

# CAS SciFinder Discovery Platform

## 全面高效获取科研信息



刘子露 博士

Zilu@acs-i.org

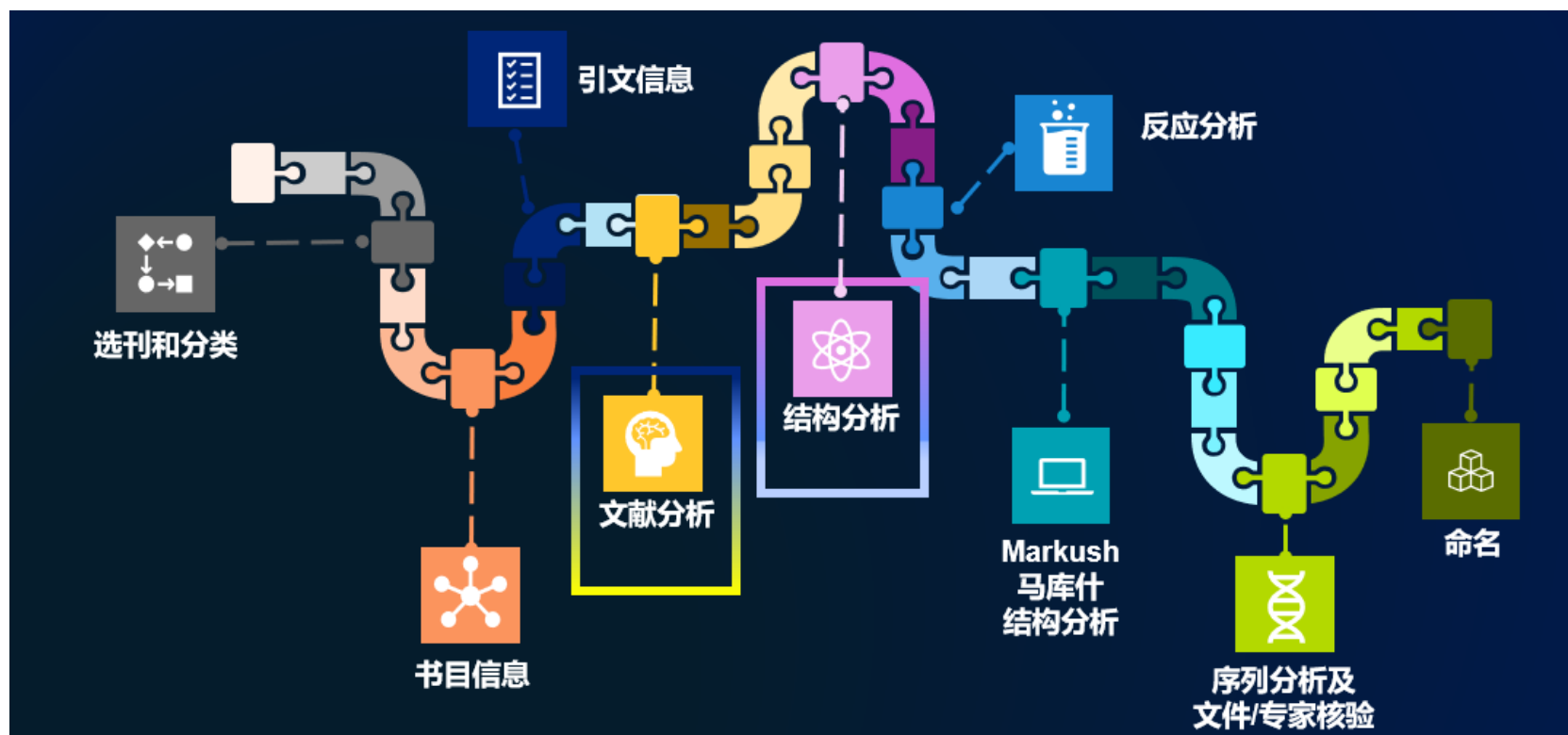
美国化学文摘社(CAS)北京代表处

# 大纲

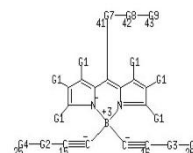
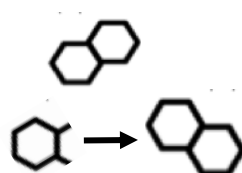
- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 如何拓展文献调研?
  - 如何调研某类物质?
  - 如何调研反应信息?
  - 怎么查、怎么选具体的实验方案?
- 常见问题Q&A



# CAS 科学家的智力标引



1990  
Smith, M.  
anthracene



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

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘



# CAS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**

Article  
pubs.acs.org/jmc

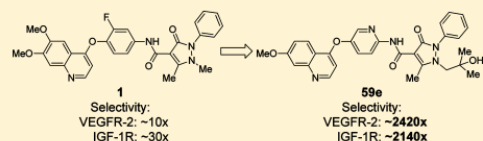
## Structure-Based Design of Novel Class II c-Met Inhibitors: 2. SAR and Kinase Selectivity Profiles of the Pyrazolone Series

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>

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<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).<sup>1</sup> 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 overexpression 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 multitargeted kinase 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

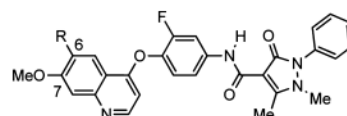
ACS Publications | © 2012 American Chemical Society | 1868

[doi.org/10.1021/jm201331s](https://doi.org/10.1021/jm201331s) | J. Med. Chem. 2012, 55, 1868–1897

Journal of Medicinal Chemistry

Article

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

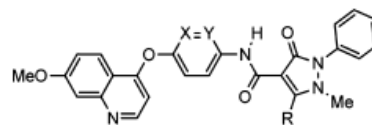


compd	R	c-Met	VEGFR-2		IGF-1R		PC3
		K <sub>i</sub>	K <sub>i</sub>	fold	K <sub>i</sub>	fold	
<b>1</b>	OMe	1	7.8	8	32.1	32	20.2
<b>11a</b>	Br	5.1	78.9	16	149	29	652
<b>11b</b>	Me	3.4	—	—	146	43	461
<b>11c</b>	Et	2.4	38	16	70.2	29	534
<b>11d</b>	H	1.1	23.7	22	178	162	37.1

<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.

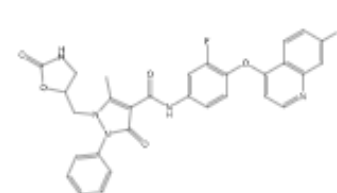
Journal of Medicinal Chemistry

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



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

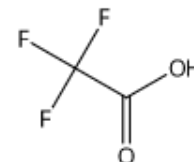
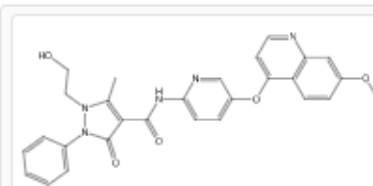
1361236-60-3



**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, Preparation, Uses

1374343-52-8



**C<sub>28</sub>H<sub>25</sub>N<sub>5</sub>O<sub>5</sub>·xC<sub>2</sub>H<sub>5</sub>F<sub>3</sub>O<sub>2</sub>**  
*1H*-Pyrazole-4-carboxamide, 2,3-dihydro-1-(2-hydroxyethyl)-*N*-[(7-methoxy-4-qui...

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

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

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

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

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

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<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

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First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username:  [Tips](#)

Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer:  [Why?](#)

请注意：

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

- - (破折号)
  - \_ (下划线)
  - . (句点)
  - @ (表示“at”的符号)
- 3.密码必须包含 7-15 个字符，并且至少包含**三种以下字符**：
- 字母
  - 混合的大小写字母
  - 数字
  - 非字母数字的字符（例如 @、#、%、&、\*）

例：abc@123

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

## Registration Already Complete


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

点击激活链接后注册成功

通过<https://SciFinder-n.cas.org>访问



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




**CAS**  
SciFinder

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Log In

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使用CAS SciFinder账号登录

# CAS SciFinder主界面

The screenshot displays the CAS SciFinder homepage. On the left is a sidebar menu with categories: LIFE SCIENCES (CAS BioFinder), CAS SCIFINDER DISCOVERY PLATFORM (CAS SciFinder, CAS Analytical Methods, CAS Formulus), STN IP PROTECTION SUITE (CAS STNext, CAS Scientific Patent Explorer), REGULATORY (CAS Chemical Compliance Index), and ACCOUNT MANAGEMENT (CAS Profile). The main header includes the CAS SciFinder logo, a notification bell, a settings icon, and a user profile icon, with a blue box labeled '更新结果提醒' (Update results reminder) above the bell. Below the header, a personalized greeting 'Good Afternoon,' is followed by a search bar containing the text 'Proton nmr spectral data for C13H13Br'. To the right of the search bar is a 'Draw' button with a structure icon, highlighted by a yellow box and labeled '结构绘制面板' (Structure drawing panel). Below the search bar is a 'Featured Search' section with six tiles: 'Prior Art Discovery' (highlighted with a purple box and labeled '现有技术探索'), 'Patent Markush' (highlighted with a blue box and labeled '专利Markush检索'), 'Advanced Search' (highlighted with a blue box and labeled '高级检索选项'), 'Retrosynthetic Analysis' (highlighted with a blue box and labeled '逆合成路线设计'), 'Search CAS Lexicon' (highlighted with a blue box and labeled 'CAS词库'), and 'Search CAS Sequences' (highlighted with a blue box and labeled 'CAS序列检索'). At the bottom, the 'History' tab is selected, showing a 'Recent Search History' section with a table of search results. The first entry is dated 'September 9, 2025' and has the search text 'reduction of aldehyde catalysed by cobalt'. A blue box labeled '近期检索历史' (Recent search history) points to this section. A 'Rerun Search' button is located at the end of the search entry.

CAS SciFinder

更新结果提醒

检索结果管理和账号设置

结构绘制面板

Good Afternoon,

Proton nmr spectral data for C13H13Br

Featured Search

Prior Art Discovery  
Discover prior art in patents and non-patent literature using AI-enhanced search technologies.

Patent Markush  
Search Patent Markush by structure and view associated references.

Advanced Search  
Select data fields and search operators to create a focused query.

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

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

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

现有技术探索

专利Markush检索

高级检索选项

逆合成路线设计

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History For You

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View All Search History

September 9, 2025

Search All

reduction of aldehyde catalysed by cobalt

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？

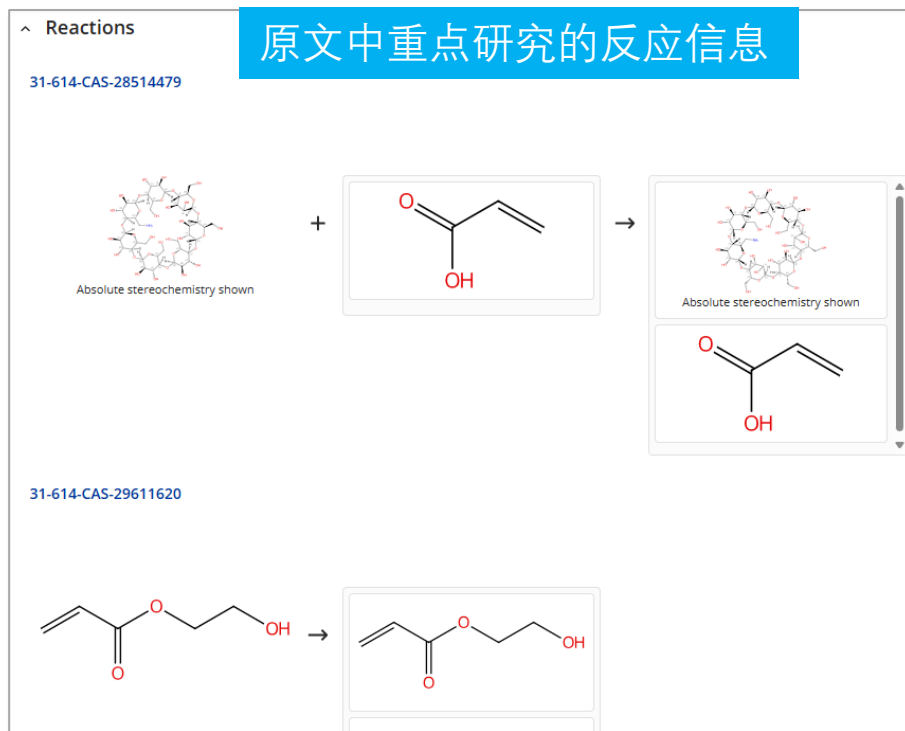
# 已知文献标识符

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 displays the CAS SciFinder web interface. At the top, the CAS SciFinder logo is on the left, and navigation tools like 'References', 'Draw', and a search bar are on the right. The main search bar contains the query '"Elasticity dependent fast underwater adhesion demonstrated by macroscopic"'. Below the search bar, there's a 'View Related Results' button and a 'View: Full Abstract' dropdown. On the left side, a 'Filter Results' panel is visible, with options to 'Analyze Results' and 'Filter by' (selected) or 'Exclude'. The search results section shows '1 Result' and a list of results. The first result is highlighted with a blue box and contains the title 'Elasticity-Dependent Fast Underwater Adhesion Demonstrated by Macroscopic Supramolecular Assembly'. Below the title, the authors are listed: 'By: Ju, Guannan; Cheng, Mengjiao; Guo, Fengli; Zhang, Qian; Shi, Feng'. The journal information is 'Angewandte Chemie, International Edition (2018), 57(29), 8963-8967 | Language: English, Database: CAPLUS and MEDLINE'. The abstract text follows: '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)'. At the bottom of the result, there's a 'Full Text' dropdown and a row of icons with counts: a cube icon with '14', a flask icon with '2', a quote icon with '82', and a circular arrow 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



## 原文中重点研究的反应信息

^ Substances

原文中重点研究的物质信息

1200829-09-9

1122464-65-6

59765-68-3

57033-29-1

$C_{10}H_{17}N.C_3H_4O_2$   
2-Propenoic acid, compd. with tricyclo[3.3.1.1<sup>3,7</sup>]decan-1-amine (1:1)  
Role: Properties

$C_{42}H_{71}NO_{34}.x(C_3H_4O_2)_x$   
 $\beta$ -Cyclodextrin, 6<sup>A</sup>-amino-6<sup>A</sup>-deoxy-, compd. with 2-propenoic acid homopolymer  
Role: Reactant, Reactant or Reagent

$(C_7H_{10}N_2O_2.C_5H_8O_3.C_3H_5NO)_x$   
2-Propenoic acid, 2-hydroxyethyl ester, polymer with *N,N'*-methylenebis[2-propenoic acid]  
Role: Properties, Synthetic Preparation, Preparation

$(C_7H_{10}N_2O_2.C_5H_8O_3)_x$   
2-Propenoic acid, 2-hydroxyethyl ester, polymer with *N,N'*-methylenebis[2-propenoic acid]  
Role: Properties, Synthetic Preparation, Preparation

## 物质角色

## ^ Concepts

## CAS科学家提供的标准技术术语

Adhesion, physical

Modifier: **underwater**

Elasticity

Gelatin

Modifier: copolymer with dimethylacrylamide

Role: Properties

Hydrogels

Multilayers

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-tetrafluoropropane

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-tetrafluoropropane (HCFC-244bb) from a reactant stream including 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-trifluoropropane (HCFC-253db), which may be separated from the product composition. 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
IN2020754-12-1		

CAS RN 754-12-1  
CAS Name 2,3,3,3-Tetrafluoropropene

Get Substance Details  
Get Bioactivity Data  
Get Reactions (1,467)  
Synthesize (1,150)  
Start Retrosynthetic Analysis  
Get References (3,783)  
Get Suppliers (23)

Edit Structure Reset

C=C(F)(F)F(F)F

CAS PatentPak

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### Key Substances in Patent

CAS RN 754-12-1

C=C(F)(F)F(F)F

Analyst Markup Locations (1)  
Page 7

CAS RN 421-73-8

CC(F)(F)C(F)(F)Cl

Analyst Markup Locations (1)  
Page 8

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 (Na<sub>2</sub>CO<sub>3</sub>/H<sub>2</sub>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

modified within the spirit and scope of this disclosure. Further, this application is intended to cover such departures from the present disclosure as come within known or customary practice in the art to which this disclosure pertains.

The invention claimed is:

1. A method for producing 2-chloro-1,1,1,2-tetrafluoropropane (HCFC-244bb), comprising the steps of: providing a reactant stream including a mixture of HCFC-244bb and 2-chloro-3,3,3-trifluoropropene (HCFO-1233xf), the amount of HCFO-1233xf between 5 wt. % and 25 wt. % based on a total weight of the reactant stream; and hydrogenating the HCFO-1233xf of the reactant stream in a vapor phase in the presence of hydrogen gas and a

US 10,125,066 B1

13

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-trifluoropropane (HCFC-253db).

14

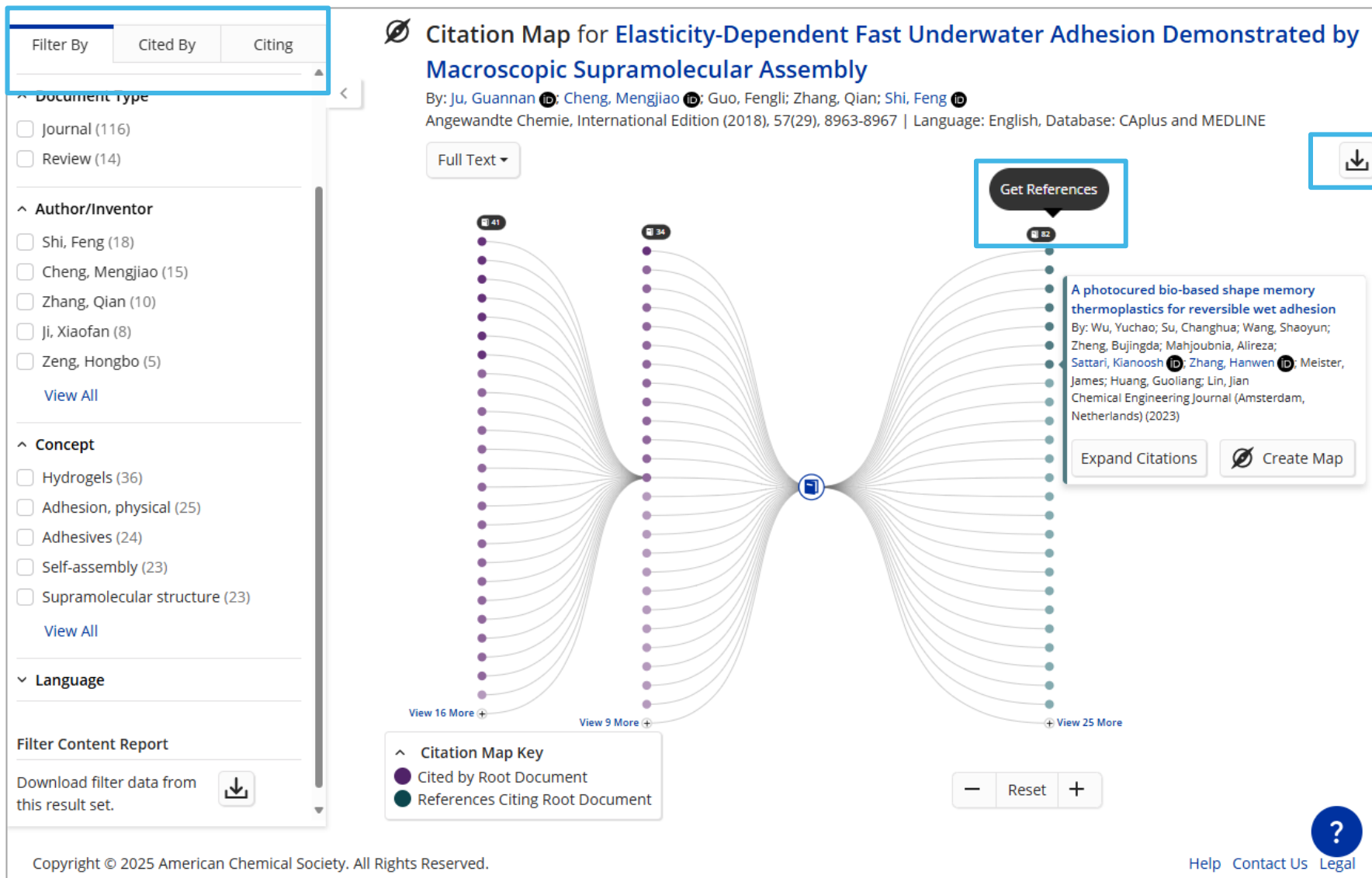
catalyst and the alpha aluminum support, at a temperature between 100° C. and 250° C. to generate a product composition including unreacted HCFC-244bb and 2-chloro-1,1,1-trifluoropropane (HCFC-253db); and separating the HCFC-244bb and the HCFC-253db.

11. The method of claim 10, further comprising the

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- 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）

在CAS Lexicon词库层级中选择适合的主题词：

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

The screenshot displays the 'Search CAS Lexicon' interface. At the top, there is a search bar containing 'Neoplasm' and a 'Search Concept' button. Below the search bar, the results for 'Neoplasm' are shown under the 'Preferred Concept' section. The results include a list of synonyms and a list of broader concepts (1) and narrower concepts (76). A blue box highlights the 'Personalized medicine - Preferred Concept' section, which is added to the query. Below this, a blue box highlights the 'Preferred Concept' section for 'Personalized medicine', showing its synonyms and a 'View fewer synonyms' link. At the bottom, there are buttons for 'AND', 'OR', 'NOT', 'Add to Query', 'Clear Query', and 'Search'.

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

Neoplasm [Search Concept](#)

^ 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

Personalized medicine - Preferred Concept

AND [Remove All](#)

Neoplasm - Preferred Concept

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

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

# 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



Good Evening

("Boron nitride" or BN) and (2D or "two dimensional")

porous

Porous Zol  
Porous COF  
Porous HOF  
Porousblack  
Porous Star  
Porous MOFs  
Porous COFs  
Porous film  
Porous HOFs  
Porous SiLK

自动提示检索词,  
启发检索思路

# 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 ▾

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

12,503 Results

Sort: Relevance ▾ View: Full Abstract ▾

1

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

By: Du, Chunyan; Zhang, Zhuo; Yu, Guanlong; Wu, Haipeng; Chemosphere (2021), 272, 129501 | Language: English, Database: CAPLUS and MEDLINE

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 adsorption for researchers intending to use MOFs to remove antibiotics from water.

Full Text ▾ 0 0 262

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](#)

Filter Results <

Analyze Results

Behavior

Filter by Exclude

Search Within Results

Concept

224 Results

Sort: Relevance ▾ View: Full Abstract ▾

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: CAPLUS 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 methodology.

Full Text ▾ 4 0 415

2

**Polyoxovanadometalate-catalyzed selective epoxidation of alkenes with hydrogen peroxide**

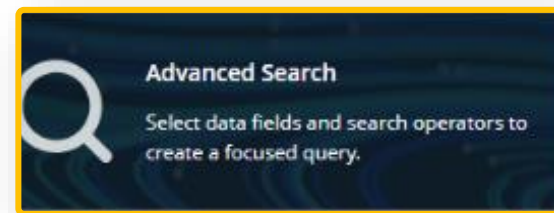
By: Nakagawa, Yoshinori; Kamata, Keigo; Kotani, Miyuki; Yamaguchi, Kazuya; Mizuno, Noritaka Angewandte Chemie, International Edition (2005), 44(32), 5136-5141 | Language: English, Database: CAPLUS and MEDLINE



# 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）



AND  
OR  
NOT

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

**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

CO2 and "catalytic hydrogenation" × Draw Q

AND

Publication Name

Chem

×

Volume (Optional)  
Chem  
Chemisches Zentralblatt

AND

Abstract/Keywords

Chemical Engineering Journal (Amsterdam, Netherlands)  
Chemical Physics Letters  
Chemical Communications (Cambridge, United Kingdom)  
Chemosphere  
Chemistry - A European Journal  
ChemRxiv  
Chemical Engineering Science  
Chemistry Letters

×

AND

Title

×

AND

Concept

×

+ Add Advanced Search Field

Search

# 1.3 文献结果：最新 & 引用最多 & 早期科学研究

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

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, 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: CAPus 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.

Full Text ▾ 13 0

Filter Results

Analyze Results

Behavior

Filter by Exclude

Search Within Results

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

排序方式：  
相关性  
引用次数  
收录号  
发表时间

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CAS SciFinder

References ▾ solar cell

Filter Behavior

Filter by Exclude

Search Within Results

Concept

Database

☐ CAPus (374K)  
☐ MEDLINE (31K)  
☒ **CHEMZENT (2,238)**

Filtering: Database: CHEMZENT X

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. Hypogeic 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

# 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

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

Substances

Reactions

Citing

Filter Results

Analyze Results

Behavior

Filter by

Exclude

Search Within Results

Concept

Formulation Purpose

CA Section

CAS Content

Publication Year

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, 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: CAlus 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

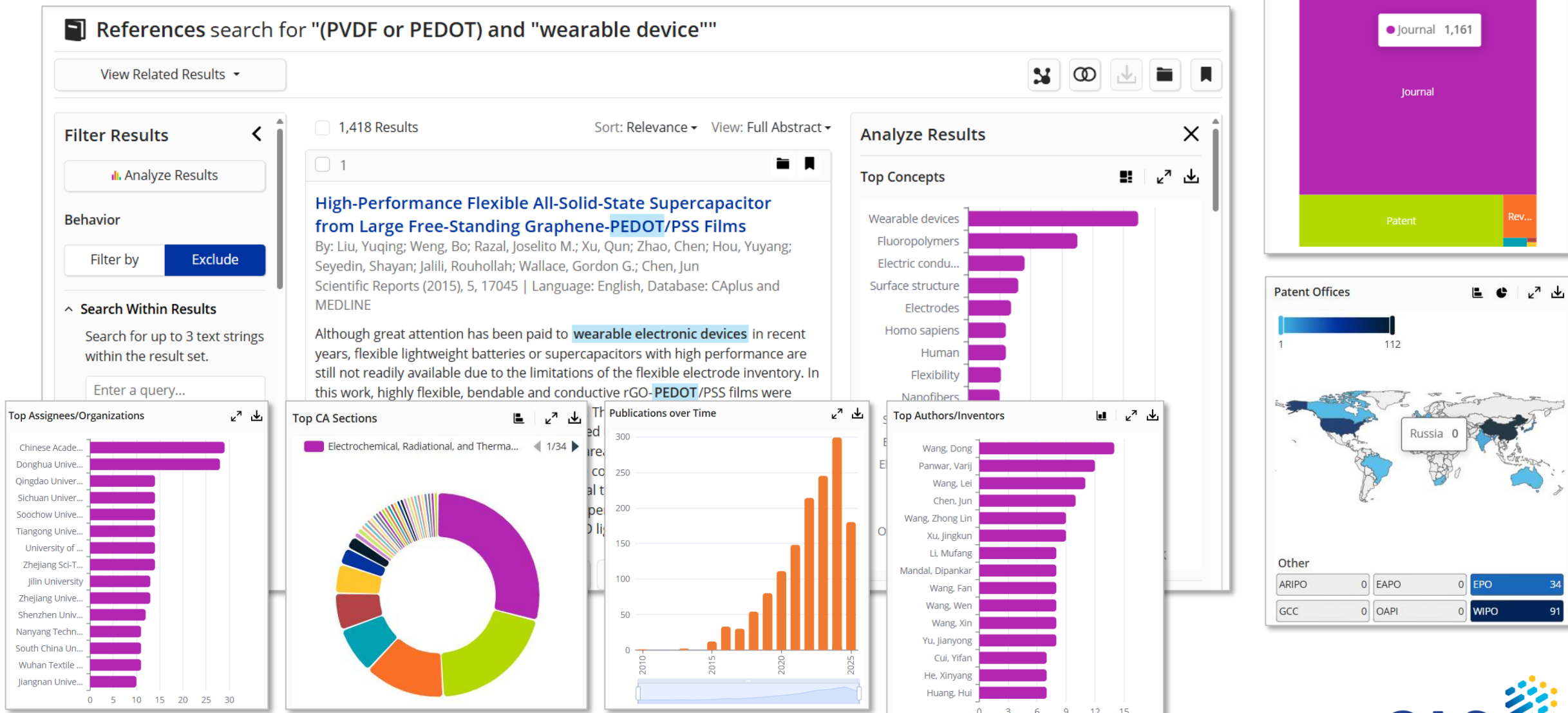
Biosensors & Bioelectronics (2021), 175, 112879 | Language: English, Database: CAlus and MEDLINE

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 portable anal. tools that remove the need for external detection systems. This work describes the construction, by screen-printing, of a self-powered

数据关联

可视化分析

# 可视化的结果筛选和分析



# 筛选工具 CAS Section & Concept

CA Section

By CountAlphanumeric

学科研究方向

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)

☐ 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 CountAlphanumericSearch

纵览并精准定位核心研究点

7 Selected

☐ Wearable devices (501)

☒ Current density (50)

☒ Coating materials (30)

☐ Fluoropolymers (343)

☒ Hydrogels (50)

☐ Electrolytes (29)

☐ Electric conductivity (155)

☐ Humans (48)

☐ Sheet resistance (29)

☐ Electrodes (128)

☒ Surface structure (124)

☐ Homo sapiens (117)

☐ Human (117)

☐ Nanofibers (101)

☐ Electric current-potential relationship (100)

☐ Polyesters (92)

☐ Carbon nanotubes (86)

☒ Flexibility (84)

☐ Stress-strain relationship (83)

☐ Electrospinning (82)

Apply

Cancel

Concept

Top CountAlphanumericSearch

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)

☐ Cellulosic nanofibers (1)

☒ Core-shell nanoparticles (1)

☐ Electric nanogenerators (24)

☒ Metal Nanoparticles (3)

☐ Nanofibril (2)

☒ Nanofilms (6)

☐ Nanofilters (1)

☒ Nanoflakes (2)

☐ 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

合并、交集和去重

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

View Related Results ▾

## Filter Results

Analyze Results

## Behavior

Filter by

Exclude

## Search Within Results

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

Enter a query...

Search

Searching for...

Clear All

dop\*

×

✓ Concept

✓ CA Section

✓ CAS Content

Filtering: Concept: Hydrogels ✕

Excluding: Search Within Results: dop\* ✕

104 Results

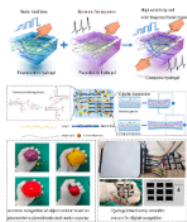
Sort: Relevance ▾ View: Full Abstract ▾

1

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

By: Hu, Zhirui; Li, Jie; Wei, Xiaotong; Wang, Chen; Cao, Yang; Gao, Zhiqiang; Han, Jing; Li, Yingchun

ACS Applied Materials & Interfaces (2022), 14(40), 45853-45868 | Language: English, Database: CAPLUS and MEDLINE



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

0

Save Results

定题追踪

Name

Wearable device

Search Options

☐ Query Only ☐ Selected Answers ☒ All Answers (Up to 20,000)

Add Existing Tags (Optional)

☐ Aero  
☐ Alloys  
☐ Archaeology  
☐ Biotech  
☐ catalyst

New Tag (Optional)

Add tag name

Tag Color

Light Blue

Alerts

Frequency

As Available

Add Email(s)

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

Save

Cancel

# 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

CAS SciFinder

References Organic photovoltaic cell

References search for "Organic photovoltaic cell" + drawn structure

View Related Results

Structure Match

As Drawn (0)

Substructure (1,303)

Behavior

Filter by Exclude

Search Within Results

Concept

CA Section

Publication Year

Language

English (136)

Chinese (25)

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: CAPlus

Patent Status: Alive

Substance Role

Uses (1,203)

Properties (712)

Preparation (180)

Process (170)

Synthetic Preparation (167)

Nanoscale (5)

View All

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

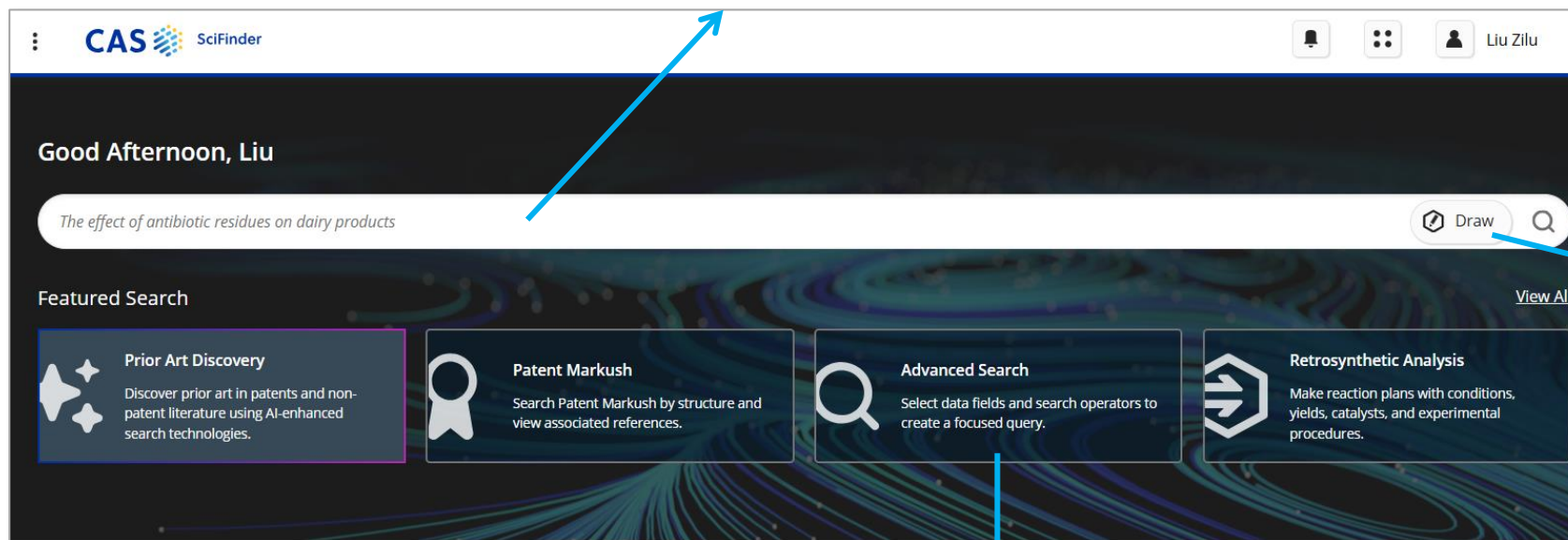
1. 利用引文地图拓展文献检索
2. 检索词的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
3. 利用丰富的筛选工具，快速获得目标文献
4. 主题词+结构联合检索快速获得文献

## 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



- 使用结构绘制面板进行结构检索

- 高级检索

## 检索策略推荐

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



# 物质检索—物质/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

CAS SciFinder Substances search for "isotac\*" + drawn structure

View Related Results

Filter Results

Structure Match

As Drawn (24)

Substructure (69)

Similarity (47)

Analyze Structure Precision

Behavior

Filter by Exclude

Search Within Results

Reference Role

Preparation (24)

Synthetic Preparation (23)

Properties (18)

24 Results

1 25086-18-4 (C<sub>8</sub>H<sub>8</sub>)<sub>x</sub> Isotactic polystyrene

2 114028-92-1 (C<sub>8</sub>H<sub>8</sub>, C<sub>3</sub>H<sub>6</sub>)<sub>x</sub> Components: 2 Isotactic propylene-styrene graft copolymer

3 198351 (C<sub>8</sub>H<sub>8</sub>, C<sub>2</sub>H<sub>4</sub>)<sub>x</sub> Components: 2 Isotactic propylene-styrene graft copolymer

1,070 60 8

64 17 0

20 1 0

CAS SciFinder Substances search for "10.1039/c3py00121k"

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Reference Role

Preparation (15)

Synthetic Preparation (15)

Properties (12)

Technical or Engineered Material Use (12)

Uses (12)

View All

Substance Class

Aromatic Rings

Reaction Role

Element

Functional Group

Polymer Class

15 Results

1 68-12-2 C<sub>3</sub>H<sub>7</sub>NO Formamide, N,N-dimethyl-

2 109-72-8 C<sub>4</sub>H<sub>9</sub>Li Lithium, butyl-

3 609771-63-3 C<sub>82</sub>H<sub>14</sub>O<sub>2</sub> 3'-H-Cyclopropa[8.25][5.6]fullerene-C70-D5N(6)-3'-butan oic acid, 3'-phenyl-, meth...

4 79-40-3 C<sub>2</sub>H<sub>4</sub>N<sub>2</sub>S<sub>2</sub> Ethanedithioamide

5 C<sub>74</sub>H<sub>90</sub>S<sub>4</sub>Sn<sub>2</sub> Stannane, 1,1'-[6,6,12,12-tetrakis(4-hexylphenyl)]-6,12 -dihydrodithieno[2.3-d:2'...

200K 4.7M 308

30K 611K

7,698 69 62

2,009 1,008 78

128 160 16

Relevance

CAS RN: Ascending

CAS RN: Descending

Molecular Formula: Ascending

Molecular Formula: Descending

Molecular Weight: Ascending

Molecular Weight: Descending

Number of References: Ascending

Number of References: Descending

Number of Suppliers

物质排序：相关度、CAS RN、分子式、分子量、文献量、供应商数量

## 2.1 分子式检索： 高效检索聚合物或无机化合物

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：高熵碳化物 C.Hf.Nb.Ta.Ti.Zr
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性  $\text{Na}_2\text{SO}_4$ :  $\text{H}_2\text{O}_4\text{S}.2\text{Na}$

$(\text{C}_2\text{H}_4\text{O})_n\text{H}_2\text{O}$ : 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](#) [Q](#)

**Search Fields:**

- Molecular Formula** (Examples: C<sub>6</sub>H<sub>6</sub> | (C<sub>8</sub>H<sub>8</sub>)<sub>x</sub> | C<sub>22</sub>H<sub>26</sub>CuN<sub>2</sub>O<sub>5</sub>.C<sub>2</sub>H<sub>3</sub>N)
- Substance RN** (Examples: 57-88-5 | 101600)
- Component RN** (Examples: 120-12-7 | 71432)
- Chemical Name**

**Advanced Search Fields:**

- Experimental Spectra**
  - Proton NMR
  - Carbon-13 NMR
  - Nitrogen-15 NMR
  - Fluorine-19 NMR
  - Phosphorus-31 NMR
- Life Science Data
- Biological
- Chemical Properties
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal

**Chemical Properties:**

- 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：<sup>1</sup>H, <sup>13</sup>C, <sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>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℃

Substances References Clear All

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

Filter by Exclude

Search Within Results

Reference Role

Substance Class

- ☒ Polymer (33)
- ☐ Element (19)
- ☐ Alloy (9)
- ☐ Manual Registration (8)
- ☐ Organic/Inorganic Small Molecule (5)

View All

Aromatic Rings

Reaction Role

Element

Functional Group

Polymer Class

Number of Components

Filtering: Substance Class: Polymer X Clear All Filters

33 Results

Sort: Number of References: Descending View: Partial

1 9002-88-4 (C<sub>2</sub>H<sub>4</sub>)<sub>x</sub> Ethene, homopolymer 529K 25K 112

2 9004-34-6 Unspecified Cellulose 404K 14K 120

3 9003-07-0 (C<sub>3</sub>H<sub>6</sub>)<sub>x</sub> 1-Propene, homopolymer 357K 9,299 49

4 9002-89-5 25038-59-9 9002-84-0

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 Exclude

Search Within Results

Reference Role

Preparation (86)

Synthetic Preparation (86)

Reactant (37)

Reactant or Reagent (37)

Properties (22)

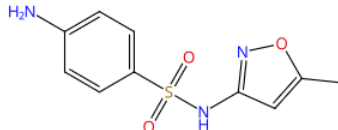
View All

86 Results

Sort: Number of References: Descending View: Partial

1

723-46-6



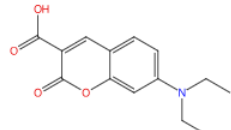
C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S

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

31K 1,090 116

2

50995-74-9



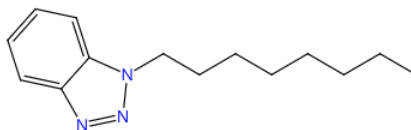
C<sub>14</sub>H<sub>15</sub>NO<sub>4</sub>

2H-1-Benzopyran-3-carboxylic acid, 7-(diethylamino)-2-oxo-

784 1,007 79

3

59046-27-4



C<sub>14</sub>H<sub>21</sub>N<sub>3</sub>

1H-Benzotriazole, 1-octyl-

25 21 3



# 物质详情

CAS Registry Number: 723-46-6

31K 1,079 123 View in CAS BioFinder

Nc1ccc(cc1)S(=O)(=O)Nc2ccoc2C

C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S

Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)-

Properties

Molecular Weight

Melting Point (Experimental)

Boiling Point (Predicted)

Density (Experimental)

pKa (Experimental)

Experimental Properties | Spectra

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 peroxymonosulfate 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

View All Patents

723-46-6

Nc1ccc(cc1)S(=O)(=O)Nc2ccoc2C

C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S

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

Experimental Spectra

1H NMR

13C NMR

Hetero NMR

View Proton NMR Spectrum (Image Available)

View Proton NMR Spectrum (Image Available)

View Proton NMR Spectrum (Image Available)

View Proton NMR Spectrum (Image Available)

View Proton NMR Spectrum (Image Available)

Solvent

Dimethyl sulfoxide; Carbon tetrachloride

Source

(1) LC

Solvent

-

Source

(2) ENAMINE

Solvent

-

Source

(2) ENAMINE

Solvent

-

Source

(3) BIORAD

Solvent

Chloroform-*d*; DMSO-*d*<sub>6</sub> (1:1)

Source

(3) BIORAD

Other Names and Identifiers

Experimental Properties

Experimental Spectra

Pharmacological Data

ADME

Toxicity

Predicted Properties

Predicted Spectra

Bioactivity Indicators

Target Indicators

Regulatory Information

GHS Hazard Statements

Additional Details

Condition

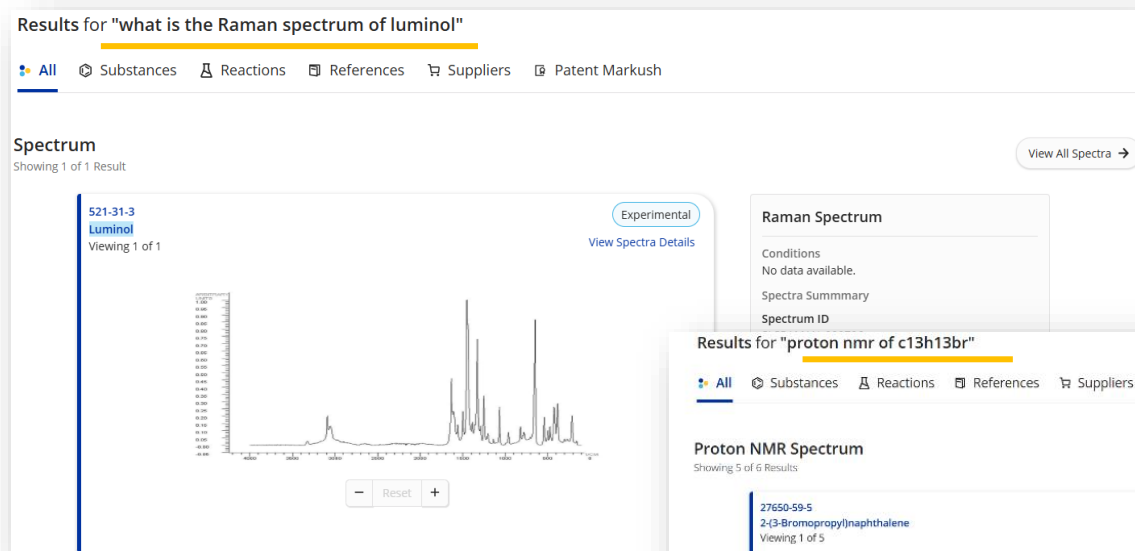
-

Press: 760.00 Torr

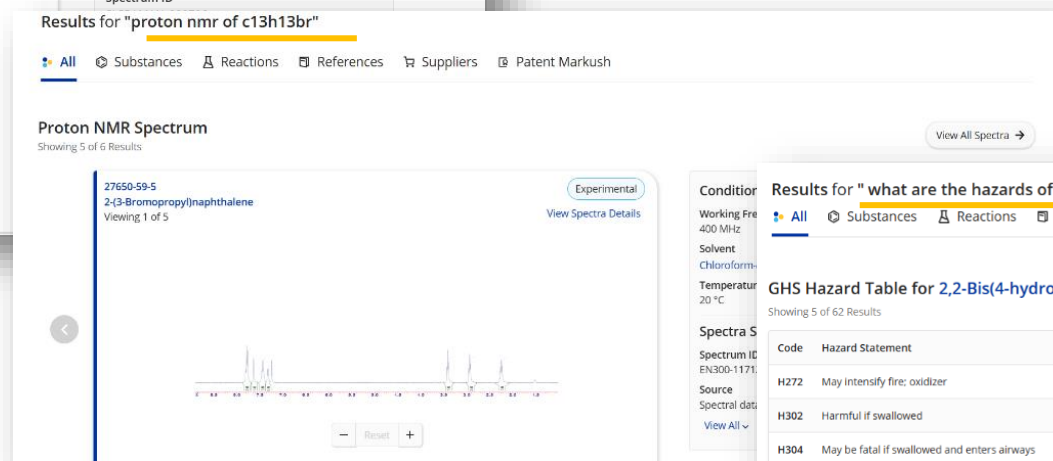
-

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



自然语言直接查阅Raman谱图



自然语言直接查阅NMR谱图

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

All Substances Reactions References Suppliers

Condition  
Working Fre  
400 MHz  
Solvent  
Chloroform  
Temperature  
20 °C

Spectra S  
Spectrum ID  
EN300-1171  
Source  
Spectral data  
View All

GHS Hazard Table for 2,2-Bis(4-hydroxyph...  
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

AIIC, AREC, CANL, CLP, DSL, EECL, EINECS, ENCS, FDA, HAP, HHAZ, HTU, IECSC, INSQ, ITC, IUR, JDATA, NZIO, PICCS, PIL, PROP, REACH, RSTR, S313, SIDS, State\_CA, PROP65, State\_MA, State\_MN, State\_NJ, State\_OR, State\_PA, State\_VT, State\_WA, STOR, STY, TCSL, 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

Value	Condition	Source
78.5 °C	-	"Hazardous Substances Data Bank" data were obtained from the ...
181.27 °C	Pressure: 15200 Torr	Camacho, I. D.; Theoretical Foundations of Chemical Engineering
110 °C (approx)	-	-
85 °C (approx)	-	-
80 °C	-	-

[View in Detail Page →](#)

自然语言直接查阅物质沸点

Results for "what is the pKa of benzene"

All Substances Reactions References Suppliers

71-43-2  
**Benzene**

pKa  
**43**

Source  
CAS

**pKa Properties**  
Showing 5 of 5 results

Value	Condition	Source
43	-	CAS

[View in Detail Page →](#)

自然语言直接查阅pKa值

Results for "melting point of mercury"

All Substances Reactions References Suppliers Patent Markush

7439-97-6  
**Mercury**

Melting Point  
**-38.87 °C**

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

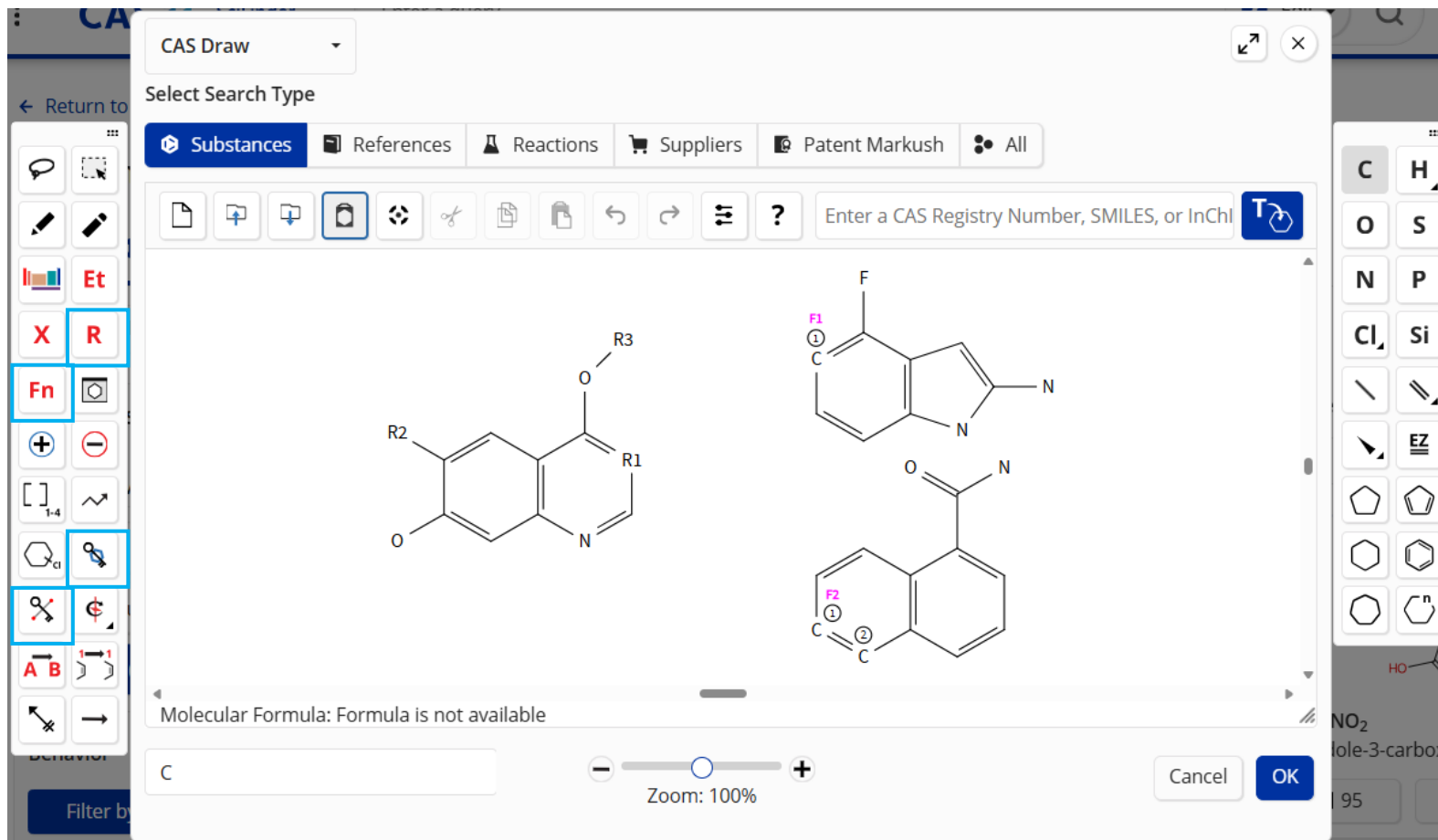
**Melting Point Properties**  
Showing 5 of 30 Results

Value	Condition	Source
-38.87 °C	-	"Hazardous Substances Data Bank" data were obtained from the ...
>350 °C (decomp)	-	Niamnont, Nakorn; Organic Letters, (2009), 11(13), 2768-2771, CA...
39.25 °C	-	Connolly, James A. D.; Journal of Geophysical Research: Planets, (...)
38.8 °C	-	Vega, Cesar; Journal of Food Science, (2005), 70(3), E244-E251, CA...
-38.4 °C	-	Cicogna, Francesca; Reactive & Functional Polymers, (2012), 72(10...

[View in Detail Page →](#)

自然语言直接查阅熔点

## 2.4 结构检索



氢同位素：氕、氘和氚

双键、三键和不确定化学键

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

Ring Lock

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

Atom Lock

原子锁定工具

被锁定的原子或官能团不发生非氢取代

# 结构检索

例：已知结构片段的物质检索

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

**Substances search for drawn structure**

View Related Results ▾

Filter Results

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

1 3031025-06-3

2 1421448-06-7

3 1421448-0

$C_{28}H_{30}NNiP_2$

$C_{28}H_{53}NNiP_2$   
Nickel, [2-(dicyclohexylphosphino-κP)-N-[2-(dicyclohexylphosphino-κP)ethyl]ethan...

$C_{28}H_{54}NNiP_2$   
Nickel(1+), [2-(dicyclohexylphosphino-κP)-N-[2-(dicyclohexylphosphino-κP)ethyl]e...

1 0 0

3 7 0

2 0 0

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

R1 Ni, Cu, Co

Cy P Cy

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

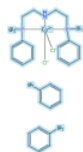
- ☐ Preparation (515)
- ☐ Synthetic Preparation (513)
- ☐ Properties (297)
- ☐ Uses (138)
- ☐ Catalyst Use (123)
- ☐ Reactant (104)
- ☐ Reactant or Reagent (104)
- ☐ Process (36)
- ☐ Physical, Engineering, or Chemical Process (35)
- ☐ Substance Claimed (15)
- ☐ Technical or Engineered Material Use (12)
- ☒ 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

1

1087216-22-5



$C_{28}H_{29}Cl_2CoNP_2$   
Cobalt, dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]ethan...

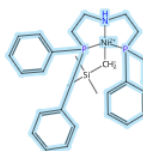
10

106

0

2

2924724-62-7



$C_{32}H_{40}NNiP_2Si$

1

1

4

579490-58

## Reaction Role

- ☐ Product (234)
- ☐ Reactant (58)
- ☐ Reagent (3)
- ☒ Catalyst (38)

## Element

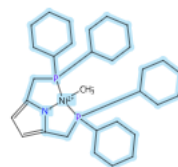
## Functional Group

## Number of Components

## Commercial Availability

4

1449235-31-7



$C_{31}H_{53}NNiP_2$   
Nickel, [2,5-bis[(dicyclohexylphosphino-κP)methyl]-1H-pyrrolato-κN]methyl-, (SP-...

2

4

0

## Reaction Role: 物质在反应中的角色

Filtering:

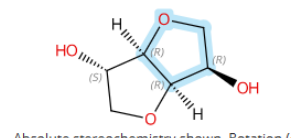
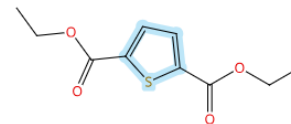
Substance Class: Polymer X

Number of Components: 4 X

138 Results

## Substance Class: 物质类别

2757996-73-7



Absolute stereochemistry shown, Rotation (+)

$(C_{10}H_{12}O_4S.C_8H_{14}O_4.C_6H_{10}O...$

Components: 4

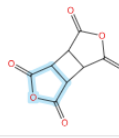
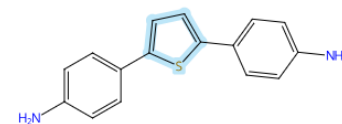
D-Glucitol, 1,4:3,6-dianhydro-, polymer with 1,4-diethyl butanedioate, 2,5-dieth...

1

1

0

2226925-66-0



$H_2N$

$(C_{16}H_{14}N_2S.C_{13}H_{14}N_2.C_{10}H_2...$

Components: 4

1H,3H-Benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone, polymer with 4,4'-methylenebis...

1

0

0

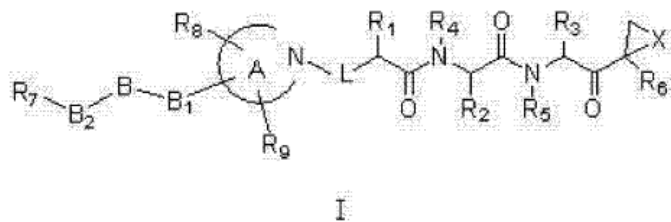
## 2.5 CAS Markush检索，助力结构查新

CN 104945470 A

权 利 要 求 书

1/3 页

1. 一种杂环构建的三肽环氧化物类化合物，具有下述结构通式 I：



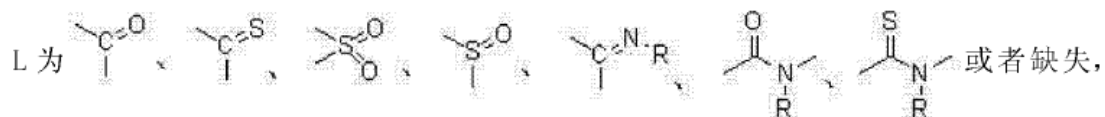
其中：

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

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

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

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



其中 R 选自 H、 $C_{1-6}$  烷基或卤代的  $C_{1-6}$  烷基；

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

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

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

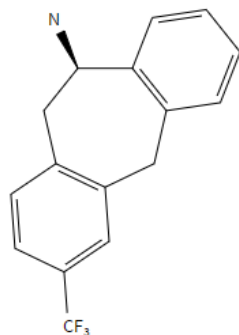
预测性物质[Prophetic Substance]：

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

# CAS Markush检索

第一步：物质结构检索

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



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

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

2 146364-18-3

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

Filter Results

Structure Match

As Drawn (0)

Substructure (2)

Similarity (6,054)

Behavior

Filter by Exclude

Search Within Results

Similarity

85-89 (1)

80-84 (2)

75-79 (23)

70-74 (148)

65-69 (998)

60-64 (4,497)

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

174 Results

1 87 ...

38506-20-6

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

2 84 ...

1705598-88-4

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

4 79 ...

13055-66-8

C17H13F3O  
5H-Dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)-5-one

5 79 ...

1644159-08-9

C18H15F3N  
5H-Dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)-5-methylene-N-methyl-

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

The screenshot displays the CAS SciFinder Patent Markush search interface. At the top, the CAS SciFinder logo and a search bar are visible. The main heading is "Patent Markush search for drawn structure". Below this, there is a "View Related Results" button. The left sidebar contains "Filter Results" with options for "Patent Markush Match" (As Drawn (4), Substructure (33)) and "Behavior" (Filter by, Exclude). The main area shows 4 results. The first result, EP502788, is highlighted. It includes a chemical structure diagram, the title "Preparation of triaminotriazines and analogs as antitumor and antiparasitic adjuncts", the assignee "Adir et Cie.", the patent status "Dead", and the patent claim "11". The second result, WO2015082046, is partially visible below. The interface also includes a "Search Patent Markush" button and a "Full Text" dropdown menu.

# 物质检索小结

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

Behavior

Filter by Exclude

Search Within Results

Yield

99,804 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction)

Steps: 1 Yield: 100%

resin-bound

Reactions search for "10.1021/ja027603q"

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

Reagent

Solvent

Experimental Protocols

Reaction Mapping

10 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction)

Steps: 1 Yield: 95%

Suppliers (109)

Suppliers (99)

Suppliers (91)

Suppliers (13)

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 ▾

## 醋酸酐合成紫杉醇

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

Scheme 1 (10 Reactions) Steps: 1 Yield: 85-96% ...

Suppliers (68)

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)

1.1 Reagents: [Hexamethyldisilazane](#)  
Catalysts: [4-\(Dimethylamino\)pyridine](#)  
Solvents: [Acetonitrile](#); rt

1.2 Reagents: [Hydrochloric acid](#)  
Solvents: [Water](#); rt

- “**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

Reactions search for "synthesis of paclitaxel catalyzed by triphenylphosphine"

View Related Results ▾

## 三苯基膦催化合成紫杉醇

7,007 Results Group: By Scheme ▾ Sort: Relevance ▾ View: Collapsed ▾

Scheme 1 (1 Reaction) Steps: 1 Yield: 60% ...

Suppliers (83)

Suppliers (139)

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

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: Ensui Sugar Refining Co., Ltd.  
World Intellectual Property Organization, WO2017006573 A1 2017-01-12

PatentPak ▾ Full Text ▾

# 自然语言检索反应

Reactions search for "synthesis of paclitaxel in tetrahydrofuran"

View Related Results

在四氢呋喃中合成紫杉醇

82 Results

Group: By Scheme Sort: Relevance View: Collapsed

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

Absolute stereochemistry shown, Rotation (-)

31-049-CAS-15414262 Steps: 1 Yield: 100%

1.1 Reagents: Pyridine  
Solvents: Ethanol, Tetrahydrofuran

Filter Results

Behavior

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

Catalyst

Reagent

Solvent

“in”连接物质指定溶剂

“mediated by”连接物质指定试剂

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

View Related Results

盐酸作为试剂参与合成紫杉醇

8,768 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (2 Reactions) Steps: 1 Yield: 100%

Absolute stereochemistry shown, Rotation (-)

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

Experimental Protocols

PatentPak Full Text

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

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)

# 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 ▾

Filter Results

Behavior

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

Catalyst

Reagent

Solvent

Experimental Protocols

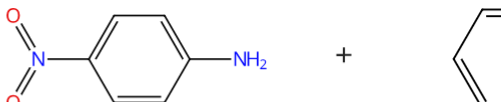
Non-Participating Functional Groups

Reaction Mapping

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 more relevant results. Continue to develop this feature, your feedback is important in making this tool even 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

Reactions search for "suzuki coupling reaction"

View Related Results ▾

Filter Results

Behavior

Filter by Exclude

Search Within Results

Yield

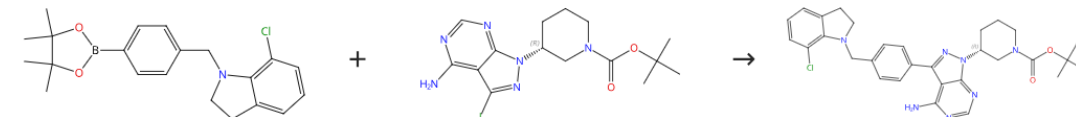
Reaction Scale

View All

1,469,847 Results

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

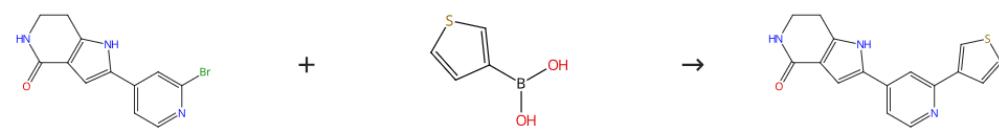
Scheme 1 (1 Reaction) Steps: 1 Yield: 100% ⋮



Supplier (1) Suppliers (50)

Expand Scheme ▾

Scheme 2 (1 Reaction) Steps: 1 Yield: 100% ⋮



Suppliers (4) Suppliers (101) Suppliers (3)

Expand Scheme ▾

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 ▾

乙酸钯催化合成醛类化合物

🔗 ⬇️ 📌 Save ▾

113,811 Results Group: By Scheme ▾ Sort: Relevance ▾ View: Collapsed ▾

**Filter Results** <

Behavior

Filter by Exclude

▼ Search Within Results

▼ Yield

^ Reaction Scale

☐ Milligram (78K)

☐ Gram (73K)

☐ Kilogram (48)

☐ No Scale Provided (32K)

^ Reaction Notes

☐ Stereoselective (29K)

☐ Regioselective (16K)

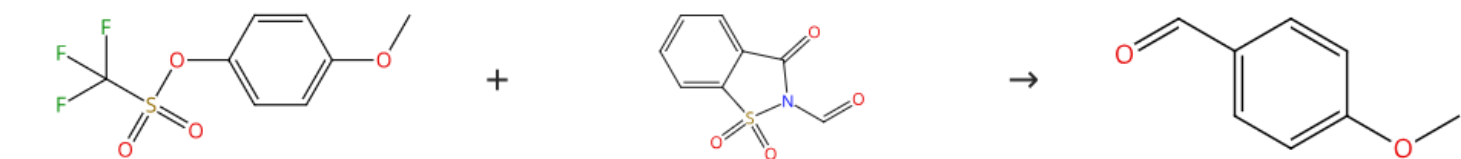
☐ Chemoselective (6,079)


☐ Thermal (4,585)


☐ High Pressure (2,137)


[View All](#)

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



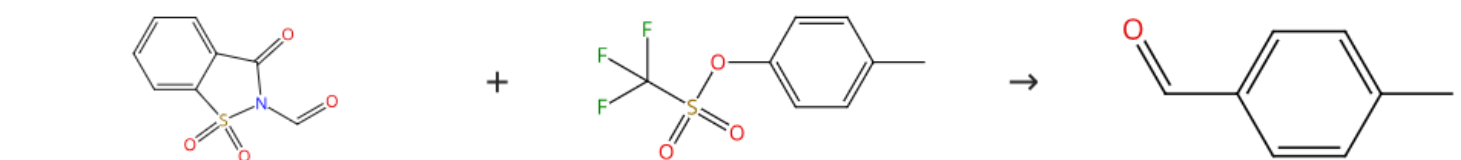
 Suppliers (58)


 Suppliers (77)


 Suppliers (135)


[Expand Scheme ▾](#)

**Scheme 2 (1 Reaction)** Steps: 1 Yield: 100% ⋮



 Suppliers (77)

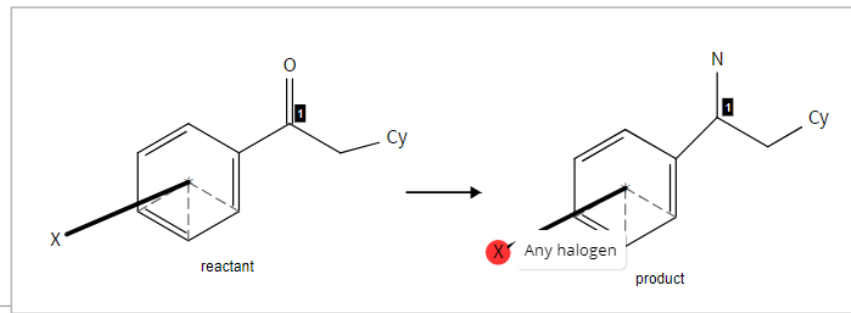
 Suppliers (63)

 Suppliers (104)

[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

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

**Scheme 1 (5 Reactions)**

Suppliers (79) Suppliers (13)

Expand Scheme ▾

**Scheme 2 (1 Reaction)**

Suppliers (45) Suppliers (3)

Steps: 1 Yield: 76% ...

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

Filter Results

Structure Match

As Drawn (34)

Substructure (8,806)

Similarity (0)

Behavior

Filter by

Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

Catalyst

Reagent

Solvent

Experimental Protocols

Non-Participating Functional Groups

Reaction Mapping

Source Reference

Document Type

Language

Publication Year

Organization

Publication Name

CA Section

Filter Content Report

Download filter data from this result set.

8,806 Results

Group: By Transformation

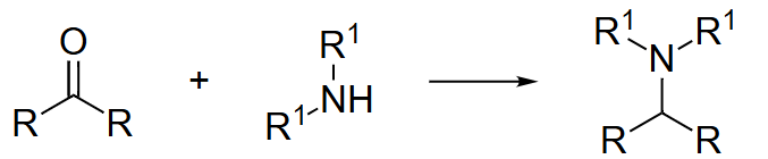
Sort: Reaction Count: Descending

View: Collapsed

1

Reductive Alkylation of Ammonia or Amines

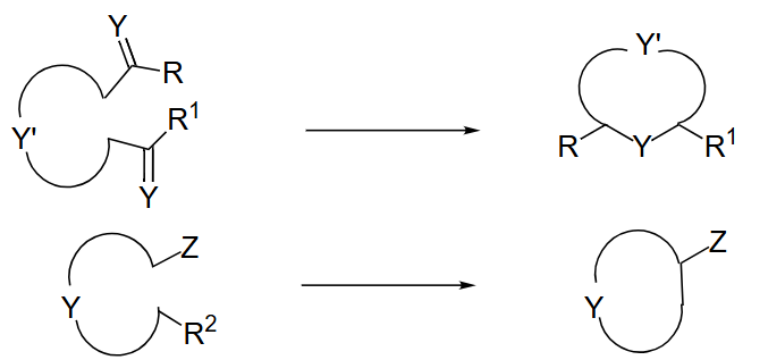
View 120 Related Reactions



2

Formation of N/O/S Heterocycles

View 64 Related Reactions



Y, Y' = NH, O, S

# 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: 1Yield: 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

**CAS SciFinder** | References | Reaction mechanism

References search for "Reaction mechanism" + drawn structure

View Related Results ▾

**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

6 Results

1

**Friedel-Crafts Hydroxyalkylation of Indoles with  $\alpha$ -Keto Amides using Reusable Catalytic System in Water**

By: Muthukumar, Alagesan; Sekar, Govindasamy

Journal of Organic Chemistry (2018), 83(16), 8827-8839 | Language: English, Database: CPlus and M

In the presence of  $K_3PO_4$  and tetrabutylammonium bromide,  $\alpha$ -keto amides underwent green Friedel-Crafts hydroxyalkylation reactions with indoles to give  $\alpha$ -aryl- $\alpha$ -hydroxyindoleacetamides. The method relies on reaction at the solid-liquid interface. The reaction was studied;  $^1H$  NMR experiments indicated that the reaction proceeds via a

Full Text ▾ 82 65 25

2

**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

Scheme 1 (1 Reaction) Steps: 1 Yield: 97%

Scheme 2 (1 Reaction) Steps: 1 Yield: 96%

Chemical reaction schemes showing the Friedel-Crafts hydroxyalkylation of indoles with  $\alpha$ -keto amides, and the  $\alpha$ -amylase catalyzed Friedel-Crafts reaction of isatin.

## 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

CAS Registry Number  
**2628280-40-8**

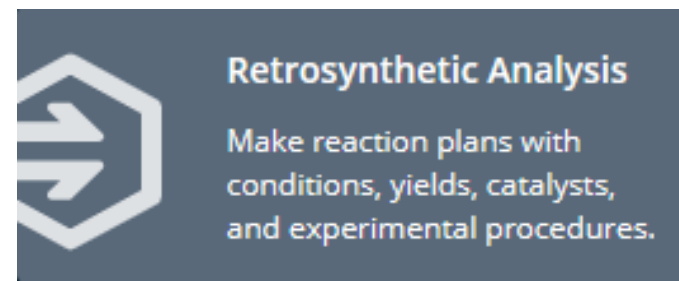
CAS Name  
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrrolidinyl]ethyl]-3-[(2S)-3,3-dimethyl-1-oxo-2-[(2,2,2-trifluoroethyl)amin...

Get Substance Details  
Get Life Science Data  
Get Reactions (356)  
Synthesize (351)  
**Start Retrosynthetic Analysis**  
Get References (1,589)  
Get Suppliers (49)  
View in CAS BioFinder

Absolute stereochemistry shown

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](#)

### Break and Protect Bonds (Optional)

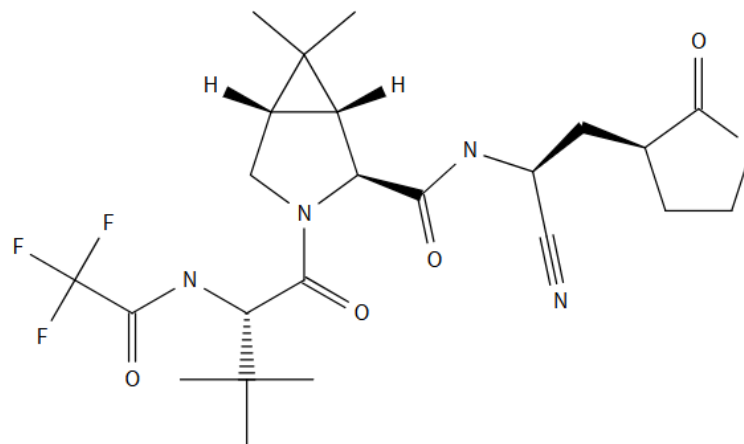
断裂键或保护键

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.

#### Starting Material Cost Limit

200 USD/mol ▼

Reset filter Apply

**起始原料费用**

## 逆合成路线详情

**Retrosynthesis Plan for drawn structure**

Build Status: Complete ✓ Estimated Yield: 11% Overall Price: \$1047.98 ⓘ

**已知反应**

**预测型反应**

**Viewing All Steps**

**A ⇒ B + C**

1.1 Reagents : Diisopropylet  
[bis(dimethylamino)met  
Solvents : Dichlorometh  
[View All](#) [Experimental Pr](#)

**Evidence Alternative Steps**

**B ⇒ D + E**

1.1 Reagents : Lithium hydro  
Solvents : 1,2-Dimethoxy  
[View All](#)

**D ⇒ F**

**Scheme 1 (1 Reaction)**

Steps: 2 Yield: 0

[31-367-CAS-9815976](#)

1.1 Reagents : Triethylamine, 1-Hydroxybenzotriazole, 1H-Benzotriazolium, 1-[  
[bis(dimethylamino)methylene]-, 3-oxide  
Catalysts : 4-(Dimethylamino)pyridine  
Solvents : Dimethylformamideovernight, rt; 17 h, rt

[Get Experimental Protocols](#)

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- 可查看每步反应的文献支持与详细条件

# 路线优化，考虑替换路线？

drawn structure

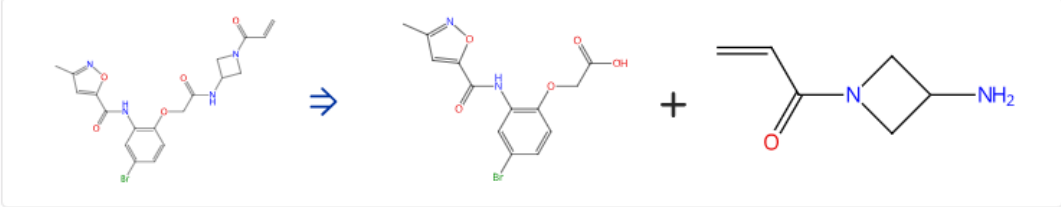
Build Status: Complete ✔ Estimated Yield: 11% Overall Price: \$1047.98 ⓘ

[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

Evidence Alternative Steps (37) Exclude Step

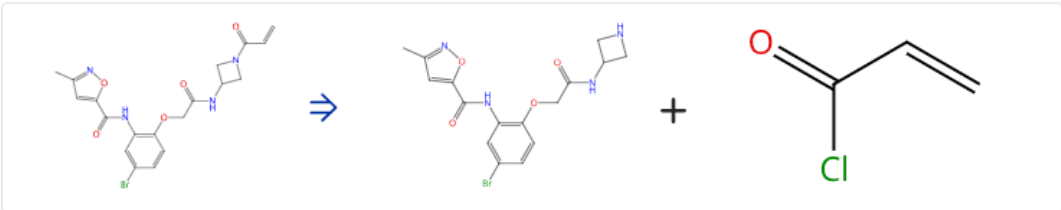
Filters

2 of 37 Predicted Step Average Yield: 63%



Evidence ▼ Replace Step

3 of 37 Predicted Step Average Yield: 63%



Evidence ▼ Replace Step

Reset

# 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](#)

Suppliers (25)      Suppliers (97)      98%

3. Maintain the reaction temperature between 30 and 50°C for 2 hours.
4. Quench the mixture by the slow addition of water (260 mL).
5. Pour the reaction mixture into a separating funnel.
6. Extract the mixture with ethyl acetate (4 x 140 mL).
7. Pool the organic fractions.
8. Wash the organic fractions with NaHCO<sub>3</sub> (3 x 60 mL) and NaHSO<sub>3</sub> (3 x 100 mL).
9. Dry the organic fractions with sodium sulfate (Na<sub>2</sub>SO<sub>4</sub>).
10. Concentrate the solvent under reduced pressure to obtain a thick yellow syrup.
11. Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully.
12. Dry the resulting yellow syrup under high vacuum to obtain product.

#### Filter Behavior

Filter by
Exclude

---

☒ Yield

☒ Number of Steps

☒ Non-Participating Functional Groups

☒ Reaction Mapping

☒ Experimental Protocols

☐ Experimental Procedure (83)

view

Yield: 98%

ation Empowers the  
eparation of  
lly Pure [<sup>18</sup>F]Tala  
n Vivo Evaluation as  
racer  
regory D. et al

linal Chemistry  
15690-15701

Organization  
ns Imaging Center,  
Preclinical Imaging  
macy  
s University

Tuebingen 72076  
Germany

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	<a href="#">Hydrochloric acid</a> <a href="#">Titanium chloride (TiCl<sub>3</sub>)</a>	-	<a href="#">Methanol</a> <a href="#">Tetrahydrofuran</a> <a href="#">Water</a>	rt; 30 min, rt; 2 h, 30 - 50 °C
2	<a href="#">Water</a>	-	-	-

Experimental Protocols

**Synthetic Methods**

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

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

**Reagents** [Hydrochloric acid](#)  
[Titanium chloride \(TiCl<sub>3</sub>\)](#)  
[Water](#)

**Solvents** [Methanol](#)  
[Tetrahydrofuran](#)  
[Water](#)

#### Transformation

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

#### Scale

gram

#### Characterization Data

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

State: yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

#### Transformations

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



## 4.2 CAS分析实验方法详情

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

### Analysis of Vanadium in Stainless steel by Electrochemical extraction

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

CAS Method Number  
1-119-CAS-292609

**实验原料**

Analyte  
Vanadium

Matrix  
Stainless steel

Method Category  
Element Detection

Technique  
Electrothermal atomic absorption spectroscopy; Electrochemical extraction

**分析仪器**

**Validation**

Linearity Range	0-400 µg/L
Recovery	0.03 wt% (0.05 wt% reference value, sample data)

**数据有效性**

**Equipment Used**

Cutting machine, Secotom-10, Struers

Ultrasonic cleaning unit, P 30 H, Elmasonic

Grinding machine, Labopol-6, Struers

Potentiostat, SP-150, BioLogic

Vacuum pump, BUSCHI

Graphite furnace atomic absorption spectrometer, AAnalyst 600, PerkinElmer

Autosampler, AS-800, PerkinElmer

**Conditions**

**Instrument**

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

**分析条件**

**Instructions**

**Preparation of stainless steel process samples**

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

**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.

**操作步骤**

# 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方法

The screenshot shows the CAS SciFinder interface for a search titled "References search for 'steel and impurity'". The left sidebar contains a "Behavior" section with a "Filter by" button and an "Exclude" button. Under "Search Within Results", the "CAS Content" section is expanded, showing "Analytical Methods (29)" selected and "Formulations (18)" unselected. The main results area shows 29 results, sorted by Relevance, with a view of Full Abstract. The first result is titled "Portable capillary electrophoresis coupled with swab-based extraction device for cleaning validation in pharmaceutical facilities" by Atia, Mostafa A. et al. The second result is titled "Validation of an HPLC method for analysis of nifedipine residues on stainless-steel surfaces in the manufacture of pharmaceuticals" by Milenovic, D. M. et al. A tooltip is visible over the first result, showing the "Analytical Methods" section with the "Method Title" and two links to the analysis of Lidocaine hydrochloride in Medical cotton swabs by Capillary electrophoresis.

References search for "steel and impurity"

View Related Results ▾

We are displaying the most relevant results.  
[Learn about result relevance.](#)

[Load All Results](#)

Filtering: CAS Content: Analytical Methods ✕ [Clear All Filters](#)

29 Results Sort: Relevance ▾ View: Full Abstract ▾

1

**Portable capillary electrophoresis coupled with swab-based extraction device for cleaning validation in pharmaceutical facilities**  
By: Atia, Mostafa A. ; Amuno, Ria Marni; Kalsoom, Umme; Ollerton, Samantha; Rhoden, Alan; Haddad, Paul R.; Breadmore, Michael C.   
Journal of Chromatography A (2023), 1688, 463666 | Language: English, Database: CAPlus and MEDLINE

All pharmaceutical manufacturers are required to verify that their production equipment is free of contamination. This is achieved by the use of a fully automated portable capillary electrophoresis instrument with an integrated detection of pharmaceutical residues on surfaces of manufacturing equipment. Lidocaine was detected on a surface by swabbing, extracted from the swab, and analyzed within 1 min. The recovery was 81.3%, with a LOD of 0.13µg/swab. This fast, sensitive, and simple method implements the need for manual sample pre-treatment provides the possibility for on-site rapid detection in the industry.

[Full Text ▾](#) 2 0 9

**Analytical Methods**

**Method Title**

[Analysis of Lidocaine hydrochloride in Medical cotton swabs by Capillary electrophoresis](#)

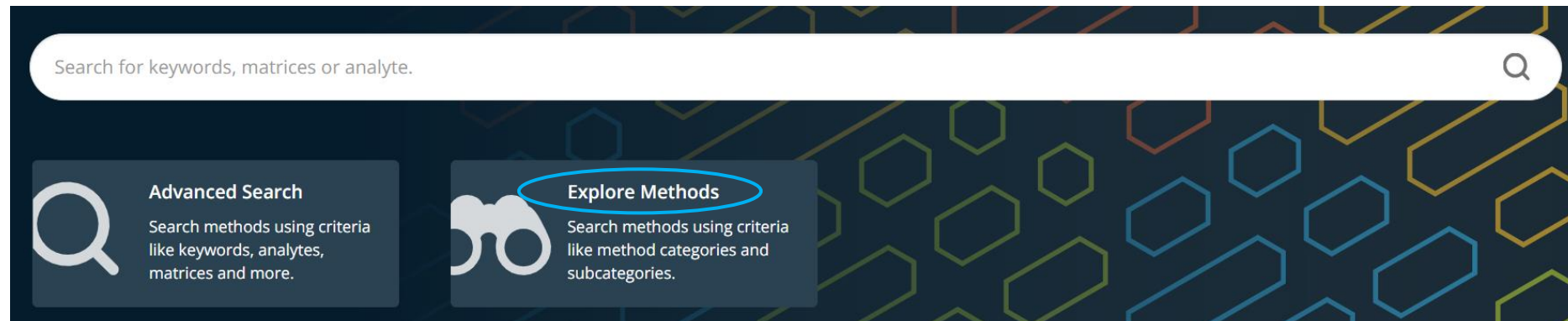
[Analysis of Lidocaine hydrochloride in Medical cotton swabs by Capillary electrophoresis](#)

2

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

# 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



方法分类: 13大类, 45小类

农业应用、生物鉴定、生物分子分离、环境、食品、考古、有机物、药学、毒理学等

### 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?

## Advanced Search

Keyword ▼ steel

AND ▼ Keyword ▼ sulfur

Add Search Criteria

Filter By

^ Analyte

☒ Sulfur (22)

☐ Carbon (12)

☐ Manganese (8)

☐ Chromium (7)

☐ Copper (7)

View All

^ Matrix

☒ Steel (22)

☐ Leaf (14)

☐ Air (8)

☐ Airborne particles (7)

☐ Soils (7)

View All

^ Method Category

^ Technique

^ Validation

☐ Limit of Detection (15)

☐ Sensitivity (5)

☐ Concentration (4)

☐ Precision (4)

☐ Recovery (4)

View All

22 Results

Sort: Relevance ▼ Group: By Method ▼

1

Analysis of Carbon in Steel by Laser induced breakdown spectroscopy

JOURNAL

By: Jiang, X.; Hayden, P.; Costello, J. T.; Kennedy, E. T.  
Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet:  
Optimization of parameters for detection of carbon and sulfur in steel  
Spectrochimica Acta, Part B: Atomic Spectroscopy (2014), 101, 106-113. Elsevier B.V.

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

View Abstract ▼

Full Text ▼

View in CAS SciFinder

2

Analysis of Carbon in Steel by Laser induced breakdown spectroscopy

JOURNAL

By: Jiang, X.; Hayden, P.; Costello, J. T.; Kennedy, E. T.  
Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet:  
Optimization of parameters for detection of carbon and sulfur in steel  
Spectrochimica Acta, Part B: Atomic Spectroscopy (2014), 101, 106-113. Elsevier B.V.

Analyte

Sulfur; Carbon

Matrix

Steel

Other Materials

Material: Spectron laser

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

69

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

# 如何选择合适的分析方法？

Comparing your 2 selected Methods			
<div>Expand All Collapse All</div>			
	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	
CAS Method Number	1-119-CAS-266812	1-119-CAS-101987	
Method Category	Element Detection	Element Detection	
Technique	Laser induced breakdown spectroscopy	Time-of-flight mass spectrometry; Glow discharge spectrometry	
Analyte	Carbon; <b>Sulfur</b>	Tantalum; Cobalt; Molybdenum; Manganese; Vanadium; Phosphorus; Copper; Tin; Magnesium; Lead; Tungsten; Titanium; Nickel; Boron; Arsenic; Chromium; Silver	
Matrix	<b>Steel</b>	<b>Steel</b>	
Other Materials	Spectron laser	Grimm-type chamber (with a 4 mm diameter and inner diameter flow tube)	
Equipment Used	Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer, VM-521, Acton Research Corporation; CCD camera.	Orthogonal time-of-flight mass spectrometer, ToF MS, Switzerland; Dry pump, Triscroll 300, Varian Inc., Fisons; Radio frequency glow discharge orthogonal time-of-flight mass spectrometer, ToF MS, Switzerland	

0.3 µg/g, Boron, 0.2 µg/g, Magnesium, 0.3 µg/g, Aluminum, 1.9 µg/g, Silicon, 1.6 µg/g, Phosphorus, 1.0 µg/g, **Sulfur**, 2.3 µg/g, Titanium, 1.1 µg/g, Vanadium, 1.0 µg/g, Chromium, 5.5 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

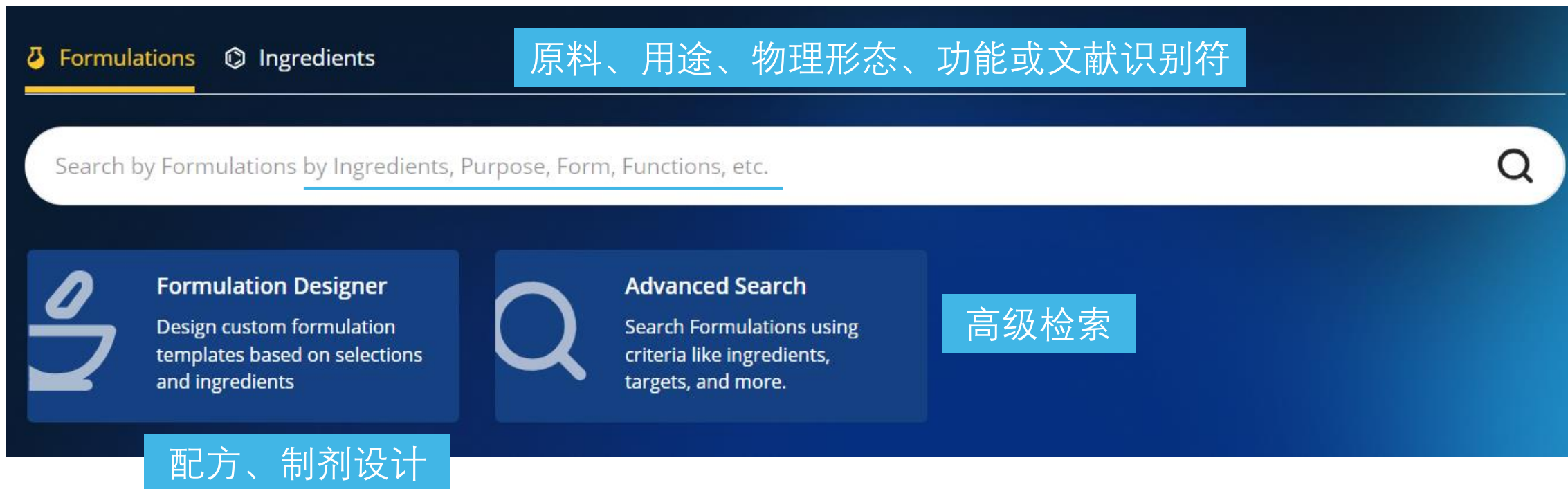
[View Less ^](#)

Method	Laser-induced breakdown spectroscopic analysis using helium as ambient gas in single pulse mode 1. Perform the analysis using LIBS setup containing the laser	Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode 1. Collect the NIST 1262b certified reference <b>steel</b> .
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.
Precision	-	12% (RSD, reproducibility), Boron, 28% (RSD, reproducibility), Magnesium, 2% (RSD, reproducibility), Aluminum, 6% (RSD, reproducibility), Silicon, 5% (RSD, reproducibility), Phosphorus, 6% (RSD, reproducibility)
Sensitivity	-	6 - 165 cps/(µg/g)
Source	<div>JOURNAL</div> <div>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></div> <div>By: Jiang, X.; Hayden, P.; Costello, J. T.; Kennedy, E. T.</div> <div>Spectrochimica Acta, Part B: Atomic Spectroscopy (2014), 101, 106 - 113.</div> <div><div>Full Text</div><div>View in CAS SciFinder</div></div>	<div>JOURNAL</div> <div>A comparison of non-pulsed radiofrequency and pulsed radiofrequency glow discharge orthogonal time-of-flight mass spectrometry for analytical purposes</div> <div>By: Lobo, L.; Pisonero, J.; Bordel, N.; Pereiro, R.; Tempez, A.; Chapon, P.; Michler, J.; Hohl, M.; Sanz-Medel, A.</div> <div>Journal of Analytical Atomic Spectrometry (2009), 24 (10), 1373 - 1381.</div> <div><div>Full Text</div><div>View in CAS SciFinder</div></div>



## 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



- 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

- Industry
  - ☐ Cosmetics & Personal Care
  - ☐ Inks, Paints, & Coatings
  - ☒ Pharmaceutical
  - ☐ Unclassified
- Purpose
  - ☒ Pharmaceutical implants (1,154)
  - ☐ Gels (365)
  - ☐ Tablets (349)
  - ☐ Capsules (247)
  - ☐ Powders (213)
- View All
- State of Matter
- Delivery Route
- Information Included
  - ☐ Component Amount (1,517)
  - ☒ Process (1,154)
  - ☐ Experimental Activity (765)
  - ☐ Effective Dose (186)
- Document Type
- Organization
- Language
- Publication Year

1,154 Results

Sort: Relevance Group: By Family

1

**Implants: Antitumor Agents** [Compare](#)

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

Purpose: Antitumor agents

Physical Form: **implant**

Component	Function	Amount Reported
Group: Ti-TNTs wire implants	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** [Compare](#)

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？

- 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

**Implants: Antitumor Agents**

Formulation Ingredients

Component	Function	Amount Reported	Optionality
Group: Ti-TNTs wire implants	Pharmaceutical implants	-	Mandatory
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

Nopioic-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

Nopioic-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

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 ▼	Optional ▼	Anticorrosion
Ex: binder, surfactant, carrier		

Search For	Operator	Enter one term
All Fields ▼	Optional ▼	coating
General search of all fields		

Add Another Term

 Search

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

- Optional ▼
- Required
- Optional
- Excluded

Clear All

# 检索原料

Ingredients search for "Propylene glycol"

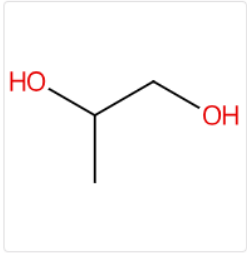
Filter by

- Industry
  - ☐ Agrochemical
  - ☐ Cleaning & Surfactant Products
  - ☐ Cosmetics & Personal Care
  - ☐ Food & Related
  - ☐ Inks, Paints, & Coatings
  - ☒ Pharmaceutical
- Regulatory Information
  - ☐ REACH (4)
  - ☐ Cosing: Cosmetic Ingredient Inventory (2)
  - ☐ EPA Pesticide Inactive Ingredients (2)
  - ☒ FDA Inactive Ingredients Database (2)
  - ☐ ANMAT (1)
- Experimental Properties
- Commercial Availability
- Toxicity/Ecological Toxicity

2 Results

1

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



C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>

(±)-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](#)

2

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	<input type="text" value="Vitamin A"/> 
<b>Cosmetics &amp; Personal Care</b>	Skin conditioners	Cream preparations	<input type="text" value="Polyethylene glycol"/> 
Agrochemical	Sunscreens	Cosmetic lotions	
Cleaning & Surfactant Products	Hair dyes	Cosmetic packs	
Inks, Paints, & Coatings	Hair preparations	<b>Gels</b>	 <a href="#">Add Another Ingredient</a>
Food & Related	Antiperspirants	Liquids	
	Cleaning compositions	Powders	
	Skin cleansers	Solutions	
	Skin-lightening cosmetics	Nanospheres	
	Oral hygiene products	Pastes	
	<b>Skin care products</b>	<a href="#">- View More Physical Forms -</a>	
	<a href="#">- View More Purposes -</a>		

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

Your Template

Unit Size  mg

Function	Ingredient	Regulatory	Top Alternatives	Amounts
Active or Featured Ingredient:	Vitamin A	ANMAT; NMPA	-	Amount not available <input type="button" value="x"/>
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 <input type="button" value="x"/>
Carriers	Ethylene glycol <div>View More Alternatives</div>	CosIng: Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database	Water; Polyethylene glycol	Approximate Range
Skin conditioners	Ethylene glycol <div>View More Alternatives</div>	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

- 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

Allantoin

1,2-Octanediol

Tricaprin

Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated

Glyceryl polyacrylate

N-(2-Hydroxyethyl)acetamide



# 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.](#)

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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

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: CAPLUS 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 ± 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: CAPLUS 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)

[View All](#)

# 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

3 0 55 Citation Map

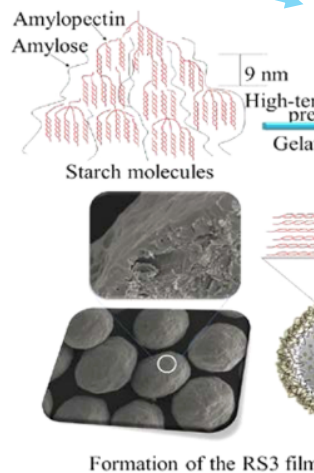
In this Reference

- [Concepts](#)
- [Substances](#)
- [Formulations](#)
- [Cited Documents](#)

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 hypoglycemia system has been demonstrated for the accurate delivery of bioactive po



**Keywords:** starch film coated microparticle colon polypeptide delivery

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[Full Text](#)

[View in CAS Formulus](#)

### 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](#)
- [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](#)

# 实验方案检索小结

1. 利用Synthetic Methods™查看文献中合成方法详情
2. 利用CAS Analytical Methods进行主题检索或分类浏览获得分析方法，或通过文献查看关联的分析实验及数据详情
3. 利用CAS Formulus检索原料、配方/制剂，或通过文献结果集获得关联的配方/制剂信息；利用配方设计工具启发产品配方的开发

# 大纲

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



# CAS SciFinder检索浏览器推荐

浏览器推荐:

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

# 常见登录问题

## Unauthorized IP Address

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

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



There was a problem verifying your account.

Try Again

Contact Us

Or [Log Out](#) and try again.

Reference Id: GU75LMf9iZnhTq6mymUog

- 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



# 学习资源

微信公众号：ACS美国化学学会



线上学习短视频：



CAS SciFinder 学习中心



内容包括：基础演示短视频，专题培训录屏、综合应用案例等

# 使用注意事项

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

# THANK YOU!



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