

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

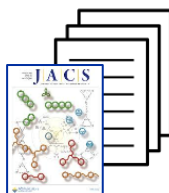
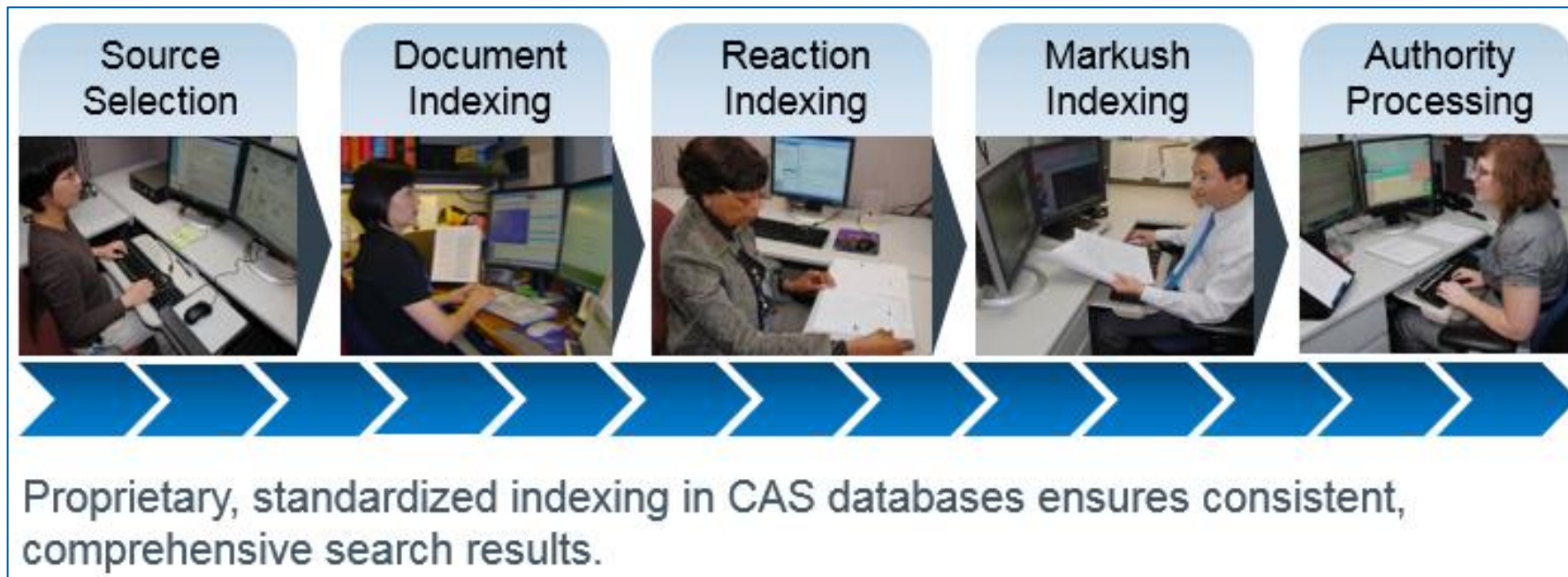


来源：

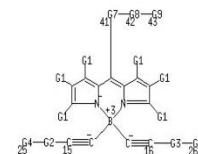
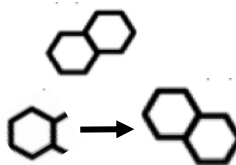
<https://www.cas.org/cas-data>

<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-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

CAS 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 ServicesSM

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 SciFinderⁿ ——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 MethodsTM ——借助CAS科学家深度加工的科学方法，提升研究效率

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

CAS Formulus[®] ——助力开发安全、有效的产品

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

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




Log in to SciFinder®

Username or Email Address

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

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



Log in to SciFinder®

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

Password

☐ Keep me signed in

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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 CAS SciFinder login main interface. On the left is a sidebar menu with categories like SCIFINDER DISCOVERY PLATFORM, STN IP PROTECTION SUITE, REGULATORY, and ACCOUNT MANAGEMENT. The main area features a top navigation bar with tabs for All, Substances, Reactions, References, and Suppliers. A search bar is prominently displayed with a 'Draw' button highlighted by a yellow box and labeled '结构绘制面板' (Structure Drawing Panel). Below the search bar is a 'Molecular Formula' input field with a dropdown menu and a label '高级检索选项' (Advanced Search Options). The interface also includes three main service tiles: 'Retrosynthetic Analysis' (逆合成路线设计), 'Search CAS Lexicon' (CAS词库), and 'Search CAS Sequences' (CAS序列检索). At the bottom, there is a 'Recent Search History' section labeled '近期检索历史' and a 'View All Search History' link. The top right corner contains a '更新结果提醒' (Update Results Reminder) button and user profile icons.

大纲

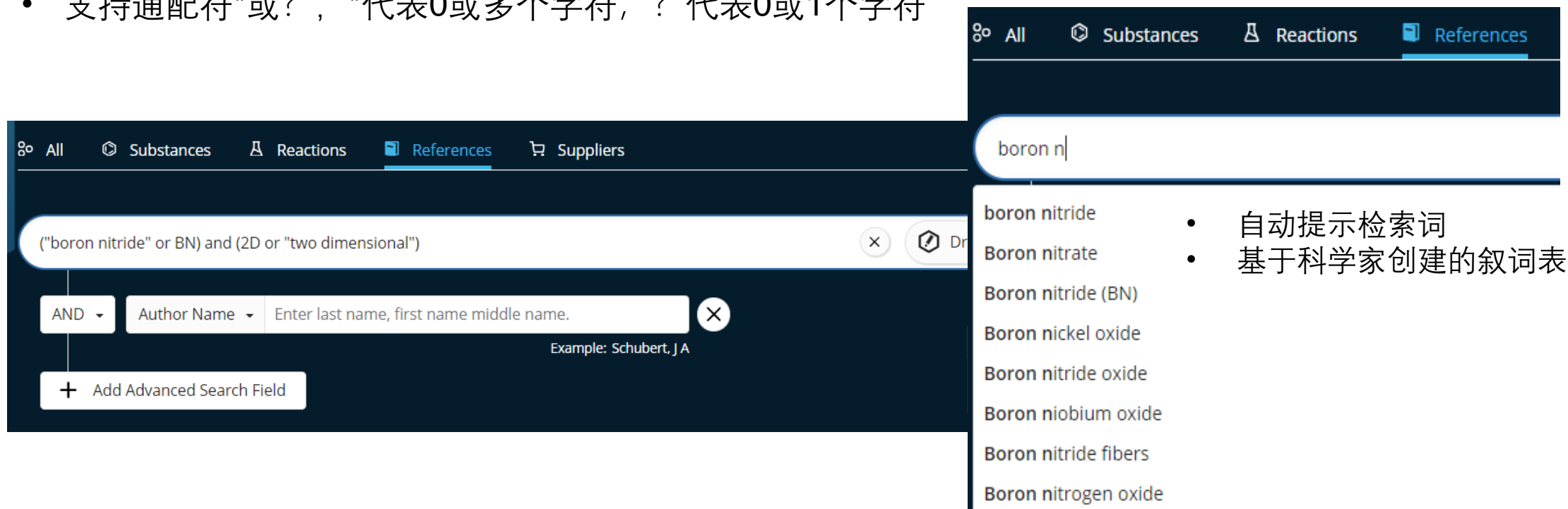
- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
 - 如何开展文献调研？
 - 如何聚焦某类物质？
 - 如何调研反应信息？
 - 怎么查、怎么选具体的实验方案？
- 常见问题Q&A

1. 如何开展文献检索？

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

1.1 如何精准构建检索主题？

- 支持使用：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
- 布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not
- “ ”不允许词形变化，但可出现单数或复数；() 优先运算，括号中表达式还可以和其他术语交互
- 支持通配符*或?，*代表0或多个字符；? 代表0或1个字符



The screenshot displays the CAS search interface. The main search bar contains the query: `("boron nitride" or BN) and (2D or "two dimensional")`. Below the search bar, there are fields for `AND` and `Author Name`, with a placeholder text: `Enter last name, first name middle name.` and an example: `Example: Schubert, J A`. A button labeled `+ Add Advanced Search Field` is also visible.

On the right side, a dropdown menu shows suggestions for the query `boron n`:

- boron nitride
- Boron nitrate
- Boron nitride (BN)
- Boron nickel oxide
- Boron nitride oxide
- Boron niobium oxide
- Boron nitride fibers
- Boron nitrogen oxide

Two bullet points are listed next to the suggestions:

- 自动提示检索词
- 基于科学家创建的叙词表

1.1 如何精准构建检索主题？

主题词示例：

(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

Filter by Exclude

Search Within Results

Document Type

Substance Role

Language

Publication Year

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Bioactivity Data

Formulation Purpose

Database

20,116,548 Results

1

Electrophoretic transfer of proteins from p
Procedure and some applications
By: Towbin, Harry; Staehelin, Theophil; Gordon, Julian
Proceedings of the National Academy of Sciences of the U
Database: CAPLUS and MEDLINE

A method was devised for the electrophoretic transfer of p
results in quant. transfer of ribosomal proteins from gels c
obtained with no loss of resolution, but the transfer was n
simpler than conventional procedures. The immobilized p
capacity on the nitrocellulose was blocked with excess pro

View More

Full Text

Subst

2

Polymer photovoltaic cells: enhanced effici
heterojunctions
By: Yu, G.; Gao, J.; Hummelen, J. C.; Wudl, F.; Heeger, A. J.
Science (Washington, D. C.) (1995), 270(5243), 1789-91 | Le

The carrier collection efficiency (η_c) and energy conversion
of the semiconducting polymer with C₆₀ or its functional
hexyloxy-1,4-phenylene vinylene (MEH-PPV) and fullerene
2.9 percent, efficiencies that are better by more than two
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

Sort: Relevance View: Partial Abstract

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: CAPLUS

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 (EGaln) into microgels of marine polysaccharides. During sonicating bulk EGaln in aqueous alginate solution, alginate not only facilitates th...

View More

Full Text

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

2

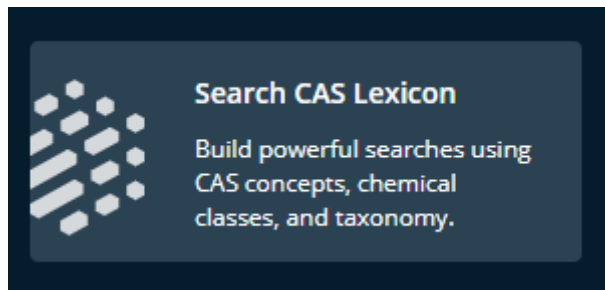
Conductive polymers and devices
By: Vannikov, A. V.
Vysokomolekulyarnye Soedineniya, Seriya A i Seriya B (2009), 51(4), 547-571 | Language: Russian, Database: CAPLUS

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

Primary batteries - Preferred Concept ⓘ [×](#)

OR [Remove All](#)

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

AND OR NOT [Add to Query](#) [Clear Query](#) [Search](#)

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

The screenshot displays the CAS search interface with the 'References' tab selected. The search bar prompts the user to search by keyword, substance name, CAS RN, patent number, PubMed ID, AN, CAN, and/or DOI. Below the search bar, there is a section for 'Author Name' with a text input field and a dropdown menu. A yellow box highlights the '+ Add Advanced Search Field' button. Another yellow box highlights a dropdown menu showing logical operators: AND, OR, and NOT. A third yellow box highlights a dropdown menu showing various search fields: Authors, Publication Name, Organization, Title, Abstract/Keywords, Concept, Substances, Bioactivity Data (marked as NEW), Publication Year, Document Identifier, Patent Identifier, and Publisher. An example search term 'Schubert, J A' is shown next to the author name input field.

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

文本与结构是“and”关系

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)

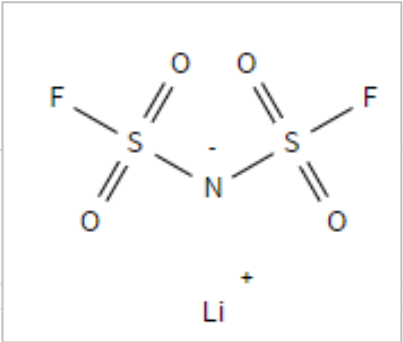
☐ Nanoscale (5)

☐ Purification or Recovery (4)

☐ Analyte (2)

Apply

Cancel



Li⁺

定位物质在文献中的研究角色

CAS SciFinder

References

("lithium battery" or "lithium-ion battery" or "Li-ion batt

Edit

Search

1

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)

1,454 Results

Sort: Relevance

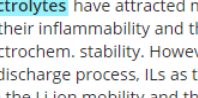
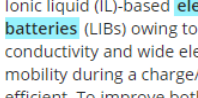
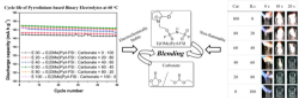
View: Partial Abstract

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, Taeun; Kim, Young Gyu

ACS Sustainable Chemistry & Engineering (2016), 4(2), 497-505 | Language: English, Database: Caplus



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 electrochem. 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 task-s...

View More

Full Text

Substances (11)

Reactions (3)

Citing (30)

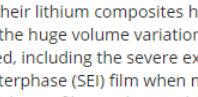
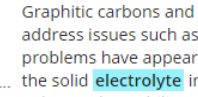
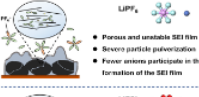
Citation Map

2

Anionic Effect on Enhancing the Stability of a Solid Electrolyte Interphase Film for Lithium Deposition on Graphite

By: Yang, Gaojing; Zhang, Simeng; Weng, Suting; Li, Xiaoyun; Wang, Xuefeng; Wang, Zhaoxiang; Chen, Lique

Nano Letters (2021), 21(12), 5316-5323 | Language: English, Database: Caplus 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.

80,812 Results

Sort: Relevance View: Partial Abstract

1

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

By: Chen, Xiaorong; Yu, Xinmeng; 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_xN/CNT) is rationally designed by the thermal of corresponding hydroxide/carbontubes at low temperature, following nitridation. The synergistic effect between Ni-Co ternary nitrides (Ni₄N, Co_{5.47}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.

PatentPak Full Text

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

AI技术支持的相关度排序

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

Relevance

Times Cited

Accession Number: Ascending

Accession Number: Descending

Publication Date: Newest

Publication Date: Oldest

排序方式

Search Within Results

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

结果集的二次检索

Search

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

<input checked="" type="checkbox"/> Electrochemical, Radiational, and Thermal Energy Technology (56K)	<input type="checkbox"/> Inorganic Analytical Chemistry (51)	<input type="checkbox"/> Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (12)
<input checked="" type="checkbox"/> Electrochemistry (775)	<input type="checkbox"/> Physical Properties of Synthetic High Polymers (48)	<input type="checkbox"/> Thermodynamics, Thermochemistry, and Thermal Properties (10)
<input checked="" type="checkbox"/> Industrial Inorganic Chemicals (493)	<input type="checkbox"/> Biochemical Methods (45)	<input type="checkbox"/> Magnetic Phenomena (7)
<input type="checkbox"/> Plastics Fabrication and Uses (402)	<input type="checkbox"/> Optical, Electron, and Mass Spectroscopy and Other Related Properties (42)	<input type="checkbox"/> Nuclear Technology (6)
<input type="checkbox"/> Electric Phenomena (374)	<input type="checkbox"/> Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms (40)	<input type="checkbox"/> Propellants and Explosives (6)
<input type="checkbox"/> Plastics Manufacture and Processing (205)	<input type="checkbox"/> Pharmaceuticals (38)	<input type="checkbox"/> Cement, Concrete, and Related Building Materials (5)
<input type="checkbox"/> Ceramics (184)	<input type="checkbox"/> Textiles and Fibers (36)	<input type="checkbox"/> Surface Active Agents and Detergents (5)
<input type="checkbox"/> Chemistry of Synthetic High Polymers (140)	<input type="checkbox"/> Air Pollution and Industrial Hygiene (34)	<input type="checkbox"/> Toxicology (5)
<input type="checkbox"/> Heterocyclic Compounds (More Than One Hetero Atom) (120)	<input type="checkbox"/> General Physical Chemistry (32)	<input type="checkbox"/> Food and Feed Chemistry (4)
<input type="checkbox"/> Nonferrous Metals and Alloys (110)	<input type="checkbox"/> Fossil Fuels, Derivatives, and Related Products (31)	<input type="checkbox"/> Industrial Carbohydrates (4)
		<input type="checkbox"/> 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)
- ☐ 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 (1,666)
- ☐ Binding energy (1,666)
- ☐ Sodium-ion secondary batteries (1,646)
- ☐ Electric conductors (1,622)
- ☐ Electric resistance (1,582)
- ☐ Electric transfer (1,562)

OK Cancel

Concept

Top Count Alphanumeric Search

Concept Name

nano*

3 Selected

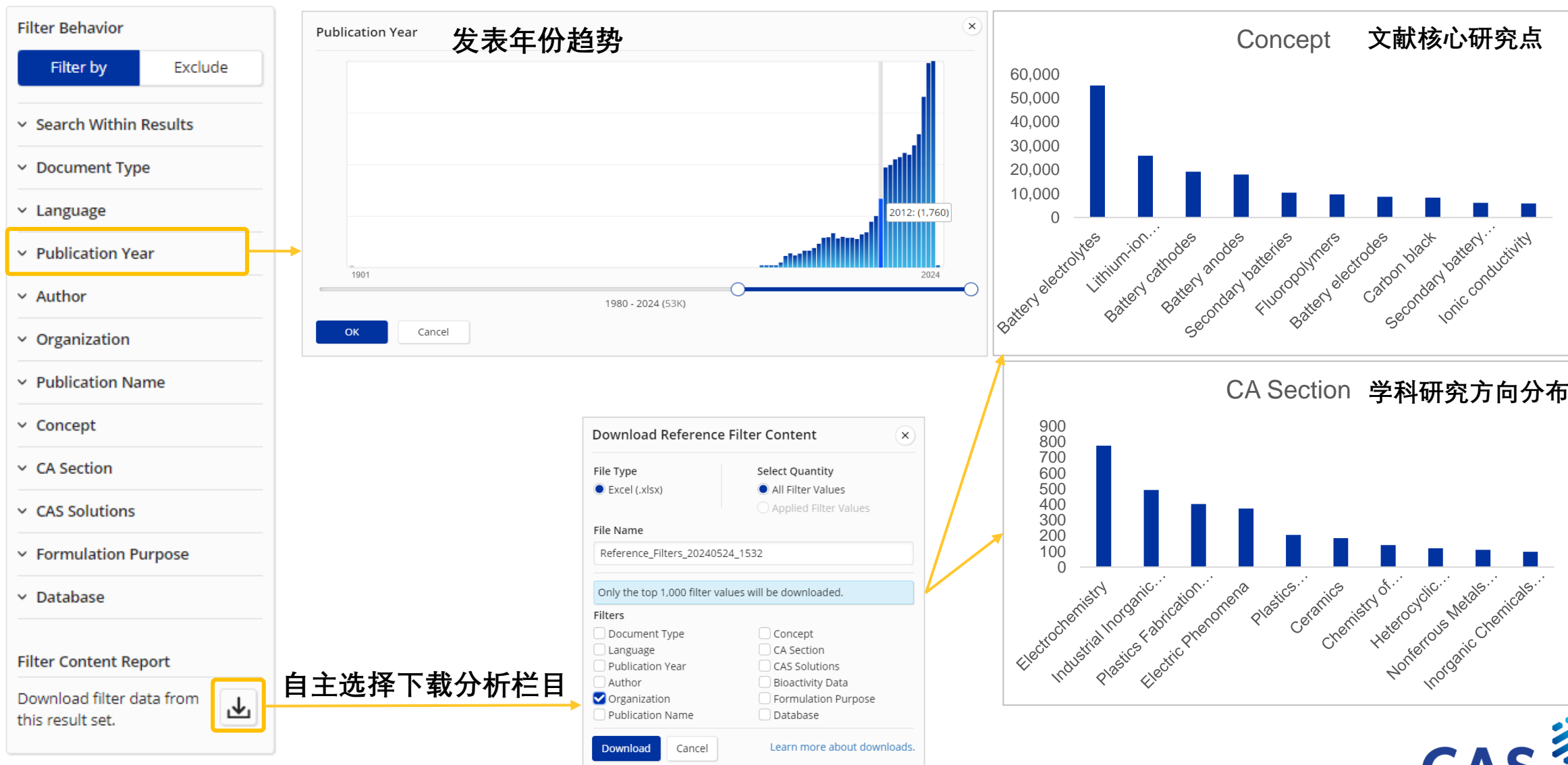
支持使用通配符

精准定位核心研究点

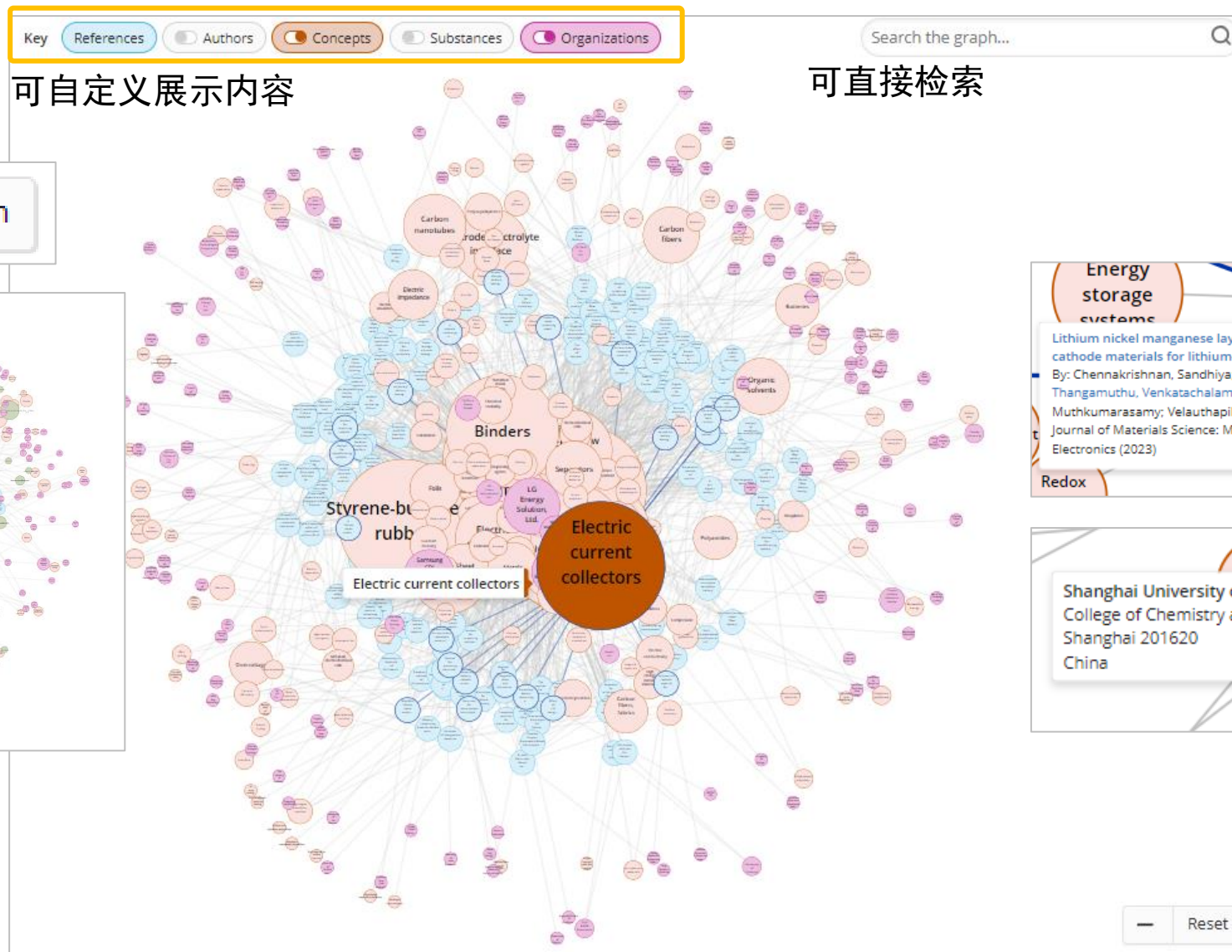
- ☐ Carbon nanofibers (376)
- ☒ Carbon nanostructured materials (20)
- ☐ Carbon nanotube fibers (39)
- ☐ Carbon nanotubes (2,175)
- ☐ Cellulosic nanofibers (23)
- ☐ Core-shell nanoparticles (60)
- ☐ Electric nanogenerators (3)
- ☐ Ferromagnetic nanoparticles (1)
- ☐ Graphite nanofibers (40)
- ☐ Halloysite nanotubes (3)
- ☐ Nanocrystallites (7)
- ☐ Nanocrystallization (3)
- ☐ Nanocrystals (197)
- ☐ Nanocubes (39)
- ☐ Nanocylinders (1)
- ☐ Nanodevices (9)
- ☐ Nanodisks (18)
- ☐ Nanodispersions (2)
- ☐ 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

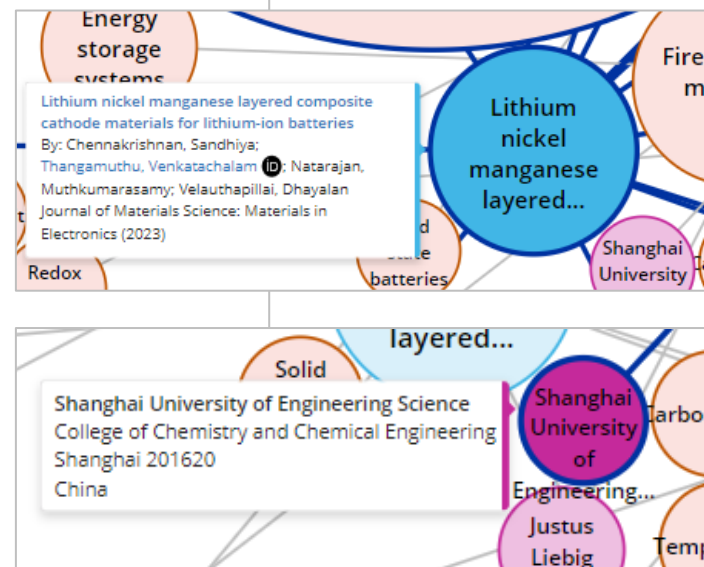
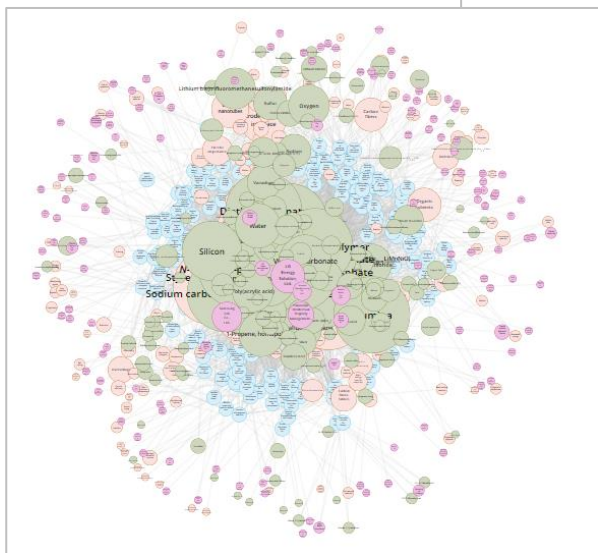


1.4 可视化分析——知识图谱



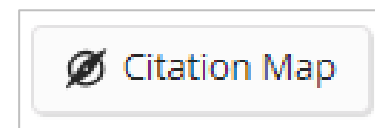
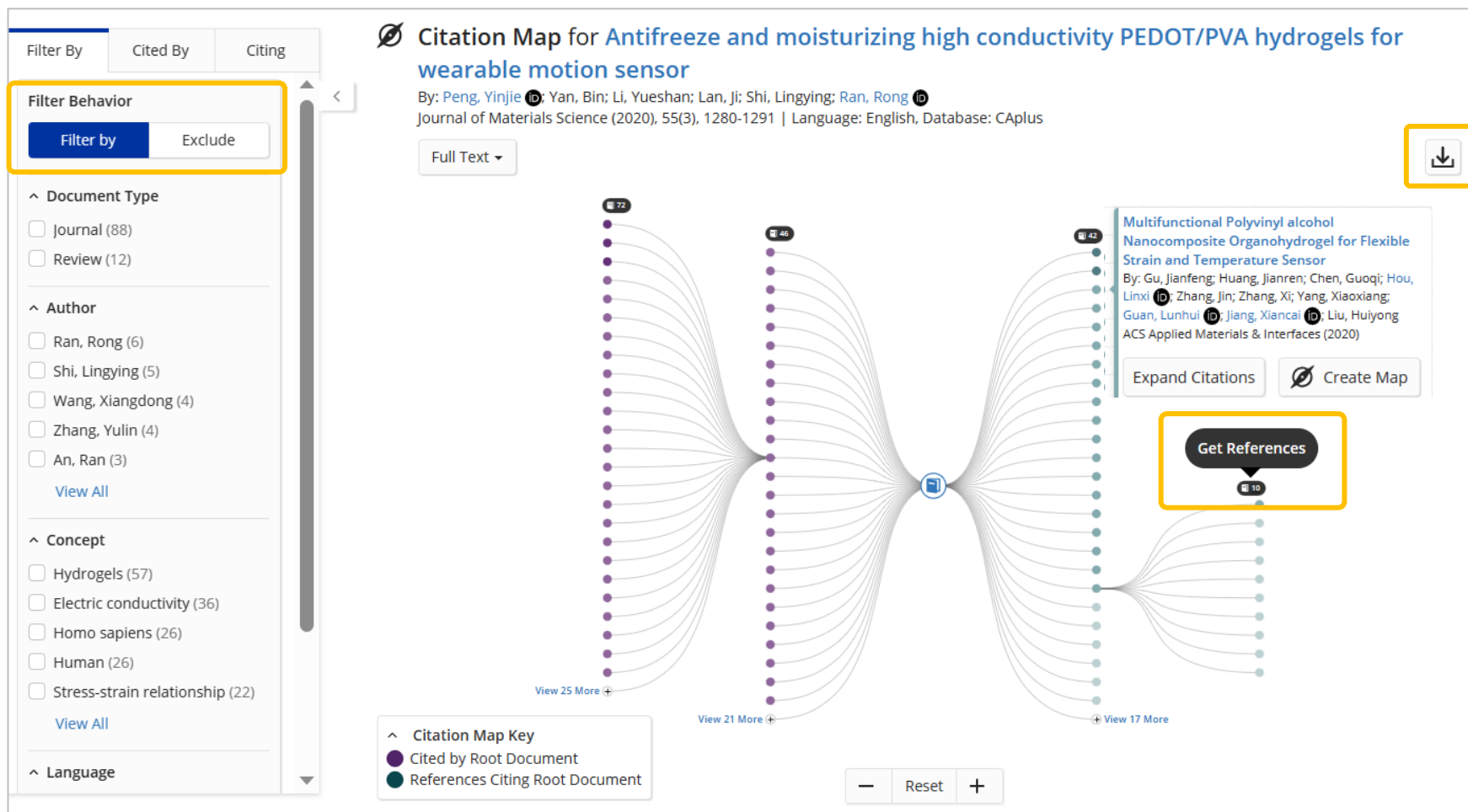
可自定义展示内容

可直接检索

 Knowledge Graph

1.4 可视化分析——引文地图

便捷获得相关文献



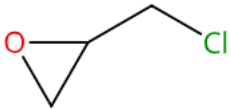
- Cited By: 参考文献
- Citing: 引用当前文献的文献
- 通过聚类选项筛选引文
- 可下载引文地图
- 显示引文和被引文献的数量，点击可链接至对应的文献结果页面

1.5 深入文献详情

内容合集间彼此关联

1

106-89-8



C₃H₅ClO

Epichlorohydrin

53K

32K

84

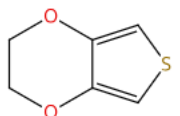
References

Reactions

Suppliers

2

126213-51-2



(C₆H₆O₂S)_x

Poly(3,4-ethylenedioxythiophene)

48K

1,505

7

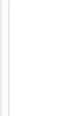
References

Reactions

Suppliers

3

50851-5



(C₈H₈O₃S)_x

Poly(styrenesulfonic acid)

40K

882

2

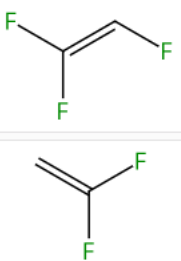
References

Reactions

Suppliers

4

28960-88-5



(C₂H₂F₂·C₂HF₃)_x

Components: 2

P(VDF-TrFE)

5,483

63

7

References

Reactions

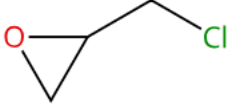
Suppliers

5

2839834-68-1

106602-18-0

Image Not Available



(C₃H₅ClO.Unspecified)_x

Components: 2

2

1

0

References

Reaction

Suppliers

6

106602-18-0

Image Not Available

Unspecified

N-[2-Hydroxy-3-(trimethylammonium)propyl]chitosan chloride

500

247

0


References

Reactions

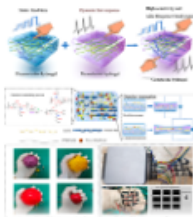
Suppliers

1

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 piezoelec. 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 fluori...

View More

Full Text

Substances (7)


Reaction (1)

Citing (9)

Citation Map

106602-18-0

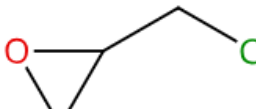
Image Not Available

+ 

→

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

23

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1.5 深入文献详情

巧用CAS PatentPak浏览专利

13

Polymerization with living characteristics with controlled dispersity, polythereby, 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: CAS

This invention concerns a free radical **polymerization** process, selected chain transfer agents and **polymers** made thereby, in which the process comprises preparing **polymers** (ZCS₂Q_q)_pR (I) or Z(CS₂Q_q)_pR (II) by contacting: (i) a monomer having repeating units Q, selected from vinyl monomers of structure C₂H₃Q, alkylmaleimide, N-arylmaleimide, dialkyl fumarate and cyclopolymerizable monomers; (ii) a thiocarbonyl compound from (ZCS₂)_pR (III) and Z'(CS₂R)_m (IV) having a chain transfer constant ≥0.1; and (iii) free radicals p.

[View More](#)

PatentPak Full Text ▾

Substances (83) Reactions (0) Citing (39)

Patent	Language	Kind Code	PatentPak Options
WO9801478	English	A1	PDF PDF+ Viewer
CN1137144	Chinese	C	PDF
CN1500813	Undetermined	A	PDF
CN1673216	Chinese	A	PDF
CN1331851	Chinese	C	PDF

CAS PatentPak

PAGE 28 / 88 ZOOM 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 32

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.

15 **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).

20 **Procedure 2**
Preparation of benzyl dithiobenzoate (3) (C, p=1, R = CH₂Ph, 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

25 ¹H-nmr (CDCl₃) δ (ppm) 1.43 (t, 6H); 4.38 (s, 2H), 4.65 (q, 4H) and 7.30-7.45 (m, 5H).

5 **Procedure 8**
Preparation of tert-butyl trithioperbenzoate (21) (C, p=1; R = (CH₃)₃CS; 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. ¹H-nmr (CDCl₃) δ (ppm) 1.32 (s, 9H), 7.45 (m, 3H) and 8.00 (m, 2H).

10 **Example 13**
Preparation of 2-phenylprop-2-yl 4-chlorodithiobenzoate (22) (C, p=1, R = C(CH₃)₂Ph; Z = *p*-ClC₆H₄)
A mixture of 4-chlorodithiobenzoic acid (13 g) and *o*-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 %). ¹H-nmr (CDCl₃) δ (ppm) 2.00 (s, 6H); 7.30 (m, 5H); 7.55 (d, 2H) and 7.83 (d, 2H).

15 20

文献检索小结

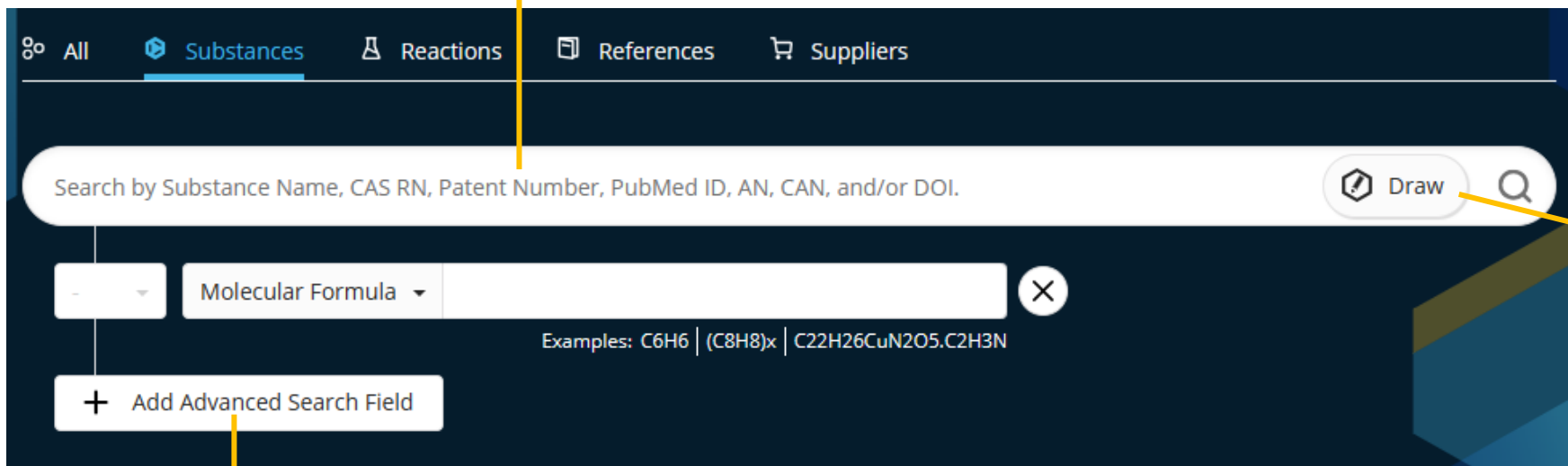
1. 检索主题的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
2. 主题词+结构联合检索，快速获得文献
3. 利用丰富的筛选工具，缩小范围，锁定目标文献
4. 检索结果趋势分析、知识图谱、引文地图
5. 文献详情，CAS PatentPak浏览专利详情

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



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

- 使用结构绘制面板进行结构检索

- 高级检索

检索策略推荐

- 有机化合物，金属配合物，天然产物：结构检索
- 无机物，合金：分子式检索
- 高分子化合物：分子式检索和结构检索

物质检索——物质标识符

Substances search for "Paxlovid 2628280-40-8"

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

Absolute stereochemistry shown

C23H32F3N5O4

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

319 References 106 Reactions 39 Suppliers

2

2803933-60-8

Absolute stereochemistry shown

C37H48N6O5S2.C23H32F3N5O4

Components: 2

Paxlovid

39 References 0 Reactions 0 Suppliers

- 可同时检索多个物质标识符（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

Navigation: All Substances Reactions References

Search: PEG

- 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

Sort: Relevance View: Partial

1 25322-68-3 $\text{HO}-(\text{C}_2\text{H}_4\text{O})_n\text{H}$ PEG 455K References 63K Reactions 792 Suppliers

2 1370345-22-4 Oxirane, homopolymer Preferred RN: 25322-68-3 0 References 0 Reactions 0 Suppliers

3 934660-23-8 $(\text{C}_2\text{H}_4\text{O})_n(\text{C}_2\text{H}_4\text{O})_n\text{C}_2\text{H}_6\text{O}_2$ 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 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 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

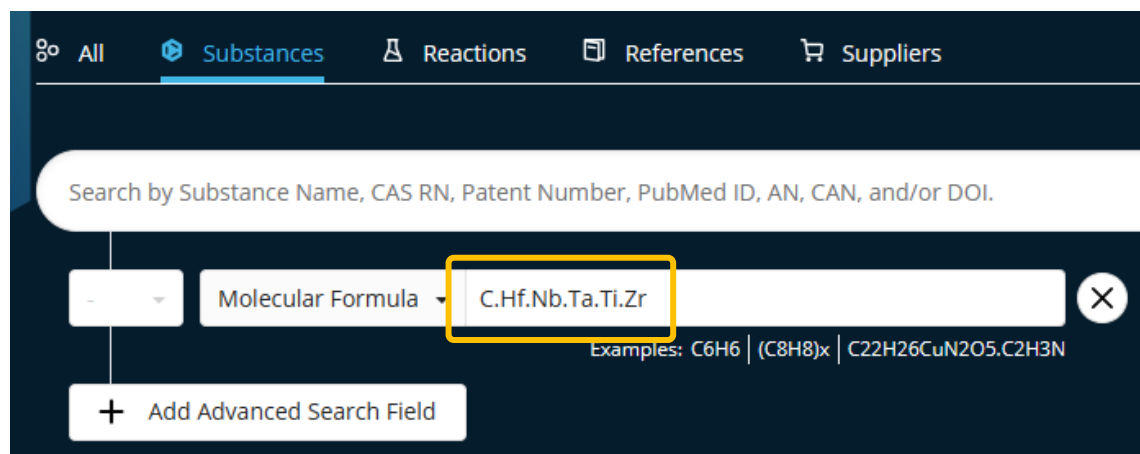
The screenshot displays the CAS Substances search interface. On the left, the search bar is set to "Substances" and the search criteria are "Component RN" with values "115-07-1" and "74-85-1". A dropdown menu for "Component RN" is open, showing options: "Molecular Formula", "CAS Registry Number" (highlighted), "Chemical Identifier", "Substance RN", and "Component RN".

On the right, the "Substances search for 2 Advanced Fields" panel is shown. The "Filter Behavior" section has "Filter by" selected. The "Filtering" section shows "Number of Components: 2" and "Substance Class: Polymer". The "Number of Components" filter is expanded, showing "2 (24)" selected. The "Substance Class" filter is also expanded, showing "Polymer (24)" selected. The search results are displayed in a grid, showing the first three results:

- Result 1: 725713-40-6, (C₃H₆.C₂H₄)_x, Components: 2, 1-Propene, polymer with ethene, diblock. 314 References, 169 Reactions, 0 Suppliers.
- Result 2: 935748-32-6, (C₃H₆.C₂H₄)_x, Components: 2, 1-Propene, polymer with ethene, alternating, diblock. 6 References, 0 Reactions, 0 Suppliers.
- Result 3: 9010-79-1, (C₃H₆.C₂H₄)_x, Components: 2, Ethylene-propylene copolymer. 66K References, 3,665 Reactions, 13 Suppliers.

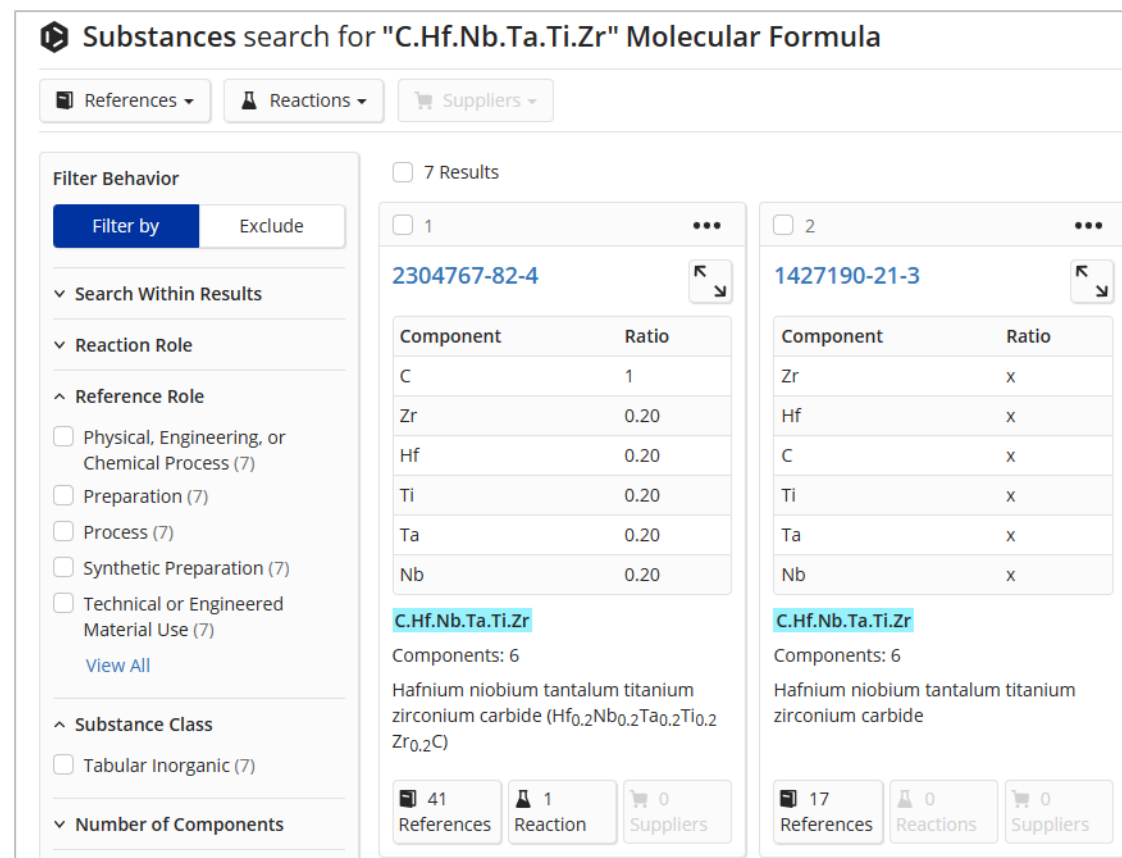
2.1 分子式检索：高效检索聚合物或无机化合物

- 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_2SO_4 : $\text{H}_2\text{O}_4\text{S}.2\text{Na}$



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



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

References Reactions Suppliers

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

Physical, Engineering, or Chemical Process (7)

Preparation (7)

Process (7)

Synthetic Preparation (7)

Technical or Engineered Material Use (7)

View All

Substance Class

Tabular Inorganic (7)

Number of Components

7 Results

1

2304767-82-4

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

C.Hf.Nb.Ta.Ti.Zr

Components: 6

Hafnium niobium tantalum titanium zirconium carbide ($\text{Hf}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2}\text{Ti}_{0.2}\text{Zr}_{0.2}\text{C}$)

41 References 1 Reaction 0 Suppliers

2

1427190-21-3

Component	Ratio
Zr	x
Hf	x
C	x
Ti	x
Ta	x
Nb	x

C.Hf.Nb.Ta.Ti.Zr

Components: 6

Hafnium niobium tantalum titanium zirconium carbide

17 References 0 Reactions 0 Suppliers

2.1 分子式检索：高效检索聚合物或无机化合物

All Substances Reactions References Suppliers

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

-

Molecular Formula

(C₂H₄O)_nC₄H₈O

Examples: C₆H₆ | (C₈H₈)_x |

+ Add Advanced Search Field

Substances search for "(C₂H₄O)_nC₄H₈O" Molecular Formula

References Reactions Suppliers

Filter Behavior
Filter by Exclude

Search Within Results
Reaction Role
Reference Role
Commercial Availability
Number of Components
Element
Functional Group

12 Results

31497-33-3

(C₂H₄O)_nC₄H₈O
Poly(oxy-1,2-ethanediyl), alpha-(2-methyl-2-propen-1-yl)-omega-hydroxy-
1,667 References 1,562 Reactions 6 Suppliers

27252-80-8

(C₂H₄O)_nC₄H₈O
Polyethylene glycol allyl methyl ether
917 References 511 Reactions 11 Suppliers

85600-94-8

(C₂H₄O)_nC₄H₈O
Poly(oxy-1,2-ethanediyl), alpha-3-buten-1-yl-omega-hydroxy-
44 References 21 Reactions 0 Suppliers

All Substances Reactions References Suppliers

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

-

Molecular Formula

(C₅H₆O₄.C₄H₆O₂.C₃H₄O₂)_x

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

+ Add Advanced Search Field

Substances search for "(C₅H₆O₄.C₄H₆O₂.C₃H₄O₂)_x" Molecular Formula

References Reactions Suppliers

Filter Behavior
Filter by Exclude

Search Within Results
Reaction Role
Reference Role
Commercial Availability
Number of Components
Molecular Weight
Stereochemistry
Element
Functional Group
Aromatic Rings
Substance Class
Isotopes
Metals

6 Results

97384-95-7

(C₅H₆O₄.C₄H₆O₂.C₃H₄O₂)_x
Components: 3
Butanedioic acid, 2-methylene-, polymer with 2-methyl-2-propenoic acid and 2-propanoic acid...
28 References 4 Reactions 0 Suppliers

63899-49-0

(C₅H₆O₄.C₄H₆O₂.C₃H₄O₂)_x
Components: 3
Butanedioic acid, 2-methylene-, polymer with ethenyl acetate and 2-propanoic acid...
7 References 2 Reactions 0 Suppliers

56280-96-7

(C₅H₆O₄.C₄H₆O₂.C₃H₄O₂)_x
Components: 3
2-Butenedioic acid (Z)-, 1-methyl ester, polymer with ethenyl acetate and 2-propanoic acid...
3 References 0 Reactions 0 Suppliers

- (C₂H₄O)_nC₄H₈O: 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

32

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2.2 属性值联用检索物质

The screenshot displays the CAS search interface. At the top, there are tabs for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. Below these is a search bar with the text 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' A dropdown menu is open, showing various search criteria: 'Molecular Formula', 'CAS Registry Number', 'Chemical Identifier', 'Document Identifier', 'Patent Identifier', 'Experimental Spectra' (highlighted), 'Bioactivity Data' (marked with a 'NEW' tag), 'Biological', 'Chemical Properties', 'Density', 'Electrical', 'Lipinski', 'Magnetic', 'Mechanical', 'Optical and Scattering', 'Structure Related', and 'Thermal'. The 'Experimental Spectra' dropdown is further expanded, showing 'Proton NMR', 'Carbon-13 NMR', 'Nitrogen-15 NMR', 'Fluorine-19 NMR', and 'Phosphorus-31 NMR'. In the background, there are sections for 'Search CAS Lexicon' and 'Search CAS Sequences'. At the bottom left, there is a 'Recent Searches' section. On the right side of the interface, there are examples of molecular formulas: C₆H₆, (C₈H₈)_x, and C₂₂H₂₆CuN₂O₅.C₂H₃N. Below the search bar, there are two main search areas: 'Search CAS Lexicon' and 'Search CAS Sequences'. The 'Search CAS Lexicon' section includes the text 'Build powerful searches using concepts, chemical and taxonomy.' The 'Search CAS Sequences' section includes the text 'Query BLAST, CDR, and algorithms for nucleotide protein based sequence'. At the bottom right, there is a 'Recent Searches' section with a date 'August 15' and a time '10:44 AM'. Below this, there is a 'Substance' section with a chemical structure and the text 'As Drawn (2) Substructure (6,704) Similarity (242K)'.

实验核磁谱图数值助力结构解析

高级检索字段：

- CAS RN (物质、组份)、物质标识符、分子式、文献号、专利号
- 实验谱图：¹H, ¹³C, ¹⁵N, ¹⁹F, ³¹P 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

The screenshot displays the CAS search interface. At the top, there are tabs for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. Below these is a search bar with the text 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' A dropdown menu is open, showing various search criteria: 'Molecular Formula', 'CAS Registry Number', 'Chemical Identifier', 'Document Identifier', 'Patent Identifier', 'Experimental Spectra', 'Bioactivity Data' (marked with a 'NEW' tag), 'Biological', 'Chemical Properties' (highlighted), 'Density', 'Electrical', 'Lipinski', 'Magnetic', 'Mechanical', 'Optical and Scattering', 'Structure Related', and 'Thermal'. The 'Chemical Properties' dropdown is further expanded, showing 'Koc', 'logD', 'logP', 'Mass Intrinsic Solubility (g/L)', 'Mass Solubility (g/L)', 'Molar Intrinsic Solubility (mol/L)', 'Molar Solubility (mol/L)', 'Molecular Weight', 'pKa', and 'Vapor Pressure (Torr)'. In the background, there are sections for 'Search CAS Lexicon' and 'Search CAS Sequences'. The 'Search CAS Lexicon' section includes the text 'Build powerful searches using concepts, chemical and taxonomy.' The 'Search CAS Sequences' section includes the text 'Query BLAST, CDR, and algorithms for nucleotide protein based sequence'. At the bottom left, there is a 'Recent Searches' section. On the right side of the interface, there are examples of molecular formulas: C₆H₆, (C₈H₈)_x, and C₂₂H₂₆CuN₂O₅.C₂H₃N. Below the search bar, there are two main search areas: 'Search CAS Lexicon' and 'Search CAS Sequences'. The 'Search CAS Lexicon' section includes the text 'Build powerful searches using concepts, chemical and taxonomy.' The 'Search CAS Sequences' section includes the text 'Query BLAST, CDR, and algorithms for nucleotide protein based sequence'. At the bottom right, there is a 'Recent Searches' section with a date 'August 15' and a time '10:44 AM'. Below this, there is a 'Substance' section with a chemical structure and the text 'As Drawn (2) Substructure (6,704) Similarity (242K)'.

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/cm³、拉伸强度>1000MPa、熔点>600℃。

Substances search for 3 Advanced Fields

Filter Behavior: **Filter by** Exclude

Search Within Results

Reaction Role

Reference Role

Bioactivity Data

Commercial Availability

Number of Components

Element

Aromatic Rings

Substance Class

- ☒ Alloy (18)
- ☐ Element (9)
- ☐ Polymer (9)
- ☐ Manual Registration (4)
- ☐ Mineral (1)
- [View All](#)
- ☐ Isotopes

Filtering: Substance Class: Alloy X Clear All Filters

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

1	2	3																																																												
11134-23-9	12634-55-8	12627-49-5																																																												
<table><thead><tr><th>Component</th><th>Percent</th></tr></thead><tbody><tr><td>Fe</td><td>62-72</td></tr><tr><td>Cr</td><td>16.00-18.00</td></tr><tr><td>Ni</td><td>10.00-14.00</td></tr><tr><td>Mo</td><td>2.00-3.00</td></tr><tr><td>Mn</td><td>0-2.00</td></tr><tr><td>Si</td><td>0-1.00</td></tr><tr><td>P</td><td>0-0.045</td></tr><tr><td>S</td><td>0-0.030</td></tr><tr><td>C</td><td>0-0.030</td></tr></tbody></table> <p>C.Cr.Fe.Mn.Mo.Ni.P.S.Si Components: 9 AlSi 316L</p> <p>25K References 17 Reactions 5 Suppliers</p>	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	<table><thead><tr><th>Component</th><th>Percent</th></tr></thead><tbody><tr><td>Mg</td><td>95-97</td></tr><tr><td>Al</td><td>2.5-3.5</td></tr><tr><td>Zn</td><td>0.6-1.4</td></tr><tr><td>Mn</td><td>0.20</td></tr><tr><td>Si</td><td>0-0.10</td></tr><tr><td>Cu</td><td>0-0.05</td></tr><tr><td>Ca</td><td>0-0.04</td></tr><tr><td>Ni</td><td>0-0.005</td></tr><tr><td>Fe</td><td>0-0.005</td></tr></tbody></table> <p>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...</p> <p>12K References 8 Reactions 0 Suppliers</p>	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	<table><thead><tr><th>Component</th><th>Percent</th></tr></thead><tbody><tr><td>Al</td><td>87-91</td></tr><tr><td>Zn</td><td>5.1-6.1</td></tr><tr><td>Mg</td><td>2.1-2.9</td></tr><tr><td>Cu</td><td>1.2-2.0</td></tr><tr><td>Cr</td><td>0.18-0.28</td></tr><tr><td>Fe</td><td>0-0.50</td></tr><tr><td>Si</td><td>0-0.40</td></tr><tr><td>Mn</td><td>0-0.30</td></tr><tr><td>Ti</td><td>0-0.20</td></tr></tbody></table> <p>Al.Cr.Cu.Fe.Mg.Mn.Si.Ti.Z... Components: 9 AA 7075</p> <p>11K References 1 Reaction 1 Supplier</p>	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
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																																																													
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Ca	0-0.04																																																													
Ni	0-0.005																																																													
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Component	Percent																																																													
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Si	0-0.40																																																													
Mn	0-0.30																																																													
Ti	0-0.20																																																													

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

AllSubstancesReactionsReferencesSuppliers

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

Molecular Weight220 to 280

Predicted values only. Examples: 46.07 | 125 to 350 | >300

ANDpKa1.3 to 1.8

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

ANDCarbon-13 NMR114 to 171, 96, 11.5

Allowance of ± 2 ppm. Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187

+ Add Advanced Search Field

Substances search for 3 Advanced Fields

ReferencesReactionsSuppliers

Filter Behavior

Filter by

Exclude

Reaction Role

☐ Product (15)

☐ Reactant (11)

☐ Reagent (1)

☐ Catalyst (1)

Reference Role

☐ Preparation (15)

☐ Synthetic Preparation (15)

☐ Biological Study (14)

☐ Pharmacological Activity (14)

☐ Uses (14)

View All

Bioactivity Data

☒ Structure Activity Relationships (15)

☒ Toxicity (2)

☒ Absorption, Distribution, Metabolism, Excretion (1)

Filtering: Bioactivity Data: 3 Selected X

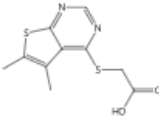
Clear All Filters

15 Results

Sort: Molecular Formula: Ascending View: Partial

1

296262-16-3



C10H10N2O2S2
2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]acetic acid

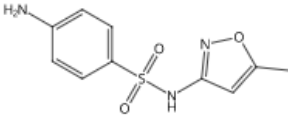
5References

42Reactions

44Suppliers

2

723-46-6



C10H11N3O3S
Sulfamethoxazole

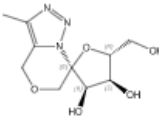
24KReferences

961Reactions

120Suppliers

3

1631737-39-7



C10H15N3O5
(2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxymethyl)-3'-methylspiro[furan-2(3H),7'(6'H)]-...

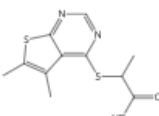
2References

22Reactions

0Suppliers

4

442571-27-9



C10H10N2O2S2
2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]acetic acid

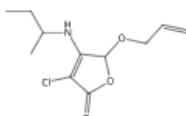
5References

42Reactions

44Suppliers

5

1927010-88-5



C10H11ClO2
1-allyl-4-chloro-5-methyl-2H-pyran-2-one

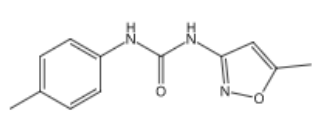
24KReferences

961Reactions

120Suppliers

6

697787-29-4



C10H11ClO2
1-allyl-4-chloro-5-methyl-2H-pyran-2-one

24KReferences

961Reactions

120Suppliers

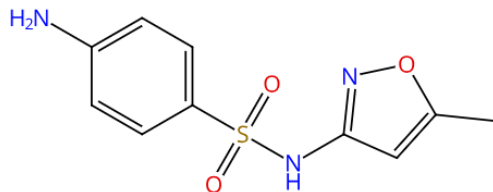
- 分子量：220至280之间
- pKa：1.3至1.8之间
- C谱特征峰：114至171之间，96，11.5

物质详情

CAS Registry Number: 723-46-6

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

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



$C_{10}H_{11}N_3O_3S$

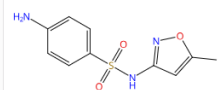
Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-

Boiling Point Carbon-13 NMR Spectrum for 723-46-6

Density (Ex)
pKa (Predi
Experimen

723-46-6



$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

Solvent

DMSO- d_6 (2206-27-1)

Standard

Tetramethylsilane (75-76-3)

Spectrum Summary

Spectrum ID

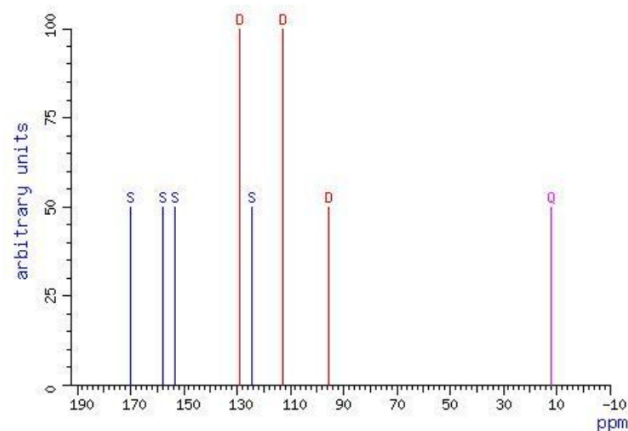
CNCC-59959-233D

Spectrometer

JEOL GX-270

Source

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



Other Names and Identifiers

Experimental Properties

Experimental Spectra

折叠菜单显示物质各类信息

1H NMR

^{13}C NMR

Hetero NMR

IR

Mass

Raman

UV and Visible

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

Carbon-13 NMR Spectrum - 1 Source

Solvent

DMSO- d_6

DMSO- d_6

-

Methanol- d_4

DMSO- d_6

-

DMSO- d_6

-

Source

(1) WSS

(2) WSS

(2) WSS

(3) CAS

(4) CAS

(5) BIORAD

(6) AIST

(7) CAS

Sources

(1) Kartashov, V. S.; Khimiko-Farmatsevticheskii 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, Nareesh; 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) Blasoli, 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

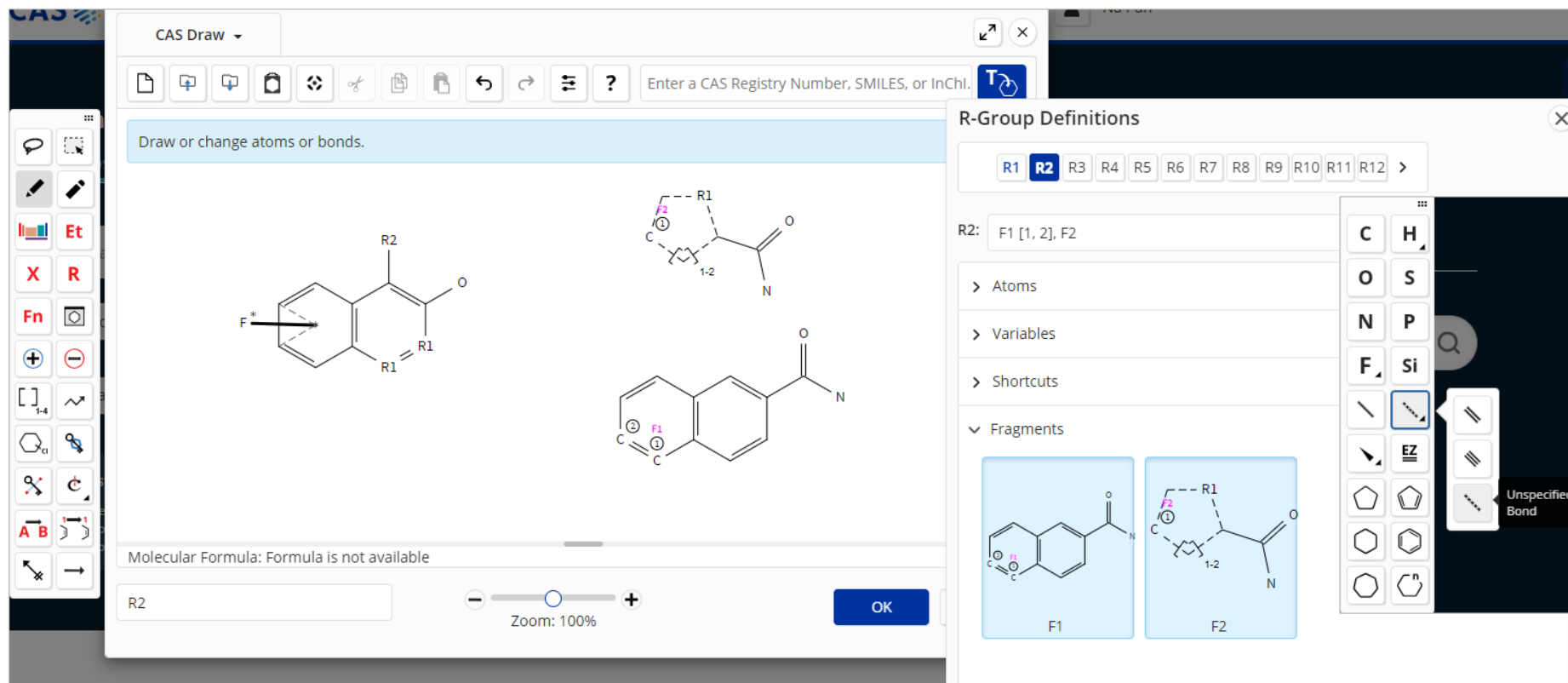
GHS Hazard Statements

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

The screenshot displays the CAS Substances search interface. At the top, the search bar is labeled "Substances search for drawn structure". Below it, there are tabs for "References", "Reactions", and "Suppliers". The search results are displayed in a grid format, showing chemical structures and their corresponding CAS numbers. The "Structure Match" section on the left highlights the search criteria: "As Drawn (0)", "Substructure (732)", and "Similarity (9)". The "Filter Behavior" section on the right allows users to filter results by various criteria, including "Reaction Role", "Reference Role", "Commercial Availability", "Number of Components", "Molecular Weight", "Stereochemistry", "Element", "Substance Class", "Isotopes", "Metals", "Experimental Property", "Bioactivity Indicator", and "Search Within Results".

Chemical structure of the search fragment (R1) is shown above the results grid:

C1CCNCC1P(C)(C)C2=CC=CC=C2

The results grid shows the following entries:

- 685504-28-3: $C_{31}H_{35}Cl_3CoNP_2$ (7-4)-Trichloro[N-[2-(diphenylphosphino- κP)ethyl]-N-[2-(diphenylphosphino)ethyl]...
- 807307-30-8: $C_{31}H_{35}Cl_3CoNOP_2$ Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- κP)ethyl]-N-[2-(diphenylphosphino)ethyl]...
- 635299-07-9: $C_{31}H_{35}Cl_3CoNOP_2 \cdot H$ Components: 2 Component RN: 807307-30-8 Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- κP)ethyl]-N-[2-(diphenylphosphino)ethyl]...
- 635299-08-0
- 16827-53-5
- 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

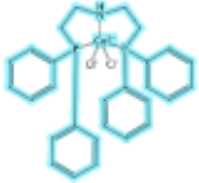
Commercial Availability

Number of Components

Molecular Weight

4

1087216-22-5



$C_{28}H_{29}Cl_2CoNP_2$

Dichloro[2-(diphenylphosphino- κP)-N-[2-(diphenylphosphino- κP)ethyl]ethanamine- κN ...

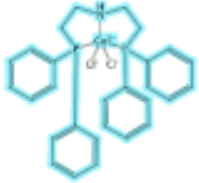
8References

105Reactions

0Suppliers

5

2170923-58-5



$C_{28}H_{29}Cl_2CoNP_2$

8References

105Reactions

0Suppliers

Reference Role:
物质在文献中的研究角色

Filter by

Exclude

Reaction Role

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)

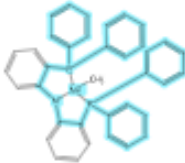
8References

105Reactions

0Suppliers

4

579490-58-7



$C_{37}H_{31}NNiP_2$

(SP-4-1)-[2-(Diphenylphosphino- κP)-N-[2-(diphenylphosphino- κP)phenyl]benzenamine...

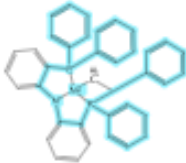
7References

22Reactions

0Suppliers

5

579490-62-3



$C_{38}H_{33}NNiP_2$

(SP-4-1)-[2-(Diphenylphosphino- κP)-N-[2-(diphenylphosphino- κP)phenyl]benzenamine...

6References

21Reactions

0Suppliers

Reaction Role:
物质在反应中的角色

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)

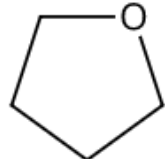

☐ Salt and Compound With (9)

☐ General Derivative (3)

^ Isotopes

☐ 4

849402-50-2



$(C_4H_8O.C_4H_4S)_x.xCH_4O$

Components: 3

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

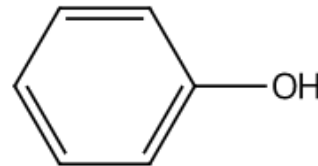
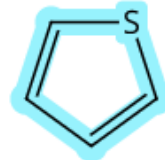
☐ 1 Reference

☐ 0 Reactions

☐ 0 Suppliers

☐ 5

62306-29-0



$(C_6H_6O.C_4H_4S.CH_2O)_x$

Components: 3

Formaldehyde, polymer with phenol and thiophene

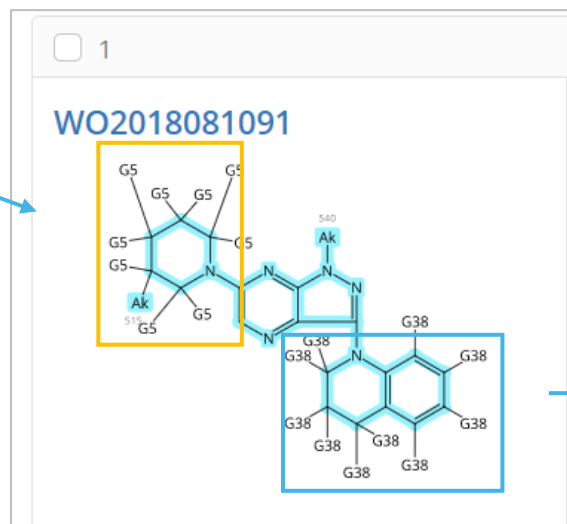
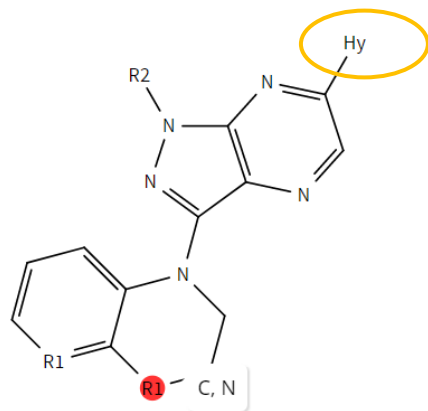
☐ 2 References

☐ 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



命中的Markush结构及解读

WO2018081091

☒ Search Patent Markush

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

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

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

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

Patent claim 1

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

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

专利中的定位，专利权人、命中结构的特点等等

WO 2018/081091

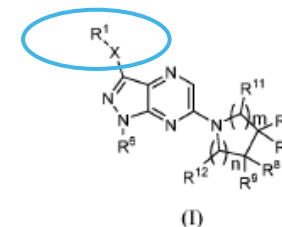
PCT/US2017/058048

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-R⁶⁶, O, S, S(O), SO₂, CR¹³R¹⁴, -O-C(R¹³R¹⁴)-, -C(R¹³R¹⁴)O-, C(O), or C=C(R¹³R¹⁴);

- 15 R⁶⁶ is selected from the group consisting of H, -(C₁-C₆)alkyl and phenyl, or together with R¹ bicyclic aryl or
- and the nitrogen to which they are attached form a nitrogen ring moiety selected from the group substituted with one or
- consisting of 5-7 membered monocyclic heteroaryl, a 8-12 membered bicyclic moiety with one
- saturated ring and one aromatic or heteroaromatic ring, a 8-12 membered bicyclic heteroaryl,
- and a 4-7 membered heterocycle, wherein the nitrogen ring moiety is optionally substituted
- 20 with one, two or more substituents each independently selected from the group consisting of
- R¹⁰, -OR¹⁰, -S(O)_wR¹⁰ (wherein w is 0, 1 or 2), -N(R¹⁰)₂, -OS(O)_wR¹⁰ (wherein w is 0, 1, or
- 2), -S(O)_w-N(R¹⁰)₂ (wherein w is 0, 1 or 2), -S(O)(NH)R¹⁰, -P(O)(R¹⁰)₂, -C(O)R¹⁰, -
- C(O)N(R¹⁰)₂, oxo, halogen, nitrile, phenyl (optionally substituted with one, two or three halo,
- C₁₋₃alkyl or C₁₋₃haloalkyl), C₁₋₃alkyl, C₁₋₃haloalkyl, and heteroaryl (optionally substituted with
- 25 one, two or three halo, C₁₋₃alkyl or C₁₋₃haloalkyl);

CAS 结构层面的数据集

What is claimed is:

1. Compound represented by the following Chemical formula 1 or Chemical formula 2, an enantiomer thereof, a diastereomer thereof, or a pharmaceutically acceptable salt thereof:

[Chemical formula 1]

or

[Chemical formula 2]

wherein

X¹ is O, S or —N(CH₂CH₃)—,

X² and X³ are each independently N or CH,

Y is absent, or, is —CH₂—; —CH₂NH—; —C(=O)—; —CH₂CH₂—; —NH—; —NHC(=O)—; —C(=O)—NH—; —CH(CH₃)—; —CF₂—; —CH(OCH₃)—; —CH₂O—; —N(CH₃)—; or —CH₂NHC(=O)—,

Z is absent, or, is —CH₂S—; —CH₂S(=O)—; —CH₂NH—; —CH(R')S—; —CH₂CH₂S—; —CH₂N(CH₃)—;

$$\text{—CH}_2\text{N}(\text{C}(\text{CH}_3)_2)\text{—}$$

—CH=CH—; —S—; —CH₂—; —O—; —CH₂S(=O)—; —C(=O)—; —SCH₂—; —CH₂CH₂—; —CH(OH)—; —CH(CH₃)CH₂—; —OCH₂—; —C(=O)—

PAGE 120 ZOOM 120% PDF+ PGP+

Key Substances in Patent

CAS RN 7272-84-6

Analyt. Markap Locations (1)
Page 120

CAS RN 178330-98-3

Analyt. Markap Locations (1)
Page 120

CAS RN 780774-34-7

Analyt. Markap Locations (1)

WO 2016/081554

PCT/US2015/061260

a. an inhibitor selected from the group consisting of a ROCK inhibitor, a PTEN inhibitor and a combination thereof;

b. a growth factor selected from the group consisting of FGF2, HGF, IGF1, KGF1, KGF2, KGF3, KGF4, KGF5, KGF6, KGF7, KGF8, KGF9, KGF10, KGF11, KGF12, KGF13, KGF14, KGF15, KGF16, KGF17, KGF18, KGF19, KGF20, KGF21, KGF22, KGF23, KGF24, KGF25, KGF26, KGF27, KGF28, KGF29, KGF30, KGF31, KGF32, KGF33, KGF34, KGF35, KGF36, KGF37, KGF38, KGF39, KGF40, KGF41, KGF42, KGF43, KGF44, KGF45, KGF46, KGF47, KGF48, KGF49, KGF50, KGF51, KGF52, KGF53, KGF54, KGF55, KGF56, KGF57, KGF58, KGF59, KGF60, KGF61, KGF62, KGF63, KGF64, KGF65, KGF66, KGF67, KGF68, KGF69, KGF70, KGF71, KGF72, KGF73, KGF74, KGF75, KGF76, KGF77, KGF78, KGF79, KGF80, KGF81, KGF82, KGF83, KGF84, KGF85, KGF86, KGF87, KGF88, KGF89, KGF90, KGF91, KGF92, KGF93, KGF94, KGF95, KGF96, KGF97, KGF98, KGF99, KGF100, KGF101, KGF102, KGF103, KGF104, KGF105, KGF106, KGF107, KGF108, KGF109, KGF110, KGF111, KGF112, KGF113, KGF114, KGF115, KGF116, KGF117, KGF118, KGF119, KGF120, KGF121, KGF122, KGF123, KGF124, KGF125, KGF126, KGF127, KGF128, KGF129, KGF130, KGF131, KGF132, KGF133, KGF134, KGF135, KGF136, KGF137, KGF138, KGF139, KGF140, KGF141, KGF142, KGF143, KGF144, KGF145, KGF146, KGF147, KGF148, KGF149, KGF150, KGF151, KGF152, KGF153, KGF154, KGF155, KGF156, KGF157, KGF158, KGF159, KGF160, KGF161, KGF162, KGF163, KGF164, KGF165, KGF166, KGF167, KGF168, KGF169, KGF170, KGF171, KGF172, KGF173, KGF174, KGF175, KGF176, KGF177, KGF178, KGF179, KGF180, KGF181, KGF182, KGF183, KGF184, KGF185, KGF186, KGF187, KGF188, KGF189, KGF190, KGF191, KGF192, KGF193, KGF194, KGF195, KGF196, KGF197, KGF198, KGF199, KGF200, KGF201, KGF202, KGF203, KGF204, KGF205, KGF206, KGF207, KGF208, KGF209, KGF210, KGF211, KGF212, KGF213, KGF214, KGF215, KGF216, KGF217, KGF218, KGF219, KGF220, KGF221, KGF222, KGF223, KGF224, KGF225, KGF226, KGF227, KGF228, KGF229, KGF230, KGF231, KGF232, KGF233, KGF234, KGF235, KGF236, KGF237, KGF238, KGF239, KGF240, KGF241, KGF242, KGF243, KGF244, KGF245, KGF246, KGF247, KGF248, KGF249, KGF250, KGF251, KGF252, KGF253, KGF254, KGF255, KGF256, KGF257, KGF258, KGF259, KGF260, KGF261, KGF262, KGF263, KGF264, KGF265, KGF266, KGF267, KGF268, KGF269, KGF270, KGF271, KGF272, KGF273, KGF274, KGF275, KGF276, KGF277, KGF278, KGF279, KGF280, KGF281, KGF282, KGF283, KGF284, KGF285, KGF286, KGF287, KGF288, KGF289, KGF290, KGF291, KGF292, KGF293, KGF294, KGF295, KGF296, KGF297, KGF298, KGF299, KGF300, KGF301, KGF302, KGF303, KGF304, KGF305, KGF306, KGF307, KGF308, KGF309, KGF310, KGF311, KGF312, KGF313, KGF314, KGF315, KGF316, KGF317, KGF318, KGF319, KGF320, KGF321, KGF322, KGF323, KGF324, KGF325, KGF326, KGF327, KGF328, KGF329, KGF330, KGF331, KGF332, KGF333, KGF334, KGF335, KGF336, KGF337, KGF338, KGF339, KGF340, KGF341, KGF342, KGF343, KGF344, KGF345, KGF346, KGF347, KGF348, KGF349, KGF350, KGF351, KGF352, KGF353, KGF354, KGF355, KGF356, KGF357, KGF358, KGF359, KGF360, KGF361, KGF362, KGF363, KGF364, KGF365, KGF366, KGF367, KGF368, KGF369, KGF370, KGF371, KGF372, KGF373, KGF374, KGF375, KGF376, KGF377, KGF378, KGF379, KGF380, KGF381, KGF382, KGF383, KGF384, KGF385, KGF386, KGF387, KGF388, KGF389, KGF390, KGF391, KGF392, KGF393, KGF394, KGF395, KGF396, KGF397, KGF398, KGF399, KGF400, KGF401, KGF402, KGF403, KGF404, KGF405, KGF406, KGF407, KGF408, KGF409, KGF410, KGF411, KGF412, KGF413, KGF414, KGF415, KGF416, KGF417, KGF418, KGF419, KGF420, KGF421, KGF422, KGF423, KGF424, KGF425, KGF426, KGF427, KGF428, KGF429, KGF430, KGF431, KGF432, KGF433, KGF434, KGF435, KGF436, KGF437, KGF438, KGF439, KGF440, KGF441, KGF442, KGF443, KGF444, KGF445, KGF446, KGF447, KGF448, KGF449, KGF450, KGF451, KGF452, KGF453, KGF454, KGF455, KGF456, KGF457, KGF458, KGF459, KGF460, KGF461, KGF462, KGF463, KGF464, KGF465, KGF466, KGF467, KGF468, KGF469, KGF470, KGF471, KGF472, KGF473, KGF474, KGF475, KGF476, KGF477, KGF478, KGF479, KGF480, KGF481, KGF482, KGF483, KGF484, KGF485, KGF486, KGF487, KGF488, KGF489, KGF490, KGF491, KGF492, KGF493, KGF494, KGF495, KGF496, KGF497, KGF498, KGF499, KGF500, KGF501, KGF502, KGF503, KGF504, KGF505, KGF506, KGF507, KGF508, KGF509, KGF510, KGF511, KGF512, KGF513, KGF514, KGF515, KGF516, KGF517, KGF518, KGF519, KGF520, KGF521, KGF522, KGF523, KGF524, KGF525, KGF526, KGF527, KGF528, KGF529, KGF530, KGF531, KGF532, KGF533, KGF534, KGF535, KGF536, KGF537, KGF538, KGF539, KGF540, KGF541, KGF542, KGF543, KGF544, KGF545, KGF546, KGF547, KGF548, KGF549, KGF550, KGF551, KGF552, KGF553, KGF554, KGF555, KGF556, KGF557, KGF558, KGF559, KGF560, KGF561, KGF562, KGF563, KGF564, KGF565, KGF566, KGF567, KGF568, KGF569, KGF570, KGF571, KGF572, KGF573, KGF574, KGF575, KGF576, KGF577, KGF578, KGF579, KGF580, KGF581, KGF582, KGF583, KGF584, KGF585, KGF586, KGF587, KGF588, KGF589, KGF590, KGF591, KGF592, KGF593, KGF594, KGF595, KGF596, KGF597, KGF598, KGF599, KGF600, KGF601, KGF602, KGF603, KGF604, KGF605, KGF606, KGF607, KGF

Chemistry & Biology
388

A Phagocytosis

B

3-(4-pyridyl)indole
Rocutout

C

Rocutout
100 μ M 50 μ M 25 μ M 12.5 μ M

Assays Used:

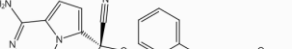
- Phagocytosis Assay:** Cells were incubated with *E. coli* labeled with Dil. Cells were then treated with 3-(4-pyridyl)indole or DMSO. Cells were stained with Calcein. Cells were imaged by fluorescence microscopy.
- Wound Healing Assay:** Cells were seeded into 96-well plates. Cells were treated with 3-(4-pyridyl)indole or DMSO. Cells were imaged by phase-contrast microscopy.

Results:

- Phagocytosis Assay:** 3-(4-pyridyl)indole treatment significantly reduced phagocytosis of Dil-labeled *E. coli* by cells.
- Wound Healing Assay:** 3-(4-pyridyl)indole treatment significantly accelerated wound healing in cells.


CAS Registry Number: [1809249-37-3](#)




References (3,472) **Reactions** (643) **Suppliers** (51)

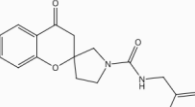

Absolute stereochemistry shown

Additional Details

- Document Types
 - Journal, Patent, Preprint
- Source of Registration
 - CAS Client Services
- Substance Classes
 - Small Molecule

 CAS Registry Number: **1704613-20-6**

 References (0)  Reactions (0)  Suppliers (2)



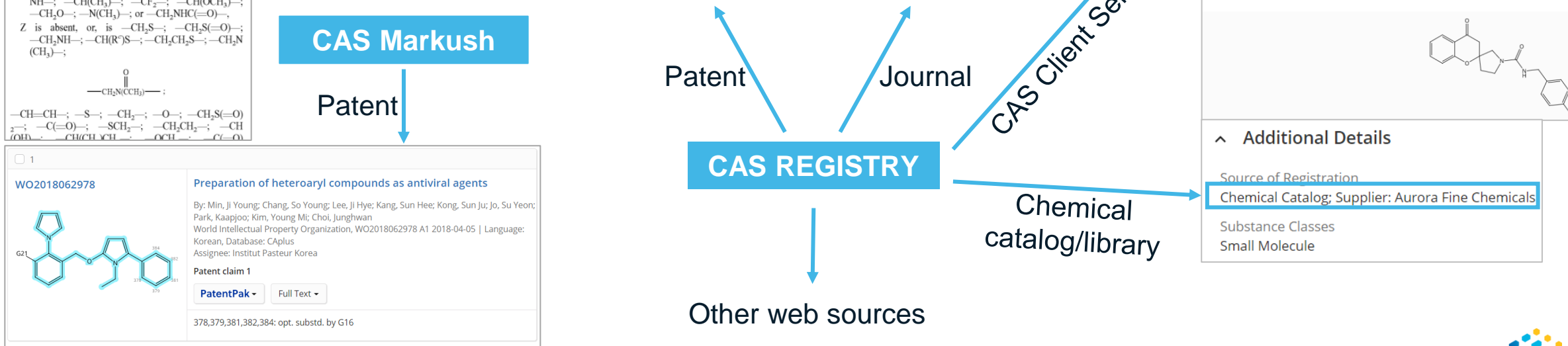
Additional Details

Source of Registration

Chemical Catalog; Supplier: Aurora Fine Chemicals

Substance Classes

Small Molecule



如何进行完整的分子结构检索？

Substances search for drawn structure

References ▾ Reactions ▾ Suppliers ▾

Structure Match

As Drawn (0)

Substructure (0)

Similarity (101K)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.
[Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

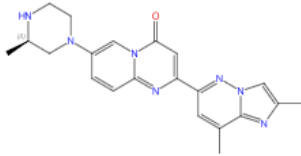
Filtering: Similarity: 3 Selected ✕ Number of Components: 1 ✕ [Clear All Filters](#)

286 Results

Sort: Relevance ▾ View: Partial ▾

1 95 ...

1825352-54-2



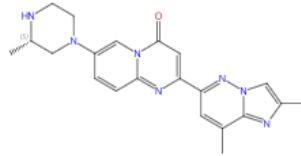
Absolute stereochemistry shown

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

5 References 25 Reactions 1 Supplier

2 95 ...

1825352-53-1



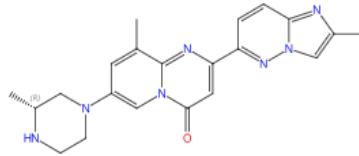
Absolute stereochemistry shown

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

5 References 25 Reactions 1 Supplier

3 95 ...

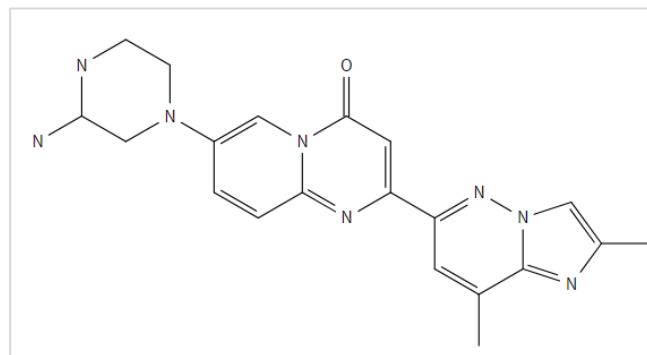
1825352-79-1



Absolute stereochemistry shown

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

5 References 19 Reactions 1 Supplier



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

如何进行完整的分子结构检索？

Substances search for drawn structure

References ▾ Reactions ▾ Suppliers ▾

Structure Match

As Drawn (0)

Substructure (0)

Similarity (101K)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.
[Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

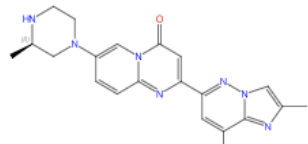
Filtering: Similarity: 3 Selected ✕ Number of Components: 1 ✕ [Clear All Filters](#)

286 Results

Sort: Relevance ▾ View: Partial ▾

1 95 ...

1825352-54-2



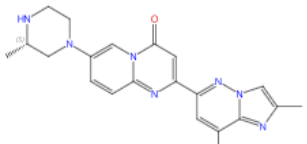
Absolute stereochemistry shown

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

5 References 25 Reactions 1 Supplier

2 95 ...

1825352-53-1



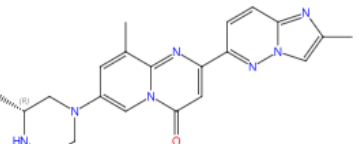
Absolute stereochemistry shown

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

5 References 25 Reactions 1 Supplier

3 95 ...

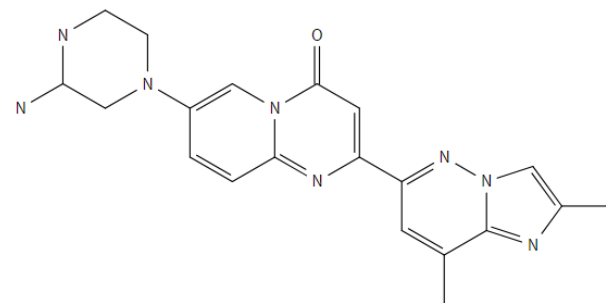
1825352-79-1



Absolute stereochemistry shown

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

5 References 19 Reactions 1 Supplier



查看相似结构，可参考
Similarity score

如何进行完整的分子结构检索？

CAS SciFinder[®]

Substances Enter a query...

Edit

Return to Home

Patent Markush search for drawn structure

References

Patent Markush Match

As Drawn (1)

Substructure (1)

Filter Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (1)

CA Section

1 Result

1

WO2017081111

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

Assignees: Hoffmann-La Roche AG; Hoffmann-La Roche Inc.

World Intellectual Property Organization, WO2017081111 A1 2017-05-18 | Language: English, Database: CAplus

Patent claim 1

PatentPak Full Text

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

629: opt. substd.

Chemical structure diagram of a complex molecule, likely a substituted pyrido-pyrimidinone derivative.

- 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



Search CAS Sequences

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



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 search for "Semaglutide"

References

Filter Behavior

Filter by Exclude

Substance Role

Product (222)

Reactant (10)

Yield

90-100% (3)

228 Results

Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (1 Reaction) Steps: 7

Absolute stereochemistry shown, Rotation (+)

Suppliers (98)

Suppliers (64)

910463-68-2
Image Not Available

Suppliers (28)

Reactions search for "175:621496"

References

Filter Behavior

Filter by Exclude

Yield

90-100% (3)

80-89% (5)

70-79% (2)

50-69% (3)

No Yield Available (120)

133 Results

Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (2 Reactions) Steps: 7-8

Absolute stereochemistry shown

Suppliers (145)

Suppliers (77)

204656-20-2
Image Not Available

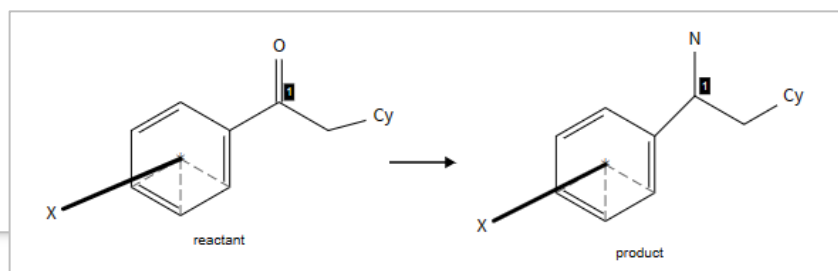
Suppliers (37)

Reactions References Suppliers

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

Draw

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

References

Structure Match

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

Filter Behavior

Filter by Exclude

Search Within Results

Yield

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

Reaction Scale

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

Non-Participating Functional Groups

Filtering: Reaction Mapping: Mapping Data Available

16 Results

Group: By Scheme

- By Scheme
- By Document
- By Transformation

Sort: Relevance

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

View: Collapsed

Scheme 1 (5 Reactions)

Suppliers (93) Suppliers (15)

Expand Scheme

Scheme 2 (1 Reaction)

Steps: 1 Yield: 76%

Suppliers (53) Suppliers (3)

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

1.1 Reagents: [O-Methylhydroxylamine hydrochloride](#)

Solvents: [Pyridine](#); rt; 1 h, 50 °C

Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

By: Heidelbaugh, Todd M.; et al

反应分组:

- 按反应式
- 按文献
- 按转化类型

反应排序:

- 相关度
- 公布时间
- 产率
- 步数

3.2 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

The screenshot displays the CAS Reaxys search interface. On the left, a sidebar contains various filter categories. The 'Structure Match' section has 'Substructure (8,044)' selected. The 'Filter Behavior' section has 'Filter by' selected. The 'Search Within Results' section is expanded, showing filters for Yield, Reaction Scale, Non-Participating Functional Groups, Number of Steps, Reaction Mapping, Experimental Protocols, Reaction Type, Stereochemistry, Reagent, Catalyst, and Solvent. The 'Commercial Availability' and 'Reaction Notes' sections are also visible. The main results area shows a list of reactions. The first reaction is 'Reductive Alkylation of Ammonia or Amines', which is highlighted with a yellow box. Below it is 'Formation of N/O/S Heterocycles', also highlighted. The third reaction is '1,3-Dipolar Addition'. The interface includes a 'Download filter data from this result set' button at the bottom left of the sidebar.

Structure Match

As Drawn (34)

Substructure (8,044)

Similarity (0)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Milligram (268)

Gram (292)

No Scale Provided (7,680)

Non-Participating Functional Groups

Number of Steps

Reaction Mapping

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

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.

8,044 Results

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

1

Reductive Alkylation of Ammonia or Amines

View 108 Related Reactions

2

Formation of N/O/S Heterocycles

View 47 Related Reactions

3

1,3-Dipolar Addition

View 37 Related Reactions

Y, Y' = NH, O, S

Z = Electron withdrawing group

筛选工具：不参与反应官能团

不参与反应官能团：出现在反应前后，但未发生变化的官能团

Structure Match

As Drawn (34)

Substructure (8,044)

Similarity (0)

Filter Behavior

Filter by

Exclude

Search Within Results

Yield

Reaction Scale

Non-Participating Functional Groups

☒ Halide (205)

☐ Phenyl halide (203)

☐ Amide (66)

☐ Alkene (62)

☐ Cyclic alkene (58)

View All

Number of Steps

Reaction Mapping

Experimental Protocols

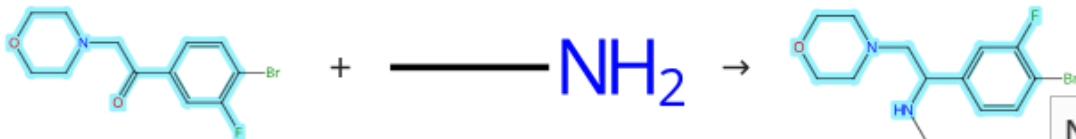
Filtering: Non-Participating Functional Groups: Halide X

Clear All Filters

205 Results

Group: By Scheme Sort: Relevance View: Collapsed

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



Suppliers (122)

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

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

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

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

Experimental Protocols


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

By: Neeb, Michael J.; et al
World Intellectual Property Organization, WO2008-01-24

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)

☐ Carboxamide (14)

☐ Urea (12)

☐ Carboxylic ester (9)

☐ Carbamate (8)

☐ Imine (8)

☐ Acyclic ketone (7)

☐ Ketone (7)

OK

Cancel

3.3 联用检索——结构与关键词

关注人名反应？

联用检索提高检索效率

Search interface showing a query for "Friedel-Crafts acylation". The search bar includes filters for "AND", "Author Name", and "Add Advanced Search Field". A chemical structure of indole is shown, with a yellow arrow pointing to the "References" tab in the bottom screenshot.

References search for "Friedel-Crafts acylation" + drawn structure. The search results show 1,100 results. The "Reactions" tab is selected, showing 1,100 results. The search results include a list of reactions, with the first result being "ZrCl₄-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole".

Reactions search for "2011:601374". The search results show 21 results. The "Reactions" tab is selected, showing 21 results. The search results include a list of reactions, with the first result being "Scheme 1 (1 Reaction)" showing a reaction of a bicyclic ketone with indole to form a 3-acylindole derivative.

3.4 如何获得逆合成路线？

先进AI技术与CAS科学家标引的丰富反应信息相结合

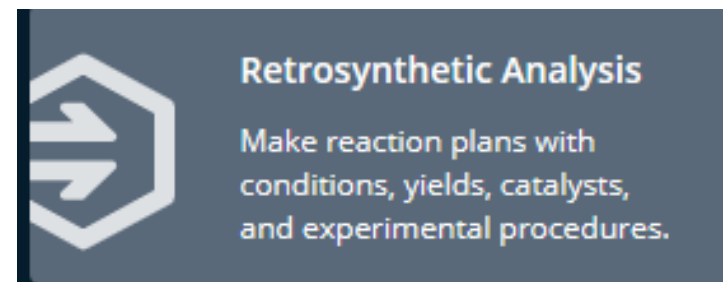
(1) 已知化合物：点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis

The screenshot displays the CAS Retrosynthesis Tool interface. On the left, a search bar shows the CAS RN 2628280-40-8. Below it, the chemical structure of 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli... is shown with absolute stereochemistry. The molecular formula is C₂₃H₃₂F₃N₅O₄. Below the structure, there are buttons for 236 References, 53 Reactions, and 39 Suppliers. On the right, a detailed view of the same molecule is shown, with the 'Start Retrosynthetic Analysis' button highlighted in orange. The interface also includes a 'Substance Detail' section with links to Reactions (53), Synthesize (52), References (236), and Suppliers (39). At the bottom right, there are buttons for 'Edit Structure', 'Reset', and a download icon.

CAS Retrosynthesis Tool:

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

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

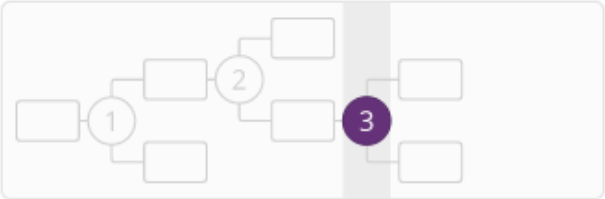


逆合成分析的预设参数

Retrosynthesis Plan Options for drawn structure

Select Synthetic Depth **反应深度** [Learn more.](#)

☐ 1
☐ 2
☒ 3
☐ 4



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

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

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

100 **起始原料费用** USD/mol ▼

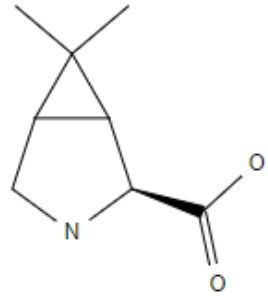
☐ Email me when my plan is complete

[Create Retrosynthesis Plan](#)

Break and Protect Bonds

[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)

Scoring Profiles

Complexity Reduction

Convergence

Evidence

Cost

Yield

Atom Efficiency

Apply Reset Scoring

路线概览

调节参数

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

Max Yield 97%

Max Yield 68%

Max Yield 77%

Max Yield 97%

Reset

Off Low Medium High



逆合成路线详情

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Key Experimental Steps Predicted Steps Edit Plan Options

已知反应

预测型反应

View all alternatives (20)
View evidence (15,146)
Exclude this step

Reactions from Retrosynthesis Plan Evidence

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Non-Participating Functional Groups

15,146 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction)

Steps: 1 Yield: 88%

Scheme 2 (1 Reaction)

Steps: 1

- 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)

Suppliers (15)

Suppliers (89)

98%

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrochloric acid Titanium chloride (TiCl₃)	-	Methanol Tetrahydrofuran Water	rt; 30 min, rt; 2 h, 30 - 50 °C
2	Water	-	-	-

Alternative Steps (2)

Experimental Protocols

Synthetic Methods

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

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

Reagents [Hydrochloric acid](#)
[Titanium chloride \(TiCl₃\)](#)
[Water](#)

Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

View PDF Full Text

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

Procedure

1. Suspend methyl 5-Fluoro-2-(2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl)-3-nitrobenzoate (8.1 g, 25.2 mmol) and 4-bromobenzaldehyde (8.9 g, 50.5 mmol) in THF (50 mL) and MeOH (10 mL).
2. Add titanium(III) chloride solution [20% wt solution in HCl (2 M), 130 mL, 6 equiv] to the resulting mixture in dropwise fashion over 30 minutes at room temperature.
3. Maintain the reaction temperature between 30 and 50°C for 2 hours.
4. Quench the mixture by the slow addition of water (260 mL).
5. Pour the reaction mixture into a separating funnel.
6. Extract the mixture with ethyl acetate (4 x 140 mL).
7. Pool the organic fractions.
8. Wash the organic fractions with NaHCO₃ (3 x 60 mL) and NaHSO₃ (3 x 100 mL).
9. Dry the organic fractions with sodium sulfate (Na₂SO₄).
10. Concentrate the solvent under reduced pressure to obtain a thick yellow syrup.
11. Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully.
12. Dry the resulting yellow syrup under high vacuum to obtain product.

Transformation

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

Scale

gram

Characterization Data

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

State

yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

Transformations

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

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	View Structure	7440-62-2
Stainless steel	matrix		12597-68-1
Al ₂ O ₃ 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	View Structure	7697-37-2
Hydrofluoric acid	reagent	View Structure	7664-39-3
Acetylacetone	reagent	View Structure	123-54-6
Chromium	reagent	View Structure	7440-47-3
Methanol	reagent	View Structure	67-56-1
Tetramethylammonium chloride	reagent	View Structure	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; Alatarvas, 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®

Abstract ^

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

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

分析仪器

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 Al₂O₃ 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.

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

References search for "steel and impurity"

Substances Reactions Citing Knowledge Graph

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

Filtering: CAS Solutions: Analytical Methods X Clear All Filters

23 Results Sort: Relevance View: Partial Abstract

1

Validation of an HPLC method for analysis of nifedipine residues on stainless-steel surfaces in the manufacture of pharmaceuticals
By: Milenovic, D. M.; Lazic, M. L.; Veljkovic, V. B.; Todorovic, Z. B.
Acta Chromatographica (2008), 20(2), 183-194 | Language: English, Database: CPlus
[Analytical Methods](#)

A simple, sensitive, and convenient HPLC method has been developed, validated, and applied to anal. of stainless-steel surfaces of equipment used in drug manufacture Cotton swabs moistened with methanol residues of the drug from the surfaces; recoveries were 82.26, 86.88, and 88.95% for 25, 125, and 250 µg the results, as relative standard deviation (RSD), was <5%. The method was validated over the concentration range of 25-250 µg/L. Small quantities of residues of the drug and its main impurities were determined by HPLC.

electrolyte and arsenic in 10% acetylacetone electrolyte were in good agreement with industrial data. Titanium and aluminum were measured from the dissolved steel matrix but titanium was also detected in the inclusions. It was concluded that the anal. results for titanium and aluminum measured using an optical emission spectrometer is affected by the inclusions within the stainless steel.

Keywords: double stabilized stainless steel alloying impurity element inclusion

[Open Access](#) [Full Text](#)

[Expand All](#) [Collapse All](#)

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

Document Type
Substance Role
Language
Publication Year
Availability

Full Text

Substances (2) Reactions (0) Citing

^ CAS Content

☒ Analytical Methods (28)

☐ Formulations (15)

Concepts
Substances
Analytical Methods

Title	CAS Method Number
Analysis of Aluminum in Stainless steel by Electrochemical extraction	1-119-CAS-285768
Analysis of Aluminum in Stainless steel by Electrochemical extraction	1-119-CAS-286264
Analysis of Vanadium in Stainless steel by Electrochemical extraction	1-119-CAS-286328
Analysis of Vanadium in Stainless steel by Electrochemical extraction	1-119-CAS-286333
Analysis of Arsenic in Stainless steel by Electrochemical extraction	1-119-CAS-286759
Analysis of Copper in Stainless steel by Electrochemical extraction	1-119-CAS-286842
Analysis of Arsenic in Stainless steel by Electrochemical extraction	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

CAS Analytical Methods

Good Afternoon, Na

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

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

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

高级检索 **浏览不同类别分析方法**

Recent Searches **近期检索**

Explore : Organometallic Compound Analysis

Advanced : analyte : olaparib, matrix : blood plasma

CAS
A division of the
American Chemical Society

CAS Analytical Methods分析方法类别

目前涵盖13个大类，45个小类；某些子分类属于多种方法分类。

Agricultural Applications / Analysis: 除草剂分析…

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

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

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

Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析…

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

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

Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析…

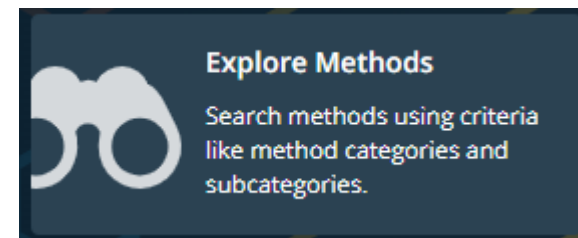
Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…

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

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

Polymer: 塑料加工

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

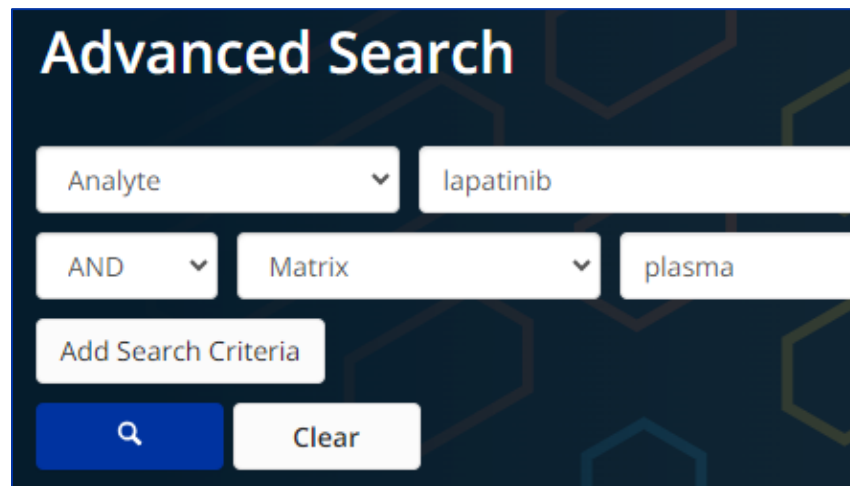


关键词检索分析方法

- 直接检索示例：
lapatinib 拉帕替尼



- 高级检索示例：
分析拉帕替尼血药浓度的方法



检索结果分析与精炼

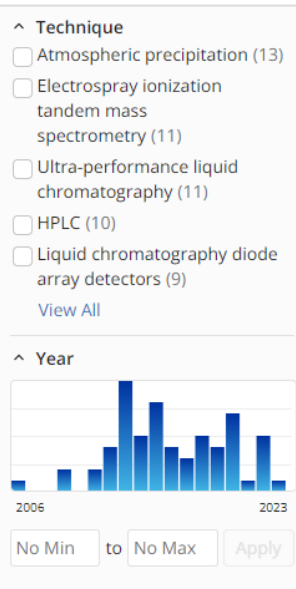
分析物

基质

方法分类

技术&仪器

年份



Results for lapatinib

62 Results

Sort: Relevance Group: By Method

Compare (2/3) Compare Save

对比不同分析方法

1

Analysis of Lapatinib by Microplate spectroscopy

JOURNAL

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

JOURNAL

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 C₁₈ column (250 × 4.5 mm, 5 μ); Nylon membrane filters of 0.45 μ size

Method Category Active Pharmaceutical Ingredient and Metabolite Analysis

对照多个感兴趣的分析方法详情

Method 1		Method 2	
CAS Method Number	1-101-CAS-187473	1-101-CAS-157505	
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis	
Technique	HPLC-tandem mass spectrometry	Atmospheric precipitation; High-performance liquid chromatography-mass spectrometry	
Analyte	Lapatinib	Lapatinib	
Matrix	Blood plasma	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- 10 psi; dry gas temperature- 350 °C; capillary voltage- 1.5 kV; mode target ions: m/z 581 (or lapatinib), m/z 231 (or lapatinib-d3) 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 daily or in View All	

Format

☒ PDF

☐ XLS

Download Cancel

Method	Sample extraction	Protein precipitation
	1. Spike 250 µl of plasma sample with 5 µl of internal standard working solution and acidify with 20 µl of concentrated formic acid. View All	1. Thaw the plasma sample to room temperature. 2. Add an aliquot of 10 µL of the internal standard working solution. View All
Linearity Range	5 - 5000 ng/ml	10 - 2000 ng/mL
Limit of Quantitation	5 ng/mL	10 ng/mL
Recovery	43% ± 14%, 42% ± 10% and 48% ± 12% (recovery), for 5, 15, 800 and 4000 ng/mL spiked sample, respectively.	-
Accuracy	102.1%, 98.6%, 102.5% and 98.3% (recovery), for 5, 15, 800 and 4000 ng/mL QC sample, respectively.	98.3 - 109.2% (recovery, intra-day); 93.0 - 104.1% (recovery, inter-day)
Precision	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, respectively.	5.6 - 12.0% (CV, intra-day); 6.8 - 11.5% (CV, inter-day)
Concentration	-	14816.6 ng/mL (at 30 mg/kg)
Source	<p>JOURNAL</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; LoRusso, Patricia; Li, Jing</p> <p>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 941, 100 - 108.</p> <p>Full Text View in CAS SciFinder</p>	<p>JOURNAL</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</p> <p>Latin American Journal of Pharmacy (2014), 33 (1), 158 - 162.</p> <p>Full Text View in CAS SciFinder</p>

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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 displays the CAS Formulus homepage. At the top, it says "Good Evening, Na" and has tabs for "Formulations" and "Ingredients". Below this is a search bar with the placeholder text "Search by Formulations by Ingredients, Purpose, Form, Functions, etc." and a magnifying glass icon. To the right of the search bar is a blue button labeled "直接检索" (Direct Search). Below the search bar are two main options: "Formulation Designer" with a description "Design custom formulation templates based on selections and ingredients" and a blue button labeled "制剂、配方设计" (Formulation Design); and "Advanced Search" with a description "Search Formulations using criteria like ingredients, targets, and more." and a blue button labeled "高级检索" (Advanced Search). Below these options is a section titled "Recent Search History" with a blue button labeled "近期检索" (Recent Search). To the right of this section is a link "View Search History". The search history shows a search from December 22, 2023, at 2:16 PM, for "Formulations" with the criteria "+Ingredient:'Olaparib' +Form:'Tablets' (135)". There are two buttons for this search: "Rerun Search" and "Edit Search".

Good Evening, Na

Formulations Ingredients

Search by Formulations by Ingredients, Purpose, Form, Functions, etc. 直接检索

Formulation Designer
Design custom formulation templates based on selections and ingredients
制剂、配方设计

Advanced Search
Search Formulations using criteria like ingredients, targets, and more.
高级检索

Recent Search History 近期检索 View Search History

December 22, 2023

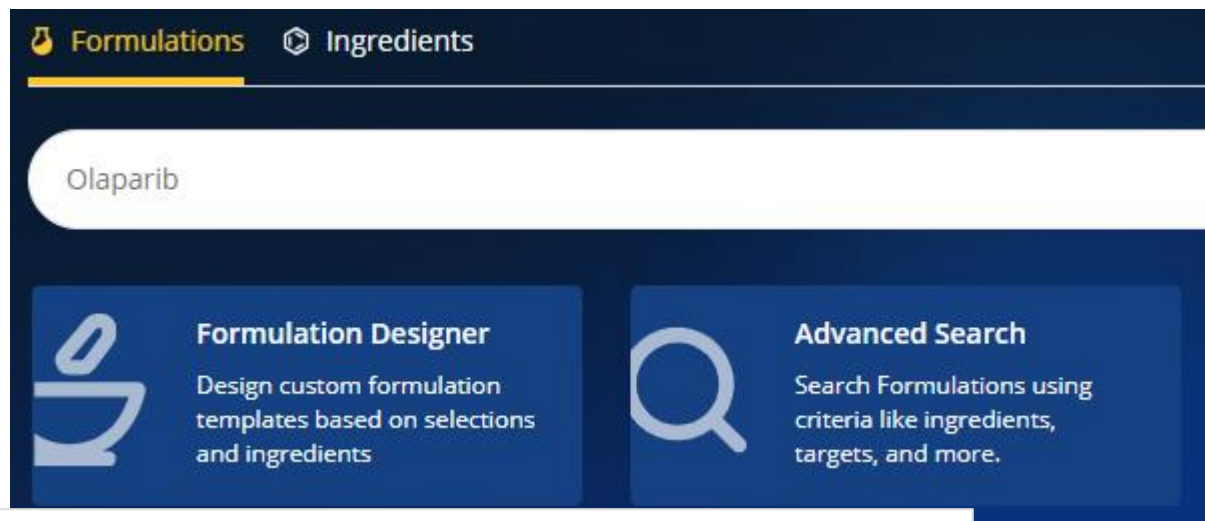
2:16 PM

Formulations +Ingredient:"Olaparib" +Form:"Tablets" (135)

Rerun Search Edit Search

关键词检索制剂/配方

- 直接检索示例：
Olaparib 奥拉帕尼



- 高级检索示例：
奥拉帕尼片剂

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

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

[Add Another Term](#)

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

检索结果分析与精炼

应用领域

目的/用途

物理形态

物质状态

作用方式

制剂信息

文献类型

机构名

发表年份

Document Type

☐ Journal (7)

☐ Article (7)

☐ Patent (627)

☐ Claim (392)

☐ Comparative Example (30)

☐ Example (203)

☐ Table (2)

☐ Product Insert (5)

Organization

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

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

☐ Sunshine Lake Pharma Co., Ltd. (29)

☐ AstraZeneca UK Ltd. (22)

☐ Immunomedics, Inc. (21)

Publication Year

2007

2023

No Min

to

No Max

Apply

State of Matter

☐ Solid (100)

☐ Liquid (26)

☐ Semisolid (5)

Delivery Route

☐ Oral drug delivery systems (128)

☐ Pharmaceutical intravenous injections (35)

☐ Intraperitoneal injections (34)

☐ Mucosal drug delivery systems (30)

☐ Intramuscular injections (26)

View All

Information Included

☐ Component Amount (269)

☐ Process (196)

☐ Experimental Activity (162)

☐ Effective Dose (49)

Industry

☐ Food & Related

☐ Pharmaceutical

☐ Unclassified

Purpose

☐ Antitumor agents (415)

☐ Drug delivery systems (86)

☐ Pharmaceutical formulations (34)

☐ Antiproliferative agents (23)

☐ Anti-inflammatory agents (22)

View All

Physical Form

☐ Tablets (128)

☐ Capsules (66)

☐ Pharmaceutical injections (19)

☐ Particles (18)

☐ Powders (15)

View All

Formulations search for "Olaparib"

Get Additional References

一键获取相关文献

639 Results

Sort: Relevance ▼

1

Mixture: Pharmaceutical Mixture

Location: Article page 2

Purpose: pharmaceutical mixture

Add to Compare

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

View Formulation Detail

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	View

 Predicted value

Formulation Ingredients

制剂成分、功能、用量

Component	Function	Amount Reported	Optionality
Olaparib	poly(ADP-ribose) polymerase inhibitor [Ⓢ]	200 g	Mandatory
Vinyl acetate-vinylpyrrolidone copolymer	carrier [Ⓢ] , polymeric stabilizer [Ⓢ]	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...

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.

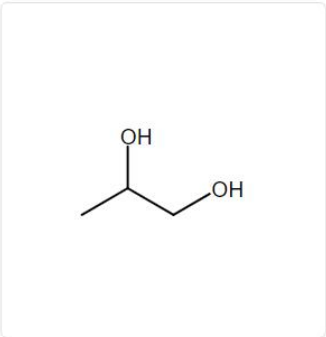
检索原料



- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至设计工具
Formulation Designer

- 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](#)



C₃H₈O₂

(±)-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 ³	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](#)

设计配方/制剂

🔧 Formulation Designer ?

Clear All Selections

Industry

Pharmaceutical
Cosmetics & Personal Care
Agrochemical
Cleaning & Surfactant Products
Inks, Paints, & Coatings
Food & Related

Purpose

Coating materials
Adhesives
Jet-printing inks
Water-thinned coating materials
Antifouling coating materials
Powder coating materials
Printing inks
Anticorrosive coating materials
Paints
Photocurable coating materials
[- View More Purposes -](#)

Physical Form

Solutions
Paints
Powders
Films
Coating materials
Liquids
Emulsions
Disperse systems
Tablets
Resins
[- View More Physical Forms -](#)

Add up to 5 Ingredients

Water



Ethanol



+ [Add Another Ingredient](#)

Create Template



Formulation Designer

Design custom formulation
templates based on selections
and ingredients

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

SaveDownload

Your Template

Unit SizemgGoClear

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 ⓘ
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 ⓘ
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% ⓘ
Surfactants	Sorbitan mono-(9Z)-9- octadecenoate	Drug Master File List; EPA Pesticide Inactive	Sodium dodecyl sulfate; Sodium dodecylbenzenesulfonate;	Approximately 2% ⓘ

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	γ-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

Filter Behavior

Filter by Exclude

Document Type

Language

Publication Year

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Content

Analytical Methods (5)

Formulus (3)

Bioactivity Data

Formulation Purpose

Database

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: CAlplus 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-β1, and inflammatory factors were measured by ELISA. Myocardial injury and myo...

View More

Full Text

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

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: CAlplus 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

^ 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

0

0

0

Citation Map

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

In this Reference

[IPC Data](#)

[CAS Concepts](#)

[Formulations](#)

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

The invention relates to the field of medicines, in particular to an application of a traditional Chinese medicine composition for preparing a medicine for preventing and/or treating myocardial hypertrophy and an application to preparation of 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 treating 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	Publication Date	Application Number	Application Date	Kind Code
CN112190652	2021-01-08	CN2020-11207191	2020-11-03	A
Assignee	Source	Database Information	Language	
Capital Medical University, China	China CODEN: CNXXEV	AN: 2021:56481 CAN: 176:120018 CAplus	Chinese	

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Appli
CN112190652	Chinese	A	PDF	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	Function	Amount Reported
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

85

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CAS

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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)

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First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username: [Tips](#)

Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: [Why?](#)

请注意：

1.必须输入真实姓名和**学校**邮箱。
2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- - (破折号)
- _ (下划线)
- . (句点)
- @ (表示“at”的符号)

3.密码必须包含 7-15 个字符，并且至少包含**三种以下字符**：

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

例：abc@123

4.从下拉列表中选择一个密码提示问题并给出答案。

单击 Register（注册）。

Registration Already Complete

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

点击激活链接后注册成功

通过<https://scifinder-n.cas.org/>访问

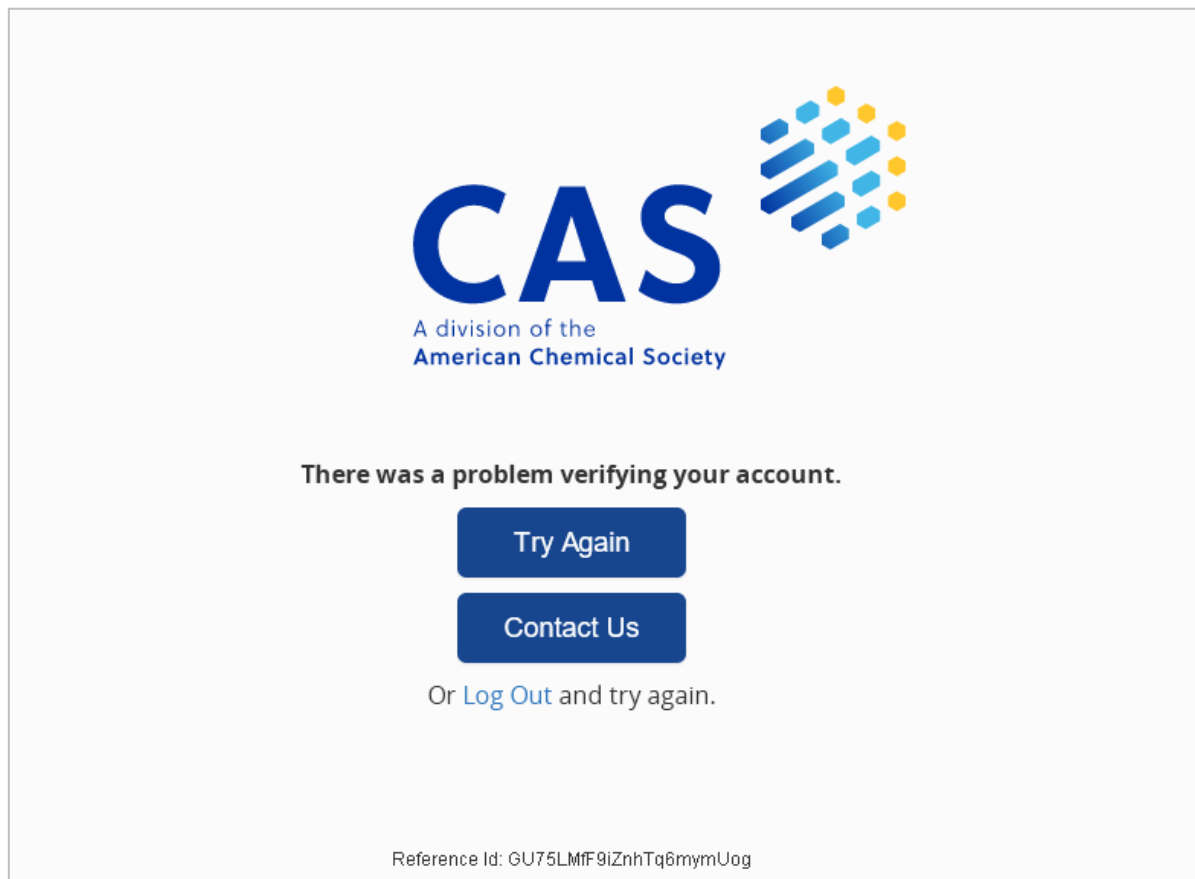
常见注册问题

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

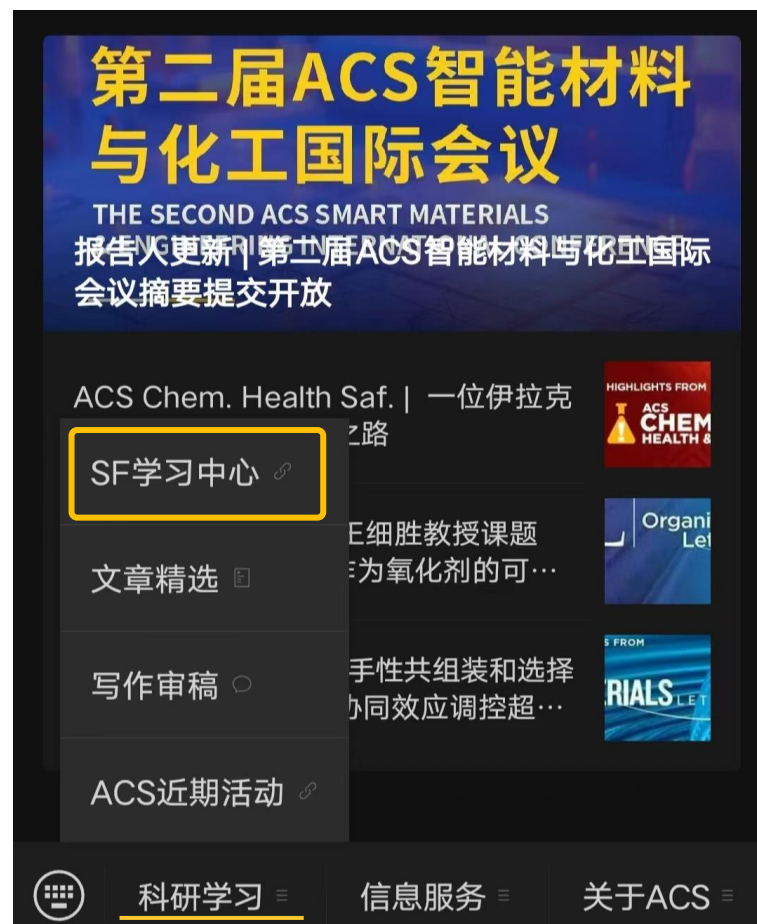
线上学习资源

“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 SCIFINDER DISCOVERY PLATFORM™

2024专题论坛直播时间表

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

9月26日 | 药物立项调研策略



11月14日 | 电池及电化学能源材料



10月24日 | 聚合物的研发与应用



12月19日 | 专利查新与规避专利侵权风险



CAS SciFinder Discovery Platform

9月至12月的四场专题论坛

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

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

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

扫码参赛：



使用注意事项

- 一人注册一个帐号
- 实名注册，需提供真实姓名信息（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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