

# 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及CAS SciFinder Discovery Platform (Academic)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



# CAS 具有最全面的学科连接内容合集



Over  
**50K**  
scientific journals  
and documents

Over  
**274**  
million substances

Over  
**50**  
languages  
translated

Over  
**109**  
patent offices  
worldwide

# CAS 独特的内容合集

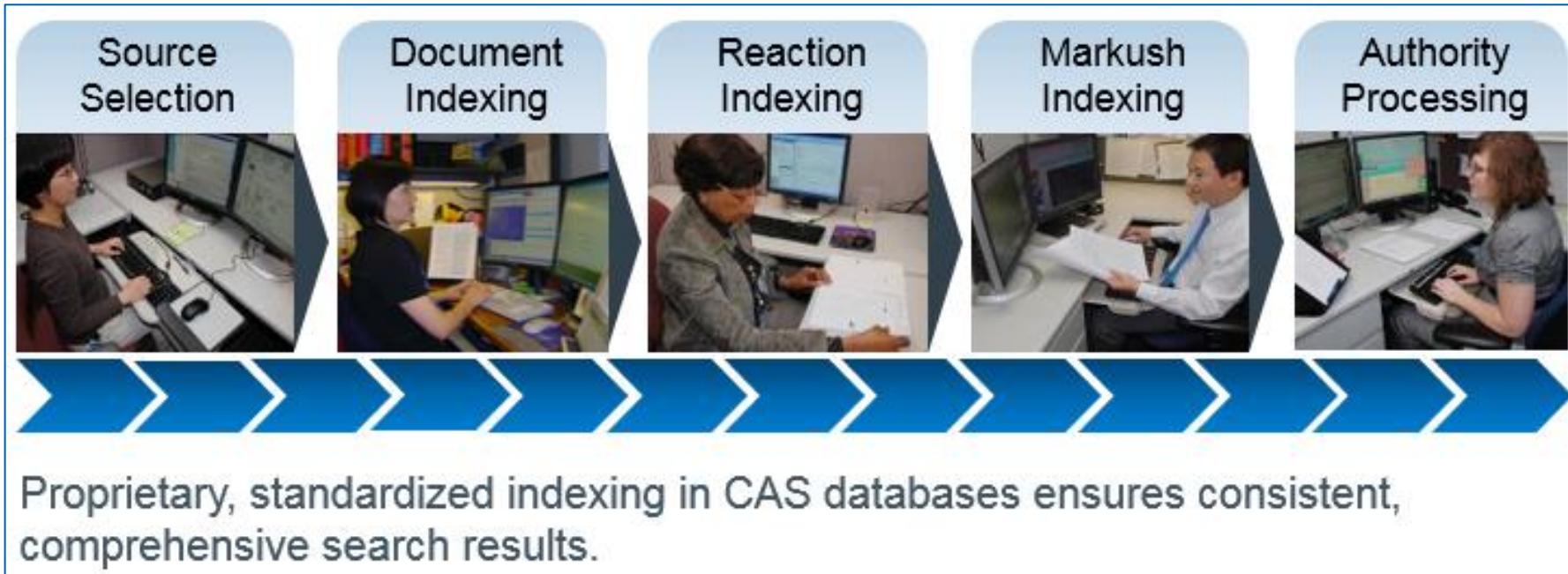


来源：

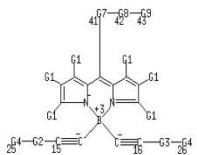
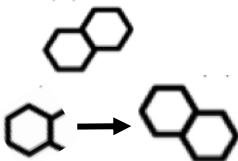
<https://www.cas.org/cas-data>

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

# CAS 科学家的智力标引



1990  
Smith, M.  
anthracene



Androst-4-en-3-one,  
17-hydroxy-17-  
methyl-, (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 解决方案与服务



Discovery

## CAS SciFinder Discovery Platform™

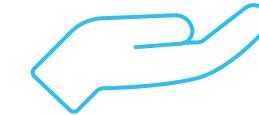
Get discoveries to market faster and optimize margins by giving researchers the information they need



Intellectual Property

## STN IP Protection Suite™

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



Custom Solutions

## CAS Custom Services™

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

# CAS SciFinder Discovery Platform 解决方案

## CAS SciFinder<sup>n</sup> —— 加速科学发现的业界领先的科学工具

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

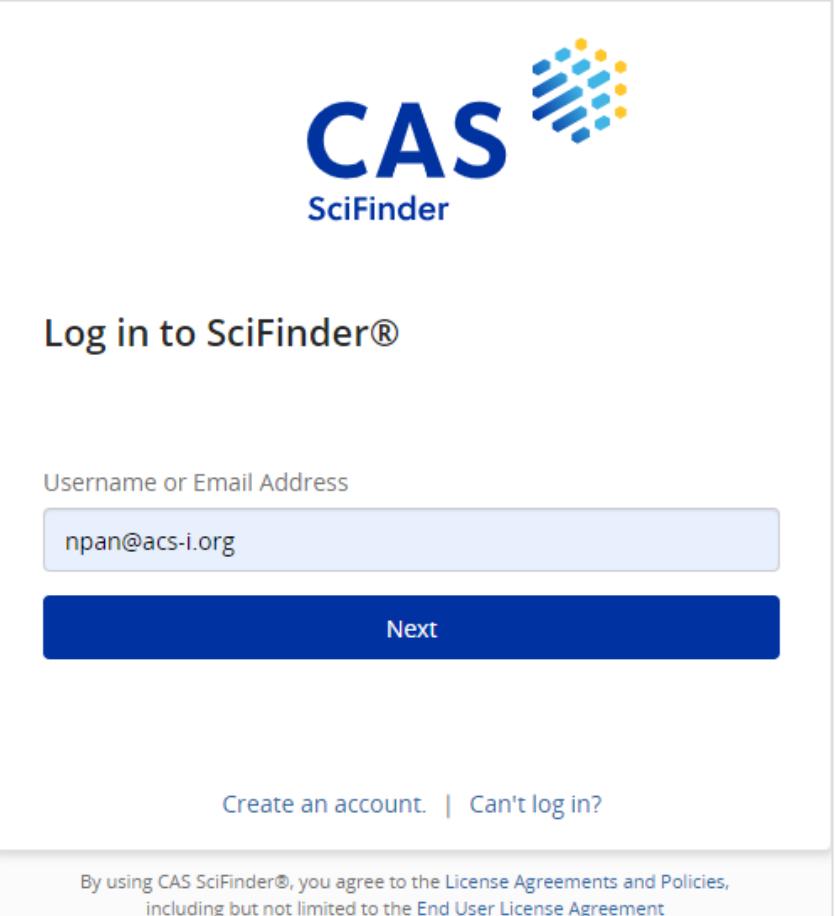
## CAS Analytical Methods<sup>TM</sup> —— 借助CAS科学家深度加工的科学方法，提升研究效率

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

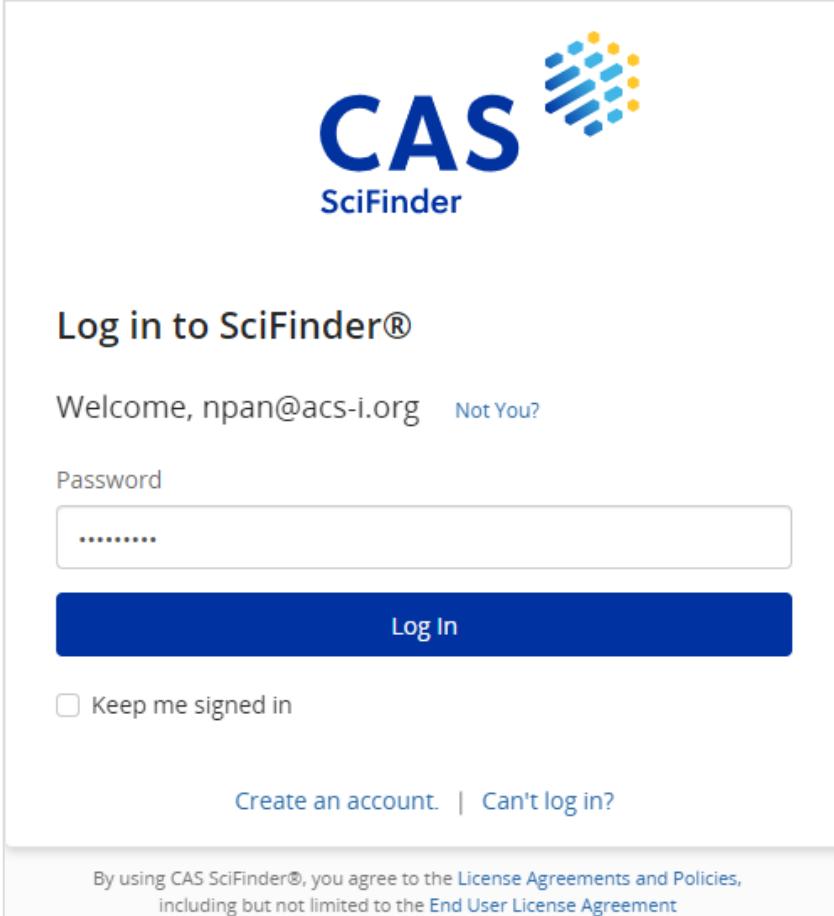
## CAS Formulus<sup>®</sup> —— 助力开发安全、有效的产品

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

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



The screenshot shows the first step of the login process. It features the CAS SciFinder logo at the top left. Below it is a large "Log in to SciFinder®" button. Underneath this button is a text input field labeled "Username or Email Address" containing "npan@acs-i.org". A blue "Next" button is positioned below the input field. At the bottom of the screen, there are links for "Create an account." and "Can't log in?". A small note at the very bottom states: "By using CAS SciFinder®, you agree to the License Agreements and Policies, including but not limited to the End User License Agreement".



The screenshot shows the second step of the login process. It features the CAS SciFinder logo at the top left. Below it is a large "Log in to SciFinder®" button. Underneath this button is a text input field labeled "Password" showing a masked password. To the right of the password field is a link "Not You?". A blue "Log In" button is positioned below the password field. Below the "Log In" button is a checkbox labeled "Keep me signed in". At the bottom of the screen, there are links for "Create an account." and "Can't log in?". A small note at the very bottom states: "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 登录主界面

丰富的CAS解决方案，灵活的检索角度

The screenshot displays the main interface of the CAS SciFinder 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 area features a "Good Morning, [User]" greeting and a search bar for substances, reactions, references, and suppliers. A yellow arrow points to the three-dot menu icon in the top right. Other highlighted features include "更新结果提醒" (Update results reminder), "结构绘制面板" (Structure drawing panel) with a "Draw" button, "高级检索选项" (Advanced search options), "逆合成路线设计" (Retrosynthetic analysis), "CAS词库" (CAS Lexicon), "CAS序列检索" (Search CAS Sequences), and "Recent Search History" (近期检索历史) with a "View All Search History" link.



# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)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?
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  - 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 the following elements:

- Top navigation bar: All, Substances, Reactions, References (highlighted), Suppliers.
- Search bar: "boron n".
- Search results dropdown:
  - boron nitride
  - Boron nitrate
  - Boron nitride (BN)
  - Boron nickel oxide
  - Boron nitride oxide
  - Boron niobium oxide
  - Boron nitride fibers
  - Boron nitrogen oxide
- Main search area:
  - Search query: ("boron nitride" or BN) and (2D or "two dimensional")
  - Boolean operator: AND
  - Author Name field: Enter last name, first name middle name. Example: Schubert, J A
  - Add Advanced Search Field button

# 1.1 如何精准构建检索主题?

主题词示例：

(poly\* not polyethylene) and “conductive device” (聚合物但排除聚乙烯，导电装置)

References search for "poly\* not polyethylene"

Substances Reactions Citing Knowledge Graph

Filter Behavior

20,116,548 Results

1

Electrophoretic transfer of proteins from procedure and some applications

By: Towbin, Harry; Staehelin, Theophil; Gordon, Julian  
Proceedings of the National Academy of Sciences of the U.S.A., 1980, 77(12), 7200-7204 | Language: English, Database: CPlus and MEDLINE  
A method was devised for the electrophoretic transfer of proteins in quant. transfer of ribosomal proteins from gels obtained with no loss of resolution, but the transfer was not simpler than conventional procedures. The immobilization capacity on the nitrocellulose was blocked with excess pro

View More

Full Text Substances

2

Polymer photovoltaic cells: enhanced efficiency heterojunctions

By: Yu, G.; Gao, J.; Hummelen, J. C.; Wudl, F.; Heeger, A. J. Science (Washington, D. C.) (1995), 270(5243), 1789-91 | Language: English, Database: CPlus  
The carrier collection efficiency ( $\eta_c$ ) and energy conversion of the semiconducting polymer with  $C_{60}$  or its functionalized hexyloxy)-1,4-phenylene vinylene (MEH-PPV) and fullerene 2.9 percent, efficiencies that are better by more than two times made with pure MEH-PPV. The efficient charge separation

View More

References search for "(poly\* not polyethylene) and "conductive device""

Substances Reactions Citing Knowledge Graph

199 Results

1

Liquid Metal Droplets Wrapped with Polysaccharide Microgel as Biocompatible Aqueous Ink for Flexible Conductive Devices

By: Li, Xiankai; Li, Mingjie; Zong, Lu; Wu, Xiaochen; You, Jun; Du, Peikang; Li, Chaoxu | Advanced Functional Materials (2018), 28(39), n/a | Language: English, Database: CPlus  
Nanometerization of liquid metal in organic systems can facilitate deposition of liquid metals onto substrates and then recover its conductivity through sintering. Although having broader potential applications, producing stable aqueous inks of liquid metals keeps challenging because of rapid oxidation of liquid metal when exposing to water and oxygen. Here, a biocompatible aqueous ink is produced by encapsulating alloy nanodroplets of gallium and indium (EGaIn) into microgels of marine polysaccharides. During sonication bulk EGaIn in aqueous alginate solution, alginate not only facilitates th...

View More

Full Text Substances (4) Reactions (0) Citing (48) Citation Map

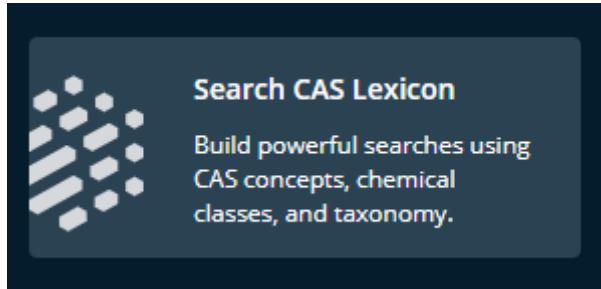
2

Conductive polymers and devices

By: Vannikov, A. V. | Vysokomolekulyarnye Soedineniya, Seriya A i Seriya B (2009), 51(4), 547-571 | Language: Russian, Database: CPlus  
A review. Classes of polymeric conductors, mechanisms of conductivity, optical properties, and photophys. properties of thin polymeric films and devices based on them were considered.

Full Text Substances (0) Reactions (0) Citing (9) Citation Map

# 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

Primary batteries ?  
This will search synonyms: Nonrechargeable **batteries**; Primary bat...

Broader Concepts (1) Select All  
 Batteries ?

Narrower Concepts (10) Select All  
 Button-type primary batteries  
 Dry cell primary batteries  
 Lithium primary batteries ?  
 Nuclear batteries  
 Primary batteries, reserve  
[View All](#)

Related Concepts (4) Select All  
 Battery electrodes ?  
 Battery electrolytes  
 Electrolytic capacitors

AND OR NOT Add to Query Clear Query Search

Primary batteries - Preferred Concept ? X

OR Remove All

Primary batteries - Narrower Concept (1)  
 Primary batteries - Related Concept (1)

主题词示例：  
primary batteries (干电池)

- 干电池的上位词
- 干电池的下位词
- 干电池相关词汇

# 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)

**+ 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

Example: Schubert, J A

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：关注锂电池技术中特定的热点材料

策略：从References出发，主题词+结构联用检索

Substance Role

By Count Alphanumeric

1 Selected

Uses (1,368)

Technical or Engineered Material Use (1,237)

Properties (255)

Physical, Engineering, or Chemical Process (178)

Process (178)

Modifier or Additive Use (83)

Other Use, Unclassified (72)

Reactant or Reagent (56)

Reactant (50)

Preparation (39)

Industrial Manufacture (20)

Synthetic Preparation (19)

Reagent (6)

Nanoscale (5)

Purification or Recovery (4)

Analyte (2)

Apply Cancel

定位物质在文献中的研究角色

文本与结构是“and”关系

CAS SciFinder References ("lithium battery" or "lithium-ion battery" or "Li-ion batt") Edit Q

Return to Home References search for ("lithium battery" or "lithium-ion battery") Substances Reactions Citing Knowledge Graph

Structure Match As Drawn (1,454) Substructure (1,454)

Filter Behavior Filter by Exclude

Document Type Journal (348) Patent (1,098) Review (7) Preprint (8)

Substance Role Uses (1,368) Properties (255) Process (178) Reactant or Reagent (56) Preparation (39) View All Language English (673)

1 Pyrrolinium-based Ionic Liquid as a Flame Retardant for Binary Electrolytes of Lithium-ion Batteries By: Kim, Hyung-Tae; Kang, Jaesik; Mun, Junyoung; Oh, Seung M.; Yim, Tae-eun; Kim, Young Gyu ACS Sustainable Chemistry & Engineering (2016), 4(2), 497-505 | Language: English, Database: CPlus Ionic liquid (IL)-based electrolytes have attracted much attention to enable safe Li ion batteries (LIBs) owing to their inflammability and thermal stability as well as their high conductivity and wide electrochemical stability. However, because of the interruption of Li ion mobility during a charge/discharge process, ILs as the only electrolyte solvent could not be efficient. To improve both the Li ion mobility and the safety issue of LIBs, the authors suggest new binary electrolytes that consist of pyrrolinium-based IL and com. carbonate. The pyrrolinium-based IL is characterized by some tasks... View More Full Text

2 Anionic Effect on Enhancing the Stability of a Solid Electrolyte Interphase Film for Lithium Deposition on Graphite By: Yang, Gaojing ID; Zhang, Simeng; Weng, Suting; Li, Xiaoyun; Wang, Xuefeng ID; Wang, Zhaoxiang ID; Chen, Liqian Nano Letters (2021), 21(12), 5316-5323 | Language: English, Database: CPlus and MEDLINE Graphitic carbons and their lithium composites have been utilized as lithium deposition substrates to address issues such as the huge volume variation and dendritic growth of lithium. However, new problems have appeared, including the severe exfoliation of the graphite particles and the instability of the solid electrolyte interphase (SEI) film when metallic lithium is plated on the graphite. Herein, we enhance the stability of the SEI film on the graphite substrate for lithium deposition in an electrolyte of lithium bis(fluorosulfonyl)imide (LiFSI) dissolved in the carbonate solvent, thereby ...

# 1.3 文献结果分析与筛选

References search for 3 CAS Lexicon Concepts

Substances Reactions Citing Knowledge Graph

Filter Behavior Filter by Exclude

Search Within Results

Document Type Language Publication Year Author Organization Publication Name Concept CA Section CAS Solutions Formulation Purpose Database

Filter Content Report Download filter data from this result set

PatentPak Full Text Substances (13) Reactions (0) Citing (0) Citation Map

AI技术支持的相关度排序

Sort: Relevance View: Partial Abstract

80,812 Results

1 Ni-Co ternary nitrides with multiple surface oxides as bifunctional oxygen electrocatalysts for metal-air batteries

By: Chen, Xiaorong; Yu, Xinxing; Zhang, Guixin; Wei, Sisi; Huang, Youguo; Wang, Hongqiang; Jiang, Juantao; Ma, Zhaoling; Li, Qingyu  
Journal of Electroanalytical Chemistry (2024), 958, 118162 | Language: English, Database: CAplus

The bifunctional non-noble metal catalysts based on the metal nitrides with high activity and high efficiency is very challenging for the development of high-performance metal-air batteries. Herein, a new Ni-Co ternary nitrides anchored on nitrogen-doped carbontubes (denoted as NiCo<sub>x</sub>N/CNT) is rationally designed by the thermal of corresponding hydroxide/carbontubes at low temperature, following nitridation. The synergistic effect between Ni-Co ternary nitrides (Ni<sub>4</sub>N, Co<sub>5.47</sub>N, CoN) effectively regulates the electronic configuration of the active site, thereby optimizing the chemisorption energy...

View More

Full Text Substances (13) Reactions (0) Citing (0) Citation Map

2 Purification method for lithium bis(fluorosulfonyl)imide

Assignee: Novel Cosmos Advanced Material (Anhui) Co., Ltd.  
World Intellectual Property Organization, WO2024046025 A1 2024-03-07 | Language: Chinese, Database: CAplus

A purification method for Li bis(fluorosulfonyl)imide, comprising the following steps: adding a dehydrating agent into a pretreatment solution containing crude Li bis(fluorosulfonyl)imide, carrying out a dehydration reaction at 20°-40°, reacting for 1-6 h after no acidic gas escapes in the reaction system, and filtering to obtain a filtrate, wherein the dehydrating agent is Bi trichloride or Sb trichloride; and evaporating and concentrating the filtrate, and recrystallizing to obtain high-purity Li bis(fluorosulfonyl)imide.

Substances (18) Reactions (0) Citing (0) Citation Map

Save Results

Name: Battery

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

Add Existing Tags (Optional): Chinese Medicine Food Material Polymer SJTU Test

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.

结果集的二次检索



# 筛选工具 CA Section

## 纵览学科研究方向

- ^ CA Section
  - Electrochemical, Radiational, and Thermal Energy Technology (56K)
  - Electrochemistry (775)
  - Industrial Inorganic Chemicals (493)
  - Plastics Fabrication and Uses (402)
  - Electric Phenomena (374)

[View All](#) 

CA Section

By Count Alphanumeric

3 Selected

- Electrochemical, Radiational, and Thermal Energy Technology (56K)
- Electrochemistry (775)
- Industrial Inorganic Chemicals (493)
- Plastics Fabrication and Uses (402)
- Electric Phenomena (374)
- Plastics Manufacture and Processing (205)
- Ceramics (184)
- Chemistry of Synthetic High Polymers (140)
- Heterocyclic Compounds (More Than One Hetero Atom) (120)
- Nonferrous Metals and Alloys (110)
- Inorganic Analytical Chemistry (51)
- Physical Properties of Synthetic High Polymers (48)
- Biochemical Methods (45)
- Optical, Electron, and Mass Spectroscopy and Other Related Properties (42)
- Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms (40)
- Pharmaceuticals (38)
- Textiles and Fibers (36)
- Air Pollution and Industrial Hygiene (34)
- General Physical Chemistry (32)
- Fossil Fuels, Derivatives, and Related Products (31)
- Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (12)
- Thermodynamics, Thermochemistry, and Thermal Properties (10)
- Magnetic Phenomena (7)
- Nuclear Technology (6)
- Propellants and Explosives (6)
- Cement, Concrete, and Related Building Materials (5)
- Surface Active Agents and Detergents (5)
- Toxicology (5)
- Food and Feed Chemistry (4)
- Industrial Carbohydrates (4)
- Fertilizers, Soils, and Plant Nutrition (3)

OK Cancel

# 筛选工具 Concept

聚焦核心研究点

## ^ Concept

- Battery electrolytes (55K)
- Lithium-ion secondary batteries (25K)
- Battery cathodes (19K)
- Battery anodes (18K)
- Secondary batteries (10K)
- Ionic conductivity (5,913)
- Carbon nanostructured materials (20)

[View All](#)

Concept

Top Count   Alphanumeric   Search

2 Selected

- Battery electrolytes (55K)
- Lithium-ion secondary batteries (25K)
- Battery cathodes (19K)
- Battery anodes (18K)
- Secondary batteries (10K)
- Fluoropolymers (9,709)
- Battery electrodes (8,656)
- Carbon black (8,317)
- Secondary battery separators (6,196)
- Ionic conductivity (5,913)
- Lithium primary batteries (5,907)
- Solid electrolytes (4,625)
- Electric impedance (4,307)

OK   Cancel

Concept

Top Count   Alphanumeric   Search

精准定位核心研究点

支持使用通配符

Concept Name

nano\*

3 Selected

- Carbon nanofibers (376)
- Carbon nanostructured materials (20)
- Nanoparticles (2,011)
- Coating materials (1,850)
- Electric capacitance relationship (1,850)
- Solid-state secondary batteries (1,808)
- Diffusion (1,706)
- Thermal stability (1,666)
- Density functional (1,666)
- Raman spectra (1,646)
- Binding energy (1,646)
- Sodium-ion secondary batteries (1,646)
- Electric conductors (1,622)
- Electric resistance (1,582)
- Electrodeposition (1,520)
- Nanocrystallites (7)
- Nanocrystallization (3)
- Nanocrystals (197)
- Nanocubes (39)
- Nanocylinders (1)
- Nanodevices (9)
- Nanodisks (18)
- Nanodispersions (2)
- Ferromagnetic nanoparticles (1)
- Nanodots (20)
- Nanodroplets (1)
- Nanoelectrodes (10)
- Nanoplates (50)
- Nanopore (94)
- Nanopores (1)
- Nanoporous films (8)
- Nanoporous materials (87)
- Nanopowders (69)
- Nanoreactors (7)
- Nanoribbons (52)
- Nanorings (3)
- Nanorods (274)
- Nanoscale analysis (3)

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 Solutions

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

1901 2024 (53K)

OK Cancel

Concept 文献核心研究点

Battery electrolytes, Lithium-ion..., Battery cathodes, Secondary batteries, Fluoropolymers, Battery electrodes, Carbon black, Secondary battery..., Ionic conductivity

CA Section 学科研究方向分布

Electrochemistry, Industrial Inorganic..., Plastics Fabrication..., Electric Phenomena, Ceramics, Chemistry of..., Heterocyclic..., Nonferrous Metals..., Inorganic Chemicals...

Download Reference Filter Content

File Type: Excel (.xlsx) Select Quantity: All Filter Values

File Name: Reference\_Filters\_20240524\_1532

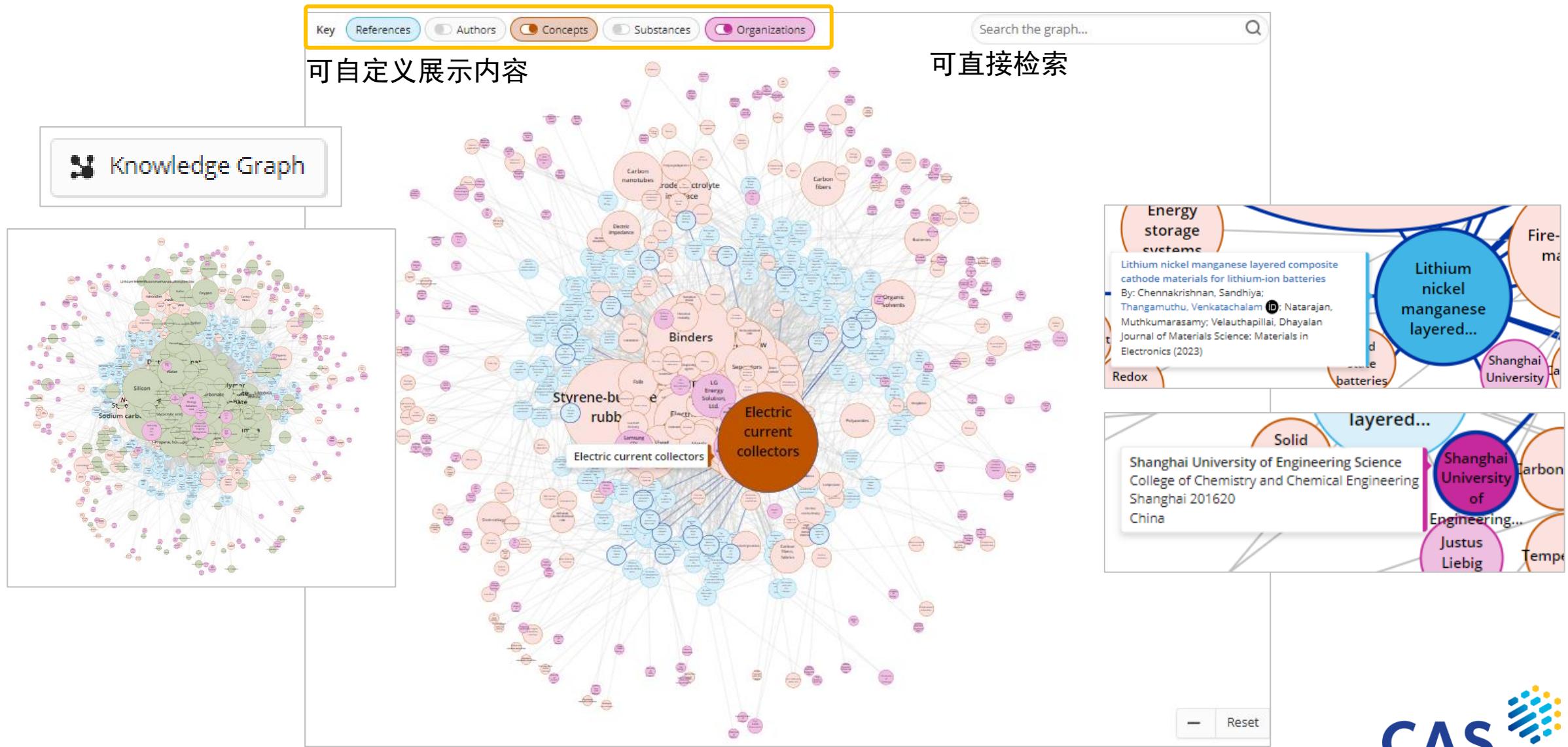
Only the top 1,000 filter values will be downloaded.

Filters:

Document Type  Concept  
 Language  CA Section  
 Publication Year  CAS Solutions  
 Author  Bioactivity Data  
 Organization  Formulation Purpose  
 Publication Name  Database

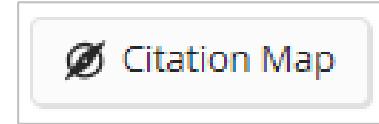
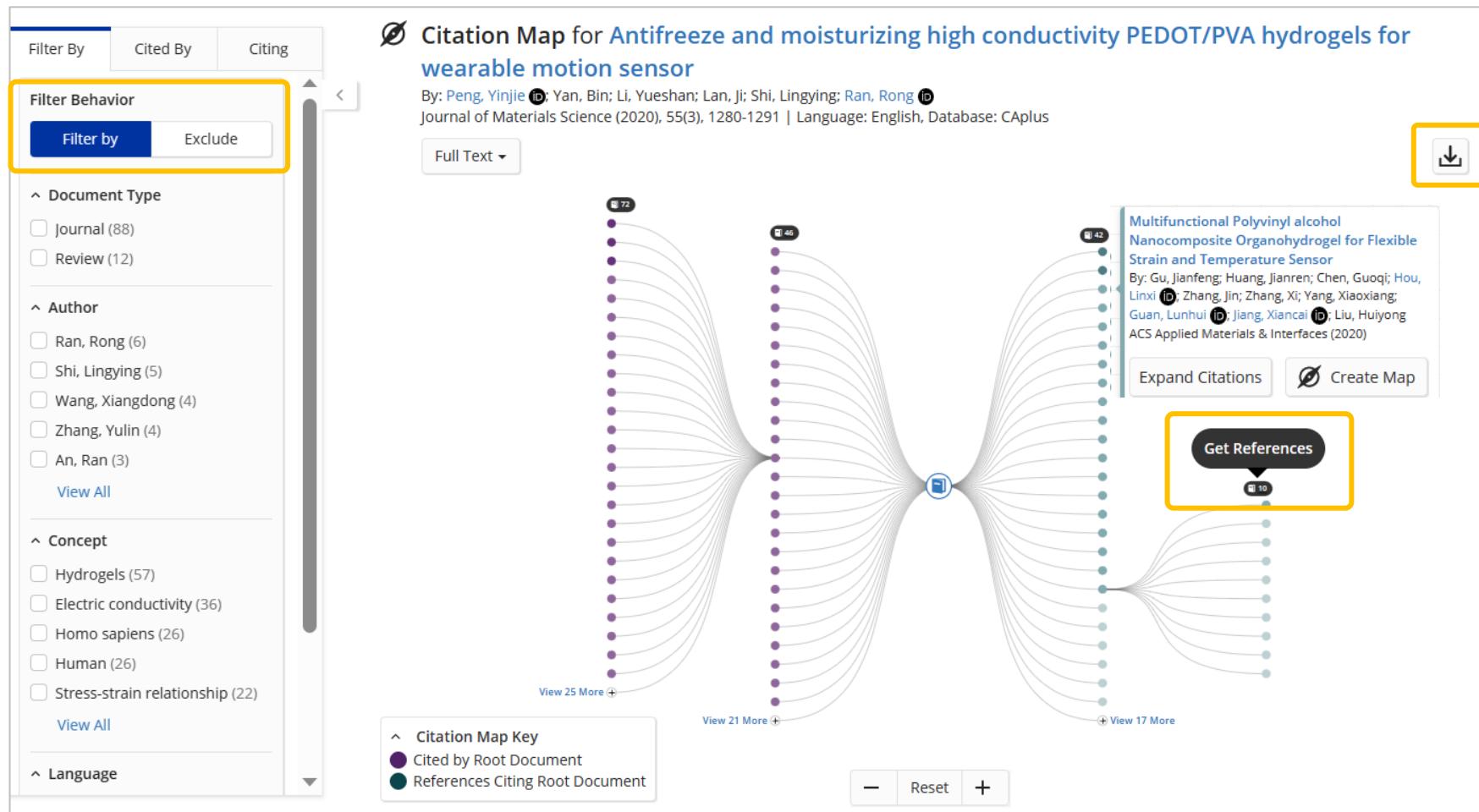
Download Cancel Learn more about downloads.

# 1.4 可视化分析——知识图谱



# 1.4 可视化分析——引文地图

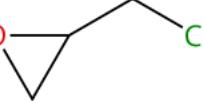
便捷获得相关文献

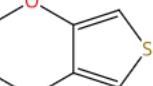


- Cited By: 参考文献
- Citing: 引用当前文献的文献
- 通过聚类选项筛选引文
- 可下载引文地图
- 显示引文和被引文献的数量，点击可链接至对应的文献结果页面

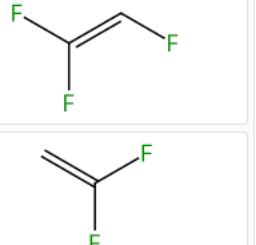
# 1.5 深入文献详情

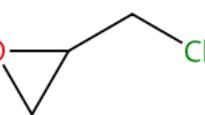
内容合集间彼此关联

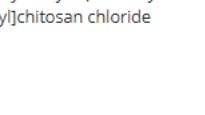
1 106-89-8  
  
C<sub>3</sub>H<sub>5</sub>ClO  
Epichlorohydrin

2 126213-51-2  


3 50851-5  
  
View More ▾

4 28960-88-5  


5 2839834-68-1  
  
(C<sub>3</sub>H<sub>5</sub>ClO.Unspecified)<sub>x</sub>  
Components: 2

6 106602-18-0  
  
Image Not Available  
Unspecified  
N-[2-Hydroxy-3-(trimethylammonium) propyl]chitosan chloride

53K References 32K Reactions 84 Suppliers

48K References 1,505 Reactions 7 Suppliers

40K References 882 Reactions 2 Suppliers

5,483 References 63 Reactions 7 Suppliers

2 References 1 Reaction 0 Suppliers

500 References 247 Reactions 0 Suppliers

Enhancing Strain-Sensing Properties of the Conductive Hydrogel by Introducing PVDF-TrFE

By: Hu, Zhirui; Li, Jie ; Wei, Xiaotong; Wang, Chen; Cao, Yang; Gao, Zhiqiang; Han, Jing; Li, Yingchun  
ACS Applied Materials & Interfaces (2022), 14(40), 45853-45868 | Language: English, Database: CAplus and MEDLINE

Conductive hydrogels have attracted attention because of their wide application in wearable devices. However, it is still a challenge to achieve conductive hydrogels with high sensitivity and wide frequency band response for smart wearable strain sensors. Here, we report a composite hydrogel with piezoresistive and piezoelectric sensing for flexible strain sensors. The composite hydrogel consists of cross-linked chitosan quaternary ammonium salt (CHACC) as the hydrogel matrix, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT: PSS) as the conductive filler, and poly(vinylidene fluoride)...

Substances (7) Reaction (1) Citing (9) Citation Map

106602-18-0 Image Not Available

+  → 

Suppliers (84)

31-614-CAS-34510937 Steps: 1

1.1 Reagents: [Poly\(styrenesulfonic acid\)](#), [Poly\(3,4-ethylenedioxythiophene\)](#)  
Solvents: [Water](#); 12 h, rt

1.2 4 h, 70 °C

1.3 Reagents: [Sodium hydroxide](#); pH 10, 70 °C

1.4 Solvents: [Dimethyl sulfoxide](#); 60 min, rt; 60 min

1.5 Reagents: [Hydrochloric acid](#)  
Solvents: [Water](#); pH 7

# 1.5 深入文献详情

## 巧用CAS PatentPak浏览专利

13

### Polymerization with living characteristics with controlled dispersity, polymers thereby, and chain-transfer agents used in the same

By: Le, Tam Phuong; Moad, Graeme; Rizzardo, Ezio; Thang, San Hoa

World Intellectual Property Organization, WO9801478 A1 1998-01-15 | Language: English, Database:

This invention concerns a free radical polymerization process, selected chain transfer agents enabling polymers made thereby, in which the process comprises preparing polymers ( $ZCS_2Q_q)_pR$  (I) or  $Z'(CS_2R)_m$  (II) by contacting: (i) a monomer having repeating units Q, selected from vinyl monomers of structure C=CH<sub>2</sub>-R, alkylmaleimide, N-arylmaleimide, dialkyl fumarate and cyclopolymerizable monomers; (ii) a thiocarbonylthio agent from  $(ZCS_2)_pR$  (III) and  $Z'(CS_2R)_m$  (IV) having a chain transfer constant  $\geq 0.1$ ; and (iii) free radicals produced by a reducing agent.

[View More ▾](#)

[PatentPak](#) ▾

Full Text ▾

Substances (83)

Reactions (0)

Citing (39)

Patent

Language

Kind Code

PatentPak Options

WO9801478	English	A1	PDF   PDF+   <a href="#">Viewer</a>
CN1137144	Chinese	C	PDF
CN1500813	Undetermined	A	PDF
CN1673216	Chinese	A	PDF
CN1331851	Chinese	C	PDF

Maintaining the ratio of fluidized bulk g. to settled bulk g. above 0.5. Ethylene and 1-butene were copolymerized at 50°C.

**CAS PatentPak** PAGE 28 /88 ZOOM DOWNLOAD PDF | PDF+

Key Substances in Patent

CAS RN 2168-82-3

Analyst Markup Locations (2)  
Page 28 | Page 35

CAS RN 108-86-1

Analyst Markup Locations (2)  
Page 28 | Page 32

CAS RN 100-58-3

Analyst Markup Locations (2)  
Page 28 | Page 35

PREPARATION OF THIOCARBONYLTHIO COMPOUNDS

The processes for making compounds (3) to (29) are as follows: Procedures 1-11 describe the preparation of known CTA compounds. Examples 1-18 describe the synthesis of novel CTA compounds.

**Procedure 1**

**Preparation of Dithiobenzoic acid and 4-chlorodithiobenzoic acid**

Dithiobenzoic acid and 4-chlorodithiobenzoic acid were prepared according to known procedures. For instance, see the method described in German Patent 1,274,121 (1968); (CA70: 3573v).

**Procedure 2**

**Preparation of benzyl dithiobenzoate (3) (C, p=1, R = CH<sub>2</sub>Ph, Z = Ph)**

This title compound was prepared by a modification of the one-pot procedure described in Recueil, 92, 601 (1973). Phenyl magnesium bromide was prepared from bromobenzene (62.8 g) and magnesium turnings (10 g) in dry tetrahydrofuran (300 mL). The solution was warmed to 40 °C and carbon disulfide (30.44 g) was added over 15 minutes whilst maintaining the reaction temperature at 40°C. To the resultant dark brown mixture was added benzyl

**CAS PatentPak** PAGE 35 /88 ZOOM DOWNLOAD PDF | PDF+

Key Substances in Patent

CAS RN 2168-82-3

Analyst Markup Locations (2)  
Page 28 | Page 35

CAS RN 108-86-1

Analyst Markup Locations (2)  
Page 28 | Page 32

CAS RN 100-58-3

Analyst Markup Locations (2)  
Page 28 | Page 35

**Procedure 8**

**Preparation of tert-butyl trithioperbenzoate (21) (C, p=1; R = (CH<sub>3</sub>)<sub>3</sub>CS; Z = P)**

The title compound (21) was prepared according to the procedure described by Aycock and Jurch, *J. Org. Chem.*, 44, 569-572, (1979). The residue was subjected to column chromatography (Kieselgel-60, 70-230 mesh, *n*-hexane eluent) to give the product, *tert*-butyl trithioperbenzoate (21) as a dark purple oil in 60 % yield. <sup>1</sup>H-nmr (CDCl<sub>3</sub>) δ (ppm) 1.32 (s, 9H), 7.45 (m, 3H) and 8.00 (m, 2H).

**Example 13**

**Preparation of 2-phenylprop-2-yl 4-chlorodithiobenzoate (22) (C, p=1, R = C(CH<sub>3</sub>)<sub>2</sub>Ph; Z = *n*-C<sub>16</sub>H<sub>4</sub>)**

A mixture of 4-chlorodithiobenzoic acid (13 g) and *a*-methylstyrene (15 mL) were heated at 70°C for 1 hour. To the reaction mixture was added *n*-hexane (30 mL) and heating was continued at 70°C for 16 hours. The resultant mixture was reduced to a crude oil. Purification, of the oil by chromatography (aluminium oxide column (activity II-III) *n*-hexane eluent) gave the title compound (22) as a purple oil (8.5 g, 40 %). <sup>1</sup>H-nmr (CDCl<sub>3</sub>) δ (ppm) 2.00 (s, 6H); 7.30 (m, 5H); 7.55 (d, 2H) and 7.83 (d, 2H).

24

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# 文献检索小结

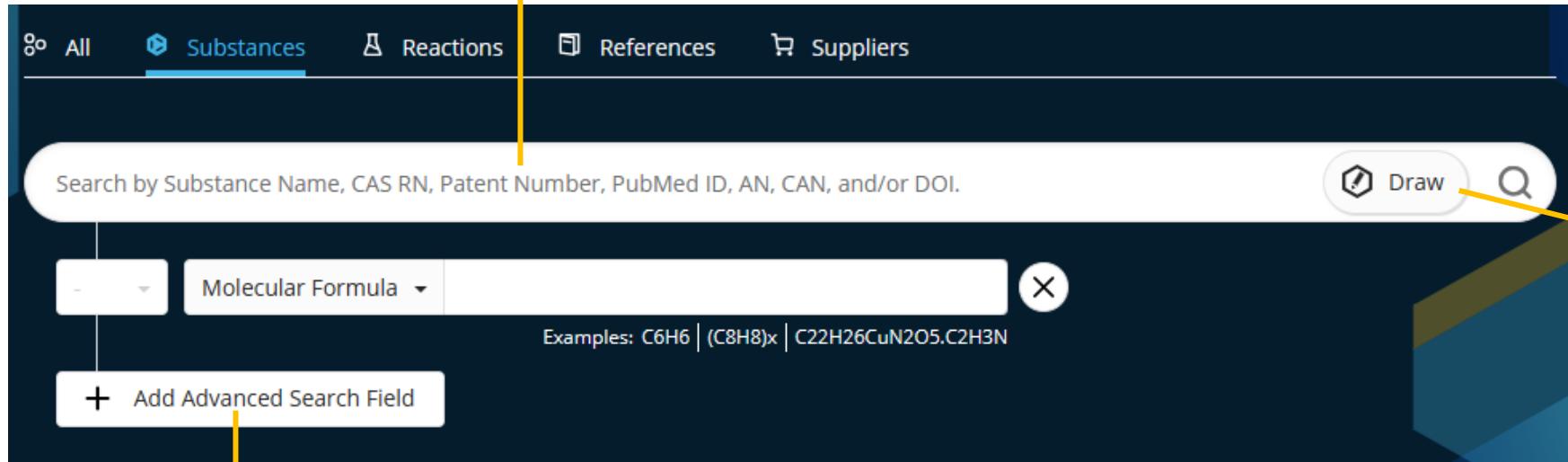
1. 检索主题的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
2. 主题词+结构联合检索，快速获得文献
3. 利用丰富的筛选工具，缩小范围，锁定目标文献
4. 检索结果趋势分析、知识图谱、引文地图
5. 文献详情，CAS PatentPak浏览专利详情

## 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

Reaction Role

Product (1)

Reactant (1)

Reference Role

Adverse Effect (2)

Analyte (2)

Analytical Study (2)

Biological Study (2)

Biological Study, Unclassified (2)

[View All](#)

Commercial Availability

Number of Components

Molecular Weight

2 Results

1 2628280-40-8

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

Absolute stereochemistry shown

319 References 106 Reactions 39 Suppliers

2 2803933-60-8

C37H48N6O5S2.C23H32F3N5O4  
Components: 2  
Paxlovid

Absolute stereochemistry shown

39 References 0 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

# 物质检索——物质标识符

示例：PEG

All    Substances    Reactions    References

PEG

PEG 58-01-4  
Pegafix  
PEG (polyglycol)  
PEG 055  
PEG 0810  
PEG 100  
PEG 1000  
PEG 1000-60L  
PEG 10000

Substances search for "PEG"

References    Reactions    Suppliers

Filter Behavior

Filter by    Exclude

Search Within Results

Reaction Role

Reference Role

Bioactivity Data

Commercial Availability

Number of Components

Molecular Weight

LogP

Element

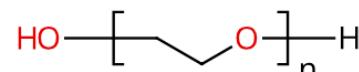
Functional Group

Aromatic Rings

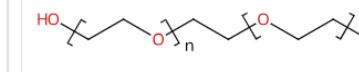
Substance Class

Isotopes

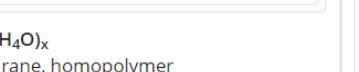
597 Results

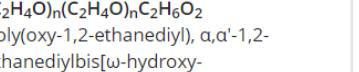
1 25322-68-3   
(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>H<sub>2</sub>O  
PEG  
455K References    63K Reactions    792 Suppliers

2 1370345-22-4   
(C<sub>2</sub>H<sub>4</sub>O)<sub>x</sub>  
Oxirane, homopolymer  
Preferred RN: 25322-68-3  
0 References    0 Reactions    0 Suppliers

3 934660-23-8   
(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>  
Poly(oxy-1,2-ethanediyl), α,α'-1,2-ethanediylbis[ω-hydroxy-]  
Preferred RN: 25322-68-3  
0 References    0 Reactions    0 Suppliers

4 6812-36-8   
Image Not Available  
Notes: A PEG monoalkylether  
Unspecified  
AEO 23  
0 References    0 Reactions    0 Suppliers

5 873815-37-3   
Image Not Available  
Notes: A blend of PEG castor oil and PE  
G oleate (Rhodia)  
Unspecified  
DV 3317  
0 References    0 Reactions    0 Suppliers

6 854918-94-8   
Image Not Available  
Notes: A blend of PEG castor oil and PE  
G oleate (Rhodia)  
Unspecified  
DV 3317  
0 References    0 Reactions    0 Suppliers

# 物质检索——组分的CAS登记号

示例：含有乙烯和丙烯为单体的聚合物

The screenshot shows the CAS Substances search interface. The search bar at the top contains the placeholder "Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/...". Below the search bar, there are four tabs: All, Substances (selected), Reactions, and References. The main search area has two "Component RN" fields. The first field has "115-07-1" selected. The second field has "74-85-1" selected and is highlighted with a yellow arrow pointing from the left side of the screen. Below these fields are dropdown menus for "AND" and "Add". The "Add" menu is expanded, showing options: Molecular Formula, CAS Registry Number (highlighted with a yellow box), and Chemical Identifier. The "CAS Registry Number" option is currently selected. To the right of the search area is a sidebar with filter options: Filter Behavior (Filter by selected, Exclude), Search Within Results, Reaction Role, Reference Role, Bioactivity Data, Commercial Availability (Number of Components: 2 (24) is checked, other options: 3 (1,194), 4 (1,458), 5 or more (1,622)), Molecular Weight, Element, Functional Group, Aromatic Rings, and Substance Class (Polymer (24) is checked). The sidebar also includes filtering for "Number of Components: 2" and "Substance Class: Polymer".

The screenshot shows the search results for substances meeting the criteria: Number of Components: 2 and Substance Class: Polymer. There are 24 results listed. The first result is 725713-40-6, which is 1-Propene, polymer with ethene, diblock. It has 314 References, 169 Reactions, and 0 Suppliers. The second result is 935748-32-6, which is 1-Propene, polymer with ethene, alternating, diblock. It has 6 References, 0 Reactions, and 0 Suppliers. The third result is 9010-79-1, which is Ethylene-propylene copolymer. It has 66K References, 3,665 Reactions, and 13 Suppliers. Other results include (C<sub>3</sub>H<sub>6</sub>.C<sub>2</sub>H<sub>4</sub>)<sub>x</sub>, Components: 2, and (C<sub>3</sub>H<sub>6</sub>.C<sub>2</sub>H<sub>4</sub>)<sub>x</sub>, Components: 2, both of which have 1-Propene, polymer with ethene, alternating, diblock as their description.

## 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：高熵碳化物 C.Hf.Nb.Ta.Ti.Zr
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性 Na<sub>2</sub>SO<sub>4</sub>: H<sub>2</sub>O<sub>4</sub>S.2Na

The screenshot shows a dark-themed search interface. At the top, there are tabs for All, Substances (which is selected), Reactions, References, and Suppliers. Below the tabs is a search bar with placeholder text: "Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.". Underneath the search bar is a "Molecular Formula" input field containing "C.Hf.Nb.Ta.Ti.Zr". This input field is highlighted with a yellow box. Below the input field, there is some example text: "Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N". At the bottom left of the search area is a button labeled "+ Add Advanced Search Field".

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

The screenshot shows a search results page for the molecular formula "C.Hf.Nb.Ta.Ti.Zr". The title of the page is "Substances search for 'C.Hf.Nb.Ta.Ti.Zr' Molecular Formula". There are three tabs at the top: References, Reactions, and Suppliers. The "References" tab is selected. On the left, there is a "Filter Behavior" section with "Filter by" and "Exclude" buttons, and a "Search Within Results" dropdown. Below that are sections for "Reaction Role" and "Reference Role", each with several filter options. The main results area shows two entries:

Component	Ratio
C	1
Zr	0.20
Hf	0.20
Ti	0.20
Ta	0.20
Nb	0.20

Below the results are detailed descriptions for each entry, showing components and their ratios, and a note that they are carbides.

## 2.1 分子式检索：高效检索聚合物或无机化合物

**Substances search for "(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>C<sub>4</sub>H<sub>8</sub>O" Molecular Formula**

Molecular Formula: (C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>C<sub>4</sub>H<sub>8</sub>O

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

**Substances search for "(C<sub>5</sub>H<sub>6</sub>O<sub>4</sub>.C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>.C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>)<sub>x</sub>" Molecular Formula**

Molecular Formula: (C<sub>5</sub>H<sub>6</sub>O<sub>4</sub>.C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>.C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>)<sub>x</sub>

Examples: C<sub>6</sub>H<sub>6</sub> | (C<sub>8</sub>H<sub>8</sub>)<sub>x</sub> | C<sub>22</sub>H<sub>26</sub>CuN<sub>2</sub>O<sub>5</sub>.C<sub>2</sub>H<sub>3</sub>N

- (C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>C<sub>4</sub>H<sub>8</sub>O: 括号中是重复结构单元, 括号外为n  
- (C<sub>5</sub>H<sub>6</sub>O<sub>4</sub>.C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>.C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>)<sub>x</sub> : 括号中是单体, 括号外为x

- (C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub>C<sub>4</sub>H<sub>8</sub>O: 括号中是重复结构单元, 括号外为n

- (C5H6O4.C4H6O2.C3H4O2)x : 括号中是单体，括号外为x

## 2.2 属性值联用检索物质

The screenshot shows the CAS Substances search interface. At the top, there are tabs for All, Substances (selected), Reactions, References, and Suppliers. Below the tabs is a search bar with placeholder text: "Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." To the left, a sidebar lists recent searches and categories like Molecular Formula, Experimental Spectra (highlighted), Bioactivity Data (NEW), and various physical properties. A dropdown menu for "Molecular Formula" is open, showing options like Molecular Formula, CAS Registry Number, Chemical Identifier, Document Identifier, Patent Identifier, and Experimental Spectra. The main search area displays a chemical structure of a molecule and search results for "As Drawn (2)", "Substructure (6,704)", and "Similarity (242K)". On the right, a large list of "高级检索字段" (Advanced Search Fields) is shown, each with a corresponding icon.

高级检索字段:

- CAS RN (物质、组份)、物质标识符、分子式、文献号、专利号
- 实验谱图:  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$  NMR
- 化学标识符: 化学名称、InChI key
- 生物: 生物富集因子、LD50
- 化学: Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压
- 密度属性: 密度、摩尔体积
- 电学: 电导/电导率、电阻/电阻率
- Lipinski: 自由旋转键、H受体/供体
- 磁: 磁力矩
- 机械属性: 拉伸强度
- 光散射: 旋光性、折射率
- 结构: 极性表面积
- 热学: 熔点、沸点、闪电、玻璃转化温度、蒸发焓

Chemical Properties > Koc

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

实验核磁共振图数值助力结构解析

# 属性值联用检索物质

检索示例：

满足多属性值要求的轻质合金，密度<7g/cm<sup>3</sup>、拉伸强度>1000MPa、熔点>600°C。

All    Substances    Reactions    References

Search by Substance Name, CAS RN, Patent Number, PubMed ID, etc.

Density (g/cm<sup>3</sup>) < 7  
Include predicted values.  
Search key property values only.

AND    Tensile Strength (Mpa) 1000 to 2500  
Search key property values only.

AND    Melting Point (°C) > 600  
Search key property values only.

+ Add Advanced Search Field

### Substances search for 3 Advanced Fields

References    Reactions    Suppliers    Save and Alert

Filter Behavior: Filter by    Exclude

Filtering: Substance Class: Alloy

18 Results    Sort: Number of References: Descending    View: Partial

Component	Percent
Fe	62.72
Cr	16.00-18.00
Ni	10.00-14.00
Mo	2.00-3.00
Mn	0-2.00
Si	0-1.00
P	0-0.045
S	0-0.030
C	0-0.030

11134-23-9

Component Percent

Fe 62.72

Cr 16.00-18.00

Ni 10.00-14.00

Mo 2.00-3.00

Mn 0-2.00

Si 0-1.00

P 0-0.045

S 0-0.030

C 0-0.030

C.Cr.Fe.Mn.Mo.Ni.P.S.Si

Components: 9

AISI 316L

25K References    17 Reactions    5 Suppliers

Component	Percent
Mg	95.97
Al	2.5-3.5
Zn	0.6-1.4
Mn	0.20
Si	0-0.10
Cu	0-0.05
Ca	0-0.04
Ni	0-0.005
Fe	0-0.005

12634-55-8

Component Percent

Mg 95.97

Al 2.5-3.5

Zn 0.6-1.4

Mn 0.20

Si 0-0.10

Cu 0-0.05

Ca 0-0.04

Ni 0-0.005

Fe 0-0.005

Al.Ca.Cu.Fe.Mg.Mn.Ni.Si.Z...

Components: 9

Magnesium alloy, base, Mg 95.97, Al 2.5-3.5, Zn 0.6-1.4, Mn 0.2, Si 0-0.10, Cu 0-0.05...

12K References    8 Reactions    0 Suppliers

Component	Percent
Al	87.91
Zn	5.1-6.1
Mg	2.1-2.9
Cu	1.2-2.0
Cr	0.18-0.28
Fe	0-0.50
Si	0-0.40
Mn	0-0.30
Ti	0-0.20

12627-49-5

Component Percent

Al 87.91

Zn 5.1-6.1

Mg 2.1-2.9

Cu 1.2-2.0

Cr 0.18-0.28

Fe 0-0.50

Si 0-0.40

Mn 0-0.30

Ti 0-0.20

Al.Cr.Cu.Fe.Mg.Mn.Si.Ti.Z...

Components: 9

AA 7075

11K References    1 Reaction    1 Supplier

在物质类别 Substance Class 中，锁定合金 Alloy。

# 属性值、谱图数值联用检索物质

Substances search interface showing search filters and results.

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

Filter section:

- Molecular Weight: 220 to 280 (Predicted values only. Examples: 46.07 | 125 to 350 | >300)
- AND pKa: 1.3 to 1.8 (Predicted values only. Examples: -1.77 | <9.25 | >2.4 | 5.25 to 8.25)
- AND Carbon-13 NMR: 114 to 171, 96, 11.5 (Allowance of  $\pm 2$  ppm. Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59)

+ Add Advanced Search Field

Substances search for 3 Advanced Fields

Filter Behavior: Filter by

Filtering: Bioactivity Data: 3 Selected

Sort: Molecular Formula: Ascending

View: Partial

15 Results

1 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

2 723-46-6 C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S Sulfamethoxazole

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

4 442571-27-9 C<sub>10</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub>S 2-((2-Chlorophenyl)methyl)thiomethylbenzoic acid

5 1927010-88-5 C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub> 2-(2-Chlorophenyl)-N-(2-methylpropyl)benzimidazolidine-1,3-dione

6 697787-29-4 C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub> 2-(2-Chlorophenyl)-N-(2-methylpropyl)benzimidazolidine-1,3-dione

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

# 物质详情

CAS Registry Number: 723-46-6

References (26K) Reactions (997) Suppliers (126) Save

This substance contains CAS Bioactivity data, such as SAR, ADME, or Toxicity tables. Explore this information below. Learn more about CAS life sciences.

Nc1ccc(cc1)S(=O)(=O)Nc2cc(C)c3oc(c3)nc2

$C_{10}H_{11}N_3O_3S$

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

Key Physical Properties

	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point		
Density (Experimental)		
pKa (Predicted)		
Experimental		

Carbon-13 NMR Spectrum for 723-46-6

723-46-6

Nc1ccc(cc1)S(=O)(=O)Nc2cc(C)c3oc(c3)nc2

$C_{10}H_{11}N_3O_3S$

CAS Name: Sulfamethoxazole

Conditions: Solvent DMSO-d<sub>6</sub> (2206-27-1), Standard Tetramethylsilane (75-76-3)

Spectrum Summary: Spectrum ID CNCC-59959-23D, Spectrometer JEOL GX-270, Source: Spectral data were obtained from John Wiley & Sons, Inc.

Figure: Carbon-13 NMR Spectrum showing peaks at approximately 145 ppm (S), 135 ppm (SS), 115 ppm (S), 110 ppm (D), 95 ppm (D), and 10 ppm (Q).

- 折叠菜单显示物质各类信息

Other Names and Identifiers

Experimental Properties

Experimental Spectra

1<sup>H</sup> NMR    1<sup>3</sup>C NMR    Hetero NMR    IR    Mass    Raman    UV and Visible

Solvent    Source

View Carbon-13 NMR Spectrum    DMSO-d<sub>6</sub>    (1) WSS

View Carbon-13 NMR Spectrum    DMSO-d<sub>6</sub>    (2) WSS

View Carbon-13 NMR Spectrum    -    (2) WSS

View Carbon-13 NMR Spectrum    Methanol-d<sub>4</sub>    (3) CAS

View Carbon-13 NMR Spectrum    DMSO-d<sub>6</sub>    (4) CAS

View Carbon-13 NMR Spectrum    -    (5) BIORAD

View Carbon-13 NMR Spectrum    DMSO-d<sub>6</sub>    (6) AIST

Carbon-13 NMR Spectrum - 1 Source    -    (7) CAS

Sources

(1) Kartashov, V. S.; Khimiko-Farmatsevicheskii Zhurnal, (1992), 26(11-12), 107-9, CAplus  
(2) Fruttero, Roberta; Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999), (1988)(10), 1863-6, CAplus  
(3) Ham, Won Seok; Angewandte Chemie, International Edition, (2019), 58(2), 532-536, CAplus  
(4) Sunduru, Naresh; European Journal of Medicinal Chemistry, (2015), 101, 595-603, CAplus  
(5) Copyright Bio-Rad Laboratories. All Rights Reserved.  
(6) "Integrated Spectral Data Base System of Organic Compounds" data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan)  
(7) Blasioli, Sonia; Journal of Colloid and Interface Science, (2014), 419, 148-159, CAplus

Structure Activity Relationships    CAS LIFE SCIENCES

Absorption, Distribution, Metabolism, and Excretion Data    CAS LIFE SCIENCES

Toxicity    CAS LIFE SCIENCES

Predicted Properties

Predicted Spectra

Bioactivity Indicators

Target Indicators

Regulatory Information

GHS Hazard Statements

Additional Details

# 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



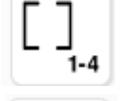
选择可变基团



自定义R基团



片段结构



重复工具



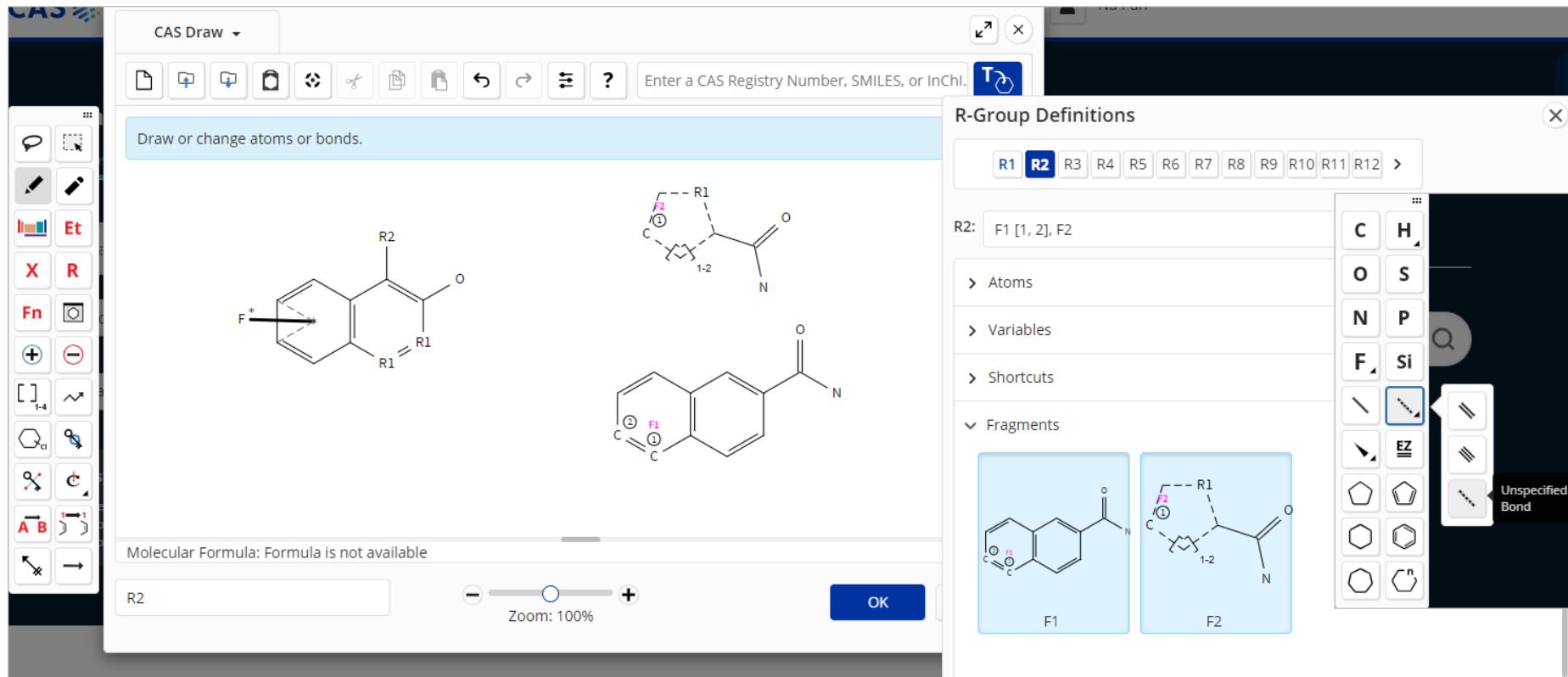
取代位置可变



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

# 结构检索

例：已知结构片段的物质检索

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

Substances search for drawn structure

Structure Match

As Drawn (0)

**Substructure (732)**

Similarity (9)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Reaction Role

732 Results

R1

Save and Alert

Sort: Relevance View: Partial

Filter Behavior

Filter by Exclude

Reaction Role

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Stereochemistry

Element

Substance Class

Isotopes

Metals

Experimental Property

Bioactivity Indicator

Search Within Results

732 Results

1 685504-28-3

C<sub>31</sub>H<sub>35</sub>Cl<sub>3</sub>CoNP<sub>2</sub>  
(T-4)-Trichloro[N-[2-(diphenylphosphino- $\kappa$ P)ethyl]-N-[2-(diphenylphosphino)ethyl]]...

2 807307-30-8

C<sub>31</sub>H<sub>35</sub>Cl<sub>3</sub>CoNOP<sub>2</sub>  
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- $\kappa$ P)ethyl]-N-[2-(diphenylphosphino)ethyl]]...

3 635299-07-9

C<sub>31</sub>H<sub>35</sub>Cl<sub>3</sub>CoNOP<sub>2</sub>.H  
Components: 2  
Component RN: 807307-30-8  
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- $\kappa$ P)ethyl]-N-[2-(diphenylphosphino)ethyl]]...

4 635299-08-0

5 16827-53-5

6 635299-09-1

物质筛选类别：

反应角色

文献角色

立体化学

物质类别

同位素

金属包含

实验物性数据

二次检索……

# 物质检索结果的筛选

Filter by

Exclude

## Reaction Role

Product (216)

Reactant (53)

Reagent (3)

Catalyst (36)

## Reference Role

Commercial Availability

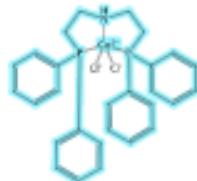
Number of Components

Molecular Weight

**Reaction Role:**  
物质在反应中的角色

4

1087216-22-5



C<sub>28</sub>H<sub>29</sub>Cl<sub>2</sub>CoNP<sub>2</sub>

Dichloro[2-(diphenylphosphino- $\kappa P$ )-N-[2-(diphenylphosphino- $\kappa P$ )ethyl]ethanamine- $\kappa N...$

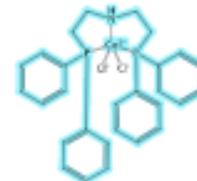
8  
References

105  
Reactions

0  
Suppliers

5

2170923-58-5



C<sub>28</sub>H<sub>29</sub>Cl<sub>2</sub>CoNP<sub>2</sub>

Reference Role

Preparation (489)

Synthetic Preparation (488)

Properties (245)

Reactant (98)

Reactant or Reagent (98)

Industrial Manufacture (9)

[View All](#)

Commercial Availability

Not Available (9)

**Reference Role:**  
物质在文献中的研究角色

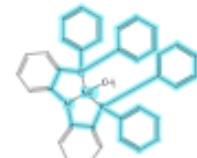
8  
References

105  
Reactions

0  
Suppliers

4

579490-58-7



C<sub>37</sub>H<sub>31</sub>NNiP<sub>2</sub>

(SP-4-1)-[2-(Diphenylphosphino- $\kappa P$ )-N-[2-(diphenylphosphino- $\kappa P$ )phenyl]benzenamina...

7  
References

22  
Reactions

0  
Suppliers

3  
References

8  
Reactions

0  
Suppliers

5

579490-62-3



C<sub>38</sub>H<sub>33</sub>NNiP<sub>2</sub>

(SP-4-1)-[2-(Diphenylphosphino- $\kappa P$ )-N-[2-(diphenylphosphino- $\kappa P$ )phenyl]benzenamina...

6  
References

21  
Reactions

0  
Suppliers

# 物质检索结果的筛选

## Substance Class: 物质类别

^ Number of Components

1 (23)  
 2 (285)  
 3 (92)  
 4 (12)  
 5 or more (11)

▼ Molecular Weight

▼ Stereochemistry

▼ Element

^ Substance Class

Polymer (92)  
 Coordination Compound (42)  
 Salt and Compound With (9)  
 General Derivative (3)

▼ Isotopes

4

849402-50-2

(C<sub>4</sub>H<sub>8</sub>O.C<sub>4</sub>H<sub>4</sub>S)<sub>x</sub>.xCH<sub>4</sub>O

Components: 3

Furan, tetrahydro-, polymer with thiophene, methyl ether, graft

1 Reference 0 Reactions 0 Suppliers

5

62306-29-0

(C<sub>6</sub>H<sub>6</sub>O.C<sub>4</sub>H<sub>4</sub>S.CH<sub>2</sub>O)<sub>x</sub>

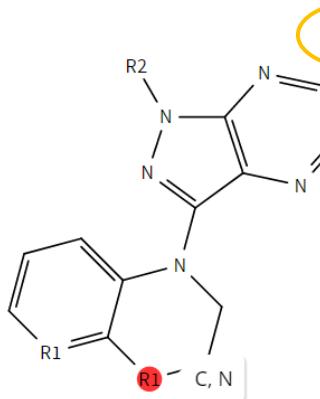
Components: 3

Formaldehyde, polymer with phenol and thiophene

2 References 0 Reactions 0 Suppliers

# 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



1  
WO2018081091  
The screenshot shows a search result for WO2018081091. It displays the claimed structure (a complex polycyclic compound) and its mapping to the detailed chemical structure below it. The mapping uses labels like G5, G38, AK, and S16 to identify specific atoms or groups in the structure.

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

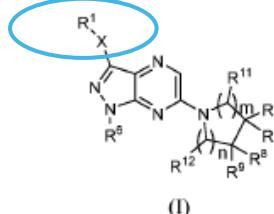
PCT/US2017/058048

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,



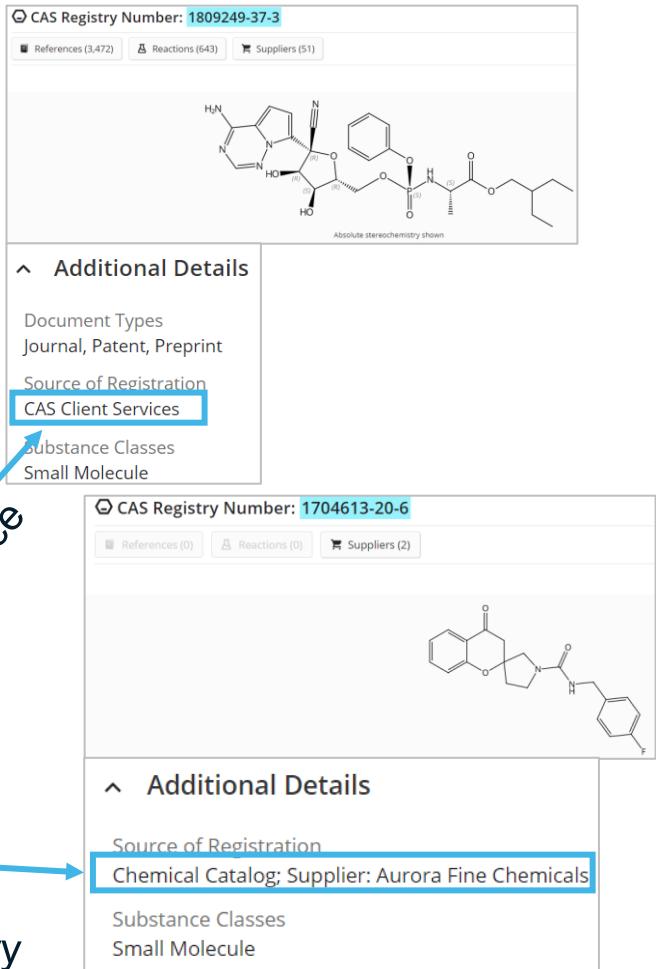
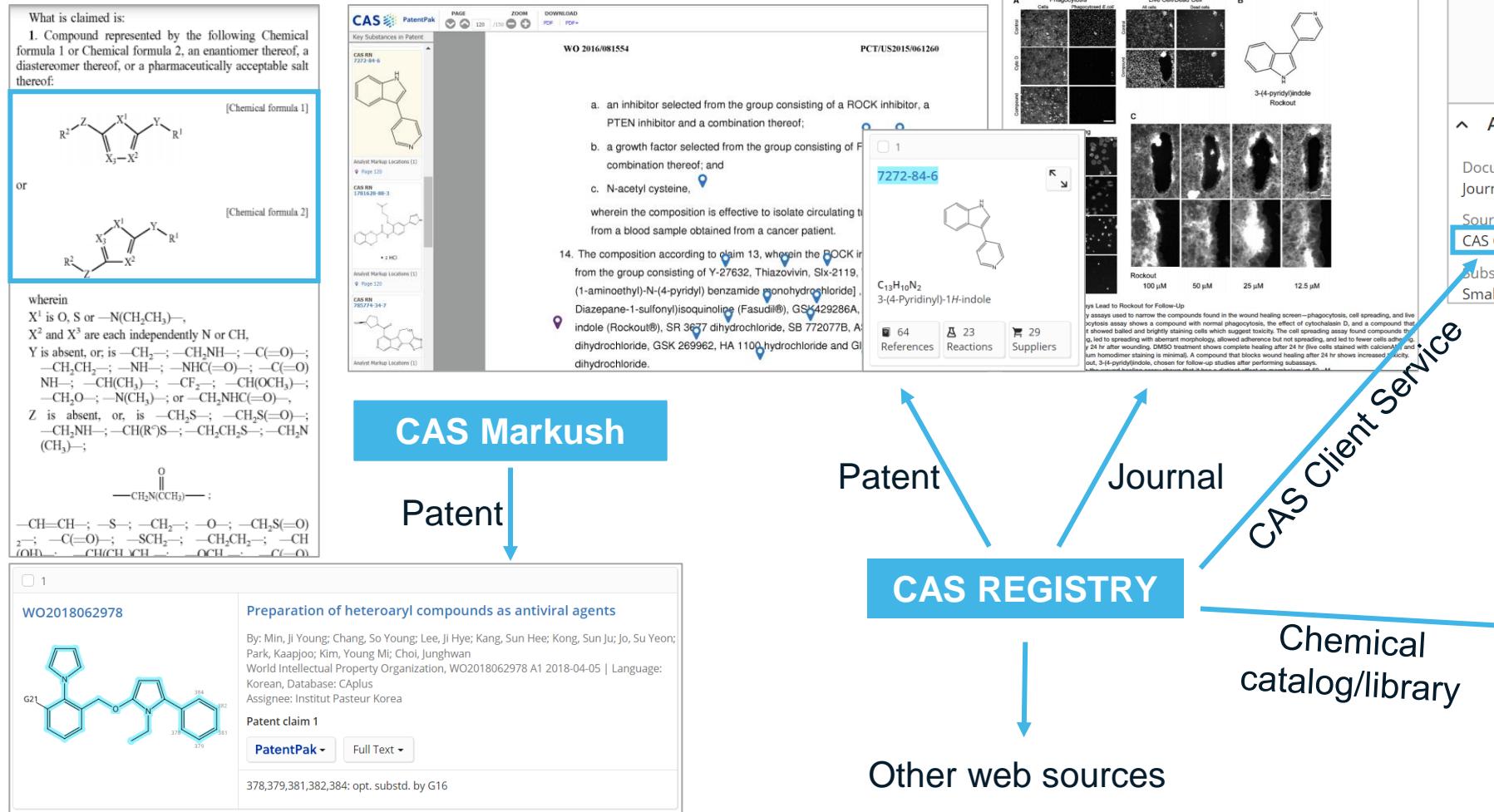
5

wherein

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

- 15 R<sup>66</sup> is selected from the group consisting of H, -(C<sub>1</sub>-C<sub>6</sub>)alkyl and phenyl, or together with R<sup>1</sup> 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<sup>10</sup>, -OR<sup>10</sup>, -S(O)<sub>w</sub>R<sup>10</sup> (wherein w is 0, 1 or 2), -N(R<sup>10</sup>)<sub>2</sub>, -OS(O)<sub>w</sub>R<sup>10</sup> (wherein w is 0, 1, or 2), -S(O)<sub>w</sub>N(R<sup>10</sup>)<sub>2</sub> (wherein w is 0, 1 or 2), -S(O)(NH)R<sup>10</sup>, -P(O)(R<sup>10</sup>)<sub>2</sub>, -C(O)R<sup>10</sup>, -C(O)N(R<sup>10</sup>)<sub>2</sub>, oxo, halogen, nitrile, phenyl (optionally substituted with one, two or three halo, C<sub>1</sub>-alkyl or C<sub>1</sub>-haloalkyl), C<sub>1</sub>-alkyl, C<sub>1</sub>-haloalkyl, and heteroaryl (optionally substituted with one, two or three halo, C<sub>1</sub>-alkyl or C<sub>1</sub>-haloalkyl);
- 20 with one, two or more substituents each independently selected from the group consisting of R<sup>10</sup>, -OR<sup>10</sup>, -S(O)<sub>w</sub>R<sup>10</sup> (wherein w is 0, 1 or 2), -N(R<sup>10</sup>)<sub>2</sub>, -OS(O)<sub>w</sub>R<sup>10</sup> (wherein w is 0, 1, or 2), -S(O)<sub>w</sub>N(R<sup>10</sup>)<sub>2</sub> (wherein w is 0, 1 or 2), -S(O)(NH)R<sup>10</sup>, -P(O)(R<sup>10</sup>)<sub>2</sub>, -C(O)R<sup>10</sup>, -C(O)N(R<sup>10</sup>)<sub>2</sub>, oxo, halogen, nitrile, phenyl (optionally substituted with one, two or three halo, C<sub>1</sub>-alkyl or C<sub>1</sub>-haloalkyl), C<sub>1</sub>-alkyl, C<sub>1</sub>-haloalkyl, and heteroaryl (optionally substituted with one, two or three halo, C<sub>1</sub>-alkyl or C<sub>1</sub>-haloalkyl);
- 25

# CAS 结构层面的数据集



# 如何进行完整的分子结构检索？

S Substances search for drawn structure

References Reactions Suppliers

Structure Match

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

As Drawn (0)

Substructure (0)

Similarity (101K)

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

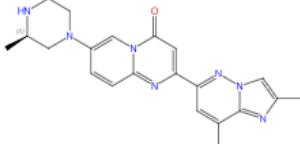
286 Results

Sort: Relevance View: Partial

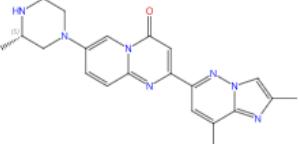
1 1825352-54-2 95 ...

2 1825352-53-1 95 ...

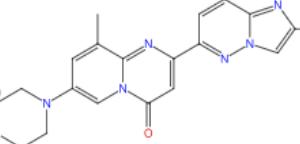
3 1825352-79-1 95 ...

  
Absolute stereochemistry shown

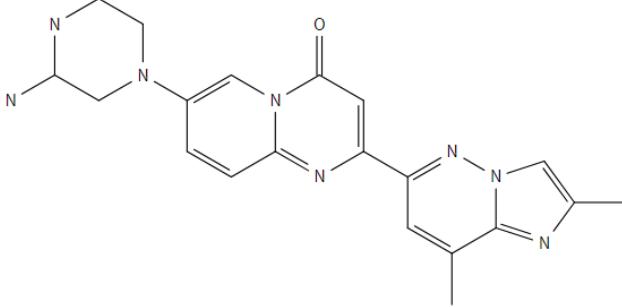
C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>O  
2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-4H-1,2-dihydroimidazo[1,2-b]pyridazine-2,8-dione

  
Absolute stereochemistry shown

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

  
Absolute stereochemistry shown

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-[(3R)-3-methyl-1-piperazinyl]-4H-1,2-dihydroimidazo[1,2-b]pyridazine-2,8-dione



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

# 如何进行完整的分子结构检索？

**Substances search for drawn structure**

References ▾ Reactions ▾ Suppliers ▾

Structure Match

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

Sort: Relevance ▾ View: Partial ▾

As Drawn (0)

Substructure (0)

Similar (101K) **Similarity (101K)**

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

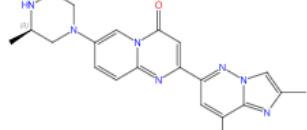
Search Within Results

286 Results

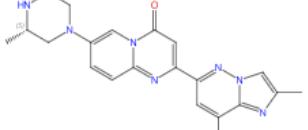
1 1825352-54-2 95 •••

2 1825352-53-1 95 •••

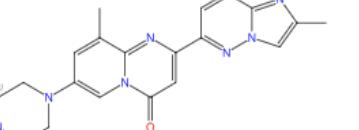
3 1825352-79-1 95 •••

  
Absolute stereochemistry shown

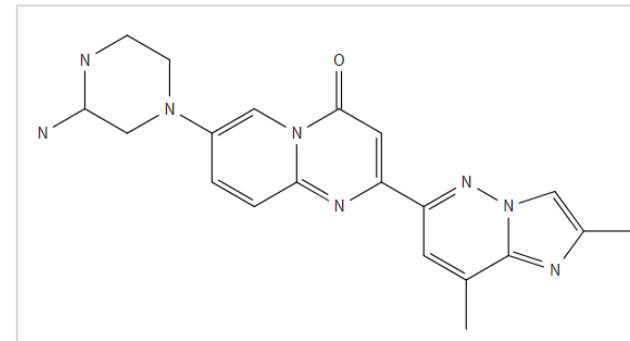
C21H23N7O  
2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-4H-1,2-dihydroimidazo[1,2-b]pyridazine-6,8-dione

  
Absolute stereochemistry shown

C21H23N7O  
2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]-4H-1,2-dihydroimidazo[1,2-b]pyridazine-6,8-dione

  
Absolute stereochemistry shown

C21H23N7O  
9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-4H-1,2-dihydroimidazo[1,2-b]pyridazine-6,8-dione



查看相似结构，可参考  
Similarity score

# 如何进行完整的分子结构检索？

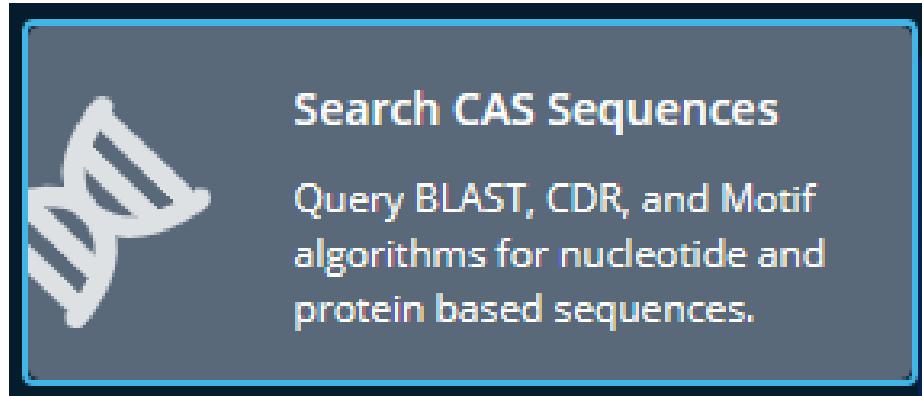
The screenshot shows the SciFinder interface for a Patent Markush search. At the top, there is a search bar with the placeholder "Enter a query..." and a "Substances" dropdown. Below the search bar, a "Return to Home" link is visible. The main area is titled "Patent Markush search for drawn structure". On the left, there is a sidebar with "Patent Markush Match" filters: "As Drawn (1)" (selected), "Substructure (1)", and "Filter Behavior" with options "Filter by" and "Exclude". Under "Filter by", there are sections for "Patent Office" (World Intellectual Property Organization (1)) and "CA Section". In the center, a search bar contains a chemical structure of a tricyclic compound. Below the search bar are buttons for "Edit Drawing", "Remove", "Save and Alert", and a checked "Search Patent Markush" button. The search results show one result for patent WO2017081111. The patent title is "Preparation of substituted 2-(imidazo[1,2-b]pyridazin-6-yl)-pyrido[1,2-a]pyrimidin-4-ones for treating amyotrophic lateral sclerosis". The assignees are Hoffmann-La Roche AG and Hoffmann-La Roche Inc. The patent claim 1 is shown, mentioning "PatentPak", "Full Text", and specific substituents: 453,454,455,456,457: opt. subst. by G22 and 629: opt. subst.

- 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

## 2.5 CAS SciFinder中的序列检索

- BLAST
- CDR
- Motif



# 物质检索小结

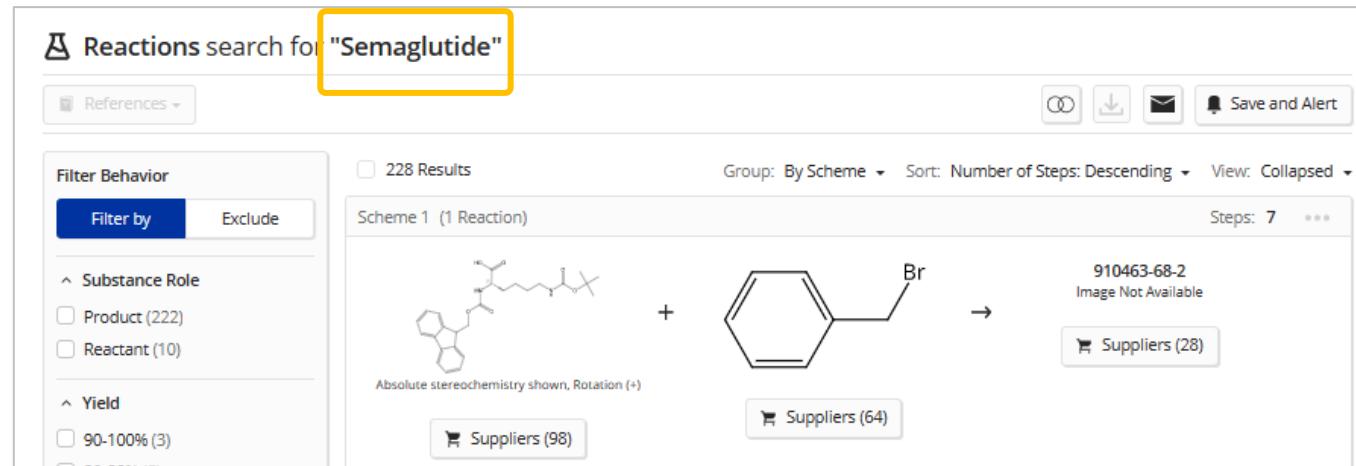
1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
3. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
4. 利用CAS Markush检索尽可能全面的获得结构的公开信息

### 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？

# 研究某类反应？

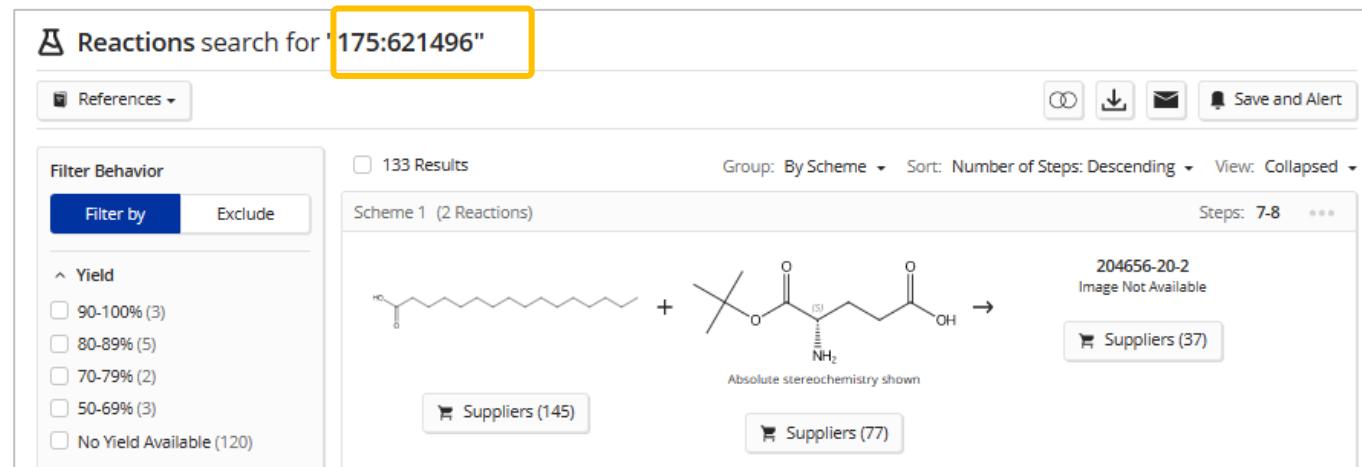
- 反应检索方法
  - 物质或文献标识符
  - 结构式
  - 关键词与结构联用



1  
910463-68-2  
Image Not Available

Unspecified  
Semaglutide  
Protein/Peptide Sequence  
Sequence Length: 34

1,527 References, 259 Reactions, 32 Suppliers



Reactions, References, Suppliers

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

Draw, Search

CAS A division of the American Chemical Society

# 3.1 查找亚结构反应

As Drawn  
亚结构反应  
相似反应

Reactions search for drawn structure

Structure Match

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

Filter Behavior

- Filter by
- Exclude

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

Scheme 1 (5 Reactions)

Suppliers (93)      Suppliers (15)

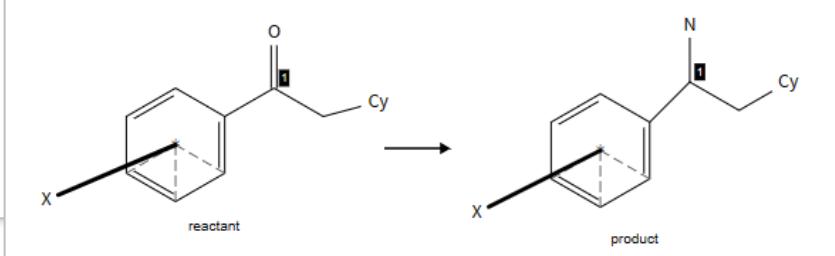
Scheme 2 (1 Reaction)

Suppliers (53)      Suppliers (3)

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

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

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

## 3.2 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

Commercial Availability

- Reaction Notes

Source Reference

- Document Type
- Language
- Publication Year
- Organization
- Publication Name
- CA Section

Filter Content Report

Download filter data from this result set.

Structure Match

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

Filter Behavior

- Filter by
- Exclude

8,044 Results Group: By Transformation ▾ Sort: Reaction Count: Descending ▾ View: Collapsed ▾

1 Reductive Alkylation of Ammonia or Amines [View 108 Related Reactions](#)

$\text{R}-\text{C}(=\text{O})-\text{R} + \text{R}'-\text{NH} \rightarrow \text{R}-\text{N}(\text{R}')-\text{R}$

2 Formation of N/O/S Heterocycles [View 47 Related Reactions](#)

$\text{Y}, \text{Y}' = \text{NH}, \text{O}, \text{S}$

$\text{Z} = \text{Electron withdrawing group}$

3 1,3-Dipolar Addition [View 37 Related Reactions](#)

# 筛选工具：不参与反应官能团

不参与反应官能团：出现在反应前后，但未发生变化的官能团

Structure Match

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

Filter Behavior

- Filter by
- Exclude

Search Within Results

Yield

Reaction Scale

- Non-Participating Functional Groups
  - Halide (205)
  - Phenyl halide (203)
  - Amide (66)
  - Alkene (62)
  - Cyclic alkene (58)
- [View All](#)

Number of Steps

Reaction Mapping

Experimental Protocols

Filtering: Non-Participating Functional Groups: Halide

205 Results Group: By Scheme ▾ Sort: Relevance ▾ View: Collapsed ▾

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

31-313-CAS-11425767 Steps: 1 Yield: 100% Preparation of N-[1-biphenyl]-N-(4-fluorophenyl)-N-(4-fluorobiphenyl)amidine derivatives as antagonists of urotensin II  
By: Neeb, Michael J.; et al  
World Intellectual Property Organization, WO2008-01-24

1.1 Solvents: Tetrahydrofuran; 15 min, rt  
1.2 Reagents: Acetic acid, Sodium cyanoborohydride; rt → 40 °C; 24 h, 40 °C  
1.3 Reagents: Sodium carbonate  
Solvents: Water

Experimental Protocols

PatentPak ▾ Full Text ▾

Collapse Scheme ▾

Scheme 2 (1 Reaction) Steps: 1 Yield:

Non-Participating Functional Groups

By Count Alphanumeric

1 Selected

Halide (205)

Phenyl halide (203)

Amide (66)

Alkene (62)

Cyclic alkene (58)

Diene (45)

Ether (37)

Amine (15)

Tertiary amine (15)

Carboxamidine (14)

Urea (12)

Carboxylic ester (9)

Carbamate (8)

Imine (8)

Acyclic ketone (7)

Ketone (7)

# 3.3 联用检索——结构与关键词

关注人名反应?

All Substances Reactions References Suppliers

Friedel-crafts acylation

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

+ Add Advanced Search Field

Edit Drawing Remove

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

Substances Reactions Citing Knowledge Graph

Structure Match

As Drawn (1,100) Substructure (2,270)

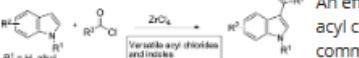
Filter Behavior

Document Type

- Journal (996)
- Patent (68)
- Review (31)
- Conference (27)

1,100 Results Sort: Relevance View: P

1 ZrCl<sub>4</sub>-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole By: Guchhait, Sankar K; Kashyap, Maneesh; Kamble, Harshad Journal of Organic Chemistry (2011), 76(11), 4753-4758 | Language: English, Database: CAplus and MEDLINE



An efficient method for regio- and chemoselective Friedel-Crafts acylation of acyl chlorides in the presence of ZrCl<sub>4</sub> has been discovered. It minimizes/eliminates common competing reactions that occur due to high and multiatom-nucleophilicity of indole. In this method, a wide range of aryl, heteroaryl, alkenoyl, and alkanoyl chlorides undergo smooth acylation of indoles without NH protection and afford 3-acetylindoles in good to high yields.

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

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

联用检索提高检索效率

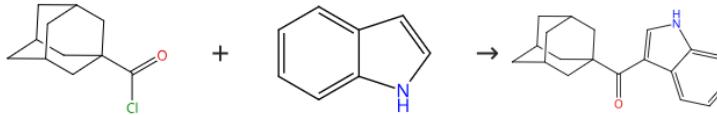
Reactions search for "2011:601374"

References

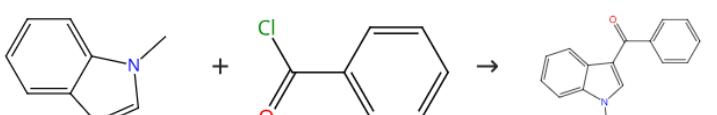
Filter Behavior

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

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



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



# 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

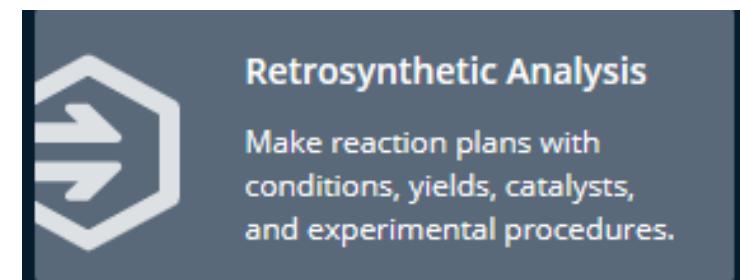
(1) 已知化合物：点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis

The screenshot shows a detailed view of a compound's properties and available actions. At the top left is the CAS Registry Number (RN) 2628280-40-8. Below it is the chemical structure with absolute stereochemistry shown. To the right of the structure is its name: 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...]. Below the name are several buttons: Substance Detail, Reactions (53), Synthesize (52), Start Retrosynthetic Analysis (which is highlighted with a yellow box), References (236), and Suppliers (39). At the bottom are Edit Structure, Reset, and a zoom-in button.

(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 P

Select Synthetic Depth 反应深度 Learn more.

1  
 2  
 3  
 4



Set Rules Supporting Predicted Reactions Learn more.

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

反応規則常见性

Set Starting Materials Cost Limit Learn more.

100 起始原料費用 USD/mol ▾

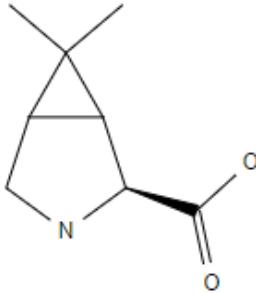
Email me when my plan is complete

>Create Retrosynthesis Plan

Break and Protect Bonds

Break Bond  Protect Bond  Clear All Bond Selections

断裂键或保护键



# 逆合成分析的调节参数

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Key Experimental Steps Predicted Steps Edit Plan Options

Plan Information

Estimated Yield: 51% Overall Price: \$29.90 (USD per 100 grams)

路线概览

Scoring Profiles

Complexity Reduction Convergence Evidence Cost Yield Atom Efficiency

Scoring Profiles:

- 降低每步原料结构的复杂性
- 逆合成路线中前体的数量
- 支持预测路线的文献数量多少
- 预测路线大概成本
- 每步的产率
- 每步的原子转化效率

Off Low Medium High

The screenshot shows a retrosynthesis planning interface. At the top, it says "Retrosynthesis Plan for drawn structure" and "Powered by ChemPlanner®". Below that are tabs for "Key", "Experimental Steps" (which is selected), "Predicted Steps", and "Edit Plan Options". There are also download, email, and save buttons. On the left, there's a sidebar with "Plan Information" showing an estimated yield of 51% and an overall price of \$29.90 (USD per 100 grams). It also lists "Scoring Profiles" with sliders for Complexity Reduction, Convergence, Evidence, Cost, Yield, and Atom Efficiency. Buttons for "Apply" and "Reset Scoring" are at the bottom of this sidebar. The main area displays a reaction scheme with six steps (A-F) and their corresponding structures. Step A is a bicyclic amine with a hydroxyl group. Step B is a substituted cyclopentane. Step C is a brominated alkene. Step D is a cyclic amide. Step E is a ketone. Step F is a cyclic ester. Each step has a flask icon indicating the number of experimental routes (e.g., 4, 25, 19) and a shopping cart icon indicating the number of supporting references (e.g., 48, 53, 57). The right side of the interface has a "Scoring Profiles:" section with a bulleted list of six items, each corresponding to one of the scoring profile sliders.

# 逆合成路线详情

已知反应

预测型反应

Retrosynthesis Plan for drawn structure

Key Experimental Steps Predicted Steps Edit Plan Options

View Excluded Options Save

Step Evidence

A  $\Rightarrow$  B + C  
Reagents: Triethylamine, Hydrogen sulfide  
Solvents: Dichloromethane  
View All

B  $\Rightarrow$  D + E  
Reagents: Triethylamine  
Solvents: Dichloromethane; 24 h, rt

Reactions from Retrosynthesis Plan Evidence

15,146 Results

Scheme 1 (1 Reaction)

Yield: 88%

Supplier: 18, 92, 9

Scheme 2 (1 Reaction)

Yield: 100%

Supplier: 136, 66, 51

Chemical structures and reaction conditions are displayed throughout the interface.

- 可查看每步反应的文献支持与详细条件

# 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. 关键词与反应式的联合检索
4. 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

## 4. 具体的实验方案怎么查、怎么选？



- 如何获取获得具体的实验操作和表征数据等信息？
- 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？

# 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-Quinolinicarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-5-quinolinemethyl 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

# 4.2 CAS分析实验方法详情

- CAS科学家标引的分析实验详情
- 无需下载全文，高效获得所需的分析实验信息

## Analysis of Vanadium in Stainless steel by Electrochemical extraction

CAS MN: 1-119-CAS-286328

Method Category: Element Detection

Technique: Electrothermal atomic absorption spectroscopy; Decomposition; Electrochemical extraction

Materials	Role	Image	CAS RN
Vanadium	analyte	<a href="#">View Structure</a>	7440-62-2
Stainless steel	matrix		12597-68-1
Al <sub>2</sub> O <sub>3</sub> cutting wheel	material		
SiC grinding paper	material		
0.05 µm pore size polycarbonate filter	material		
Standard calomel reference electrode	material		
Platinum ring counter electrode	material		
Hollow cathode lamps	material		
Electrodeless discharge lamp	material		
THGA graphite tubes	material		
Nitric acid	reagent	<a href="#">View Structure</a>	7697-37-2
Hydrofluoric acid	reagent	<a href="#">View Structure</a>	7664-39-3
Acetylacetone	reagent	<a href="#">View Structure</a>	123-54-6
Chromium	reagent	<a href="#">View Structure</a>	7440-47-3
Methanol	reagent	<a href="#">View Structure</a>	67-56-1
Tetramethylammonium chloride	reagent	<a href="#">View Structure</a>	75-57-0

## 实验原料

### Source

Determination of alloying and impurity elements from matrix and inclusions from a process sample of a double stabilized stainless steel

Sipola, Teija; Alatarvaa, Tuomas; Fabritius, Timo; Peramaki, Paavo

ISIJ International (2016), 56 (8), 1445 - 1451. Iron and Steel Institute of Japan

CODEN: IINTEY | ISSN: 09151559 | DOI: 10.2355/isijinternational.isijint-2016-071

[Full Text ▾](#)

[View in CAS SciFinder®](#)

## 文献来源

### Equipment Used

Cutting machine, Secotom-10, Struers

Ultrasonic cleaning unit, P 30 H, Elmasonic

Grinding machine, Labopol-6, Struers

Potentiostat, SP-150, BioLogic

Vacuum pump, BUSCHI

Graphite furnace atomic absorption spectrometer, AAnalyst 600, PerkinElmer

Autosampler, AS-800, PerkinElmer

## 分析仪器

### Conditions

#### Instrument

internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm; injection volume: 10 µL

## 分析条件

### Instructions

#### Preparation of stainless steel process samples

1. Cut stainless steel pieces from a corner piece of different slabs using a Struers Secotom-10 cutting machine with an Al<sub>2</sub>O<sub>3</sub> cutting wheel.
2. Grind and polish the steel samples using a Struers Labopol-6 grinding machine with SiC grinding paper to a size of approximately 15 x 10 x 5 mm.
3. Clean the sample from grinding paper traces using an Elmasonic P 30 H ultrasonic cleaning unit (frequency 37 kHz, room temperature).
4. Clean all glassware in an acid bath, rinse with ultrapure water and methanol sequentially.

## 操作步骤

#### Electrolytic extraction of stainless steel using 10% acetylacetone

1. Perform electrolytic extraction on a BioLogic SP-150 potentiostat.
2. Use 10% acetylacetone (10 v/v% acetylacetone, 1 w/v% tetramethylammonium chloride and methanol) as the electrolyte.
3. Use the sample as the working electrode and set the potential to 0.150 V vs. the standard calomel electrode (SCE).
4. Suspend the sample in the electrolyte in a platinum basket and use a platinum ring as a counter electrode.
5. Filter the electrolyte through a 0.05 µm pore size polycarbonate filter with the help of a BUSCHI vacuum pump.
6. Expose the sample to ultrasound in methanol and filter the methanol with the electrolyte.

#### Decomposition of inclusions

1. Dry the polycarbonate filter containing the extracted inclusions overnight in a desiccator.
2. Place the dry filter in a PTFE container with 5 mL concentrated nitric acid and 2 mL HF and close gently.
3. Perform decomposition for 30 minutes at 120 °C (393.15 K).
4. Cool the containers to room temperature, remove the filter and dilute to the volume with water.
5. Prepare a blank sample similarly by filtering a fresh electrolyte through a polycarbonate filter.

#### Quantification of inclusions using graphite furnace atomic absorption spectrometry (GFAAS) with Cr as a matrix modifier

1. Perform GFAAS on a PerkinElmer AAnalyst 600 graphite furnace atomic absorption spectrometer equipped with an AS-800 autosampler and PerkinElmer THGA graphite tubes (standard platform B0504033).
2. Use a hollow cathode lamp (HCL) as the radiation source.
3. Use the following furnace program: ramp for 10 s to 110 °C, hold for 30 s; ramp for 10 s to 140 °C, hold for 30 s; ramp for 10 s to 1300 °C, hold for 20 s; perform atomization at 2400 °C for 6 s; ramp for 1 s to 2500 °C and hold for 5 s.
4. Set the instrument parameters as follows: internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm.
5. Add 0.05 µg Cr as a matrix modifier.
6. Inject 10 µL of the sample and perform measurements.

### Validation

Linearity Range	0-400 µg/L
Concentration	< 1 µg

## 数据有效性

# 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获得有具体分析实验方法的文献, 从文献详情页中链接至分析实验方法

The screenshot shows the CAS SciFinder interface with the following details:

- Search Bar:** References search for "steel and impurity".
- Filtering:** CAS Solutions: Analytical Methods.
- Results:** 23 Results, Sort: Relevance, View: Partial Abstract.
- Document:** Validation of an HPLC method for analysis of nifedipine residues on stainless-steel surfaces in the manufacture of pharmaceuticals. By: Milenovic, D. M.; Lazić, M. L.; Veljković, V. B.; Todorović, Z. B. Acta Chromatographica (2008), 20(2), 183-194 | Language: English, Database: CPlus
- Keywords:** double stabilized stainless steel alloying impurity element inclusion
- Access:** Open Access, Full Text.
- CAS Content Filter:** A yellow box highlights the "Analytical Methods" option under the "CAS Content" section, which is checked.
- Table:** A table on the right lists analytical methods for stainless steel, each with a CAS Method Number:

CAS Method Number
1-119-CAS-285768
1-119-CAS-286264
1-119-CAS-286328
1-119-CAS-286333
1-119-CAS-286759
1-119-CAS-286842
1-119-CAS-287300

# 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 "Good Afternoon, Na", and a "Saved" button. Below the header, there are two main search options: "Advanced Search" (represented by a magnifying glass icon) and "Explore Methods" (represented by binoculars icon). The "Advanced Search" box contains the text: "Search methods using criteria like keywords, analytes, matrices and more." The "Explore Methods" box contains the text: "Search methods using criteria like method categories and subcategories." Below these boxes, there are two large blue buttons: "直接检索" (Direct Search) and "浏览不同类别分析方法" (Browse different categories of analytical methods). In the bottom left corner, there is a "Recent Searches" section with entries: "近期检索" (Recent Search), "Explore : Organometallic Compound Analysis", and "Advanced : analyte : olaparib, matrix : blood plasma".

# 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…

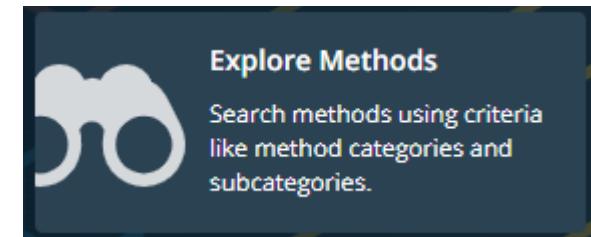
**Organic Compound Analysis:** 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…

**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

Advanced Search

Analyte: lapatinib

Matrix: plasma

AND

Add Search Criteria

Clear

# 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



Results for lapatinib

Compare (2/3) Compare Save

Sort: Relevance Group: By Method

对比不同分析方法

1

**Analysis of Lapatinib by Microplate spectroscopy**

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

In vitro effects of **lapatinib** with gemcitabine for pancreatic cancer cells

Hepato-Gastroenterology (2013), 60 (126), 1484-1487. H.G.E. Update Medical Publishing S.A.

Analyte: **Lapatinib**; Gemcitabine

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

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

View All

Method Category: Bioassay

Technique: Microplate spectroscopy

Equipment Used: Microplate reader

View Abstract Full Text View in CAS SciFinder

2

**Analysis of Lapatinib ditosylate in Pharmaceutical tablets by Reversed-phase HPLC**

By: Murthy, T. E. Gopala Krishna; Deepthi, E. Naga

Stability indicating RP-HPLC method for determination of **Lapatinib** ditosylate

Indian Pharmacist (New Delhi, India) (2011), 10 (6), 35-36, 39-41. Bazaz Publications

Analyte: **Lapatinib ditosylate**

Matrix: Pharmaceutical tablets

Other Materials: Reagent: Methanol

Material: Luna C<sub>18</sub> column (250 × 4.5 mm, 5 μ); Nylon membrane filters of 0.45 μ size

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

JOURNAL

View Abstract Full Text View in CAS SciFinder

# 对照多个感兴趣的分析方法详情

				 Format <input checked="" type="radio"/> PDF <input type="radio"/> XLS <a href="#">Download</a> <a href="#">Cancel</a>	
	Method 1	x	Method 2	x	
CAS Method Number	Analysis of Lapatinib in Blood plasma by HPLC-tandem mass spectrometry		Analysis of Lapatinib in Blood plasma by High-performance liquid chromatography-mass spectrometry		
Method Category	1-101-CAS-187473		1-101-CAS-157505		
Technique	Active Pharmaceutical Ingredient and Metabolite Analysis		Active Pharmaceutical Ingredient and Metabolite Analysis		
Analyte	HPLC-tandem mass spectrometry		Atmospheric precipitation; High-performance liquid chromatography-mass spectrometry		
Matrix	Lapatinib	Blood plasma	Lapatinib	Blood plasma	
Other Materials	Ethyl acetate; Formic acid; Methanol; XBridge C18 column (3.5 µm, 50 mm × 2.1 mm i.d.)		Acetonitrile; Formic acid; Zorbax SB-C18 column (5 µm)		
Equipment Used	LC system., Alliance2695, Waters, Milford, MA, USA; Triple quadrupole mass spectrometer, Quattro Micromass, Waters		Liquid chromatograph, 1200 Series, Agilent Technologies, Waldbronn, Germany; Ion-trap mass spectrometer, HCT, Bruker Technologies, Bremen, Germany		
Conditions	Instrument: ionization mode-Positive; heated nebulized probe- 350 °C; pressure of collision gas (Argon) (mbar)- 5.92E-003, 5.92E-003 and 5.92E-003 for lapatinib, lapatinib-d3 and zileuton; dwell time (s)- View All▼		Instrument: drying gas flow rate- 6 L/min; nebulizer pressure- 350 °C; dry gas temperature- 350 °C; capillary voltage mode target ions: m/z 581 (or lapatinib), m/z 231 (View All▼		
Preparation	Patient sample. 1. Obtain the blood sample from the patients with HER2 positive metastatic breast cancer treated with oral lapatinib daily or in View All▼		Sample Preparation 1. Orally administer the rats with lapatinib at a dose of 100 mg/kg within 0.5 min. View All▼		
					<p><b>Method</b></p> <p><b>Linearity Range</b></p> <p><b>Limit of Quantitation</b></p> <p><b>Recovery</b></p> <p><b>Accuracy</b></p> <p><b>Precision</b></p> <p><b>Concentration</b></p> <p><b>Source</b></p> <p><b>Sample extraction</b></p> <p>1. Spike 250 µl of plasma sample with 5 µl of internal standard working solution and acidify with 20 µl of concentrated formic acid.</p> <p><a href="#">View All▼</a></p> <p>5 - 5000 ng/ml</p> <p>5 ng/mL</p> <p>43% ± 14%, 42% ± 10% and 48% ± 12% (recovery), for 5, 15, 800 and 4000 ng/mL spiked sample, repectively.</p> <p>102.1%, 98.6%, 102.5% and 98.3% (recovery), for 5, 15, 800 and 4000 ng/mL QC sample, repectively.</p> <p>4.6%, 3.4%, 2.3% and 2.4% (RSD, intra-day); 4.0%, 2.9% and 3.1% (RSD, inter-day), for 5, 15, 800 and 4000 ng/mL QC sample, repectively.</p> <p>-</p> <p>14816.6 ng/mL (at 30 mg/kg)</p> <p><b>JOURNAL</b></p> <p>A stable isotope-labeled internal standard is essential for correcting for the interindividual variability in the recovery of lapatinib from cancer patient plasma in quantitative LC-MS/MS analysis</p> <p>By: Wu, Jianmei; Wiegand, Richard; Lo Russo, Patricia; Li, Jing Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 941, 100 - 108.</p> <p><a href="#">Full Text▼</a> <a href="#">View in CAS SciFinder</a></p> <p><b>Protein precipitation</b></p> <p>1. Thaw the plasma sample to room temperature. 2. Add an aliquot of 10 µl of the internal standard working solution.</p> <p><a href="#">View All▼</a></p> <p>10 - 2000 ng/mL</p> <p>10 ng/mL</p> <p>-</p> <p>98.3 - 109.2% (recovery, intra-day); 93.0 - 104.1% (recovery, inter-day)</p> <p>5.6 - 12.0% (CV, intra-day); 6.8 - 11.5% (CV, inter-day)</p> <p>14816.6 ng/mL (at 30 mg/kg)</p> <p><b>JOURNAL</b></p> <p>Quantification of lapatinib in rat plasma by liquid chromatography mass spectrometry</p> <p>By: Zhu, Jiayin; He, Yan; Wang, Yilong; Wen, Congcong; Zhang, Qingwei; Lin, Guanyang Latin American Journal of Pharmacy (2014), 33 (1), 158 - 162.</p> <p><a href="#">Full Text▼</a> <a href="#">View in CAS SciFinder</a></p>

## 4.3 研究课题在产品中的应用？配方/制剂的检索与设计

方法（1）：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 a greeting "Good Evening, Na", navigation links for "Formulations" (highlighted in yellow) and "Ingredients", and a search bar with the placeholder "Search by Formulations by Ingredients, Purpose, Form, Functions, etc." Below the search bar are two buttons: "直接检索" (Direct Search) and "Advanced Search". The "Advanced Search" button has a magnifying glass icon and the text "Search Formulations using criteria like ingredients, targets, and more." To the left is a "Formulation Designer" section with a mortar and pestle icon and the text "Design custom formulation templates based on selections and ingredients". To the right is a "制剂、配方设计" (Formulation Design) section with a magnifying glass icon and the text "高级检索" (Advanced Search). The main content area shows a "Recent Search History" section for December 22, 2023, at 2:16 PM, under the "Formulations" category. The search query is "+Ingredient:'Olaparib' +Form:'Tablets'" (135 results). Buttons for "Rerun Search" and "Edit Search" are visible. A "View Search History" link is also present.

Good Evening, Na

Formulations Ingredients

Search by Formulations by Ingredients, Purpose, Form, Functions, etc.

直接检索

Advanced Search

Formulation Designer

Design custom formulation templates based on selections and ingredients

制剂、配方设计

高级检索

Recent Search History

December 22, 2023

2:16 PM

Formulations

+Ingredient:'Olaparib' +Form:'Tablets' (135)

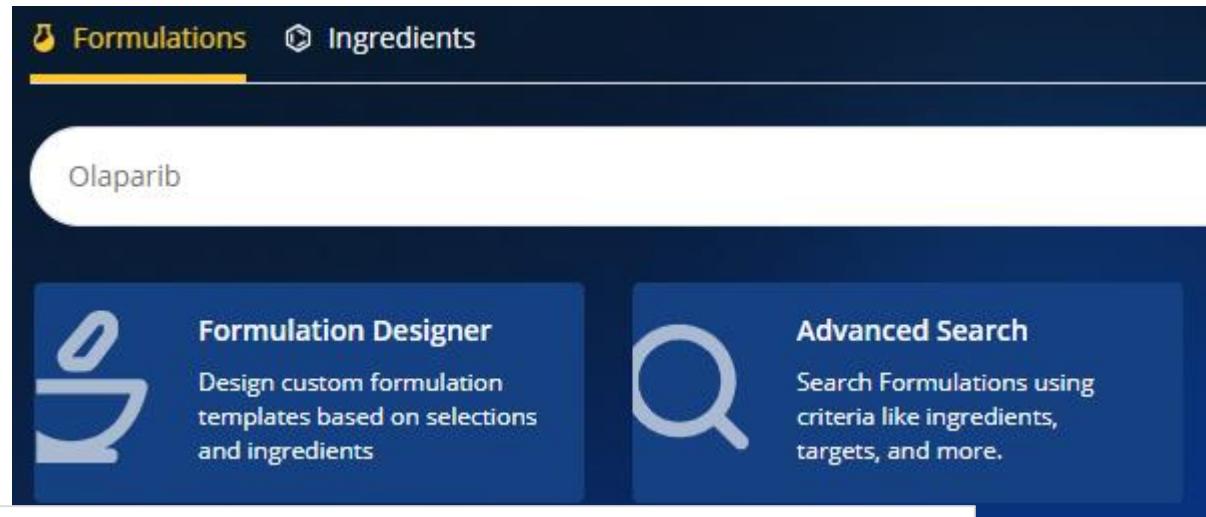
Rerun Search

Edit Search

View Search History

# 关键词检索制剂/配方

- 直接检索示例：  
Olaparib 奥拉帕尼



- 高级检索示例：  
奥拉帕尼片剂

The screenshot shows the 'Advanced Formulations Search' interface. It displays two search fields. The first field has 'Ingredient' selected as the search type, 'Required' as the operator, and 'Olaparib' entered as the term. The second field has 'Form' selected as the search type, 'Required' as the operator, and 'Tablets' entered as the term. There is also an 'Add Another Term' button and a 'Search' button at the bottom.

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

Search For      Operator      Enter one term  
Ingredient      Required      Olaparib  
Ex: caffeine, sodium, 50-00-0

Search For      Operator      Enter one term  
Form      Required      Tablets  
Ex: spray, granule, powder

Add Another Term

Search      Clear All

# 检索结果分析与精炼

应用领域

目的/用途

物理形态

物质状态

作用方式

制剂信息

文献类型

机构名

发表年份

Document Type

- Journal (7)
  - Article (7)
- Patent (627)
  - Claim (392)
  - Comparative Example (30)
  - Example (203)
  - Table (2)
- Product Insert (5)

Organization

- CSPC Zhongqi Pharmaceutical Technology (Shijiazhuang) Co., Ltd. (34)
- Shanghai Institute of Materia Medica, Chinese Academy of Sciences (33)
- Sunshine Lake Pharma Co., Ltd. (29)
- AstraZeneca UK Ltd. (22)
- Immunomedics, Inc. (21)

View All

Information Included

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

View All



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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

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...

[Lincomycin Solid Dispersion: Veterinary Drug](#)

Purpose: Veterinary drugs  
Target: Homo sapiens, Livestock, Poultry  
Delivery Route: -  
Physical Form: Pharmaceutical solid di...

[Olaparib Dispersible Tablets: Antitumor Agents](#)

Purpose: Antitumor agents  
Target: Homo sapiens, Mammary glan...  
Delivery Route: Oral drug delivery syst...  
Physical Form: Pharmaceutical orally d...

[Olaparib Dispersible Tablets: Antitumor Agents](#)

Purpose: Antitumor agents  
Target: Homo sapiens, Mammary glan...  
Delivery Route: Oral drug delivery syst...  
Physical Form: Pharmaceutical orally d...

[Lincomycin Solid Dispersion: Veterinary Drug](#)

Purpose: Veterinary drugs  
Target: Homo sapiens, Livestock, Poultry  
Delivery Route: -  
Physical Form: Pharmaceutical solid di...

### Source Patent

[Olaparib solid dispersion and preparation method 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.

80

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# 检索原料

Formulations Ingredients

Propylene Glycol

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

CAS RN: 57-55-6  
View Details

(±)-Propylene glycol Propylene glycol

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

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

Similar Ingredients with Regulatory Information

27194-74-7 Propylene glycol monolaurate  
29387-86-8 Propylene glycol butyl ether  
30136-13-1 Propylene glycol monopropyl ether  
[View 14 More](#)

Commonly Formulated With | Regulatory Information | Experimental Properties

Get Formulations Suppliers Add to Formulation Designer

81

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# 设计配方/制剂

## Formulation Designer ?

[Clear All Selections](#)

Industry	Purpose	Physical Form	Add up to 5 Ingredients
Pharmaceutical	<b>Coating materials</b>	Solutions	Water
Cosmetics & Personal Care	Adhesives	Paints	Ethanol
Agrochemical	Jet-printing inks	Powders	
Cleaning & Surfactant Products	Water-thinned coating materials	Films	
<b>Inks, Paints, &amp; Coatings</b>	Antifouling coating materials	Coating materials	
Food & Related	Powder coating materials	<b>Liquids</b>	+ Add Another Ingredient
	<b>Printing inks</b>	<b>Emulsions</b>	
	Anticorrosive coating materials	Disperse systems	
	Paints	Tablets	
	Photocurable coating materials	Resins	
	<a href="#">- View More Purposes -</a>	<a href="#">- View More Physical Forms -</a>	

 **Formulation Designer**  
Design custom formulation  
templates based on selections  
and ingredients

[Create Template](#)



# 设计配方/制剂

Formulation Designer [?](#)

Clear All Selections

Industry	Purpose	Physical Form	Active or Featured Ingredient
Inks, Paints, & Coatings	Coating materials Printing inks	Emulsions Liquids	Water Ethanol

[Edit Selections](#) [Save](#) [Download](#)

Your Template

Unit Size  mg [Go](#) [Clear](#)

Function	Ingredient	Regulatory	Top Alternatives	Amounts
Active or Featured Ingredient:	Water	ANMAT; CosIng: Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; NMPA	-	Amount not available <a href="#">X</a>
Active or Featured Ingredient:	Ethanol	CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; EU Active Substances in Pesticides; FDA GRAS (Part 184); FDA Inactive Ingredients Database; FDA Orange Book; Japanese Approved Drugs List	-	Am <a href="#">X</a>
Solvents	1,3-Butanediol	Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients	Toluene; Tetrahydrofuran; 2- Butoxyethanol; Butyl acetate; Propylene glycol monomethyl ether	Approximate Range: 10 - 17% <a href="#">X</a>
Surfactants	Sorbitan mono-(92)-9- octadecenoate	Drug Master File List; EPA Pesticide Inactive	Sodium dodecyl sulfate; Sodium dodecylbenzenesulfonate;	Approximately 2% <a href="#">X</a>

[View More Alternatives](#)

Alternative Ingredients (Showing all 23)

Select the ingredient you would like to use:

Toluene	Methanol	Water
Tetrahydrofuran	1-Butanol	Methyl isobutyl ketone
2-Butoxyethanol	Silica	Propylene glycol methyl ether acetate
Butyl acetate	Methyl ethyl ketone	Carbitol acetate
Propylene glycol monomethyl ether	Soya lecithins	Propyl acetate
Xylene	N-Methyl-2-pyrrolidone	2-Heptanone
Ethyl acetate	Cyclohexane	$\gamma$ -Butyrolactone
Isopropanol	Ethanol	

- 原料详情
- 原料管制信息
- 可替代的原料选项

# 文献关联的配方/制剂

方法（2）：在CAS SciFinder的文献结果集页面，点击CAS Content中的 Formulus 获得有具体配方或制剂信息的文献，从文献详情页中链接获取

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

Substances Reactions Citing Knowledge Graph

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

1 XinLi formula, a traditional Chinese decoction, alleviates chronic heart failure via regulating the interaction of AGTR1 and AQP1

By: Wei, Xiao-Hong; Liu, Wen-Jing; Jiang, Wei; Lan, Tao-Hua; Pan, Hai'e; Ma, Ming-Yue; You, Liang-Zhen; Shang, Hong-Cai  
Phytomedicine (2023), 113, 154722 | Language: English, Database: Cplus and MEDLINE

XinLi formula (XLF) is a traditional Chinese medicine used in clin. practice to treat chronic heart failure (CHF) in humans, with remarkable curative effect. However, the mechanism remains unknown. The goal of the current investigation was to determine how XLF affected CHF in a rat model of the condition brought on by ligation of the left anterior descending coronary artery, and to investigate the underlying mechanism. Cardiac function was detected by echocardiog. The contents of myocardial enzymes, Ang II, ALD, TGF- $\beta$ 1, and inflammatory factors were measured by ELISA. Myocardial injury and myo...

[View More](#)

2 Comparative pharmacokinetics of seven bioactive components after oral administration of crude and processed Qixue Shuangbu Prescription in chronic heart failure rats by microdialysis combined with UPLC-MS/MS

By: Chen, Linwei; Wei, Nina; Jiang, Yong; Yuan, Chengye; Xu, Luwei; Li, Jindong; Kong, Min; Chen, Yan; Wang, Qin  
Journal of Ethnopharmacology (2023), 303, 116035 | Language: English, Database: Cplus and MEDLINE

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

[View More](#)

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

CAS Content

Analytical Methods (5)

Formulus (3)

Formulation Purpose

Cardiovascular agents (3)

## 定位配方或制剂的功能目标

# 文献关联的配方/制剂

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



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

## In this Reference

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 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 mechanism for myocardial hypertrophy resistance are studied. A new thought and a new choice are provided for treatment of 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 ▾](#)

## Publication Information • Patent

Patent Number  
CN112190652

Publication Date  
2021-01-08

Application Number  
CN2020-11207191

Application Date  
2020-11-03

Kind Code  
A

Assignee  
Capital Medical University,  
China

Source  
China  
CODEN: CNXXEV

Database Information  
AN: 202156481  
CAN: 176:120018  
CAplus

Language  
Chinese

## Patent Family

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

## Formulations

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

[View CAS Formulus® Detail](#)

Location: Claim 1, 2, 3, 4, 5, 6, 7, 8, 9

Purpose: Cardiovascular agents

Target: myocardial hypertrophy, human

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

Additional Components Reported in Full Text

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

[View CAS Formulus® Detail](#)

Location: Example

Purpose: Cardiovascular agents

Target: myocardial hypertrophy, human

Component	Function	Amount Reported
Panax ginseng	-	200 wt. parts



# 实验方案检索小结

1. 利用**Synthetic Methods™**查看文献中合成方法详情
2. 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
3. 利用**CAS Formulus**检索原料、配方/制剂，或通过文献结果集获得关联的配方/制剂信息；利用配方设计工具启发产品配方的开发

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
- 常见问题Q&A



# CAS SciFinder 检索浏览器推荐

浏览器推荐：

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

# 如何获取CAS SciFinder账号

(登录图书馆网站，查看注册相关的链接和说明)

The screenshot shows the registration process for CAS SciFinder. It consists of three stacked sections:

- Contact Information:** Fields for First Name, Last Name, Email, Confirm Email, Phone Number, Fax Number, Area of Research (dropdown), and Job Title (dropdown).
- Username and Password:** Fields for Username, Password, and Re-enter Password.
- Security Information:** Fields for Security Question (dropdown) and Answer.

At the bottom left are "Register>>" and "Clear All" buttons.

## Registration Already Complete

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

请注意：

- 必须输入真实姓名和学校邮箱。
  - 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)
  - 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)。

点击激活链接后注册成功

通过<https://scifinder-n.cas.org/>访问



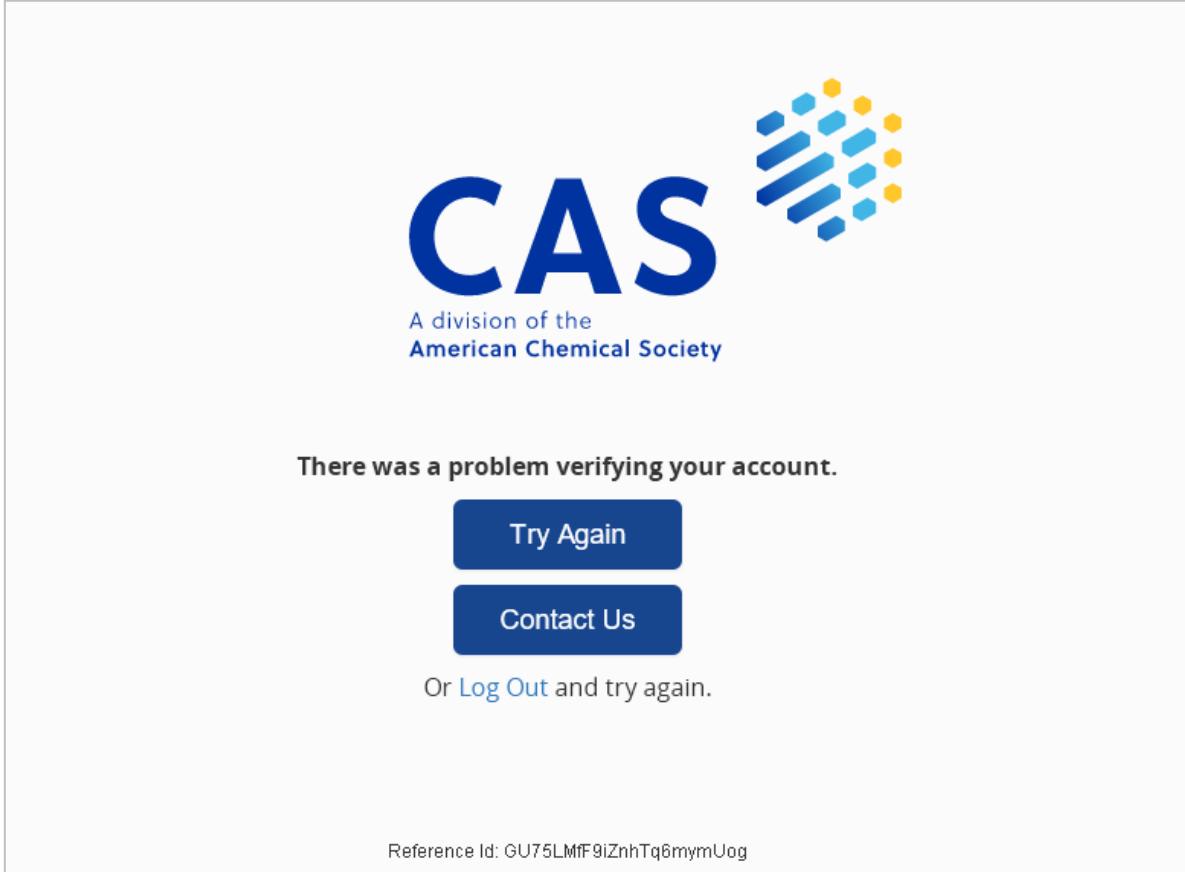
# 常见注册问题

## 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.

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

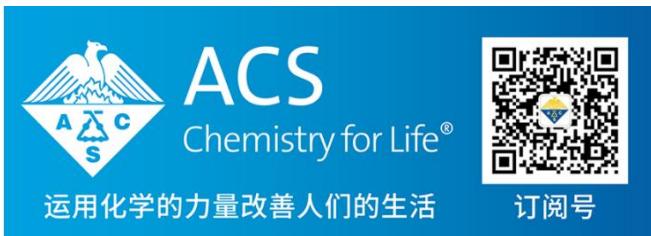
# 常见登录问题



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

# 线上学习资源

“ACS美国化学会”  
微信公众号



学习中心：短视频、专题论坛、使用技巧

历史文章：按标签分类的检索技巧及案例等

# CAS SCIINDER DISCOVERY PLATFORM™

## 2024专题论坛直播时间表

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

9月26日 | 药物立项调研策略



11月14日 | 电池及电化学能源材料



10月24日 | 聚合物的研发与应用



12月19日 | 专利查新与规避专利侵权风险



**CAS SciFinder Discovery Platform**

**9月至12月的四场专题论坛**

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

CAS SCIFINDER

# 2024 检索技能大赛

第一阶段：4月8日 - 5月10日

在线学习检索技能，并参加线上考试。

第二阶段：5月11日 - 6月8日\*

分享检索体验，赢取全国大奖：



一等奖：1名  
Macbook Air®



二等奖：3名  
九号电动滑板车（配头盔）



三等奖：10名  
索尼耳机  
WH-CH720N



入围奖：30名  
JBL音箱

扫码参赛：



所有获奖者都将获得CAS官方获奖证书。

参赛有机会获得CAS定制礼盒。更多信息请扫描参赛二维码

\*需要完成第一阶段且成绩不低于85分

# 使用注意事项

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

# Thank You For Your Attention !



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