

# CAS SciFinder Discovery Platform

## 全面高效获取科研信息



刘子露 博士

Zilu@acs-i.org

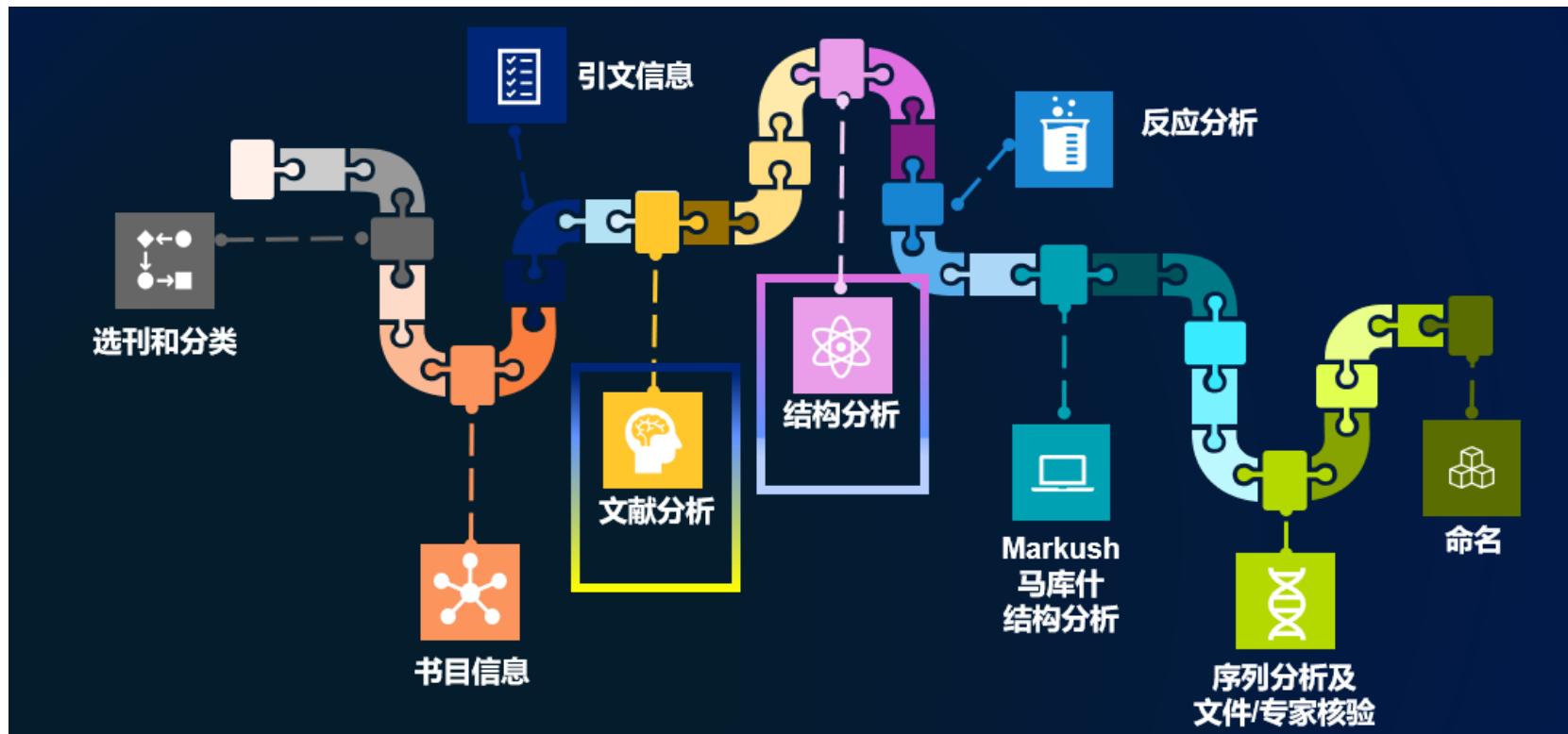
美国化学文摘社(CAS)北京代表处

# 大纲

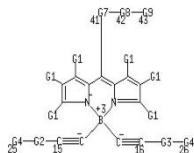
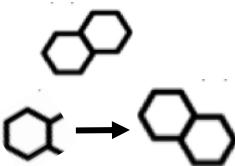
- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 如何拓展文献调研?
  - 如何调研某类物质?
  - 如何调研反应信息?
  - 怎么查、怎么选具体的实验方案?
- 常见问题Q&A



# CAS 科学家的智力标引



1990  
Smith, M.  
anthracene



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

# CAS科学家增值的文献研究

J. Med. Chem. 2012, 55, 5, 1868–1897

<https://doi.org/10.1021/jm201331s>

Journal of  
Medicinal  
Chemistry

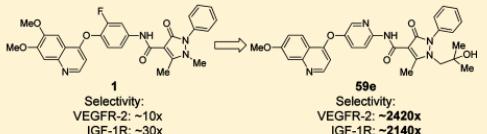
## Structure-Based Design of Novel Class II c-Met Inhibitors: 2. SAR and Kinase Selectivity Profiles of the Pyrazolone Series

Longbin Liu,<sup>\*†</sup> Mark H. Norman,<sup>†</sup> Matthew Lee,<sup>§</sup> Ning Xi,<sup>†</sup> Aaron Siegmund,<sup>†</sup> Alessandro A. Boezio,<sup>||</sup> Shon Booker,<sup>†</sup> Debbie Choquette,<sup>||</sup> Noel D. D'Angelo,<sup>†</sup> Julie Germain,<sup>†</sup> Kevin Yang,<sup>†</sup> Yajing Yang,<sup>†</sup> Yihong Zhang,<sup>†</sup> Steven F. Bellon,<sup>†</sup> Douglas A. Whittington,<sup>†</sup> Jean-Christophe Harmange,<sup>†</sup> Celia Dominguez,<sup>†</sup> Tae-Seong Kim,<sup>†</sup> and Isabelle Dussault<sup>†</sup>

<sup>†</sup>Departments of Medicinal Chemistry, <sup>§</sup>Oncology Research, and <sup>||</sup>Molecular Structure, Amgen Inc., One Amgen Center Drive, Thousand Oaks, California 91320, United States

<sup>†</sup>Departments of Medicinal Chemistry and <sup>||</sup>Molecular Structure, Amgen Inc., 360 Binney Street, Cambridge, Massachusetts 02142, United States

Supporting Information



**ABSTRACT:** As part of our effort toward developing an effective therapeutic agent for c-Met-dependent tumors, a pyrazolone-based class II c-Met inhibitor, *N*-(4-((6,7-dimethoxyquinolin-4-yl)oxy)-3-fluorophenyl)-1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazole-4-carboxamide (1), was identified. Knowledge of the binding mode of this molecule in both c-Met and VEGFR-2 proteins led to a novel strategy for designing more selective analogues of 1. Along with detailed SAR information, we demonstrate that the low kinase selectivity associated with class II c-Met inhibitors can be improved significantly. This work resulted in the discovery of potent c-Met inhibitors with improved selectivity profiles over VEGFR-2 and IGF-1R that could serve as useful tools to probe the relationship between kinase selectivity and *in vivo* efficacy in tumor xenograft models. Compound 59e (AMG 458) was ultimately advanced into preclinical safety studies.

## INTRODUCTION

The receptor tyrosine kinase (RTK) c-Met is mainly expressed by epithelial cells. Activation of c-Met is regulated by its ligand, hepatocyte growth factor (HGF), also known as scatter factor (SF). Upon binding of HGF at the extracellular domain, c-Met receptor undergoes dimerization that results in transphosphorylation of the intracellular tyrosine residues (Y1234, Y1235) within the catalytic site.<sup>2</sup> Further phosphorylation of residues Y1349 and Y1356 mobilizes the intracellular C-terminal docking domain that recruits and subsequently activates a wide range of downstream signaling molecules (e.g., Grb2, Gab1, PI3K, Akt, Ras, Erk, and STAT3) that modulate the survival, proliferation, migration, and invasion of cells. As such, normal HGF/c-Met signaling plays an important role during embryogenesis and tissue injury repair.<sup>3</sup> On the other hand, dysregulation of this pathway (through, e.g., either over-expression of HGF/c-Met or activating mutation of MET gene) can render many cellular processes unchecked and promote tumorigenesis. It has been established that aberrant signaling of the HGF/c-Met pathway correlates with aggressive tumor growth and poor prognosis in cancer patients.<sup>4</sup> Different

approaches to inhibition of the HGF/c-Met pathway in cancer cells have been documented.<sup>5</sup> These include antagonistic ligands to c-Met, antibodies against either HGF or c-Met, and small molecule kinase inhibitors targeting the intracellular kinase domain. Numerous c-Met kinase inhibitors have been reported in the literature.<sup>6</sup> These inhibitors can be categorized into either class I or class II based on their binding mode in the c-Met kinase domain (vide infra). While class I molecules tend to be very selective for c-Met, thus far, a majority of the class II molecules are multitarget inhibitors. Improving the selectivity of class II c-Met inhibitors has been a significant challenge. In fact, until recently, no selective class II c-Met inhibitors have been reported and little is known as to whether the kinase selectivity profiles of class II c-Met inhibitors can be improved. Schroeder et al. reported the design of a pyridone-based c-Met inhibitor that was selective over a number of kinases, including IGF-1R.<sup>7</sup> The selectivity over VEGFR-2 was modest (46-fold). We postulated that knowledge from kinase structural analysis

Received: October 6, 2011  
Published: February 9, 2012

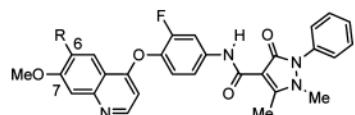
ACS Publications

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Journal of Medicinal Chemistry

Article

Table 1. Modification of the Quinoline Ring<sup>a</sup>



compd	R	c-Met		VEGFR-2		IGF-1R		PC3
		<i>K</i> <sub>i</sub>	fold	<i>K</i> <sub>i</sub>	fold	<i>K</i> <sub>i</sub>	fold	
1	OMe	1		7.8	8	32.1	32	20.2
11a	Br	5.1		78.9	16	149	29	652
11b	Me	3.4		—	—	146	43	461
11c	Et	2.4		38	16	70.2	29	534
11d	H	1.1		23.7	22	178	162	37.1

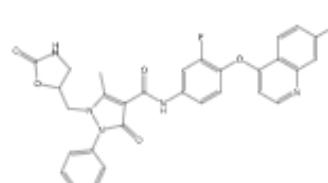
<sup>a</sup>*K*<sub>i</sub> (nM): inhibitory constant for the phosphorylation of gastrin by c-Met, VEGFR-2, or IGF-1R. Fold: ratio of *K*<sub>i</sub>(kinase)/*K*<sub>i</sub>(c-Met). PC3 IC<sub>50</sub> (nM): inhibitory concentration for HGF-mediated c-Met phosphorylation in PC3 cells. Both *K*<sub>i</sub> and IC<sub>50</sub> values are reported as an average for *n* > 2. See Supporting Information for standard deviations.

Journal of Medicinal Chemistry

Table 3. Effects of C5-Substituents on Selectivity Profiles<sup>a</sup>

compd	R	X	Y	c-Met		VEGFR-2		IGF-1R		PC3
				<i>K</i> <sub>i</sub>	<i>K</i> <sub>i</sub>	Fold	<i>K</i> <sub>i</sub>	Fold	<i>K</i> <sub>i</sub>	
11d	CH <sub>3</sub> <sup>-</sup>	CF	CH	1.1	23.7	22	178	162	37.1	
22a	CH <sub>3</sub> <sup>-</sup>	CH	N	1.2	42	35	618	515	83	
26b	NH <sub>2</sub> CH <sub>2</sub> <sup>-</sup>	CF	CH	1.4	541	378	928	649	42	
26a	BocNHCH <sub>2</sub> <sup>-</sup>	CF	CH	29	1240	43	>6600	>230	—	
26c	Et(Me)NCH <sub>2</sub> <sup>-</sup>	CF	CH	2.3	903	386	744	317	76.7	
26d		CF	CH	1.5	1310	879	1800	1206	83.9	

1361236-60-3

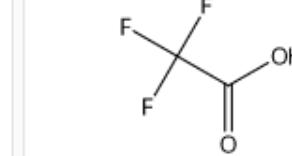
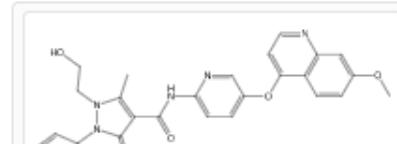


C<sub>31</sub>H<sub>26</sub>FN<sub>5</sub>O<sub>6</sub>

*N*-(3-Fluoro-4-[(7-methoxy-4-quinolinyl)oxy]phenyl)-2,3-dihydro-5-methyl-3-oxo-1...

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Reactant or Reagent, Preparation, Uses

1374343-52-8



Role: Pharmacological Activity, Reactant, Synthetic Preparation, Therapeutic Use, Biological Study, Reactant or Reagent, Preparation, Uses

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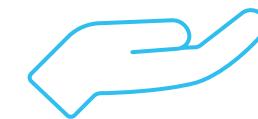


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# CAS SciFinder Discovery Platform (Academic)平台解决方案

## CAS SciFinder —— 加速科学发现的业界领先的科学工具

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

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

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

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

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**CAS SciFinder Discovery Platform (Academic) (化学文摘)**

发布时间: 2018-03-03 浏览次数: 128927 文章来源: 齐鲁工业大学图书馆

**CAS SciFinder Discovery Platform (Academic)账号注册须知:**

个人账号申请方式采用机构邮箱注册的方式使用。

读者在使用CAS SciFinder Discovery Platform (Academic)各解决方案之前须用机构域名邮箱地址注册账号，在我校有效ip范围内，点击下列网址注册：

[https://scifinder.cas.org/registration/index.html?  
corpKey=B9FBBDF6X86F35040X545FC0711B6A0B1C87](https://scifinder.cas.org/registration/index.html?corpKey=B9FBBDF6X86F35040X545FC0711B6A0B1C87)

进入注册链接后，“At which site are you located?” 齐鲁工业大学的师生选择“Qilu Univ of Technology (Jinan, )”，请用后缀为`xx@qlu.edu.cn`或者`xx@stu.qlu.edu.cn`注册帐号；山东省科学院师生选择“Shandong Academy of Sciences (Jinan, )” 请用邮箱`xx@sdas.org`

注册帐号。根据提示输入相应信息，提交注册申请后系统将自动发送一个链接到您所填写的邮箱中，进入邮箱激活此链接即可完成注册。注册参考《CAS SciFinder Discovery Platform (Academic) 用户注册指南》。

需在校园IP范围内，保持邮箱、注册链接二者的一致性才可以注册成功

注册指南: [CAS SciFinder Discovery Platform \(Academic\) 用户注册指南2023.pdf](#)

# 如何获取CAS SciFinder账号

--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:

Tips

--SECURITY INFORMATION--

Security Question:

Answer:

Why?

## Registration Already Complete

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

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 @、#、%、&、\*)

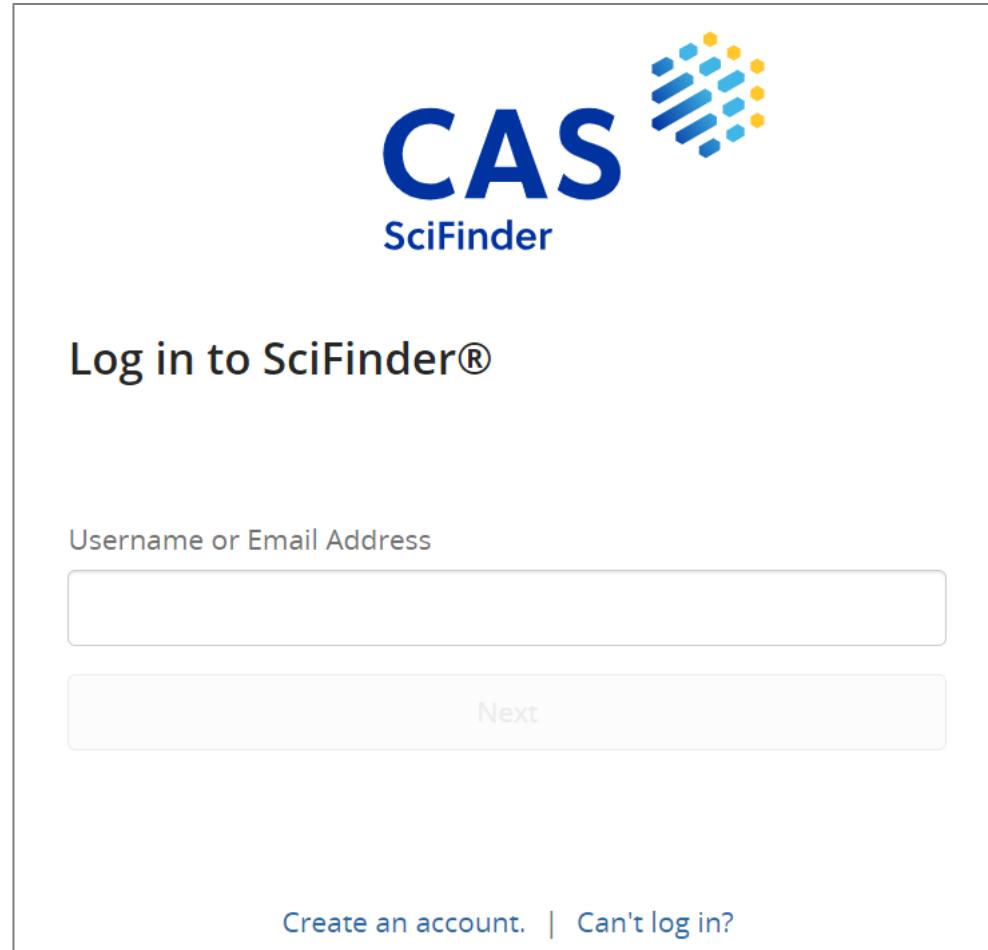
例：abc@123

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)。

点击激活链接后注册成功

通过<https://SciFinder-n.cas.org>访问

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



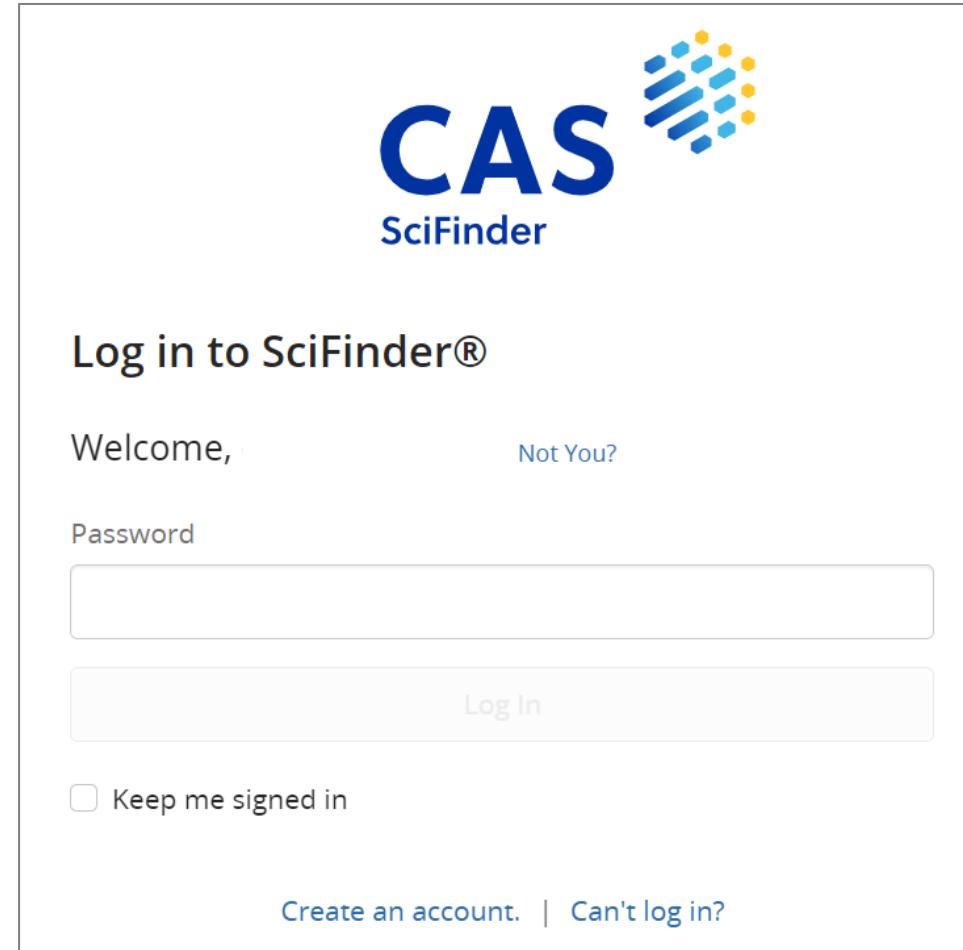
The image shows the initial step of a two-step login process for CAS SciFinder. It features the CAS SciFinder logo at the top. Below it, the text "Log in to SciFinder®" is displayed. A large input field is labeled "Username or Email Address". Below this field is a "Next" button. At the bottom of the page are links for "Create an account." and "Can't log in?".

Log in to SciFinder®

Username or Email Address

Next

Create an account. | Can't log in?



The image shows the second step of the two-step login process for CAS SciFinder. It features the CAS SciFinder logo at the top. Below it, the text "Log in to SciFinder®" is displayed. To the left is the text "Welcome," and to the right is a "Not You?" link. Below these are "Password" and "Log In" fields. A "Keep me signed in" checkbox is located between the fields. At the bottom of the page are links for "Create an account." and "Can't log in?".

Log in to SciFinder®

Welcome, 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 main interface of the CAS SciFinder application. On the left, a sidebar lists various services under 'LIFE SCIENCES' and 'REGULATORY'. The main area features a 'Featured Search' section with several options: 'Prior Art Discovery', 'Patent Markush', 'Advanced Search', 'Retrosynthetic Analysis', 'Search CAS Lexicon', 'Search CAS Sequences', and 'CAS Profile'. The 'Search CAS Sequences' and 'Search CAS Lexicon' sections are highlighted with blue boxes. Below this is a 'Recent Search History' section for 'September 9, 2025', showing a search for 'reduction of aldehyde catalysed by cobalt'.

更新结果提醒

检索结果管理和账号设置

结构绘制面板

Draw

现有技术探索

专利Markush检索

高级检索选项

逆合成路线设计

CAS词库

CAS序列检索

近期检索历史

View All Search History

Rerun Search

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 如何拓展文献调研?
  - 如何调研某类物质?
  - 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



# 如何拓展文献检索？

- 关注某篇文献的被引文献和引文——引文地图
- 主题词怎么选择？如何构建？
- 如何筛选文献？追踪最新进展？
- 研究某结构相关的文献？

# 已知文献标识符

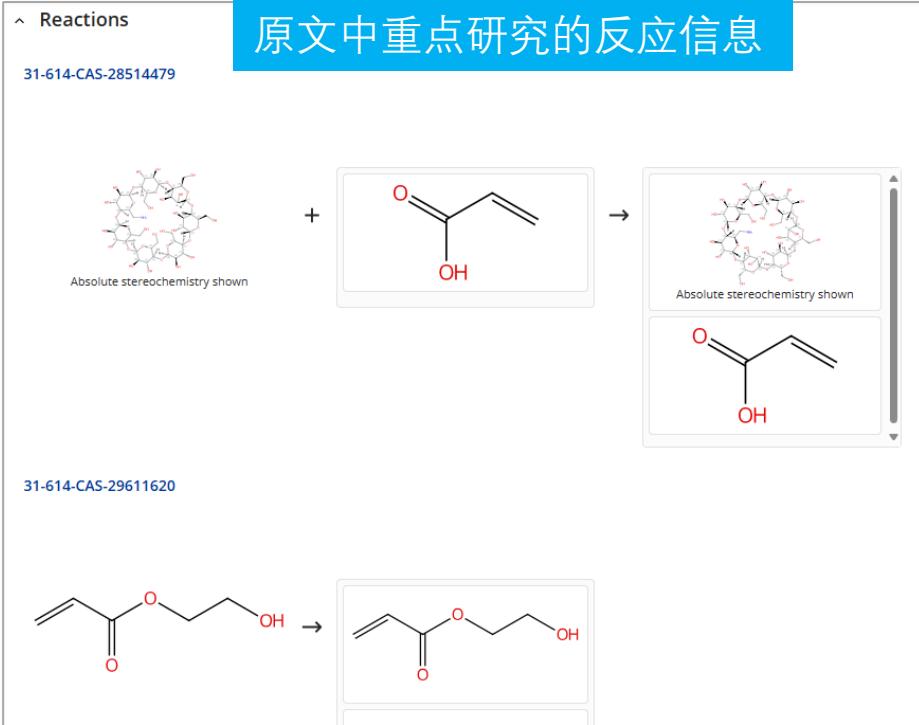
支持使用：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI

The screenshot shows the SciFinder interface with the following details:

- Header:** CAS SciFinder, References dropdown, search bar containing "Elasticity dependent fast underwater adhesion demonstrated by mac", and a notification icon showing 445.
- Left Sidebar (Filter Results):**
  - Behavior:** Filter by (selected), Exclude.
  - Search Within Results:** Search bar and dropdown.
  - Concept:** Search bar and dropdown.
  - CA Section:** Search bar and dropdown.
  - Publication Year:** Search bar and dropdown.
  - Language:** Search bar and dropdown.
- Search Results:**
  - 1 Result found.
  - Title:** Elasticity-Dependent Fast Underwater Adhesion Demonstrated by Macroscopic Supramolecular Assembly
  - Authors:** By: Ju, Guannan; Cheng, Mengjiao; Guo, Fengli; Zhang, Qian; Shi, Feng
  - Journal:** Angewandte Chemie, International Edition (2018), 57(29), 8963-8967
  - Language:** English, Database: CPlus and MEDLINE
  - Abstract:** Macroscopic supramol. assembly (MSA) is a recent development in supramol. chem. to associate visible building blocks through non-covalent interactions in a multivalent manner. Although various substrates (e.g. hydrogels, rigid materials) have been used, a general design rule of building blocks in MSA systems and interpretation of the assembly mechanism are lacking and are required. Herein we design three model systems with varied elastic modulus and correlated the MSA probability with the elasticity. Based on the effects of substrate deformability on multivalency, we have proposed an elastic-modulus-dependent rule that building blocks below a critical modulus of 2.5 MPa can achieve MSA for the used host/guest system. Moreover, this MSA rule applies well to the design of materials for fast underwater adhesion: soft substrates (0.5 MPa) can achieve underwater adhesion within 10 s with one order of magnitude higher strength than that of rigid substrates (2.5 MPa).
  - Buttons at the bottom:** Full Text, 14, 2, 82, and a magnifying glass icon.

# 文献详情

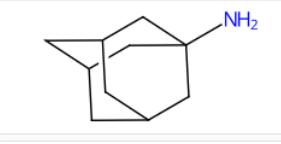
标题、摘要、重要的技术术语、引文地图、文献中重要的物质、反应、参考文献、原文链接



Substances

原文中重点研究的物质信息

1200829-09-9

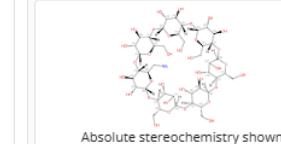


CC=CC(=O)O

C10H17N.C3H4O2  
2-Propenoic acid, compd. with tricyclo[3.3.1<sup>3,7</sup>]decan-1-amine (1:1)

Role: Properties

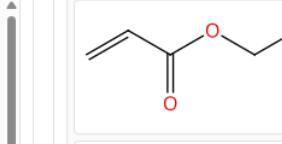
1122464-65-6



C42H71NO34.X(C3H4O2)x  
β-Cyclodextrin, 6<sup>A</sup>-amino-6<sup>A</sup>-deoxy-, com pd. with 2-propenoic acid homopolymer

Role: Reactant, Reactant or Reagent

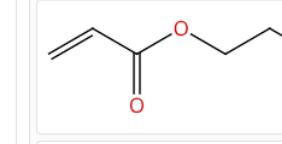
59765-68-3



C7H10N2O2.C5H8O3.C3H5NOx  
2-Propenoic acid, 2-hydroxyethyl ester, p olymer with *N,N*-methylenebis[2-propen a...]

Role: Properties, Synthetic Preparation, Preparation

57033-29-1



C7H10N2O2.C5H8O3.x  
2-Propenoic acid, 2-hydroxyethyl ester, p olymer with *N,N*-methylenebis[2-propen a...]

Role: Properties, Synthetic Preparation, Preparation

物质角色

View Experimental Protocols  
Steps: 1

1.1 Reagents: [Methylenebisacrylamide](#)  
Catalysts: [N,N,N',N'-Tetramethylethylenediamine](#), [Ammonium persulfate](#)  
Solvents: Water: 20 min. 60 °C  
[View All](#)

Concepts

CAS科学家提供的标准技术术语

Adhesion, physical  
Modifier: [underwater](#)

Hydrogels

Elasticity

Multilayers

Gelatins  
Modifier: copolymer with dimethylacrylamide

Polyelectrolytes

Stress-strain relationship

Young's modulus

# 专利文献详情

1

## Process for manufacturing high purity 2-chloro-1,1,1,2-tetrafluoro

Assignee: Honeywell International Inc.

United States, US10125066 B1 2018-11-13 | Language: English, Database: CAplus

Patent Status: Dead, Family Members: WO CN JP IN

A method for producing 2-chloro-1,1,1,2-tetrafluoro (HCFC-244bb) from a reactant 2-chloro-3,3,3-trifluoropropene (HCFO-1233xf) by selectively hydrogenating the HCFO-1233xf in the presence of hydrogen gas and a catalyst to generate a product composition including unreacted HCFO-1233xf, such as 2-chloro-1,1,1-trifluoropropene (HCFC-253db), which may be separated. HCFC-244bb may then be purified by subsequent acid neutralization and drying steps.

PatentPak Full Text 11 2 1

Patent	Language	Full Text
US10125066 B1	English	PatentPak PDF
WO2019108574 A1	English	PatentPak PDF
CN111479792 A	Chinese	PatentPak PDF
JP2021504365 T	Japanese	PatentPak PDF
IN2020504365 T		

2-chloro-1,1,1,2-tetrafluoro

Get Substance Details Get Bioactivity Data Get Reactions (1,467) Start Retrosynthetic Analysis Get References (3,783) Get Suppliers (23)

Get Structure Reset +

CAS PatentPak Key Substances in Patent

CAS RN 754-12-1

Analyst Markup Locations (1) Page 7

CAS RN 421-73-8

Analyst Markup Locations (1) Page 8

distillation ranged from 90-95%.

Example 4

Batch Acid Neutralization with 10 pH Solution of Soda Ash in Water, Followed by Drying

The acid neutralization step was conducted using a 10 gallon (3.9 L) vessel equipped with an agitator. All distilled HCFC-244bb, at 99.94% purity and <10 ppm acidity, was washed using a 10 pH solution of soda ash in water ( $\text{Na}_2\text{CO}_3/\text{H}_2\text{O}$ ). The wash procedure entailed charging 15 lb (6.8 kg) of the 10 pH soda ash solution into the 10 gallon (3.9 L) vessel, followed by 50 lb (22.7 kg) of HCFC-244bb. This addition sequence allows HCFC-244bb to sieve

55

13 US 10,125,066 B1 14

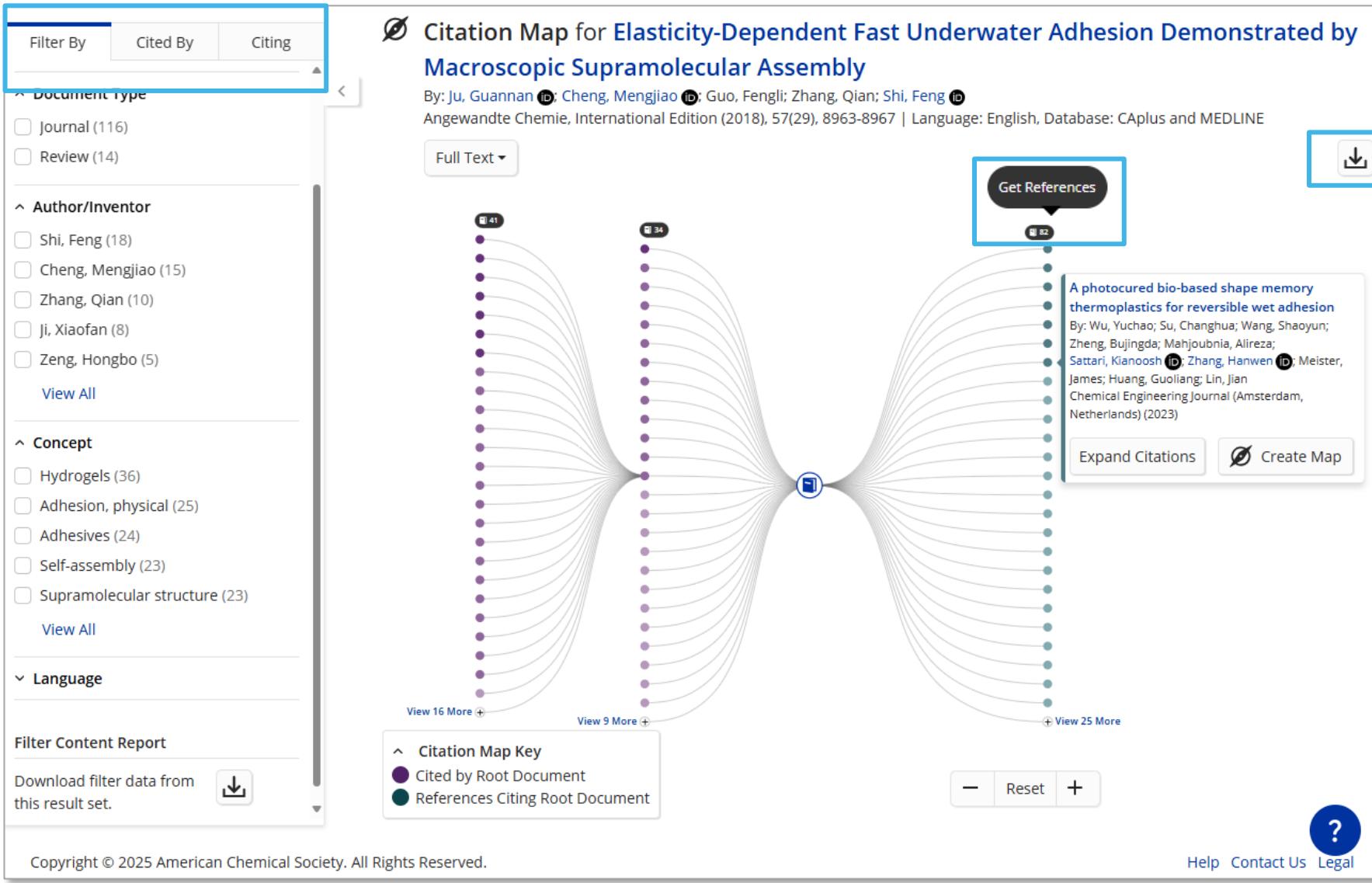
palladium catalyst diluted in an alpha aluminum support to a palladium loading between 0.3 wt. % and 0.5 wt. %, based on the total weight of the palladium catalyst and the alpha aluminum support, to generate a product composition including unreacted HCFC-244bb and 2-chloro-1,1,1-trifluoropropene (HCFC-253db).

11. The method of claim 10, further comprising the

CAS PatentPak®:

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- 一键下载原文
- 快速定位专利中的物质
- 阅读其他语言撰写的等同专利

# 1.1 引文地图: 便捷地获取关联文献



- Citing: 引用当前文献 (root document) 的文献
- Cited By: 当前文献 (root document) 所引用的参考文献
- 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

# 1.2 如何选择概念词？借助CAS Lexicon词库

- 在CAS词库层级中浏览CAS标引的概念词（Concepts）和物质
- 建立用于检索文献的检索式（最多可用1000个词）

Search CAS Lexicon

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

Preferred Concept

Neoplasm

This will search synonyms: Animal tumors; MeSH ID: D009370; Neoplasia; **Neoplasm** by histologic type; **Neoplasm** by site; Neoplastic disease; Neoplastic disorder; Neoplastic disorders; Oncological disease; Oncological diseases; Oncological disorder; Oncologic disorder; Organ, **neoplasm**; Organ tumors; Tumor cell; Tumor cells; Tumor disease; Tumors (animal); Tumour; Tumours

[View fewer synonyms](#)

Broader Concepts (1) [Select All](#)

Proliferative disorders

Narrower Concepts (76) [Select All](#)

Abdominal neoplasm

Acanthoma

Adenolymphoma

Ascitic neoplasm

Benign neoplasm

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

Personalized medicine - Preferred Concept

AND

Neoplasm - Preferred Concept

Remove All

一次检索Preferred Concept中所有同义词相关的文献

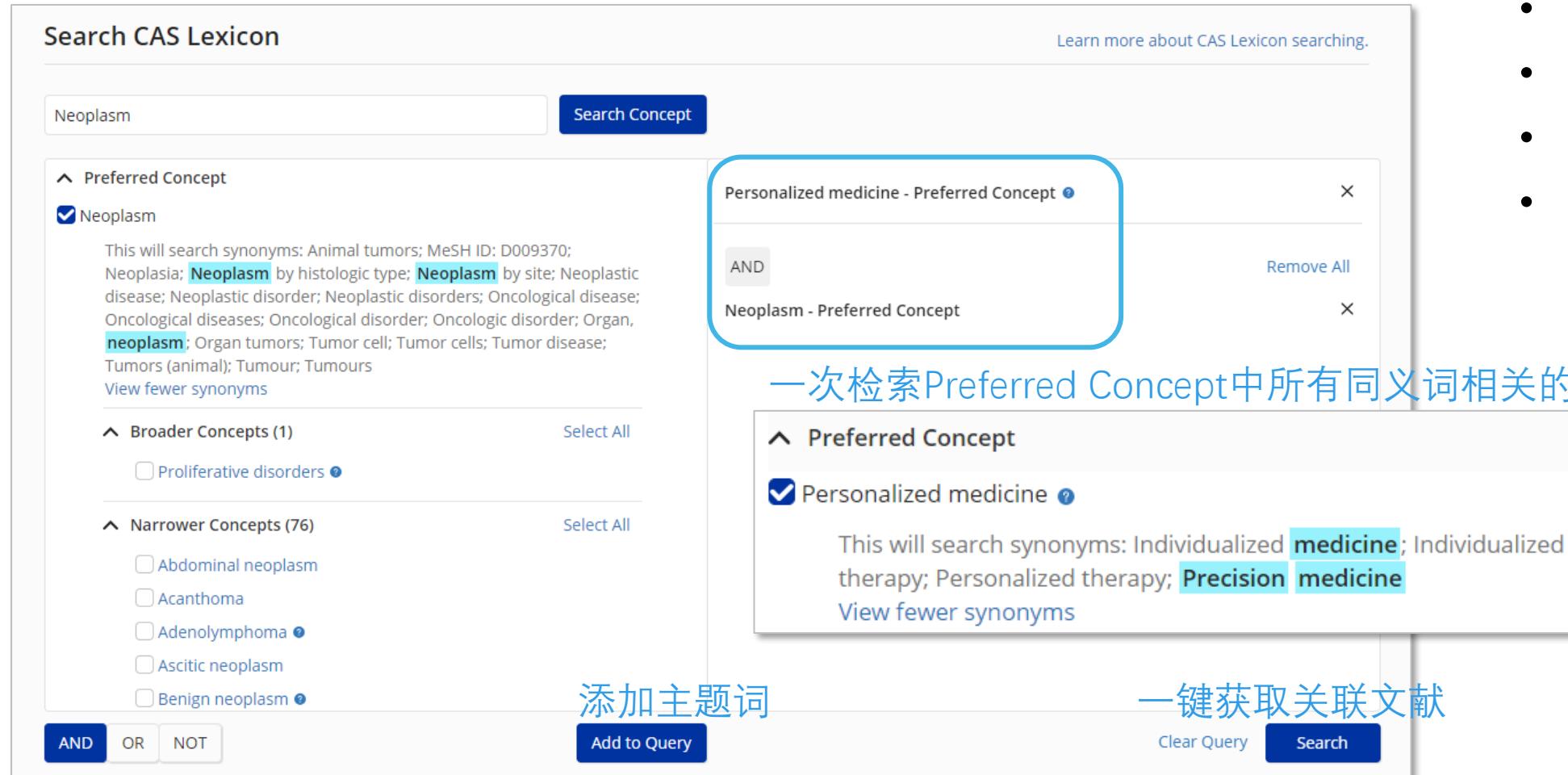
Preferred Concept

Personalized medicine

This will search synonyms: Individualized **medicine**; Individualized therapy; Personalized therapy; **Precision** **medicine**

[View fewer synonyms](#)

添加主题词 一键获取关联文献

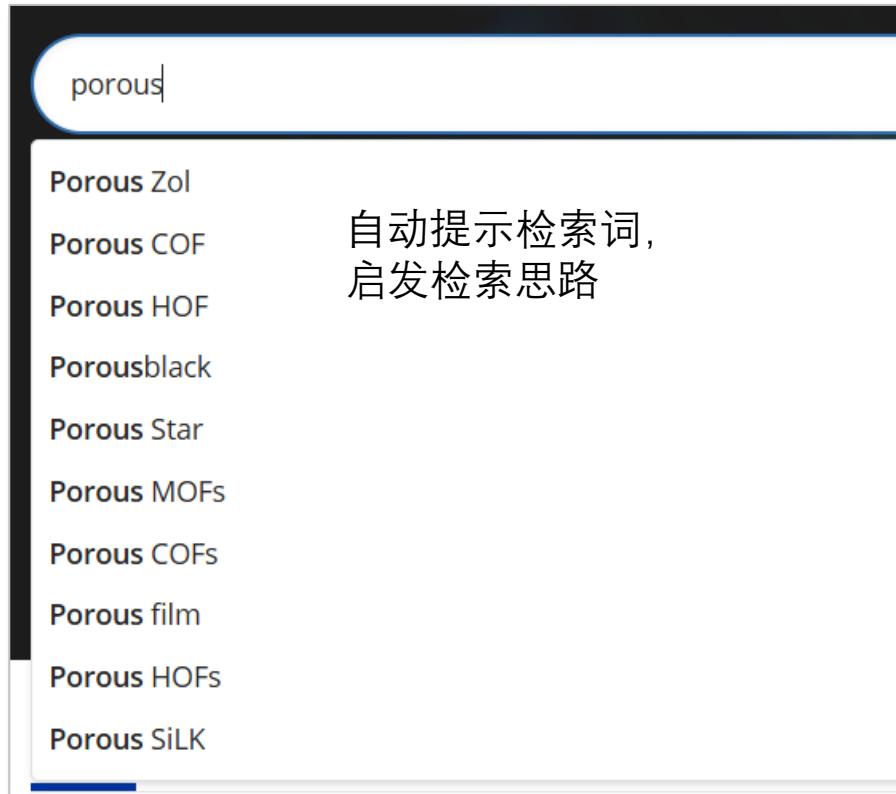
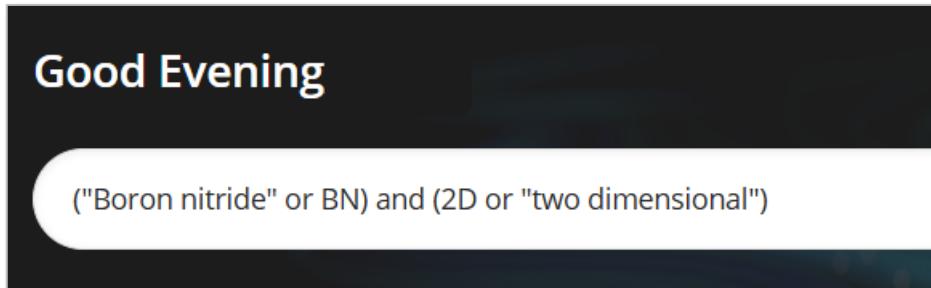


在CAS Lexicon词库层级中选择适合的主题词：

- Preferred Concept
- Broader Concepts
- Narrower Concepts
- Related Concepts

# 如何精准构建检索主题？

- 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? , 如 poly\*可代表polymer, polymerization, polyethylene等 (\*代表0或多个字符; ?代表0或1个字符)



AND  
OR  
NOT



# 精准构建检索主题

(“Metal Organic Frameworks” or MOFs) and photocataly\*  
检索： 金属有机框架和光催化

References search for ("Metal Organic Frameworks" or MOFs) and photocataly\*

[View Related Results](#)

12,503 Results

1

**A review of metal organic framework (MOFs)-b photocatalysis**

By: Du, Chunyan; Zhang, Zhuo; Yu, Guanlong; Wu, Haipeng; Ch Chemosphere (2021), 272, 129501 | Language: English, Databa

A review. Antibiotic abuse has led to serious water pollution and removal from water sources. Adsorption and photodegradation operate, and reusable. Metal organic frameworks (MOFs) are adaptable, and good crystal form. The aim of this study is to treatment methods by reviewing previous applications of MOFs; these processes are also discussed, as well as the various adsorbents for researchers intending to use MOFs to remove antibiotics from

[Load All Results](#)

**Filter Results**

[Analyze Results](#)

**Behavior**

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

[Search Within Results](#)

224 Results

1

**Regioselective and enantioselective**

By: Collman, James P.; Zhang, Xumu; Lee, V. Science (Washington, DC, United States) (1)

A review with 41 references Recent progress here, with an explanation of the biomimetic have been studied allows useful conclusions and practical catalysts have arisen from sys

[View Related Results](#)

12,503 Results

1

**A review of metal organic framework (MOFs)-b photocatalysis**

By: Du, Chunyan; Zhang, Zhuo; Yu, Guanlong; Wu, Haipeng; Ch Chemosphere (2021), 272, 129501 | Language: English, Databa

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**Filter Results**

[Analyze Results](#)

**Behavior**

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

[Search Within Results](#)

224 Results

1

**Regioselective and enantioselective**

By: Collman, James P.; Zhang, Xumu; Lee, V. Science (Washington, DC, United States) (1)

A review with 41 references Recent progress here, with an explanation of the biomimetic have been studied allows useful conclusions and practical catalysts have arisen from sys

# epoxidation and alkene and regioselective 检索：烯烃、选择性和环氧化

References search for "epoxidation and alkene and regioselective"

[View Related Results](#)

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

[Load All Results](#)

224 Results

1

**Regioselective and enantioselective epoxidation catalyzed by metalloporphyrins**  
By: Collman, James P.; Zhang, Xumu; Lee, Virgil J.; Uffelman, Erich S.; Brauman, John I.  
Science (Washington, DC, United States) (1993), 261(5127), 1404-11 | Language: English, Database: Cplus and MEDLINE  
A review with 41 references Recent progress in **regioselective** and enantioselective **epoxidations** catalyzed by metalloporphyrins is discussed here, with an explanation of the biomimetic antecedents of this area and its relevance to synthetic applications. Classification of the catalysts that have been studied allows useful conclusions to be drawn about the development of this field. In particular, both the most promising biomimetic and practical catalysts have arisen from systems that can be systematically modified by convenient synthetic methods.

415

[Full Text](#)

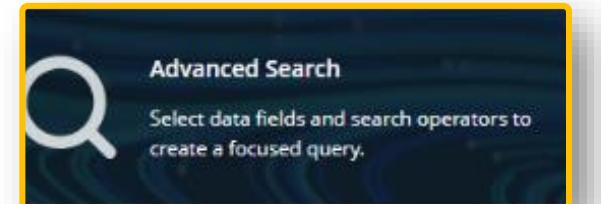
2

**Polyoxovanadometalate-catalyzed selective epoxidation of alkenes with hydrogen peroxide**  
By: Nakagawa, Yoshinao; Kamata, Keigo; Kotani, Miyuki; Yamaguchi, Kazuya; Mizuno, Noritaka  
Angewandte Chemie, International Edition (2005), 44(32), 5136-5141 | Language: English, Database: Cplus and MEDLINE

# 自定义组合检索

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）；
- 结构检索（包括物质结构和反应式）



Advanced Search

Select a search type, and then add multiple search fields to build a query. [?](#)

[Learn more about Advanced Search.](#)

Substances References Clear All

CO<sub>2</sub> and "catalytic hydrogenation"

AND Substances References Clear All

Publication Name AND Chem  
Chem  
Chemisches Zentralblatt  
Chemical Engineering Journal (Amsterdam, Netherlands)  
Chemical Physics Letters  
Chemical Communications (Cambridge, United Kingdom)  
Chemosphere  
Chemistry - A European Journal  
ChemRxiv  
Chemical Engineering Science  
Chemistry Letters

OR

NOT

Authors/Inventors  
Publication Name  
Organization  
Title  
Abstract/Keywords  
Concept  
Substances  
Life Science Data   
Publication Year  
Document Identifier  
Patent Identifier  
Publisher

+ Add Advanced Search Field

Search

?

CAS

A division of the American Chemical Society

# 1.3 文献结果：最新 & 引用最多 & 早期科学的研究

References search for "(PVDF or PEDOT) and "wearable device""

View Related Results ▾

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

Filter Results

Analyze Results

Behavior

Filter by Exclude

Search Within Results

1,418 Results

Sort: Relevance ▾ View: Full Abstract ▾

1. High-Performance Flexible All-Solid-State Supercapacitor from Large Free-Standing Graphene-PEDOT/PSS Films  
By: Liu, Yuqing; Weng, Bo; Razal, Jaselito M.; Xu, Qun; Zhao, Chen; Hou, Yuyang; Seyedin, Shayan; Jalili, Rouhollah; Wallace, Gordon G.; Chen, Jun  
Scientific Reports (2015), 5, 17045 | Language: English, Database: Cplus and MEDLINE

Although great attention has been paid to **wearable electronic devices** in recent years, flexible lightweight batteries or supercapacitors with high performance are still not readily available due to the limitations of the flexible electrode inventory. In this work, highly flexible, bendable and conductive rGO-**PEDOT/PSS** films were prepared using a simple bar-coating method. The assembled **device** using rGO-**PEDOT/PSS** electrode could be bent and rolled up without any decrease in electrochem. performance. A relatively high areal capacitance of  $448 \text{ mF cm}^{-2}$  was achieved at a scan rate of  $10 \text{ mV s}^{-1}$  using the composite electrode with a high mass loading ( $8.49 \text{ mg cm}^{-2}$ ), indicating the potential to be used in practical applications. To demonstrate this applicability, a roll-up supercapacitor **device** was constructed, which illustrated the operation of a green LED light for 20 s when fully charged.

Relevance

Times Cited

Accession Number: Ascending

Accession Number: Descending

**Publication Date: Newest**

Publication Date: Oldest

**CAS SciFinder** References ▾ solar cell

Full Text ▾ 13 0

Filter Behavior

Filter by Exclude

Search Within Results

Concept

Filtering: Database: CHEMZENT X

Clear All Filters

2,238 Results

Sort: Publication Date: Oldest ▾ View: Partial Abstract ▾

1. On the Selbstaufladung of **photo cells** in the dark and the active radiation of potassium  
By: Thirring, Hans  
Chemisches Zentralblatt (1913), 84 Book 2(1), 7-7 | Language: German, Database: CHEMZENT

Machine Translated: The self-charging in the dark at K-Photozellen is to unite Volta effect due. Hypogic acid act as galvanic elements with one electromotive force of about EUR volts and an internal resistance of the order 10tz ohms. One can only to a weak ionisation in the interior of the **cell** close, as with other observations via radio activity of K consistent.

ChemZent Full Text ▾

Substance (1) Reactions (0) Citing (0) Citation Map

- ChemZent®: 最早期的化学文摘——德国化学文摘的英文版，唯一提供可用英文获取德国化学文摘的解决方案，将化学研究相关文献回溯至十九世纪初。

排序方式：  
相关性  
引用次数  
收录号  
发表时间

# 筛选目标文献

文献类型、语言、作者  
发表机构、发表年份  
CAS标引的技术术语  
CAS标引的学科研究方向  
二次检索  
下载数据分析报告

...

- Language
- Publication Name
- Organization
- Author
- Document Type
- Substance Role
- Database

Filter Content Report

Download filter data from this result set.

Apply Filters

References search for "(PVDF or PEDOT) and "wearable device""

**View Related Results** (circled in blue)

How are these results different? [Learn more.](#)

**Substances**

- Reactions
- Citing

**Filter Results**

- Analyze Results
- Behavior

**Filter by** (highlighted with yellow arrows)

**Exclude**

**Search Within Results**

**Concept**

**Formulation Purpose**

**CA Section**

**CAS Content**

**Publication Year**

**数据关联**

1,418 Results

1

**High-Performance Flexible All-Solid-State Supercapacitor from Large Free-Standing Graphene-PEDOT/PSS Films**

By: Liu, Yuqing; Weng, Bo; Razal, Joselito M.; Xu, Qun; Zhao, Chen; Hou, Yuyang; Seyedin, Shayan; Jalili, Rouhollah; Wallace, Gordon G.; Chen, Jun  
Scientific Reports (2015), 5, 17045 | Language: English, Database: CAplus and MEDLINE

Although great attention has been paid to **wearable electronic devices** in recent years, flexible lightweight batteries or supercapacitors with high performance are still not readily available due to the limitations of the flexible electrode inventory. In this work, highly flexible, bendable and conductive rGO-**PEDOT**/PSS films were prepared using a simple bar-coating method. The assembled **device** using rGO-**PEDOT**/PSS electrode could be bent and rolled up without any decrease in electrochem. performance. A relatively high areal capacitance of 448 mF cm<sup>-2</sup> was achieved at a scan rate of 10 mV s<sup>-1</sup> using the composite electrode with a high mass loading (8.49 mg cm<sup>-2</sup>), indicating the potential to be used in practical applications. To demonstrate this applicability, a roll-up supercapacitor **device** was constructed, which illustrated the operation of a green LED light for 20 s when fully charged.

Full Text 13 0 211

2

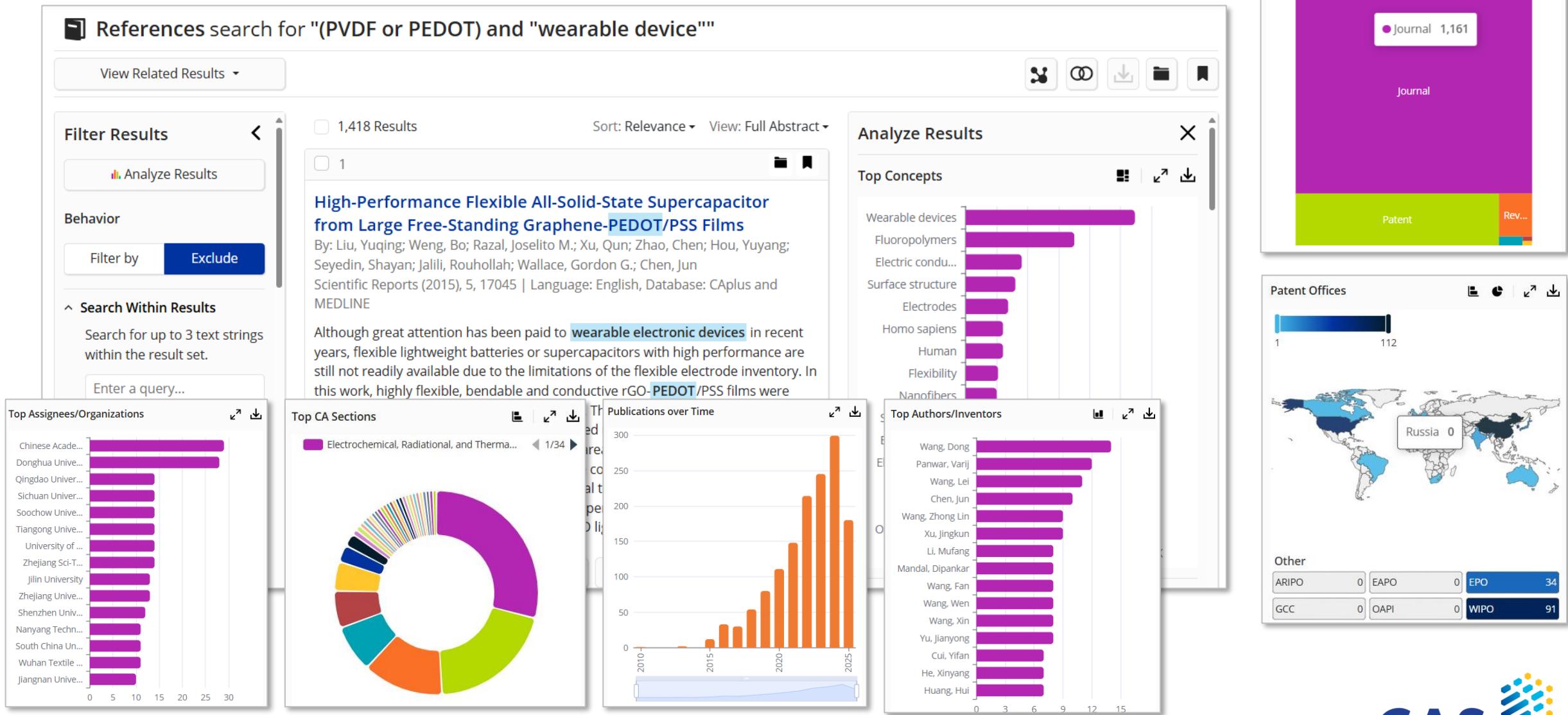
**A self-powered skin-patch electrochromic biosensor**

By: Santiago-Malagon, Sara; Rio-Colin, Diego; Azizkhani, Haniyeh; Aller-Pellitero, Miguel; Guirado, Gonzalo; del Campo, F. Javier  
Biosensors & Bioelectronics (2021), 175, 112879 | Language: English, Database: CAplus and MEDLINE

One of the limitations of many skin-patch **wearable** sensors today is their dependence on silicon-based electronics, increasing their complexity and unit cost. Self-powered sensors, in combination with electrochromic materials, allow simplifying the construction of these **devices**, leading to power anal. tools that remove the need for external detection systems. This work describes the construction, by screen-printing, of a self-powered

?

# 可视化的结果筛选和分析



# 筛选工具 CAS Section & Concept

CA Section

学科研究方向

纵览并精准定位核心研究点

6 Selected

- Electrochemical, Radiational, and Thermal Energy Technology (210)
- Electric Phenomena (169)
- Biochemical Methods (83)
- Textiles and Fibers (55)
- Plastics Fabrication and Uses (52)
- Pharmaceuticals (22)
- Plastics Manufacture and Processing (20)
- Optical, Electron, and Mass Spectroscopy and Other Related Properties (18)
- Unavailable (8)
- Electrochemistry (7)

By Count Alphanumeric

Apply Cancel

Concept

Top Count Alphanumeric Search

7 Selected

- Inorganic Analytical Chemistry (5)
- Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (5)
- Surface Chemistry and Colloids (5)
- Synthetic Elastomers and Natural Rubber (4)
- Air Pollution and Industrial Hygiene (3)
- Chemistry of Synthetic High Polymers (3)
- Magnetic Phenomena (3)
- Coatings, Inks, and Related Products (2)

Apply Cancel

Concept

Top Count Alphanumeric Search

精准定位感兴趣的核心研究点

Concept Name

nano\*

Search

17 Selected

- Carbon nanofibers (14)
- Carbon nanotube fibers (4)
- Carbon nanotubes (86)
- Flexibility (84)
- Stress-strain relationship (83)
- Electrospinning (82)
- Nanofibril (2)
- Nanofilms (6)
- Nanofilters (1)
- Nanoflakes (2)
- Core-shell nanoparticles (1)
- Electric nanogenerators (24)
- Metal Nanoparticles (3)
- Nanoflowers (2)
- Nanohorns (1)
- Nanoimprint lithography (1)
- Nanosheets (23)
- Nanospheres (1)
- Nanostructured materials (9)
- Nanostructures (18)
- Nanotechnology (4)
- Nanotubes (12)
- Nanotubes, Carbon (11)

# 筛选工具Search within results

References search for "(PVDF or PEDOT) and "wearable device""

合并、交集和去重

Save Results **定题追踪**

Filter Results **Exclude**

Filtering: Concept: Hydrogels

Excluding: Search Within Results: dop\*

104 Results

Sort: Relevance View: Full Abstract

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: CPlus 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 fluoride-co-trifluoroethylene) (**PVDF-TrFE**) as the piezoelec. filler. A one-pot thermoforming and solution **exchange** method was used to synthesize the CHACC/ **PEDOT**: PSS/**PVDF-TrFE** hydrogel. The hydrogel-based strain sensor exhibits high sensitivity (**GF**: 19.3), fast response (response time: 63.2 ms), and wide frequency range (response frequency: 5-25 Hz), while maintaining excellent mech. properties (elongation at break up to 293%). It can be concluded that enhanced strain-sensing properties of the hydrogel are contributed to both greater change in the relative resistance under stress and wider response to dynamic and static stimulus by adding **PVDF-TrFE**. This has a broad application in monitoring human motion, detecting subtle movements, and identifying object contours and a hydrogel-based array sensor. This work provides an insight into the design of composite hydrogels based on piezoelec. and piezoresistive sensing with applications for **wearable** sensors.

Full Text 7 1 40

Save Cancel

Search Within Results

Enter a query...

Search

Searching for... Clear All

dop\* X

Concept

CA Section

CAS Content

Alerts

Frequency

As Available

Add Email(s)

china@acs-i.org \*\*\*@gmail.com

Aero Alloys Archaeology Biotech catalyst

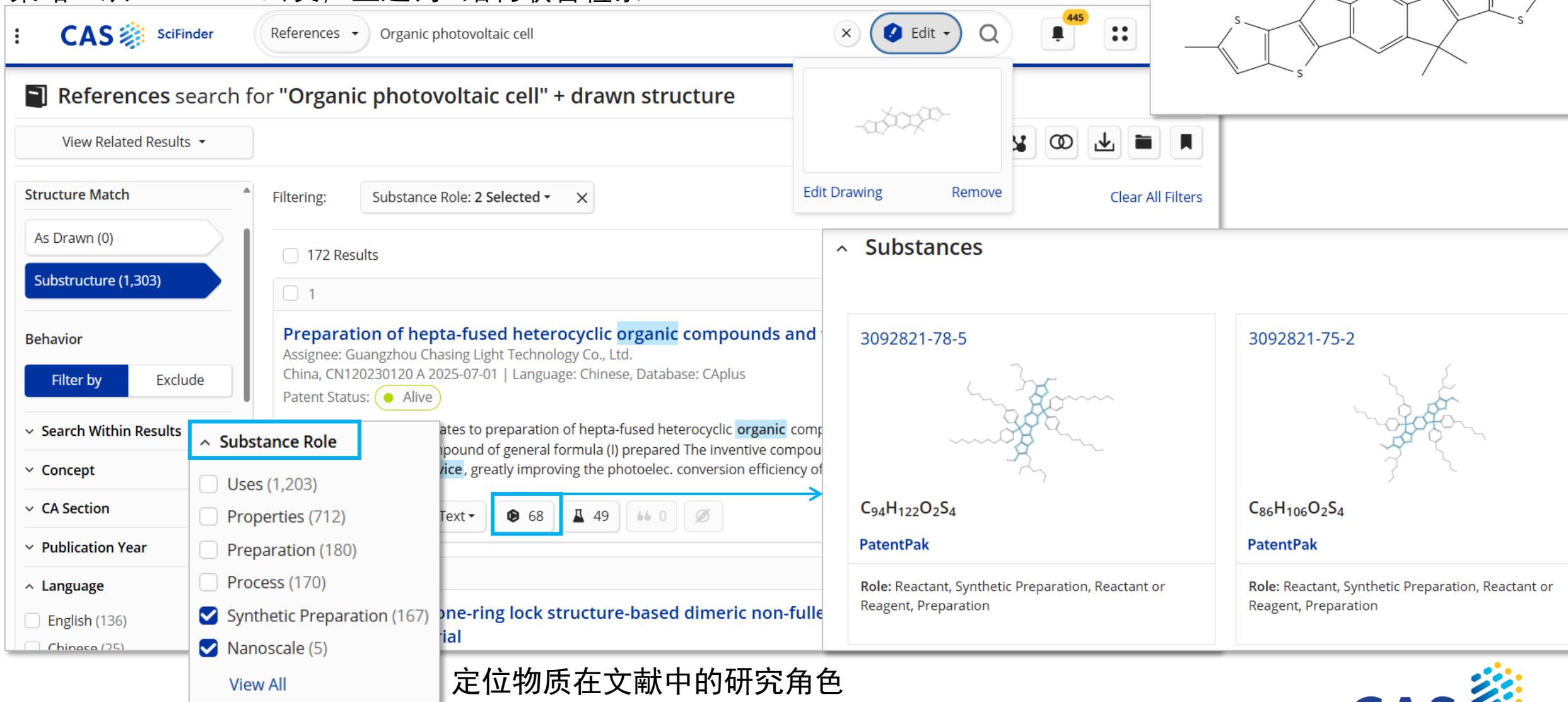
New Tag (Optional)

Add tag name Tag Color Light Blue

?

# 1.4 如何获得结构相关的文献?

策略: 从Reference出发, 主题词+结构联合检索



References search for "Organic photovoltaic cell" + drawn structure

View Related Results

Structure Match

As Drawn (0)

Substructure (1,303)

Filtering: Substance Role: 2 Selected

172 Results

1

**Preparation of hepta-fused heterocyclic organic compounds and**  
Assignee: Guangzhou Chasing Light Technology Co., Ltd.  
China, CN120230120 A 2025-07-01 | Language: Chinese, Database: Cplus  
Patent Status: Alive

ates to preparation of hepta-fused heterocyclic organic compound of general formula (I) prepared The inventive compound, greatly improving the photoelec. conversion efficiency of

Text ▾ 68 49 0

**Substances**

3092821-78-5

C94H122O2S4

PatentPak

Role: Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

3092821-75-2

C86H106O2S4

PatentPak

Role: Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

定位物质在文献中的研究角色

# 文献检索小结

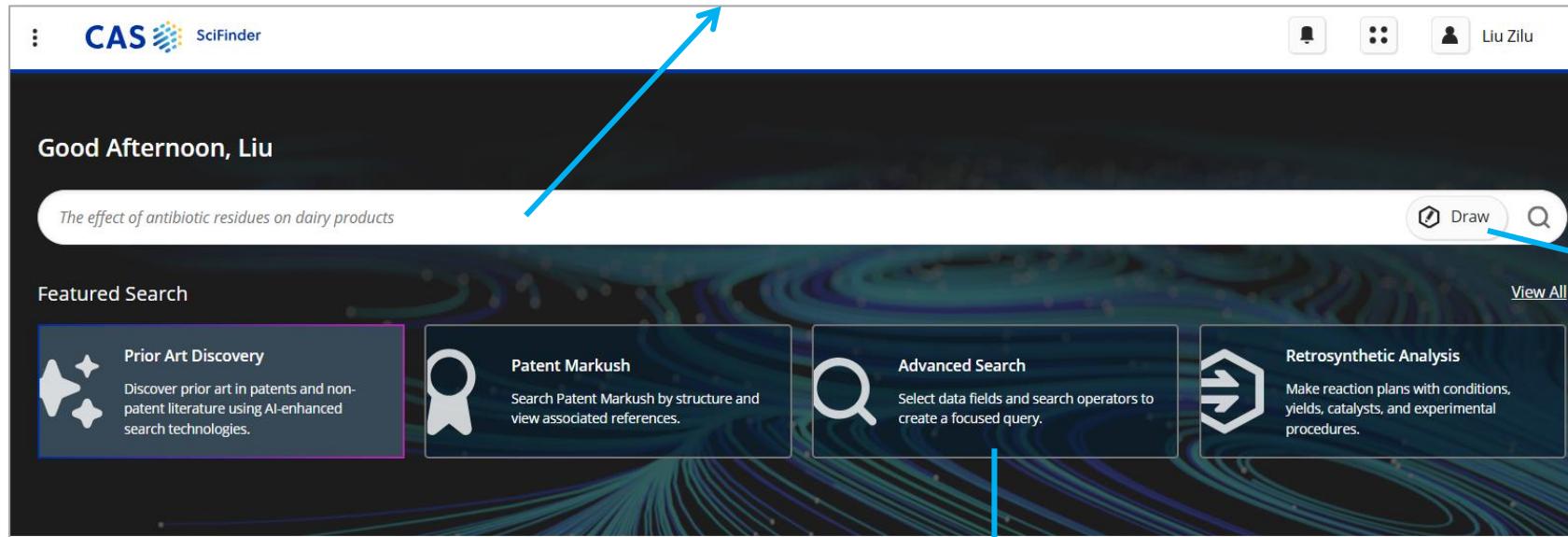
1. 利用引文地图拓展文献检索
2. 检索词的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
3. 利用丰富的筛选工具，快速获得目标文献
4. 主题词+结构联合检索快速获得文献

## 2.如何调研某类物质?

- 快速检索聚合物或无机化合物?
- 利用谱图数值确认产物或杂质? 从属性值出发, 调研某类材料?
- 检索完整分子结构? 通式结构? 或含有某些片段的物质?
- 如何确认结构新颖性?
- 如何查找相似的序列?

# 研究某种/某类物质？

- 通过物质标识符、文献标识符检索物质



The screenshot shows the SciFinder interface. At the top, there is a search bar with the placeholder text "The effect of antibiotic residues on dairy products". To the right of the search bar are icons for a bell, a menu, and a user profile labeled "Liu Zilu". Below the search bar, there is a "Good Afternoon, Liu" greeting and a "Featured Search" section. The "Featured Search" section includes five cards: "Prior Art Discovery", "Patent Markush", "Advanced Search", and "Retrosynthetic Analysis". The "Advanced Search" card is highlighted with a blue arrow pointing to it from the text "高级检索". To the right of the "Advanced Search" card is a "Draw" icon with a magnifying glass and a "Search" icon. A blue arrow points from the text "使用结构绘制面板进行结构检索" to the "Draw" icon.

- 高级检索

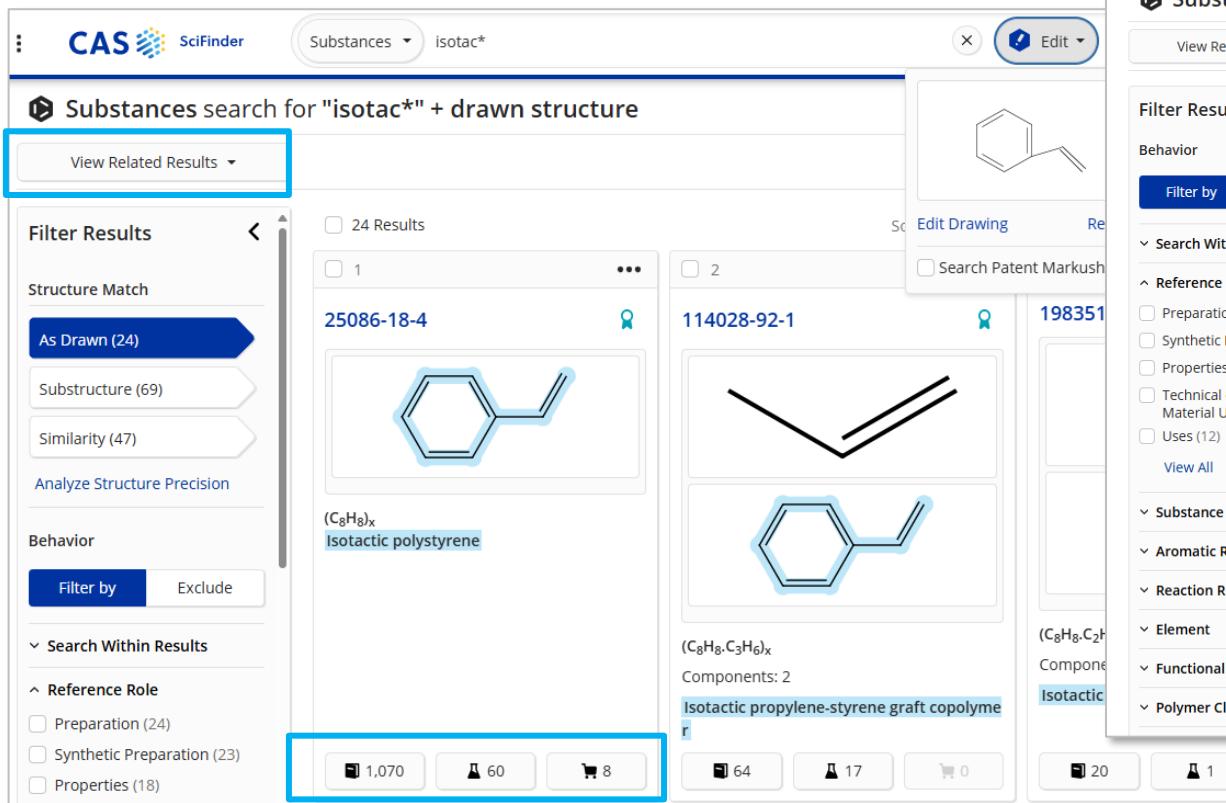
- 使用结构绘制面板进行结构检索

- 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

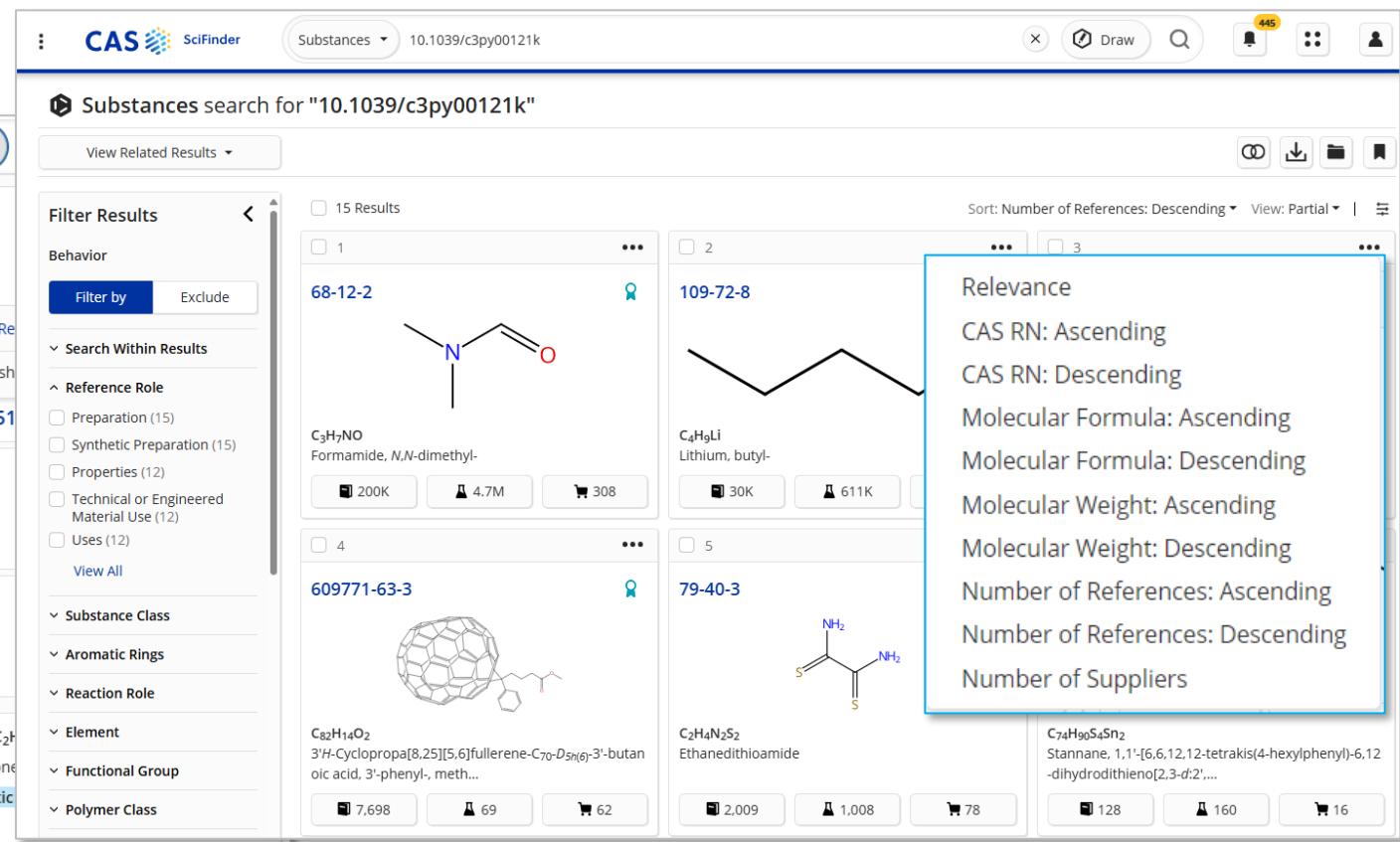
# 物质检索—物质/文献标识符

- 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)

- 迅速获得关注文献中的物质信息



The screenshot shows the SciFinder interface with a search bar containing 'isotac\*'. The results are filtered by 'As Drawn (24)'. The first result is '25086-18-4' with a structure of a benzene ring attached to a vinyl group. The second result is '114028-92-1' with a structure of a propylene-styrene graft copolymer. The third result is '198351' with a structure of isotactic polystyrene. The interface includes a 'View Related Results' button, a 'Filter Results' sidebar, and a 'View' section at the bottom.



The screenshot shows the SciFinder interface with a search bar containing '10.1039/c3py00121k'. The results are filtered by 'View Related Results'. The first result is '68-12-2' with a structure of formamide, N,N-dimethyl-, and the second is '109-72-8' with a structure of lithium, butyl-. The interface includes a 'Filter Results' sidebar, a 'Relevance' sidebar, and a 'View' section at the bottom.

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

Substances search for " $(\text{CH}_2\text{O})_n$ "

View Related Results ▾

Filter Results

Behavior

Filter by  Exclude

5 Results

Sort: Number of References: Descending ▾ View: Partial ▾

Rank	Chemical Identifier	Chemical Structure	Chemical Name	Number of References	Number of Publications	Number of Substances
1	9002-81-7		$(\text{CH}_2\text{O})_n$ Poly(oxymethylene)	8,936	312	12
2	32008-59-6		$(\text{CD}_2\text{O})_n$ Poly(oxymethylene-d <sub>2</sub> )	40	38	30
3	32107-82-7		$(\text{CH}_2\text{O})_n$ Poly(hydroxymethylene)	37	3	0

$(\text{C}_2\text{H}_4\text{O})_n\text{H}_2\text{O}$ : 括号中是重复结构单元，括号外为n  
 $(\text{C}_2\text{H}_6\text{O}_2)_x$ : 括号中是单体，括号外为x

## 2.2 属性值、谱图数值联用检索物质

Advanced Search  
Select a search type, and then add multiple search fields to build a query.

Learn more about Advanced Search.

Substances References Clear All

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

Draw 

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

AND Substance RN  Examples: 57-88-5 | 101600 

AND Component RN  Examples: 120-12-7 | 71432 

AND Chemical Name  Examples: Life Science Data | Biological | Chemical Properties | Density | Electrical | Lipinski | Magnetic | Mechanical | Optical and Scattering | Structure Related | Thermal 

+ Add Advanced Search Field

Molecular Formula  
CAS Registry Number  
Chemical Identifier  
Document Identifier  
Patent Identifier  
Experimental Spectra  
Life Science Data  
Biological  
Chemical Properties  
Density  
Electrical  
Lipinski  
Magnetic  
Mechanical  
Optical and Scattering  
Structure Related  
Thermal

Proton NMR  
Carbon-13 NMR  
Nitrogen-15 NMR  
Fluorine-19 NMR  
Phosphorus-31 NMR

Chemical Properties  
Density  
Electrical  
Lipinski  
Magnetic  
Mechanical  
Optical and Scattering  
Structure Related  
Thermal

Koc  
logD  
logP  
Mass Intrinsic Solubility (g/L)  
Mass Solubility (g/L)  
Molar Intrinsic Solubility (mol/L)  
Molar Solubility (mol/L)  
Molecular Weight  
pKa  
Vapor Pressure (Torr)

### 高级检索字段:

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

# 属性值联用检索物质

例如检索满足多属性值要求的聚合物：密度1-2g/cm<sup>3</sup>、拉伸强度>1000 MPa、熔点>150℃

在物质类别 Substance Class 中，锁定polymer

The screenshot shows the ChEMBL search interface with the following details:

- Substances** tab is selected.
- Search Bar:** Search by Substance Name, Functional Group, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.
- Filtering:** Substance Class: Polymer
- Search Results:** 33 Results
- Results List:** The first result is 9002-88-4, which is Unspecified Cellulose. It shows a chemical structure of a branched polymer chain with hydroxyl groups (OH) and a label "(C<sub>2</sub>H<sub>4</sub>)<sub>x</sub> Ethene, homopolymer". Metrics: 529K, 25K, 112.
- Second Result:** 9004-34-6, Unspecified Cellulose. It shows a chemical structure of a branched polymer chain. Metrics: 404K, 14K, 120.
- Third Result:** 9003-07-0, (C<sub>3</sub>H<sub>6</sub>)<sub>x</sub> 1-Propene, homopolymer. It shows a chemical structure of a branched polymer chain. Metrics: 357K, 9,299, 49.
- Fourth Result:** 9002-89-5, showing a chemical structure of a branched polymer chain with a hydroxyl group (OH).
- Fifth Result:** 25038-59-9, showing a chemical structure of a polymer chain with a carbonyl group and an oxygen atom.
- Sixth Result:** 9002-84-0, showing a chemical structure of a polymer chain with a fluorine atom.

在物质类别 Substance Class 中, 锁定polymer

# 属性值、谱图数值联用检索物质

- 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

Substances Advanced Search Edit

Enter a query...

Molecular Weight: 220 to 280  
Predicted values only.

AND: pKa: 1.3 to 1.8  
Predicted values only.

AND: Carbon-13 NMR: 114 to 171, 96, 11.5  
Allowance of  $\pm 2$  ppm.

+ Add Advanced Search Field

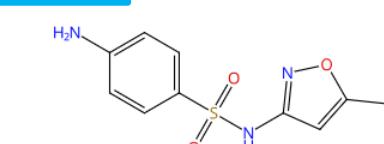
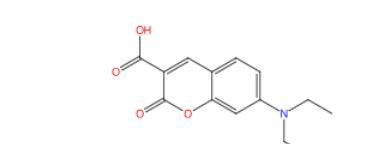
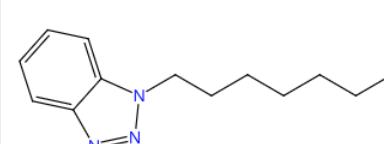
Substances Advanced search for 3 fields

View Related Results

Behavior: Filter by (selected) Exclude

86 Results

Sort: Number of References: Descending | View: Partial

Rank	Chemical Structure	Chemical Name	Chemical Formula	Number of References	Number of Citations	Number of Publications
1		723-46-6 Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)-	C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S	31K	1,090	116
2		50995-74-9 2H-1-Benzopyran-3-carboxylic acid, 7-(diethylamino)-2-oxo-	C <sub>14</sub> H <sub>15</sub> NO <sub>4</sub>	784	1,007	79
3		59046-27-4 1H-Benzotriazole, 1-octyl-	C <sub>14</sub> H <sub>21</sub> N <sub>3</sub>	25	21	3

# 物质详情

CAS Registry Number: 723-46-6

31K 1,079 123 View in CAS BioFinder

该物质被专利Claims  
保护的系列专利信息

**Patents Claimed In**

Triazine desulfurizer containing triazine methoxazole and tetracarboxylic acid oxazolidine used for desulfurization of crude oil  
Role: Reactant  
Patent Number: CN120349810  
Publication Date: 2025-07-22

Method for co-treating organic wastewater using peroxyomonosulfate and peroxydisulfate  
Role: Pollutant  
Patent Number: CN120349021  
Publication Date: 2025-07-22

External antibacterial liquid containing sulfamethoxazole, alcohol and water  
Role: Therapeutic Use  
Patent Number: CN120305271  
Publication Date: 2025-07-15

**Chemical Structure**

C10H11N3O3S

**Properties**

Molecular Weight  
Melting Point (Experimental)  
Boiling Point (Predicted)  
Density (Experimental)  
pKa (Experimental)

**Experimental Properties | Spectra**

**Other Names and Identifiers**

**Experimental Properties**

**Experimental Spectra** (highlighted with a blue arrow)

**Pharmacological Data**

**ADME**

**Toxicity**

**Predicted Properties**

**Predicted Spectra**

**Bioactivity Indicators**

**Target Indicators**

**Regulatory Information**

**GHS Hazard Statements**

**Additional Details**

**Condition**

Press: 760.00 Torr

**Experimental Spectra**

**1H NMR** (highlighted with a blue arrow)

**13C NMR**

**Hetero NMR**

**Spectrum Summary**

**723-46-6**

C10H11N3O3S

**CAS Name**  
Sulfamethoxazole

**Conditions**

Working Frequency  
400 MHz

Solvent  
[Dimethyl sulfoxide \(67-68-5\)](#)  
[Carbon tetrachloride \(56-23-5\)](#)

Temperature  
20 °C

**Spectrum Summary**

**Spectrum ID**  
F0175-0013

**Source**  
Spectral data were obtained from Life Chemicals

**Solvent**  
Dimethyl sulfoxide; Carbon tetrachloride

**Source**

(1) LC

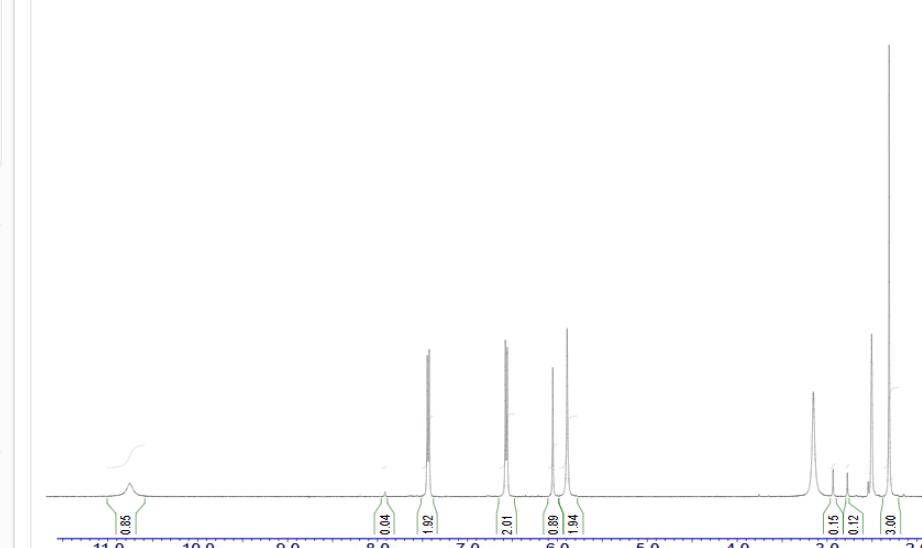
(2) ENAMINE

(2) ENAMINE

(3) BIORAD

(3) BIORAD

**1H NMR Spectrum**



- 折叠菜单显示物质各类信息

# 扩展问答类型，快速聚焦物质谱图和安全信息

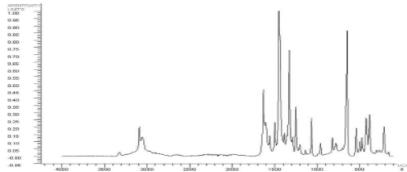
Results for "what is the Raman spectrum of luminol"

All Substances Reactions References Suppliers Patent Markush

## Spectrum

Showing 1 of 1 Result

521-31-3  
Luminol  
Viewing 1 of 1



Experimental  
View Spectra Details

Raman Spectrum  
Conditions  
No data available.  
Spectra Summary  
Spectrum ID

[View All Spectra](#)

Results for "proton nmr of c13h13br"

All Substances Reactions References Suppliers Patent Markush

## Proton NMR Spectrum

Showing 5 of 6 Results

27650-59-5  
2-(3-Bromopropyl)naphthalene  
Viewing 1 of 5



Experimental  
View Spectra Details

Condition

Working Fre

400 MHz

Solvent

Chloroform-

Temperatur

20 °C

Spectra S

Spectrum ID

EN300-1171

Source

Spectral data

[View All](#)

Results for "what are the hazards of bisphenol a?"

All Substances Reactions References Suppliers

## GHS Hazard Table for 2,2-Bis(4-hydroxyphe...

Showing 5 of 62 Results

Code Hazard Statement

H272 May intensify fire; oxidizer

H302 Harmful if swallowed

H304 May be fatal if swallowed and enters airways

H313 May be harmful in contact with skin

H317 May cause allergic skin reaction

## Regulatory List

[View in Detail Page](#)

AIC, APEC, CANL, CLP, DSL, ECL, EINECS, ENCS, FDA, HAP, HHAZ, HTU, IECSC, INSG, ITC, IUR, JDATA, NZIoC, PICCS, PII, PROP, REACH, RSTR, S313, SIDS, State\_CA\_PROP65, State\_MA, State\_MN, State\_NJ, State\_OR, State\_PA, State\_VT, State\_WA, STOR, STY, TCSI, TDCA, TSCA, VNECI, VOC, WGK

Confidential Business Information: Public

Regulatory Synonyms (35)

Details by Country/International & Other Lists



Suggested based on your search

自然语言直接查阅物质安全信息



# 支持自然语言直接检索物质理化性质，直观高效

Results for "what is the boiling point of ethanol"

All Substances Reactions References Suppliers Patent Markush

64-17-5

Ethanol

Boiling Point

78.5 °C

Source

"Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)

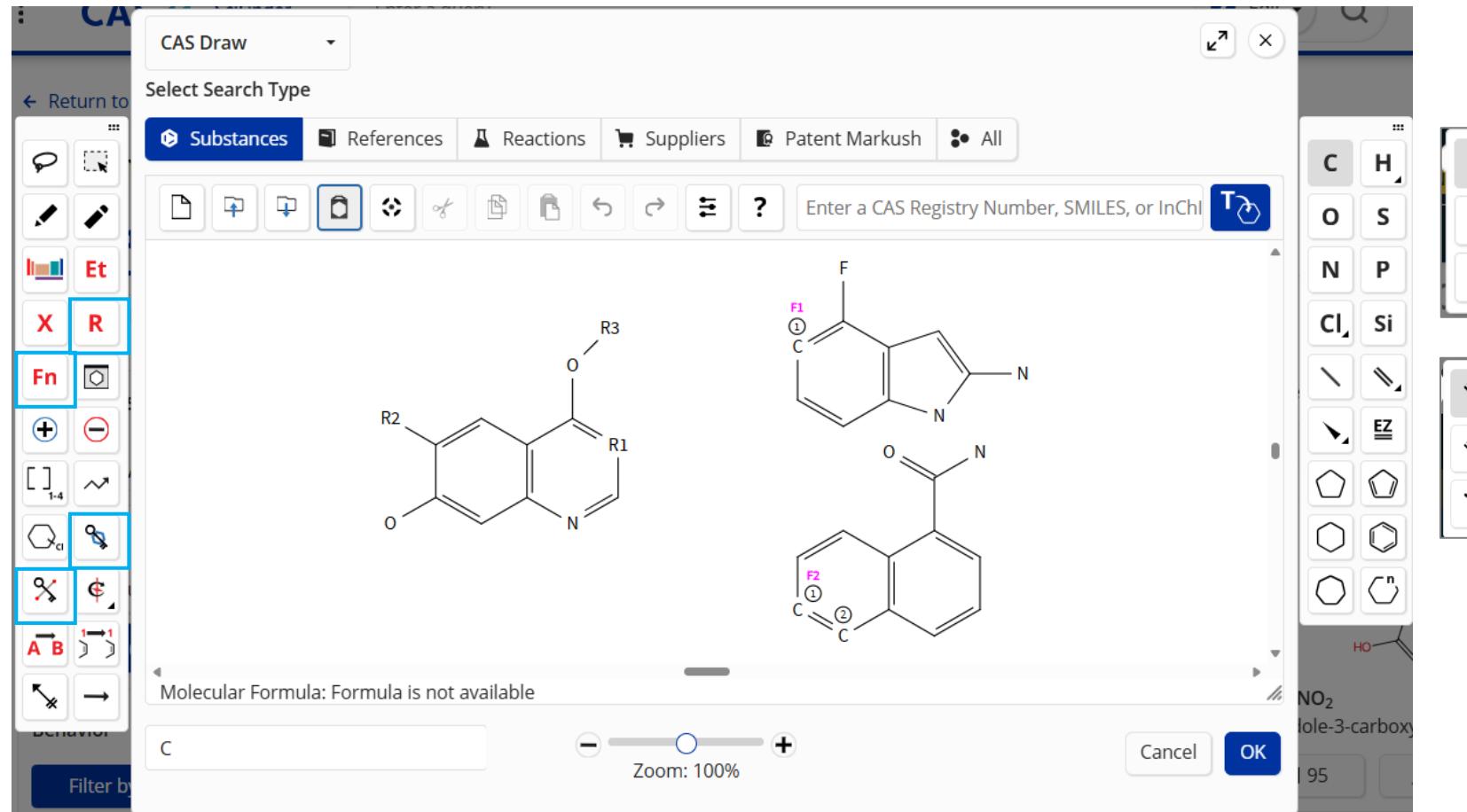
## Boiling Point Properties

Showing 5 of 415 Results

[View in Detail Page →](#)

Value	Condition	Source
78.5 °C	-	"Hazardous Substances Data Bank" data were obtained from the ...
181.27 °C	-	
110 °C (approx)	-	
85 °C (approx)	-	
80 °C	-	

## 2.4 结构检索



### R 自定义 R 基团

R基团可设置为原子、可变基团、常用官能团，也可以是自定义的片段结构

### Fn 片段结构标记

定义R基团中特定的片段结构，且一个片段可设置多个连结位点

### 环锁定工具

锁定的环无法成为更大环系的组成部分，锁定的链键无法成为环上的键

### 原子锁定工具

被锁定的原子或官能团不发生非氢取代

氢同位素：氕、氘和氚

双键、三键和不确定化学键

# 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

41 © 2025 American Chemical Society. All rights reserved.

### Substances search for drawn structure

View Related Results ▾

**Filter Results** Filter by Exclude

**Structure Match**

- As Drawn (0)
- Substructure (797)**
- Similarity (9)

Analyze Structure Precision

Behavior

**Filter by** Exclude

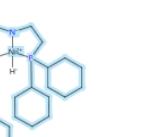
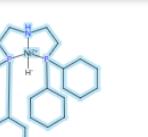
797 Results

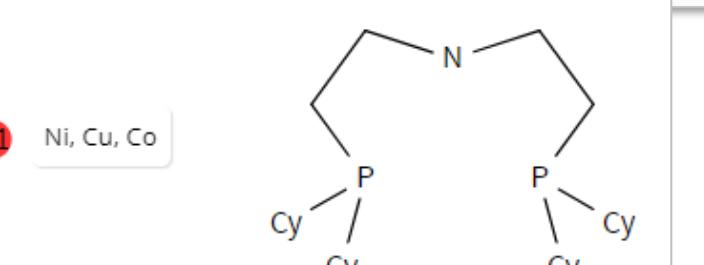
Sort: Molecular Weight: Asc

Save and Alert

Share Results

Copy Search to Clipboard

Result	Number	Chemical Structure	Chemical Formula	Description	Count	Count	Count
1	3031025-06-3		C <sub>28</sub> H <sub>30</sub> NNiP <sub>2</sub>	Nickel, [2-(dicyclohexylphosphino- $\kappa P$ )-N-[2-(dicyclohexylphosphino- $\kappa P$ ethyl]ethan...	1	0	0
2	1421448-06-7		C <sub>28</sub> H <sub>53</sub> NNiP <sub>2</sub>	Nickel, [2-(dicyclohexylphosphino- $\kappa P$ )-N-[2-(dicyclohexylphosphino- $\kappa P$ ethyl]ethan...	3	7	0
3	1421448-0		C <sub>28</sub> H <sub>54</sub> NNiP <sub>2</sub>	Nickel(1+), [2-(dicyclohexylphosphino- $\kappa P$ )-N-[2-(dicyclohexylphosphino- $\kappa P$ ethyl]ethan...	2	0	0

**R1** Ni, Cu, Co 

Filter Behavior

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

物质筛选类别:  
二次检索 (结构)  
文献角色  
物质类别  
芳环数  
**反应角色**  
元素  
官能团  
生物活性数据  
分子量  
立体化学  
同位素  
金属包含  
实验物性数据  
.....



# 结构检索

## 结构检索类别:

- As Drawn  
绘制结构中可出现R基团、可变基团；绘制结构中价态未达饱和的原子只能接氢；如有环系，不与其他环稠合或成桥环
- Substructure 亚结构  
包括As Drawn检索结果；价态未达饱和的原子可以连接氢以外的其他原子；如有环系，可形成其他环
- Similarity 相似结构  
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变  
注：如果关注相似结构检索结果，请不要绘制通式结构

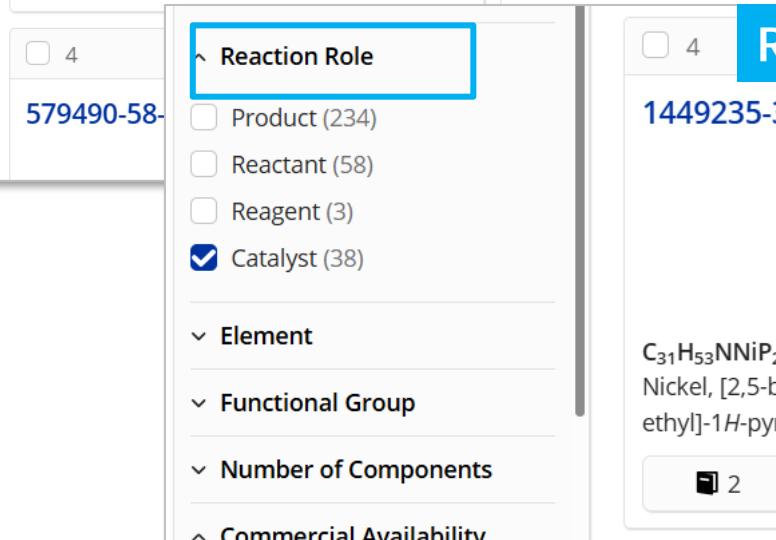
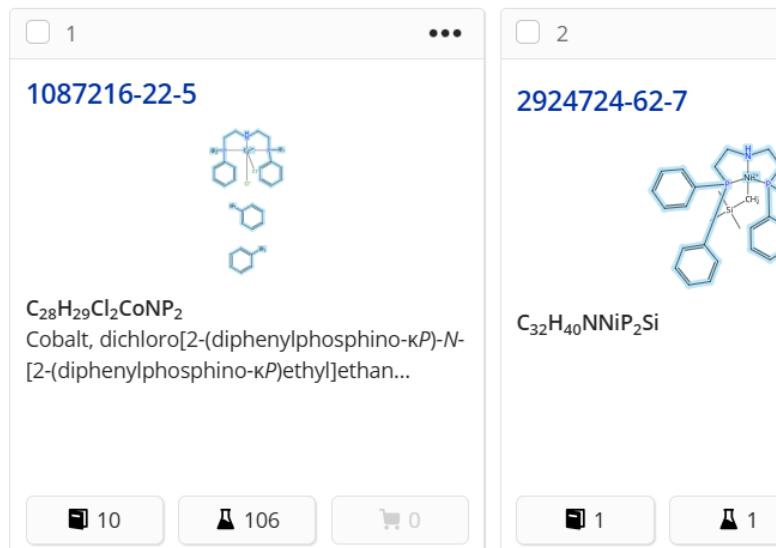
## 物质检索结果的筛选

## ^ Reference Role

- Preparation (515)
  - Synthetic Preparation (513)
  - Properties (297)
  - Uses (138)
  - Catalyst Use (123)
  - Reactant (104)
  - Reactant or Reagent (104)
  - Process (36)
  - Physical, Engineering, or Chemical Process (35)
  - Substance Claimed (15)
  - Technical or Engineered Material Use (12)
  - Industrial Manufacture (10)
  - Formation, Non-preparative (6)
  - Biological Study (4)
  - Pharmacological Activity (4)

[View All](#)

## Reference Role: 物质在文献中的研究角色



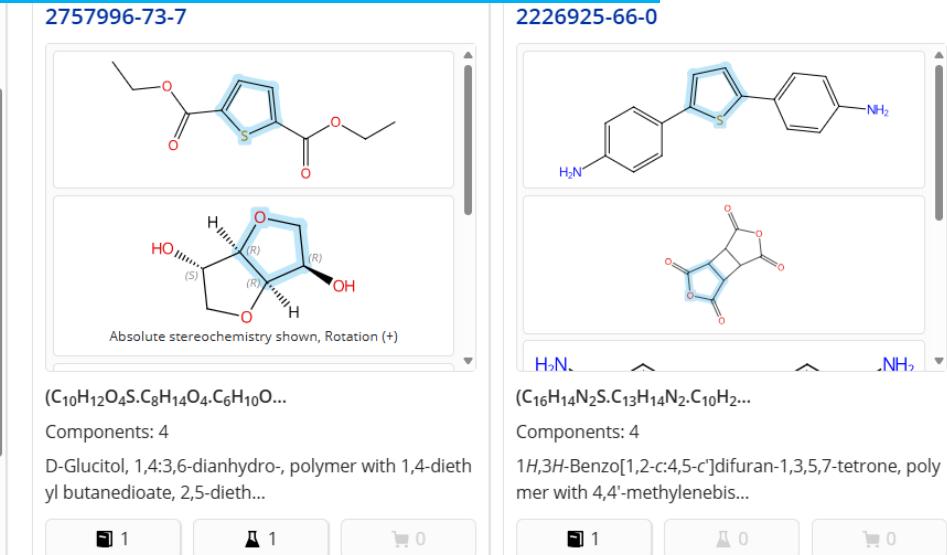
- Polymer (138)**
- Mixture (27)
- Coordination Compound
- General Derivative (2)
- Salt and Compound With
- ▼ Aromatic Rings**
- ▼ Reaction Role**
- ▼ Element**
- ▼ Functional Group**
- ▼ Polymer Class**
- ▲ Number of Components**

- 1 (233)
  - 2 (494)
  - 3 (189)
  - 4 (138)
  - 5 or more (480)

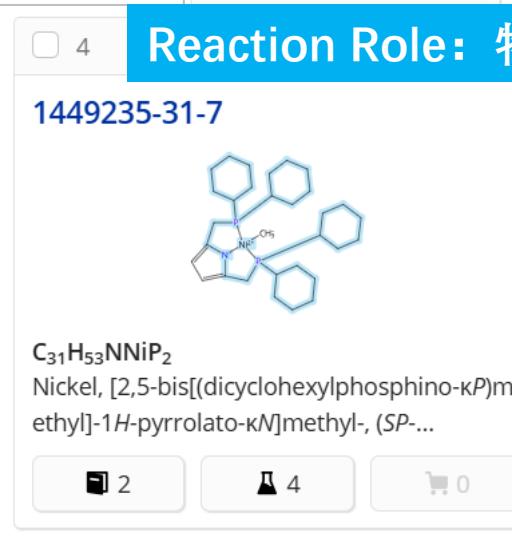
Filtering: Substance Class: Polymer X Number of Components: 4 X

138 Results

## Substance Class: 物质类别



## Reaction Role: 物质在反应中的角色



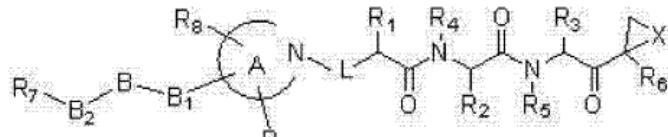
# 2.5 CAS Markush检索，助力结构查新

CN 104945470 A

## 权利要求书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



I

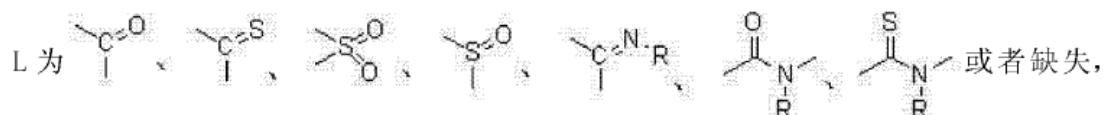
其中：

R<sub>1</sub>、R<sub>2</sub>、R<sub>3</sub>各自独立选自H、C<sub>1-6</sub>烷基-D、卤代的C<sub>1-6</sub>烷基-D、C<sub>1-6</sub>羟基烷基、C<sub>1-6</sub>巯基烷基、C<sub>1-6</sub>烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D为N(R<sub>a</sub>)(R<sub>b</sub>)或缺失，R<sub>a</sub>、R<sub>b</sub>各自独立选自H、OH、C<sub>1-6</sub>烷基、卤代的C<sub>1-6</sub>烷基或N末端保护基；

R<sub>4</sub>、R<sub>5</sub>各自独立选自H、OH、C<sub>1-6</sub>烷基、卤代的C<sub>1-6</sub>烷基或芳烷基；

R<sub>6</sub>选自H、C<sub>1-6</sub>烷基，卤代的C<sub>1-6</sub>烷基，C<sub>1-6</sub>羟基烷基，C<sub>1-6</sub>烷氧基，卤代的C<sub>1-6</sub>烷氧基，C(=O)O-C<sub>1-6</sub>烷基，C(=O)NH-C<sub>1-6</sub>烷基，芳烷基；

X为O、S、NH、N-C<sub>1-6</sub>烷基或N-卤代的C<sub>1-6</sub>烷基；



其中R选自H、C<sub>1-6</sub>烷基或卤代的C<sub>1-6</sub>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<sub>8</sub>、R<sub>9</sub>和B<sub>1</sub>基团取代；

R<sub>8</sub>、R<sub>9</sub>分别独立选自H、OH、C<sub>1-6</sub>烷基，C<sub>1-6</sub>烷氧基，C<sub>1-6</sub>羟基烷基，C<sub>1-6</sub>巯基烷基，C<sub>1-6</sub>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

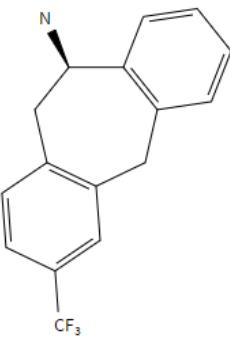
预测性物质[Prophetic Substance]：

- 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%



Substances search for drawn structure

View Related Results

Filter Results

Structure Match

As Drawn (0)

Substructure (2)

Similarity (6,054)

Analyze Structure Precision

Behavior

Filter by

Exclude

2 Results

1 146364-17-2

146364-17-2

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

1 1 0 0

2 146364-18-3

146364-18-3

C18H16F3N  
10,5-(Iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-12-n-

1 1 0 0

Filter Results

Filtering: Similarity: 4 Selected X Number of Components: 1 X

Structure Match

As Drawn (0)

Substructure (2)

Similarity (6,054)

Behavior

Filter by

Exclude

174 Results

1 87 ...

38506-20-6

C16H13F3  
5H-Dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)-

1 0 0

2 84 ...

1705598-88-4

C17H13F3  
5H-Dibenzo[a,d]cycloheptene, 10,11-dihydro-5-methylene-3-(trifluoromethyl)-

1 2 0

4 79 ...

13055-66-8

C17H13F3  
5H-Dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)-

1 0 0

5 79 ...

1644159-08-9

C17H13F3  
5H-Dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)-

1 2 0

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；  
根据需要，可进行文献检索补充

# CAS Markush检索

## 第二步：Markush结构检索 获得四项专利文献

- 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

# 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，根据需要可进行文献检索补充

### 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？

# 研究某种/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
  - 文本

1

910463-68-2

Image Not Available

Unspecified

Semaglutide

Protein/Peptide Sequence

Sequence Length: 34

3,074

378

46

Reactions search for "29022-11-5"

View Related Results

Filter Results

99,804 Results

Scheme 1 (1 Reaction)

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

Steps: 1 Yield: 100% ▾

resin-bound

Reactions search for "10.1021/ja027603q"

View Related Results

Filter Results

10 Results

Scheme 1 (1 Reaction)

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

Steps: 1 Yield: 95% ▾

Absolute stereochemistry shown, Rotation (-)

Suppliers (109)

Absolute stereochemistry shown, Rotation (-)

Suppliers (99)

Absolute stereochemistry shown

Suppliers (91)

Absolute stereochemistry shown, Rotation (-)

Suppliers (13)

Absolute stereochemistry shown

Suppliers (81)

# 利用自然语言检索反应

支持反应转化类型名称、物质类别、物质官能团和反应参与角色（包括溶剂、试剂和催化剂）

Reactions search for "synthesis of paclitaxel from acetic anhydride"

View Related Results

Filter Results

Behavior

Filter by

Exclude

Search Within Results

Yield

90-100% (2)

80-89% (3)

50-69% (5)

No Yield Available (249)

Reaction Scale

Milligram (83)

Gram (65)

259 Results

Scheme 1 (10 Reactions)

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

Steps: 1 Yield: 85-96% ⋮

Absolute stereochemistry shown

Suppliers (85)

31-355-CAS-20587342 Steps: 1

1.1 Reagents: Hexamethyldisilazane  
Catalysts: 4-(Dimethylamino)pyridine  
Solvents: Acetonitrile; rt

1.2 Reagents: Hydrochloric acid  
Solvents: Water; rt

Reactions search for "synthesis of paclitaxel catalyzed by triphenylphosphine"

View Related Results

Filter Results

Behavior

Filter by

Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

1 (1)

2 (2)

3 (3)

4 (3)

5 (3)

View All

7,002 Results

Scheme 1 (1 Reaction)

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

Steps: 1 Yield: 60% ⋮

Absolute stereochemistry shown, Rotation (-)

Suppliers (83)

Suppliers (139)

31-049-CAS-18450406 Steps: 1 Yield: 60% ⋮

1.1 Reagents: Hydrochloric acid  
Solvents: Ethanol, Tetrahydrofuran; 24 h, rt

1.2 Reagents: Formic acid, Triethylamine  
Catalysts: Triphenylphosphine, Palladium diacetate  
Solvents: Tetrahydrofuran; 5 h, rt

1.3 Reagents: Pyridinium p-toluenesulfonate  
Solvents: Methanol; 24 h, rt

1.4 Reagents: Sodium bicarbonate  
Solvents: Ethyl acetate, Water; 2 h, rt

Method for producing side chain precursor of paclitaxel and docetaxel

Assignee: Ensuko Sugar Refining Co., Ltd.

World Intellectual Property Organization, WO2017006573 A1 2017-01-12

PatentPak ▾ Full Text ▾

醋酸酐合成紫杉醇

三苯基膦催化合成紫杉醇

- “**of**”连接特定关键词指定反应产物，如 synthesis（合成），preparation（制备）和 manufacture（生产）。
- “**from**”连接物质指定反应物或试剂
- “**catalyzed by**”连接物质指定催化剂

# 自然语言检索反应

Reactions search for "synthesis of paclitaxel in tetrahydrofuran"

在四氢呋喃中合成紫杉醇

Filter Results

Behavior

Filter by

Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

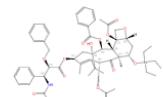
Catalyst

Reagent

Solvent

82 Results

Scheme 1 (1 Reaction)



→



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

Steps: 1 Yield: 100% ⋮

“in”连接物质指定溶剂

Reactions search for "synthesis of paclitaxel mediated by hydrochloric acid"

盐酸作为试剂参与合成紫杉醇

Filter Results

Behavior

Filter by

Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

1 (58)

2 (74)

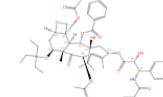
3 (90)

4 (93)

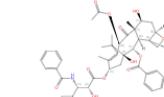
5 (69)

8,768 Results

Scheme 1 (2 Reactions)



→



Suppliers (34)

Suppliers (139)

31-049-CAS-347948

Steps: 1 Yield: 100% ⋮

1. Reagents: Hydrochloric acid

Solvents: Ethanol, Water; 0 °C; 145 min, 0 °C → rt

A catalytic asymmetric method for the preparation of the paclitaxel (taxol) C13 side-chain derivatives and its use in the preparation of taxane derivatives

Assignee: Unknown

World Intellectual Property Organization, WO2010062239 A1 2010-06-03

PatentPak ▾ Full Text ▾

“mediated by”连接物质指定试剂

# AI识别检索意向，提供最相关反应检索结果

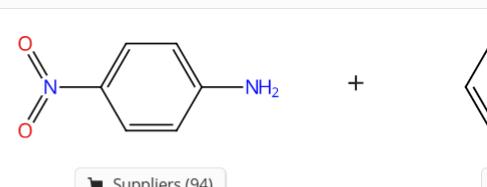
Reactions search for "reactions between 4-Nitroaniline and phenol"

View Related Results Save

Filter Results 152 Results

AI-Driven Enhancements in Reactions Searching: We've leveraged CAS-owned data and AI to optimize your reaction query. This feature is designed to identify the intent of your query more accurately, providing you with the most relevant results. Please continue to develop this feature, your feedback is important in making it better. [Learn more](#) | [Suggest Improvements](#)

Scheme 1 (28 Reactions)



Suppliers (94)

31-078-CAS-11681850 Steps: 1 Yield: 100%

1.1 Reagents: Sodium nitrite, Hydrochloric acid  
Solvents: Water; 1 h, rt; 30 min, 2 °C  
1.2 Reagents: Sodium hydroxide  
Solvents: Water; 1 h, 2 °C; 3 h, 2 °C; 24 h, 2 °C → rt

View All

Yield

- 90-100% (111K)
- 80-89% (129K)
- 70-79% (141K)
- 50-69% (191K)
- 30-49% (108K)

Reaction Scale

- Milligram (132K)
- Gram (35K)
- Kilogram (97)
- No Scale Provided (1.3M)

Expand Scheme

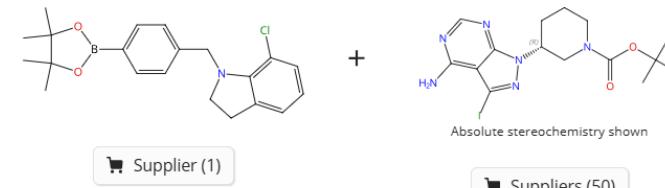
Reactions search for "suzuki coupling reaction"

View Related Results Save

Filter Results 1,469,847 Results

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

Scheme 1 (1 Reaction)

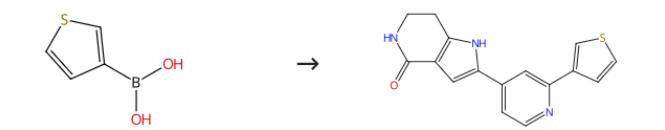


Supplier (1)

Suppliers (50)

Absolute stereochemistry shown

Scheme 2 (1 Reaction)



Supplier (4)

Suppliers (101)

Absolute stereochemistry shown

Steps: 1 Yield: 100% ...

Supplier (3)

?

文献检索时识别反应检索意向，  
便捷获取目标反应信息

# 不止具体反应，还可便捷检索某一类反应

Reactions search for "synthesis of aldehyde catalyzed by Palladium diacetate"

View Related Results ▾

Filter Results < ▾

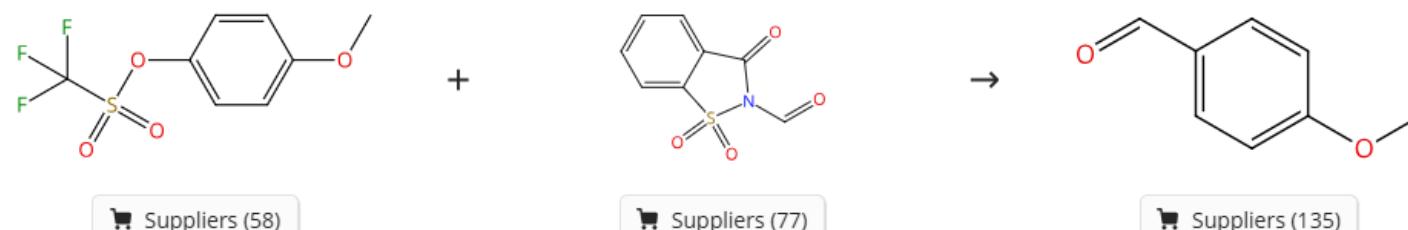
113,811 Results

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

乙酸钯催化合成醛类化合物

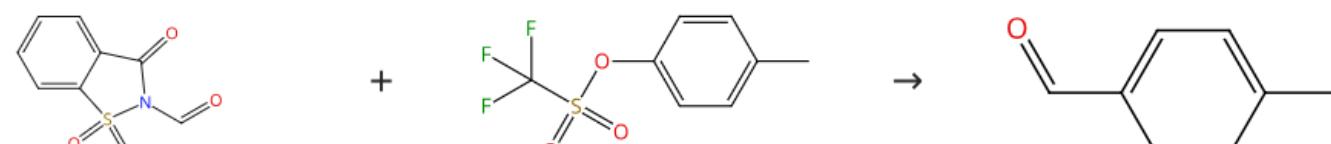
Steps: 1 Yield: 100% ⚙

**Scheme 1 (1 Reaction)**



Suppliers (58)   Suppliers (77)   Suppliers (135)

**Scheme 2 (1 Reaction)**



Suppliers (77)   Suppliers (63)   Suppliers (104)

Expand Scheme ▾

Expand Scheme ▾

## 3.2 查找亚结构反应或相似反应

As Drawn  
亚结构反应  
相似反应

Reactions search for drawn structure

View Related Results ▾

Filter Results

Structure Match

- As Drawn (34)**
- Substructure (8,806)
- Similarity (0)

Behavior

Filter by Exclude

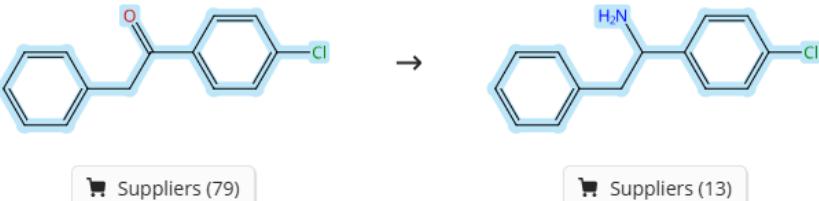
Search Within Results

Yield

- 80-89% (4)
- 70-79% (2)
- 50-69% (1)
- No Yield Available (27)

34 Results

Scheme 1 (5 Reactions)



Suppliers (79)

Suppliers (13)

Expand Scheme ▾

Scheme 2 (1 Reaction)



Suppliers (45)

Suppliers (3)

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

By Scheme

By Document

By Transformation

Relevance

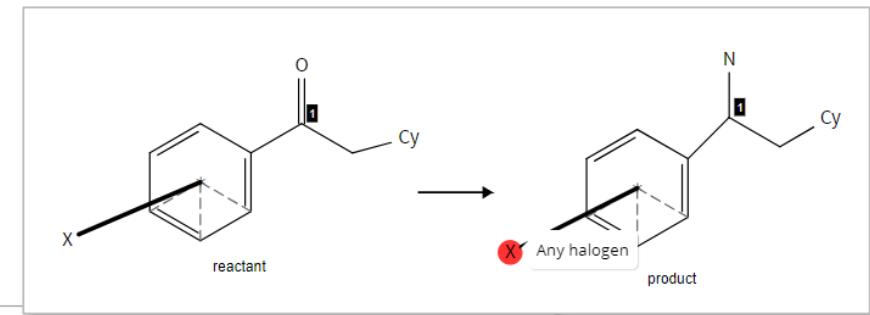
Publication Date: Newest

Publication Date: Oldest

Yield

Number of Steps: Ascending

Number of Steps: Descending



反应分组：  
按反应式  
按文献  
按转化类型

反应排序：  
相关度  
公布时间  
产率  
步数

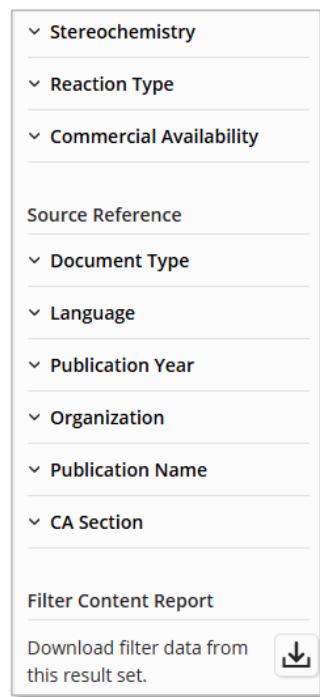
### 3.3 高效筛选目标反应

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、商品信息等

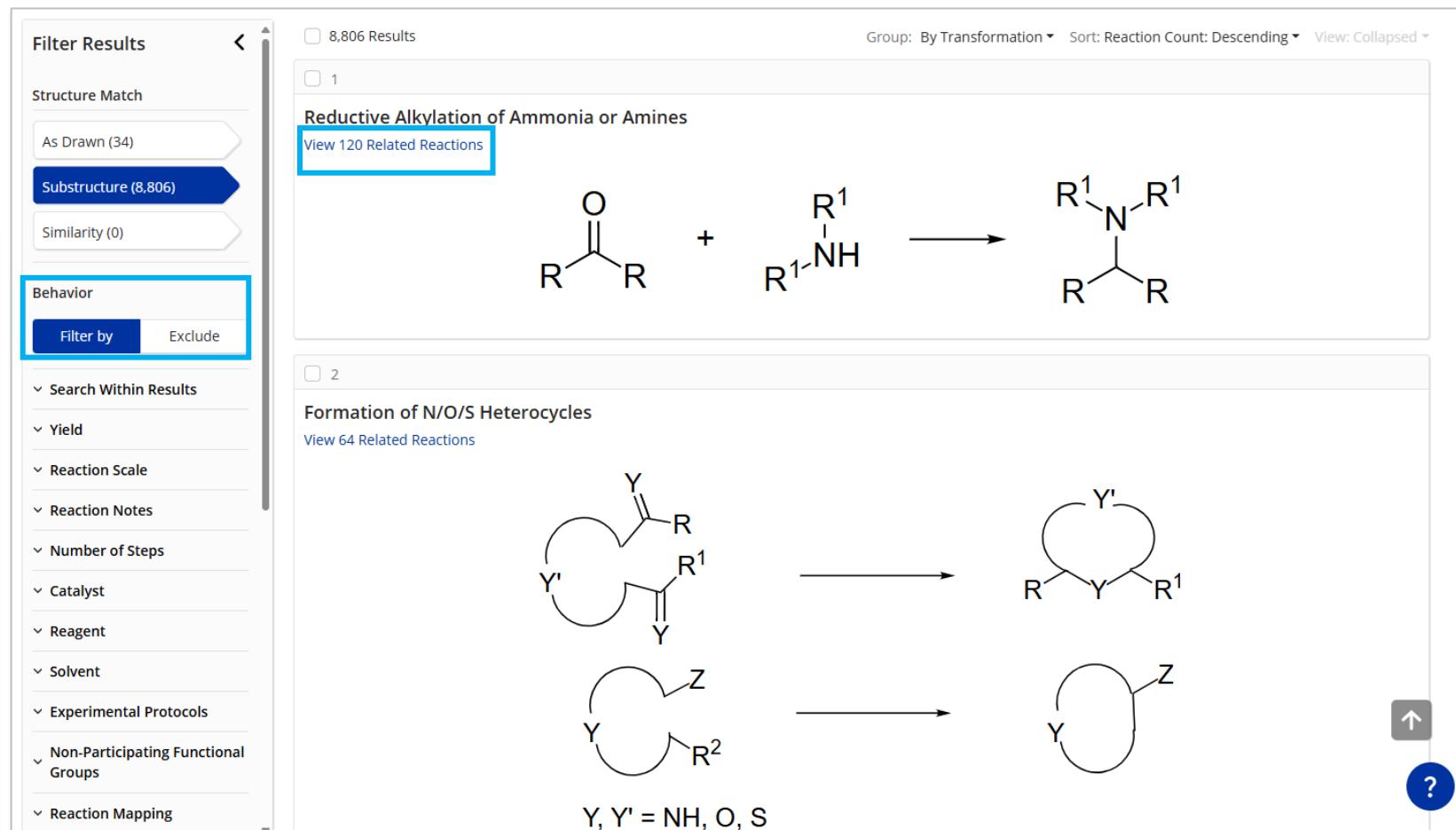
文献筛选类别：

文献类型、语言、出版年份、刊物名等



The sidebar includes sections for Stereochemistry, Reaction Type, Commercial Availability, Source Reference, Document Type, Language, Publication Year, Organization, Publication Name, CA Section, Filter Content Report, and a download link for filter data.

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



The interface shows a search results page with a 'Filter Results' sidebar. The main area displays two reaction examples: 'Reductive Alkylation of Ammonia or Amines' and 'Formation of N/O/S Heterocycles'. The 'Reductive Alkylation' reaction shows a carbonyl group reacting with an amine to form a secondary amine. The 'Formation of N/O/S Heterocycles' reaction shows the cyclization of a substituted alkene to form a heterocyclic ring. The interface includes checkboxes for results (8,806 and 1), a group dropdown (By Transformation), a sort dropdown (Reaction Count: Descending), and a collapsed view option.

# 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

Reaction Notes

Number of Steps

Catalyst

Reagent

Solvent

Experimental Protocols

Non-Participating Functional Groups

Halide (214)

Phenyl halide (212)

Amide (66)

Alkene (62)

Cyclic alkene (58)

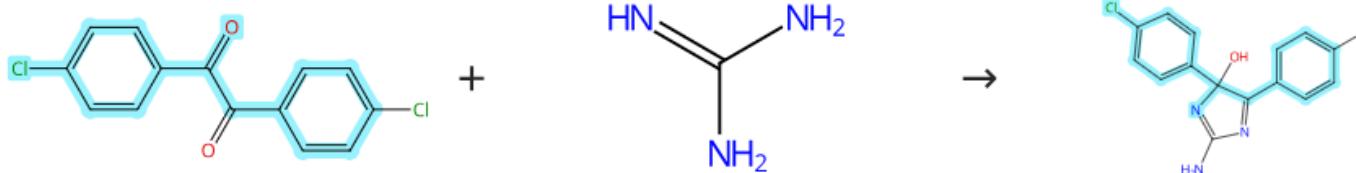
[View All](#)

Reaction Mapping

Stereochemistry

Scheme 2 (2 Reactions)

Steps: 1



[Suppliers \(71\)](#)

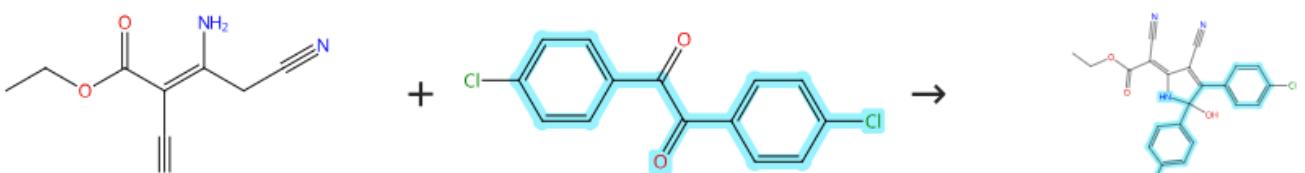
[Suppliers \(18\)](#)

[Suppliers \(2\)](#)

[Expand Scheme](#)

Scheme 3 (1 Reaction)

Steps: 1 Yield: 64%



[Suppliers \(6\)](#)

[Suppliers \(71\)](#)

[Supplier \(1\)](#)

[Expand Scheme](#)

# 3.4 联用检索——结构与关键词

关注反应的机理研究？ 联用检索提高检索效率

Chemical reaction scheme showing the Friedel-Crafts Hydroxyalkylation of Indoles with  $\alpha$ -Keto Amides using Reusa in Water. The scheme shows two reaction pathways (Scheme 1 and Scheme 2) for the synthesis of  $\alpha$ -arylo- $\alpha$ -hydroxyindoleacetamides.

**Scheme 1 (1 Reaction):** Indole +  $\alpha$ -Keto Amide  $\xrightarrow{\text{Reusa in Water}}$   $\alpha$ -arylo- $\alpha$ -hydroxyindoleacetamide

**Scheme 2 (1 Reaction):** Indole +  $\alpha$ -Keto Amide  $\xrightarrow{\text{Reusa in Water}}$   $\alpha$ -arylo- $\alpha$ -hydroxyindoleacetamide

The search interface on the left shows the following filters:

- Filter Results:
  - Analyze Results
  - Structure Match
  - As Drawn (0)
  - Substructure (6)**
- Behavior:
  - Filter by
  - Exclude
  - Search Within Results
  - Concept
  - CA Section
  - Publication Year
  - Language
  - Publication Name
  - Organization

The search results list the following entries:

- Friedel-Crafts Hydroxyalkylation of Indoles with  $\alpha$ -Keto Amides using Reusa in Water**  
By: Muthukumar, Alagesan; Sekar, Govindasamy   
Journal of Organic Chemistry (2018), 83(16), 8827-8839 | Language: English, Database: Cplus and Mplus  
In the presence of  $K_3PO_4$  and tetrabutylammonium bromide under went green Friedel-Crafts hydroxyalkylation **reactions** using  $PhCOCONHPh$  to give  $\alpha$ -aryl- $\alpha$ -hydroxyindoleacetamides such as the method relies on **reaction** at the solid-liquid interface. 11 examples were studied;  $^1H$  NMR experiments indicated that the **reaction** proceeded with high selectivity and yield.
- Experimental and computational investigation of the  $\alpha$ -amylase catalyzed Friedel-Crafts **reaction** of isatin to access symmetrical and unsymmetrical 3,3',3''-trisindoles**  
By: Kamboj, Priya; Mohapatra, Abinash; Mandal, Debasish; Tyagi, Vikas

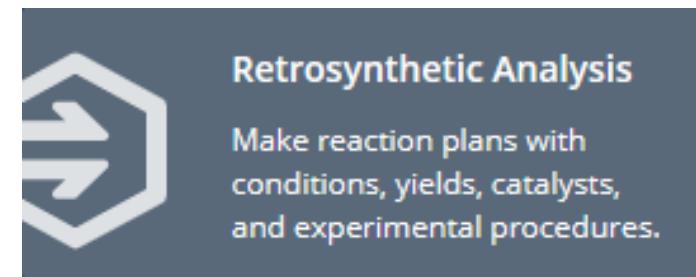
# 3.5 如何获得逆合成路线？

(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 shows a chemical structure of a complex molecule with a trifluoroethyl group, a cyclopentanone ring, and a pyrrolidine ring. The structure is annotated with stereochemistry labels (S, R, H). To the left, a sidebar displays the CAS Registry Number (2628280-40-8), the CAS Name (3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...]), and the chemical formula C<sub>23</sub>H<sub>32</sub>F<sub>3</sub>N<sub>5</sub>O<sub>4</sub>. Below these are buttons for '1,589' references, '356' suppliers, and '49' suppliers. A vertical menu on the right includes 'Get Substance Details', 'Get Life Science Data', 'Get Reactions (356)', 'Synthesize (351)', and 'Start Retrosynthetic Analysis', with the last option highlighted. At the bottom are buttons for 'Edit Structure', 'Reset', and 'Download'.

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

# 预设参数

## Retrosynthesis Plan Options for drawn structure

### Set Rules Supporting Predicted Reactions

[Learn more](#)

- Common **反应规则常见性**
- Uncommon *(includes common rules)*
- Rare *(includes common and uncommon rules)*

[Continue to Retrosynthesis Plan](#)

[Edit Structure](#)

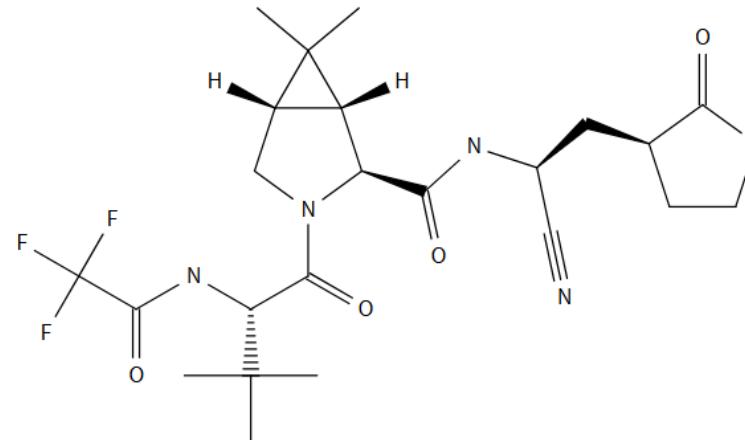
### 断裂键或保护键

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

Break Bond

Protect Bond

[Clear All Bond Selections](#)



## 逆合成路线详情

## ⇒ Retrosynthesis Plan for drawn structure

Build Status: Complete ✓    Estimated Yield: 9%    Overall Price: \$5137.82 ⓘ

## Customize Plan

Selected Options  Edit

### Predicted Rules: Common

Break and Protect Bonds: None

## Filters

 [View Excluded Options](#)

## Step Type

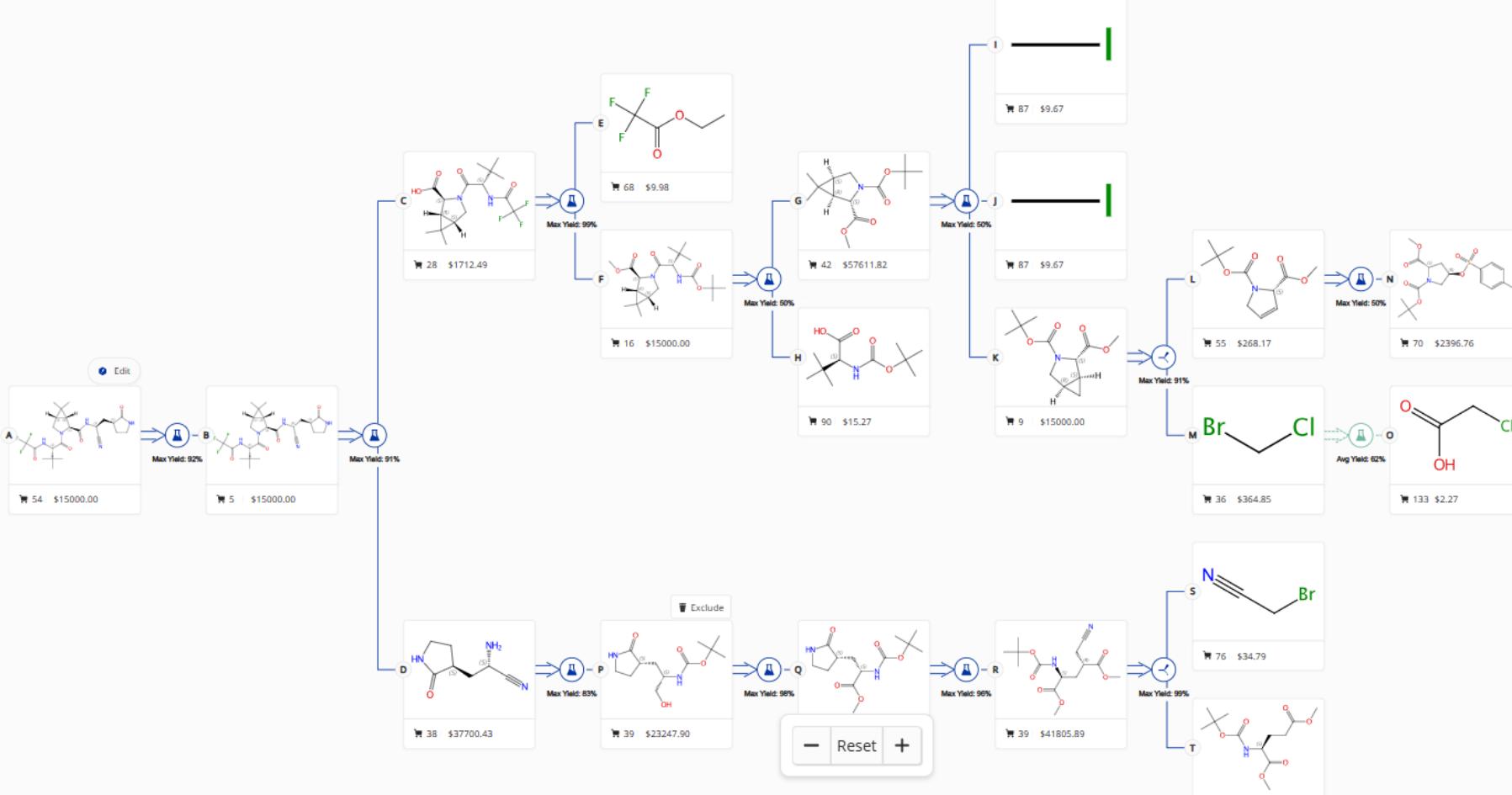
## Experimental Steps

## Predicted Steps

At least one step type must be turned on to display a plan.

300

## 起始原料费用



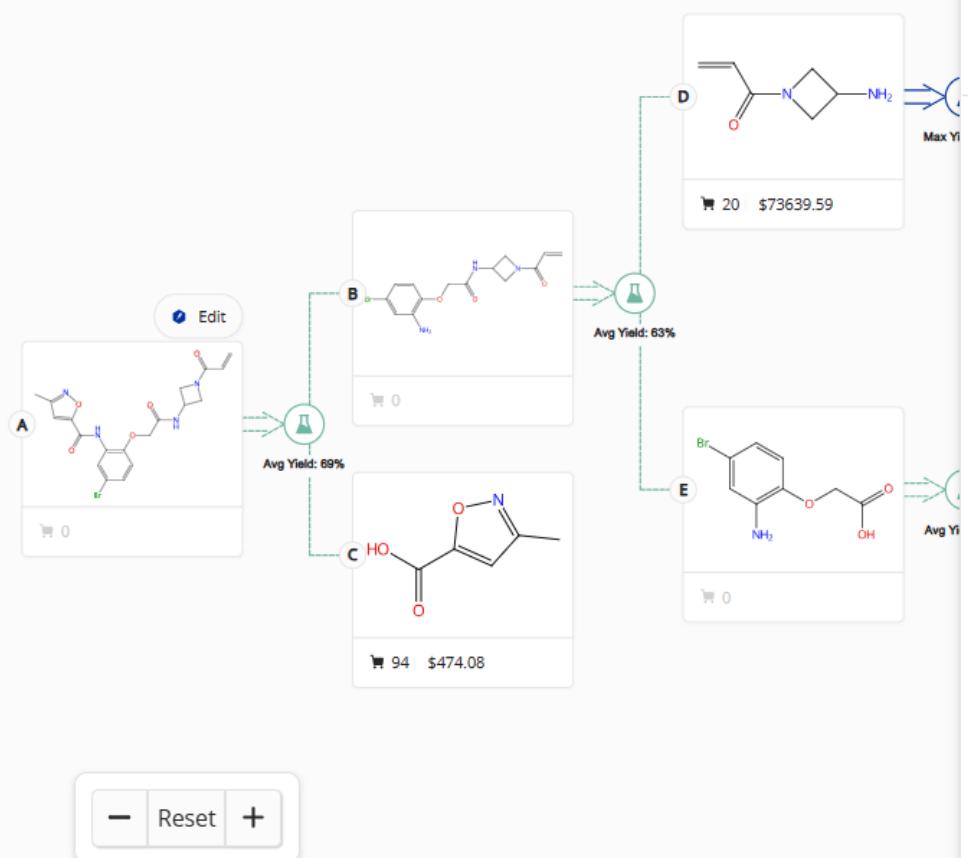


# 路线优化，考虑替换路线？

drawn structure

Build Status: Complete

Estimated Yield: 11% Overall Price: \$1047.98



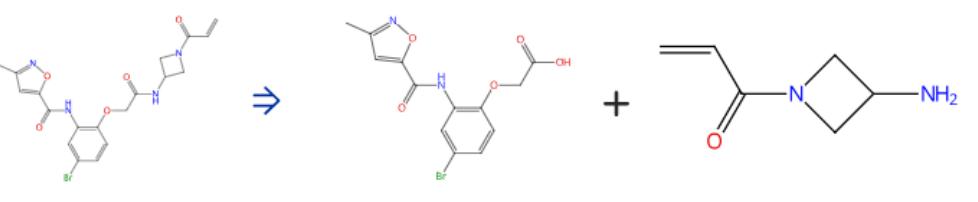
[Return to All Steps](#) 点击Alternative Steps查看并选择替换路线，得到自定义的合成路线  
  $A \Rightarrow B + C$

Evidence Alternative Steps (37)

Filters

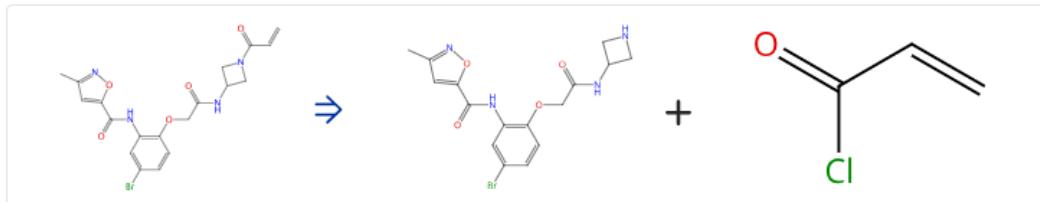
2 of 37

Predicted Step | Average Yield: 63%



3 of 37

Predicted Step | Average Yield: 63%



# 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

Get Similar Reactions

Filter Behavior

Filter by  Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (40)

Experimental Procedure (83)

Tuebingen 72076  
Germany

View: Yield: 98%

Step 1

Reaction Empowers the preparation of allyl Pure [<sup>18</sup>F]Talazoxin Vivo Evaluation as a tracer

Reagents: Hydrochloric acid, Titanium chloride (TiCl<sub>3</sub>)

Catalysts: -

Solvents: Methanol, Tetrahydrofuran, Water

Conditions: rt; 30 min, rt; 2 h, 30 - 50 °C

2

Water

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-quinoinecarboxylate, Yield: 98%

Reactants: 4-Bromobenzaldehyde, Benzoic acid, 5-fluoro-2-[2-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-5-quinoinecarboxylate, methyl ester

Reagents: Hydrochloric acid, Titanium chloride (TiCl<sub>3</sub>), Water

Solvents: Methanol, Tetrahydrofuran, Water



Procedure

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

Transformation

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

Scale

gram

Characterization Data

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

State: yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

Transformations

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

# 4.2 CAS分析实验方法详情

## Analysis of Vanadium in Stainless steel by Electrochemical extraction

CAS Method Number  
1-119-CAS-292609

Method Category  
Element Detection

Technique  
Electrothermal atomic absorption  
spectroscopy; Electrochemical  
extraction

### 实验原料

Analyte	Matrix
Vanadium	Stainless steel

Material
Al <sub>2</sub> O <sub>3</sub> cutting wheel
SiC grinding paper
0.05 μm pore size
polycarbonate filter
Standard calomel referen
<a href="#">View All</a>

### 分析仪器

#### 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

### 操作步骤

#### Instructions

##### Preparation of stainless steel process samples

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

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

1. Perform electrolytic extraction on a BioLogic SP-150 potentiostat.
2. Use 10% HCl (10 v/v% HCl, 1 w/v% tartaric acid and methanol) (~200 mL) 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.
7. Dry and weigh the steel sample.
8. Dilute the filtered electrolyte to the volume with water in a volumetric flask and subject to analysis.
9. Prepare a blank sample by filtering the blank electrolyte through a polycarbonate filter.

##### Quantification 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.

### 数据有效性

#### Validation

Linearity Range 0-400 μg/L

Recovery 0.03 wt% (0.05 wt% reference value, sample data)

### 分析条件

#### Conditions

##### Instrument

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

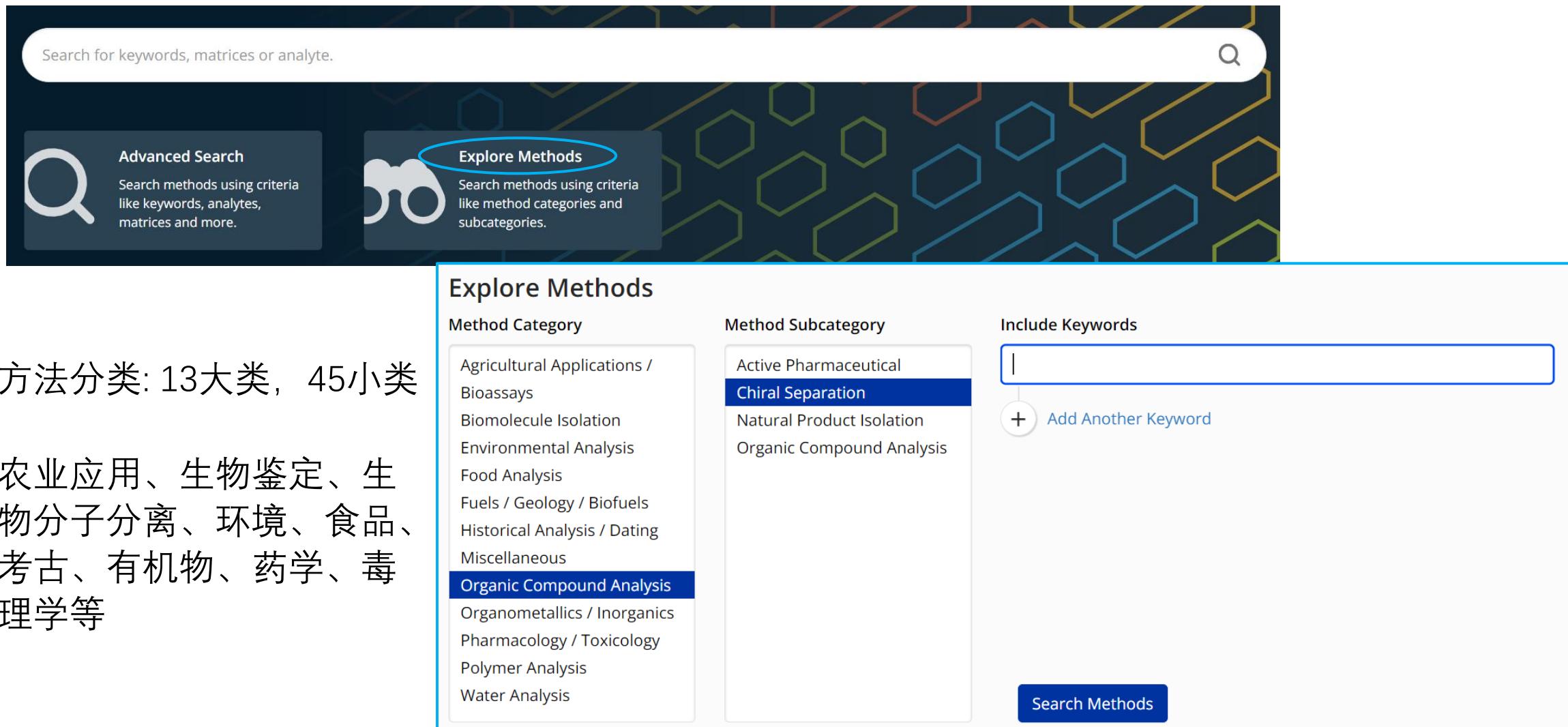
# 关注文献关联的分析方法？

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

The screenshot shows the CAS SciFinder interface. A search for "steel and impurity" has been performed, and the results are filtered by "CAS Content: Analytical Methods". There are 29 results displayed, with the first one expanded to show details. The expanded result is titled "Portable capillary electrophoresis coupled with swab-based extraction device for cleaning validation in pharmaceutical facilities" by Atia, Mostafa A. and others. The abstract discusses a method for detecting pharmaceutical residues on surfaces using a portable capillary electrophoresis instrument. The "Analytical Methods" section of the result page is highlighted, showing two links: "Analysis of Lidocaine hydrochloride in Medical cotton swabs by Capillary electrophoresis" and "Analysis of Lidocaine hydrochloride in Medical cotton swabs by Capillary electrophoresis". The left sidebar shows various filter options, with "CAS Content: Analytical Methods" selected. The bottom of the screenshot shows the footer with the CAS logo and a question mark icon.

# 直接检索感兴趣的分析实验方法

方法(1): 登录<https://methods.cas.org>, 主题检索或分类浏览



Search for keywords, matrices or analyte.

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

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

Include Keywords

**Explore Methods**

Method Category

- Agricultural Applications / 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

Method Subcategory

- Active Pharmaceutical
- Chiral Separation**
- Natural Product Isolation
- Organic Compound Analysis

Include Keywords   
+ Add Another Keyword

Search Methods

# 如何选择合适的分析方法？

The screenshot shows a search interface with the following details:

- Advanced Search:** The search terms 'steel' and 'sulfur' are entered in the 'Keyword' fields. The 'AND' operator is selected between the two terms.
- Filter By:** The results are filtered by 'Analyte' (Sulfur, Carbon, Manganese, Chromium, Copper) and 'Matrix' (Steel, Leaf, Air, Airborne particles, Soils). The 'Steel' matrix filter is selected.
- Results:** There are 22 results. The first result is a journal article titled 'Analysis of Carbon in Steel by Laser induced breakdown spectroscopy' by Jiang, X.; Hayden, P.; Costello, J. T.; Kennedy, E. T. The article discusses the use of double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet for the optimization of parameters for detection of carbon and sulfur in steel. It is published in Spectrochimica Acta, Part B: Atomic Spectroscopy (2014), 101, 106-113. Elsevier B.V.
- Article Details:** Analyte: Carbon; Sulfur; Matrix: Steel; Other Materials: Material: Spectron laser; Method Category: Element Detection; Technique: Laser induced breakdown spectroscopy; Equipment Used: Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer; CCD camera; Gas environment controls.
- Options:** View Abstract, Full Text, View in CAS SciFinder.
- Second Result:** Another article with the same title and authors, also using the same method and matrix, is listed as result 2.

关注特定的：

- ✓ 分析目标物
- ✓ 介质
- ✓ 方法类别
- ✓ 分析技术
- ✓ 验证信息类型
- ✓ 发表年份

# 如何选择合适的分析方法?

Comparing your 2 selected Methods

				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, <b>Sulfur</b> , 2.3 µg/g, Titanium, 1.1 µg/g, Vanadium, 1.0 µg/g, Chromium, 5.5 µg/g, Manganese, 8.3 µg/g, Cobalt, 12 µg/g, Nickel, 1.2 µg/g, Copper, 0.8 µg/g, Arsenic, 2.2 µg/g, Zirconium, 1.6 µg/g, Niobium, 0.2 µg/g, Molybdenum, 0.5 µg/g, Silver, 0.6 µg/g, Tin, 0.8 µg/g, Antimony, 0.5 µg/g, Tantalum, 0.9 µg/g, Tungsten, 0.4 µg/g, Lead				
				View Less ^				
Method 1		Method 2						
Analysis of Carbon in <b>Steel</b> by Laser induced breakdown spectroscopy		Analysis of Silver in <b>Steel</b> by Glow discharge spectrometry		Method	Laser-induced breakdown spectroscopic analysis using helium as ambient gas in single pulse mode		Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode	
1-119-CAS-266812		1-119-CAS-101987			1. Perform the analysis using LIBS setup containing the laser			
CAS Method Number				View All ^		View All ^		
Method Category		Element Detection		Limit of Detection	17.2 ppm, Carbon, 12.4 ppm, <b>Sulfur</b>		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, <b>Sulfur</b> , 2.3 µg/g, Titanium, 1.1 µg/g, Vanadium, 1.0 µg/g, Chromium, 5.5 µg/g, Manganese, 8.3 µg/g, Cobalt, 12 µg/g, Nickel, 1.2 µg/g, Copper, 0.8 µg/g, Arsenic, 2.2 µg/g, Zirconium, 1.6 µg/g, Niobium, 0.2 µg/g, Molybdenum, 0.5 µg/g, Silver, 0.6 µg/g, Tin, 0.8 µg/g, Antimony, 0.5 µg/g, Tantalum, 0.9 µg/g, Tungsten, 0.4 µg/g, Lead	
Technique		Laser induced breakdown spectroscopy			View All ^			
Analyte		Carbon; <b>Sulfur</b>		Precision	- 12% (RSD, reproducibility), Boron, 28% (RSD, reproducibility), Magnesium, 2% (RSD, reproducibility), Aluminum, 6% (RSD, reproducibility), Silicon, 5% (RSD, reproducibility), Phosphorus, 6% (RSD, reproducibility)		View All ^	
Matrix		<b>Steel</b>			View All ^			
Other Materials		Spectron laser		Sensitivity	- 6 - 165 cps/(µg/g)		View All ^	
Equipment Used		Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer: VM-521, Acton Research Corporation; CCD camera, <a href="#">View All ^</a>			JOURNAL			
				Source	Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet: Optimization of parameters for detection of carbon and <b>sulfur</b> in <b>steel</b>		View All ^	
					By: Jiang, X.; Hayden, P.; Costello, J. T.; Kennedy, E. T. Spectrochimica Acta, Part B: Atomic Spectroscopy (2014), 101, 106 - 113.			
				<a href="#">Full Text</a> ▾ <a href="#">View in CAS SciFinder</a>		<a href="#">Full Text</a> ▾ <a href="#">View in CAS SciFinder</a>		

## 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

The screenshot shows the CAS Formulus homepage. At the top, there are two navigation links: 'Formulations' (highlighted with a yellow underline) and 'Ingredients'. Below the navigation is a search bar with the placeholder text '原料、用途、物理形态、功能或文献识别符' (Raw material, purpose, physical form, function or literature identifier). Underneath the search bar is another search bar with the placeholder 'Search by Formulations by Ingredients, Purpose, Form, Functions, etc.' (Search by Formulations by Ingredients, Purpose, Form, Functions, etc.). To the right of this search bar is a magnifying glass icon. Below the search bars are two main sections: 'Formulation Designer' (with a dropper icon) and 'Advanced Search' (with a magnifying glass icon). The 'Formulation Designer' section includes the text 'Design custom formulation templates based on selections and ingredients'. The 'Advanced Search' section includes the text 'Search Formulations using criteria like ingredients, targets, and more.' Below these sections is a large blue button with the text '配方、制剂设计' (Formulation Design). The background of the page is dark blue.

- 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 implant"

Get Additional References

Filter by  1,154 Results Sort: Relevance ▾ Group: By Family ▾

**Industry**  Cosmetics & Personal Care  Inks, Paints, & Coatings  Pharmaceutical  Unclassified

**Purpose**  Physical Form  Pharmaceutical implants (1,154)  Gels (365)  Tablets (349)  Capsules (247)  Powders (213)

**Physical Form**  Pharmaceutical implants  Ti-TNTs wire  Acetone  Ethanol  Perchloric acid

**State of Matter**  Component Amount (1,517)  Process (1,154)  Experimental Activity (765)  Effective Dose (186)

**Delivery Route**  Document Type  Organization  Language  Publication Year

**Information Included**  Component Amount (1,517)  Process (1,154)  Experimental Activity (765)  Effective Dose (186)

1 **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	Pharmaceutical implants	-
Ti wires	Formulation excipients	-
Acetone	Solvents	-
Ethanol	Solvents	-
Perchloric acid	Formulation excipients	1

Additional group components reported

Group: Additional ingredients

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

[View Formulation Detail](#)

2 **Ophthalmic Composition: Therapy--Controlled Release, Extended-Release**  Location: Example 1, 2 Purpose: therapy Target: Homo sapiens

**JOURNAL**  
Titanium wire implants with nanotube arrays: A study model for localized cancer treatment  
Biomaterials  
Language: English  
[Full Text](#) [View in CAS SciFinder](#)

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

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

### Formulation Ingredients

Component	Function	Amount Reported	Optionality
<b>▲ Group: Ti-TNTs wire implants</b>			
Ti wires	Formulation excipients	-	Mandatory
Acetone	Solvents	-	Mandatory
Ethanol	Solvents	-	Mandatory
Perchloric acid	Formulation excipients	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...

Alimta: Folate Analog Metabolic Inhibitor  
Purpose: folate analog metabolic inhib...  
Target: Mesothelioma, non-squamous ...  
Delivery Route: intravenous  
Physical Form: Powders

Nlopoid-LMC Cyclobenzaprine Hydrochloride: Lidocaine and Menthol Kit Cyclobenzaprine...  
Purpose: Muscle relaxants  
Target: Homo sapiens, Muscle spasm, ...  
Delivery Route: Oral drug delivery syst...  
Physical Form: Tablets

Nlopoid-LMC Cyclobenzaprine Hydrochloride; Lidocaine and Menthol Kit Lidocaine 4% Menth...  
Purpose: Analgesics  
Target: Arthritis, Back pain, Homo sapi...  
Delivery Route: Topical drug delivery s...  
Physical Form: Pharmaceutical patches

Zontivity-Vorapaxar Tablet; Film Coated: Protease-Activated Receptor-1 Antagonist  
Purpose: protease-activated receptor-...  
Target: Death, Homo sapiens, ML, Stro...  
Delivery Route: Oral drug delivery syst...  
Physical Form: film coated tablet

- 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

### 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.

### 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    
Ex: binder, surfactant, carrier

Search For  Operator  Enter one term

All Fields    
General search of all fields

- 
- 
- 
- 
- 
- 
- 

- 
- 
-

# 检索原料

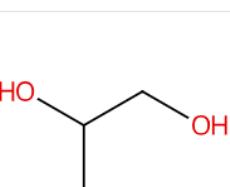
Ingredients search for "Propylene glycol"

Filter by

- 2 Results
- 1

CAS RN: 57-55-6

[View Details](#)



C3H8O2

(±)-Propylene glycol 

Propylene glycol

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

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

Similar Ingredients with Regulatory Information

- 37321-62-3 Lauroglycol
- 27194-74-7 Propylene glycol monolaurate
- 29387-86-8 Propylene glycol butyl ether

[View 14 More](#)

Commonly Formulated With | Regulatory Information | Experimental Properties

[Get Formulations](#) [Get Suppliers](#) [Add to Formulation Designer](#)

CAS RN: 107-21-1

Ethylene glycol

Formulations  Ingredients

Propylene glycol

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

- 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

# 设计配方/制剂

Formulation Designer ?

Clear All Selections

Industry	Purpose	Physical Form	Add up to 5 Ingredients
Pharmaceutical	Cosmetics and Personal care products	Emulsions	Vitamin A
<b>Cosmetics &amp; Personal Care</b>	Skin conditioners	Cream preparations	Polyethylene glycol
Agrochemical	Sunscreens	Cosmetic lotions	
Cleaning & Surfactant Products	Hair dyes	Cosmetic packs	
Inks, Paints, & Coatings	Hair preparations	<b>Gels</b>	+ Add Another Ingredient
Food & Related	Antiperspirants	Liquids	
	Cleaning compositions	Powders	
	Skin cleansers	Solutions	
	Skin-lightening cosmetics	Nanospheres	
	Oral hygiene products	Pastes	
	<b>Skin care products</b>	- View More Physical Forms -	
	- View More Purposes -		

**Create Template**

# 设计配方/制剂

Formulation Designer [?](#)

Clear All Selections

Industry	Purpose	Physical Form	Active or Featured Ingredient
Cosmetics & Personal Care	Skin care products	Gels	Vitamin A Polyethylene glycol

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

Your Template

Function	Ingredient	Regulatory	Top Alternatives	Amounts
Active or Featured Ingredient:	Vitamin A	ANMAT; NMPA	-	Amount not available <a href="#">X</a>
Active or Featured Ingredient:	Polyethylene glycol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available <a href="#">X</a>

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

Carriers	Ingredient	Regulatory	Top Alternatives	Amounts
	Ethylene glycol	Cosing: Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Water; Polyethylene glycol	Approximate Range
	<a href="#">View More Alternatives</a>			

Skin conditioners	Ingredient	Regulatory	Top Alternatives	Amounts
	Ethylene glycol	Cosing: Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Glycerol; Allantoin; 1,2-Octanediol; Tricaprin; Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated	Approximate Range
	<a href="#">View More Alternatives</a>			

- 原料详情
- 原料管制信息
- 可替代的原料选项

## Alternative Ingredients (Showing all 7)

Select the ingredient you would like to use:

Glycerol	Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated	Glyceryl polyacrylate <i>N</i> -(2-Hydroxyethyl)acetamide
Allantoin		
1,2-Octanediol		
Tricaprin		

# 文献关联的配方/制剂

方法 (2) : 在CAS SciFinder的文献结果集页面, 点击CAS Content中的 Formulations 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""

View Related Results ▾

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

Load All Results

Filter Results

Analyze Results

Behavior

Filter by Exclude

Search Within Results

Concept

Formulation Purpose

CA Section

CAS Content

Formulations (37)

Analytical Methods (7)

Filtering: CAS Content: Formulations X

Clear All Filters

37 Results

Sort: Relevance ▾ View: Full Abstract ▾

1

**Preparation and characterization of alginate and alginate-resistant starch microparticles containing nisin**

By: Hosseini, Seyede Marzieh; Hosseini, Hedayat; Mohammadifar, Mohammad Amin; German, J. Bruce; Mortazavian, Amir Mohammad; Mohammadi, Abdorreza; Khosravi-Darani, Kianoosh; Shojaee-Aliabadi, Saeedeh; Khaksar, Ramin  
Carbohydrate Polymers (2014), 103, 573-580 | Language: English, Database: CPlus and MEDLINE

Delivery systems with sustained release of nisin have been proposed to improve stability and long-term effectiveness of this bacteriocin in foods. In this study, nisin was encapsulated in alginate (Alg) and alginate-resistant starch (Alg-RS) microparticles and its release was investigated. Studies found that the nisin concentration has significant influence on encapsulation efficiency (EE), loading capacity (LC) and size of both microparticles. Furthermore, encapsulation efficiency and loading capacity values were more increased by the addition of resistant starch to the alginate formulation. The highest encapsulation efficiency was obtained with Alg-RS microparticles prepared using initial nisin to alginate weight ratio of 25% weight/weight ( $59.77 \pm 2.26\%$ ). Fourier transform-IR (FT-IR) spectroscopy, X-ray diffraction (XRD) and differential scanning calorimetry (DSC) results confirmed the presence of nisin in the microparticles. The in vitro nisin release from these microparticles followed a controlled-release pattern consistent with a Fickian diffusion mechanism. The release rate from Alg-RS microparticles was less than that from the Alg microparticles.

Full Text ▾ 3 0 96

2

**Maize and resistant starch enriched breads reduce postprandial glycemic responses in rats**

By: Brites, Carla M.; Trigo, Maria J.; Carrapico, Belmira; Alvina, Marcela; Bessa, Rui J.  
Nutrition Research (New York, NY, United States) (2011), 31(4), 302-308 | Language: English, Database: CPlus and MEDLINE

White wheat bread is a poor source of dietary fiber, typically containing less than 2%. A demand exists for the development of breads with starch that is slowly digestible or partially resistant to the digestive process. The utilization of maize flour and resistant starch is expected to reduce the release and absorption of glucose and, hence,

定位配方或制剂的功能目标

## Formulation Purpose

- Food (7)
- Antidiabetic agents (6)
- Dietary supplements (6)
- Drug delivery systems (4)
- Antimicrobial agents (2)

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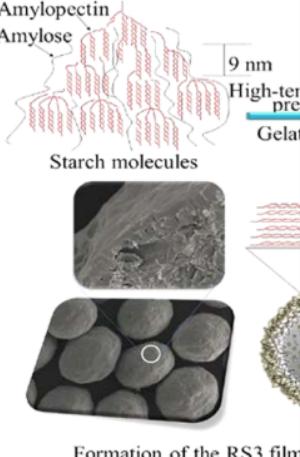
# 文献关联的配方/制剂

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

By: Situ, Wenbei; Chen, Ling; Wang, Xueyu; Li, Xiaoxi  
DOI: 10.1021/jf500472b

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 with different insulin dosages after oral administration; no glycopenia system has been demonstrated for the accurate delivery of bioactive po

**Formation of the RS3 film**



**Formulations**

**Formulation Title**

- Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems
- Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems
- Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems or Antidiabetic Agents--Controlled Release Drug Delivery Systems
- Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems
- Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems
- Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems
- Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems
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**Keywords:** starch film coated microparticle colon polypeptide delivery

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1. 利用Synthetic Methods™查看文献中合成方法详情
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# 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



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浏览器推荐：

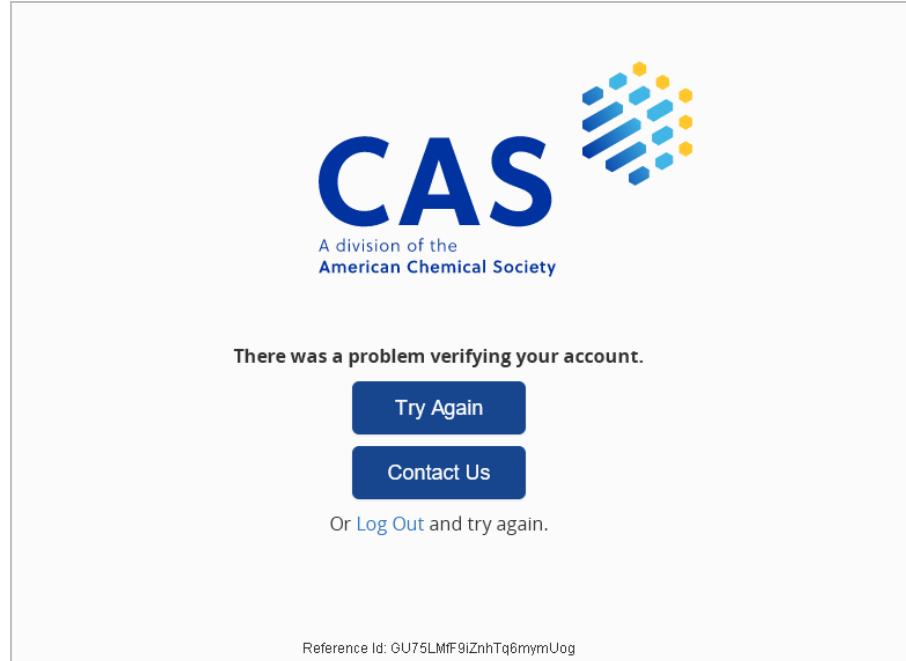
- Windows (7, 8.1, 10): Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13): Safari 9.3及更高版本, Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)
- **不建议使用360浏览器，相关功能或插件会被自动拦截**

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

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



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

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- 不得账号分享
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# THANK YOU!



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