

# 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



# 大纲

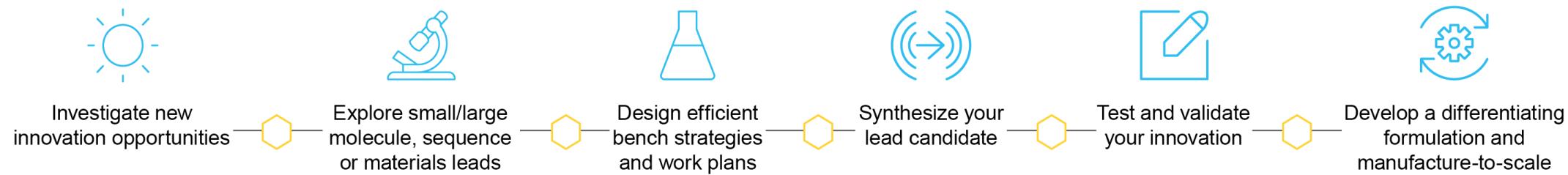
- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查找分析实验方法和制剂/配方详情?
- 常见问题Q&A



# 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

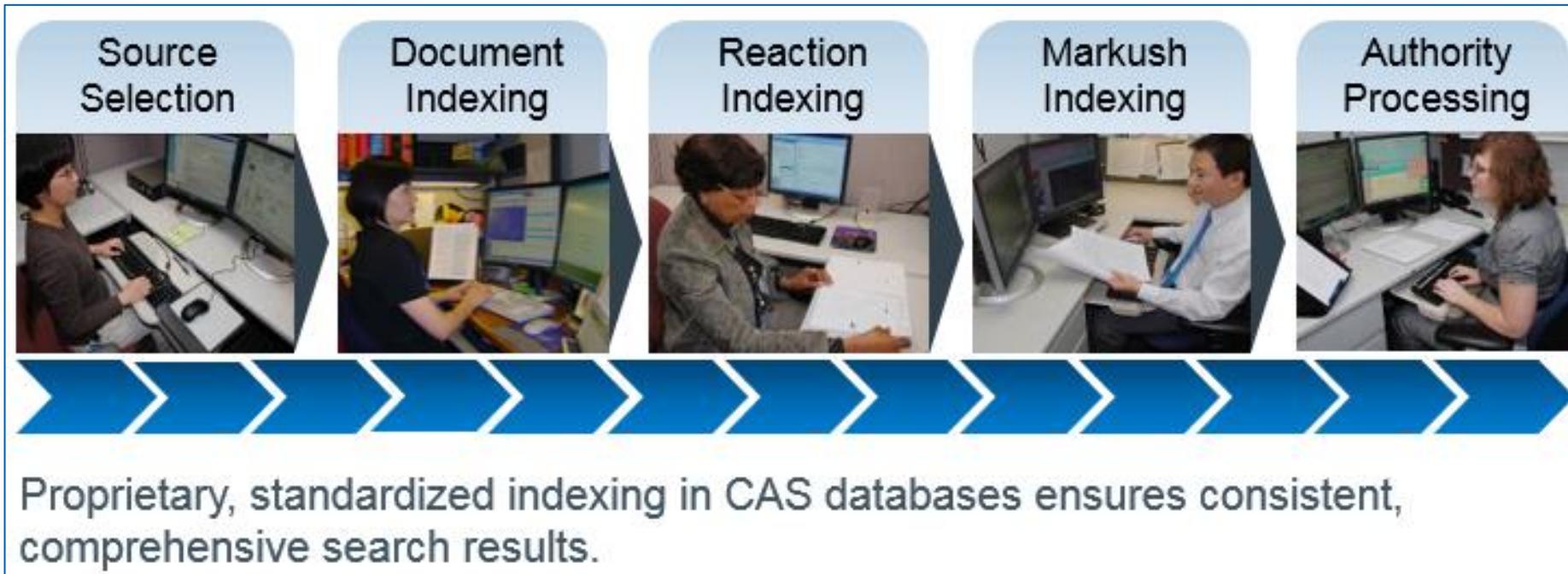


来源：

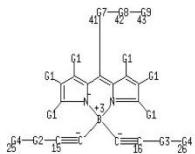
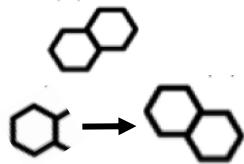
<https://www.cas.org/cas-data>

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

# CAS 科学家的智力标引



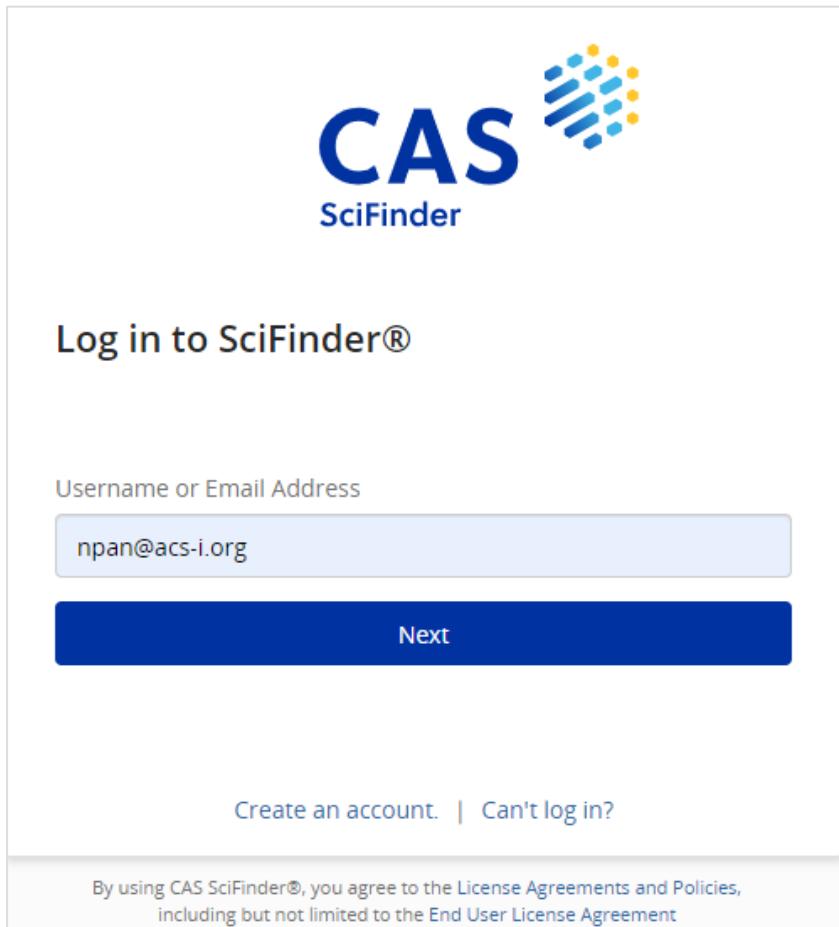
1990  
Smith, M.  
anthracene



Androst-4-en-3-one,  
17-hydroxy-17-  
methyl-, (17 $\beta$ )-

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®

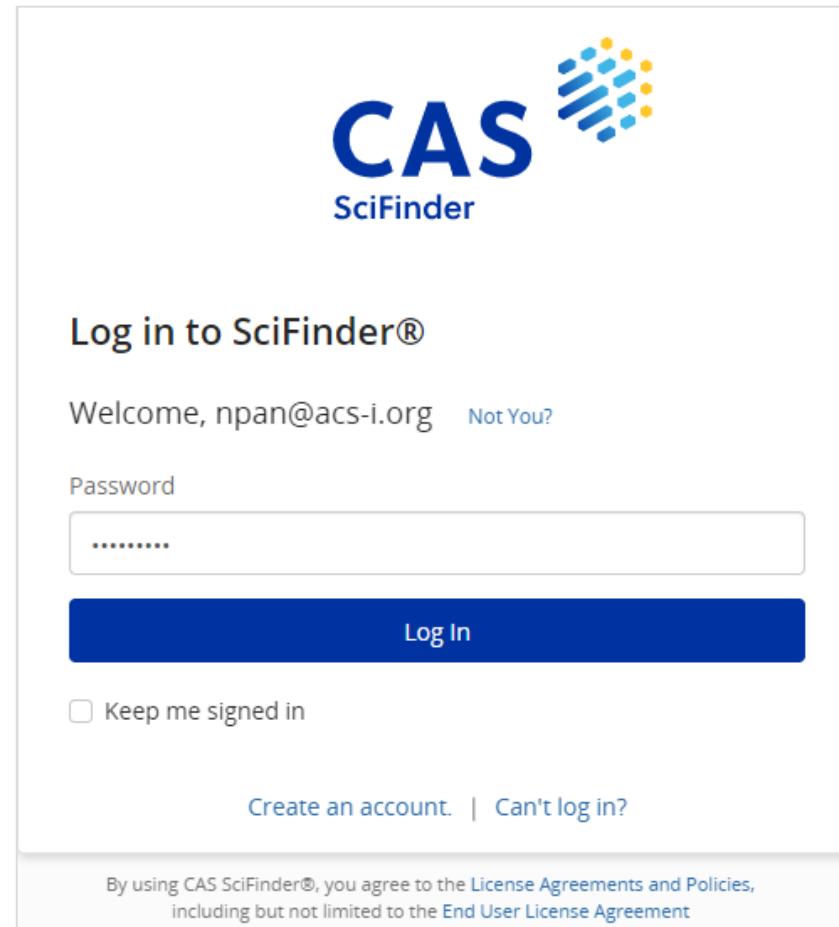
Username or Email Address

npan@acs-i.org

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?

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

使用CAS SciFinder账号登录

# CAS SciFinder 主界面

The screenshot shows the main interface of the CAS SciFinder Discovery Platform. On the left, a sidebar lists various services: SCIFINDER DISCOVERY PLATFORM (CAS SciFinder, CAS Analytical Methods, CAS Formulus), STN IP PROTECTION SUITE (STNext, CAS Scientific Patent Explorer), REGULATORY, ACCOUNT MANAGEMENT (CAS Profile). The main search area features a 'Good Morning' greeting and tabs for All, Substances (highlighted with a yellow arrow), Reactions, References, and Suppliers. A search bar allows searching by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Below the search bar are 'Molecular Formula' and 'Add Advanced Search Field' dropdowns, with '高级检索选项' (Advanced Search Options) highlighted. To the right of the search bar are buttons for Projects, Saved, History, Downloads, and Submit Feedback. A 'Draw' button with a chemical structure icon is highlighted with a yellow box. Below the search area are three cards: 'Retrosynthetic Analysis' (逆合成路线设计), 'Search CAS Lexicon' (CAS词库), and 'Search CAS Sequences' (CAS序列检索). At the bottom, a 'Recent Search History' section is shown, with '近期检索历史' (Recent Search History) highlighted in blue, and a 'View All Search History' link. A blue box labeled '结构绘制面板' (Structure Drawing Panel) covers the 'Draw' button and the search bar area.

# 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

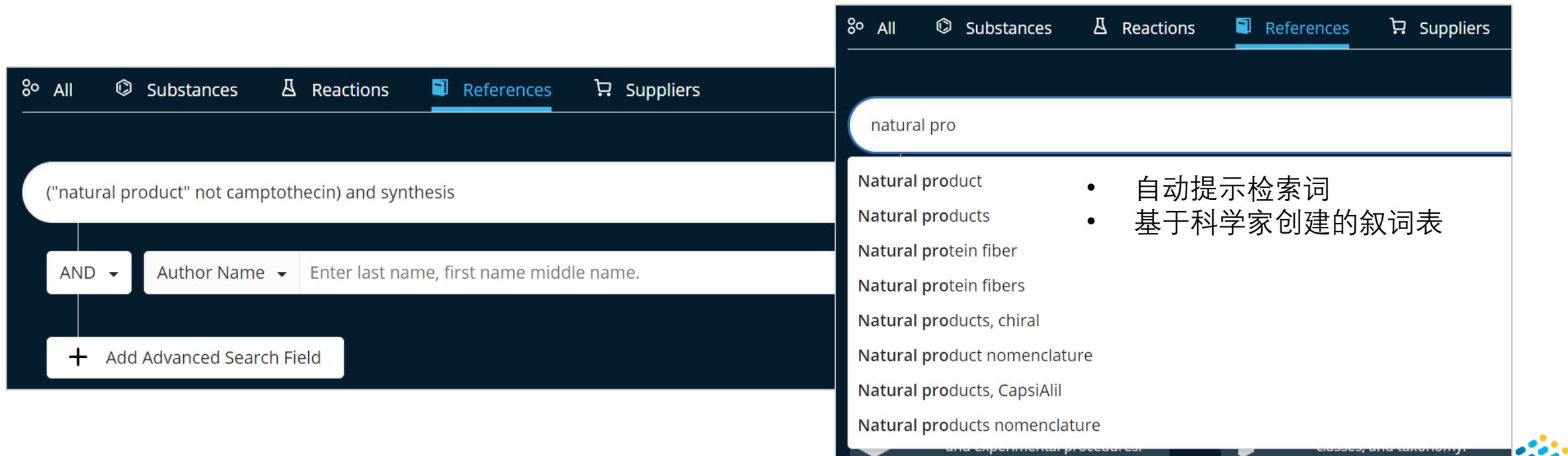


# 1. 如何开展文献检索?

- 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 shows a search interface with a navigation bar at the top and a search form below. The navigation bar includes tabs for All, Substances, Reactions, References (which is selected and highlighted in blue), and Suppliers. The search form has a search bar containing the query "natural pro". Below the search bar, the text "("natural product" not camptothecin) and synthesis" is displayed. The search form also includes dropdowns for "AND" and "Author Name", and a button to "Enter last name, first name middle name." A "Add Advanced Search Field" button is located at the bottom of the form. To the right of the search form, a dropdown menu is open, listing various search terms related to "natural product". The listed terms are: Natural product, Natural products, Natural protein fiber, Natural protein fibers, Natural products, chiral, Natural product nomenclature, Natural products, CapsiAil, and Natural products nomenclature. The text "and experimental procedures, classes, and taxonomy." is visible at the bottom of the dropdown menu. To the right of the dropdown, there is a bulleted list: "自动提示检索词" and "基于科学家创建的叙词表".

- 自动提示检索词
- 基于科学家创建的叙词表

# 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

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 environment has led to the introduction of new pesticide registration rules in the United States. These new regulations have reduced the number of synthetic routes currently available for the production of chems. for pest control. View More

Full Text Substances (0)

2

**Natural product isolation**  
By: Sticher, Otto *Natural Product Reports* (2008), 25(3), 517-554 | Language: English, Database: CPlus and MEDLINE

A review. Covering: 2000 to mid-2007. Since the 1990s, interest in natural product research has gained new attention for providing novel chem. e. and purification, recent extraction techniques used for natural product techniques, as well as multi-step chromatog. operations. It covers exam. 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: CPlus and MEDLINE

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

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

Substances Reactions Citing Knowledge Graph

162,825 Results

1

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

**Natural product synthesis in the age of scalability**  
By: Kutteruff, Christian A.; Eastgate, Martin D.; Baran, Phil S. *Natural Product Reports* (2014), 31(4), 419-432 | Language: English, Database: CPlus 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 mol. that yield substantial material enable collaborative investigations (such as SAR studies or eventful 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 o... 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

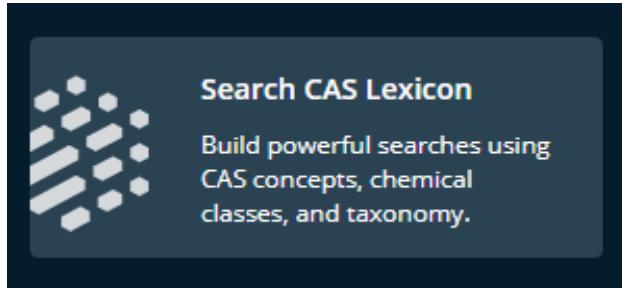
**Application of donor/acceptor-carbenoids to the synthesis of natural products**  
By: Davies, Huw M. L.; Denton, Justin R.

Sort: Relevance View: Partial Abstract

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

# 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](#)

**Steroids - Preferred Concept**

OR Remove All

**Steroids - Narrower Concepts (2)** X  
X

11-Deoxycortisol  
17-Hydroxyprogesterone

**Steroids - Related Concept (1)** X

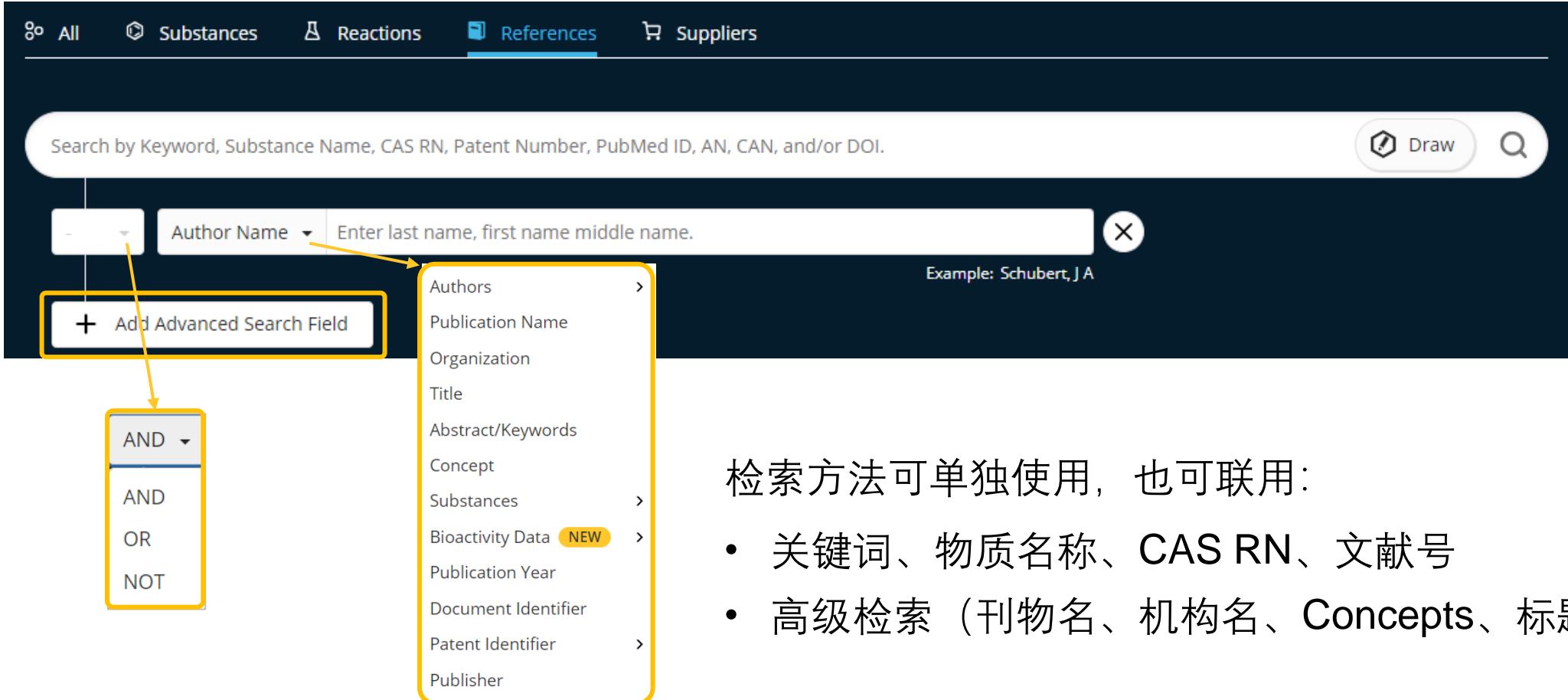
Steroid synthesis inhibitors

**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

Add to Query Clear Query Search

# 自定义组合检索



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

Author Name  (X)

Example: Schubert, J A

+ Add Advanced Search Field

Authors >

Publication Name

Organization

Title

Abstract/Keywords

Concept

Substances

Bioactivity Data NEW

Publication Year

Document Identifier

Patent Identifier

Publisher

AND

OR

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

Text: 文本与结构是“and”关系

Image: A screenshot of the SciFinder interface showing a search for "herb and medic\*" + drawn structure. The search results page displays a list of references. A chemical structure of a triterpenoid is shown in the search bar, and a callout box highlights the "Edit Drawing" and "Remove" buttons. A yellow box highlights the "Substance Role" filter in the left sidebar, and an arrow points from the text "Text与结构是“and”关系" to this filter. Another arrow points from the text "Text与结构是“and”关系" to the first reference in the list.

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

Text: By: James, Jacinda T.; Dubery, Ian A.  
Molecules (2009), 14(10), 3922-3941 | Language: English, Database: Cplus and MEDLINE

Text: A review. *Centella asiatica* accumulates large quantities of pentacyclic triterpenoid saponins, collectively known as centelloids. Triterpenoids include asiaticoside, centelloside, madecassoside, brahmoside, thankuniside, sceffoleoside, centelloside, 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 *bio*-activity of saponins has been attributed to these charac...

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

Text: 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: Cplus and MEDLINE | Analytical Methods

Text: *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.

定位物质在文献中的研究角色

Text: Substance Role

Text: By Count Alphanumeric

Text: 8 Selected

Image: A screenshot of the "Substance Role" filter dialog box. It shows a list of research roles with checkboxes. Several checkboxes are checked, including "Natural Product Occurrence (33)", "Therapeutic Use (204)", "Pharmacological Activity (132)", "Analyte (83)", "Cosmetic Use (15)", "Pharmacokinetics (15)", and "Purification or Recovery (43)". A yellow box highlights the "Apply" and "Cancel" buttons at the bottom.

Text:  Biological Study (334)

Text:  Uses (214)

Text:  Therapeutic Use (204)

Text:  Pharmacological Activity (132)

Text:  Biological Study, Unclassified (127)

Text:  Analyte (83)

Text:  Analytical Study (83)

Text:  Preparation (49)

Text:  Purification or Recovery (43)

Text:  Natural Product Occurrence (33)

Text:  Occurrence (33)

Text:  Properties (23)

Text:  Food or Feed Use (16)

Text:  Cosmetic Use (15)

Text:  Pharmacokinetics (15)

Text:  Adverse Effect (6)

Text:  Reactant (6)

Text:  Reactant or Reagent (6)

Text: 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 (selected), Exclude

Search Within Results (selected)

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

AI技术支持的相关度排序

**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  
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 o...

**Synthesis of natural product inspired compound collections**  
By: Kumar, Kama; Waldmann, Herbert  
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**Application of donor/acceptor-carbenoids to the synthesis of natural products**  
By: Davies, Huw M. L.; Denton, Justin R.

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): Add tag name, Tag Color: Light Blue

Alerts: Frequency: As Available, Add Email(s), Add Recipient(s)

Save, Cancel

定题追踪

排序方式

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

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

- Pharmaceutical natural products (113K)
- Homo sapiens (29K)
- Human (29K)
- Pharmaceutical tablets (16K)
- Pharmaceutical capsules (14K)

[View All](#)

### Concept

Top Count Alphanumeric Search

精准定位核心研究点

Concept Name

deliver\*

支持使用通配符

4 Selected

- Safflower (5,231)
- Oral drug delivery system (5,162)
- Humans (5,125)
- Astragalus membranaceus (5,110)
- Zingiber officinale (4,992)
- Plant extracts (4,718)
- Rehmannia (4,712)
- Fermentation (4,676)
- Citrus reticulata (4,665)
- Mandarin (4,665)
- Panax (4,621)
- Topical drug delivery system (4,612)
- Panax notoginseng (4,537)
- Scutellaria baicalensis (4,537)

OK Cancel

### Concept

Top Count Alphanumeric Search

精准定位核心研究点

Concept Name

deliver\*

支持使用通配符

4 Selected

- Biodegradable polymeric drug delivery systems (1)
- Intradermal drug delivery systems (5)
- Parenteral drug delivery systems (162)
- Intragastric drug delivery systems (55)
- Parenteral drug delivery systems, intraadiposal (1)
- Buccal drug delivery systems (199)
- Intrahepatic drug delivery systems (1)
- Parenteral drug delivery systems, intralesional (3)
- Intrapercardial drug delivery systems (1)
- Parenteral drug delivery systems, intrapleural (2)
- Intraperitoneal drug delivery systems (22)
- Parenteral drug delivery systems, intraprostatic (1)
- Controlled-release drug delivery systems (922)
- Intrathecal drug delivery systems (21)
- Parenteral drug delivery systems, intravesical (4)
- Controlled-release floating drug delivery systems (11)
- Intrathoracic drug delivery systems (1)
- Pharmaceutical injections, freeze-dried injectable drug delivery systems (573)
- Delivery of Health Care (2)
- 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.

自主选择下载分析栏目

Publication Year **发表年份趋势**

1971 - 2023 (3,594)

2017: (384)

OK Cancel

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

Document Type

Language

Publication Year

Author

Organization

Publication Name

Concept

CA Section

CAS Content

Life Science Data

Formulation Purpose

Database

Download Cancel Learn more about downloads.

Concepts 核心研究点分布

Epidermal... Humans Antitumor agents Female Mammary gland... Epidermal... Breast Neoplasms Receptor, ErBB-2 Signal... Cell proliferation Cell Line, Tumor Animals Neoplasm Antineoplastic... Combination...

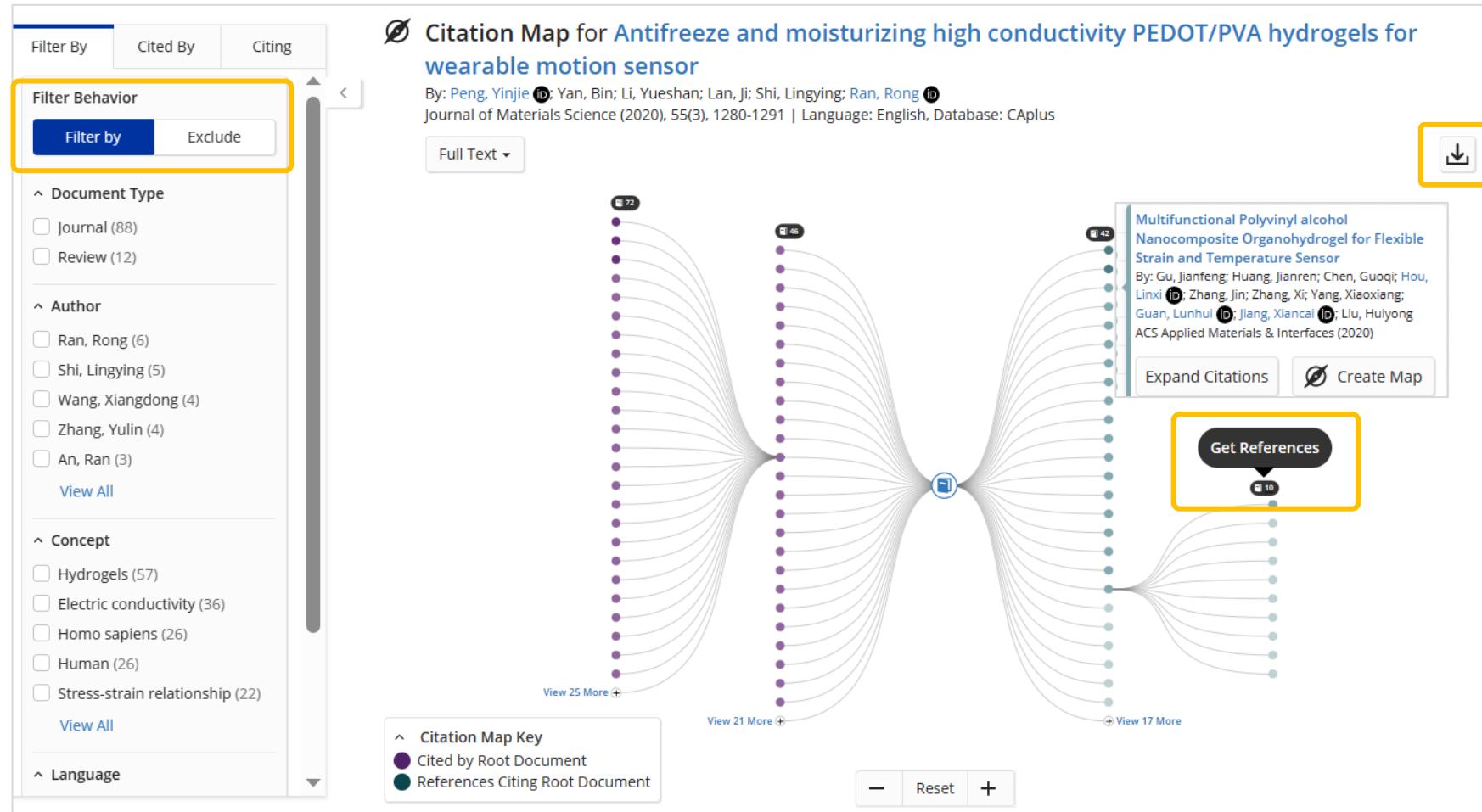
# 1.4 可视化分析——知识图谱

## Knowledge Graph

**CAS**   
A division of the  
American Chemical Society

# 1.4 可视化分析——引文地图

便捷获得相关文献



- 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

## 内容导航速览

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 study was to determine whether celecoxib, a selective Cox-2 inhibitor, protected against HER-2/neu-induced exp protein was detected in breast carcinomas from mouse mammary tumor virus (MMTV)/neu mice. Treatment with significantly reduced the incidence of mammary tumors in MMTV/neu mice ( $P = 0.003$ ) and caused about a 50% re prostaglandin E<sub>2</sub> (PGE<sub>2</sub>) levels. Because mammary glands from MMTV/neu mice expressed all four PGE<sub>2</sub> receptor that signaling through PGE<sub>2</sub> receptors is important for mammary tumorigenesis. These results strengthen the rat clin. trials to determine whether selective Cox-2 inhibitors possess anticancer properties in humans at risk for br

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 Ass for Cancer Re

## 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 EP1

Role: Biological Study, Unclassified

### Human

Prostanoid receptors, type EP3

Role: Biological Study, Unclassified

## 文献中的核心研究物质

### Substances

Substances (3)

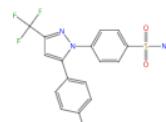
329900-75-6

Image Not Available

Unspecified  
Cyclooxygenase 2

Role: Biological Study, Unclassified, Biological Study

169590-42-5

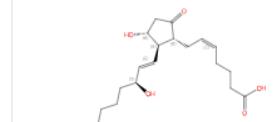


C<sub>17</sub>H<sub>14</sub>F<sub>3</sub>N<sub>3</sub>O<sub>2</sub>S  
Celecoxib

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 E2

Role: Biological Study, Unclassified, Biological Study

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# 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, alkenylsulfonyloxy, mesyloxy or tosylxy)], especially diastereomer II, synthesis of the same and intermediates theret = SiMe<sub>2</sub>CMe<sub>3</sub>, PG<sup>3</sup> = COCMe<sub>3</sub>, LG<sup>1</sup> = OMs, Ms = SO<sub>2</sub>-Me, R<sup>1</sup> = OMe] was ...

[View More](#)

**PatentPak** Full Text Substances (152) Reactions (1,160) Viewer

Patent	Language	Kind Code	PatentPak Options
WO2005118565	English	A1	PDF   PDF+ <span style="border: 1px solid yellow; padding: 2px;">Viewer</span>
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](#)

thereof

of making and using and synthetic techniques. For example formed with solutions of plant contaminants from soil and ground, the invention comprises me formed using green chem. te

Actions (0) Citing (13)

**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

Reaction scheme:

ER-812930 (TMSO<sub>2</sub> group) → ER-812933 (AcO group) → ER-812934 (MeO<sub>2</sub>C group) → ER-812935 (MeO<sub>2</sub>C group) → ER-816961 (HO group) → ER-818937 (MsO group)

Reagents: DIBALH, Toluene, Ac<sub>2</sub>O, AcOH, BF<sub>3</sub>OEt<sub>2</sub>, TFAA, CH<sub>3</sub>CN, rt, NaOMe, MeOH, THF, LAH, THF, MsCl, Et<sub>3</sub>N, HCl, MeOH, KCN, EtOH.

**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

Reaction scheme:

ER-812930 (TMSO<sub>2</sub> group) → ER-812933 (AcO group) → ER-812934 (MeO<sub>2</sub>C group) → ER-812935 (MeO<sub>2</sub>C group) → ER-816961 (HO group) → ER-818937 (MsO group)

Reagents: DIBALH, Toluene, Ac<sub>2</sub>O, AcOH, BF<sub>3</sub>OEt<sub>2</sub>, TFAA, CH<sub>3</sub>CN, rt, NaOMe, MeOH, THF, LAH, THF, MsCl, Et<sub>3</sub>N, HCl, MeOH, KCN, EtOH.

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.

22

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American Chemical Society

# 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

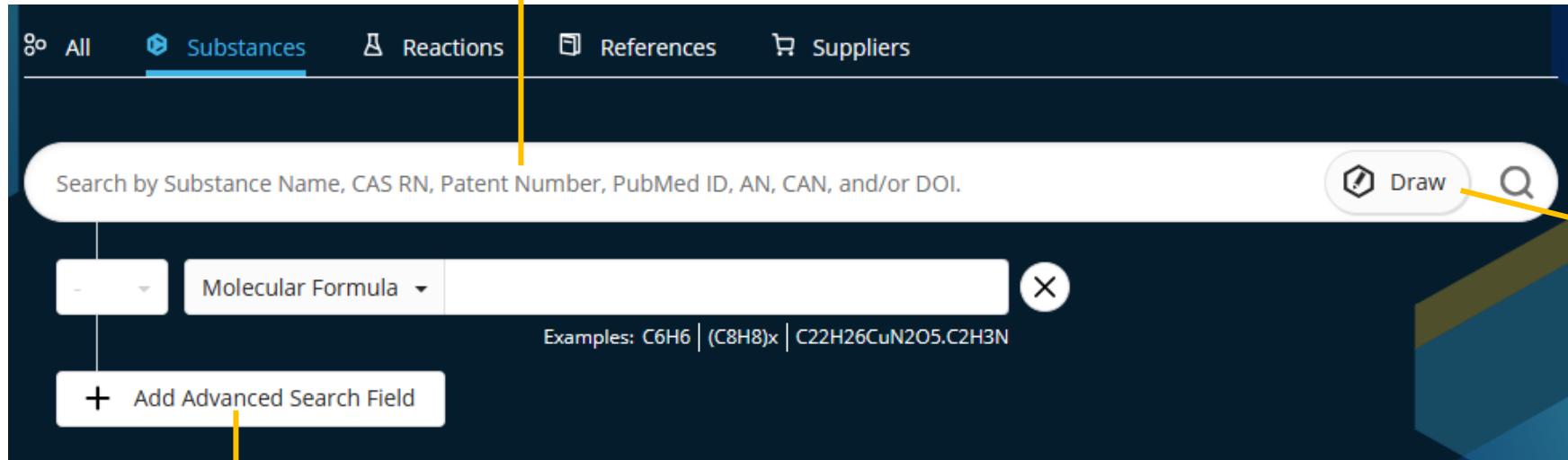


## 2. 如何聚焦某类物质?

- 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



- 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"

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)

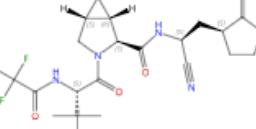
[View All](#)

Life Science Data

Commercial Availability

2 Results

1 2628280-40-8 ...

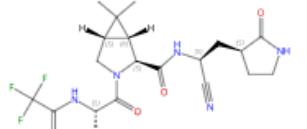


Absolute stereochemistry shown

C23H32F3N5O4

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

2 2803933-60-8 ...



Absolute stereochemistry shown

C37H48N6O5S2.C23H32F3N5O4

Components: 2

Paxlovid

999 References 320 Reactions 42 Suppliers

283 References 3 Reactions 0 Suppliers

- 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)

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

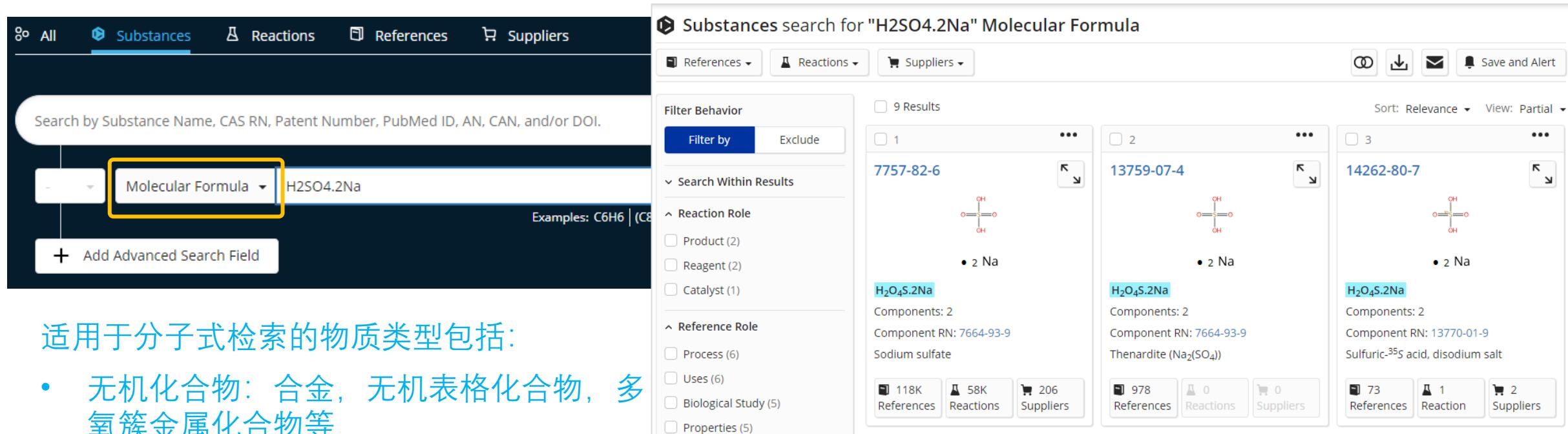
Number of References: Descending

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  $\text{Na}_2\text{SO}_4$ :  $\text{H}_2\text{O}_4\text{S}.2\text{Na}$



The screenshot shows the CAS Substances search interface. The search bar at the top contains the query "H2SO4.2Na". The search results page displays 9 results for the molecular formula  $\text{H}_2\text{O}_4\text{S}.2\text{Na}$ . Each result card includes the CAS number, a chemical structure, the formula  $\text{H}_2\text{O}_4\text{S}.2\text{Na}$ , the number of components (2), the component RN (7664-93-9), the component name (Sodium sulfate/Thenardite ( $\text{Na}_2(\text{SO}_4)$ )), and links to references, reactions, and suppliers. The results are sorted by relevance and viewed in partial mode.

Result	CAS Number	Chemical Structure	Formula	Components	Component RN	Component Name	References	Reactions	Suppliers
1	7757-82-6		$\text{H}_2\text{O}_4\text{S}.2\text{Na}$	2	7664-93-9	Sodium sulfate	118K	58K	206
2	13759-07-4		$\text{H}_2\text{O}_4\text{S}.2\text{Na}$	2	7664-93-9	Thenardite ( $\text{Na}_2(\text{SO}_4)$ )	978	0	0
3	14262-80-7		$\text{H}_2\text{O}_4\text{S}.2\text{Na}$	2	13770-01-9	Sulfuric- <sup>35</sup> S acid, disodium salt	73	1	2

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

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

Molecular Formula

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

Search CAS Lexicon

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

Search CAS Sequence

Query BLAST, CDR, and other sequence analysis algorithms for nucleotide and protein based sequences.

Recent Searches

August 15, 2023

Substance 10:44 AM

实验核磁谱图数值助力结构解析

As Drawn (2)  
Substructure (6,704)  
Similarity (242K)

Chemical Properties

- Koc
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal

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

# 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  
Examples: 46.07 | 125 to 350 | >300

AND pKa: 1.3 to 1.8  
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, 155.02 to 187.133.1 | 207.59

+ Add Advanced Search Field

Substances search for 3 Advanced Fields

References | Reactions | Suppliers

Filtering: Life Science Data: 3 Selected | Clear All Filters

Sort: Molecular Formula: Ascending | View: Partial

Filter Behavior: Filter by | Exclude

13 Results

1 1628224-40-7  
C<sub>9</sub>H<sub>13</sub>N<sub>3</sub>O<sub>5</sub>  
( $\alpha$ S)- $\alpha$ -Amino-3-(carboxymethoxy)-5-methyl-1H-pyrazole-4-propanoic acid

2 296262-16-3  
C<sub>10</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>  
2-[(5,6-Dimethylthieno[2,3-*d*]pyrimidin-4-yl)thio]acetic acid

3 723-46-6  
C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S  
Sulfamethoxazole

4 1631737-39-7  
C<sub>10</sub>H<sub>15</sub>N<sub>3</sub>O<sub>5</sub>  
(*2R,3R,4S,5R*)-4,5-Dihydro-5-(hydroxymethyl)-3'-methylspiro[furan-2(3*H*),7'(6*H*)-...]

5 442571-27-9  
C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>  
2-[(5,6-Dimethylthieno[2,3-*d*]pyrimidin-4-yl)thio]propanoic acid

6 1927010-88-5  
C<sub>11</sub>H<sub>16</sub>ClNO<sub>3</sub>  
3-Chloro-4-[(1-methylpropyl)amino]-5-(2-propen-1-oxyl)-2(5*H*)-furanone

View All

1 Reference | 4 Reactions | 0 Suppliers

5 References | 42 Reactions | 48 Suppliers

30K References | 1,047 Reactions | 112 Suppliers

2 References | 22 Reactions | 0 Suppliers

2 References | 4 Reactions | 27 Suppliers

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



# 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



选择可变基团



自定义R基团



片段结构



重复工具



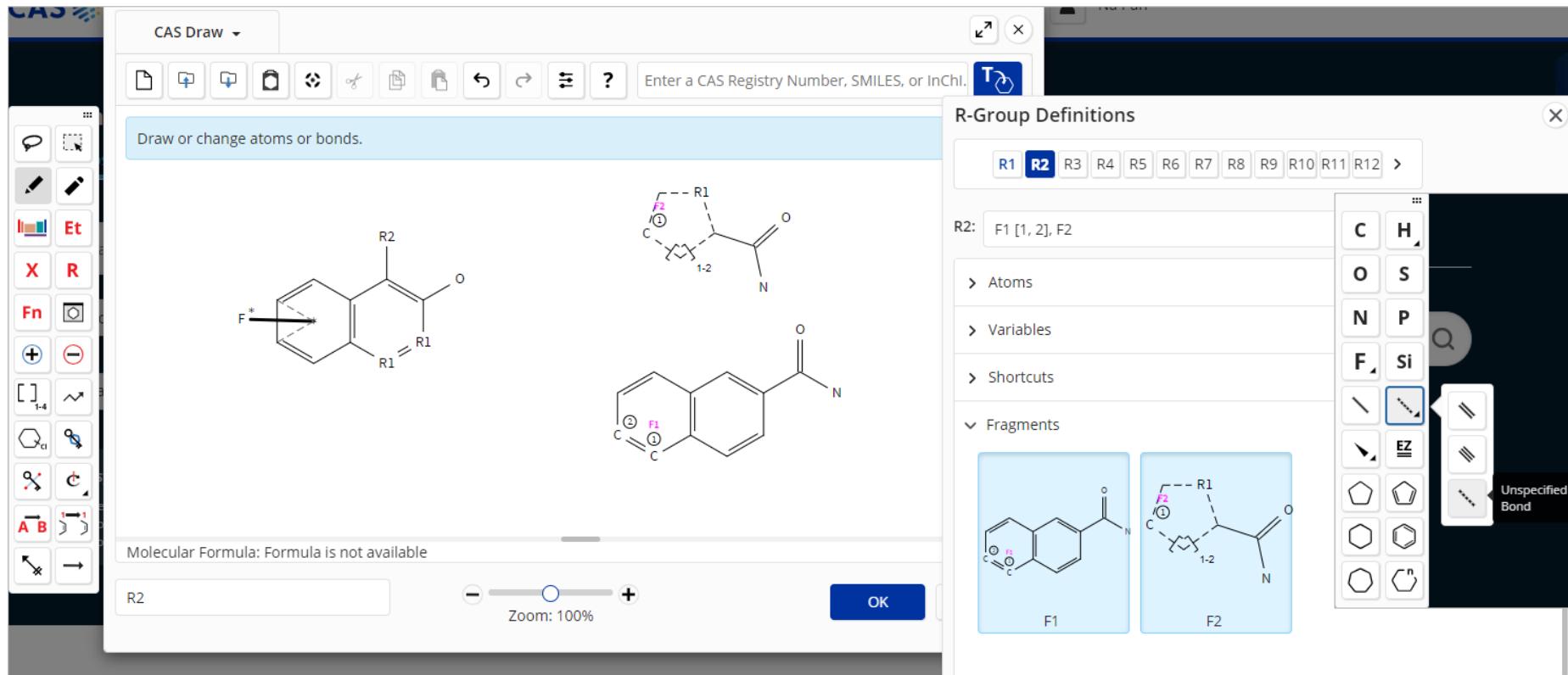
取代位置可变



环锁定工具



原子锁定工具



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

Structure Match: As Drawn (2) Substructure (62K) Similarity (596)

Filtering: Number of Components: 1

57,950 Results

Sort: Relevance View: Partial

Clear All Filters

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

Filter Behavior: Filter by Exclude

- Search Within Results
- Reaction Role
- Reference Role
- Life Science Data
- Commercial Availability
- Number of Components: 1 (57K)

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

组分数量

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？

Reaction Role:  
物质在反应中的角色

Reference Role:  
物质在文献中的研究角色

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 [...  
1845745-84-7 \[...  
2 201214-57-5 \\[...  
3 679395-52-9 \\\[...  
4 468733-27-9 \\\\[...  
5 138605-81-9 \\\\\[...  
6 1432622-95-1 \\\\\\[...  
7 81771-19-9 \\\\\\\[...  
8 179464-13-2 \\\\\\\\[...  
9\\\\\\\\]\\\\\\\\(#\\\\\\\\)\\\\\\\]\\\\\\\(#\\\\\\\)\\\\\\]\\\\\\(#\\\\\\)\\\\\]\\\\\(#\\\\\)\\\\]\\\\(#\\\\)\\\]\\\(#\\\)\\]\\(#\\)\]\(#\)](#)

Enzyme inhibitors (2)

Nervous system agents (2)

Membrane transport modulators (1)

Bioactivity Indicator

Enzymes (2)

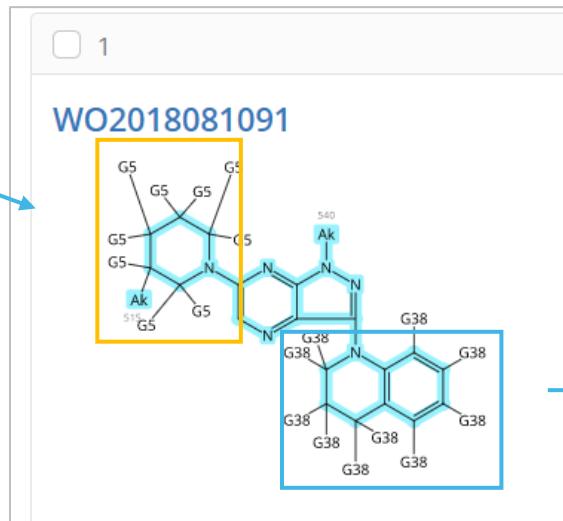
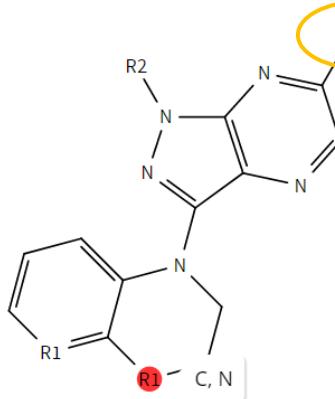
Membrane proteins (1)

Transport proteins (1)

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# 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

1  
WO2018081091

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

Patent claim 1

PatentPak ▾ Full Text ▾

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

专利中的定位，专利权人、命中结构的特点等等

WO 2018/081091

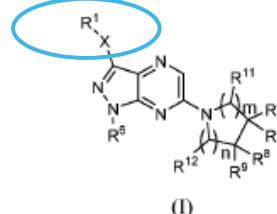
PCT/US2017/058048

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,



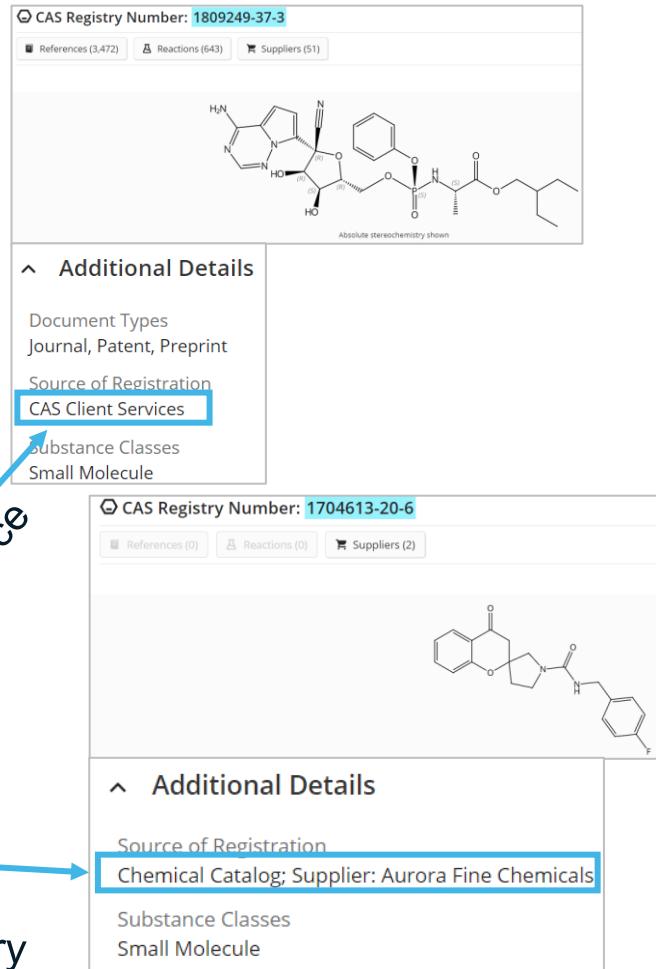
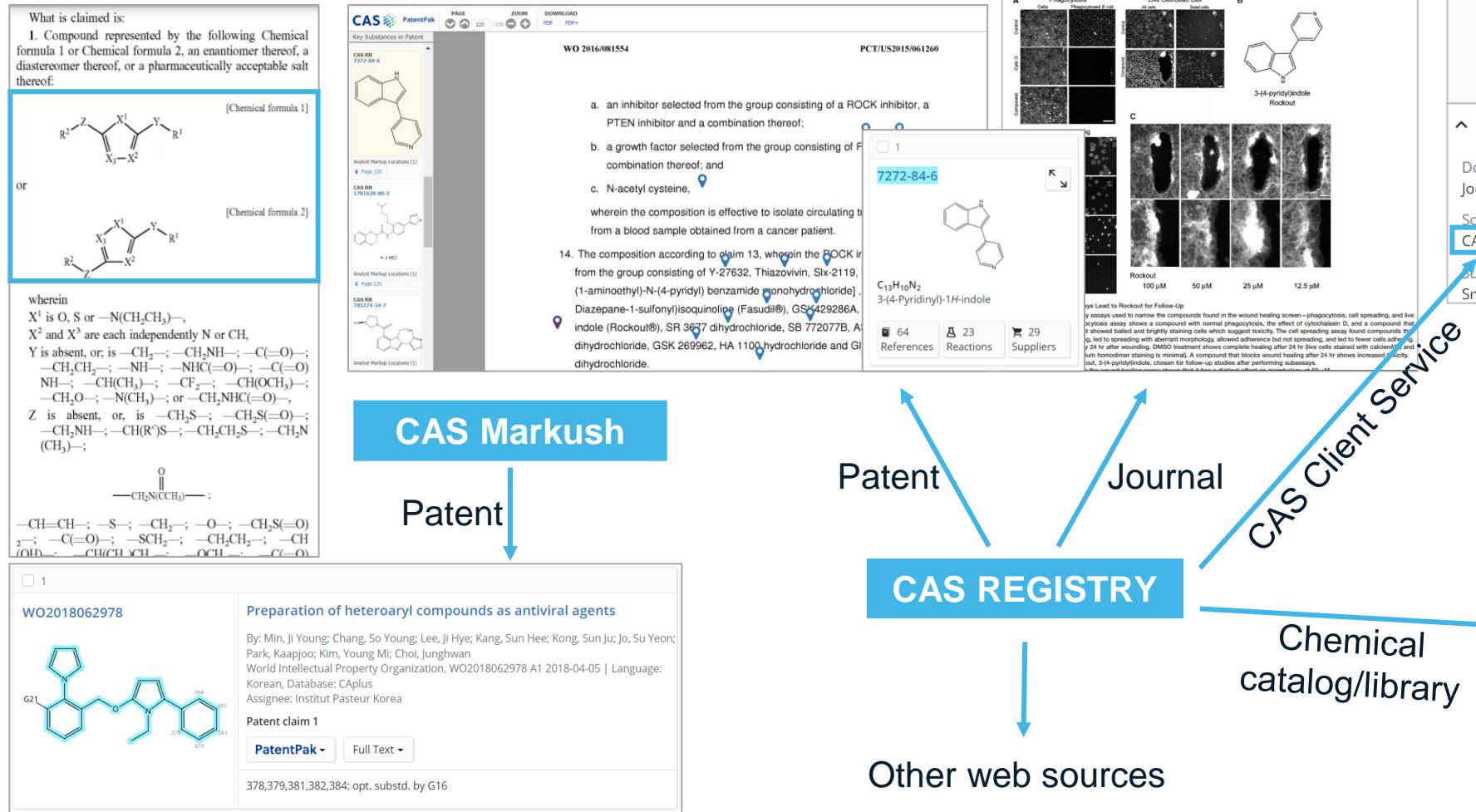
5

wherein

X is  $N-R^{66}$ ,  $O$ ,  $S$ ,  $S(O)$ ,  $SO_2$ ,  $CR^{13}R^{14}$ ,  $-O-C(R^{13}R^{14})-$ ,  $-C(R^{13}R^{14})O-$ ,  $C(O)$ , or  $C=C(R^{13}R^{14})$ ;

- 15  $R^{66}$  is selected from the group consisting of  $H$ ,  $-(C_1-C_6)alkyl$  and  $phenyl$ , or together with  $R^1$  and the nitrogen to which they are attached form a nitrogen ring moiety selected from the group 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 with one, two or more substituents each independently selected from the group consisting of  $R^{10}$ ,  $-OR^{10}$ ,  $-S(O)_wR^{10}$  (wherein  $w$  is 0, 1 or 2),  $-N(R^{10})_2$ ,  $-OS(O)_wR^{10}$  (wherein  $w$  is 0, 1, or 2),  $-S(O)_wN(R^{10})_2$  (wherein  $w$  is 0, 1 or 2),  $-S(O)(NH)R^{10}$ ,  $-P(O)(R^{10})_2$ ,  $-C(O)R^{10}$ ,  $-C(O)N(R^{10})_2$ ,  $oxo$ ,  $halogen$ ,  $nitrile$ ,  $phenyl$  (optionally substituted with one, two or three halo,  $C_{1-3}alkyl$  or  $C_{1-3}haloalkyl$ ),  $C_{1-3}alkyl$ ,  $C_{1-3}haloalkyl$ , and  $heteroaryl$  (optionally substituted with one, two or three halo,  $C_{1-3}alkyl$  or  $C_{1-3}haloalkyl$ );
- 20
- 25

# 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 Save and Alert

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

**As Drawn (0)**

**Substructure (0)**

**Similar (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

286 Results

1 1825352-54-2 95 ...

2 1825352-53-1 95 ...

3 1825352-79-1 95 ...

**C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O**  
2-(2,8-Dimethylimidazo[1,2-*b*]pyridazin-6-yl)-7-[(3*R*)-3-methyl-1-piperazinyl]-4*H*...

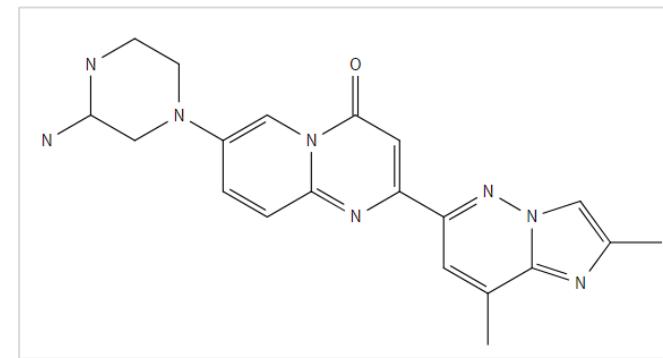
**C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O**  
2-(2,8-Dimethylimidazo[1,2-*b*]pyridazin-6-yl)-7-[(3*S*)-3-methyl-1-piperazinyl]-4*H*...

**C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O**  
9-Methyl-2-(2-methylimidazo[1,2-*b*]pyridazin-6-yl)-7-[(3*R*)-3-methyl-1-piperazinyl]...

5 References 25 Reactions 1 Supplier

5 References 25 Reactions 1 Supplier

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性检索结果

# 如何进行完整的分子结构检索？

**Substances search for drawn structure**

References ▾ Reactions ▾ Suppliers ▾

Structure Match

Filtering: Similarity: 3 Selected X Number of Components: 1 X

As Drawn (0) Substructure (0) Similarity (101K)

286 Results

Sort: Relevance ▾ View: Partial ▾

1 1825352-54-2 95 •••  
2 1825352-53-1 95 •••  
3 1825352-79-1 95 •••

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

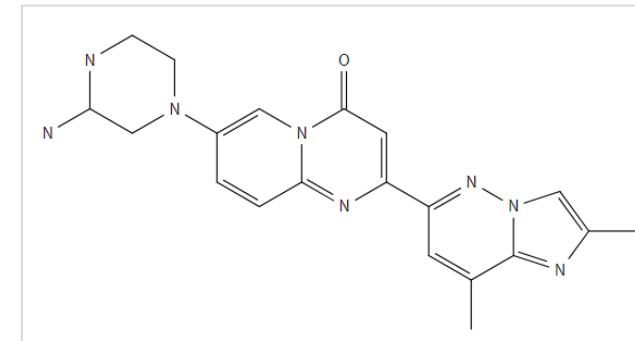
Filter by Exclude

5 References 25 Reactions 1 Supplier

5 References 25 Reactions 1 Supplier

5 References 19 Reactions 1 Supplier

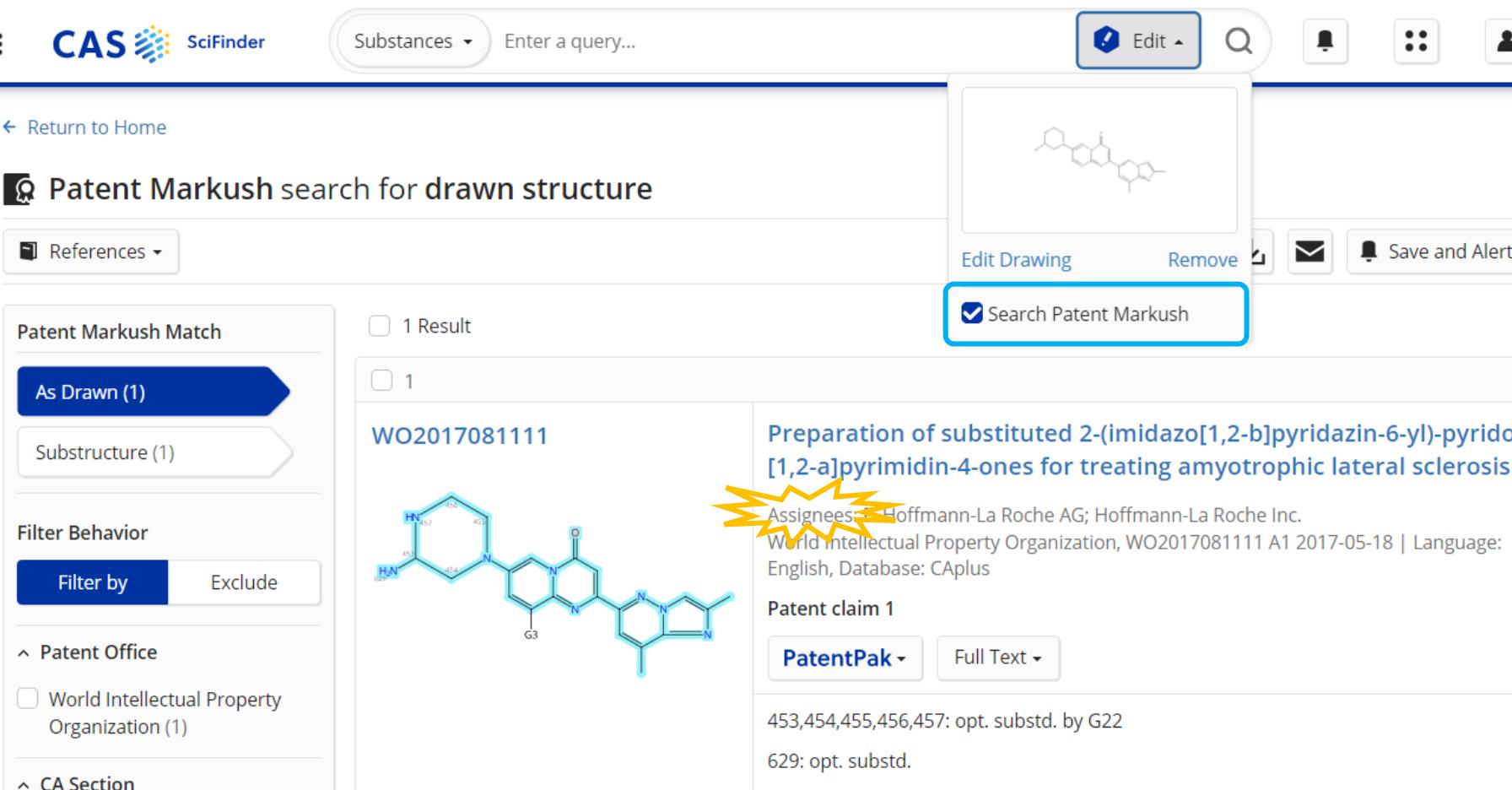
Search Within Results



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？



The screenshot shows the SciFinder interface with the following elements:

- Header:** CAS SciFinder, Substances, Enter a query...
- Search Bar:** Edit, Search icon, Notifications, More, User profile.
- Left Sidebar:** Return to Home, Patent Markush search for drawn structure, References, Patent Markush Match, As Drawn (1) (highlighted in blue), Substructure (1), Filter Behavior, Filter by (highlighted in blue), Exclude, Patent Office, World Intellectual Property Organization (1), CA Section.
- Search Results:** 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.

- 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

1,262 Results

Scheme 1 (4 Reactions)

Group: By Scheme Sort: Relevance View: Expanded

Steps: 1 Yield: 85-100% **...**

1.262 Results

Supplier (1)

Supplier (73)

Supplier (36)

31-320-CAS-19339297 Steps: 1 Yield: 100% **...**

1.1 Catalysts: Dabco 7-14 h, rt

A cascade synthesis of S-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"

人名反应智能识别

1,395,346 Results

Scheme 1 (20 Reactions)

HO-B(=O)c1ccc(Cl)cc1 + O=N(c2ccc(Cl)cc2)c3ccc(Cl)cc3  $\rightarrow$  O=N(c2ccc(Cl)cc2)c1ccc(Cl)cc1

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- $\kappa$ O')pallad(0)  
Solvents: Ethanol, Water; 20 h, 80 °C

Full Text

31-179-CAS-10541130 Steps: 1 Yield: 99% **...**

1.1 Reagents: Potassium hydroxide  
Catalysts: Palladium(1 $\pm$ ), (acetonitrile)chloro[oxybis(2,1-ethanediyl)oxy]2,1-ethanediyl[3-(1- $\mu$ )]  
Solvents: 1,4-Dioxane; 5 h, 75 °C

Full Text

31-179-CAS-8409485 Steps: 1 Yield: 98% **...**

1.1 Reagents: Potassium hydroxide  
Catalysts: Palladium(1 $\pm$ ), (acetonitrile)chloro[1,2-ethanediyl]bis[oxy-2,1-ethanediyl]3-(1-na...)

Full Text

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

Synthesis, characterization of N-heterocyclic carbene metallacrown 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

Synthesis, characterization of N-heterocyclic carbene metallacrown 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

# 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% ⋮

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

A cooperative nanoscale ZnO-NiO-Ni heterojunction for sustainable catalytic amidation of aldehydes with secondary amines  
By: Shelte, Amishwar Raysing; et al  
RSC Sustainability (2024), 2(9), 2615-2625

Experimental Protocols

Full Text ▾

31-480-CAS-16653494      Steps: 1 Yield: 100% ⋮

1.1 Reagents: Cesium carbonate, Oxygen  
Catalysts: 1648843-87-1  
Solvents: Tetrahydrofuran; 4 h, rt

Copper(II) complex of new non-innocent O-aminophenol-based ligand as biomimetic model for galactose oxidase enzyme in aerobic oxidation of alcohols  
By: Safaei, Elham; et al  
Journal of Molecular Structure (2017), 1133, 526-533

Experimental Protocols

Full Text ▾

31-480-CAS-16606643      Steps: 1 Yield: 100% ⋮

1.1 Reagents: Cesium carbonate, Oxygen  
Catalysts: 2058233-98-8  
Solvents: Tetrahydrofuran; 12 h, 298 K

Redox potential tuning by redox-inactive anions in copper(I) complexes of non-innocent o-aminophenol-based ligand containing benzoxazole: Learning from nature  
By: Safaei, Elham; et al  
Polyhedron (2017), 122, 219-227

- 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 X

Group: By Scheme ▾

By Scheme

By Document

By Transformation

Sort: Relevance ▾ View: Collapsed

Relevance

Publication Date: Newest

Publication Date: Oldest

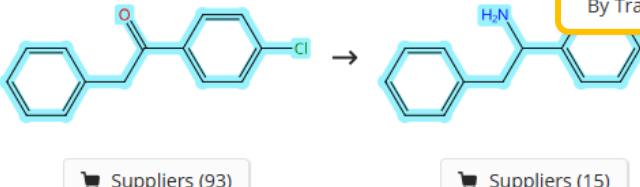
Yield

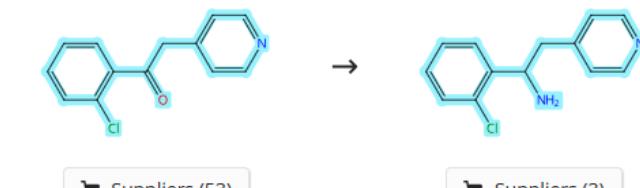
Number of Steps: Ascending

Number of Steps: Descending

16 Results

Scheme 1 (5 Reactions)

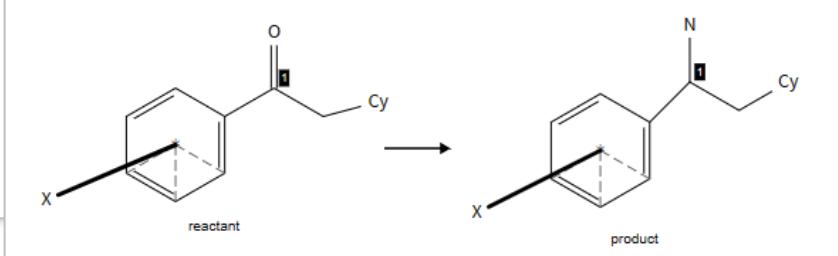




31-614-CAS-28968228 Steps: 1 Yield: 76% Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

1.1 Reagents: O-Methylhydroxylamine hydrochloride Solvents: Pyridine; rt; 1 h, 50 °C

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

# 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

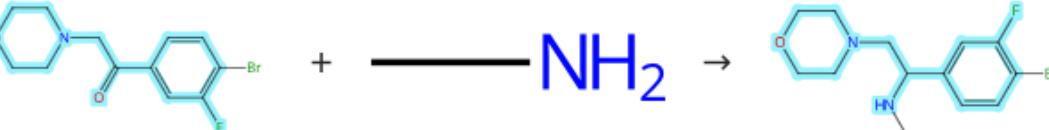
Filtering: Non-Participating Functional Groups: Halide

205 Results

Group: By Scheme

Scheme 1 (1 Reaction)

Steps: 1 Yield: 100%



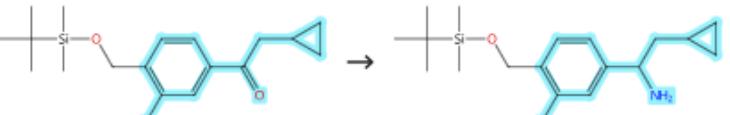
31-313-CAS-11425767 Steps: 1 Yield: 100% Preparation of N-[1-biphenylyl-(morpholinyl- and pyridinyl)ethyl]glycinamide derivatives as antagonists of urotensin II

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

By: Neeb, Michael J.; et al  
World Intellectual Property Organization, WO200801112008-01-24

Scheme 2 (1 Reaction)

Steps: 1 Yield: 100%



Non-Participating Functional Groups

Halide (205)  Tertiary amine (15)  
 Phenyl halide (203)  Carboxamidine (14)  
 Amide (66)  Urea (12)  
 Alkene (62)  Carboxylic ester (9)  
 Cyclic alkene (58)  Carbamate (8)  
 Diene (45)  Imine (8)  
 Ether (37)  Acyclic ketone (7)  
 Amine (15)  Ketone (7)

# 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)

View PDF Full Text

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

Procedure

- Suspend methyl 5-Fluoro-2-(2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl)-3-nitrobenzoate (8.1 g, 25.2 mmol) and 4-bromobenzaldehyde (8.9 g, 50.5 mmol) in THF (50 mL) and MeOH (10 mL).
- 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.
- Maintain the reaction temperature between 30 and 50°C for 2 hours.
- Quench the mixture by the slow addition of water (260 mL).
- Pour the reaction mixture into a separating funnel.
- Extract the mixture with ethyl acetate (4 x 140 mL).
- Pool the organic fractions.
- Wash the organic fractions with NaHCO<sub>3</sub> (3 x 60 mL) and NaHSO<sub>3</sub> (3 x 100 mL).
- Dry the organic fractions with sodium sulfate (Na<sub>2</sub>SO<sub>4</sub>).
- Concentrate the solvent under reduced pressure to obtain a thick yellow syrup.
- Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully.
- 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-Quinolincarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-5-quinolincarboxylate

State

yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

Transformations

- 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

# 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)

View PDF Full Text

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

Procedure

- Suspend methyl 5-Fluoro-2-(2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl)-3-nitrobenzoate (8.1 g, 25.2 mmol) and 4-bromobenzaldehyde (8.9 g, 50.5 mmol) in THF (50 mL) and MeOH (10 mL).
- 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.
- Maintain the reaction temperature between 30 and 50°C for 2 hours.
- Quench the mixture by the slow addition of water (260 mL).
- Pour the reaction mixture into a separating funnel.
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- Pool the organic fractions.
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- 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-Quinolincarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-5-methyl ester

State

yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

Transformations

- 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

# 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

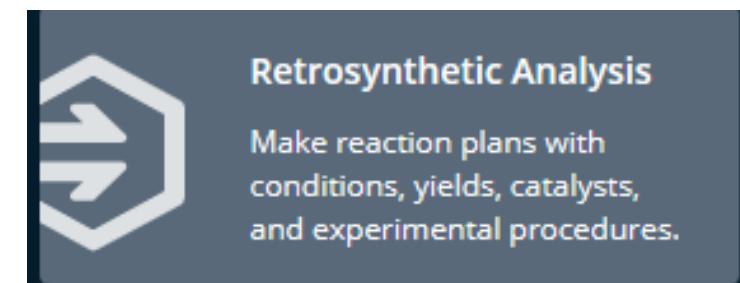
(1) 已知化合物: 点击物质结构, 弹出的物质菜单中点击 Start Retrosynthetic Analysis

The screenshot shows the CAS Retrosynthesis Tool interface. On the left, a search result for CAS RN 2628280-40-8 is displayed, showing the chemical structure of a complex molecule with absolute stereochemistry. Below the structure, the chemical formula  $C_{23}H_{32}F_3N_5O_4$  and the full name "3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...]" are shown. Below the name are buttons for "References" (236), "Reactions" (53), and "Suppliers" (39). In the center, a detailed view of the molecule is shown with stereochemistry labels (S, R) and a "Start Retrosynthetic Analysis" button, which is highlighted with a yellow box. To the right, there are buttons for "Edit Structure", "Reset", and "Suppliers (39)".

(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

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



# 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)

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](#)

Break Bond Protect Bond [Clear All Bond Selections](#)

断裂键或保护键

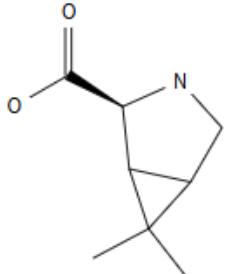
Set Starting Materials Cost Limit [Learn more](#)

Set Starting Materials Cost Limit 起始原料费用

1000 USD/mol

Email me when my plan is complete

Continue to Retrosynthesis Plan



# 逆合成路线详情

## Retrosynthesis Plan for drawn structure

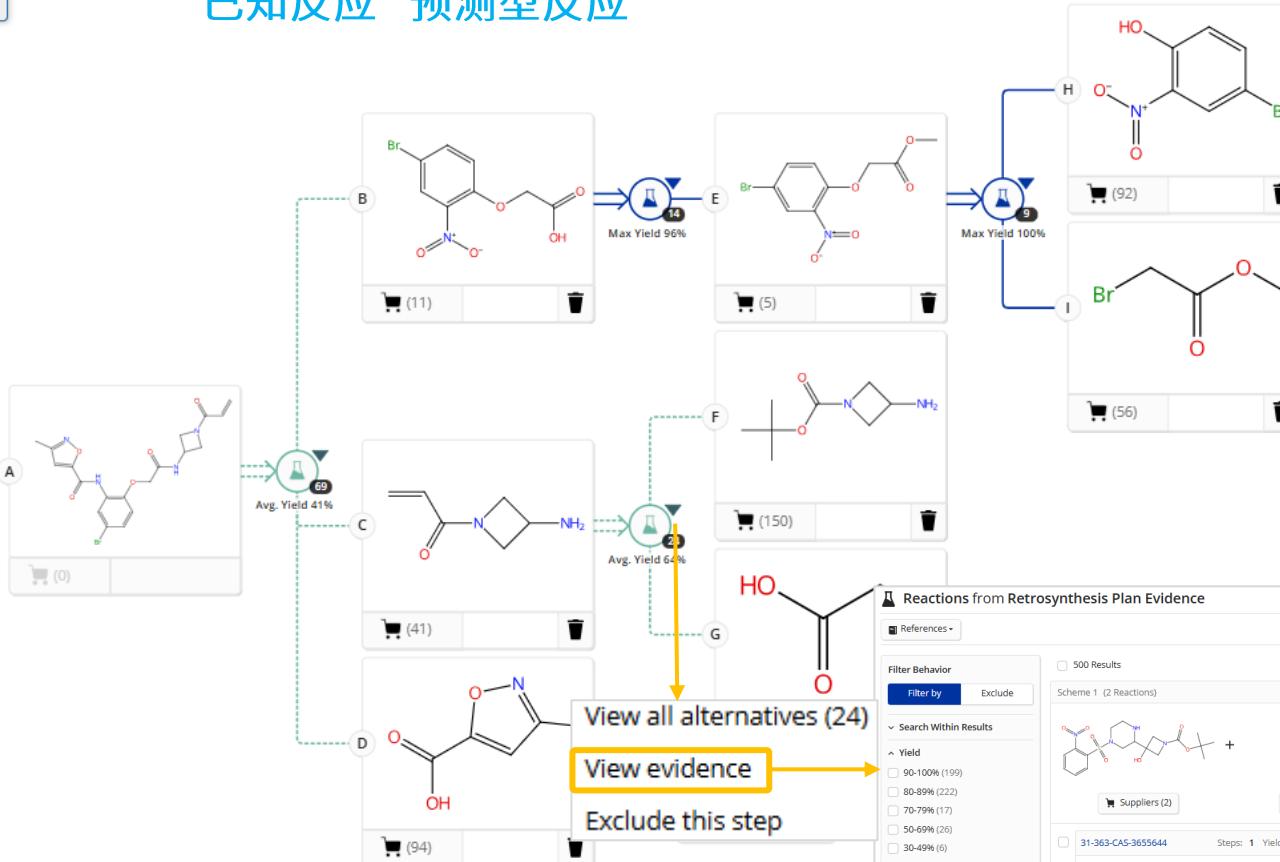
Powered by ChemPlanner®

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



Reactions from Retrosynthesis Plan Evidence

Filter Behavior: Filter by Exclude

Filter Within Results: Yield (90-100% (199), 80-89% (222), 70-79% (17), 50-69% (26), 30-49% (6))

Number of Steps: 1

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: Scheme 1 (2 Reactions)

Group: By Scheme Sort: Relevance View: Expanded

Supplier: (2) Supplier: (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

31-363-CAS-5805537: 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

Preparation of azetidines as MEK kinase inhibitors for the treatment of proliferative diseases, especially cancer

Preparation of N-acylated imidazole MEK inhibitors and 4-aryl-2-aminoimidazole JAK-2 inhibitors and their combinations useful for treating neoplasia

Preparation of azetidines as MEK kinase inhibitors for the treatment of proliferative diseases, especially cancer

**CAS**  
A division of the  
American Chemical Society

# 路线优化，考虑替换路线？

The screenshot shows a chemical synthesis planning interface. On the left, a reaction scheme shows a starting material (C) reacting with a reagent to form intermediate F. A dropdown menu for step F shows 'View all alternatives (24)'. An arrow points from this menu to a detailed view of alternative steps for the reaction C → F + G.

**Reaction C → F + G**

Maximum Yield: 96%  
Evidence  
Alternative steps (14)

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

**Reaction C → F + G Alternative Steps (24)**

Filter by: Alternative Step Type, Predicted (24)

1 of 12:  $\text{C} \Rightarrow \text{F} + \text{G}$  (Predicted Step)

Selected View 4 similar Alternatives View evidence Average yield: 64%

2 of 12:  $\text{C} \Rightarrow \text{F}' + \text{G}$  (Predicted Step)

Select View 2 similar Alternatives View evidence Average yield: 78%

3 of 12:  $\text{C} \Rightarrow \text{F}'' + \text{G}$  (Predicted Step)

**Text:** 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<sup>TM</sup>——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

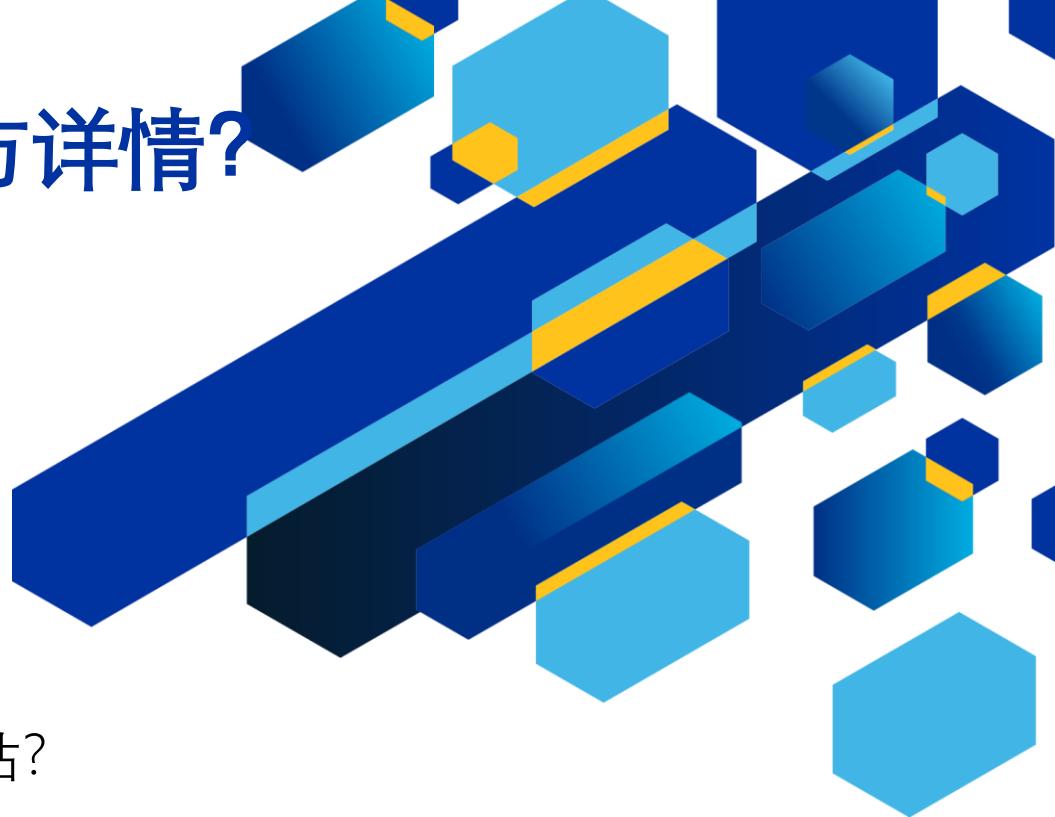
# 大纲

- 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实验方法

The screenshot shows the CAS SciFinder interface with a search bar at the top containing "References search for 'lapatinib and cancer'". Below the search bar are four buttons: "Substances", "Reactions", "Citing", and "Knowledge Graph". To the right of these are icons for search, download, and file. A message box on the left says "We are displaying the most relevant results." and "Learn about result relevance." with a "Load All Results" button. The main area is titled "Filtering: CAS Content: Analytical Methods" with a "Clear All Filters" link. It shows "28 Results" and "Sort: Relevance" and "View: Partial Abstract". The results list includes the following entries:

- 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: CPlus 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](#)
- 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: CPlus 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  $\mu$ L) were prepared using solid phase extraction (SPE) columns, and 6.0  $\mu$ L of the reconstituted eluate was injected onto a Phenomenex Curosil-PFP 3  $\mu$  anal. column (50 mm  $\times$  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...

On the left, a "Filter Behavior" sidebar shows "Filter by" selected. Below it is a list of filter categories: "Search Within Results", "Document Type", "Substance Role", "Language", "Publication Year", "Author", "Organization", "Publication Name", "Concept", "CA Section", "CAS Content" (which is highlighted with a yellow box), "Formulations (789)", and "Analytical Methods (28)". At the bottom of the sidebar, there are buttons for "Full Text", "Substances (7)", "Reactions (0)", "Citing (180)", and "Citation Map".

# 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.; Levvaz, S.; Widmer, N.; Decosterd, L. A.

DOI: [10.1016/j.jchromb.2009.04.045](https://doi.org/10.1016/j.jchromb.2009.04.045)

The treatment of some **cancer** patients has shifted from traditional, non-specific cytotoxic chemotherapies to targeted therapies. Imatinib mesylate, a selective inhibitor of tyrosine kinases (TKIs) is the most well-known TKI. It has opened the way to the development of several addnl. TKIs, including sunitinib, nilotinib, dasatinib, and sorafenib for the treatment of various hematol. **malignancies** and solid tumors. All these agents are characterized by high inter- and pharmacokinetic variability, are at risk for drug interactions, and are not devoid of toxicity. Adverse events may occur at any time periods, anticipating the careful monitoring of their plasma exposure via Therapeutic Drug Monitoring (TDM) as an important component of patients' follow-up. We have developed a liquid chromatog.-tandem mass spectrometry (LC-MS/MS) method for the simultaneous determination of the six major TKIs currently in use. Plasma samples are extracted with ethyl acetate and the supernatant is diluted in ammonium formate 20 mM (pH 4.0) 1:2. Reverse-phase chromatog. separation is performed on a C18 column with a linear gradient elution of 20 mM ammonium formate pH 2.2 and acetonitrile containing 1% formic acid. The total run time is 30 min, with a 5 min gradient from 20% acetonitrile to the initial solvent composition up to 20 min. Analyte quantification, using matrix-matched calibration curves, is performed by electrospray ionization-triple quadrupole mass spectrometry by selected reaction monitoring detection. The method is fully validated according to FDA recommendations, including assessment of extraction yield, matrix effect, precision (90.1-104.2%), accuracy (87.1-104.2%), as well as TKIs short- and long-term stability in plasma. The method is accurate (-9.2 to +9.9%) and sensitive (lower limits of quantification comprised between 1 and 10 ng/ml). This is the first assay covering the major currently in-use TKIs. It is an improvement over previous methods in terms of convenience (a single extraction step), selectivity and sensitivity. It may contribute to filling the current knowledge gaps in the pharmacokinetics/pharmacodynamics of these drugs and help to define their therapeutic ranges in different patient populations. The use of these anticancer drugs could contribute to minimize the side effects and to improve the lasting therapeutic response.

Keywords: imatinib nilotinib dasatinib sunitinib sorafenib lapatinib targeted anticancer drugs drug monitoring

[View Source](#)

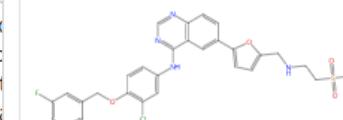
[Full Text](#)

[View in CAS Analytical Methods](#)

### Substances

#### Substances (7)

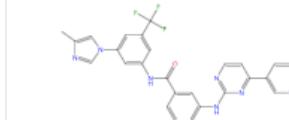
231277-92-2



C29H26ClFN4O4S  
Lapatinib

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

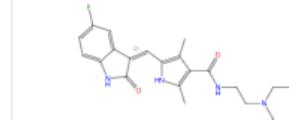
641571-10-0



C28H22F3N7O  
Nilotinib

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

557795-19-4



Double bond geometry shown

C22H27FN4O2  
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

[Download](#) [Save](#)

CAS Method Number	Method Category	Technique			
1-101-CAS-181855	Active Pharmaceutical Ingredient and Metabolite Analysis	HPLC-tandem mass spectrometry; Extraction			
Analyte	Matrix	Material	Reagent	Biological Reagent	Source
Dasatinib Imatinib mesylate Lapatinib Nilotinib Sorafenib	Blood plasma	2.1 mm x 50 mm XTerra dC18 5 $\mu$ m analytical column	-	-	<b>JOURNAL</b>  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 <a href="#">View Abstract</a> <a href="#">Full Text</a>
Validation					
<b>Linearity Range</b> 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					
<b>Limit of Detection</b> 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					
<b>Limit of Quantitation</b> 1 ng/mL, Imatinib 1 ng/mL, Dasatinib 1 ng/mL, Nilotinib 1 ng/mL, Sunitinib 10 ng/mL, Sorafenib 5 ng/mL, Lapatinib					
<b>Accuracy</b> 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					
<b>Precision</b> 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					

### 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  $\mu$ L) with a 100  $\mu$ L of internal standard solution.
2. Subject the resulting sample to protein precipitation with acetonitrile (600  $\mu$ L) 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  $\mu$ L aliquot of the supernatant and 400  $\mu$ L 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.

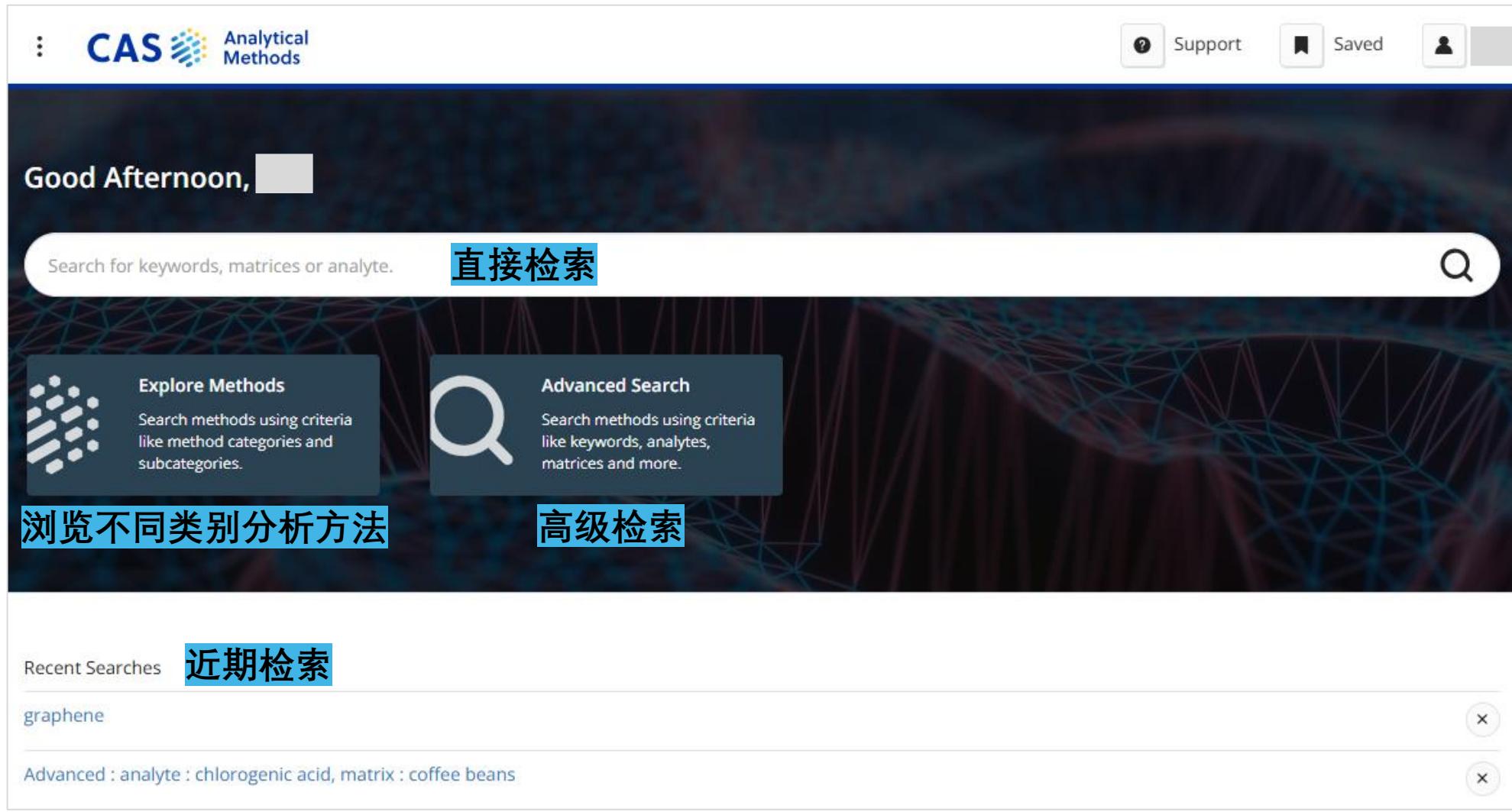
#### LC-MS/MS analysis of the extracted plasma samples

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 Fisher Scientific Inc, Waltham, MA).
2. Separate the analytes on a 2.1 mm x 50 mm XTerra dC18 5  $\mu$ m 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 Fisher 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).



# 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, a search bar containing the text "直接检索" (Direct Search), and links for "Support", "Saved", and a user profile. Below the search bar, there are two main search options: "Explore Methods" (Search methods using criteria like method categories and subcategories) and "Advanced Search" (Search methods using criteria like keywords, analytes, matrices and more). The background features a dark, abstract geometric pattern. At the bottom, there is a "Recent Searches" section with entries for "graphene" and "Advanced : analyte : chlorogenic acid, matrix : coffee beans", each with a delete button. The footer contains the text "© 2025 American Chemical Society. All rights reserved." and the CAS logo.

Good Afternoon, [redacted]

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 

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# 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…

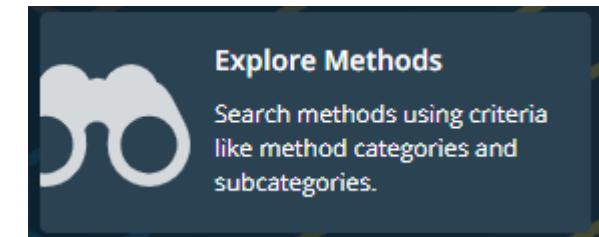
**Organic Compound Analysis:** 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…

**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…

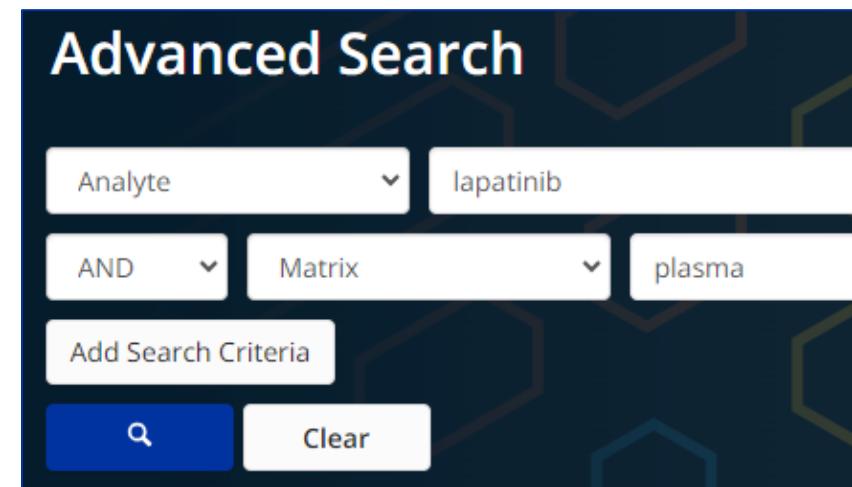


# 关键词检索分析方法

- 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

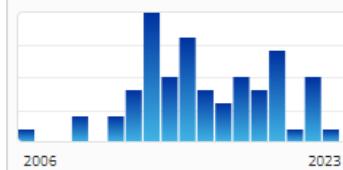
年份

^ Technique

- Atmospheric precipitation (13)
- Electrospray ionization tandem mass spectrometry (11)
- Ultra-performance liquid chromatography (11)
- HPLC (10)
- Liquid chromatography diode array detectors (9)

View All

^ Year



## Results for lapatinib

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

JOURNAL

Compare

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; Photodiode array (PDA) detector; pH

meter; Ultra Sonicator; Analytical balance

View Abstract ▾

Full Text ▾

View in CAS SciFinder

2

### Analysis of Lapatinib by Microplate spectroscopy

JOURNAL

Compare

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

对比不同分析方法

# 对照多个感兴趣的分析方法详情

Comparing your 2 selected Methods

		Format <input checked="" type="radio"/> PDF <input type="radio"/> XLS	Download	Cancel
			Download	
	Method 1	Method 2		
	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 $\mu$ )		
Equipment Used	Microplate reader, 550, Bio-Rad Laboratories, Hercules, CA, USA	Ultra performance liquid chromatography (UPLC) system, SHIMADZU; Autosampler, SHIMADZU; Phtodiode array (PDA) detector, SHIMADZU; pH meter, Labindia; Ultra Sonicator; Analytical balance, SHIMADZU		
Conditions	Instrument: detection wavelength: 570 nm	-		
Preparation	<p>Collection of <b>lapatinib</b> and gemcitabine sample</p> <ol style="list-style-type: none"> <li>1. Collect <b>lapatinib</b> and gemcitabine samples.</li> <li>2. Dissolve <b>lapatinib</b> in methanol and dissolve gemcitabine in phosphate buffered saline (PBS).</li> <li>3. Dilute in Dulbecco's modified Eagle's medium (DMEM) to the required concentrations immediately before use.</li> </ol>	<p>Preparation of 0.1% ortho phosphoric acid (OPA) buffer pH 3</p> <ol style="list-style-type: none"> <li>1. Add 1 mL of ortho phosphoric acid in 1000 mL water.</li> <li>2. Adjust this solution to pH 3 by using sodium hydroxide.</li> </ol> <p>Preparation of mobile phase</p> <ol style="list-style-type: none"> <li>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.</li> <li>2. Filter through 4.5 <math>\mu</math> filter under vacuum filtration.</li> </ol> <p>Diluents preparation</p> <ol style="list-style-type: none"> <li>1. Prepare the diluents with 0.1% OPA buffer:acetonitrile (30:70) ratio.</li> </ol>		
			<p>Instructions</p> <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) (Nikkien 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 <math>\mu</math>L/well.</li> <li>2. Expose the cell to drugs for 48 h.</li> <li>3. Add 10 <math>\mu</math>L 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 <math>\mu</math>L/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>Bioactivity</b></p> <p>7.5 <math>\mu</math>M (IC<sub>50</sub>, MiaPaca-2 cell line), <b>Lapatinib</b>, 4.5 <math>\mu</math>M (IC<sub>50</sub>, PANC-1 cell line), <b>Lapatinib</b>, 2.7 <math>\mu</math>M (IC<sub>50</sub>, MiaPaca-2 cell line), Gemcitabine, 0.25 <math>\mu</math>M (IC<sub>50</sub>, PANC-1 cell line), Gemcitabine</p> <p><b>Linearity Range</b></p> <p>-</p> <p><b>Limit of Detection</b></p> <p>-</p> <p><b>Limit of Quantitation</b></p> <p>-</p> <p><b>Accuracy</b></p> <p>-</p> <p><b>Precision</b></p> <p>-</p> <p><b>Source</b></p> <p><b>JOURNAL</b></p> <p><i>In vitro effects of <b>lapatinib</b> with gemcitabine for pancreatic cancer cells</i> By: Murata, Akihiro; Nakata, Bunzo; Komoto, Masahiro; Hirata, Keiichiro; Kimura, Kenjiro; Amano, Ryosuke; Hirakawa, Kosei Hepato-Gastroenterology (2013), 60 (126), 1484 - 1487.</p> <p><b>JOURNAL</b></p> <p><i>Analytical method validation report for assay of <b>Lapatinib</b> by UPLC</i> By: Biswal, Sabysachi; Mondal, Sumanta Pharmaceutical Methods (2019), 10 (1), 9 - 14.</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

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, Qiu-jin; Wang, Li-rong; Zhang, Xiao-nan; Ding, Yue-jia; Li, Hao; Yang, Ying-xi; Zhang, Ao; Li, Yan-yan; Lv, Shi-chao; Zhang, Jun-ping  
Pharmacological Research (2020), 151, 104552 | Language: English, Database: CPlus 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: CPlus 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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^ CAS Content

Analytical Methods (8)

Formulations (3)

^ Formulation Purpose

Cardiovascular agents (3)

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

0 0 0 Citation Map

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

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

Keywords: myocardial hypertrophy prevention traditional Chinese medicine composition

PatentPak PDF Get Prior Art Analysis Full Text View in CAS Formulus

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	PDF	2021-01-08	CN2020-11207191	2020-11-03

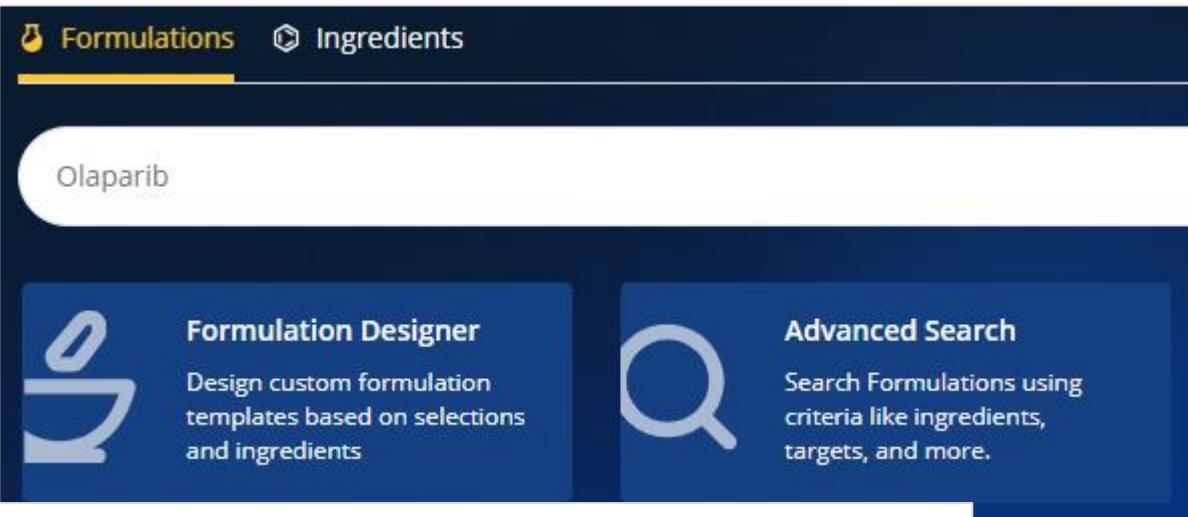
# 直接检索制剂/配方或配方成分

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 shows the CAS Formulus homepage with a dark blue header. The header includes the CAS Formulus logo, a user profile placeholder, and links for Help & Support, Alerts, Saved, and a user icon. The main content area starts with a greeting "Good Afternoon, [redacted]". Below it are two navigation tabs: "Formulations" (highlighted in yellow) and "Ingredients". A search bar contains the placeholder "Search by Formulations by Ingredients, Purpose, Form, Functions, etc." and a large blue button labeled "直接检索" (Direct Search). Below the search bar are two buttons: "Formulation Designer" (with a dropper icon) and "Advanced Search" (with a magnifying glass icon). The "Formulation Designer" button has the text "Design custom formulation templates based on selections and ingredients". The "Advanced Search" button has the text "Search Formulations using criteria like ingredients, targets, and more." At the bottom of the page, there is a "Recent Search History" section titled "近期检索" (Recent Search) with a timestamp "November 20, 2024" and a search entry "12:41 PM Formulations PEG (1020195)". It includes "Rerun Search" and "Edit Search" buttons. A "View Search History" link is also present.

# 关键词检索制剂/配方

- 直接检索示例：  
Olaparib 奥拉帕尼



The screenshot shows the 'Formulations' search interface. At the top, there are two tabs: 'Formulations' (highlighted in yellow) and 'Ingredients'. Below the tabs, the search bar contains the text 'Olaparib'. Underneath the search bar, there are two main sections: 'Formulation Designer' (with an icon of a beaker and a swirl) and 'Advanced Search' (with an icon of a magnifying glass). The 'Advanced Search' section is expanded, showing the 'Advanced Formulations Search' interface. This interface includes two search fields: the first for 'Ingredient' (set to 'Olaparib') and the second for 'Form' (set to 'Tablets'). Both fields have dropdown menus for 'Search For' and 'Operator'. Below these fields are buttons for 'Add Another Term', 'Search', and 'Clear All'.

- 高级检索示例：  
奥拉帕尼片剂

# 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)

View All

Information Included

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

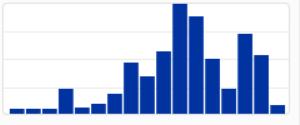
View All

Physical Form

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

View All

Publication Year



2007 2023

No Min to No Max Apply

Formulations search for "Olaparib" Get Additional References 一键获取相关文献

Compare (0/3) Save Sort: Relevance ▾

Filter by  639 Results

Industry  Food & Related  Pharmaceutical  Unclassified

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

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

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

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

Full Text ▾ View in CAS SciFinder

获取报道该配方的文献

# 制剂、配方详情

 Olaparib Solid Dispersion: Antitumor Agents

[!\[\]\(1c96958c73cc6fbd0a116c5b9f7c147f\_img.jpg\) Save](#)

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

① Predicted value

**制剂成分、功能、用量**

Component	Function	Amount Reported	Optionality
Olaparib	poly(ADP-ribose) polymerase inhibitor <sup>①</sup>	200 g	Mandatory
Vinyl acetate-vinylpyrrolidone copolymer	carrier <sup>①</sup> , polymeric stabilizer <sup>①</sup>	800 g	Mandatory

More Formulations like this...

<a href="#">Lincomycin Solid Dispersion: Veterinary Drug</a> Purpose: Veterinary drugs Target: Homo sapiens, Livestock, Poultry Delivery Route: - Physical Form: Pharmaceutical solid di...	<a href="#">Olaparib Dispersible Tablets: Antitumor Agents</a> Purpose: Antitumor agents Target: Homo sapiens, Mammary glan... Delivery Route: Oral drug delivery syst... Physical Form: Pharmaceutical orally d...	<a href="#">Olaparib Dispersible Tablets: Antitumor Agents</a> Purpose: Antitumor agents Target: Homo sapiens, Mammary glan... Delivery Route: Oral drug delivery syst... Physical Form: Pharmaceutical orally d...	<a href="#">Lincomycin Solid Dispersion: Veterinary Drug</a> Purpose: Veterinary drugs Target: Homo sapiens, Livestock, Poultry Delivery Route: - Physical Form: Pharmaceutical solid di...
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**Source Patent**

[Olaparib solid dispersion and preparation method thereof](#)

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

[Patent PDF](#) [View in CAS SciFinder](#)

**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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中文

全部  题名  作者

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维普数据库 Elsevier ScienceDirect 中华医学会期刊全文数据库(IP登录) SciFinder

1、登录学校图书馆官网，在“电子资源”中点击“SciFinder”。

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#### 一、数据库链接

访问链接: <https://scifinder-n.cas.org/>

账号注册地址: <https://scifinder.cas.org/registration/index.html?corpKey=4A9382C4X86F350ABX229D311A5663BB09AC>

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演示。

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1. 如果进入系统后20分钟没有操作，系统将自动断开您与服务器的连接。
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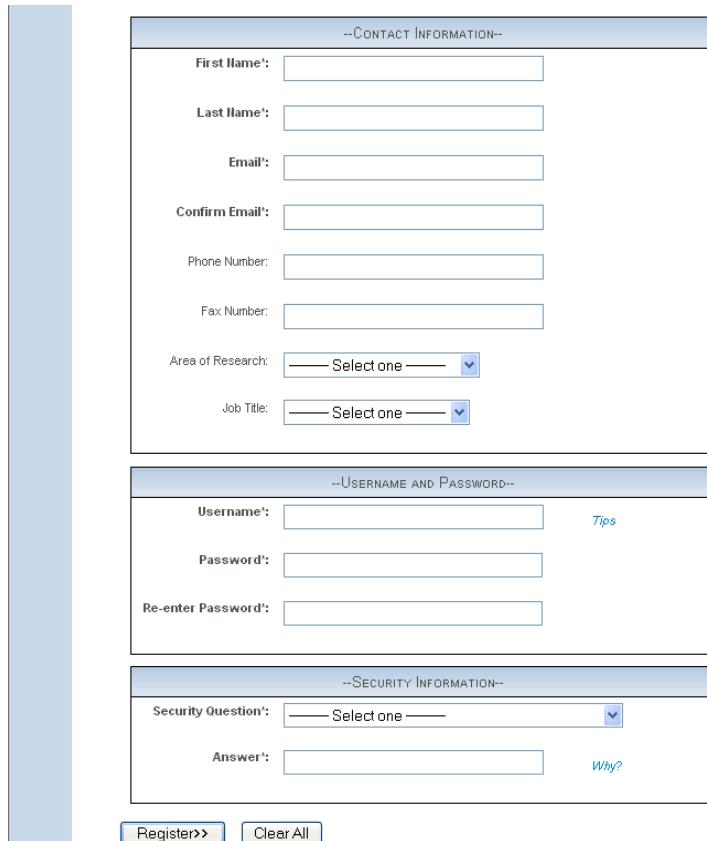
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1. 必须输入真实姓名和**学校**邮箱。
2. 用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：
  - - (破折号)
  - \_ (下划线)
  - . (句点)
  - @ (表示“at”的符号)
3. 密码必须包含 7-15 个字符，并且至少包含**三种以下字符**：
  - 字母
  - 混合的大小写字母
  - 数字
  - 非字母数字的字符 (例如 @、#、%、&、\*)

例：abc@123

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



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First Name\*:

Last Name\*:

Email\*:

Confirm Email\*:

Phone Number:

Fax Number:

Area of Research:

Job Title:

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Re-enter Password\*:

Tips

--SECURITY INFORMATION--

Security Question:

Answer\*:

Why?

Register>> Clear All

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You have already completed your registration. For assistance with accessing SciFinder, consult the key contact for your organization.

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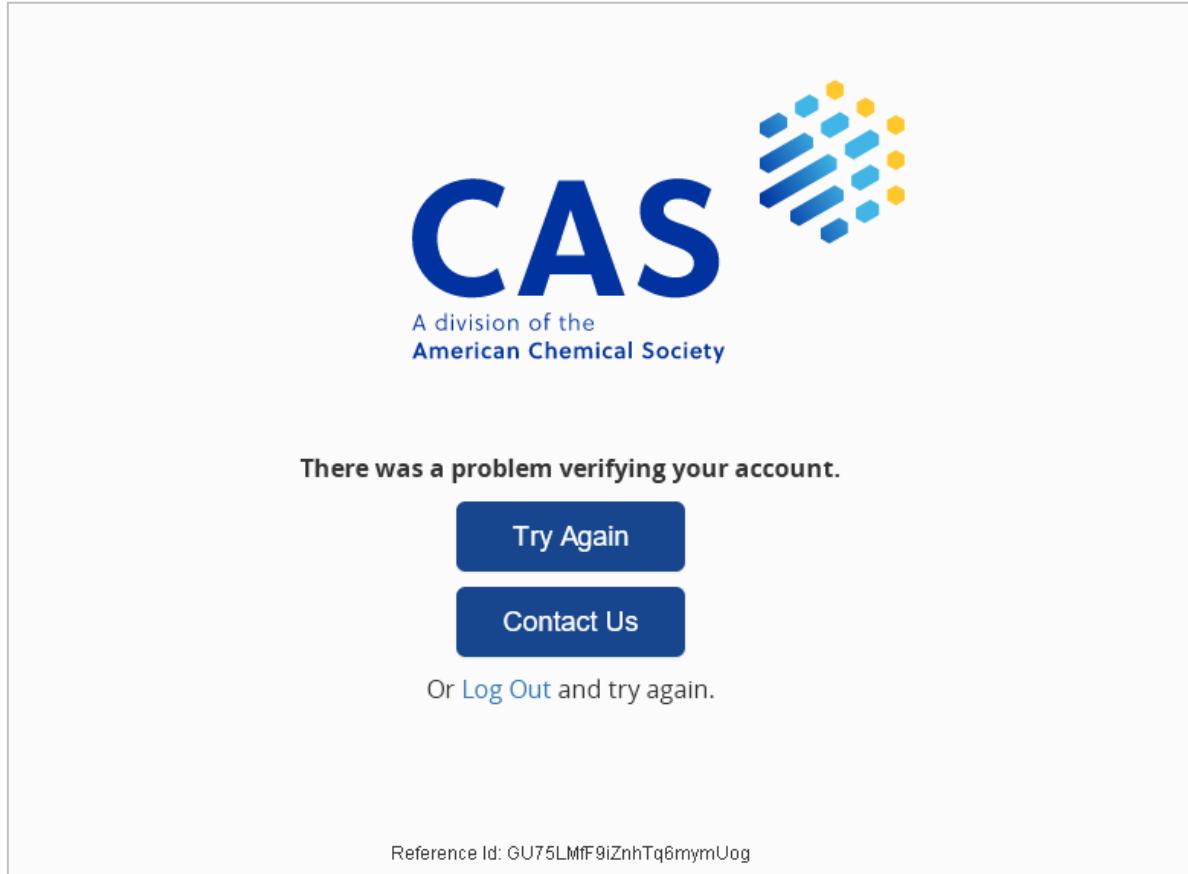
# 常见注册问题

## Unauthorized IP Address

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

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- 确认连入校园网，且不是通过VPN连接
- 如果链接正确，且在校园内，请联系图书馆或  
China@acs-i.org

# 常见登录问题



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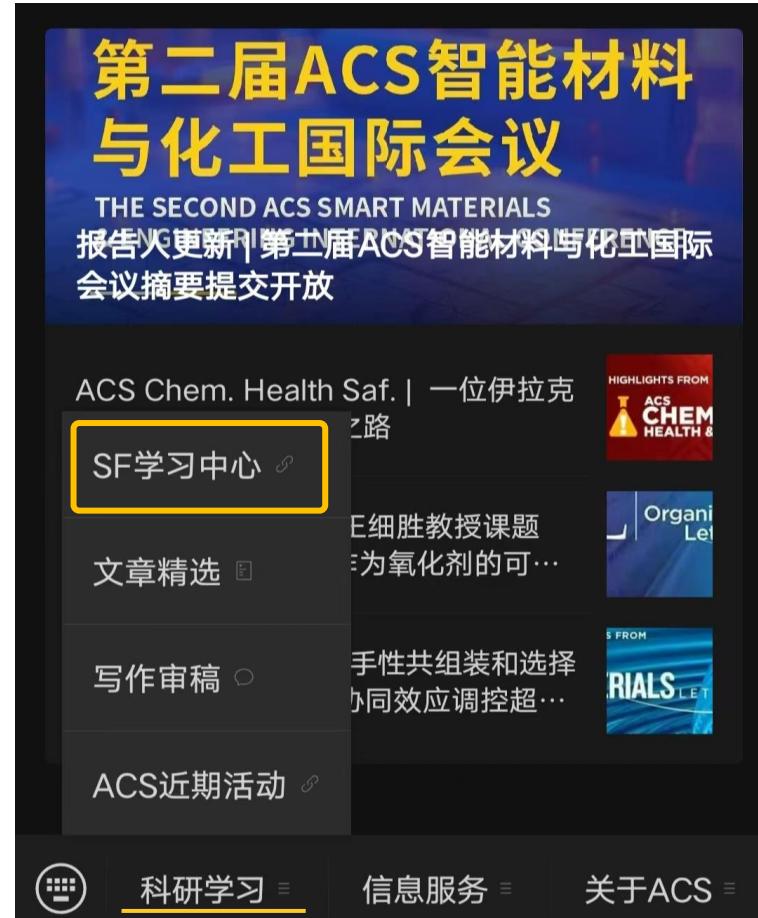
- Windows (7, 8.1, 10): Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13): Safari 9.3及更高版本, Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)
- 不建议使用360浏览器，相关功能或插件会被自动拦截

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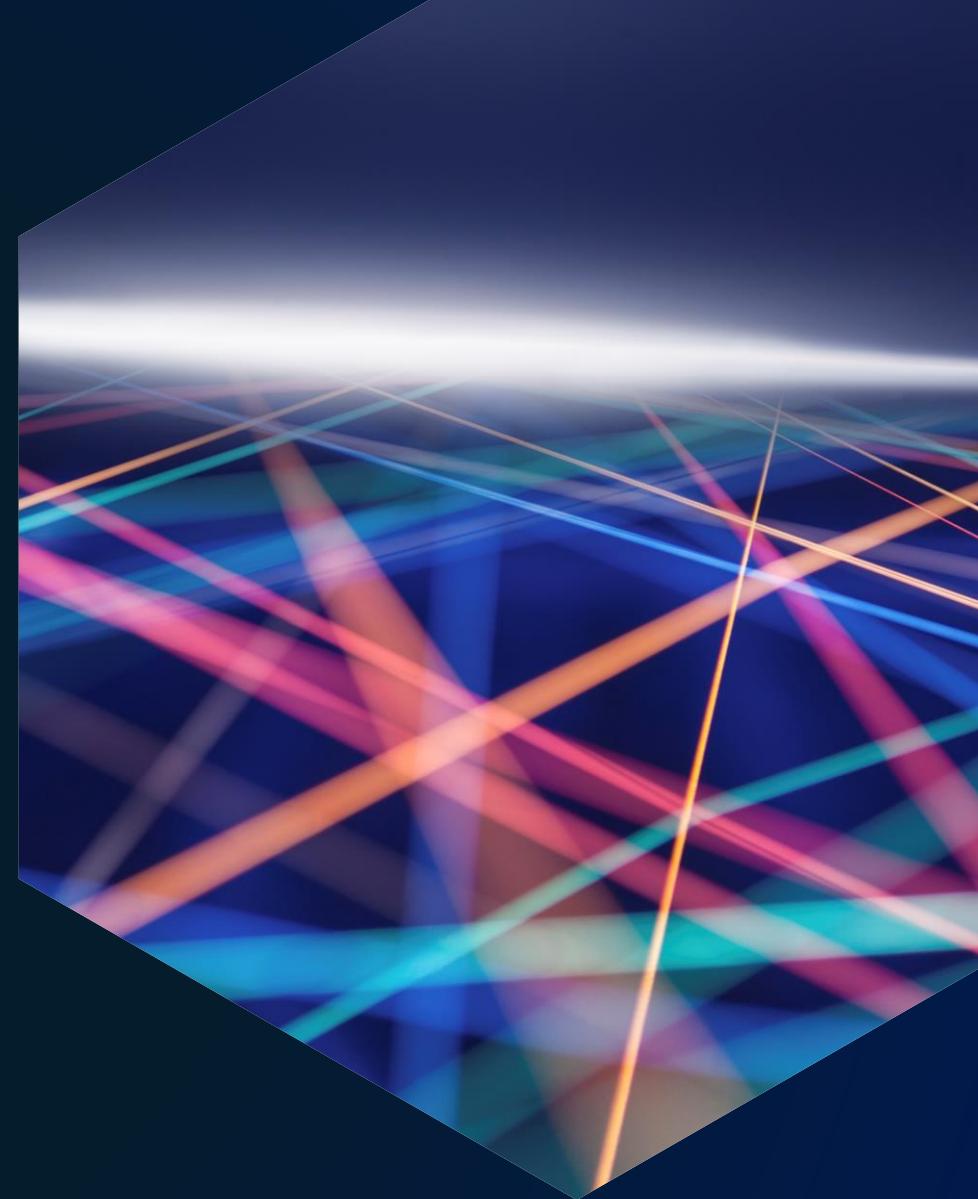
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- 各领域中特有的分子结构怎么画？
- 精心设计的分子有没有被他人报道过？
- 如何灵活绘制结构，分析目标化合物及相似结构在专利中的布局？
- 如何设计合成路线策略，优化绿色安全的制备工艺？
- 已制备的材料，如何实现应用上的突破？
- 如何高效管理和协作多个并行课题？

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# CAS SCIFINDER DISCOVERY PLATFORM™

## 2025 春季专题论坛直播时间表



3月 21 日 | 零基础入门

演讲人：刘子露 博士



3月 28 日 | 解锁新功能

演讲人：杜德鑫 博士



4月 18 日 | 助攻论文写作

演讲人：潘娜 博士



4月 25 日 | 探索科研成果转化

演讲人：钱欣 博士



5月 9 日 | 结构绘制面板  
及案例详解

演讲人：刘子露 博士



5月 23 日 | 反应检索策略及典  
型案例

演讲人：陈开乾 博士

“

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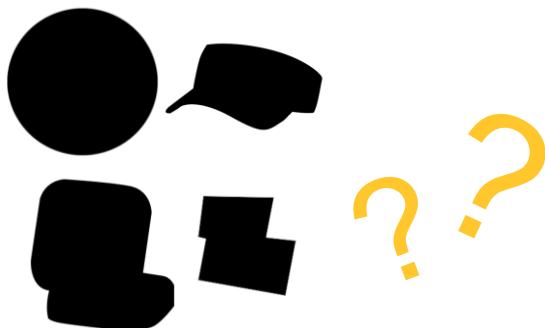
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and progress  
are connections  
that matter



谢谢！

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