

CAS SciFinder Discovery Platform (Academic)

全面高效获取科技信息



潘娜 博士

npan@acs-i.org

美国化学文摘社(CAS)北京代表处

CAS

A division of the
American Chemical Society



大纲

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



CAS 具有最全面的学科连接内容合集



Over
50K
scientific journals
and documents

Over
274
million substances

Over
50
languages
translated

Over
109
patent offices
worldwide

CAS独特的内容合集

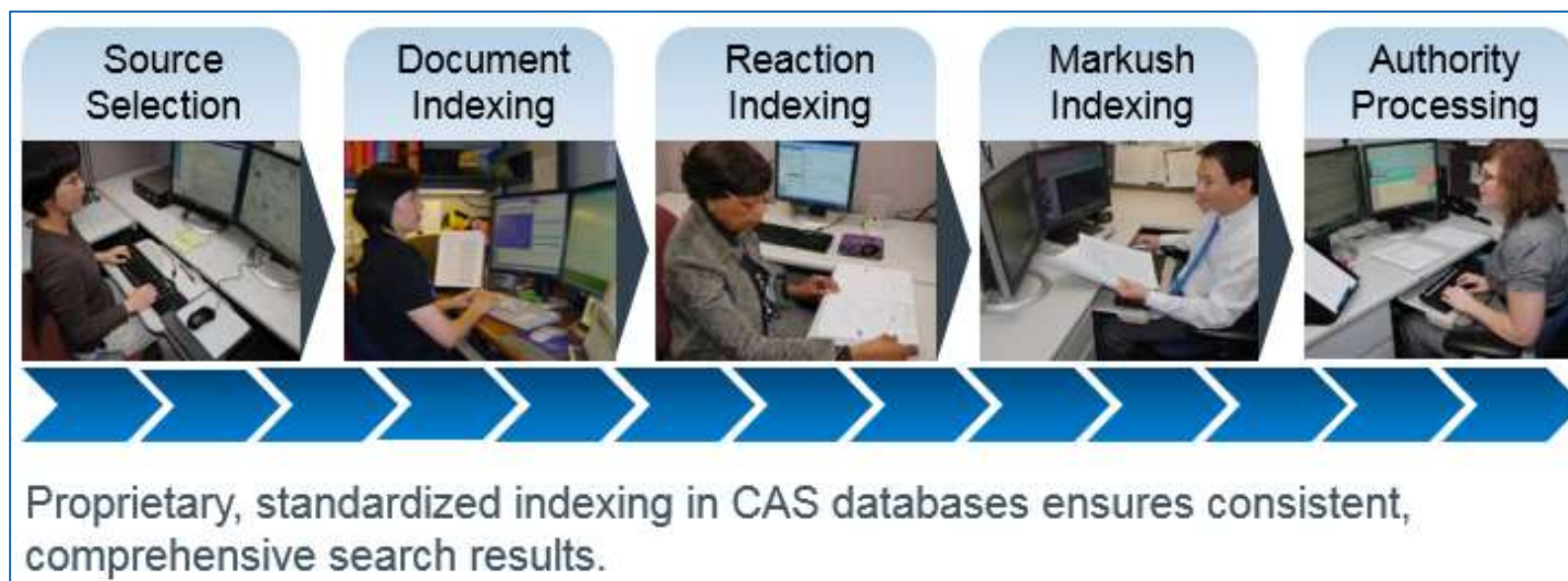


来源：

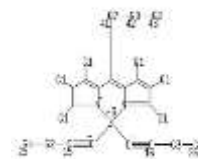
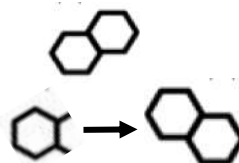
<https://www.cas.org/cas-data>

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

CAS科学家的智力标引



1990
Smith, M.
anthracene



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

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 (Academic)平台解决方案

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。

如何获取CAS SciFinderⁿ账号

(登录图书馆网站，查看注册相关的链接和说明)

Registration form fields:

- CONTACT INFORMATION:
 - First Name:
 - Last Name:
 - Email:
 - Confirm Email:
 - Phone Number:
 - Fax Number:
 - Area of Research:
 - Job Title:
- USERNAME AND PASSWORD:
 - Username:
 - Password:
 - Re-enter Password:
- SECURITY INFORMATION:
 - Security Question:
 - Answer:

Buttons: Register, Clear All

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

如何获取CAS SciFinderⁿ账号

(登录图书馆网站, 查看注册相关的链接和说明)



1、登录学校图书馆首页, 点击左下方资源导航模块。

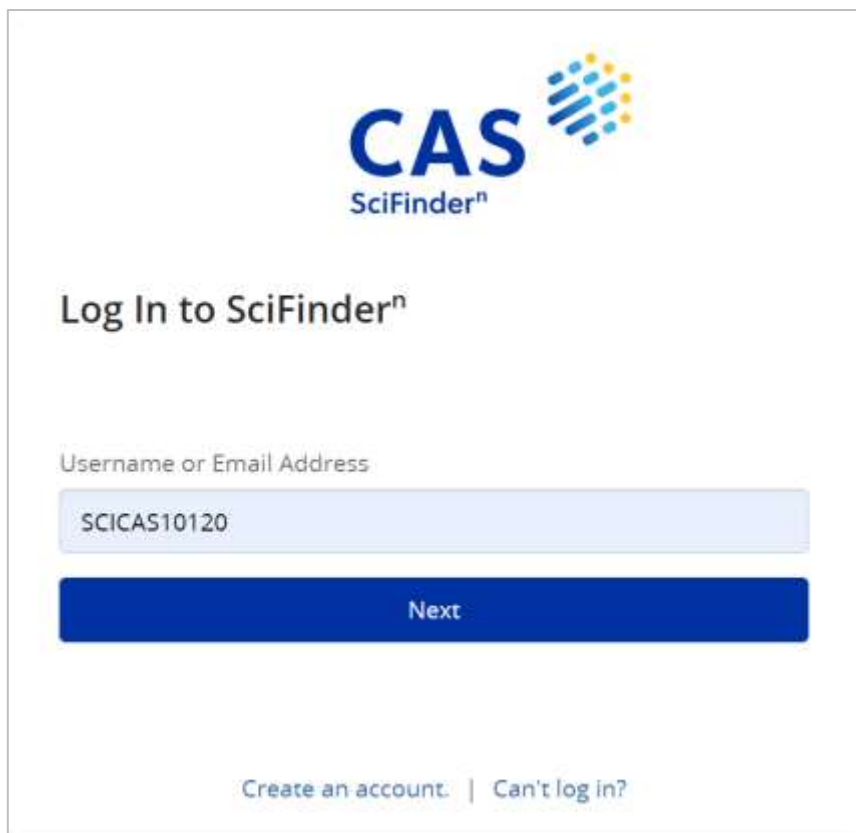
2、在列表中中找到SciFinder Scholar, 点击右侧详情。

ESI(Essential Science Indicators)	其他	综合	
INCITES数据库	其他	综合	
寻知学术文献数据检索平台	期刊 会议论文 硕博论文 专利 图书	综合	
剑桥期刊电子回溯库	电子期刊	综合	详情
美国科研出版社电子期刊库	电子期刊	综合	详情
EI village(美国工程索引)	目录/文摘/索引	综合	详情
SciFinder Scholar(CA网络版)	目录/文摘/索引	物理学 化学/化工.....	详情
Web of Science (SCI/CPCI-S)	目录/文摘/索引	综合	详情
百链搜索	搜索引擎/知识发现	综合	详情



3、点击文章中的链接进行账号注册。

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



CAS SciFinderⁿ

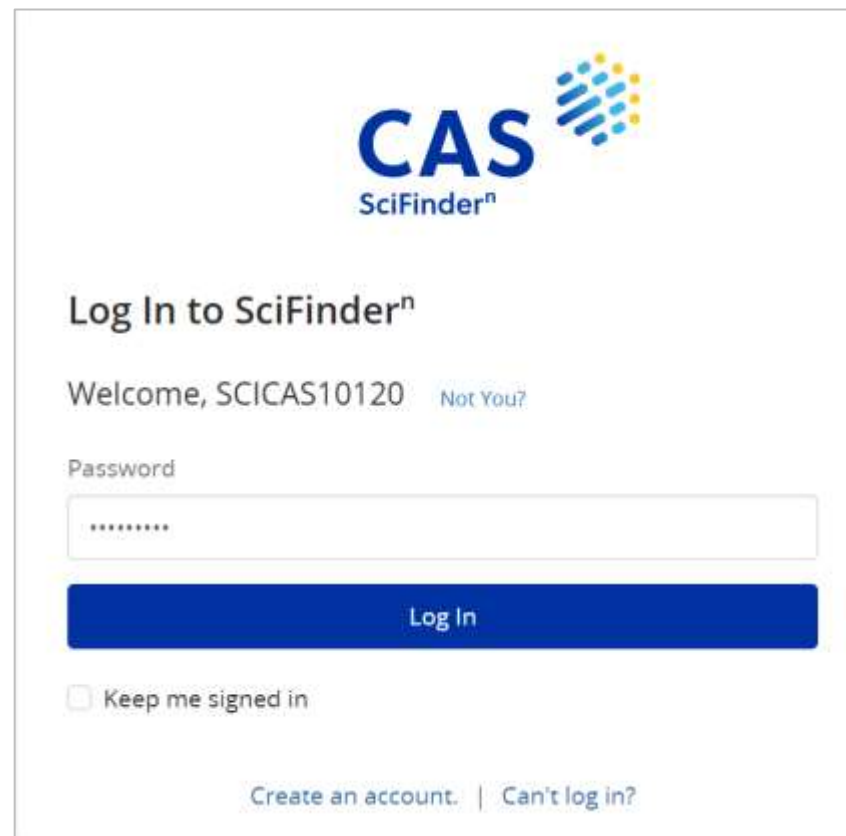
Log In to SciFinderⁿ

Username or Email Address

SCICAS10120

Next

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



CAS SciFinderⁿ

Log In to SciFinderⁿ

Welcome, SCICAS10120 [Not You?](#)

Password

.....

Log In

Keep me signed in

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

使用CAS SciFinder账号登录

CAS SciFinder[®]主界面

The screenshot shows the CAS SciFinder® main interface. On the left, a navigation menu is highlighted with a yellow box, listing various tools and services. At the top right, a user profile area is highlighted, showing 'Alerts', 'Saved', and 'Na Pan'. The main search area features a search bar with a 'Draw' button highlighted. Below the search bar, there are three featured search options: Retrosynthetic Analysis, Search CAS Lexicon, and Search CAS Sequences. At the bottom, a 'Recent Search History' section is highlighted, showing a search for 'Molecular Formula: Al2O3 (12 Results)' with 'Rerun Search' and 'Edit Search' buttons highlighted.

SCIFINDER DISCOVERY PLATFORM

- CAS SciFinder[®]
- CAS Analytical Methods
- CAS Formulus
- STN IP PROTECTION SUITE
- STNext
- CAS Scientific Patent Explorer
- REGULATORY
- CAS Chemical Compliance Index
- ACCOUNT MANAGEMENT
- CAS Profile

Good Morning, Na **灵活检索选项**

Alerts Saved Na Pan

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

Draw

Molecular Formula

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

+ Add Advanced Search Field

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

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

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

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

October 27, 2023

Substances Molecular Formula: Al2O3 (12 Results) 12:29 PM

Rerun Search Edit Search

提醒更新的结果
已保存的检索和结果集
账户信息

检索项逻辑关系
文本与结构检索便捷联用

CAS解决方案

查看全部检索历史

重新运行检索式
修改检索式



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

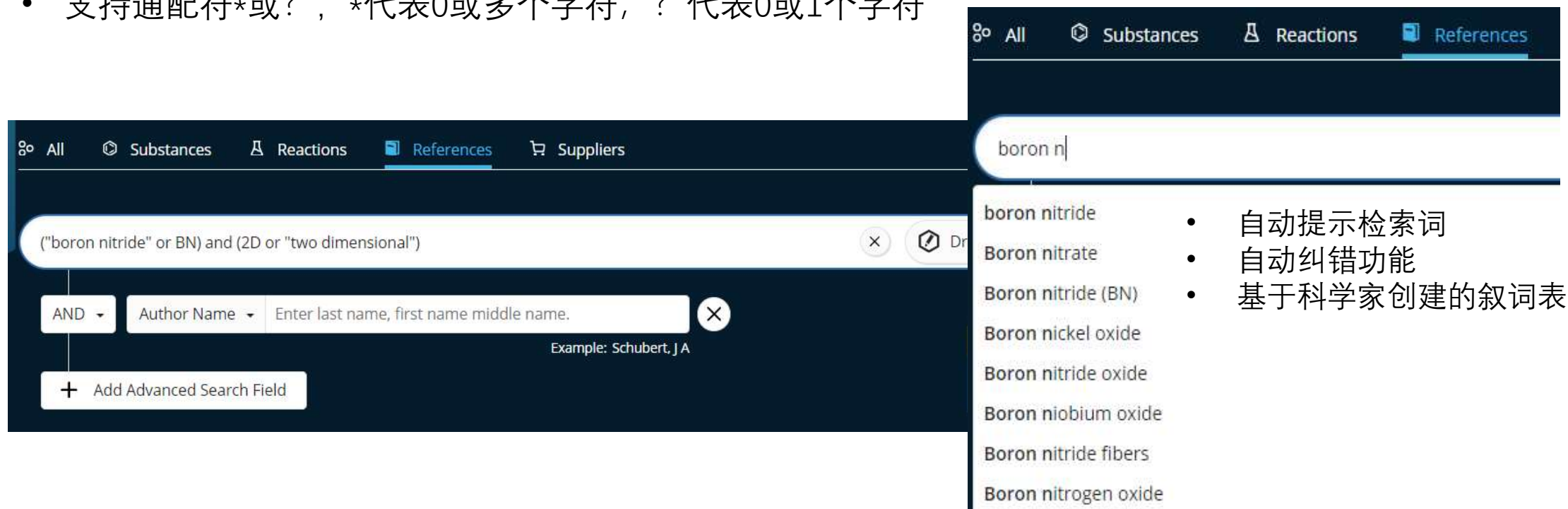


1. 如何开展文献检索？

- 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 top navigation bar includes tabs for All, Substances, Reactions, References, and Suppliers. The main search area contains a search bar with the query: ("boron nitride" or BN) and (2D or "two dimensional"). Below the search bar, there are fields for AND, Author Name, and a text input field with the placeholder "Enter last name, first name middle name." and an example "Schubert, J A". A button labeled "+ Add Advanced Search Field" is also visible.

On the right side, a dropdown menu is shown with the search term "boron n|". The dropdown list includes the following suggestions:

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

Next to the dropdown list, there are three bullet points:

- 自动提示检索词
- 自动纠错功能
- 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）

The image displays two screenshots of the CAS search interface. The left screenshot shows a search for "poly* not polyethylene" with 20,116,548 results. The right screenshot shows a search for "(poly* not polyethylene) and 'conductive device'" with 199 results. Both screenshots show a list of search results with filters on the left and a "Load More Results" button.

Left Screenshot: Search for "poly* not polyethylene"

- Search Results: 20,116,548 Results
- Filter Behavior: Filter by (selected), Exclude
- Search Within Results: Search Within Results
- Document Type: Document Type
- Substance Role: Substance Role
- Language: Language
- Publication Year: Publication Year
- Author: Author
- Organization: Organization
- Publication Name: Publication Name
- Concept: Concept
- CA Section: CA Section
- CAS Solutions: CAS Solutions
- Bioactivity Data: Bioactivity Data
- Formulation Purpose: Formulation Purpose
- Database: Database

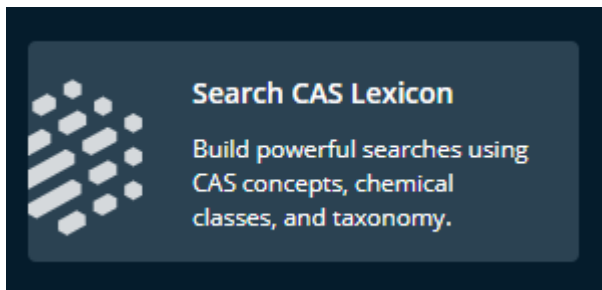
Right Screenshot: Search for "(poly* not polyethylene) and 'conductive device'"

- Search Results: 199 Results
- Sort: Relevance, View: Partial Abstract
- Filter Behavior: Filter by (selected), Exclude
- Document Type: Document Type
- Substance Role: Substance Role
- Language: Language
- Publication Year: Publication Year
- Author: Author
- Organization: Organization
- CA Section: CA Section
- CAS Solutions: CAS Solutions
- Database: Database

Search Results (Right Screenshot):

- 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 (EGain) into microgels of marine polysaccharides. [View More](#)
- 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.

如何选择概念词？借助CAS Lexicon词库



- CAS科学家标引的概念词 (Concepts) 和物质
- 直接添加概念词建立检索式 (最多可用1000个词)

Search CAS Lexicon

Primary batteries

Your Query
You may include up to 1,000 terms in a search.

Preferred Term

Primary batteries
This will search synonyms: Nonrechargeable **batteries**; **Primary** **battery**

Batteries

Button-type primary batteries
 Dry cell primary batteries
 Lithium primary batteries
 Nuclear batteries
 Primary batteries, reserve

Battery electrodes
 Battery electrolytes
 Electrolytic capacitors
 Electrolytic cells

Primary batteries
 Lithium primary batteries
 Battery electrolytes

Select a boolean operator [Learn more about CAS Lexicon searching.](#)

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. A search bar at the top contains the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' Below the search bar, a dropdown menu is open, showing various search fields: Authors, Publication Name, Organization, Title, Abstract/Keywords, Concept, Substances, Bioactivity Data (marked as NEW), Publication Year, Document Identifier, Patent Identifier, and Publisher. A yellow box highlights the 'Add Advanced Search Field' button, which is linked to a secondary dropdown menu showing logical operators: AND, OR, and NOT. The main search bar also contains the text 'Author Name' and 'Enter last name, first name middle name.' with an example 'Schubert, J A'.

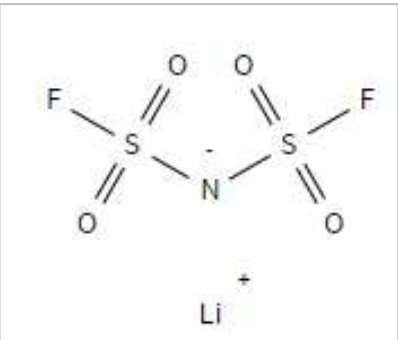
检索方法可单独使用，也可联用：

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

1.2 如何获得结构相关的文献?

示例：关注锂电池技术中特定的热点材料
策略：从References出发， 主题词+结构联用检索

文本与结构是“and”关系



Substance Role

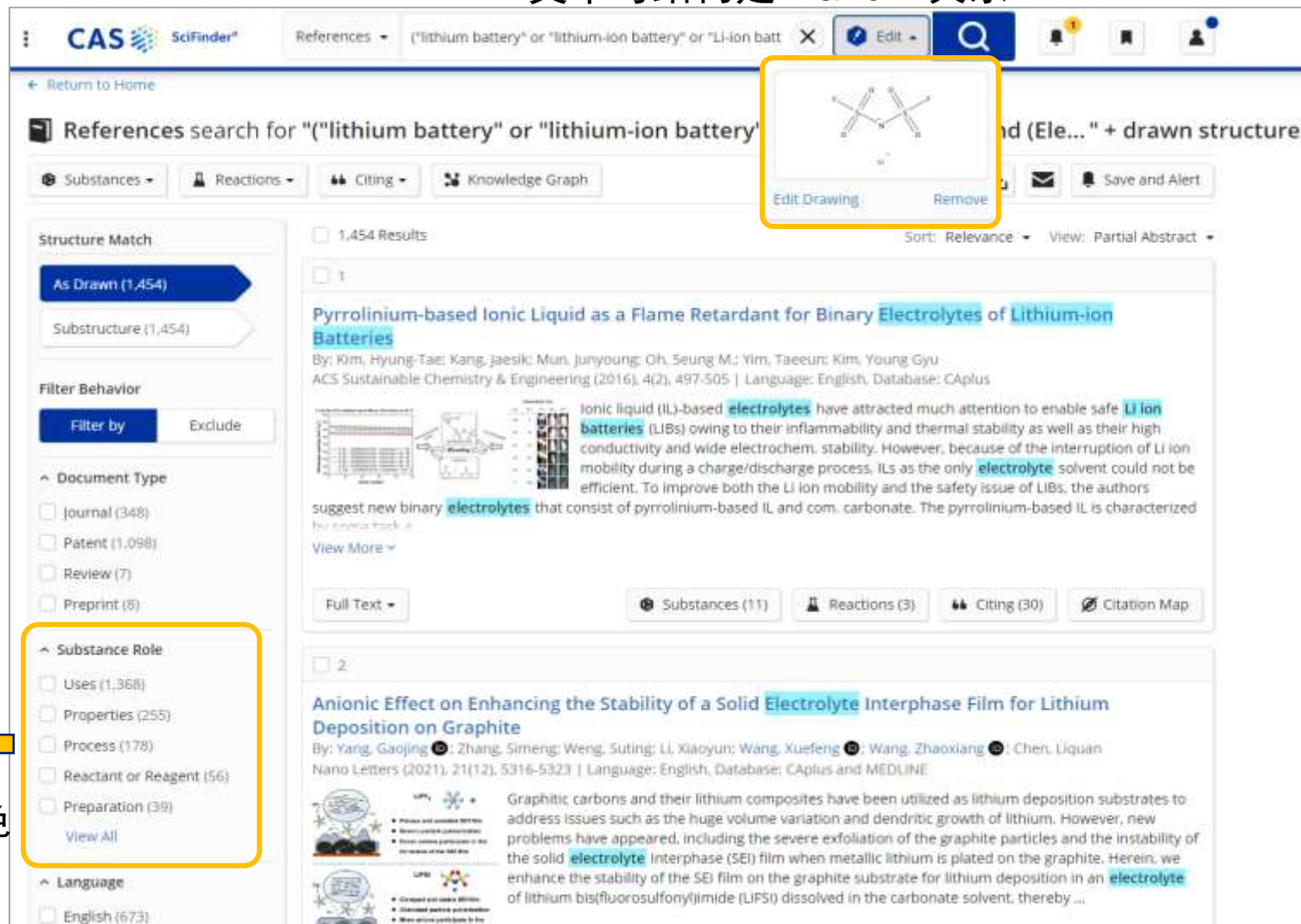
By Count | Alphanumeric

1 Selected

<input checked="" type="checkbox"/> Uses (1,368)	<input type="checkbox"/> Reactant or Reagent (56)
<input type="checkbox"/> Technical or Engineered Material Use (1,237)	<input type="checkbox"/> Reactant (50)
<input type="checkbox"/> Properties (255)	<input type="checkbox"/> Preparation (39)
<input type="checkbox"/> Physical, Engineering, or Chemical Process (178)	<input type="checkbox"/> Industrial Manufacture (20)
<input type="checkbox"/> Process (178)	<input type="checkbox"/> Synthetic Preparation (19)
<input type="checkbox"/> Modifier or Additive Use (83)	<input type="checkbox"/> Reagent (6)
<input type="checkbox"/> Other Use, Unclassified (72)	<input type="checkbox"/> Nanoscale (5)
	<input type="checkbox"/> Purification or Recovery (4)
	<input type="checkbox"/> Analyte (2)

Apply | **Cancel**

定位物质在文献中的研究角色



References search for "lithium battery" or "lithium-ion battery"

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: CAsPlus

1,454 Results

Sort: Relevance | View: Partial Abstract

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, Liqian
Nano Letters (2021), 21(12), 5316-5323 | Language: English, Database: CAsPlus and MEDLINE

1.3 文献结果分析与筛选

References search for 2 CAS Lexicon Terms

Substances Reactions Citing Knowledge Graph Save and Alert

60,503 Results Sort: Relevance View: Partial Abstract

Filter Behavior Filter by Exclude

Search Within Results

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

Filter Content Report Download filter data from this result set.

1
A p-n organic battery, a method of fabricating the battery thereof
By: Al-Sehemi, Abdullah G.; Dere, Aysegul; Al-Ghamdi, Ahmed A.; Yakuphanoglu, Fahrettin; Pannipara, Mehboobali
United States, US20230343960 A1 2023-10-26 | Language: English, Database: CAplus
In the present disclosure, a p-n organic battery comprising a p-type organic semiconductor and n-type organic semiconductor as active electrodes, anode and cathode current electrodes, separator and electrolyte and a method of fabricating the same is disclosed. The p-n organic battery has a p-type organic semiconductor separated from a n type organic semiconductor by an aqueous electrolyte solution, contained in an insulating vessel with suitable terminals (not shown) being provided in elec. contact with the anode current electrode and the cathode current electrode. The aqueous electrolyte can...
View More

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

2
Method for preparing sodium bis(fluorosulfonyl)imide and use thereof
By: Liu, Jianwen; Liu, Shiqi; Wang, Shiquan
World Intellectual Property Organization, WO2023202325 A1 2023-10-26 | Language: Chinese, Database: CAplus
The present disclosure relates to the tech. field of sodium ion battery electrolyte materials, and in particular, to a method for preparing sodium bis(fluorosulfonyl)imide and use thereof. The method comprises: in an inert atm., uniformly mixing bis(fluorosulfonyl)imide, a sodium source, and a non-aqueous solvent for reaction, and separating the solid and liquid phases after the reaction is completed to give sodium bis(fluorosulfonyl)imide. The non-aqueous solvent comprises at least one of acetonitrile, valeronitrile, pyridine, chloroethanol, chloroform, n-propanol, toluene, di-Et ether, aceto...
View More

PatentPak Full Text Substances (26) Reactions (0) Citing (0) Citation Map

Save Results and Create Alert 定题追踪

Name Battery

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

Alert Frequency
 No Alerts
 As Available
 Weekly
 Monthly

Add Existing Tags (Optional)
 Material

New Tag (Optional) Tag Color

Save Cancel

Relevance 排序方式
Times Cited
Accession Number: Ascending
Accession Number: Descending
Publication Date: Newest
Publication Date: Oldest

Search Within Results
Search for up to 3 text strings within the result set.
Enter a query...
结果集的二次检索

筛选工具CA Section

纵览学科研究方向

^ CA Section

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

[View All](#)

CA Section

By Count | Alphanumeric

3 Selected

<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 (2,010)
- 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)
- Electrotransfer (1,560)
- 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

Concept

Top Count Alphanumeric Search

Search

Concept Name

nano*

3 Selected

- 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

精准定位核心研究点


支持使用通配符

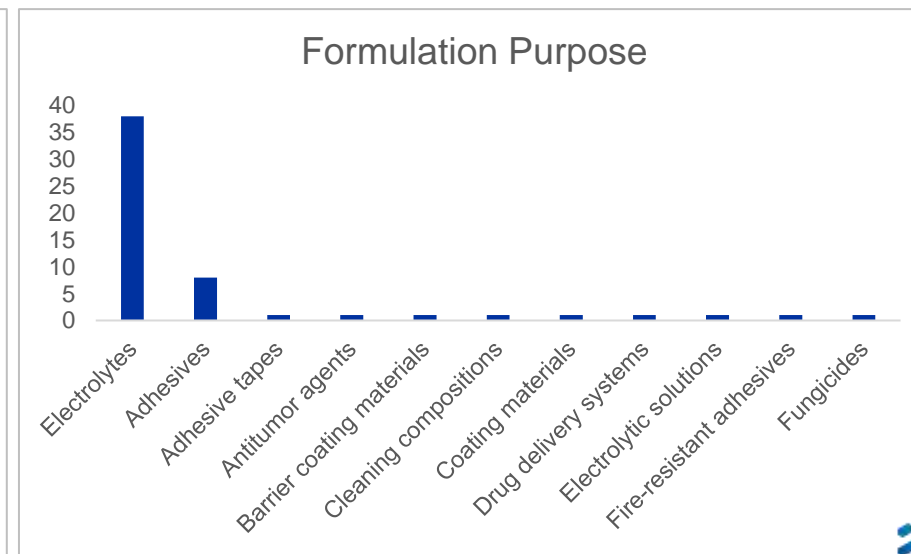
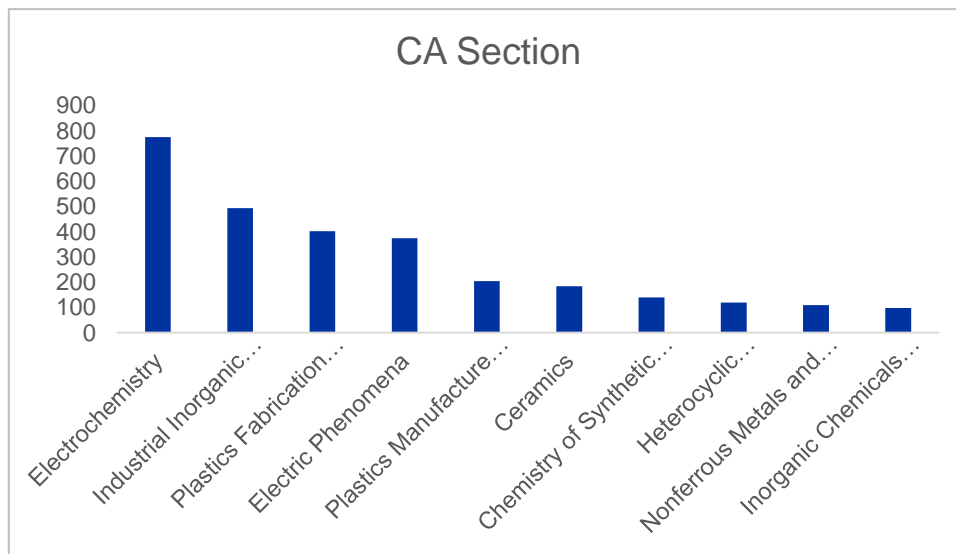
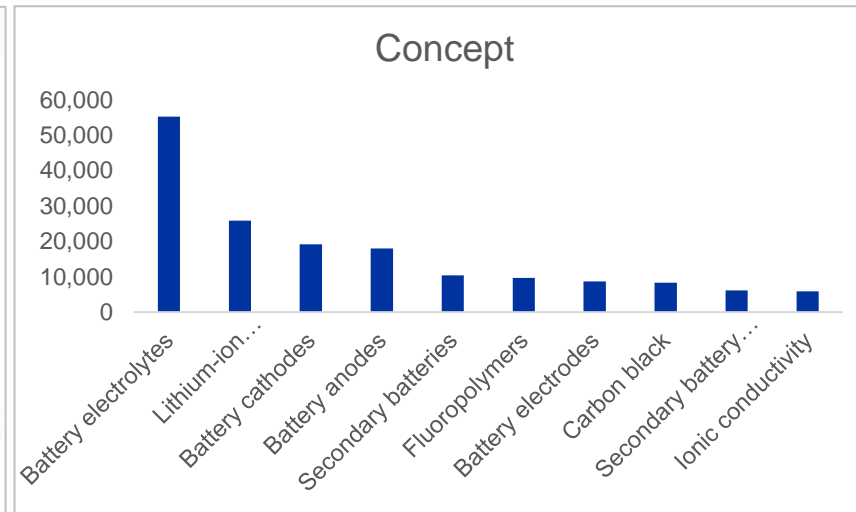
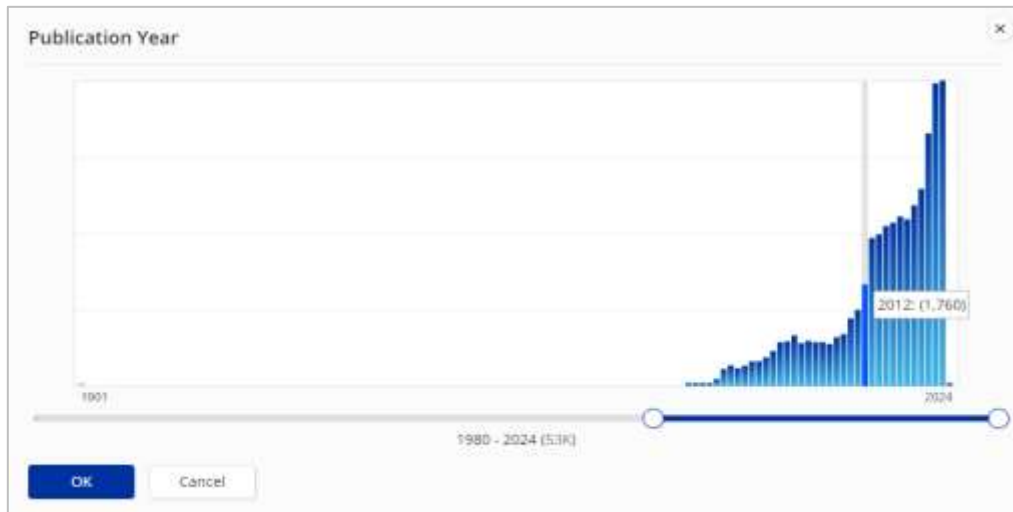
1.4 可视化分析——检索结果趋势分析

Filter Behavior

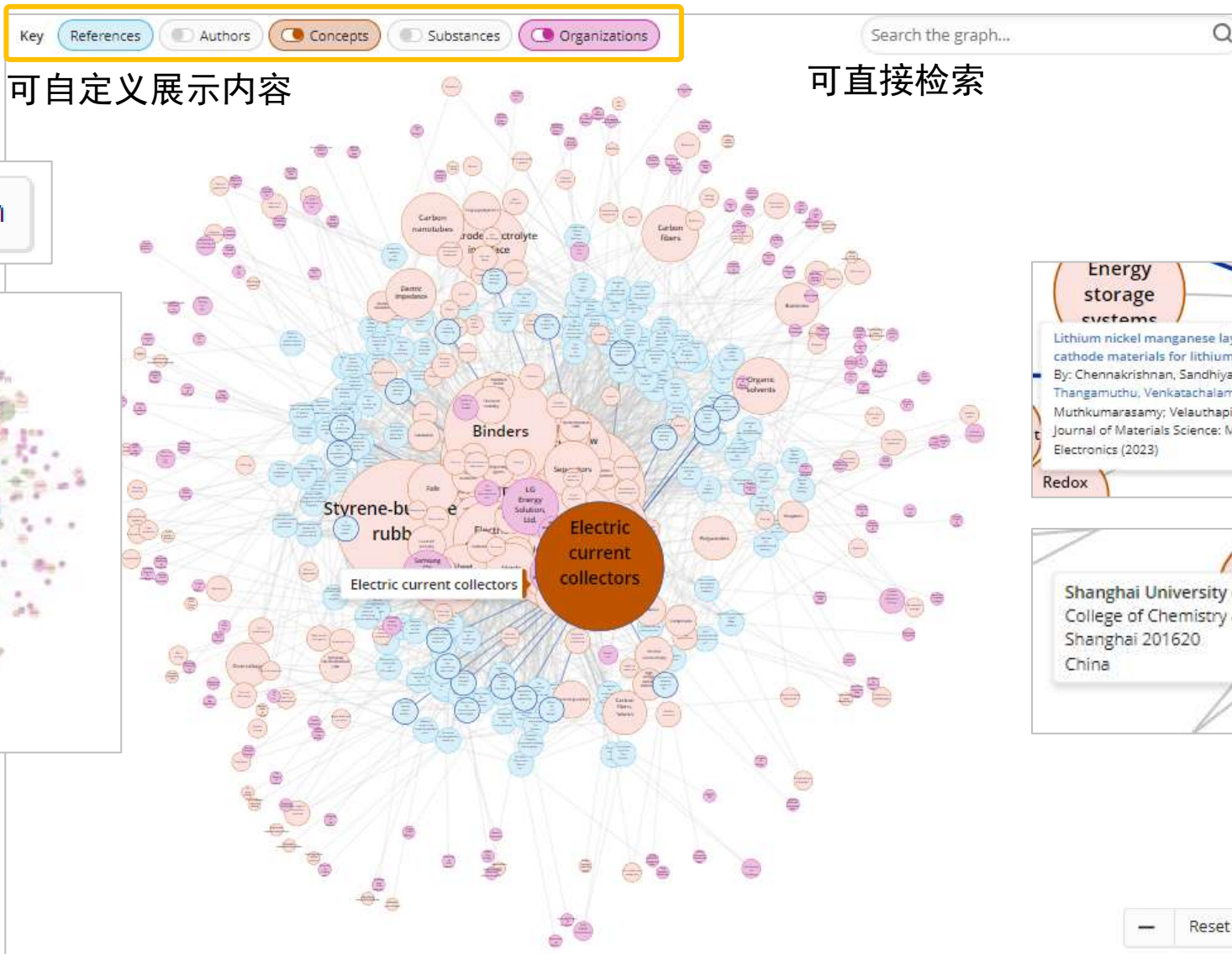
- Search Within Results
- Document Type
- Language
- Publication Year
- Author
- Organization
- Publication Name
- Concept
- CA Section
- CAS Solutions
- Formulation Purpose
- Database

Filter Content Report

Download filter data from this result set. 

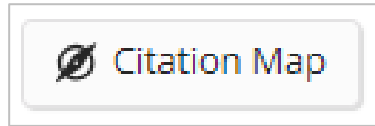
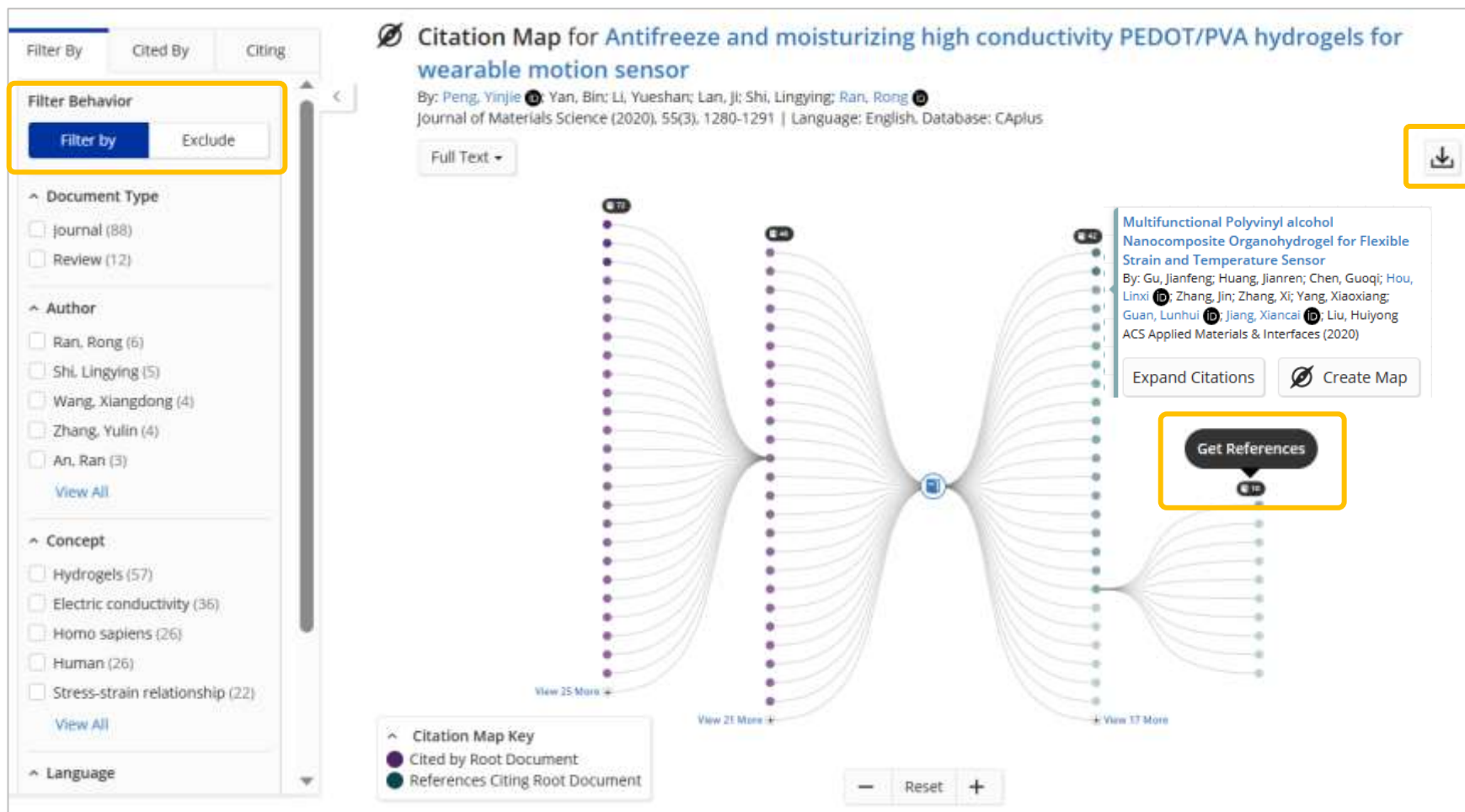


1.4 可视化分析——知识图谱



1.4 可视化分析——引文地图

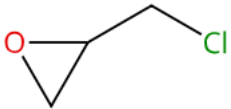
便捷获得相关文献

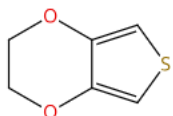



- Citations: 参考文献
- Cited By: 引用当前文献的文献
- 通过聚类选项筛选引文
- 可下载引文地图
- 显示引文和被引文献的数量，点击可链接至对应的文献结果页面

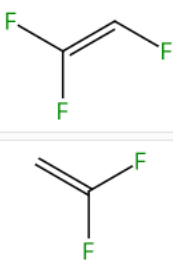
1.5 深入文献详情

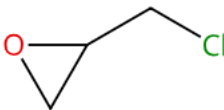
内容合集间彼此关联

1 106-89-8

C₃H₅ClO
Epichlorohydrin
53K References 32K Reactions 84 Suppliers

2 126213-51-2

(C₆H₆O₂S)_x
Poly(3,4-ethylenedioxythiophene)
48K References 1,505 Reactions 7 Suppliers

3 50851-5

(C₈H₈O₃S)_x
Poly(styrenesulfonic acid)
40K References 882 Reactions 2 Suppliers


4 28960-88-5

(C₂H₂F₂-C₂HF₃)_x
Components: 2
P(VDF-TrFE)
5,483 References 63 Reactions 7 Suppliers


5 2839834-68-1

106602-18-0
Image Not Available
(C₃H₅ClO.Unspecified)_x
Components: 2
2 References 1 Reaction 0 Suppliers

6 106602-18-0
Image Not Available
Unspecified
N-[2-Hydroxy-3-(trimethylammonium)propyl]chitosan chloride
500 References 247 Reactions 0 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



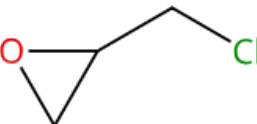
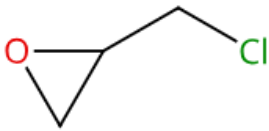
Conductive hydrogels have attracted attention because of their wide application in wearable devices. However, it is still a challenge to achieve conductive hydrogels with high sensitivity and wide frequency band response for smart wearable strain sensors. Here, we report a composite hydrogel with piezoresistive 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

+  → 

Suppliers (84)

106602-18-0
Image Not Available

31-614-CAS-34510937 Steps: 1

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

1.2
4 h, 70 °C

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

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

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

1.5 深入文献详情

巧用CAS PatentPak浏览专利

13

Polymerization with living characteristics with controlled dispersity, 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 (ZCS₂Q₀)_pR (I) or ZCS₂Q₀R (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 thiocarbonylthio compound from (ZCS₂)_pR (III) and Z'(CS₂)_pR' (IV) having a chain transfer constant >0.1; and (iii) free radicals or other initiators.

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 ZOOM /88 DOWNLOAD PDF PDF+

Key Substances in Patent

CAS RN 2168-82-3
ClC1=CC=C(C=C1)C(=S)S

Analyst Markup Locations (2)
Page 28
Page 25

CAS RN 100-86-1
BrC1=CC=CC=C1

Analyst Markup Locations (2)
Page 28
Page 32

CAS RN 100-58-3
C1=CC=CC=C1

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

CAS PatentPak PAGE 35 ZOOM /88 DOWNLOAD PDF PDF+

Key Substances in Patent

CAS RN 2168-82-3
ClC1=CC=C(C=C1)C(=S)S

Analyst Markup Locations (2)
Page 28
Page 25

CAS RN 100-86-1
BrC1=CC=CC=C1

Analyst Markup Locations (2)
Page 28
Page 32

CAS RN 100-58-3
C1=CC=CC=C1

Analyst Markup Locations (2)
Page 28
Page 32

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 = Ph)
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

15 **Example 13**
Preparation of 2-phenylprop-2-yl 4-chlorodithiobenzoate (22) (C, p=1, R = C(CH₃)₂Ph; Z = *n*-C₆H₁₄)
A mixture of 4-chlorodithiobenzoic acid (13 g) and *n*-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).

20

文献检索小结

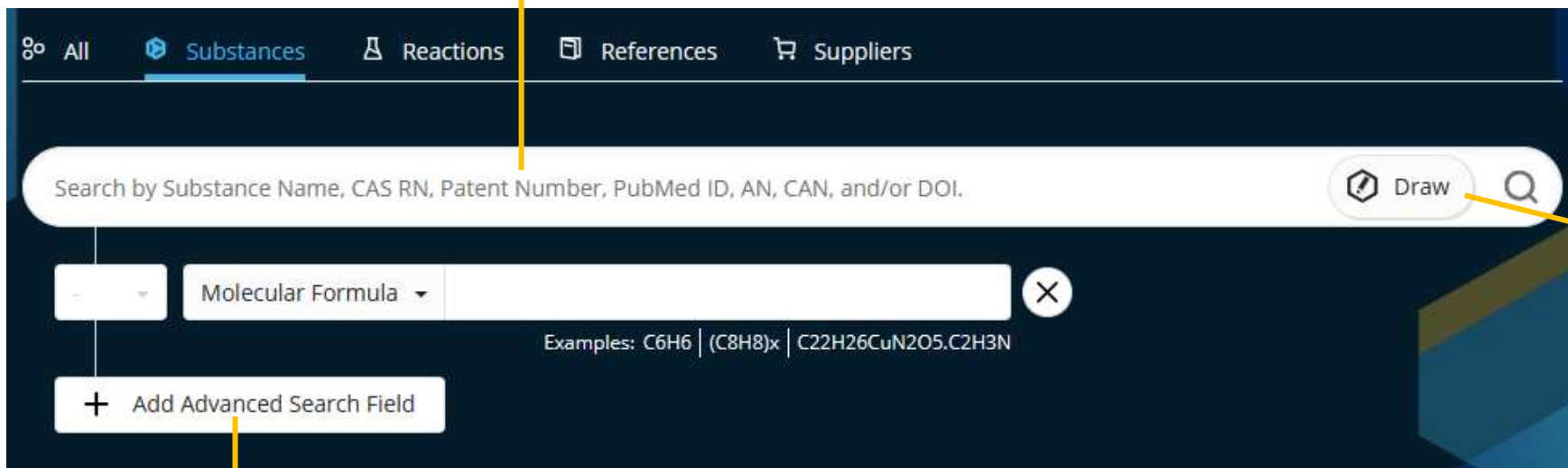
1. 检索主题的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
2. 主题词+结构联合检索，快速获得文献
3. 利用丰富的筛选工具，缩小范围，锁定目标文献
4. 检索结果趋势分析、知识图谱、引文地图
5. 文献详情，CAS PatentPak浏览专利详情

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



- 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

$C_{23}H_{32}F_3N_5O_4$
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

Absolute stereochemistry shown

$C_{37}H_{48}N_6O_5S_2 \cdot C_{23}H_{32}F_3N_5O_4$
Components: 2
Paxlovid

39 References 0 Reactions 0 Suppliers

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

Sort: Relevance

Relevance

CAS RN: Ascending

CAS RN: Descending

Molecular Formula: Ascending

Molecular Formula: Descending

Molecular Weight: Ascending

Molecular Weight: Descending

Number of References: Ascending

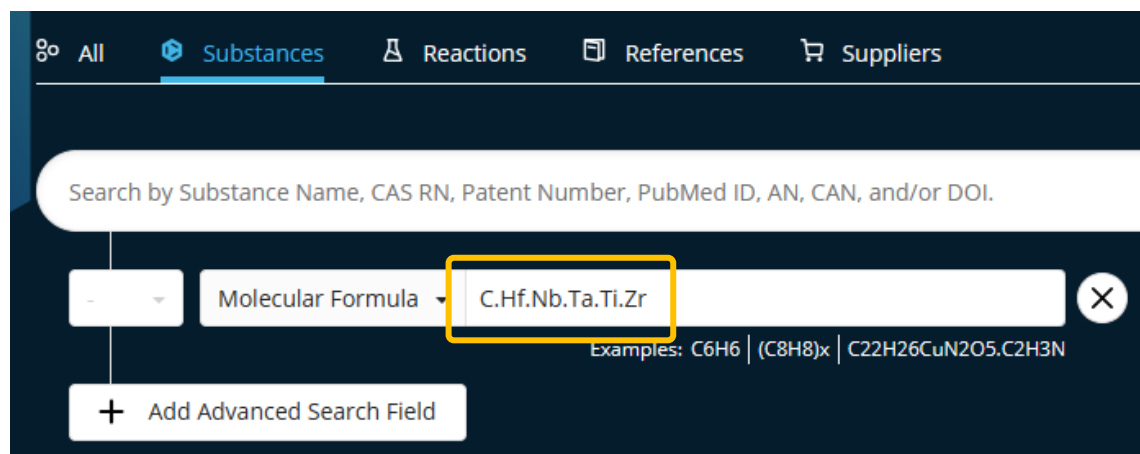
Number of References: Descending

Number of Suppliers

物质排序：相关度、CAS RN、分子式、分子量、文献量、供应商数量

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



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

The screenshot shows the search results page for the molecular formula "C.Hf.Nb.Ta.Ti.Zr". The page title is "Substances search for 'C.Hf.Nb.Ta.Ti.Zr' Molecular Formula". There are navigation tabs for "References", "Reactions", and "Suppliers". The page shows 7 results. The first result is "2304767-82-4" and the second is "1427190-21-3". Each result has a table showing the components and their ratios. The first result has components C, Zr, Hf, Ti, Ta, and Nb with ratios 1, 0.20, 0.20, 0.20, 0.20, and 0.20 respectively. The second result has components Zr, Hf, C, Ti, Ta, and Nb with ratios x, x, x, x, x, and x respectively. The page also shows a "Filter Behavior" section with options for "Filter by" and "Exclude". There are also sections for "Search Within Results", "Reaction Role", "Reference Role", "Substance Class", and "Number of Components".

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

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

2.2 属性值联用检索物质

The screenshot shows the CAS search interface with the 'Experimental Spectra' dropdown menu open. The menu lists various search criteria: Molecular Formula, CAS Registry Number, Chemical Identifier, Document Identifier, Patent Identifier, Experimental Spectra (highlighted), Bioactivity Data (NEW), Biological, Chemical Properties, Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, and Thermal. The 'Experimental Spectra' sub-menu is also visible, listing: Proton NMR, Carbon-13 NMR, Nitrogen-15 NMR, Fluorine-19 NMR, and Phosphorus-31 NMR. A chemical structure is shown at the bottom of the interface.

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

The screenshot shows the 'Chemical Properties' dropdown menu open, listing various search criteria: Chemical Properties (highlighted), Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, and Thermal. The 'Chemical Properties' sub-menu is also visible, listing: Koc, logD, logP, Mass Intrinsic Solubility (g/L), Mass Solubility (g/L), Molar Intrinsic Solubility (mol/L), Molar Solubility (mol/L), Molecular Weight, and Vapor Pressure (Torr).

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 $<7\text{g/cm}^3$ 、拉伸强度 $>1000\text{MPa}$ 、熔点 $>600^\circ\text{C}$ 。

The screenshot displays a search interface for substances. On the left, a search panel shows three criteria: Density (g/cm³) < 7, Tensile Strength (Mpa) 1000 to 2500, and Melting Point (°C) > 600. The 'Substance Class' filter is set to 'Alloy (18)'. The main search results are titled 'Substances search for 3 Advanced Fields' and show 18 results. Three results are displayed in detail:

- 11134-23-9**: Component Percent table with 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), and C (0-0.030). Components: 9. AISI 316L. 25K References, 17 Reactions, 5 Suppliers.
- 12634-55-8**: Component Percent table with 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), and Fe (0-0.005). Components: 9. Magnesium alloy, base, Mg 95-97, Al 2.5-3.5, Zn 0.6-1.4, Mn 0.2, Si 0-0.10, Cu 0-0.05... 12K References, 8 Reactions, 0 Suppliers.
- 12627-49-5** (highlighted): Component Percent table with 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), and Ti (0-0.20). Components: 9. AA 7075. 11K References, 1 Reaction, 1 Supplier.

在物质类别 Substance Class 中,
锁定合金 Alloy。

属性值、谱图数值联用检索物质

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

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

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

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

+ Add Advanced Search Field

Substances search for 3 Advanced Fields

References Reactions Suppliers Save and Alert

Filtering: Bioactivity Data: 3 Selected X Clear All Filters

15 Results Sort: Molecular Formula: Ascending View: Partial

1	2	3
296262-16-3 <chem>C10H10N2O2S2</chem> 2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]acetic acid 5 References 42 Reactions 44 Suppliers	723-46-6 <chem>C10H11N3O3S</chem> Sulfamethoxazole 24K References 961 Reactions 120 Suppliers	1631737-39-7 <chem>C10H15N3O5</chem> (2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxymethyl)-3-methylspiro[furan-2(3H),7'(6'H)]-... Absolute stereochemistry shown, Rotation (-) 2 References 22 Reactions 0 Suppliers
442571-27-9 <chem>C10H10N2O2S2</chem> 2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]acetic acid 5 References 42 Reactions 44 Suppliers	1927010-88-5 <chem>C10H17N3O2</chem> 1-(2-ethoxyethyl)pyrrolidine-2-carboxamide 24K References 961 Reactions 120 Suppliers	697787-29-4 <chem>C10H10N2O2S2</chem> 2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]acetic acid 5 References 42 Reactions 44 Suppliers


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

物质详情

CAS Registry Number: 723-46-6

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

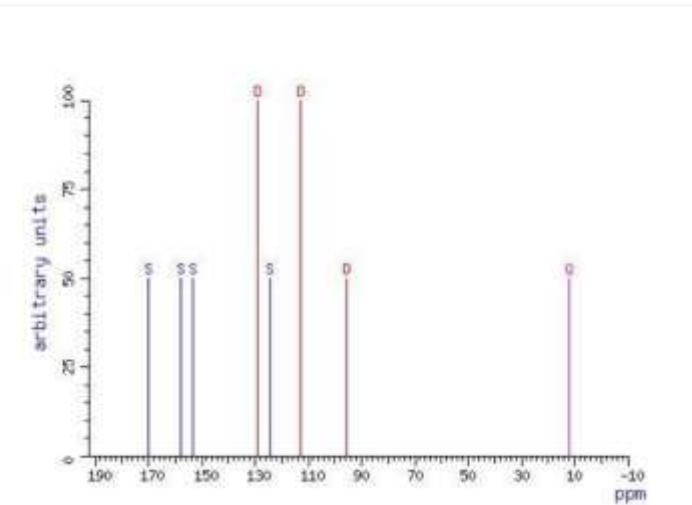
This substance contains CAS Bioactivity data, such as SAR, ADME, or Toxicity tables. Explore this information below. [Learn more about CAS life sciences.](#)



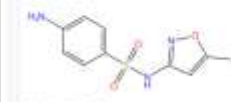
$C_{10}H_{11}N_3O_3S$
Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)- (9CI, AC)

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

Carbon-13 NMR Spectrum for 723-46-6



723-46-6



$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

- Solvent: DMSO- d_6 (72206-27-1)
- Standard: Tetramethylsilane (75-08-0)

Spectrum Summary

- Spectrum ID: CNCC-5959-2330
- Spectrometer: JEOL GX-270
- Source: Spectral data were obtained from John Wiley & Sons, Inc.

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra

1H NMR 13C NMR Hetero NMR IR Mass Raman UV and Visible

View Carbon-13 NMR Spectrum	Solvent	Source
View Carbon-13 NMR Spectrum	DMSO- d_6	(1) WSS
View Carbon-13 NMR Spectrum	DMSO- d_6	(2) WSS
View Carbon-13 NMR Spectrum	-	(2) WSS
View Carbon-13 NMR Spectrum	Methanol- d_4	(3) CAS
View Carbon-13 NMR Spectrum	DMSO- d_6	(4) CAS
View Carbon-13 NMR Spectrum	-	(5) BIORAD
View Carbon-13 NMR Spectrum	DMSO- d_6	(6) AIST
Carbon-13 NMR Spectrum - 1 Source	-	(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, Naresh; European Journal of Medicinal Chemistry, (2015), 101, 595-603, CAplus
- (5) Copyright Bio-Rad Laboratories. All Rights Reserved.
- (6) "Integrated Spectral Data Base System of Organic Compounds" data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan)
- (7) Blasioli, Sonia; Journal of Colloid and Interface Science, (2014), 419, 148-159, CAplus

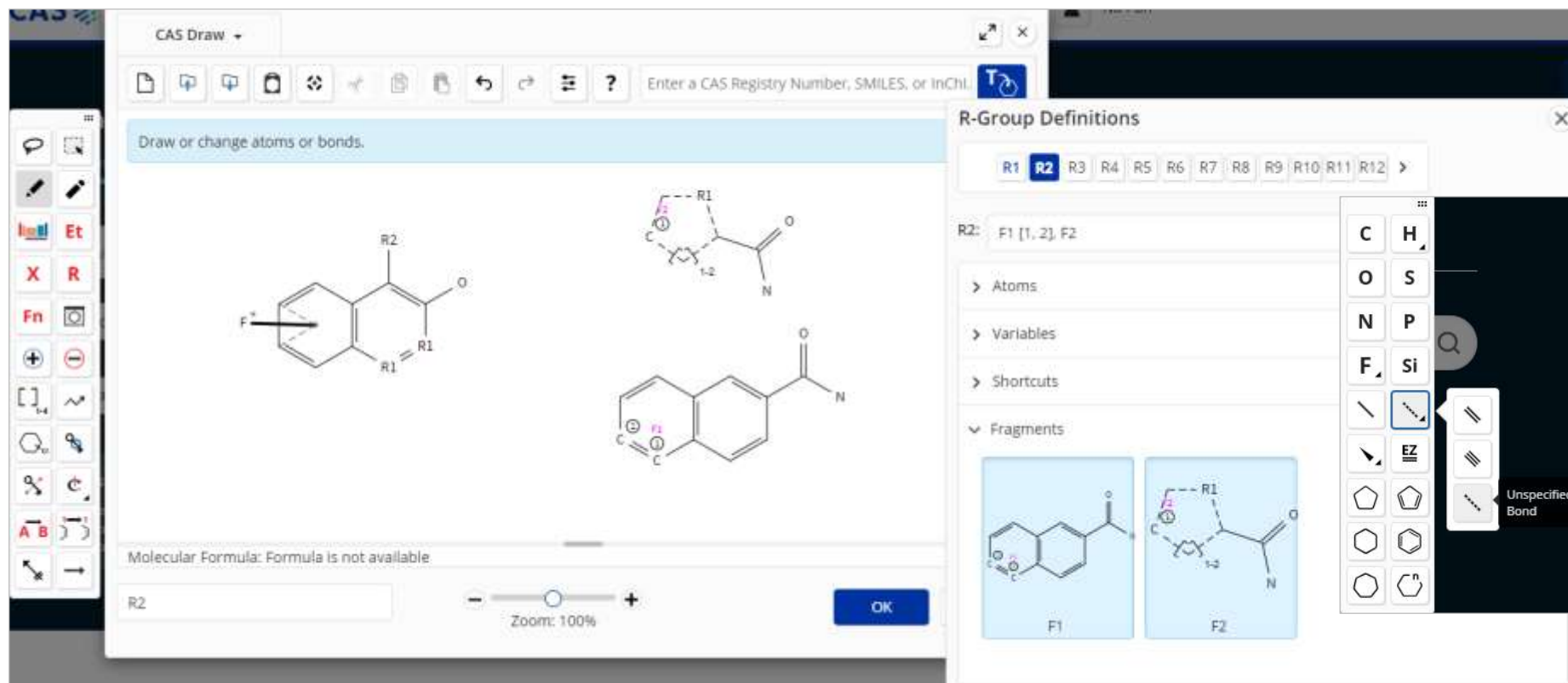
- Structure Activity Relationships CAS LIFE SCIENCES
- Absorption, Distribution, Metabolism, and Excretion Data CAS LIFE SCIENCES
- Toxicity CAS LIFE SCIENCES
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements
- Additional Details

• 折叠菜单显示物质各类信息




2.3 结构检索

灵活构建通式结构，提高物质/反应信息的检索效率

-  选择可变基团
-  自定义R基团
-  片段结构
-  重复工具
-  取代位置可变
-  环锁定工具
-  原子锁定工具



利用绘图工具自定义相似结构:

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

结构检索

例：已知结构片段的物质检索

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

Substances search for drawn structure

References Reactions Suppliers

Structure Match

- As Drawn (0)
- Substructure (732)**
- Similarity (9)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Reaction Role

R1

732 Results

1 685504-28-3

2 807307-30-8

3 635299-07-9

4 635299-08-0

5 16827-53-5

6 635299-09-1

Save and Alert

Filter Behavior

- Filter by Exclude
- Reaction Role
- Reference Role
- Commercial Availability
- Number of Components
- Molecular Weight
- Stereochemistry
- Element
- Substance Class
- Isotopes
- Metals
- Experimental Property
- Bioactivity Indicator
- Search Within Results

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

- Preparation (489)
- Synthetic Preparation (488)
- Properties (245)
- Reactant (98)
- Reactant or Reagent (98)
- Industrial Manufacture (9)

Commercial Availability

- Not Available (9)


Commercial Availability

- Not Available (9)

Reaction Role:
物质在反应中的角色

Reference Role:
物质在文献中的研究角色


1087216-22-5



$C_{28}H_{29}Cl_2CoNP_2$
Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]ethanamine-κN...

8 References 105 Reactions 0 Suppliers


2170923-58-5



$C_{28}H_{29}Cl_2CoNP_2$

8 References 105 Reactions 0 Suppliers


579490-58-7



$C_{37}H_{31}NNiP_2$
(SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzenamine-κN...

7 References 22 Reactions 0 Suppliers

579490-62-3



$C_{38}H_{33}NNiP_2$
(SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzenamine-κN...

6 References 21 Reactions 0 Suppliers

物质检索结果的筛选

Substance Class: 物质类别

Number of Components

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

Molecular Weight

Stereochemistry

Element

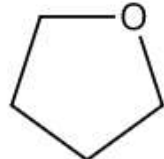

Substance Class

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

Isotopes

4

849402-50-2

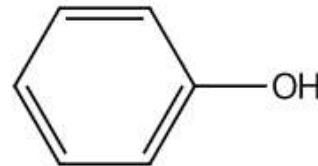



$(C_4H_8O.C_4H_4S)_x.xCH_2O$
Components: 3
Furan, tetrahydro-, polymer with thiophene, methyl ether, graft

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

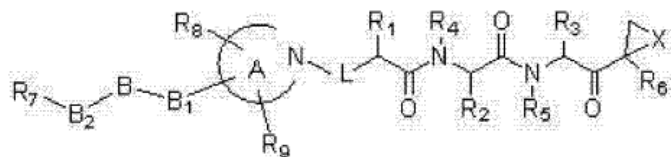
2.4 CAS Markush检索，助力结构查新

CN 104945470 A

权利要求书

1/3 页

1. 一种杂环构建的三肽环氧化物类化合物，具有下述结构通式 I：



I

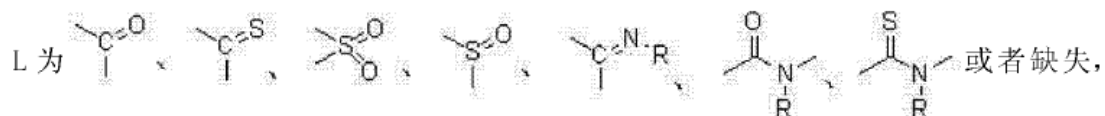
其中：

R_1, R_2, R_3 各自独立选自 H、 C_{1-6} 烷基、-D、卤代的 C_{1-6} 烷基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 $N(R_a)$ (R_b) 或缺失， R_a, R_b 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4, R_5 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 羟基烷基、 C_{1-6} 烷氧基、卤代的 C_{1-6} 烷氧基、 $C(O)O-C_{1-6}$ 烷基、 $C(O)NH-C_{1-6}$ 烷基、芳烷基；

X 为 O、S、NH、 $N-C_{1-6}$ 烷基或 $N-$ 卤代的 C_{1-6} 烷基；



其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

环 A 选自 5 ~ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ~ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ~ 3 个选自 O、N 和 S 的杂原子并任选地被 R_8, R_9 和 B_1 基团取代；

R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基、 C_{1-6} 烷氧基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷

具体物质[Specific Substance]： 以具体化学结构陈述的特定物质，会被分配CAS RN

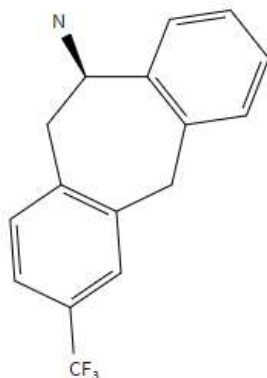
预测性物质[Prophetic Substance]：

- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

CAS Markush检索

第一步：物质结构检索

- As drawn结果为0
- Substructure结果为2
- Similarity相似度最高85-89%



Structure Match

As Drawn (0)

Substructure (2)

Similarity (5,664)

Analyze Structure Precision

Chemscrape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscrape.

Create Chemscrape Analysis

2 Results

Sort: Number of R

146364-17-2

C17H14F3N
10,5-(Iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl) derivative...

1 Reference 1 Reaction 0 Suppliers

146364-18-3

C18H16F3N
10,5-(Iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-12-methyl-3-(trifluoromethyl) derivative...

1 Reference 1 Reaction 0 Suppliers

Structure Match

As Drawn (0)

Substructure (2)

Similarity (5,664)

Chemscrape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscrape.

Create Chemscrape Analysis

Filter Behavior

Filter by Exclude

Similarity

- 85-89 (1)
- 80-84 (2)
- 75-79 (20)
- 70-74 (140)
- 65-69 (958)
- 60-64 (4,211)

Reaction Role

Reference Role

Filtering: Number of Components: 1 X

Clear All Filters

5,332 Results

Sort: Number of References: Descending View: Partial

1 61

1210-33-9

C15H13Cl
5-Chlorodibenzosuberane

143 References 130 Reactions 61 Suppliers

2 64

1057277-76-5

C16H14F3N
1,2,3,4-Tetrahydro-2-[4-(trifluoromethyl)phenyl]isoquinoline

90 References 121 Reactions 2 Suppliers

3 68

7005-53-0

C15H15N
IEM 2115

58 References 78 Reactions 14 Suppliers

4 60

3436-04-2

C18H17Br
5-(3-Bromopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene

5 62

1729-63-1

C16H13N
10,11-Dihydro-5H-dibenzo[a,d]cycloheptene-5-carbonitrile

6 64

35764-73-9

C21H24F3N
Fluotracen

Relative stereochemistry shown

Feedback

为了尽可能完整地获得公开的结构信息，需要同时进行Substance和Markush结构检索

CAS Markush检索

第二步：Markush结构检索
获得四件专利文献

- 直观呈现检索结构与专利原文中Markush匹配部分的结构；
- 标引其在专利中出现的位置；
- 详细的结构取代信息描述

The screenshot displays the CAS SciFinder interface for a Patent Markush search. At the top, the search bar contains "Substances" and "Enter a query...". The main heading is "Patent Markush search for drawn structure". A chemical structure is shown in a yellow box with "Edit Drawing" and "Remove" buttons. Below it, a "References" dropdown and "Search Patent Markush" checkbox are visible. The search results are categorized into "Patent Markush Match" and "Filter Behavior". The "Patent Markush Match" section shows "As Drawn (4)" and "Substructure (33)". The "Filter Behavior" section includes "Filter by" and "Exclude" buttons. The "Patent Office" section lists "World Intellectual Property Organization (3)", "European Patent Organization (1)", and "CA Section" with sub-categories like "Agrochemical Bioregulators (1)", "Electric Phenomena (1)", "Heterocyclic Compounds (More Than One Hetero Atom) (1)", and "Pharmacology (1)". The "Filter Content Report" button is at the bottom. The search results are displayed in a grid. The first result is "WO2011025969" with a chemical structure and a table of patent information. The second result is "EP502788" with a chemical structure and a table of patent information.

WO2011025969

Compounds that treat malaria and prevent malaria transmission

By: Su, Xin-Zhuan; Yuan, Jing; Raj, Dipak; Pattaradilokrat, Sittiporn; Johnson, Ron; Huang, Ruili
World Intellectual Property Organization, WO2011025969 A1 2011-03-03 | Language: English, Database: CAplus
Assignee: United States Dept. of Health and Human Services

Patent claim 1

Patent	Language	Kind Code	PatentPak Options
WO2011025969	English	A1	PDF PDF+ Viewer
CN102595894	Chinese	A	PDF
US20120196882	English	A1	PDF PDF+ Viewer
US9375424	English	B2	PDF
US20160303103	English	A1	PDF

EP502788

Patent claim 11

Patent	Language	Kind Code	PatentPak Options
EP502788	French	A1	PDF

2.5 CAS SciFinderⁿ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

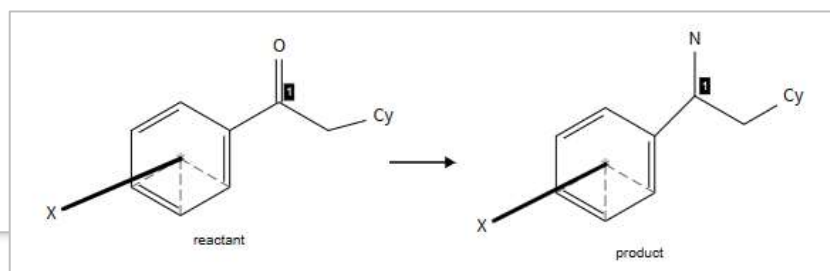
910463-68-2
Image Not Available
Unspecified
Semaglutide
Protein/Peptide Sequence
Sequence Length: 34
1,527 References | 259 Reactions | 32 Suppliers

Reactions search for "Semaglutide"
228 Results
Scheme 1 (1 Reaction)
Steps: 7
Suppliers (98) | Suppliers (64) | Suppliers (28)

Reactions search for "175:621496"
133 Results
Scheme 1 (2 Reactions)
Steps: 7-8
Suppliers (145) | Suppliers (77) | Suppliers (37)

Reactions | References | Suppliers
Search bar with Draw button

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% Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

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

By: Heidelberg, 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 a search interface for chemical reactions. On the left, there are two vertical filter panels. The top panel, 'Structure Match', includes 'As Drawn (34)', 'Substructure (8,044)' (highlighted with a blue arrow), and 'Similarity (0)'. Below it is the 'Filter Behavior' section with 'Filter by' and 'Exclude' buttons. The bottom panel, 'Search Within Results', lists various filters such as 'Yield', 'Reaction Scale' (Milligram, Gram, No Scale Provided), 'Non-Participating Functional Groups', 'Number of Steps', 'Reaction Mapping', 'Experimental Protocols', 'Reaction Type', 'Stereochemistry', 'Reagent', 'Catalyst', and 'Solvent'. A 'Filter Content Report' section at the bottom allows downloading filter data.

The main results area shows a list of reactions. The first result is 'Reductive Alkylation of Ammonia or Amines' with 8,044 results. It includes a chemical reaction scheme: $R-C(=O)-R + R^1-NH-R^1 \rightarrow R-C(R)-N(R^1)-R^1$. Below the scheme is a button 'View 108 Related Reactions'. The second result is 'Formation of N/O/S Heterocycles' with 2 results. It shows two reaction schemes for the formation of 5-membered heterocycles. The first scheme shows a cyclic structure with a carbonyl group reacting to form a heterocycle with a nitrogen atom. The second scheme shows a cyclic structure with a carbonyl group and an electron-withdrawing group (Z) reacting to form a heterocycle with a nitrogen atom. Below the schemes is the text: 'Y, Y' = NH, O, S' and 'Z = Electron withdrawing group'. The third result is '1,3-Dipolar Addition' with 3 results.

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%

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

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

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

Experimental Protocols PatentPak Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield:

Non-Participating Functional Groups

By Count Alphanumeric

1 Selected

- Halide (205)
- Phenyl halide (203)
- Amide (66)
- Alkene (62)
- Cyclic alkene (58)
- Diene (45)
- Ether (37)
- Amine (15)
- Tertiary amine (15)
- 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 bar: Friedel-crafts acylation

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

Structure: Indole

Buttons: Edit Drawing, Remove

Reactions search for "2011:601374"

Filter Behavior: Filter by Exclude

Search Within Results

Yield

Reaction Scale

Non-Participating Functional Groups

Number of Steps

Reaction Mapping

Experimental Protocols

Reaction Type

Reagent

Catalyst

Solvent

Commercial Availability

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

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

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

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

Substances Reactions Citing Knowledge Graph

Structure Match: As Drawn (1,100) Substructure (2,270)

Filter Behavior: Filter by Exclude

Document Type: Journal (996) Patent (68) Review (31) Conference (27)

1,100 Results Sort: Relevance View: P

ZrCl₄-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole

By: Guchhait, Sankar K.; Kashyap, Maneesh; Kamble, Harshad

Journal of Organic Chemistry (2011), 76(11), 4753-4758 | Language: English, Database: CPlus and MEDLINE

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

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

3.4 如何获得逆合成路线?

(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 contains 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 are buttons for 'References (236)', 'Reactions (53)', and 'Suppliers (39)'. On the right, a detailed view of the same structure is shown, with the 'Start Retrosynthetic Analysis' button highlighted in a yellow box. Other buttons include 'Edit Structure', 'Reset', and a download icon.

CAS Retrosynthesis Tool:

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

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


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

逆合成分析的预设参数

Retrosynthesis Plan Options for drawn structure

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

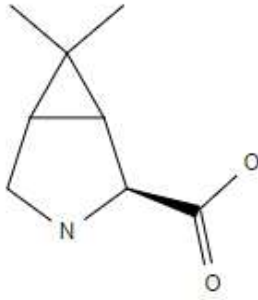
1
 2
 3
 4



Break and Protect Bonds

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

断裂键或保护键



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](#)

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

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

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 View Excluded Options Download Email Save

预测型反应

已知反应

Step	Evidence
$A \Rightarrow B + C$ Average Yield: 69% Evidence (4,925) Alternative Steps (91)	1.1 Reagents: Triethylamine Hydrogen sulfide Solvents: Dichloromethane View All
$B \Rightarrow D + E$ Average Yield: 65% Evidence (15,146) Alternative Steps (20)	1.1 Reagents: Triethylamine Solvents: Dichloromethane; 24 h, rt

Reactions from Retrosynthesis Plan Evidence

References Download Email Save

Filter Behavior Filter by Exclude

15,146 Results Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1: (1 Reaction) Steps: 1 Yield: 88%

C1CCN(C1)C(=O)CC + CCCC(=O)O >> C1CCN(C1)C(=O)CC

Suppliers (18) Suppliers (92) Suppliers (9)

Expand Scheme

Scheme 2: (1 Reaction) Steps: 1

C1CCN(C1)C(=O)CC + CCCC(=O)Cl >> C1CCN(C1)C(=O)CC

Suppliers (136) Suppliers (66) Suppliers (51)

Expand Scheme

- 可查看每步反应的文献支持与详细条件

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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-\(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
Tuebingen 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

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

CAS Method Number 3-315-CAS-33168860

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

操作步骤

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 solutions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 [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 Small quantities of residues of the drug and its main impurities were determined by HPLC...

[View More](#)

electrolyte and arsenic in 10% acetylacetonone 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
- Availability

CAS Solutions

- Analytical Methods (23)
- Formulus (9)

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 Solutions Analytical Methods

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

Browse Method Categories

- Agricultural Applications / Analysis
- Bioassays
- Biomolecule Isolation
- Environmental Analysis
- Food Analysis
- Fuels / Geology / Biofuels
- Historical Analysis / Dating
- Miscellaneous
- Organic Compound Analysis
- Organometallics / Inorganics
- Pharmacology / Toxicology
- Polymer Analysis
- Water Analysis

方法分类: 13大类, 45小类

聚合物分析、有机物分析、金属有机/无机、食品分析、药理学、毒理学、农业应用、生物分子分离等

Browse Method Categories > Agricultural Applications / Analysis

除草剂、农药残留、土壤分析

Herbicide Analysis

Pesticide Residue Analysis

Soil Analysis

如何选择合适的分析方法?

The screenshot displays the CAS Analytical Methods database interface. The search term 'steel and sulfur' is entered in the top search bar. The left sidebar contains filter categories: Analyte (Sulfur, Carbon, Manganese, Aluminum, Chromium), Matrix (Steel, Reinforced concrete), Method Category (Element Detection), Technique (Laser induced breakdown spectroscopy, Liquid scintillation counting, Neutron activation analysis, Time-of-flight mass spectrometry, Atomic emission spectrometry), and Year. The main results area shows a list of results, with the first result highlighted: 'Analysis of Carbon in Steel by Laser induced breakdown spectroscopy'. This result includes details such as Analyte (Sulfur; Carbon), Matrix (Steel), Method Category (Element Detection), and Technique (Laser induced breakdown spectroscopy). The full text and CAS SciFinder links are also visible.

关注特定的:

- ✓ 分析目标物
- ✓ 介质
- ✓ 方法类别
- ✓ 分析技术
- ✓ 发表年份

如何选择合适的分析方法?

Compare Methods

	1	2
Title	Analysis of Carbon in Steel by Laser induced breakdown spectroscopy	Analysis of Silver in Steel by Glow discharge mass spectrometry
CAS Method Number	1-119-CAS-267238	1-119-CAS-101987
Method Category	Element Detection	Element Detection
Technique	Laser induced breakdown spectroscopy	Time-of-flight mass spectrometry; Glow discharge mass spectrometry
Analyte	Sulfur ; Carbon	Titanium; Chromium; Antimony; Magnesium; Lead; Silicon; Cobalt; Sulfur ; Niobium; Tin; Nickel; Manganese; Vanadium; Boron; Molybdenum; Phosphorus; Silver; Tungsten; Copper; View All
Matrix	Steel	Steel
Other Materials	Continuum Surelite laser	Grimm-type chamber (with a 4 mm diameter anode and a 2.5 mm inner diameter flow tube)
Equipment Used	Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer, VM-521, Acton View All	Orthogonal time-of-flight mass spectrometer, ToFwerk, Thun, Switzerland; Dry pump, Triscroll 300, Varian Inc., Palo Alto, USA; Radio frequency glow discharge orthogonal time View All

Source	Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet: Optimization of parameters for detection of carbon and sulfur in steel View All	A comparison of non-pulsed radiofrequency and pulsed radiofrequency glow discharge orthogonal time-of-flight mass spectrometry for analytical purposes View All
Method	Laser-induced breakdown spectroscopic analysis using nitrogen as ambient gas in double pulse mode View All	Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode <ol style="list-style-type: none">1. Collect the NIST 1262b certified reference steel. View All
Limit of Detection	2.9 ppm, Carbon, 1.5 ppm, Sulfur	0.3 µg/g, Boron, 0.2 µg/g, Magnesium, 0.3 µg/g, Aluminum, 1.9 µg/g, Silicon, 1.6 µg/g, Phosphorus, 1.0 µg/g, Sulfur , 2.3 µg/g, Titanium, 1.1 µg/g, Vanadium, 1.0 µg/g, Chromium, 5.5 View All
Precision		12% (RSD, reproducibility), Boron, 28% (RSD, reproducibility), Magnesium, 2% (RSD, reproducibility), Aluminum, 6% (RSD, reproducibility), Silicon, 5% (RSD, View All)
Sensitivity		6 - 165 cps/(µg/g)

Method	<p>Laser-induced breakdown spectroscopic analysis using nitrogen as ambient gas in double pulse mode</p> <ol style="list-style-type: none"> 1. Perform the analysis using LIBS setup containing the laser pulse generation system (two synchronized lasers), the optical system (lenses, mirrors, polarizer and half-wave plate), an ablation chamber, spectrometer, detection system (CCD camera and computer) and finally the gas environment controls (needle valve, gauge, pressure meters). 2. Use the Q-switched Nd:YAG lasers to create the plasmas in double-pulse mode by Continuum Surelite (model III-10), operating at the fundamental wavelength of 1.06 µm with a pulse width of 6 ± 1 ns and maximum output energy of 800 mJ. 3. Operate the laser at a repetition rate of 10 Hz. 4. Insert the optical combination of a half-wave plate and a polarizer into the Surelite laser beam to vary the pulse energy incident on the sample. 5. Focus the approximately 10-mm-diameter beams produced by Surelite laser onto the steel samples by plano-convex lenses of 125 mm and 150 mm focal 	<p>Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode</p> <ol style="list-style-type: none"> 1. Collect the NIST 1262b certified reference steel. 2. Determine the performance of the pulsed RFGD-TOFMS. 3. The radiofrequency glow discharge orthogonal time-of-flight mass spectrometer (RFGD-TOFMS) includes a RFGD bay unit (RF generator, matching box, RF connector, refrigerator disc and sample mounting system with a pneumatic piston to press the sample against the source) (GD Profiler HR instrument (Horiba Jobin Yvon, Longjumeau, France)). 4. Use the GD source of a copper-based modified Grimm-type chamber with a 4 mm diameter anode and a 2.5 mm inner diameter flow tube (EMPA, Switzerland). 5. Extract the ions originating from the source at pressure of 800 Pa through a sampler of 500 µm diameter and a 1 mm diameter skimmer. 6. The following interface region includes electrostatic focusing and deflecting components and couples the
--------	---	---

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>) 输入检索式

Searching for...

Formulations 原料、用途、物理形态、功能或文献识别符

Search for Formulations by Ingredient, Purpose, Form, Function, etc.

orthopedic and implant

Try Advanced Search for a more precise search experience

高级检索

Design custom formulations templates based on selections and ingredients.

- 制药、化妆品、食品、农化、油墨、涂料等多领域中的配方
- 工艺、成分、目标成分的常见配伍成分、设计配方、探索合规要求等

配方/制剂结果集

- 利用聚类项精简结果：
行业、配方/制剂用途、物理形式、物质状态、递送方式、涵盖信息、文献类型、发表机构、发表年份
- 可查看制剂或配方成分，功能及用量
- 可查看原料详情
- 支持对比选中的制剂或配方
- 支持查看或下载专利全文
- 可查看制剂或配方详情

Formulations search for "orthopedic and implant"

Get Additional References

1,064 Results

Sort: Relevance

Filter by

- Industry
 - Pharmaceutical
- Purpose
 - Antitumor agents (107)
- Physical Form
 - Pharmaceutical implants (1,064)
- Information Included
 - Process (1,064)

Implants: Antitumor Agents

Location: Article page 3, 6, 7, 8, 9

Purpose: Antitumor agents

Physical Form: implant

Component	Function	Amount Reported
Group: Ti-TNTs wire implants	implant	-
Ti wires	additives	-
Acetone	Solvents	-
Ethanol	Solvents	-
Perchloric acid	additives	1

Additional group components reported

Trail aqueous solution	-	2 mg/mL
------------------------	---	---------

View Formulation Detail

2

Composition for Promoting Bone Formation

Location: Claim 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41

Purpose: promoting bone formation

Target: Amphibia, Ape, Aves, Bos taurus, Canis familiaris, Capra, Cavia porcellus, Equus caballus, Felis catus, Fish, Gerbil, Hamster, Homo sapiens, Monkey, Mus musculus, Oryctolagus cuniculus, Ovis aries, Rattus, Reptilia, Swine

Delivery Route: Intraosseous prosthetic implants, Intramedullary application

Physical Form: pharmaceutical implants

Add to Compare

Component	Function	Amount Reported
Group: surgical implant	-	-
Dental implants	-	-

PATENT

Use of pro-inflammatory compounds for promoting bone formation

Assignee: Imperial Innovations Limited

- 一次最多可以比较三种不同制剂或配方的信息详情

配方/制剂的制备? 实验评估?

Implants: Antitumor Agents

↓ Save

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents	-	-	implant	View

Formulation Ingredients Expand All Groups | Collapse All Groups

Component	Function	Amount Reported	Optionality
Group: Ti-TNTs wire implants	implant	-	Mandatory
Ti wires	additives	-	Mandatory
Acetone	Solvents	-	Mandatory
Ethanol	Solvents	-	Mandatory
Perchloric acid	additives	1	Mandatory
butanol	Solvents	6	Mandatory
ethylene glycol electrolyte	solid support material	9	Mandatory
Water	Solvents	-	Mandatory
Trail aqueous solution	-	2 mg/mL	Mandatory

More Formulations like this... NEW

Ha-NP with HASE: Antitumor Agents
Purpose: Antitumor agents
Target: -
Delivery Route: -
Physical Form: Particles

CIPRODEX: Antibacterial
Purpose: Antibacterial agents
Target: Haemophilus influenzae, Hom...
Delivery Route: AURICULAR (otic)
Physical Form: Liquids, Suspensions

CIPRODEX Ciprofloxacin and Dexamethasone Suspension/Drops: Antibacterial Agents or...
Purpose: Antibacterial agents, corticos...
Target: Haemophilus influenzae, Hom...
Delivery Route: AURICULAR (optic).
Physical Form: Liquids, Suspensions

Ha-NP-Loaded Microneedle Patch: Antitumor Agents
Purpose: Antitumor agents
Target: Neoplasms
Delivery Route: skin absorption
Physical Form: Pharmaceutical patches

Process

stage 1: Ti-TNTs wire implants were loaded overnight with 2 mg/mL Trail aqueous solution for in-vitro, ex-vivo and in-vivo studies. prior to loading, implants were cleaned with ethanol, dried under sterile conditions and placed in a 30 mL drops of Trail solutions placed on a parafilm strip. after overnight drug loading, implants were dabbed with a soft tissue and dried and placed in PBS solution to monitor drug release profile at 37 °C, over a range of selected time points.

- 制剂或配方原料
- 相似的制剂或配方
- 制备工艺
- 制剂或配方实验评估
- 专利来源

Experimental Activity

Descriptor	Notes	Details
Ex-vivo study	-	no caspase-3 activity was observed for PBS-TNTs samples
cell death	-	highest cell death was observed in Trail-TNTs
drug release	-	45 %
in-vitro cytotoxicity	-	luciferase activity confirmed 100% cell death in Trail-TNTs
loading amount	-	12.63 µg

Source Journal

Titanium wire implants with nanotube arrays: A study model for localized cancer treatment

Biomaterials
Language: English
Location: Article page 3, 6, 7, 8, 9

Full Text View in CAS SciFinder

高级检索

[← Return to Home](#)

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

Function **Optional** Anticorrosion
Ex: binder, surfactant, carrier

Search For **Operator** Enter one term

All Fields **Optional** coating
General search of all fields

[Add Another Term](#)

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

- All Fields
- All Fields
- Form
- Function
- Ingredient
- Purpose
- Route
- Target

检索原料

Searching for...

Formulations

Ingredients

Ingredients

Search by Ingredient Name, CAS Registry Number, or Function

propylene glycol

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

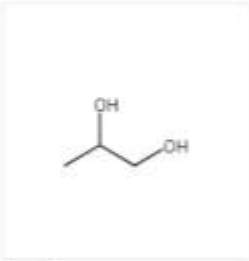
- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至设计工具
Formulation Designer

Ingredients search for "propylene glycol"

2 Selected 3 Results

1

CAS RN: 57-55-6
[View Details](#)



C3H8O2

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; Carriers; Plasticizers; Humectants; Antifreeze...

Similar Ingredients with Regulatory Information

- 27194-74-7 Propylene glycol monoaurate
- 29387-86-8 Propylene glycol butyl ether
- 30136-13-1 Propylene glycol monopropyl ether

[View 14 More](#)

Commonly Formulated With | Regulatory Information | Experimental Properties

Formulations Suppliers Add to Designer

设计配方/制剂

Formulation Designer ? Clear All Selections

Industry

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

Purpose

- Coating materials**
- Adhesives
- Jet-printing inks
- Water-thinned coating materials
- Antifouling coating materials
- Printing inks
- Paints
- Powder coating materials
- Anticorrosive coating materials
- Inks
- View More Purposes -

Physical Form

- Solutions
- Powders
- Paints
- Liquids**
- Films
- Tablets
- Emulsions
- Coating materials
- Disperse systems
- Resins
- View More Physical Forms -

Add up to 5 Ingredients

- Water
- Ethanol
- + Add Another Ingredient

Create Template

Formulation Designer

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 solutions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 "encapsulat* and resistant starch"

Substances - Reactions - Citing - Knowledge Graph

857 Results Sort: Relevance - View: Partial Abstract -

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

Filter Behavior
Filter by Exclude

- Document Type
- Substance Role
- Language
- Publication Year
- Available at My Institution
- Author
- Organ
- Public

1
Resistant starch from high-amylose maize increases insulin sensitivity in overweight and obese men
By: Maki, Kevin C.; Pelkman, Christine L.; Finocchiaro, E. Terry; Kelley, Kathleen M.; Lawless, Andrea L.; Schild, Arianne L.; Ra
Journal of Nutrition (2012), 142(4), 717-723 | Language: English, Database: CAlplus and MEDLINE

This study evaluated the effects of 2 levels of intake of high-amylose maize type 2 **resistant starch** (HAM-RS2) on insulin s (S) in participants with waist circumference ≥ 89 (women) or ≥ 102 cm (men). Participants received 0 (control starch), 15, or 3 (double-blind) of HAM-RS2 in random order for 4-wk periods separated by 3-wk washouts. Minimal model S₁ was assessed end of each period using the insulin-modified i.v. glucose tolerance test. The efficacy evaluable sample included 11 men and women (mean \pm SEM) age 49.5 \pm 1.6 y, with a BMI of 30.6 \pm 0.5 kg/m² and waist circ...

View More

Full Text - Substances (9) Reactions (0) Citing (131) Citat

2
Conserved and variable responses of the gut microbiome to resistant starch type 2
By: Bendiks, Zachary A.; Knudsen, Knud E. B.; Keenan, Michael J.; Marco, Maria L.
Microbiome (New York, NY: United States) (2020), 77, 12-28 | Language: English, Database: CAlplus and MEDLINE

2), a dietary fiber comprised solely of glucose, has been extensively studied in clin. tri...
...ove metabolic and systemic health. Because the health modulatory effects of RS2 and...
...ough modification of the gut microbiome, those studies frequently include assessme...
...icrobial composition and function. In this review, we identify the conserved respo...

CAS Solutions

- Formulus (37)
- Analytical Methods (4)

定位配方或制剂的功能目标

Formulation Purpose

By Count Alphanumeric

4 Selected

- Food (7)
- Antidiabetic agents (6)
- Dietary supplements (5)
- Diet (3)
- Drug delivery systems (3)
- Antimicrobial agents (2)
- Antibacterial agents (1)
- Antihypertensives (1)
- Antioxidants (1)
- Antitumor agents (1)
- Bakery products (1)
- Beverages (1)

Apply Cancel

文献关联的配方/制剂

- ✓ Concepts
- ✓ MEDLINE® Medical Subject Headings

Substances

Formulations

Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

[View CAS Formulus® Detail](#)

Location: SI Page 3 Article Page 2 Figure 15

Purpose: Drug delivery systems

Target: 5-aminosalicylic acid

Component 成分	Function 功能	Amount Reported 用量
<ul style="list-style-type: none"> ^ Group: bioactive component-loaded microparticle core 	model active agent	-
5-Aminosalicylic acid	-	20 %
Cellulose	additives	Ratio: 3
Starch	excipients	Ratio: 1
<ul style="list-style-type: none"> ✓ Group: RS3-based aqueous coating dispersion 	coating materials	-

Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

[View CAS Formulus® Detail](#)

Location: SI Page 3 Article Page 2 Figure 15

Purpose: Drug delivery systems

Target: 5-aminosalicylic acid

Resistant Starch Film-Coated Microparticles for an Oral Colon-Specific Polypeptide Delivery System and Its Release Behaviors

Substances (3) Reactions (0) Citing (42) Citation Map

JOURNAL

Source

Journal of Agricultural and Food Chemistry
Volume: 62
Issue: 16
Pages: 3599-3609
Journal: Evaluation Study; Article; Research Support, Non-U.S. Gov't
2014
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CAlplus and MEDLINE

Company/Organization

Ministry of Education Engineering Research Centre of Starch and Protein Processing, Guangdong Province Key Laboratory for Green Processing of Natural Products and Product Safety
South China University of Technology
Guangzhou 510640
China

Publisher

American Chemical Society

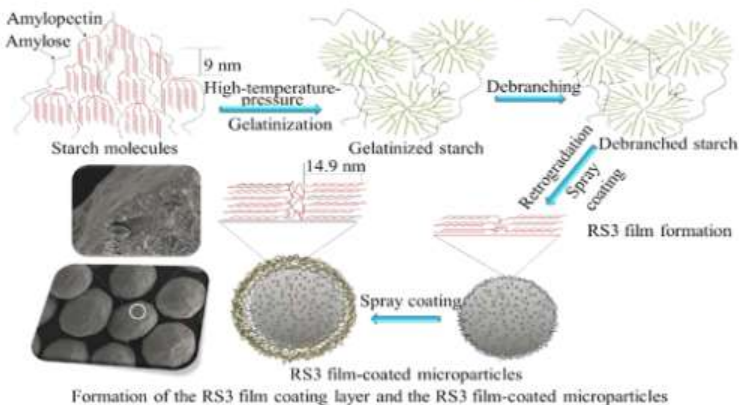
Language

English

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

By: Situ, Wenbei; Chen, Ling; Wang, Xueyu; Li, Xiaoxi

For the delivery of bioactive components to the colon, an oral colon-specific controlled release system coated with a resistant starch-based film through aqueous dispersion coating process was developed. Starch was modified by a high-temperature-pressure reaction, enzymic debranching, and retrogradation, resulting in a dramatic increase in the resistibility against enzymic digestion (meaning the formation of resistant starch, specifically RS3). This increase could be associated with an increase in the relative crystallinity, a greater amount of starch mol. aggregation structure, and the formation of a compact mass fractal structure, resulting from the treatment. The microparticles coated with this RS3 film showed an excellent controlled release property. In streptozotocin (STZ)-induced type II diabetic rats, the RS3 film-coated insulin-loaded microparticles exhibited the ability to steadily decrease the plasma glucose level initially and then maintain the plasma glucose level within the normal range for total 14-22 h with different insulin dosages after oral administration; no hypoglycemia or glycemic fluctuation was observed. Therefore, the potential of this new RS3 film-coated microparticle system has been demonstrated for the accurate delivery of bioactive polypeptides or protein to the colon.



Keywords: starch film coated microparticle colon polypeptide delivery insulin

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Concepts

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 SciFinderⁿ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

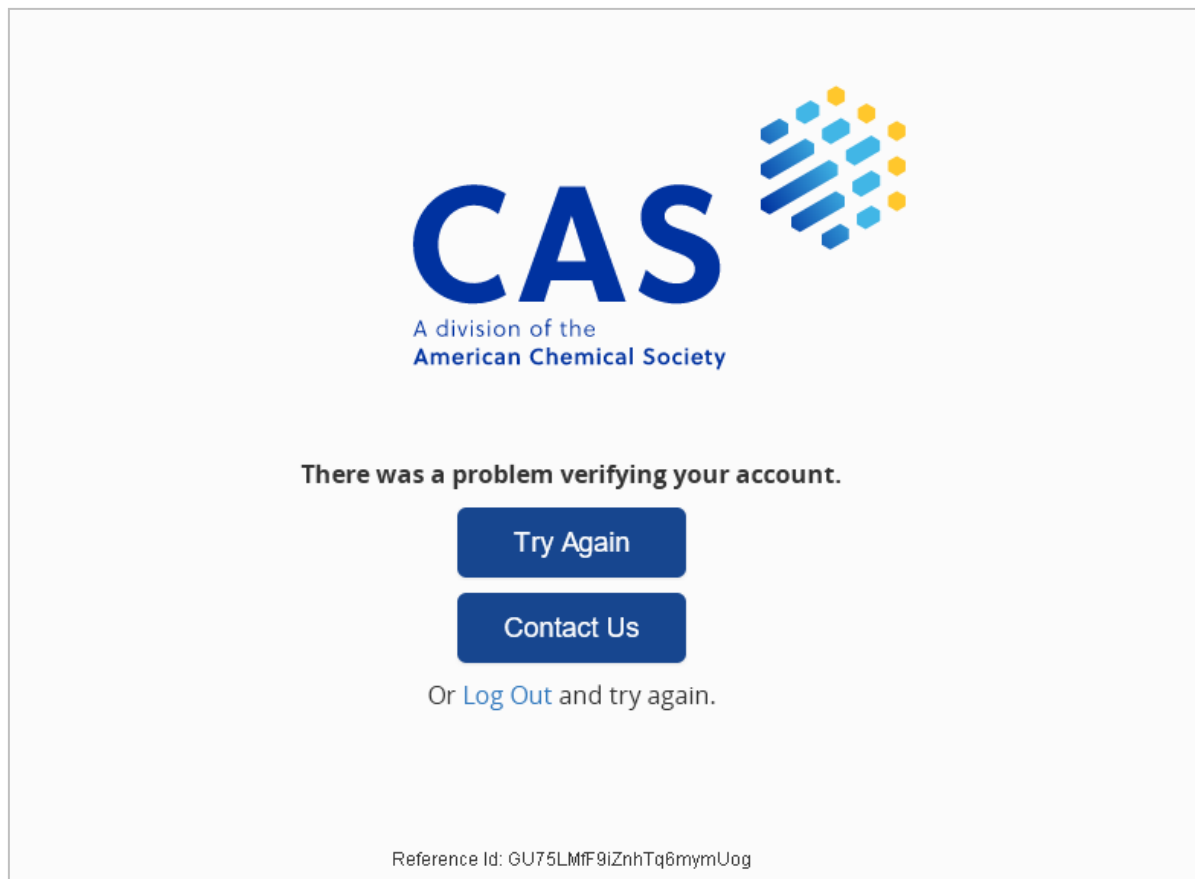
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- 检查注册链接是否正确
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线上学习资源



CAS SciFinderⁿ
学习中心



2023 CAS SciFinder Discovery Platform 专题论坛

日期	主题
3月1日	解锁CAS SciFinder Discovery Platform新功能
3月8日	巧用CAS SciFinder Discovery Platform文献检索快速进阶
3月15日	万物互联 CAS SciFinder Discovery Platform物质检索更高效
3月22日	CAS SciFinder Discovery Platform反应检索, 不止A to B
4月4日	不止化学: CAS SciFinder Discovery Platform序列检索技巧
4月12日	新手入门开题和文献综述? 巧用CAS SciFinder Discovery Platform事半功倍
4月19日	实验进展太慢? 巧用CAS SciFinder Discovery Platform寻找启发
5月10日	毕业季 CAS SciFinder Discovery Platform助力论文写作及答辩准备
5月24日	毕业季 巧用CAS SciFinder Discovery Platform 做足升学与择业准备
9月15日	专利专题论坛
9月22日	生物制药专题论坛
10月13日	高分子材料专题论坛
10月27日	金属有机与无机化学专题论坛
11月10日	食品与个人护理品专题论坛

论坛录制
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Unit 1010, Tower B, Raycom InfoTech Park
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+86-10-6250 8026/7
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