

CAS SciFinder

# 疑难检索案例分析

2021.5



# 大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略 (CAS Analytical Methods)



# CAS致力于提高创新效率

CAS的数据和服务是基于对以往知识经验的回顾，对当代前沿研究的洞察，以及对未来发展趋势的前瞻



## HINDSIGHT

Connecting past discoveries  
to build a better future

连接前人的发现，建设更美好的未来

## INSIGHT

Revealing unseen relationships that spark ideas and speed  
discovery

揭示能激发想法和加速发现的，未预见的联系

## FORESIGHT

Identifying trends and emerging opportunities to accelerate  
growth

确定加速增长的趋势和新机遇

# CAS具有最全面的学科连接内容合集



Over  
**50K**  
scientific journals  
and documents

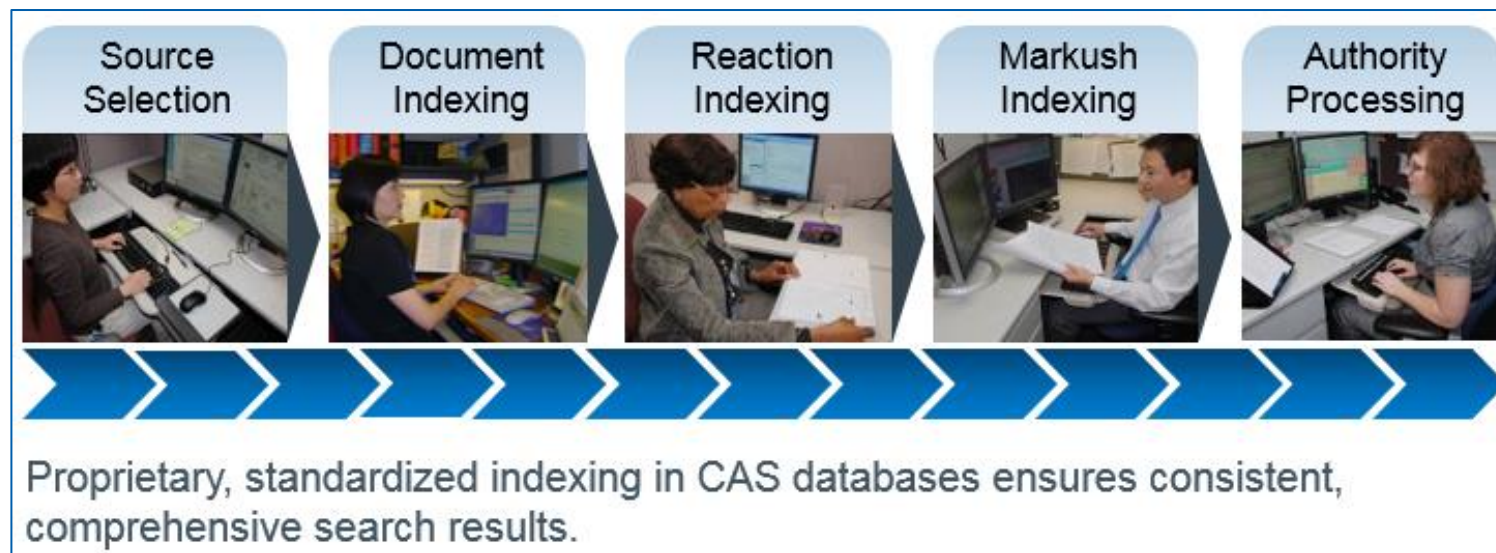
Over  
**250**  
million  
substances

Over  
**50**  
languages  
translated

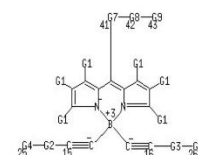
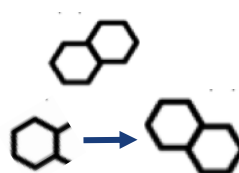
**64**  
patent offices  
worldwide



# CAS科学家的智力标引



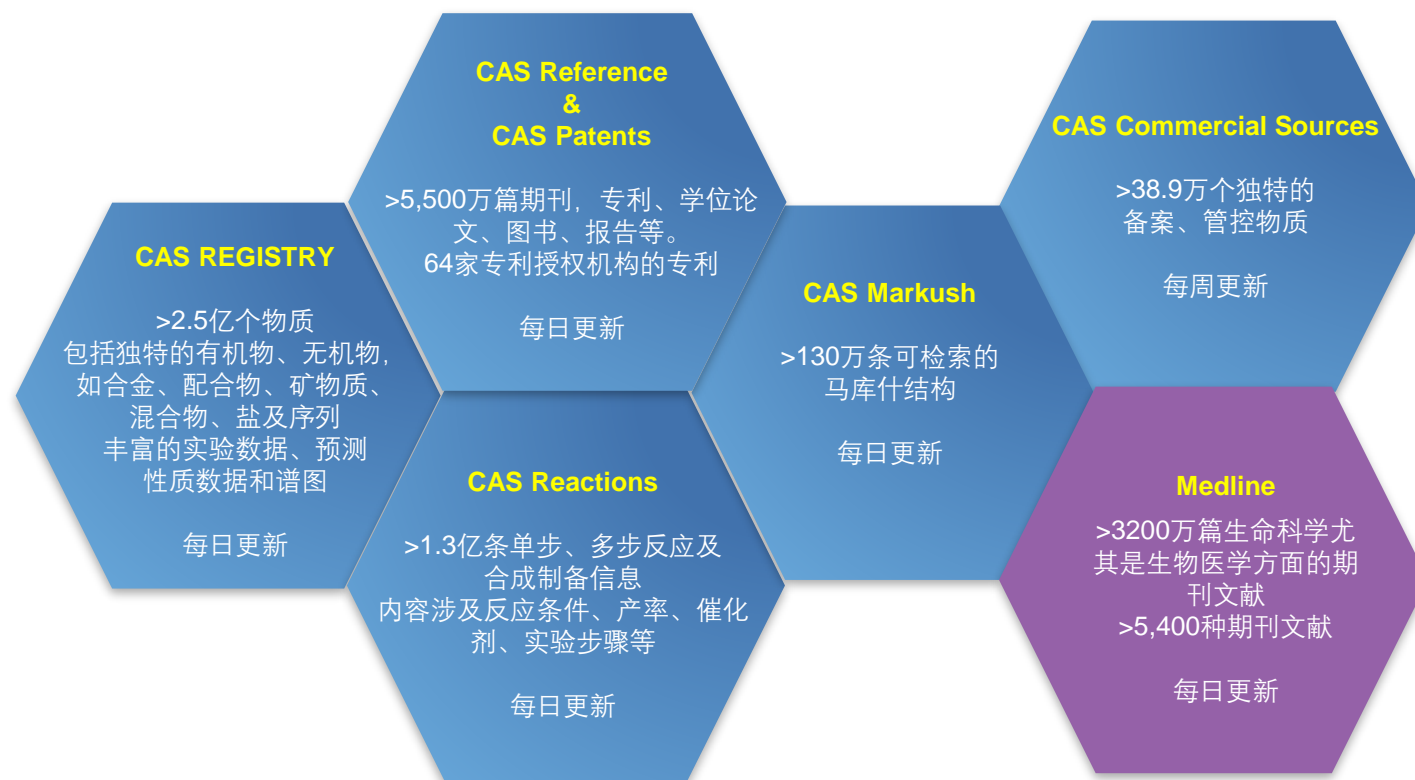
1990  
Smith, M.  
anthracene



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内容合集--CAS SciFinder



CAS SciFinder是提供经CAS科学家人工标引内容的工具型解决方案。

# CAS解决方案与服务

## DISCOVERY



### **CAS SciFinder Discovery Platform™**

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

## INTELLECTUAL PROPERTY



### **STN IP Protection Suite™**

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

## CUSTOM SOLUTIONS



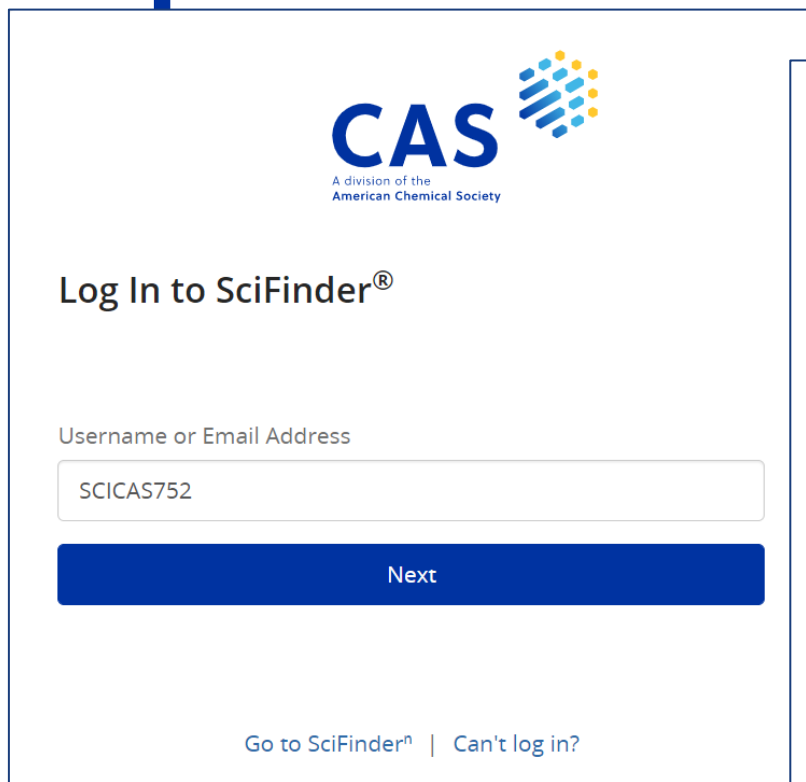
### **CAS Custom Services<sup>SM</sup>**

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

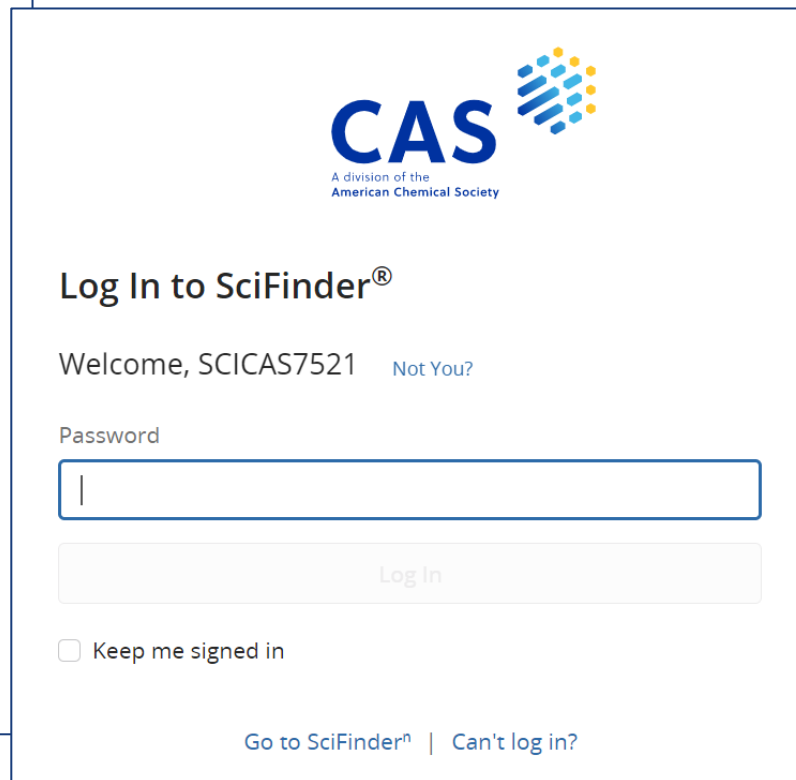


# CAS SciFinder登录网址

## https://SciFinder.cas.org



The screenshot shows the initial login page of CAS SciFinder. At the top is the CAS logo with the text "A division of the American Chemical Society". Below it is the heading "Log In to SciFinder®". There is a label "Username or Email Address" above a text input field containing "SCICAS752". Below the input field is a blue button labeled "Next". At the bottom, there are links "Go to SciFinder<sup>®</sup>" and "Can't log in?".



The screenshot shows the login page after clicking "Next". It features the same CAS logo and heading. Below the heading, it says "Welcome, SCICAS7521" followed by a link "Not You?". There is a label "Password" above a text input field. Below the input field is a grey button labeled "Log In". Below the button is a checkbox labeled "Keep me signed in". At the bottom, there are links "Go to SciFinder<sup>®</sup>" and "Can't log in?".

每个用户必须注册后才能使用



# CAS SciFinder主界面

The screenshot shows the CAS SciFinder main interface. The top navigation bar includes the SciFinder logo, a 'Tools Bar' (工具栏) annotation, and links for Preferences, SciFinder Help, and Sign Out. Below the navigation bar are tabs for Explore, Saved Searches, and SciPlanner. The left sidebar contains three main sections: REFERENCES (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), SUBSTANCES (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and REACTIONS (with sub-item: Reaction Structure). Annotations point to these sections: '文献检索' (Literature Search) for REFERENCES, '物质检索' (Substance Search) for SUBSTANCES, and '反应检索' (Reaction Search) for REACTIONS. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with examples, a 'Search' button, and a link to 'Advanced Search'. An annotation '已保存的结果集' (Saved Results) points to the search area. The right sidebar contains a 'SAVED ANSWER SETS' section with a list of saved sets (CSF1R, jmc, EP 19870107847, Daclatasvir-1, SUB result, EX result, MF result, polymer1, structure search, Autosaved Substance Set) and a 'KEEP ME POSTED' section with a message 'You have no profiles.' and a link to 'Learn how to: Create Keep Me Posted'. An annotation '定题追踪' (Topic Tracking) points to the 'KEEP ME POSTED' section.

CAS Solutions  
SciFinder®  
A CAS SOLUTION

工具栏

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

REFERENCES

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

SUBSTANCES

Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

REACTIONS

Reaction Structure

文献检索

物质检索

反应检索

REFERENCES: RESEARCH TOPIC

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

Search

Advanced Search

已保存的结果集

SAVED ANSWER SETS

CSF1R  
jmc  
EP 19870107847  
Daclatasvir-1  
SUB result  
EX result  
MF result  
polymer1  
polymer1  
structure search  
Autosaved Substance Set

View All | Import

KEEP ME POSTED

You have no profiles.

Learn how to:  
Create Keep Me Posted

定题追踪

# 大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略 (CAS Analytical Methods)



# CAS SciFinder检索--文献检索

## ■ 文献检索方法

- 主题检索
- 作者名检索
- 机构名检索
- 文献标识符检索
- 期刊名称和专利信息（公开号，申请号等）
- 从物质，反应获得文献

## ■ 检索策略推荐

- 关注某特定领域的文献：主题检索
- 关注物质有关的文献：先获得物质，再获得文献
- 关注某科研人员的文献：作者名检索
- 关注某机构科研进展：机构名检索



# 利用Index Term选词

主题检索：植物中天然活性成份的抗癌研究

检索式：Nature Active Component **with** Anti Cancer



CAS Solutions

**SCIFINDER**  
A CAS SOLUTION

SciFinder<sup>n</sup> is here! [Learn more](#) about the power of n. Participating customers <https://scifinder->

Explore ▼ Saved Searches ▼ SciPlanner

**REFERENCES**

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

**SUBSTANCES**

- Chemical Structure
- Markush

**REFERENCES: RESEARCH TOPIC ?**

Nature Active Component with Anti Cancer

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds


**Search**

Advanced Search

关键词之间用介词连接： in, with, of...



# 利用Index Term选词

CAS Solutions  **SCIFINDER<sup>®</sup>**  
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

SciFinder<sup>n</sup> is here! [Learn more](#) about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "Nature Active Component with A..."

只有253条文献吗?

REFERENCES ?

Select All Deselect All

1 of 4 Research Topic Candidates Selected

	References
<input checked="" type="checkbox"/> 253 references were found containing the two concepts "Nature Active Component" and "Anti Cancer" closely associated with one another.	253
<input type="checkbox"/> 590 references were found where the two concepts "Nature Active Component" and "Anti Cancer" were present anywhere in the reference.	590
<input type="checkbox"/> 9523 references were found containing the concept "Nature Active Component".	9523
<input type="checkbox"/> 1626328 references were found containing the concept "Anti Cancer".	1626328

Get References

“Concepts”表示对主题词做了同义词的扩展；

“Closely associated with one another”表示同时出现在一个句子中；

“were present anywhere in the reference”表示同时出现在一篇文献中；

# 利用Index Term选词

文献筛选工具

SciFinder<sup>n</sup> is here! [Learn more](https://scifinder-n.cas.org) about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Research Topic "Nature Active Component with A..." > **references (226)**

REFERENCES

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

Display Options

0 of 226 References Selected

Page: 1 of 12

Analyze by:

Author Name

Zhang Yaozhou 4

Chen Jianqing 3

Chen Yujiao 3

Cheng Jianjun 3

Cheng Yiyu 3

Cui Jinsong 3

Dou Jing 3

Gao Jiayu 3

Ge Zhiwei 3

He Qing 3

Show More

1. **Fucoidan induces apoptosis in A2058 cells through ROS-exposed activation of MAPKs signaling pathway**

Quick View Other Sources

By Ryu, Yea Seong; Hyun, Jin Won; Chung, Ha Sook

From Natural Product Sciences (2020), 26(3), 191-199. | Language: English, Database: CAPLUS

Fucoidan, a **natural component** of brown seaweed, has various biol. **activities** such as **anti-cancer activity**, **anti-oxidant**, and **anti-inflammatory** against various **cancer** cells. However, the fucoidan has been implicated in melanoma cells via apoptosis signaling pathway. Therefore, we investigated apoptosis with fucoidan in A2058 human melanoma cells with dose- and time-dependent manners. In our results, A2058 cells viability decreased at relatively short-time and low-concn. through fucoidan. This effects of fucoidan on A2058 cells appeared to be mediated by the induction of apoptosis, as manife...

2. **Traditional chinese medicine-based pharmaceutical composition [Machine Translation].**

Quick View PATENTPAK

By Cai, Haide; Cai, Xin

From Faming Zhuanli Shenqing (2021), CN 112587560 A 20210402. | Language: Chinese, Database: CAPLUS

[Machine Translation of Descriptors]. The pharmaceutical compn. provided by the present invention combines a medicine for cell nutrition and cell stabilization, a medicine for **anti-platelet** aggregation, and **anti-cancer** metastasis, and a medicine for regulating the balance of YIN and YANG of the human body, supplementing blood and clearing blood, supplementing QI and ventilating, dredging the meridians, and **reducing** blood lipid. The invention has the advantages that the **activity** of the inherent pluripotent stem cells in the blood of the human body is **activated**, the **activated** pluripotent stem ce...

3. **Exploring the self-assembly mechanism and effective synergistic antitumor chemophototherapy of a biodegradable and glutathione responsive ursolic acid prodrug mediated photosensitive nanodrug**

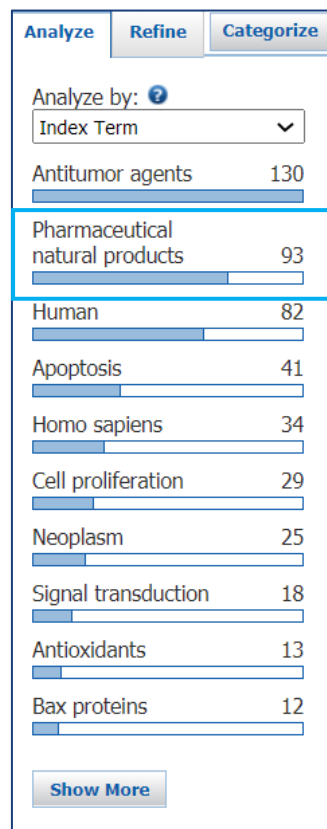
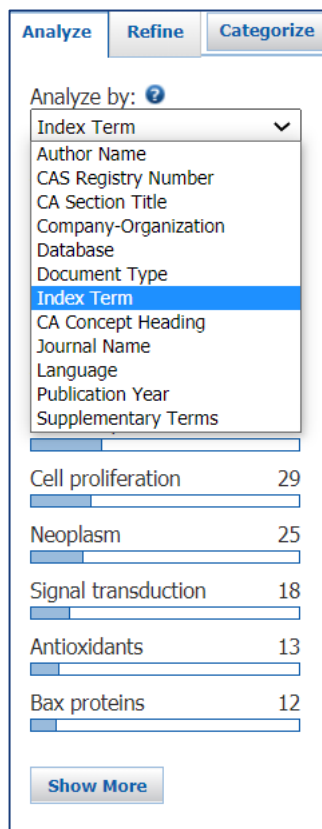
Quick View Other Sources

By Cheng, Jianjun; Wang, Shu; Zhao, Haitian; Liu, Yan; Yang, Xin

From Biomaterials Science (2021), Ahead of Print. | Language: English, Database: CAPLUS

Supramolecularly assembled photochemotherapeutic nanocomposites composed of pure drug small mols. are promising for synergistically improved **tumor** therapy, yet potential multiple challenges remain to be addressed. Herein, we rationally designed a novel multifunctional small mol. disulfide modified **natural** pentacyclic triterpene of ursolic acid (UASS) that simultaneously possesses self-assembly ability, glutathione (GSH) responsivity, **anticancer activity**, biocompatibility and biodegradability and further constructed carrier-free GSH-sensitive photosensitive nanocomposite UASS-Ce<sub>6</sub> NPs for safe ...

# 利用Index Term选词



Index Term基于内容的分析工具，发现natural products, Pharmaceutical这个和“天然活性成分”很相关的词

是否用这个词去检索，效果会更好？

# 利用Index Term选词

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "Nature Active Component with A..." > references (226)

**REFERENCES**

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

**SUBSTANCES**

- Chemical Structure
- Markush

**REFERENCES: RESEARCH TOPIC ?**

Natural Product with anti cancer

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

**Search**

Advanced Search

新的检索式：

Natural Product with anti cancer

REFERENCES ?	
Select All Deselect All	
1 of 5 Research Topic Candidates Selected	
<input type="checkbox"/> 31 references were found containing "Natural Product with anti cancer" as entered.	References 31
<input checked="" type="checkbox"/> 14631 references were found containing the two concepts "Natural Product" and "anti cancer" closely associated with one another.	14631
<input type="checkbox"/> 61310 references were found where the two concepts "Natural Product" and "anti cancer" were present anywhere in the reference.	61310
<input type="checkbox"/> 603806 references were found containing the concept "Natural Product".	603806
<input type="checkbox"/> 1626328 references were found containing the concept "anti cancer".	1626328
<b>Get References</b>	

Index Term:

帮助用户了解涉及到的重要技术术语，并修正检索词

更换检索词后，结果放大近60倍



# STN中的CAS Role

## ANST Analytical Study

Analyte	ANT
Analytical Matrix	AMX
Analytical Reagent Use	ARG
Analytical Role, Unclassified	ARU

## PREP Preparation

Bioindustrial Manufacture	BMF
Biosynthetic Preparation	BPN
Byproduct	BYP
Industrial Manufacture	IMF
Preparation, Unclassified	PNU
Purification or Recovery	PUR
Synthetic Preparation	SPN

## PROC Process

Biochemical Process	BCP
Biological Process	BPR
Geological or Astronomical Process	GPR
Physical, Engineering, or Chemical Process	PEP
Removal or Disposal	REM

## BIOL Biological Study

Adverse Effect, Including Toxicity	ADV
Agricultural Use	AGR
Biological Activity or Effector, Except Adverse	BAC
Biochemical Process	BCP
Bioindustrial Manufacture	BMF
Biological Occurrence	BOC
Biosynthetic Preparation	BPN
Biological Process	BPR
Biological Study, Unclassified	BSU
Biological Use, Unclassified	BUU
Cosmetic Use	COS
Diagnostic Use	DGN
Food or Feed Use	FFD
Natural Product Occurrence	NPO
Pharmacological Activity	PAC
Pharmacokinetics	PKT
Therapeutic Use	THU



ACS  
International



A division of the  
American Chemical Society

# STN中的CAS Role

## FORM Formation, Nonpreparative

Formation, Unclassified	FMU
Geological or Astronomical Formation	GFM

## NANO Nanomaterial

## OCCU Occurrence

Biological Occurrence	BOC
Geological or Astronomical Occurrence	GOC
Natural Product Occurrence	NPO
Occurrence, Unclassified	OCU
Pollutant	POL

## RACT Reactant or Reagent

Reactant	RCT
Reagent	RGT

## USES Uses

Agricultural Use	AGR
Analytical Reagent Use	ARG
Biological Use, Unclassified	BUU
Catalyst Use	CAT
Cosmetic Use	COS
Diagnostic Use	DGN
Food or Feed Use	FFD
Modifier or Additive Use	MOA
Other Use, Unclassified	NUU
Polymer in Formulation	POF
Technical or Engineered Material Use	TEM
Therapeutic Use	THU

# 巧用CAS Role

## 查找纯化双氧水（7722-84-1）的文献

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "Natural Product with anti canc..."

**REFERENCES**

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

**SUBSTANCES**

- Chemical Structure
- Markush

**REFERENCES: RESEARCH TOPIC ?**

purify of 7722-84-1

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

**Search**

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "purify of 7722-84-1"

**REFERENCES ?**

Select All Deselect All

1 of 4 Research Topic Candidates Selected

	References
<input checked="" type="checkbox"/> 2964 references were found containing the two concepts "purify" and "7722-84-1" closely associated with one another.	2964
<input type="checkbox"/> 23803 references were found where the two concepts "purify" and "7722-84-1" were present anywhere in the reference.	23803
<input type="checkbox"/> 2953232 references were found containing the concept "purify".	2953232
<input type="checkbox"/> 371389 references were found containing the concept "7722-84-1".	371389

**Get References**

# 巧用CAS Role

## 1. Material preparation method with visible light catalysis for purifying indoor air and sterilizing

By: Huang, Aimin

Assignee: Hebei Yuqing Environmental Protection Equipment Co., Ltd., Peop. Rep. China

The invention discloses a material prepn. method with visible light catalytic purify. of indoor air and sterilization, which has good purify. effect on formaldehyde, excellent sterilization performance, high visible light utilization rate and low cost. The material is a composite formed by loading Ag<sup>+</sup>/Cu-BiVO<sub>4</sub> on sepiolite.

### Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
CN 112691683	PDF	A		Apr 23, 2021	CN 2020-11545149	Dec 24, 2020

### Priority Application

CN 2020-11545149	Dec 24, 2020
------------------	--------------

### Indexing

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms (Section67)

### Concepts

Composites  
Heat treatment  
Stirring  
Volatile organic compounds

Drying process  
Roasting  
Vibration

material prepn. method with visible light catalysis for purifying indoor air and sterilizing

### Substances

63800-37-3 Sepiolite

Catalyst support; material prepn. method with visible light catalysis for purifying indoor air and sterilizing  
Catalyst use; Physical, engineering or chemical process; Process; Uses

14701-21-4

material prepn. method with visible light catalysis for purifying indoor air and sterilizing  
Biological use, unclassified; Modifier or additive use; Biological study; Uses

7440-50-8P Copper

material prepn. method with visible light catalysis for purifying indoor air and sterilizing  
Catalyst use; Modifier or additive use; Synthetic preparation; Preparation; Uses

7647-01-0 Hydrochloric acid  
7697-37-2 Nitric acid  
7722-84-1 Hydrogen peroxide



7761-88-8 Silver nitrate

material prepn. method with visible light catalysis for purifying indoor air and sterilizing  
Physical, engineering or chemical process; Process

噪音信息



# 巧用CAS Role

SciFinder<sup>®</sup> A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

SciFinder<sup>n</sup> is here! [Learn more](#) about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore | Saved Searches | SciPlanner

Research Topic "purify of 7722-84-1" > references (2964) > Material preparation method wi...

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Accession Number

0 of 2964 References Selected

1. **Material preparation method with visible light catalysis**  
PATENTPAK  
By Huang, Aimin  
From Faming Zhuanli Shenqing (2021), CN 112691683 A 20210422.  
The invention discloses a material prepn. method with good performance, high visible light utilization rate and low energy consumption.

2. **Hydrogels for the entrapment of bacteria and formaldehyde**  
PATENTPAK  
By Redcorn, Raymond; Winkler, Mari-Karoliina Henriikka; Godfrey, David  
From PCT Int. Appl. (2021), WO 2021076508 A1 20210422.  
Hydrogels for entrapment of live microorganisms and formaldehyde.

3. **Purification method of iron chloride**  
PATENTPAK  
By Che, Ying; He, Kaijing; Liang, Jinhua; Liang, Maojie; Chen, Hong  
From Faming Zhuanli Shenqing (2021), CN 112661196 A 20210422.  
The invention discloses a method for purifying iron chloride. The method can be applied to the fields of drinking water treatment and the like. The purification method provided by the invention comprises the following steps: oxidizing iron-contaminated water with hydrogen peroxide, adding a stripping agent for stripping to obtain a stripping solution, and the obtained iron chloride product can be used for the like. The purification method provided by the invention has good purification effect on formaldehyde, excellent sterilization effect on sepiolite.

**Save This Answer Set**

\* Required

Save:  
☒ All answers  
☐ Only selected answers

Title: \*  
purify of H2O2


Description:

OK Cancel

# 巧用CAS Role

☐ 1. 7722-84-1 🔍

~308261 📄

 ~127 🧪

OO

**H<sub>2</sub>O<sub>2</sub>**  
Hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>)  
▶ **Key Physical Properties**  
Regulatory Information  
Experimental Properties

**Get References**

**Limit results to:**

☐ Adverse Effect, including toxicity  
☐ Analytical Study  
☐ Biological Study  
☐ Combinatorial Study  
☐ Crystal Structure  
☐ Formation, nonpreparative  
☐ Miscellaneous  
☐ Occurrence

☒ Preparation  
☐ Process  
☐ Properties  
☐ Prophetic in Patents  
☐ Reactant or Reagent  
☐ Spectral Properties  
☐ Uses


**For each sequence, retrieve:**

☐ Additional related references, e.g., activity studies, disease studies.

Get

Cancel

# 巧用CAS Role

CAS Solutions


Preferences
SciFinder Help
Sign Out

Welcome Helen Zhu

SciFinder<sup>n</sup> is here! Learn more about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore
Saved Searches
SciPlanner
Save
Print
Export

⚠ Duplicates not removed. Answer set exceeds 10,000 reference limit.

Substance Identifier "7722-84-1" > substances (1) > get references (18225)

REFERENCES

Get Substances
Get Reactions
Get Related Citations
Tools

Create Keep Me Posted Alert
Send to SciPlanner

Analyze
Refine
Categorize

Sort by: Accession Number

☐ 0 of 18225 References Selected

Analyze by:
Author Name

Hutchings Graham J 63
Wang Wei 56
Wang Li 55
Edwards Jennifer K 48
Wang Erzhong 45
Brillas Enric 39
Carley Albert F 36
Kornienko V L 35
Jia Liming 33

☐ 1. Water-electrolysis bipolar plate structure for generating hydrogen peroxide

☐ 2. C70 Fullerene Catalyzed Photo...

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (18225):

Reference Answer Set Details	Date Saved
<input checked="" type="checkbox"/> purify of H2O2 (2964) Research Topic "purify of 7722-84-1" > references (2964)	May 17, 2021
<input type="checkbox"/> 黄茂 (4374) Research Topic "huangqi" > references (4374)	Dec 3, 2020
<input type="checkbox"/> synthesis of Daclatasvir (24) Substance Identifier "Daclatasvir" > substances (1) > get reactions (156) > get references (24)	Nov 9, 2020
<input type="checkbox"/> Jiangsu Univ-2001-2014 CAlus (13504) Opened saved answer set "Jiangsu Univ-2014 CAlus" (13669) > refine "2000-" (13542) > refine "2001-" (13504)	Oct 12, 2020

Select an option for combining the answer sets:

☐ Combine Include all answers from both sets

☒ Intersect Include only answers that appear in both sets

☐ Exclude Include only answers from current answer set (18225) that are not in purify of H2O2 (2964)


☐ Exclude Include only answers from purify of H2O2 (2964) that are not in current answer set (18225)


Combine Answer Sets
Cancel

electrode and a neg. electrode, and provides an electrode (GDE); a pos. electrode part including a le part to prevent elec. corrosion due to the pos.

n explored here. The developed strategy's main e. Further, sym. secondary amines can also be ctional theory studies revealed that the current

© 2021 American Chemical Society. All rights reserved.


ACS International


CAS

A division of the American Chemical Society

# 巧用CAS Role

REFERENCES

Get Substances

Get Reactions

Get Related Citations

Tools

Create Keep Me Posted Alert

Send to SciPlanner

Analyze Refine Categorize

Analyze by:

Author Name

Tanaka Fujio 7

Huo Wenzhou 6

Li Huayi 6

Liu Ye 6

Lv Qinglin 6

Minamikawa Yoshitsugu 6

Murakami Shinichi 6

Kajiware Shoichiro 5

Nagai Kazunori 5

Shi Ning 5

Show More

Sort by: Accession Number

0 of 368 References Selected

Page: 1 of 19

1. Process for providing anhydrous alkane sulfonic acids in purified form

Quick View PATENTPAK

By Ott, Timo; Biertuempel, Ingo

From PCT Int. Appl. (2020), WO 2020212298 A1 20201022. | Language: English, Database: CAPLUS

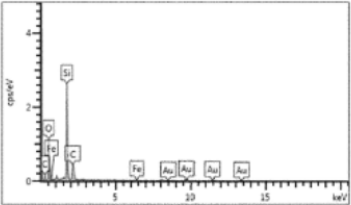
The invention is related to a process for providing an anhyd. alkane sulfonic acid in purified form comprising: (i) providing a reaction mixt. comprising hydrocarbon, alkanesulfonic acid and disulfuric acid; (ii) adding an additive to the reaction mixt., the additive reacting with disulfuric acid to form sulfuric acid as well as a reaction product of SO<sub>3</sub> and the additive, the reaction product having a b.p. higher than SO<sub>3</sub>; (iii) sepg. the hydrocarbon from the reaction mixt., followed by (iv) purifn. of the remaining reaction mixt. by distn. The advantage of the method of invention, is, that t...

2. Droplet-impingement, flow-assisted electro-fenton purification using heterogeneous silica/iron nanocomposite catalyst

Quick View PATENTPAK

By Basheer, Chanbasha; Haider, Muhammad Baseer; Nsubuga, Hakimu

From U.S. Pat. Appl. Publ. (2020), US 20200321630 A1 20201008. | Language: English, Database: CAPLUS



A droplet-impingement, flow-assisted electro-Fenton (DFEF) catalyst, system, and method can degrade to trace level org. materials, such as  $\beta$ -blockers in water. A silica/carbon-x % iron composite (RHS/C-x % Fe) can be made, e.g., from rice husks and iron ions into heterogeneous catalysts of varied iron content. The DFEF approach can improve oxygen satrn., mass transfer of  $\beta$ -blockers at the cathode, and continuous electrogeneration of hydroxyl radicals (.OH) in soln. and at boron-doped anode surfaces. A central composite design (CCD) can reduce costs and increase efficiency. Beta-blockers can...

3. Novel method for purifying hydrogen peroxide

Quick View PATENTPAK

By Wang, Gang; Guo, Fumin; Liu, Qiong; Li, Suidang; Kou, Xiaokang

From Faming Zhuanli Shenqing (2020), CN 111252740 A 20200609. | Language: Chinese, Database: CAPLUS

The invention discloses a novel method for purifying hydrogen peroxide, which has the advantages of good prodn. safety and low cost. The method comprises using multi-way conversion valve system and hydrogen peroxide purifn. resin.

4. Method for purifying hydrogen peroxide used in semiconductor device fabrication

Quick View PATENTPAK

浏览记录，判断是否符合要求

# 巧用CAS Role

## 1. Process for providing anhydrous alkane sulfonic acids in purified form

By: Ott, Timo; Bliertuempel, Ingo  
Assignee: BASF SE, Germany

The invention is related to a process for providing an anhyd. alkane sulfonic acid in purified form comprising: (i) providing a reaction mixt. comprising hydrocarbon, alkanesulfonic acid and disulfuric acid; (ii) adding an additive to the reaction mixt., the additive reacting with disulfuric acid to form sulfuric acid as well as a reaction product of SO<sub>3</sub> and the additive, the reaction product having a b.p. higher than SO<sub>3</sub>; (iii) sepg. the hydrocarbon from the reaction mixt., followed by (iv) purifn. of the remaining reaction mixt. by distn. The advantage of the method of invention, is, that the formation of sulfur trioxide is avoided by adding an additive selected from hydrogen peroxide, sulfuric acid, alkane sulfonic acid, ALK-SO<sub>2</sub>-O-O-X [ALK = Me, Et, Pr, Bu, C<sub>5-10</sub> alkyl; X = H, alkali metals, earth alk. metals, aluminum, and zinc, as well as mixts. of two or more of them], or ALK-SO<sub>2</sub>-O-O-SO<sub>2</sub>-O-X, to the reaction mixt. prior to the removal of the non-reacted hydrocarbons.

### Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
WO 2020212298	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	A1		Oct 22, 2020	WO 2020-EP60371	Apr 14, 2020

### Priority Application

EP 2019-170171	A	Apr 18, 2019
EP 2019-176382	A	May 24, 2019

### Indexing

Industrial Organic Chemicals, Leather, Fats, and Waxes (Section45-4)
Section cross-reference(s): 23

### Concepts

Sulfonic acids
alkylper-, salts, reaction products with sulfur trioxide; process for providing anhyd. alkane sulfonic acids in purified form
Industrial manufacture; Preparation
Sulfonic acids

### Substances

75-75-2P Methanesulfonic acid
7664-93-9DP Sulfuric acid, reaction products with sulfur trioxide
7722-84-1DP Hydrogen peroxide, reaction products with sulfur trioxide
process for providing anhyd. alkane sulfonic acid in purified form
Industrial manufacture; Preparation

## 5. Method for purifying hydrogen peroxide used in semiconductor device fabrication

By: Kim, Deokyun; Kim, Hyejin; Kim, Kyungyeol; Kim, Yongil  
Assignee: OCI Company Ltd., S. Korea

The present invention relates to a method for purifying H<sub>2</sub>O<sub>2</sub>. More particularly, the method comprises: a step of purifying a crude product of H<sub>2</sub>O<sub>2</sub> using a primary purifn. system; and a step of purifying the primarily-purified H<sub>2</sub>O<sub>2</sub> soln. using a secondary purifn. system. One of the primary purifn. system and the secondary purifn. system comprises an electrodeionization system, and the other of the primary purifn. system and the secondary purifn. system comprises at least one of a distn. system, a resin system, a reverse osmosis system, and a combination system thereof.

### Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
WO 2020036274	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	A1		Feb 20, 2020	WO 2019-KR1135	Jan 25, 2019
KR 2020020374	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	A	Korean	Feb 26, 2020	KR 2018-96017	Aug 17, 2018
CN 112789241		A		May 11, 2021	CN 2019-80065196	Jan 25, 2019

### Priority Application

KR 2018-96017	A	Aug 17, 2018
WO 2019-KR1135	W	Jan 25, 2019

### Indexing

Industrial Inorganic Chemicals (Section49-8)
Section cross-reference(s): 76

### Concepts

Semiconductor device fabrication
method for purifying hydrogen peroxide

### Substances

7722-84-1P Hydrogen peroxide, preparation	Page 13 in <b>PATENTPAK</b>
method for purifying hydrogen peroxide	
Purification or recovery; Technical or engineered material use; Preparation; Uses	

都是需要的文献

# 善用Categorize

检索文献：

1. 去除N-甲基甲酰胺（123-39-7）的文献？
2. 用N-甲基甲酰胺（123-39-7）作洗脱剂的文献？

# 善用Categorize

去除N-甲基甲酰胺（123-39-7）

Explore ▼

Saved Searches ▼

SciPlanner

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

REFERENCES: RESEARCH TOPIC ?

remove of 123-39-7

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

Search

REFERENCES ?

Select All Deselect All

1 of 4 Research Topic Candidates Selected

<input checked="" type="checkbox"/>	59 references were found containing the two concepts "remove" and "123-39-7" closely associated with one another.	59
<input type="checkbox"/>	325 references were found where the two concepts "remove" and "123-39-7" were present anywhere in the reference.	325
<input type="checkbox"/>	358833 references were found containing the concept "remove".	358833
<input type="checkbox"/>	5445 references were found containing the concept "123-39-7".	5445

Get References



# 善用Categorize

## 1. Efficient organic piston ring decarburization repairing agent

By: Peng, Hongbin; Xiang, Hua

Assignee: Jiangxi Longwei Environmental Protection Technology Development Co., Ltd., Peop. Rep. China

The title repairing agent comprises (by wt. parts) carbon deposit dissolving agent (N,N-dimethylformamide, N,N-dimethylacetamide, etc.) 50-80, detergent dispersant (SURFONAMINE FL1000, SURFONAMINE B100 and/or T3595) 5-20, ester type lubricating tackifier (CRODA Perfad 3336, Ketjenlube 3700, etc.) 1-5, solvent-based surfactant (N,N-dimethyl-9-decenamide and/or STEPOSOL MET-10U) 1-10, oil fouling disintegration accelerator (triphenylphosphine and/or diphenyl-2-pyridylphosphine) 1-2, and additive 0.1-1. The additive includes antioxidant (2,6-di-tert-butyl-4-methylphenol and/or 2,6-di-tert-Bu mixed phenol) and rust inhibitor (T551, T561, etc.). The invention can improve carbon **removal** efficiency, soly., stability and corrosion resistance, and has high safety, simple recycling procedure and no wastewater discharge.

### Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
CN 111925844	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	A		Nov 13, 2020	CN 2020-10654471	Jul 9, 2020

### Priority Application

CN 2020-10654471	Jul 9, 2020
------------------	-------------

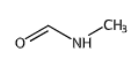
### Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-12)
Section cross-reference(s): 47

### Concepts

Internal combustion engines	Lubricating oil additives
Piston rings	
efficient piston ring org. carbon <b>removal</b> repairing agent for engine	

### Substances

68-12-2 N,N-Dimethylformamide, uses	Page 2 in <b>PATENTPAK</b>
79-16-3 N-Methylacetamide	Page 2 in <b>PATENTPAK</b>
88-12-0 N-Vinyl-2-pyrrolidone, uses	Page 2 in <b>PATENTPAK</b>
123-39-7 Methylformamide	Page 2 in <b>PATENTPAK</b>
	
127-19-5 N,N-Dimethylacetamide	Page 2 in <b>PATENTPAK</b>
128-37-0 2,6-Di-tert-butyl-4-methylphenol, uses	Page 2 in <b>PATENTPAK</b>
603-35-0 Triphenylphosphine, uses	Page 2 in <b>PATENTPAK</b>
616-45-5 2-Pyrrolidone	Page 2 in <b>PATENTPAK</b>
872-50-4 1-Methyl-2-pyrrolidone, uses	Page 2 in <b>PATENTPAK</b>
2687-91-4 1-Ethyl-2-pyrrolidone	Page 2 in <b>PATENTPAK</b>
3470-99-3 1-Propylpyrrolidin-2-one	Page 2 in <b>PATENTPAK</b>
6837-24-7 N-Cyclohexyl-2-pyrrolidone	Page 2 in <b>PATENTPAK</b>
14433-76-2 N,N-Dimethylcapramide	Page 2 in <b>PATENTPAK</b>
37943-90-1 Diphenyl-2-pyridylphosphine	Page 2 in <b>PATENTPAK</b>
150648-12-7 SURFONAMINE B100	Page 2 in <b>PATENTPAK</b>
152618-68-3 T 561	Page 2 in <b>PATENTPAK</b>
325737-17-5 T 747 (antirust additive)	Page 2 in <b>PATENTPAK</b>
1356964-77-6 N,N-Dimethyl-9-decenamide	Page 2 in <b>PATENTPAK</b>
1819965-72-4 Steposol MET 10U	Page 2 in <b>PATENTPAK</b>
1980862-50-7 T 746 (phosphate)	Page 2 in <b>PATENTPAK</b>
2566475-41-8 PE 3100 (polyester)	Page 2 in <b>PATENTPAK</b>

efficient piston ring org. carbon **removal** repairing agent for engine

Other use, unclassified; Uses

噪音信息很多，如何去除？

# 善用Categorize

CAS Solutions **SciFinder**  
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

SciFinder<sup>n</sup> is here! Learn more about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore | Saved Searches | SciPlanner

Research Topic "remove of 123-39-7" > references (59) > Efficient organic piston ring ...

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | **Categorize**

Sort by: Accession Number

0 of 59 References Selected

Analyze by: Author Name

Egbe Matthew I 4

Hara Yasushi 4

Takahashi Fumiharu 4

Bang Sun Hong 2

Hong Heon Pyo 2

Lee Dong Hoon 2

Lee Woo Ram 2

Legenza Michael Walter 2

Park Tae Moon 2

Ward Irl E 2

Show More

1. **Efficient organic piston ring decarburization repairing agent**  
PATENTPAK  
By Peng, Hongbin; Xiang, Hua  
From Faming Zhuanti Shenqing (2020), CN 111925844 A 20201113. | Language: Chinese, Database: CAPLUS  
The title repairing agent comprises (by wt. parts) carbon deposit dissolving agent (N,N-dimethylformamide, N,N-dimethylacetamide, etc.) 50-80, detergent dispersant (SURFONAMINE FL1000, SURFONAMINE B100 and/or T3595) 5-20, ester type lubricating tackifier (CRODA Perfad 3336, Ketjenlube 3700, etc.) 1-5, solvent-based surfactant (N,N-dimethyl-9-decanamide and/or STEPOSOL MET-10U) 1-10, oil fouling disintegration accelerator (triphenylphosphine and/or diphenyl-2-pyridylphosphine) 1-2, and additive 0.1-1. The additive includes antioxidant (2,6-di-tert-butyl-4-methylphenol and/or 2,6-di-tert-Bu mix...

2. **Photoresist-removing stripper composition and method for stripping photoresist using same**  
PATENTPAK  
By Park, Tae Mun; Lee, Dong Hun; Song, Hyeon U.; Lee, U. Ram  
From Repub. Korean Kongkae Taeho Kongbo (2020), KR 2020112551 A 20201005. | Language: Korean, Database: CAPLUS  
The present invention relates to a photoresist-removing stripper compn. and a method for stripping photoresist using same, wherein the photoresist-removing stripper compn. has excellent photoresist stripping power, inhibits corrosion of a lower metal film during a stripping process, and is capable of effectively removing oxides.

3. **Photoresist-removing stripper composition and method for stripping photoresist using same**  
PATENTPAK  
By Park, Tae Moon; Lee, Dong Hoon; Song, Hyun Woo; Lee, Woo Ram  
From PCT Int. Appl. (2020), WO 2020197014 A1 20201001. | Language: Korean, Database: CAPLUS  
The present invention relates to a photoresist-removing stripper compn. and a method for stripping photoresist using same, wherein the photoresist-removing stripper compn. has excellent photoresist stripping power, inhibits corrosion of a lower metal film during a stripping process, and is capable of effectively removing oxides.

4. **Self-assembled radioactive cesium removal complex, its manufacturing method, and method for removing radioactive cesium using thereof**  
PATENTPAK  
By Oh, Yeong Tak; Lee, Hui Hyeon; Kim, Myeong Gil; Won, Jong Guk; Kang, Yeo Gyeong  
From Repub. Korean Kongkae Taeho Kongbo (2020), KR 2020064526 A 20200608. | Language: Korean, Database: CAPLUS  
The present invention relates to a radioactive cesium removal complex contg. self-assembled chalcogen compds.; and an ammonium group bound to the surface of the chalcogen compd.

Chemical structures and diagrams illustrating the self-assembled radioactive cesium removal complex and its application.

# 善用Categorize

Categorize ?

1. Select a heading and category.

Category Heading

All

Technology

General chemistry

Physical chemistry

Polymer chemistry

Biotechnology

Environmental chemistry

Synthetic chemistry

Catalysis

Genetics & protein chemistry

Biology

Analytical chemistry

Category

Substances in technology (874)

Materials & products (72)

Formed, removed, & other substances (65)

Metallurgy (43)

Processes & apparatus (38)

Imaging & recording (5)

Power & fuel topics (4)

Ceramics (2)

Construction (2)

2. Select index terms of interest.

Index Terms

Select All Deselect All

☒ Formamide, N-methyl- 7
 ☐ Dimethylformamide 4
 ☐ Formamide 3
 ☐ Carbon 2
 ☐ Copper 2
 ☐ Copper alloy 2
 ☐ Dimethylamine 2
 ☐ Oxides (inorganic) 2
 ☐ Polyimides 2
 ☐ 1-Fluoro-1,2,2-trichloroethane 1
 ☐ 2,3-Dimethyl-1-butanol 1
 ☐ 2,4-Di-tert-butylphenol 1
 ☐ 2,6-Di-tert-butyl-1,4-benzoquinone 1
 ☐ 2-(Methyl mercapto)benzothiazole 1

Selected Terms

Click 'x' to remove the category from 'Selected Terms'

✱ Technology > Formed, removed, & other substances (1 Terms)

Technology > Formed, removed, & other substances > 1 Index Term(s) Selected

OK Cancel

# 高效阅读专利文献—CAS PatentPak

1. Method for removing odor of ethylene-vinyl acetate copolymer

Quick View PATENTPAK

By Ma, Qingsheng  
From Faming Zhu

The invention relates to a method for removing odor of ethylene-vinyl acetate copolymer, wherein the core component of the foaming system comprises 70-100 parts of ethylene-vinyl acetate, 1-20 parts of polyurethane, 0.5-10 parts of zinc hydroxide and 0.5-5 parts of triglyceride.

base: CAPLUS

Patent No. CN 109810370

PatentPak Options PDF | PDF+ | Viewer

Kind A

Language Chinese

PAGE 4 / 4

ZOOM

DOWNLOAD PDF

Key Substances in Patent

CAS RN 123-39-7

CCNC=O

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 4

CAS RN 68-12-2

CC(C)N(C)C=O

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 4

CAS RN 29196-72-3

OCC(O)C(=O)O

份,甘油三酯3份,利用上述配方与80份乙烯-醋酸乙烯进行发泡,发泡过程和得到的发泡制品无异味,检测结果:甲酰胺低于5ppm;乙酰苯低于5ppm;N-甲基甲酰胺低于5ppm;N,N-二甲基甲酰胺低于5ppm,均低于相关标准。

[0020] 实施例2:偶氮二异丁腈1份,过氧化二异丙苯5份,三聚磷酸铝1份,氧化锌为5份,甘油三酯5份,利用上述配方与70份乙烯-醋酸乙烯进行发泡,发泡过程和得到的发泡制品无异味,检测结果:甲酰胺低于10ppm;乙酰苯低于10ppm;N-甲基甲酰胺低于10ppm;N,N-二甲基甲酰胺低于10ppm,均低于相关标准。

跳转回SciFinder  
开启新检索

在PatentPak浏览器中点击物质  
下面的紫色灯泡，快速定位到  
PDF文件中的物质信息。也可从  
PDF文件中与PatentPak进行互动

# 文献检索小结

1. 主题检索时，使用介词 in, with, of 等作为连接词
2. 根据检索要求选择合适的候选项
3. 通过SciFinder的Analyze/Refine功能来缩小检索的范围
4. 利用Analyze-Index Term查看更好的关键词
5. 使用Categorize可以让系统来实现自动分类
6. 利用CAS Role解决问题
7. 检索思路：初检—浏览结果集—修正检索式或考虑相应的筛选策略—得到更准确的结果集

# 大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略 (CAS Analytical Methods)



# CAS SciFinder检索--物质检索

## ■ 物质检索方法

- 结构式检索
- 分子式检索
- 理化性质（物质属性）检索
- 物质标识符检索：化学名称、CAS RN
- 从文献或反应结果获得

## ■ 检索策略推荐

- 有机化合物，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



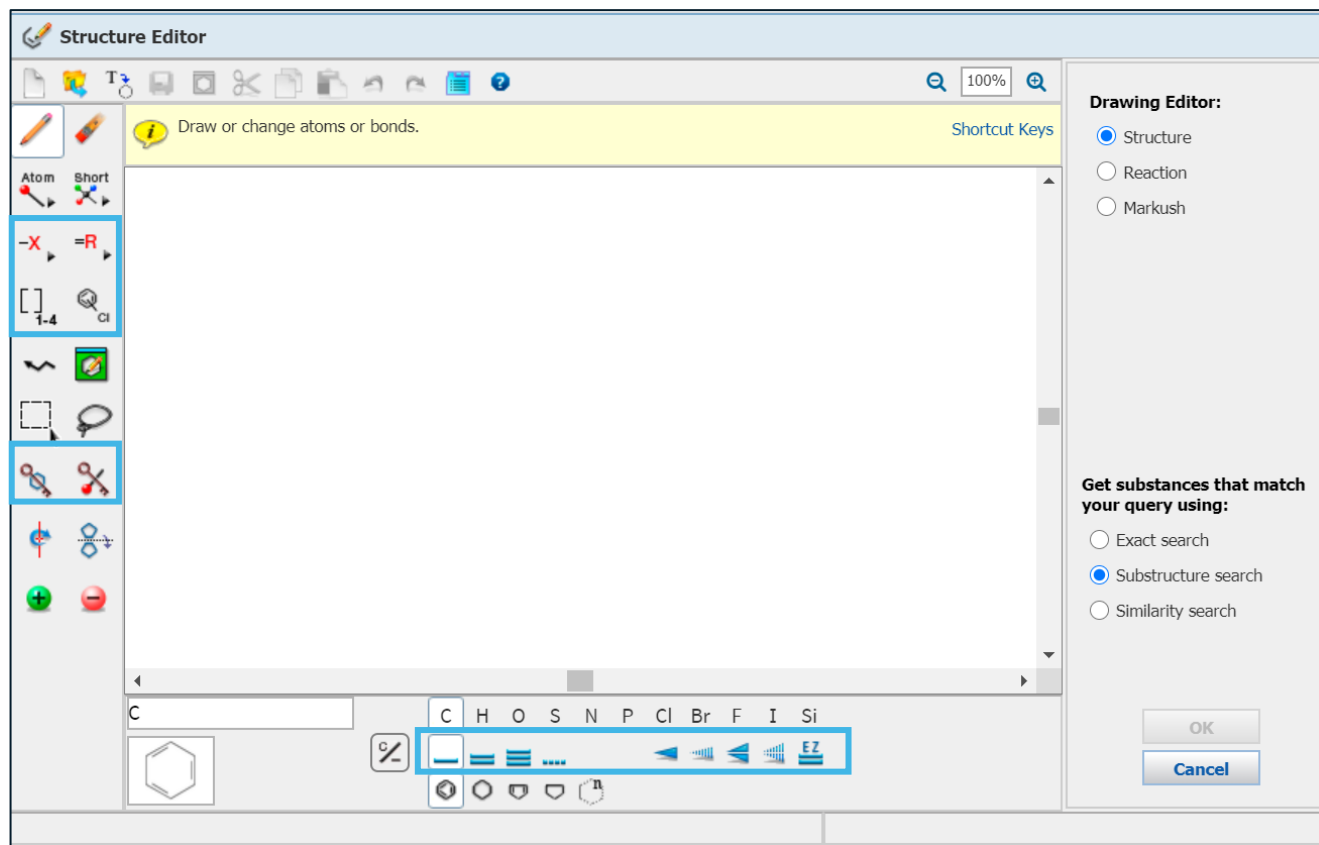
### SUBSTANCES

Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier



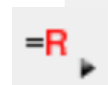


# 绘图面板




## 重要绘制工具注释

 选择可变基团

 自定义R基团

 重复工具

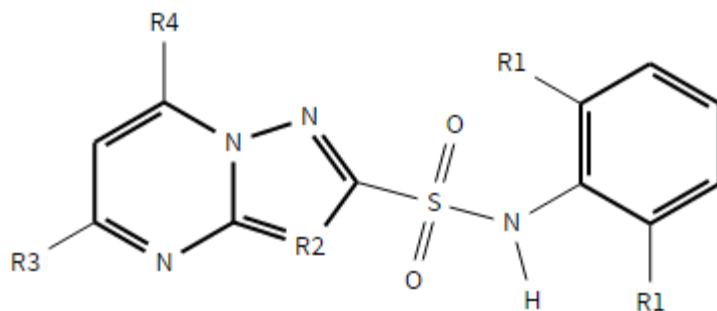
 取代位置可变

 锁环工具

 锁原子工具

# 检索具有相同结构特征的物质

找到包含如下物质的相关文献:




要求:


- R1 = X, H, -NO<sub>2</sub>, -CF<sub>3</sub>
- R2 = C 或 N
- R3 = 任意非氢原子
- R4 = 2-5个碳的碳链
- 结构中的环不发生稠环

# CAS Markush检索

(19) 中华人民共和国国家知识产权局



(12) 发明专利申请



(10) 申请公布号 CN 104945470 A

(43) 申请公布日 2015.09.30

(21) 申请号 201410122313.4

C07K 1/16(2006.01)

(22) 申请日 2014.03.30

C07K 1/06(2006.01)

(71) 申请人 浙江大学

A61K 38/06(2006.01)

地址 310027 浙江省杭州市西湖区浙大路 38 号

A61P 35/00(2006.01)

申请人 中国科学院上海药物研究所

A61P 35/02(2006.01)

(72) 发明人 胡永洲 李佳 刘滔 张建康

A61P 25/28(2006.01)

周宇波 杨波 何倩军 许磊

A61P 37/02(2006.01)

胡小蓓

(74) 专利代理机构 杭州求是专利事务有限公司

司 33200

代理人 张法高 赵杭丽

(51) Int. Cl.

C07K 5/087(2006.01)

C07K 5/083(2006.01)

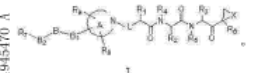
权利要求书3页 说明书24页 附图4页

(54) 发明名称

杂环构建的三肽环氧酮类化合物及制备和应用

(57) 摘要

本发明提供一种杂环构建的三肽环氧酮类化合物,以 Carfilzomib 为先导化合物,经缩合、酸性条件下脱去 Boc 保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶体抑制剂。本发明化合物具有极强的蛋白酶体抑制活性及细胞增殖抑制活性,是有前景的蛋白酶体抑制剂,为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得,路线设计合理,反应条件温和,各步产率高,操作简便,适合工业化生产。具有下述式 I 的结构通式:



CN 104945470 A

## 具体实施方式

[0026] 本发明结合附图和实施例作进一步的说明,以下实施例仅是说明本发明,而不是以任何方式限制本发明。

[0027] 制备实施例 1、4-(吡嗪-2-基氨甲酰基)哌啶-1-甲酸叔丁酯 (1a, 1b)

将 1-(叔丁氧羰基)哌啶-4-甲酸 (2.75g, 12mmol) 置于 50mL 三颈瓶中, N<sub>2</sub> 保护下加入 25mL 无水 CH<sub>2</sub>Cl<sub>2</sub>, 然后缓缓滴入吡啶 (2.5mL, 30mmol) 和二氯亚砷 (1.1mL, 14mmol), 该反应液置于室温反应半小时。随后, 2-氨基吡嗪 (0.95g, 10mmol) 和三乙胺 (5.7mL, 40mmol) 溶于 15mL CH<sub>2</sub>Cl<sub>2</sub> 后缓缓滴入上述反应液, 室温反应 6 小时。反应液加 30mL 饱和食盐水稀释, 分出有机层, 水层 CH<sub>2</sub>Cl<sub>2</sub> 提取 (15mL×3), 合并有机层, 无水硫酸钠干燥后减压除去溶剂, 柱层析分离得白色固体 2.3g, 收率 74%。m.p.: 134-136℃; <sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>): δ = 9.55 (s, 1H, pyrazine-H), 8.35 (d, 1H, J=2.0Hz, pyrazine-H), 8.23 (s, 1H, pyrazine-H), 7.97 (s, 1H, NH), 4.20 (m, 2H, CH<sub>2</sub>), 2.81 (m, 2H, CH<sub>2</sub>), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH<sub>2</sub>), 1.76 (m, 2H, CH<sub>2</sub>), 1.47 (s, 9H, CH<sub>3</sub>) ppm; ESI-MS: m/z = 307 [M+H]<sup>+</sup>。

[0028] 制备实施例 2、4-(吡嗪-2-酰基)哌啶-1-甲酸叔丁酯 (1c, 1d)

吡嗪-2-羧酸 (1.5g, 12mmol) 置于 50mL 反应瓶中, 加入 35mL 无水 CH<sub>2</sub>Cl<sub>2</sub> 溶解, 随即加入 1-羟基苯并三氮唑 (1.6g, 12mmol) 和 N-(3-二甲氨基丙基)-N'-乙基碳二亚胺盐酸盐 (3.5g, 18mmol), 室温反应半小时。随后, 哌啶-1-甲酸叔丁酯 (1.9g, 10mmol) 加入反应液中, 室温反应 3 小时。反应液加入 30mL 饱和碳酸氢钠水溶液稀释, 分出有机层, 饱和食

具体物质[Specific Substance]:

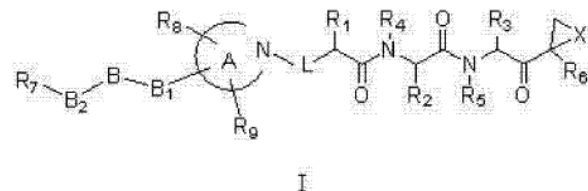
以具体化学结构陈述的特定物质, 会被分配CAS RN

# CAS Markush检索

预测性物质[Prophetic Substance]:

- 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
- 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，能检索到通过结构检索检不到的专利

1. 一种杂环构建的三肽环氧酮类化合物,具有下述结构通式 I:



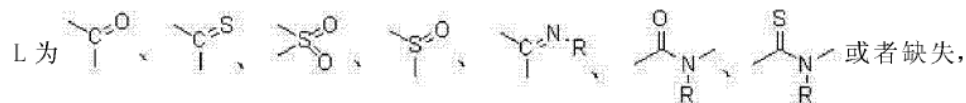
其中：

$R_1, R_2, R_3$  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<sub>4</sub>, R<sub>5</sub> 各自独立选自 H、OH、C<sub>1-6</sub> 烷基、卤代的 C<sub>1-6</sub> 烷基或芳烷基；

R<sub>5</sub> 选自 H, C<sub>1-6</sub> 烷基, 卤代的 C<sub>1-6</sub> 烷基, C<sub>1-6</sub> 羟基烷基, C<sub>1-6</sub> 烷氧基, 卤代的 C<sub>1-6</sub> 烷氧基, C(0)O-C<sub>1-6</sub> 烷基, C(0)NH-C<sub>1-6</sub> 烷基, 芳烷基;

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

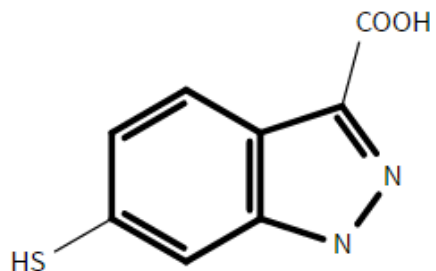


其中 R 选自 H、C<sub>1-6</sub> 烷基或卤代的 C<sub>1-6</sub> 烷基；

环A选自5~7元的饱和脂肪杂环、不饱和杂环、或者有取代的5~7元的饱和脂肪杂环、不饱和杂环,所述的杂环包含0~3个选自O、N和S的杂原子并任选地被R<sub>8</sub>、R<sub>9</sub>和B<sub>1</sub>基团取代;

$R_8, R_9$  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、 $C_{1-6}$  烷基-D、芳基、杂环芳基、环烷基和杂环基, 这些基团可以被卤素、硝基、氨基、CN、 $C_{1-6}$  烷基、卤代的  $C_{1-6}$  烷基、 $C_{1-6}$  烷氧基或卤代的  $C_{1-6}$  烷氧基取代, 每个基团可与一个或多个芳基或杂环

# CAS Markush检索



Explore ▼	Saved Searches ▼	SciPlanner
⚠ Explore Substances resulted in 0 substances <a href="#">Return</a>		
Chemical Structure substructure with limiters > <b>substances (0)</b>		
<b>SUBSTANCES</b>		
Analyze	Refine	
Analyze by: <i>No substances available</i>		

Substance检索结果为0!

# CAS Markush检索

Markush substructure > references (69)

REFERENCES

Get Substances Get Reactions Get Related Citations Tools Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

☐ 0 of 69 References Selected Page: 1 of 4

Analyze by:

Author Name

Boga Sobhana Babu 3

Deng Yongqi 3

Nan Yang 3

Paliwal Sunil 3

Shih Neng Yang 3

Shippis Gerald W Jr 3

Tsui Hon Chung 3

Alhassan Abdul Basit 2

Beier Norbert 2

Bulawa Christine Ellen 2

Show More

☐ 1. **Preparation of ethynylheterocycles as rho-associated coiled-coil kinase (ROCK) inhibitors for the treatment of diseases**  
 Quick View **PATENTPAK**  
By Li, An-Hu; Sakilam, Satish Kumar; Gadhiya, Satish Kumar; Lim, Dong Sung; Zong, Yao; Ponnala, Shashikanth; Zhang, Ying; Jung, Dawoon; Oehlen, Lambertus J. W. M.  
From PCT Int. Appl. (2021), WO 2021016256 A2 20210128. | Language: English, Database: CAPLUS  
The invention relates to prepn. of ethynylheterocycles of formula (I): and pharmaceutically acceptable salts thereof, wherein Cy<sup>1</sup>, Cy<sup>2</sup>, Cy<sup>3</sup> each independently represents an aryl, heteroaryl, or heterocyclic, which is optionally fused with a 3-8 membered cycloalkyl, 3-8 membered heterocycloalkyl, 6-membered aryl, or 5-6 membered heteroaryl; R, R<sup>1</sup>, R<sup>2</sup>, and R<sup>3</sup> each independently represents an aryl, heteroaryl, or heterocyclic, which is optionally fused with a 3-8 membered cycloalkyl, 3-8 membered heterocycloalkyl, 6-membered aryl, or 5-6 membered heteroaryl, and pharmaceutical compns. thereof, ...

☐ 2. **Indazoles and azaindazoles as LRRK2 inhibitors in the treatment of CNS disorders and their preparation**  
 Quick View **PATENTPAK**  
By Garofalo, Albert W.; De Lombaert, Stephane; Schwarz, Jacob Bradley; Andreotti, Daniele; Sabbatini, Fabio Maria; Serra, Elena; Bernardi, Silvia; Migliore, Marco; Budassi, Federica; Beato, Claudia  
From PCT Int. Appl. (2021), WO 2021007477 A1 20210114. | Language: English, Database: CAPLUS  
The invention relates compds. of formula I, their prepn. and their use as inhibitors of LRRK2 in the treatment of CNS disorders. Compd. I, wherein A is halo, (un)substituted C<sub>1-6</sub> alkyl, (un)substituted C<sub>2-6</sub> alkenyl, etc.; ring B is Ph and 5- to 10-membered heteroaryl wherein said 5- to 10-membered heteroaryl comprises 1, 2 and 3 ring-forming heteroatoms independently selected from N, O and S; X<sup>2</sup> is N and CR<sup>2</sup>; X<sup>3</sup> is N and CR<sup>3</sup>; X<sup>4</sup> is N and CR<sup>4</sup>; no more than two of X<sup>2</sup>, X<sup>3</sup> and X<sup>4</sup> are simultaneously N; R<sup>1</sup> is independently H, halo, C<sub>1-6</sub> alkyl, etc.; R<sup>2</sup> and R<sup>4</sup> are independently H, halo, C<sub>2-6</sub> alke...

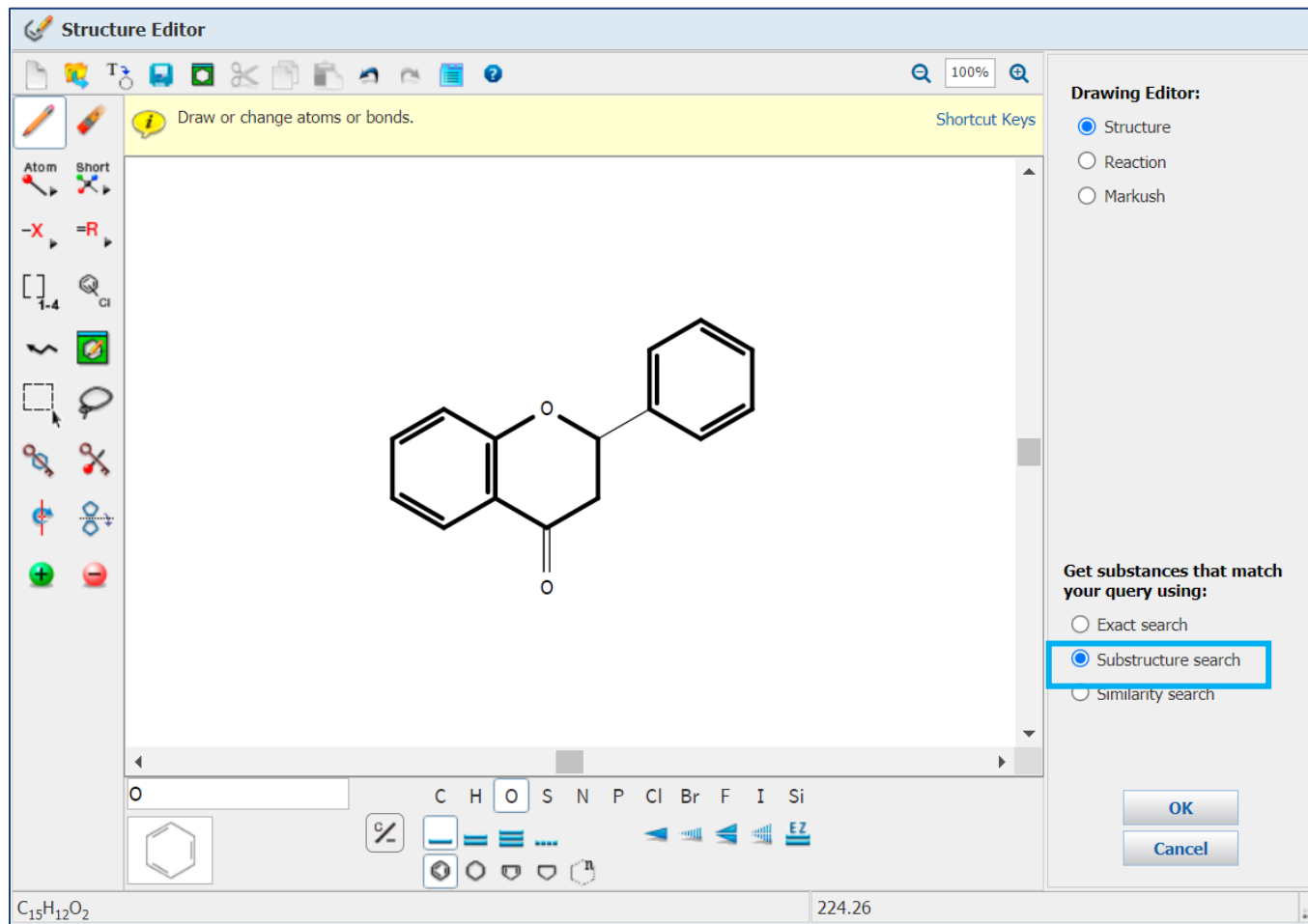
☐ 3. **Organic electroluminescent materials and devices**  
 Quick View **PATENTPAK**  
By Ji, Zhiqiang; Boudreaux, Pierre-Luc T.; Shih, Wei-Chun  
From U.S. Pat. Appl. Publ. (2020), US 20200358008 A1 20201112. | Language: English, Database: CAPLUS  
Provided are organometallic compds. comprising novel ligands represented by a general chem. formula I (Y = R, OR, SR etc.; Z = O, S, NR<sup>n</sup>; X<sup>1-5</sup> = C, N; R<sup>A</sup>, R<sup>B</sup> = substitution; R, R<sup>n</sup> = alkyl, cycloalkyl heteroalkyl etc.) as OLED materials for OLED.

Formula 1

Formula 2

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

# 天然产物的筛选



- |                 |                                     |                                 |
|-----------------|-------------------------------------|---------------------------------|
| Characteristics | <input checked="" type="checkbox"/> | Single component                |
|                 | <input type="checkbox"/>            | Commercially available          |
|                 | <input type="checkbox"/>            | Included in references          |
| Classes         | <input type="checkbox"/>            | Alloys                          |
|                 | <input type="checkbox"/>            | Coordination compounds          |
|                 | <input type="checkbox"/>            | Incompletely defined            |
|                 | <input type="checkbox"/>            | Mixtures                        |
|                 | <input type="checkbox"/>            | Polymers                        |
|                 | <input checked="" type="checkbox"/> | Organics, and others not listed |
| Studies         | <input type="checkbox"/>            | Analytical                      |
|                 | <input checked="" type="checkbox"/> | Biological                      |
|                 | <input type="checkbox"/>            | Preparation                     |
|                 | <input type="checkbox"/>            | Reactant or reagent             |



# 天然产物的筛选

Chemical Structure substructure with limiters > substances (10247)

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: Relevance

0 of 10247 Substances Selected

Page: 1 of 205

Display Options

Analyze by:

Substance Role

Biological Study 10059

Uses 5417

Preparation 5383

Properties 3972

Occurrence 2162

Analytical Study 1646

Reactant or Reagent 1520

Process 695

Formation, Nonpreparative 368

Prophetic in Patents 65

Show More

1. 487-26-3

~2770 ~89

Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$   
4/4'-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-  
▶ Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

2. 17002-31-2

~294 ~16

Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$   
4/4'-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-  
▶ Key Physical Properties  
Experimental Properties

3. 27439-12-9

~262 ~12

Absolute stereochemistry., Rotation (+).

$C_{15}H_{12}O_2$   
4/4'-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2R)-  
▶ Key Physical Properties  
Experimental Properties

4. 92496-65-6

~70 ~37

$C_{15}H_{12}O_3$   
4/4'-1-Benzopyran-4-one, 2,3-dihydro-2-(3-hydroxyphenyl)-  
▶ Key Physical Properties  
Regulatory Information  
Experimental Properties

5. 334707-47-0

~7 ~3

Absolute stereochemistry.

$C_{15}H_{12}O_3$   
4/4'-1-Benzopyran-4-one, 2,3-dihydro-2-(3-hydroxyphenyl)-, (2S)-

6. 2545-13-3

~43 ~7

Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_3$   
4/4'-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-2-phenyl-, (2S)-

7. 6515-36-2

~311 ~81

$C_{15}H_{12}O_3$   
4/4'-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-2-phenyl-

8. 41255-36-1

~84 ~5

$C_{16}H_{14}O_2$   
4/4'-1-Benzopyran-4-one, 2,3-dihydro-2-(4-methylphenyl)-

哪些物质是天然存在的呢？

# 天然产物的筛选

☐ 22. **17348-76-4**

~147 

~63

**C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>**  
**4-(4-Hydroxyphenyl)-2,3-dihydro-1H-benzoxan-4-one**

**Get References**

**Limit results to:**

☐ Adverse Effect, including toxicity  
☐ Analytical Study  
☐ Biological Study  
☐ Combinatorial Study  
☐ Crystal Structure  
☐ Formation, nonpreparative  
☐ Miscellaneous  
☒ Occurrence

☐ Preparation  
☐ Process  
☐ Properties  
☐ Prophetic in Patents  
☐ Reactant or Reagent  
☐ Spectral Properties  
☐ Uses

**For each sequence, retrieve:**

☐ Additional related references, e.g., activity studies, disease studies.


### Studies of structure-activity relationship on plant polyphenol-induced suppression of human liver cancer cells

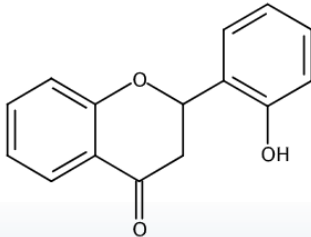
By: Loa, Jacky; Chow, Pierce; Zhang, Kai

To study anticancer activities of 68 plant polyphenols with different backbone structures and various substitutions and to analyze the structure-activity relationship, 68 polyphenols on human liver cancer cells were screened by the 3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyltetrazolium bromide method. Structure-activity relationship was analyzed with selected structures. Cell cycle progression was assayed by flow cytometry anal. and apoptosis was analyzed by DNA fragment assay. Based on the results, they were sub-classed to flavonoids (chalcones, flavanones, flavones and isoflavones), chromones and coumarins. The order of their potency to suppress the cell cycle progression was chromones > isoflavones > flavanones > coumarins. Chalcones comprise the most potent group with  $IC_{50}$  values ranging from 21.69 to 197  $\mu M$ . Top n-phenyl substituted chalcones showed the highest  $IC_{50}$  values at 2'-carbon position in B-ring. Flavones ranked second in their potencies. Quercetin, 4-hydroxyflavone and luteolin are three hydroxyflavones with the highest  $IC_{50}$  values are 30.81, 39.29 and 71.17  $\mu M$ , resp. Chromones, isoflavones, flavanones and coumarins showed much lower potencies when compared to chalcones with  $IC_{50}$  values are 131 to >400, 138 to >400 and 360.85 to >400  $\mu M$ , resp. In mechanistic studies, the most potent chalcone, 2,2'-dihydroxychalcone could induce G2/M arrest in human liver cancer cells. Anal. of structure-activity relationship showed that following structures are required for their inhibitory potencies on human liver cancer cells: (1) of the unique backbone structure of chalcones with a open C-ring; (2) within the chalcone group, hydroxyl substitution at 2'-carbon of B-ring; (3) hydroxyl substitution at 4-position of A-ring. However, some other structures were found to decrease their potencies: e.g. substitutions by sugar moieties in flavones. These data are valuable for the design of potential antiproliferative agents of cancer cells.

## Indexing

Pharmacology (Section1-3)

17348-76-4 2'-Hydroxyflavanone 

Oc1ccccc1C2=C(C(=O)O2)c3ccccc3

SAR showed that unique back bone structure of chalcones with open C-ring, within chalcone group, hydroxyl substitution of 2'-hydroxyflavanone from plant polyphenols was required for inhibiting human liver cancer cell

Natural product occurrence;  
Occurrence; Uses

Pharmacological activity; Therapeutic use; Biological study;

# 无机复合物的检索

检索YAG: Ce<sup>3+</sup>复合物及相关文献

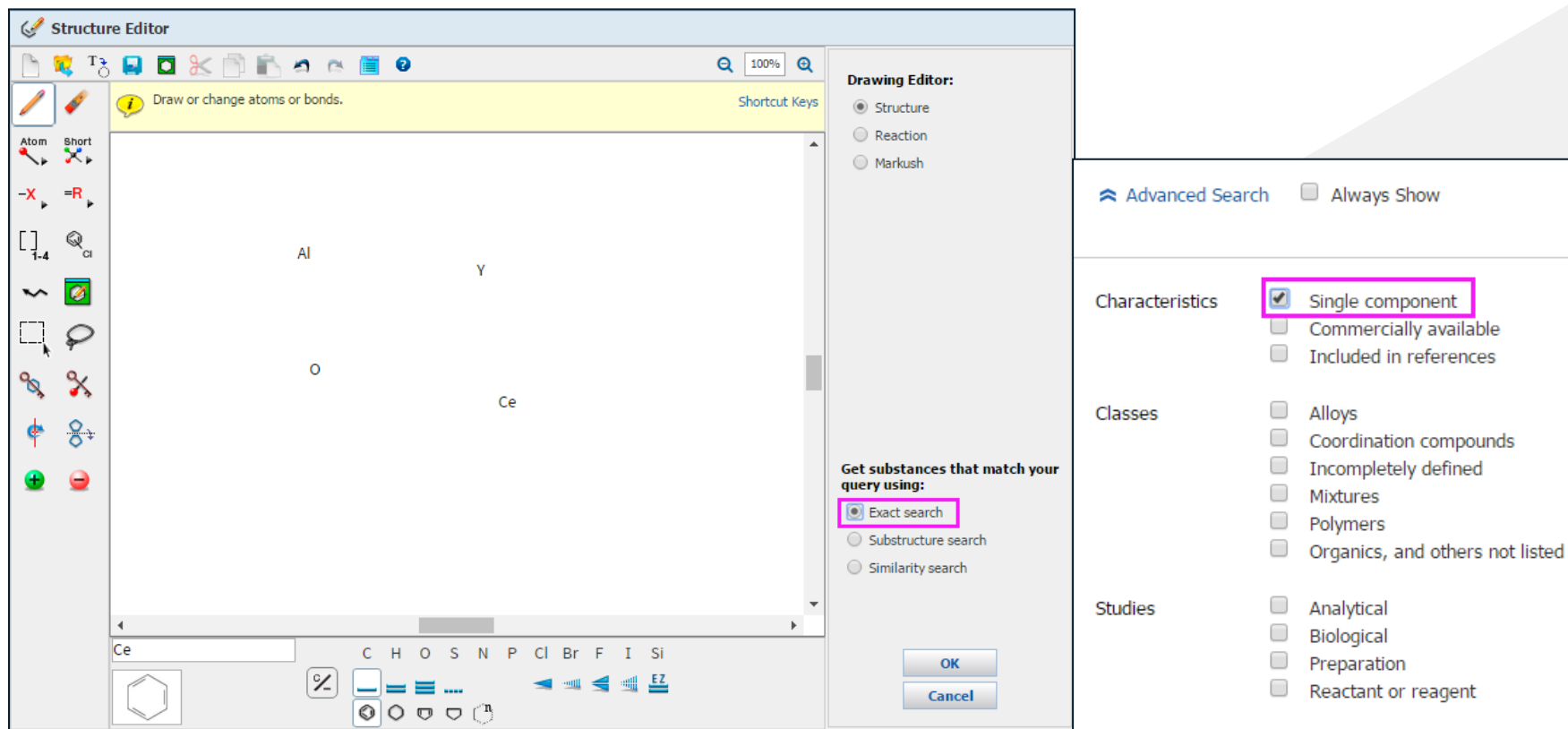
The screenshot shows the SciFinder web interface. At the top, there's a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, a breadcrumb trail reads: 'Substance Identifier "YAG" > substances (1) > get references (18553) > refine "Ce" (1338) > Phosphor plate composition co'. On the left, a sidebar lists search criteria under 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags) and 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier). The main area is titled 'SUBSTANCES: SUBSTANCE IDENTIFIER' and contains a text input field with 'YAG'. Below the field, it says 'Enter one per line. Examples: 50-00-0, 999815, Acetaminophen'. A blue 'Search' button is at the bottom.

先通过物质标识符检索底物YAG

The screenshot shows the search results for 'YAG'. At the top, it says '0 of 1 Substance Selected'. Below, there's a list item '1. 12005-21-9' with a magnifying glass icon. To the left of the item are icons for '25597' and '~14'. The main content area shows 'Substance Image Cannot Be Displayed' and the identifier '12005-21-9'. Below this, the chemical formula  $\text{Al}_5\text{O}_{12}\text{Y}_3$  is displayed, followed by the name 'Aluminum yttrium oxide ( $\text{Al}_5\text{Y}_3\text{O}_{12}$ )'. At the bottom, there are links for 'Key Physical Properties', 'Regulatory Information', and 'Experimental Properties'.

了解YAG的分子式，  
主要是元素组成 Al、O、Y

# 无机复合物的检索



画入所有原子，选择精确结构检索，随后选择单一组份



# 无机复合物的检索

0 of 1 Substance Selected

1. 12005-21-9

~25597 ~14

Substance  
Image  
Cannot Be  
Displayed  
12005-21-9

**Al<sub>5</sub>O<sub>12</sub>Y<sub>3</sub>**  
Aluminum yttrium oxide (Al<sub>5</sub>Y<sub>3</sub>O<sub>12</sub>)

► **Key Physical Properties**  
Regulatory Information  
Experimental Properties

### Get References

**Limit results to:**

<input type="checkbox"/> Adverse Effect, including toxicity	<input type="checkbox"/> Preparation
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Process
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Prophetic in Patents
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input checked="" type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

**For each sequence, retrieve:**

☐ Additional related references, e.g., activity studies, disease studies.

通过底物获得应用相关的文献

# 无机复合物的检索

Substance Identifier "YAG" > substances (1) > **get references (18553)** > refine "Ce" (1338) > Phosphor plate composition com...

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

Display Options

0 of 18553 References Selected

Refine by: ⓘ

- Research Topic
- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic

Ce

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

1. **Phosphor plate composition comprising phosphor powder and sintering agent for vehicle headlamp**

Quick View PATENTPAK

By Won, Ju Yeon; Kim, Won Jin

From Repub. Korean Kongkae Taeho Kongbo (2017), KR 2017014153 A 20170208. | Language: Korean, Database: CAPLUS

An embodiment of the present invention relates to a phosphor plate compn. having wide luminescent region while improving brightness, comprising yttrium aluminum garnet (YAG) or gadolinium yttrium aluminum garnet (GdYAG) phosphor powders doped with at least one dopant selected from cesium (Ce), gadolinium (Gd) and neodymium (Nd); and at least one sintering agent selected from any one of lithium fluoride (LiF), magnesium oxide (MgO) and spinel (MgAl<sub>2</sub>O<sub>4</sub>).

2. **Cleaning system and method for operating the cleaning system**

Quick View PATENTPAK

By Lukac, Nej; Lukac, Matjaz; Jezersek, Matija; Gregorcic, Peter

From Eur. Pat. Appl. (2017), EP 3127502 A1 20170208. | Language: English, Database: CAPLUS

The invention relates to a cleaning system being configured for cleaning, including fragmentation, debridement, material removal, irrigation, disinfection and decontamination, of cavities filled with a liq.. The cleaning system comprises an electromagnetic radiation system and the liq. A treatment handpiece and its exit component are configured to irradiate the liq. within the cavity with the radiation beam, wherein a wavelength of the radiation beam is chosen for significant absorption of the radiation beam in the liq.. The electromagnetic radiation system is adapted to generate a first va...

用Ce限定文献



# 无机复合物的检索

Substance Identifier "YAG " > substances (1) > get references (18553) > refine "Ce" (1338) > Phosphor plate composition com...

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number ↓

Display Options

0 of 1338 References Selected

Page: 1 of 67

Analyze by: ⓘ

Author Name ▼

Hirosaki Naoto 18

Takeda Takashi 14

Nikl M 12

Liang Xiaojuan 11

Xiang Weidong 11

Do Young Rag 10

Fujita Shunsuke 8

Funahashi Shiro 8

Mares J A 8

Nikl Martin 8

Show More

1. **Phosphor plate composition comprising phosphor powder and sintering agent for vehicle headlamp**

Quick View PATENTPAK

By Won, Ju Yeon; Kim, Won Jin  
From Repub. Korean Kongkae Taehe Kongbo (2017), KR 2017014153 A 20170208. | Language: Korean, Database: CAPLUS

An embodiment of the present invention relates to a phosphor plate compn. having wide luminescent region while improving brightness, comprising yttrium aluminum garnet (YAG) or gadolinium yttrium aluminum garnet (GdYAG) phosphor powders doped with at least one dopant selected from cesium (Ce), gadolinium (Gd) and neodymium (Nd); and at least one sintering agent selected from any one of lithium fluoride (LiF), magnesium oxide (MgO) and spinel ( $MgAl_2O_4$ ).

2. **Light emitting device improves heat dissipation efficiency of heat generated in wavelength converting member and illuminating device including light emitting device**

Quick View PATENTPAK

By Harada, Masamichi; Yoshimura, Kenichi; Onuma, Hiroaki  
From Jpn. Kokai Tokkyo Koho (2017), JP 2017028097 A 20170202. | Language: Japanese, Database: CAPLUS

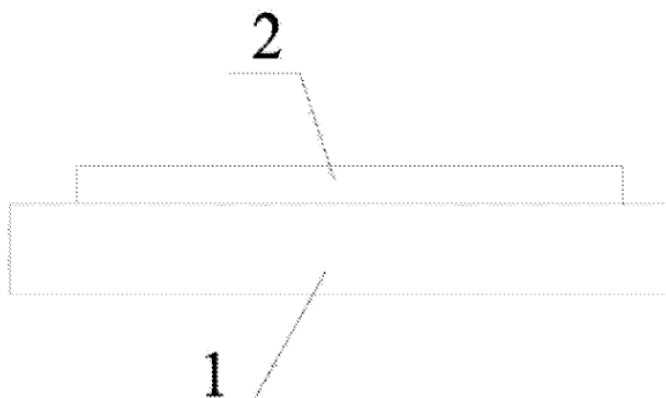
The present invention relates to a light emitting device and illuminating device including the light emitting device. Light emitting device comprises of multiple light emitting elements, substrate on which multiple light emitting elements are mounted, wavelength converting member for converting a wavelength of light emitted from multiple light emitting elements. The wavelength conversion member includes phosphor sealed with a sealing material for converting the wavelength of the light and a holding material for holding the phosphor. The holding material is characterized in that it contains ...

# 无机复合物的检索

## 5. Microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their production method

By: Cao, Dun-Hua; Dong, Yong-Jun; Liang, Yue-Shan  
Assignee: Peop. Rep. China

The present invention relates to a Ce:YAG wafer-based composite structure comprising a Ce:YAG wafer and a red light emitting layer fixed on the Ce:YAG wafer. The present invention also relates to a method for the prepn. of the Ce:YAG wafer-based composite structure. The optical composite structure realizes a wide waveband luminescence from green light to red light, and can be widely used in the fields of detection equipment and illumination devices.



该文中没有标引物质1947312-57-3,  
却是我们需要的文献

### Substances

7440-45-1 Cerium, properties 🔍 Page 7 in PATENTPAK

YAG doped with; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Modifier or additive use; Properties; Technical or engineered material use; Uses

12005-21-9 YAG 🔍 Page 7 in PATENTPAK

cerium-doped, europium-doped; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Properties; Technical or engineered material use; Uses

7440-53-1 Europium, properties 🔍 Page 6 in PATENTPAK

dopant; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method


Modifier or additive use; Properties; Technical or engineered material use; Uses

1314-36-9 Yttrium oxide (Y2O3), properties 🔍 Page 6 in PATENTPAK

europium-doped; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Properties; Technical or engineered material use; Uses

# 无机复合物的检索



PATENTPAK<sup>™</sup>  
A CAS SOLUTION

PAGE 7 / 7

ZOOM - +

DOWNLOAD PDF

Key Substances in Patent

CAS RN 7440-53-1

**Eu**

[Search in SciFinder](#) | [View Detail](#)

Analyst Markup Locations (1)

[page 6](#)

CAS RN 1314-36-9

Yttrium oxide (Y<sub>2</sub>O<sub>3</sub>)

[Search in SciFinder](#) | [View Detail](#)

Analyst Markup Locations (1)

[page 6](#)

CAS RN 7440-45-1

**Ce**

US 2016/0341832 A1

3

Nov. 24, 2016

nm~700 nm, and thus achieving a wide waveband luminescence from green light to red light.

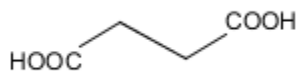
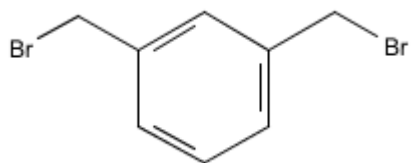
**[0042]** The purpose, technical solutions and beneficial effects of the present invention are described with reference to the above particular examples. Nevertheless, it will be understood that the above examples are not provided to limit the present invention. The invention is intended to cover various modifications and equivalent arrangements included within the spirit and scope of the claims.

1. A Ce:YAG wafer-based composite structure, wherein said composite structure comprises:  
a Ce:YAG wafer; and  
a red light emitting layer fixed on said Ce:YAG wafer.
2. The Ce:YAG wafer-based composite structure according to claim 1, wherein the main emission peak of said red light emitting layer is at 580 nm~660 nm.
3. The Ce:YAG wafer-based composite structure according to claim 2, wherein said red light emitting layer is a deposited film capable of emitting red light.
4. The Ce:YAG wafer-based composite structure according to claim 2, wherein said red light emitting layer is a transparent colloid layer doped with red fluorescent powder.
5. The Ce:YAG wafer-based composite structure according to claim 2, wherein said red light emitting layer is a crystalline, a ceramic or a glass doped with red light
6. A method for the preparation of a Ce:YAG wafer-based composite structure, comprising:  
(1) producing a Ce:YAG wafer by Czochralski process, temperature gradient process or Kyropoulos process;  
(2) grinding and polishing the Ce:YAG wafer produced in step (1) to obtain a fluorescent wafer having desired size; and  
(3) adding a red light emitting layer on the fluorescent wafer obtained in step (2).
7. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim 6, wherein the red light emitting layer added in step (3) is a red light emitting film deposited by physical or chemical vapor deposition.
8. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim 6, wherein the red light emitting layer added in step (3) is a transparent colloid layer doped with red fluorescent powder.
9. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim 6, wherein the red light emitting layer added in step (3) is a crystalline, a ceramic or a glass doped with red light luminescence center of rare earth or transition metal and fixed on the fluorescent wafer.

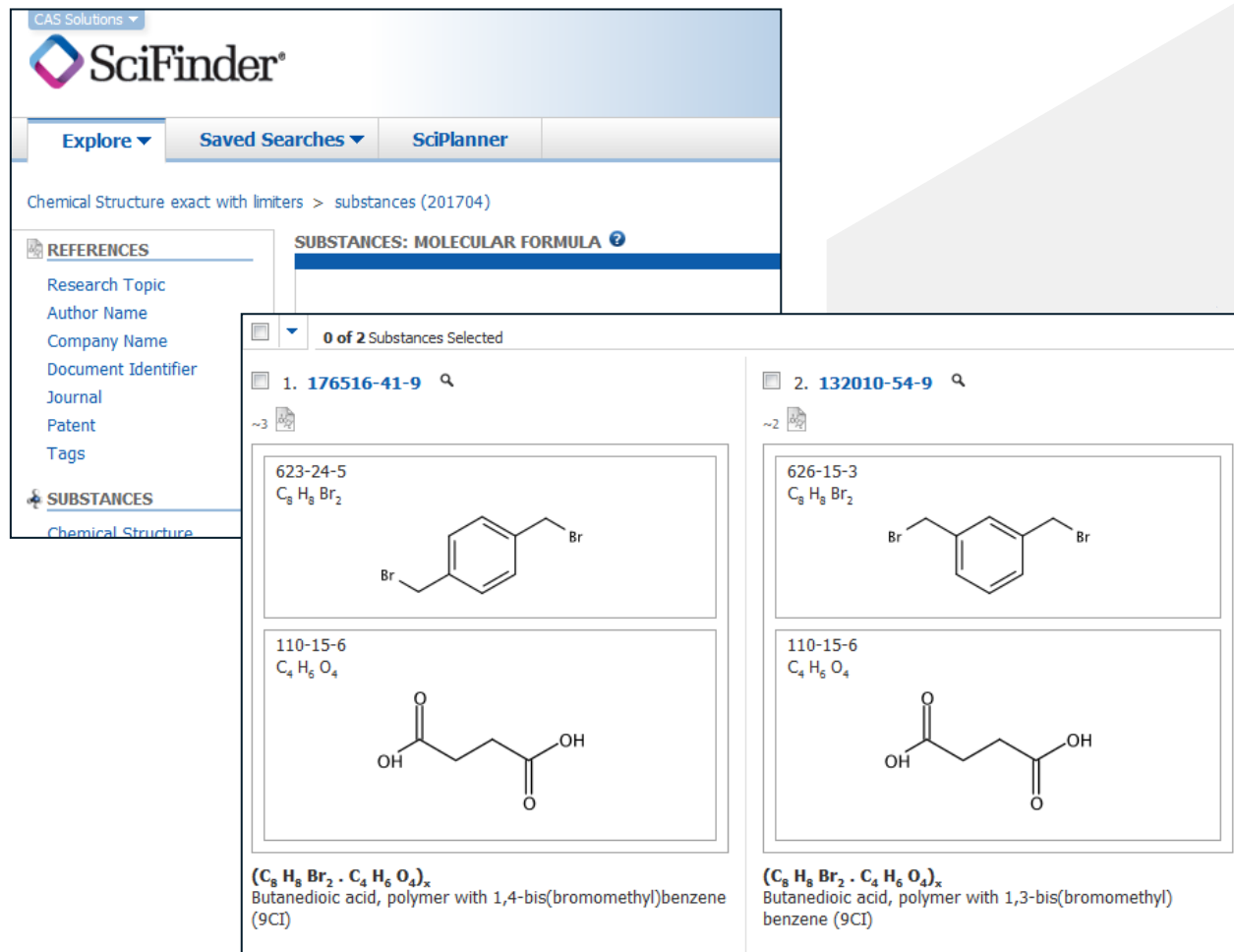
专利中仅仅以文字方式提到此物质

# 聚合物的检索

已知起始原料的聚合物



$(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$



CAS Solutions  
SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

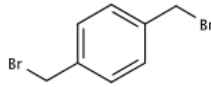
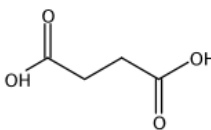
Chemical Structure exact with limiters > substances (201704)

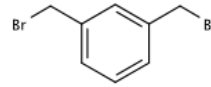
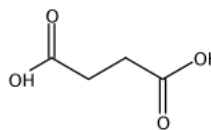
REFERENCES  
Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

SUBSTANCES  
Chemical Structure

SUBSTANCES: MOLECULAR FORMULA ?

0 of 2 Substances Selected

1. 176516-41-9  
~3  
623-24-5  
C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub>  
  
110-15-6  
C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>  
  
(C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub> · C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>)<sub>x</sub>  
Butanedioic acid, polymer with 1,4-bis(bromomethyl)benzene (9CI)

2. 132010-54-9  
~2  
626-15-3  
C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub>  
  
110-15-6  
C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>  
  
(C<sub>8</sub> H<sub>8</sub> Br<sub>2</sub> · C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>)<sub>x</sub>  
Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

分子式检索后会得到同分异构体

# 聚合物的检索

Structure Editor

Draw or change atoms or bonds.

Atom Shortcuts

Br

COOH

Scale 100

C<sub>8</sub>H<sub>8</sub>Br<sub>2</sub> · C<sub>4</sub>H<sub>6</sub>O<sub>4</sub> (query)

263.96 · 118.09

Get substances that match your query using:

- ☒ Exact search
- ☐ Substructure search
- ☐ Similarity search

OK

Cancel

Characteristics

- ☒ Single component
- ☐ Commercially available
- ☐ Included in references

Classes

- ☐ Alloys
- ☐ Coordination compounds
- ☐ Incompletely defined
- ☐ Mixtures
- ☒ Polymers
- ☐ Organics, and others not listed

Studies

- ☐ Analytical
- ☐ Biological
- ☐ Preparation
- ☐ Reactant or reagent

单一组分

聚合物

0 of 1 Substance Selected

1. 132010-54-9

~2

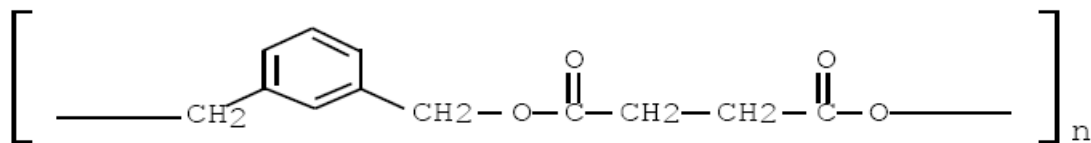
626-15-3  
C<sub>8</sub>H<sub>8</sub>Br<sub>2</sub>

110-15-6  
C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>

(C<sub>8</sub>H<sub>8</sub>Br<sub>2</sub> · C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>)<sub>x</sub>  
Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

# 聚合物的检索

已知重复单元的聚合物



(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>

# 聚合物的检索

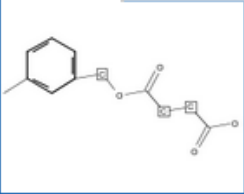
Analyze Refine

Refine by: ?

- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Structure Editor:

Java Non-Java



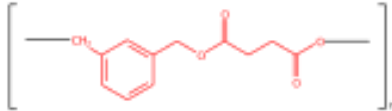
Click image to change structure or view detail.

Search type: **Substructure**

0 of 1 Substance Selected

1. 132010-11-8

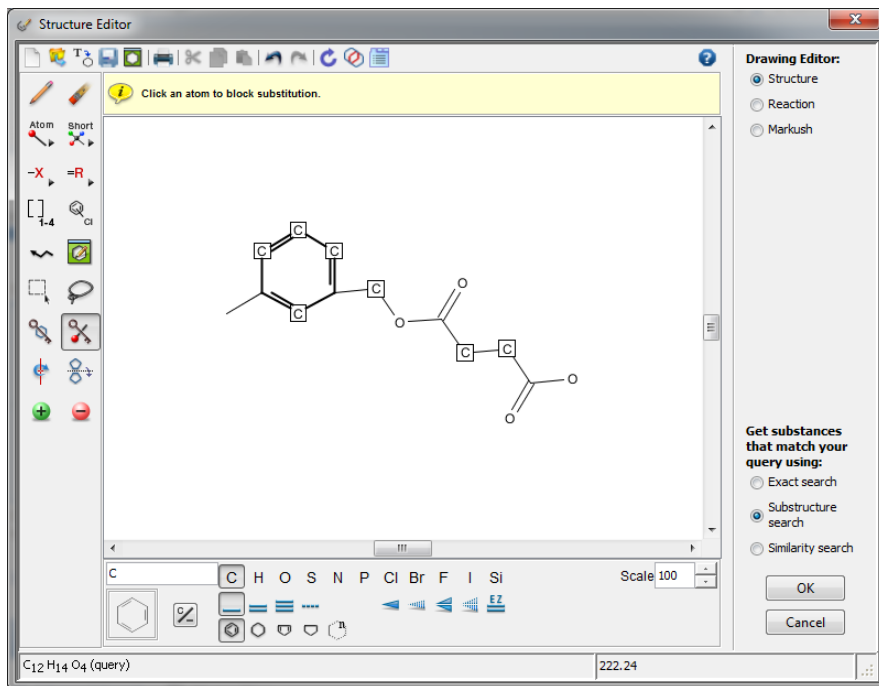
~2



$(C_{12}H_{12}O_4)_n$   
Poly[oxy(1,4-dioxo-1,4-butanediyl)oxymethylene-1,3-phenylenemethylene] (9CI)

利用结构特征进行Refine，迅速查找需要的物质

# 聚合物的检索



绘制好SRU后用亚结构检索  
因为两段为开放状态

Characteristics	<input checked="" type="checkbox"/> Single component <input type="checkbox"/> Commercially available <input type="checkbox"/> Included in references
Classes	<input type="checkbox"/> Alloys <input type="checkbox"/> Coordination compounds <input type="checkbox"/> Incompletely defined <input type="checkbox"/> Mixtures <input checked="" type="checkbox"/> Polymers <input type="checkbox"/> Organics, and others not listed
Studies	<input type="checkbox"/> Analytical <input type="checkbox"/> Biological <input type="checkbox"/> Preparation <input type="checkbox"/> Reactant or reagent

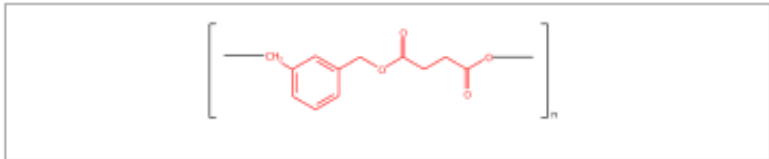
单一组分

聚合物

0 of 1 Substance Selected

1. **132010-11-8** 🔍

~2



**(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>**  
Poly[oxy(1,4-dioxo-1,4-butanediyl)oxymethylene-1,3-phenylenemethylene] (9CI)



# 聚合物的检索

含端基和SRUs的聚合物

Explore ▾ Saved Searches ▾ SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES: MOLECULAR FORMULA ?

(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub> C<sub>3</sub>H<sub>6</sub>O

Examples:  
H<sub>4</sub>SiO<sub>4</sub>  
(C<sub>3</sub>H<sub>6</sub>O.C<sub>2</sub>H<sub>4</sub>O)<sub>x</sub>

Search

SUBSTANCES

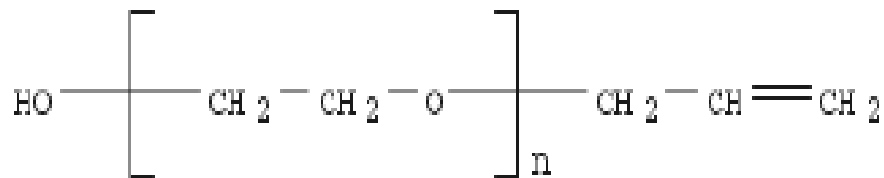
(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub> C<sub>3</sub>H<sub>6</sub>O



SRU部分



两端部分



0 of 4 Substances Selected

1. 1500029-22-0

~3

(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub> C<sub>3</sub>H<sub>6</sub>O  
Poly(oxy-1,2-ethanediyl), α-(1-methylethenyl)-ω-hydroxy-

2. 191403-44-8

~5

(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub> C<sub>3</sub>H<sub>6</sub>O  
Poly(oxy-1,2-ethanediyl), α-1-propen-1-yl-ω-hydroxy-

3. 50856-25-2

~57

(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub> C<sub>3</sub>H<sub>6</sub>O  
Poly(oxy-1,2-ethanediyl), α-ethenyl-ω-methoxy-

4. 27274-31-3

~1115 ~15

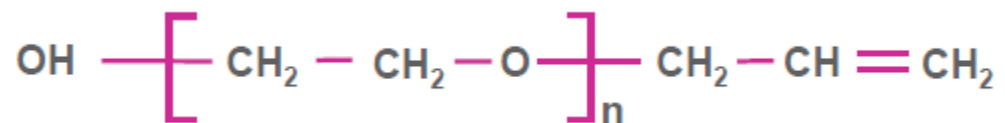
(C<sub>2</sub>H<sub>4</sub>O)<sub>n</sub> C<sub>3</sub>H<sub>6</sub>O  
Poly(oxy-1,2-ethanediyl), α-2-propen-1-yl-ω-hydroxy-

[Regulatory Information](#)

# 聚合物的检索

杂化聚合物的检索：

检索由以下聚合物和2-丙烯酸（C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>）聚合生成的聚合物



检索策略：分子式检索



丙烯酸  
部分

SRU部分

两端部分

# 聚合物的检索

Explore ▼

Saved Searches ▼

SciPlanner

Molecular Formula "(C3 H4 O2 . (C2 H4 O)n C3 H6 O..." > substances (6)

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: MOLECULAR FORMULA ?

(C3 H4 O2. (C2 H4 O)n C3 H6 O)x

Examples:  
H4SiO4  
(C3H6O.C2H4O)x

Search

# 聚合物的检索

Analyze by: Substance Role

Preparation 5

Uses 3

Occurrence 2

Properties 2

Reactant or Reagent 2

Analytical Study 1

Formation, Nonpreparative 1

Process 1

Prophetic in Patents 1

Show More

0 of 6 Substances Selected

1. 1580002-57-8

50856-25-2  
(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O

79-10-7  
C<sub>3</sub> H<sub>4</sub> O<sub>2</sub>

(C<sub>3</sub> H<sub>4</sub> O<sub>2</sub> · (C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O)<sub>x</sub>  
2-Propenoic acid, polymer with α-ethenyl-ω-methoxypoly(oxy-1,2-ethanediyl) graft

2. 1314225-78-9

191403-44-8  
(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O

79-10-7  
C<sub>3</sub> H<sub>4</sub> O<sub>2</sub>

(C<sub>3</sub> H<sub>4</sub> O<sub>2</sub> · (C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O)<sub>x</sub>  
2-Propenoic acid, polymer with α-1-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), graft

3. 1010818-79-7

27274-31-3  
(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O

79-10-7  
C<sub>3</sub> H<sub>4</sub> O<sub>2</sub>

(C<sub>3</sub> H<sub>4</sub> O<sub>2</sub> · (C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O)<sub>x</sub>  
2-Propenoic acid, polymer with α-2-propen-1-yl-ω-hydroxypoly(oxy-1,2-ethanediyl), block

4. 250591-73-2

50856-25-2  
(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O

79-10-7  
C<sub>3</sub> H<sub>4</sub> O<sub>2</sub>

(C<sub>3</sub> H<sub>4</sub> O<sub>2</sub> · (C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O)<sub>x</sub>  
2-Propenoic acid, polymer with α-ethenyl-ω-methoxypoly(oxy-1,2-ethanediyl) (9CI)

5. 185506-87-0

27274-31-3  
(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O

79-10-7  
C<sub>3</sub> H<sub>4</sub> O<sub>2</sub>

6. 82850-00-8

27274-31-3  
(C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>3</sub> H<sub>6</sub> O

79-10-7  
C<sub>3</sub> H<sub>4</sub> O<sub>2</sub>

Block: 嵌段聚合物

Graft: 接枝聚合物

# 聚合物的检索

后处理聚合物的检索：

检索对由2, 5-呋喃二酮和苯乙烯聚合而成的物质进行结构修饰的聚合物

检索策略：

1. 先检索由2, 5-呋喃二酮和苯乙烯聚合而成的物质，获得CAS登记号
2. 主题检索相应的CAS登记号加D
3. 如果有具体的修饰要求，可在topic中直接加入相应的词，  
如：sulfonated xxxx-xx-xd， ester xxxx-xx-xd

# 聚合物的检索

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Search Type:

Exact Structure

Substructure

Similarity

0 of 15 Substances Selected

Characteristics

Single component

Commercially available

Included in references

Classes

Alloys

Coordination compounds

Incompletely defined

Mixtures

Polymers

Organics, and others not listed

1. 9011-13-6	2. 31075-11-3	3. 36512-28-4	4. 96411-80-2
<p>108-31-6 C<sub>4</sub> H<sub>2</sub> O<sub>3</sub></p> <p>100-42-5 C<sub>8</sub> H<sub>8</sub></p> <p>(C<sub>8</sub> H<sub>8</sub> · C<sub>4</sub> H<sub>2</sub> O<sub>3</sub>)<sub>x</sub> 2,5-Furandione, polymer with ethenylbenzene</p> <p>Key Physical Properties</p> <p>Regulatory Information</p> <p>Spectra</p> <p>Experimental Properties</p>	<p>100-42-5 C<sub>8</sub> H<sub>8</sub></p> <p>24937-72-2 (C<sub>4</sub> H<sub>2</sub> O<sub>3</sub>)<sub>x</sub></p> <p>108-31-6 C<sub>4</sub> H<sub>2</sub> O<sub>3</sub></p> <p>C<sub>8</sub> H<sub>8</sub> · (C<sub>4</sub> H<sub>2</sub> O<sub>3</sub>)<sub>x</sub> Maleic anhydride, telomer with styrene (8CI)</p>	<p>108-31-6 C<sub>4</sub> H<sub>2</sub> O<sub>3</sub></p> <p>9003-53-6 (C<sub>8</sub> H<sub>8</sub>)<sub>x</sub></p> <p>100-42-5 C<sub>8</sub> H<sub>8</sub></p> <p>(C<sub>8</sub> H<sub>8</sub>)<sub>x</sub> · C<sub>4</sub> H<sub>2</sub> O<sub>3</sub> 2,5-Furandione, telomer with ethenylbenzene (9CI)</p>	<p>19361-62-7 C<sub>8</sub> D<sub>8</sub></p> <p>108-31-6 C<sub>4</sub> H<sub>2</sub> O<sub>3</sub></p> <p>(C<sub>8</sub> D<sub>8</sub> · C<sub>4</sub> H<sub>2</sub> O<sub>3</sub>)<sub>x</sub> 2,5-Furandione, polymer with ethenyl-d<sub>5</sub>-benzene-d<sub>5</sub> (9CI)</p>
5. 106209-33-0	6. 112020-31-2	7. 128162-14-1	8. 145678-57-5
<p>108-31-6 C<sub>4</sub> H<sub>2</sub> O<sub>3</sub></p>	<p>108-31-6 C<sub>4</sub> H<sub>2</sub> O<sub>3</sub></p>	<p>108-31-6 C<sub>4</sub> H<sub>2</sub> O<sub>3</sub></p>	<p>108-31-6 C<sub>4</sub> H<sub>2</sub> O<sub>3</sub></p>

# 聚合物的检索

Explore ▾

Saved Searches ▾

SciPlanner

Chemical Structure exact with limiters > substances (15)

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

REFERENCES: RESEARCH TOPIC ?

9011-13-6D

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

REFERENCES ?

Get Substances

Get Reactions

Get Related Citations

Tools ▾

Create Keep Me Posted Alert

Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number ▾

0 of 1013 References Selected

Display Options

Page: 1 of 101

Analyze by: Author Name ▾

Konishi Kunihiro	24
Maeda Hiroshi	20
Yagi Norio	20
Chiba Takashi	19
Kitsunai Tomoyuki	18
Tong Wei	17
Kurokawa Kinya	16
Cao Min	15
Niimura Tetsuya	15
Sun Donghai	15

Show More

1. Lubricant composition comprising branched diesters and viscosity index improver

Quick View PATENTPAK ▾

By Sanson, Julien; Champagne, Nicolas; Benard, Francois  
From PCT Int. Appl. (2017), WO 2017021332 A1 20170209. | Language: English, Database: CAPLUS

The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver. The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.

2. Thermosetting adhesive sheet with excellent dimensional stability, adhesion, heat resistance, flexibility, electrical insulation, dielectric constant and dielectric loss tangent for protecting printed wiring board

Quick View PATENTPAK ▾

By Sakaguchi, Takeshi; Ogiwara, Naoto; Tosaki, Koichi; Kishi, Hiromasa; Kobayashi, Hidenobu  
From Jpn. Tokkyo Koho (2017), JP 6074698 B1 20170208. | Language: Japanese, Database: CAPLUS

Title sheet is formed from a thermosetting compn. comprising a resin A1, an organometallic compd. and a tri or more functional epoxy group-contg. compd., wherein the resin A1 does not have an epoxy group and has a reactive functional group capable of reacting with at least one of the organometallic compd. or epoxy group-contg. compd., a functional group except a reactive functional group and a functional group with a hetero atom except halogen, a resin A2 does not have a reactive functional group and has a functional group with a hetero atom except halogen, a resin A3 has neither a reactive fu...

3. Lubricant composition comprising branched diesters and viscosity index improver

Quick View PATENTPAK ▾

By Sanson, Julien; Champagne, Nicolas; Benard, Francois  
From Eur. Pat. Appl. (2017), EP 3124579 A1 20170201. | Language: English, Database: CAPLUS

The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.

4. Thermosetting resin composition with excellent metal foil adhesiveness and dielectric and heat resistance properties for forming prepreg, laminated board and printed wiring board

Quick View PATENTPAK ▾

By Yoshino, Hiroaki; Yanagida, Makoto  
From Jpn. Kokai Tokkyo Koho (2017), JP 2017019906 A 20170126. | Language: Japanese, Database: CAPLUS

Title compn. comprises (A) a polyimide curing agent which is a polyimide compd. obtd. by reacting (a) a maleimide compd. having at least two N-substituted maleimide groups in one mol., (b) an aniline compd. having two arom. amino groups in one mol. and (c) an aminophenol compd. having one arom. amino group and at least one arom. hydroxyl group in one mol. in a mole ratio of f(a): (b): (c) 1.4:0: 0.1-1.0: 0.1-1.0, and having bonding degree of 7 calcd. from the formula: bonding degree = wt. av. mol. wt./charned av. mol.

# 聚合物的检索



## 1. Lubricant composition comprising branched diesters and viscosity index improver

By: Sanson, Julien; Champagne, Nicolas; Benard, Francois

Assignee: Total Marketing Services, Fr.

The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver. The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.

### Patent Information

Patent No.		Kind	Language	Date	Application No.	Date
WO 2017021332	 PATENTPAK	A1		Feb 9, 2017	WO 2016-EP68229	Jul 29, 2016
EP 3124579	 PATENTPAK	A1	English	Feb 1, 2017	EP 2015-179371	Jul 31, 2015

### Priority Application

EP 2015-179371	A	Jul 31, 2015
----------------	---	--------------










### Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-8)

### Concepts

Base oils	Crankcase oil
Lubricating oil additives	Transesterification
lubricant compn. comprising branched diesters and viscosity index improver	
Polyolefins	
lubricant compn. comprising branched diesters and viscosity index improver	
Modifier or additive use; Uses	
Lubricating oil additives	
viscosity improvers: lubricant compn. comprising branched diesters and viscosity index	

### Substances

78-79-5D Isoprene, polymers	
106-99-0D Butadiene, polymers	
9003-31-0D Polyisoprene, hydrogenated	
9011-13-6D Styrene-maleic anhydride copolymer, esters	
25038-32-8D Isoprene-styrene copolymer, hydrogenated	
lubricant compn. comprising branched diesters and viscosity index improver	
Modifier or additive use; Uses	
64-18-6 Formic acid	
124-07-2 Octanoic acid	
143-07-7 Dodecanoic acid	
157336-71-5	
1627033-75-4	





# 物质检索小结

1. 选择合适的检索方式
2. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
3. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
4. 正确理解Exact、Substructure、Similarity检索结果集的意义和范围
5. 利用CAS Markush检索尽可能全面的获得结构的公开信息

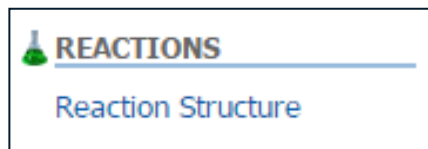
# 大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略 (CAS Analytical Methods)

# CAS SciFinder检索--反应检索

## ■ 反应检索方法

- 结构式



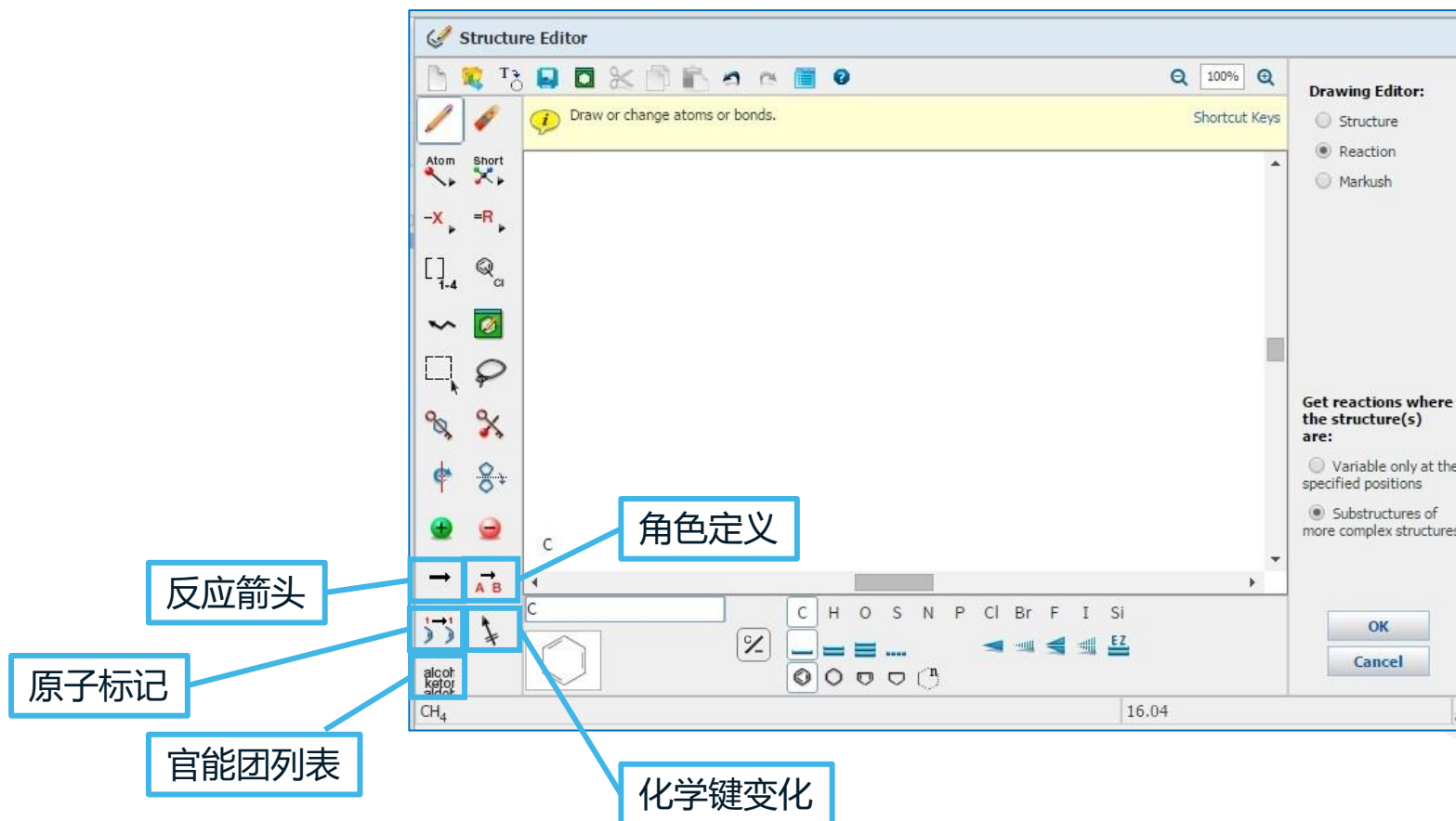
## ■ 常用获取方法

- 已知物质：由物质获取反应
- 已知文献：从文献中获取反应
- 精确结构反应检索
- 亚结构反应检索

Get reactions where  
the structure(s)  
are:

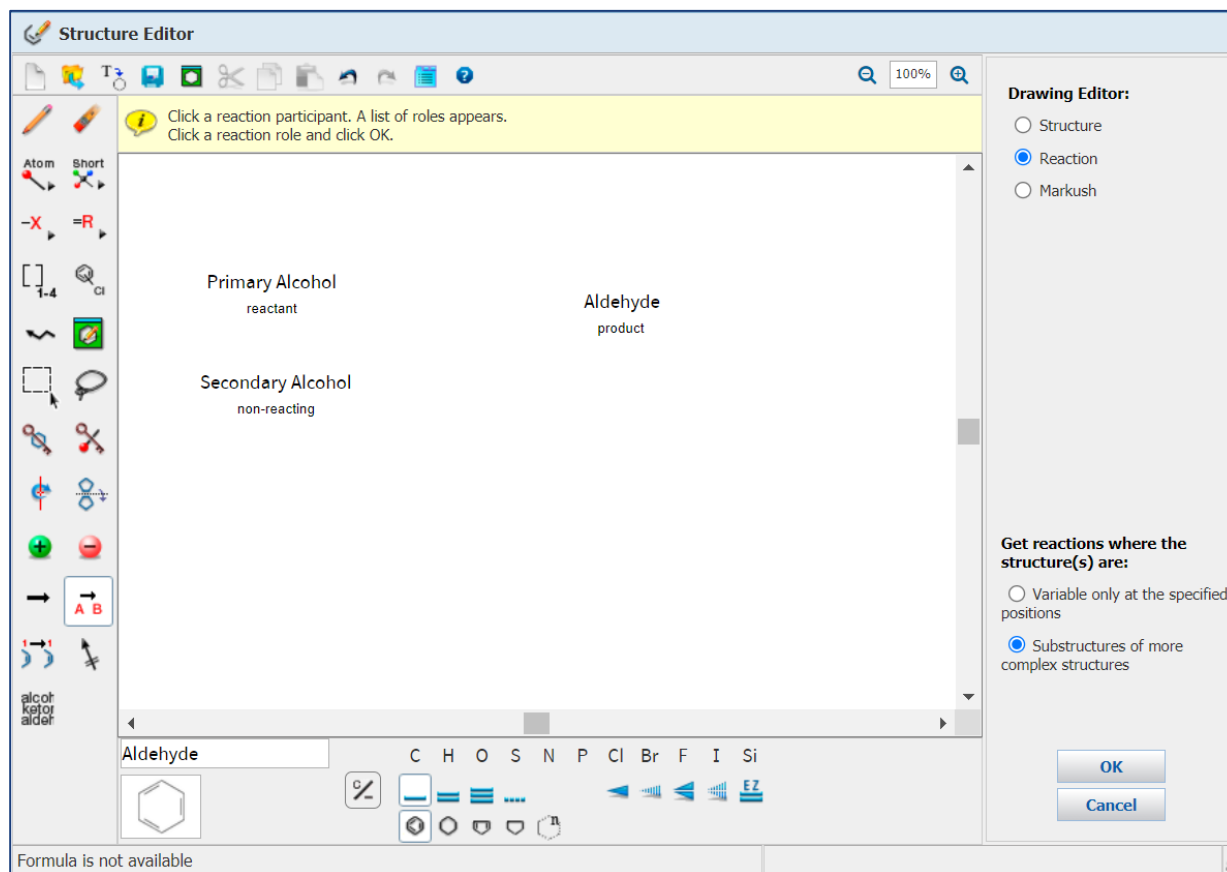
- ☐ Variable only at the  
specified positions
- ☒ Substructures of  
more complex structures

# 结构编辑器--绘制反应工具



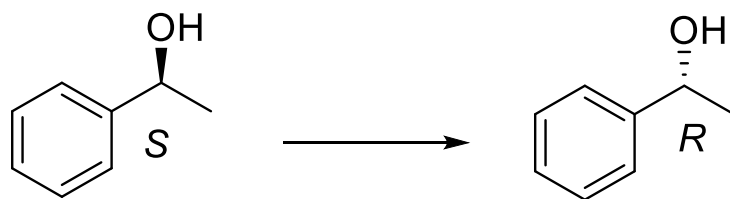
# 化学选择性反应的检索

问题：底物上有伯羟基和仲羟基，能否找到合适的氧化剂使伯羟基氧化成醛而仲羟基不受影响？



# 直接检索反应受限时如何处理

检索如下构型翻转的反应



# 新化合物合成路线设计

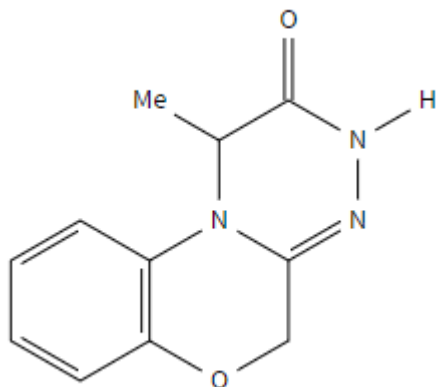
检索思路1: 检索结构相似的物质, 获得有参考价值的合成路线;

检索思路2: 检索通式结构, 获得有参考价值的合成路线;


检索思路3: 先自行做逆合成反应分析, 然后验证相关的反应。

# 新化合物合成路线设计

检索思路1：相似结构检索，获得有参考价值的合成路线



CAS Solutions ▾

 **SciFINDER**  
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

⚠ Explore Substances resulted in 0 substances [Return](#)

Chemical Structure exact > **substances (0)**

**SUBSTANCES**

Analyze Refine

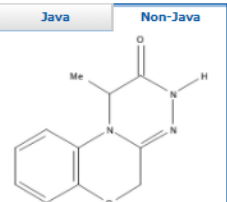
Analyze by:  
*No substances available*



# 新化合物合成路线设计

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Characteristics

- ☒ Single component
- ☐ Commercially available
- ☐ Included in references

Classes

- ☐ Alloys
- ☐ Coordination compounds
- ☐ Incompletely defined
- ☐ Mixtures
- ☐ Polymers
- ☒ Organics, and others not listed

Studies

- ☐ Analytical
- ☐ Biological
- ☒ Preparation
- ☐ Reactant or reagent

Search Type:

- ☐ Exact Structure
- ☐ Substructure
- ☒ Similarity

☐ Show precision analysis

ChemDraw  
Launch a SciFinder substance

Select All Deselect All

1 of 7 Similarity Candidates Selected

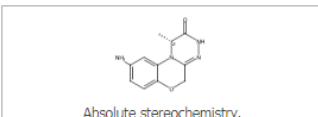
	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input checked="" type="checkbox"/> 90-94	6
<input type="checkbox"/> 85-89	6
<input type="checkbox"/> 80-84	16
<input type="checkbox"/> 75-79	26
<input type="checkbox"/> 70-74	57
<input type="checkbox"/> 65-69	103
<input type="checkbox"/> 0-64 (least similar)	309

Get Substances

0 of 6 Substances Selected

Score: 91

1. 1613721-07-5



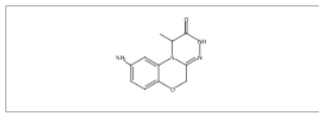
Absolute stereochemistry.

**C<sub>11</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>**  
[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1*H*)-one, 9-amino-3,5-dihydro-1-methyl-, (1*R*)-

Key Physical Properties

Score: 91

2. 1613722-60-3

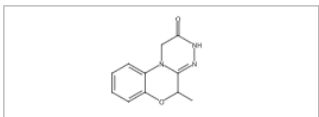


**C<sub>11</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>**  
[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1*H*)-one, 9-amino-3,5-dihydro-1-methyl-

Key Physical Properties

Score: 90

3. 139605-55-3

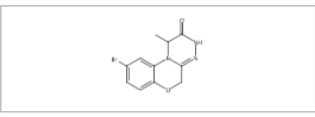


**C<sub>11</sub>H<sub>11</sub>N<sub>3</sub>O<sub>2</sub>**  
[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1*H*)-one, 3,5-dihydro-5-methyl-

Key Physical Properties

Score: 90

4. 1613721-69-9

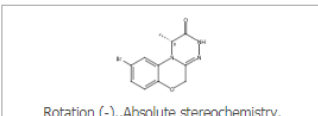


**C<sub>11</sub>H<sub>10</sub>BrN<sub>3</sub>O<sub>2</sub>**  
[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1*H*)-one, 9-bromo-3,5-dihydro-1-methyl-

Key Physical Properties

Score: 90

5. 1613721-93-9



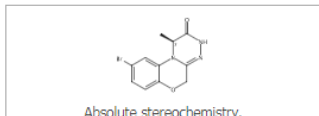
Rotation (-), Absolute stereochemistry.

**C<sub>11</sub>H<sub>10</sub>BrN<sub>3</sub>O<sub>2</sub>**  
[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1*H*)-one, 9-bromo-3,5-dihydro-1-methyl-, (1*R*)-

Key Physical Properties

Score: 90

6. 1613722-23-8



Absolute stereochemistry.

**C<sub>11</sub>H<sub>10</sub>BrN<sub>3</sub>O<sub>2</sub>**  
[1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1*H*)-one, 9-bromo-3,5-dihydro-1-methyl-, (1*S*)-

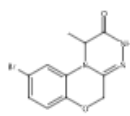
Key Physical Properties

# 新化合物合成路线设计

Score: 90

4. 1613721-69-9

~1 ~2



**C<sub>11</sub> H<sub>10</sub> Br N<sub>3</sub> O<sub>2</sub>**  
 [1,2,4]Triazino[3,4-c]  
 9-bromo-3,5-dihydro-1-  
 ▶ Key Physical Properties

CAS Registry Number: 1613721-69-9

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a

Get Commercial Sources

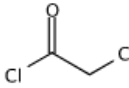
Get Regulatory Information

Get References

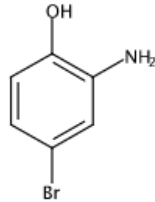
Export as Image

1. View Reaction Detail [Link](#)

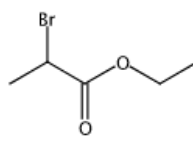
4 Steps Hover over any structure for more options.

  
 ~64

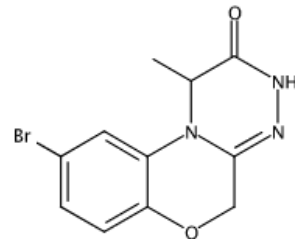
+

  
 ~156

+

  
 [Step 2.1]  
 ~103

→

  
 ~2

▼ Overview

**Steps/Stages**

1.1 R:NaHCO<sub>3</sub>, S:H<sub>2</sub>O, S:(CH<sub>2</sub>OMe)<sub>2</sub>, 0°C; 0.5 h, 15°C; overnight, 80°C; 80°C → rt

1.2 R:H<sub>2</sub>O

2.1 R:K<sub>2</sub>CO<sub>3</sub>, S:Me<sub>2</sub>CO, 5 h, 70°C

3.1 R:Lawesson's reagent, S:PhMe, 3 h, 120°C

4.1 R:N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O, S:EtOH, overnight, rt

**Notes**

1) alternate reaction conditions gave lower yield, Reactants: 3, Reagents: 5, Solvents: 5, Steps: 4, Stages: 5, Most stages in any one step: 2

**References**


Triazinone compounds as PKC kinase inhibitors and their preparation

Quick View **PATENTPAK**

By George, Dawn M. et al

From PCT Int. Appl., 2014089904, 19 Jun 2014

© 2021 American Chemical Society. All rights reserved.



ACS  
International

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

# 新化合物合成路线设计

检索思路2：通式结构检索，获得有参考价值的合成路线

The screenshot displays the 'Structure Editor' window. The central canvas shows a chemical structure of a benzimidazole derivative with an 'Ak' label. The left sidebar contains various drawing tools. The right sidebar includes search filters:

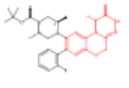
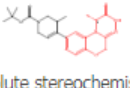
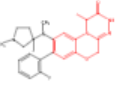
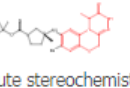
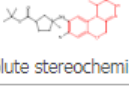
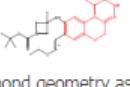
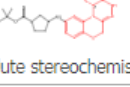
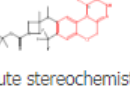
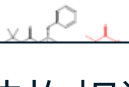
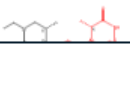
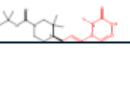
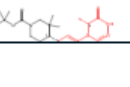
- Drawing Editor:**
  - ☒ Structure
  - ☐ Reaction
  - ☐ Markush
- Get substances that match your query using:**
  - ☐ Exact search
  - ☒ Substructure search
  - ☐ Similarity search
- Characteristics:**
  - ☒ Single component
  - ☐ Commercially available
  - ☐ Included in references
- Classes:**
  - ☐ Alloys
  - ☐ Coordination compounds
  - ☐ Incompletely defined
  - ☐ Mixtures
  - ☐ Polymers
  - ☒ Organics, and others not listed
- Studies:**
  - ☐ Analytical
  - ☐ Biological
  - ☒ Preparation
  - ☐ Reactant or reagent

Buttons for 'OK' and 'Cancel' are at the bottom right. The status bar at the bottom left indicates 'Formula is not available'.

# 新化合物合成路线设计

Sort by: CAS Registry Number    Display Options

0 of 424 Substances Selected    Page: 1 of 9

<p>1. 1654735-60-0</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>28</sub>H<sub>34</sub>FN<sub>5</sub>O<sub>4</sub></b> 1-Piperazinecarboxylic acid, 4-[(8-(2-fluorophenyl)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)-2,5-dimethyl-, 1,1-dimethylethyl ester, (2S,5R)-</p> <p>▶ Key Physical Properties</p>	<p>2. 1654735-59-7</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>22</sub>H<sub>28</sub>N<sub>4</sub>O<sub>4</sub></b> 1(2H)-Pyridinecarboxylic acid, 3,6-dihydro-3-methyl-4-[(1R)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>	<p>3. 1654735-57-5</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>24</sub>H<sub>28</sub>FN<sub>5</sub>O<sub>2</sub></b> [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1H)-one, 9-[(1,3-dimethyl-3-pyrrolidinyl)methylamino]-8-(2-fluorophenyl)-3,5-dihydro-1-methyl-</p> <p>▶ Key Physical Properties</p>	<p>4. 1654735-48-4</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>21</sub>H<sub>28</sub>BrN<sub>5</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 3-[(8-bromo-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)amino]-3-methyl-, 1,1-dimethylethyl ester, (3R)-</p> <p>▶ Key Physical Properties</p>
<p>5. 1654732-77-0</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>21</sub>H<sub>28</sub>BrN<sub>5</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 3-[(8-bromo-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)amino]-3-methyl-, 1,1-dimethylethyl ester, (3S)-</p> <p>▶ Key Physical Properties</p>	<p>6. 1654732-76-9</p>  <p>Double bond geometry as shown.</p> <p><b>C<sub>24</sub>H<sub>33</sub>N<sub>5</sub>O<sub>5</sub></b> 1-Azetidinecarboxylic acid, 3-[[8-[(1E)-2-ethoxyethenyl]-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]amino]-3-methyl-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>	<p>7. 1654728-88-7</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>26</sub>H<sub>27</sub>N<sub>5</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 3-[[[(1R)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]amino]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>	<p>8. 1654728-63-8</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>23</sub>H<sub>29</sub>F<sub>3</sub>N<sub>4</sub>O<sub>4</sub></b> 1-Azetidinecarboxylic acid, 3-methyl-3-[1-[(1R)-1,2,3,5-tetrahydro-1-methyl-2-oxo-8-(trifluoromethyl)[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]ethyl]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>
<p>9. 1654725-00-4</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>21</sub>H<sub>28</sub>BrN<sub>5</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 3-[(8-bromo-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)amino]-3-methyl-, 1,1-dimethylethyl ester, (3S)-</p> <p>▶ Key Physical Properties</p>	<p>10. 1632329-18-0</p>  <p>Double bond geometry as shown.</p> <p><b>C<sub>24</sub>H<sub>33</sub>N<sub>5</sub>O<sub>5</sub></b> 1-Azetidinecarboxylic acid, 3-[[8-[(1E)-2-ethoxyethenyl]-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]amino]-3-methyl-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>	<p>11. 1632329-17-9</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>26</sub>H<sub>27</sub>N<sub>5</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 3-[[[(1R)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]amino]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>	<p>12. 1632329-16-8</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>23</sub>H<sub>29</sub>F<sub>3</sub>N<sub>4</sub>O<sub>4</sub></b> 1-Azetidinecarboxylic acid, 3-methyl-3-[1-[(1R)-1,2,3,5-tetrahydro-1-methyl-2-oxo-8-(trifluoromethyl)[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]ethyl]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>

筛选结构相近的物质

# 新化合物合成路线设计

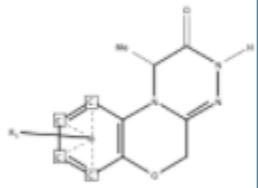
Analyze
Refine

Refine by: ?

- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

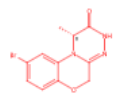
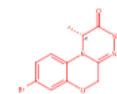
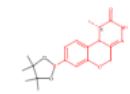
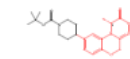
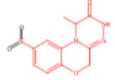
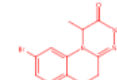
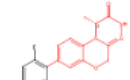
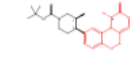
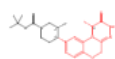
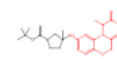
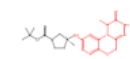
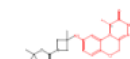
Structure Editor:

Java
Non-Java



Click image to change structure or view detail.

Search type: **Substructure**

<p>25. 1613721-93-9</p>  <p>Absolute stereochemistry., Rotation (-).</p> <p><b>C<sub>11</sub>H<sub>10</sub>BrN<sub>3</sub>O<sub>2</sub></b> [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 9-bromo-3,5-dihydro-1-methyl-, (1<i>R</i>)-</p> <p>▶ Key Physical Properties</p>	<p>26. 1613721-90-6</p>  <p>Absolute stereochemistry., Rotation (-).</p> <p><b>C<sub>11</sub>H<sub>10</sub>BrN<sub>3</sub>O<sub>2</sub></b> [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 8-bromo-3,5-dihydro-1-methyl-, (1<i>R</i>)-</p> <p>▶ Key Physical Properties</p>	<p>27. 1613721-87-1</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>17</sub>H<sub>22</sub>BN<sub>3</sub>O<sub>4</sub></b> [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 3,5-dihydro-1-methyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-, (1<i>R</i>)-</p> <p>▶ Key Physical Properties</p>	<p>28. 1613721-85-9</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>21</sub>H<sub>28</sub>N<sub>4</sub>O<sub>4</sub></b> 1-Piperidinecarboxylic acid, 4-[(1<i>R</i>)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-, 1,1-dimethylethyl ester</p> <p>▶ Key Physical Properties</p>
<p>29. 1613721-72-4</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>11</sub>H<sub>10</sub>N<sub>4</sub>O<sub>4</sub></b> [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 3,5-dihydro-1-methyl-9-nitro-</p> <p>▶ Key Physical Properties</p>	<p>30. 1613721-69-9</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>11</sub>H<sub>10</sub>BrN<sub>3</sub>O<sub>2</sub></b> [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 9-bromo-3,5-dihydro-1-methyl-</p> <p>▶ Key Physical Properties</p>	<p>31. 1613721-49-5</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>17</sub>H<sub>14</sub>FN<sub>3</sub>O<sub>2</sub></b> [1,2,4]Triazino[3,4-c][1,4]benzoxazin-2(1<i>H</i>)-one, 8-(2-fluorophenyl)-3,5-dihydro-1-methyl-, (1<i>R</i>)-</p> <p>▶ Key Physical Properties</p>	<p>32. 1613721-44-0</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>22</sub>H<sub>30</sub>N<sub>4</sub>O<sub>4</sub></b> 1-Piperidinecarboxylic acid, 3-methyl-4-[(1<i>R</i>)-1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl]-, 1,1-dimethylethyl ester, (3<i>S</i>,4<i>S</i>)-</p> <p>▶ Key Physical Properties</p>
<p>33. 1613721-38-2</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>22</sub>H<sub>30</sub>N<sub>4</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 3-methyl-3-[(1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)]-, 1,1-dimethylethyl ester</p>	<p>34. 1613721-34-8</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>21</sub>H<sub>29</sub>N<sub>5</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 2-methyl-2-[(1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)]-, 1,1-dimethylethyl ester</p>	<p>35. 1613721-25-7</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>21</sub>H<sub>29</sub>N<sub>5</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 2-methyl-2-[(1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)]-, 1,1-dimethylethyl ester</p>	<p>36. 1613721-09-7</p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>20</sub>H<sub>27</sub>N<sub>5</sub>O<sub>4</sub></b> 1-Pyrrolidinecarboxylic acid, 2-methyl-2-[(1,2,3,5-tetrahydro-1-methyl-2-oxo[1,2,4]triazino[3,4-c][1,4]benzoxazin-9-yl)]-, 1,1-dimethylethyl ester</p>

# 新化合物合成路线设计

Group by: **No Grouping** Sort by: **Accession Number** [Display Options](#)

0 of 8 Reactions Selected

1. **View Reaction Detail** [Link](#)

**4 Steps** *Hover over any structure for more options.*

**Overview**

**Experimental Procedure**

**METHODSNow™**

**Procedure**

1. Add 2-chloroacetyl chloride ( 83.6 mL, 1110 mmol ) dropwise to a solution of 2-amino-4-nitrophenol ( 114.0 g, 740 mmol ) ,  $K_2CO_3$  ( 306.2 g, 2220 mmol ) and tetrabutyl ammonium bromide ( 23.8 g, 74 mmol ) in acetonitrile ( 1.50 L ) at 0 °C.
2. Heat the reaction mixture at 80 °C for 1 h.

[View more...](#)

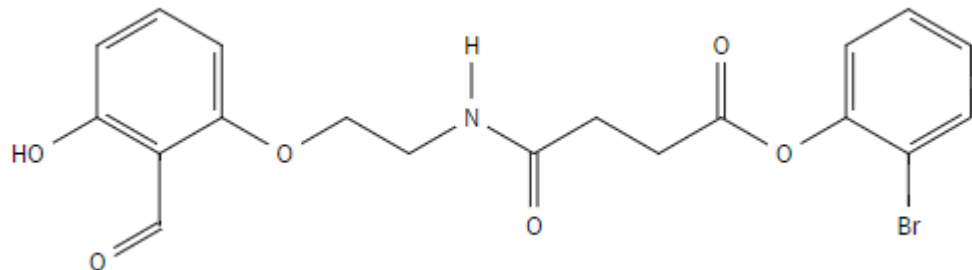
**Available Experimental Data**

$^1H$  NMR,  $R_f$ , State

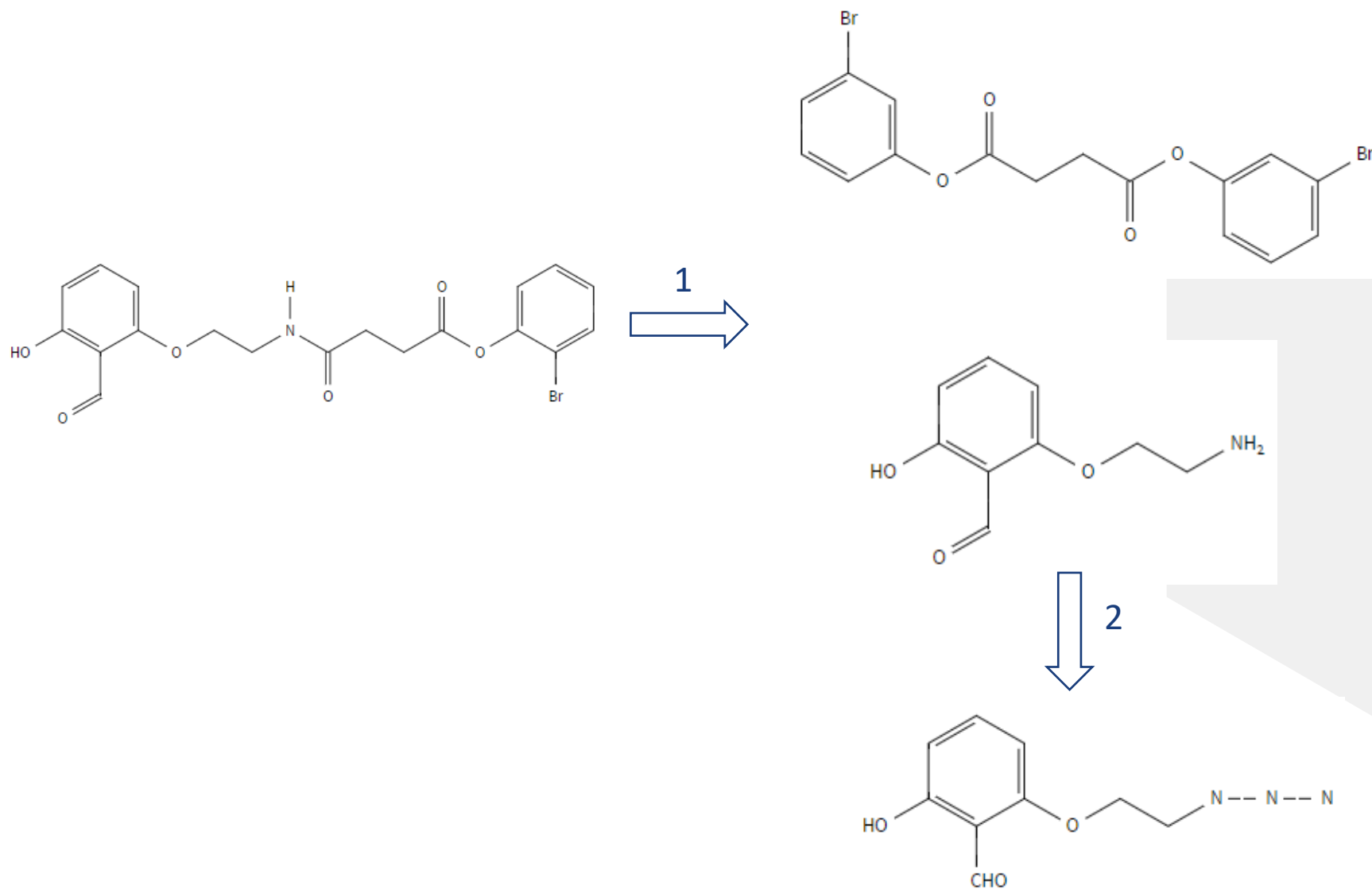
[View with MethodsNow](#)

# 新化合物合成路线设计

检索思路3：先自行做逆合成反应分析，然后验证相关的反应。



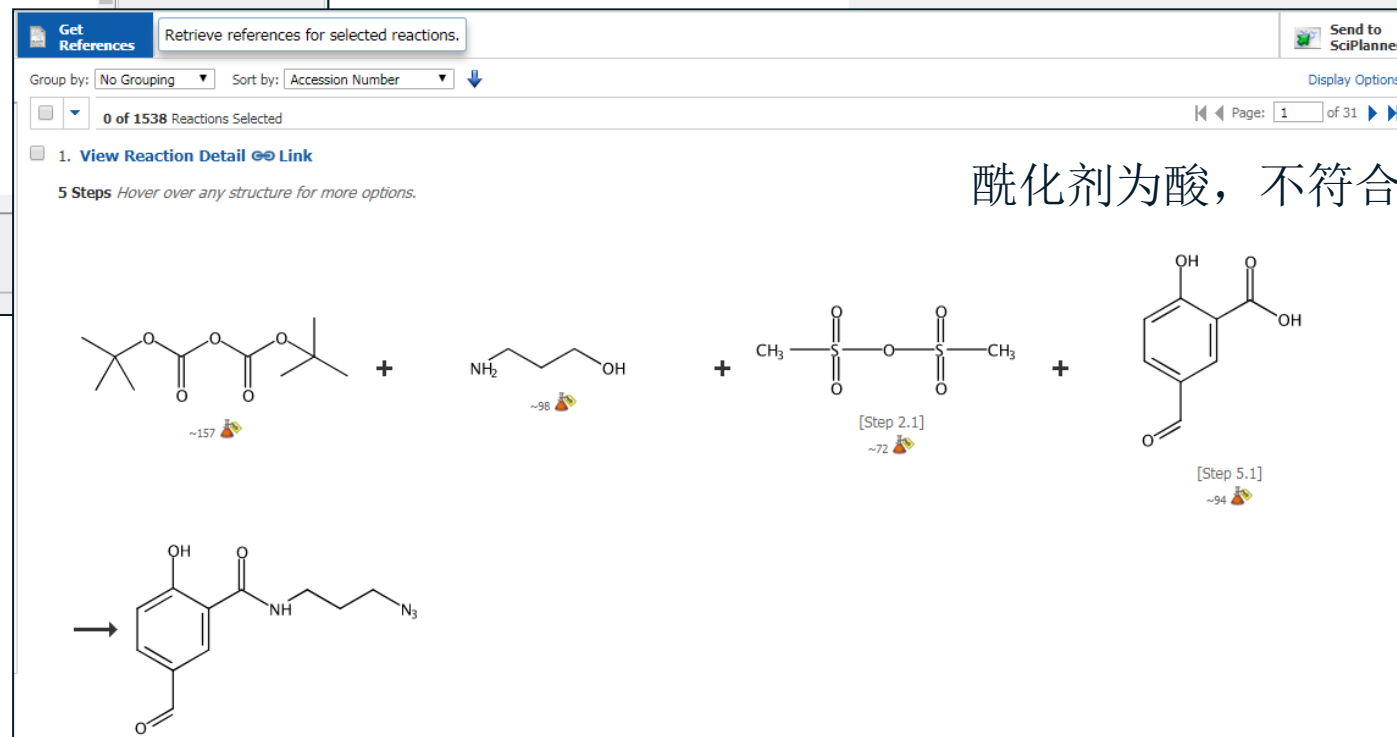
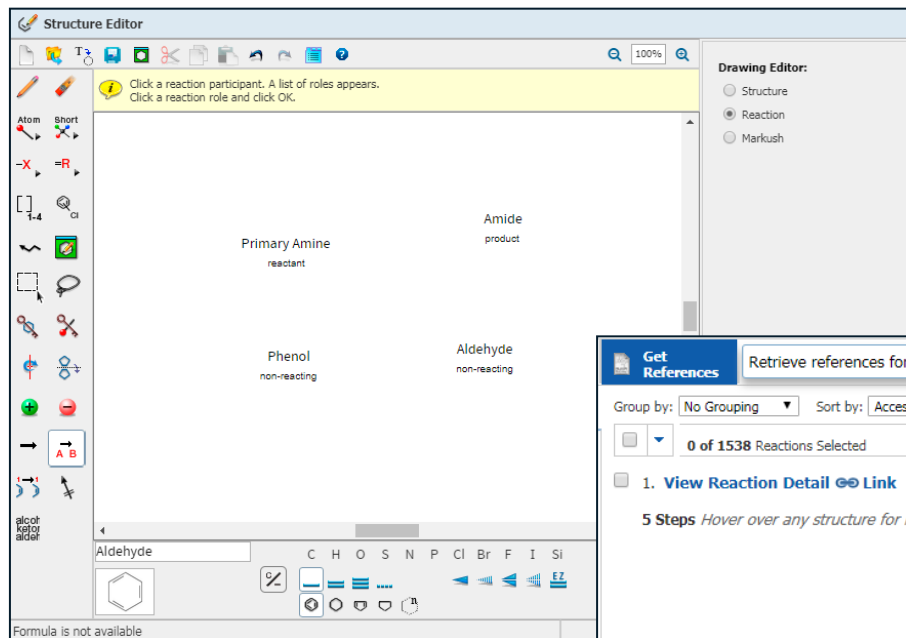
# 新化合物合成路线设计





# 新化合物合成路线设计

## 反应1:



# 新化合物合成路线设计

不理想

问题：底物太多？步数太多！

AnalyzeRefine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Structure Editor:

JavaNon-Java

Carboxylate Ester  
REACTANT

Click image to change structure or view detail.  
Search type: Substructure

Refine

Get ReferencesTools

Send to SciPlanner

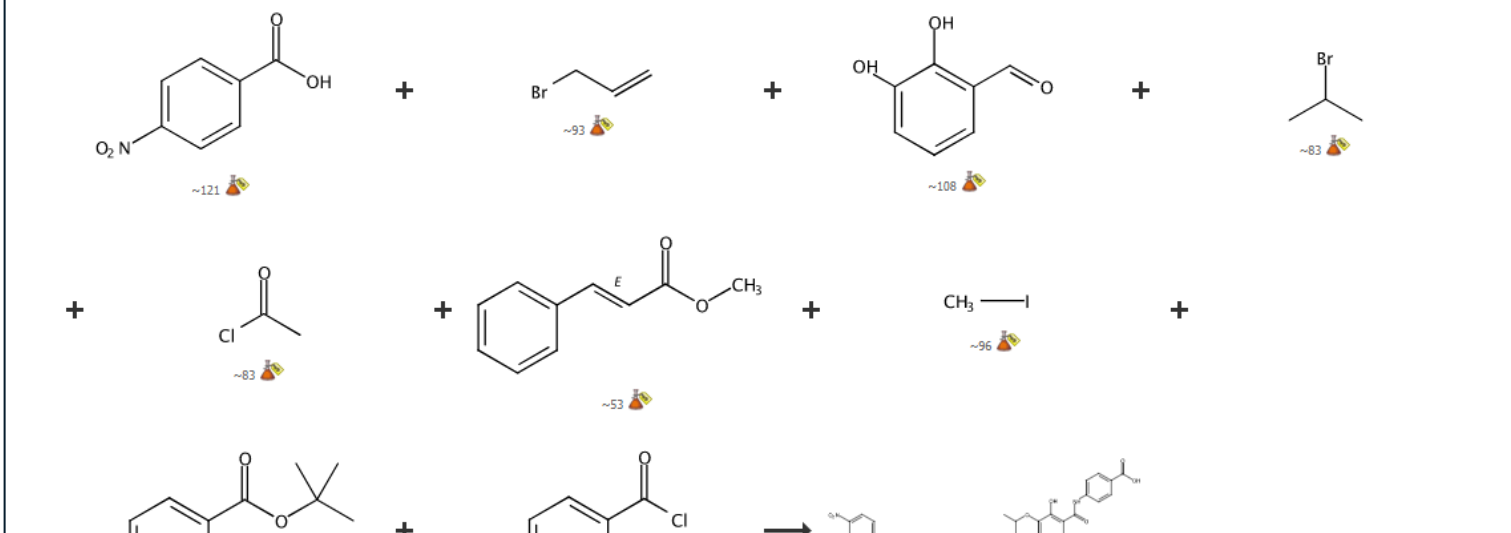
Group by: No GroupingSort by: Accession Number

0 of 855 Reactions Selected

Display Options

1. View Reaction Detail Link

22 Steps (Converging) Hover over any structure for more options.



© 2021 American Chemical Society. All rights reserved.

ACS  
International

CAS  
A division of the  
American Chemical Society

# 新化合物合成路线设计

Analyze Refine

Refine by: ?

☐ Reaction Structure

☐ Product Yield

☒ Number of Steps

☐ Reaction Classification

☐ Excluding Reaction Classification

☐ Non-participating functional groups

Number of Steps:

Examples: 1, 1 - 3, 1 -, - 3

Refine

进一步筛选

Get References Tools

Send to SciPlanner

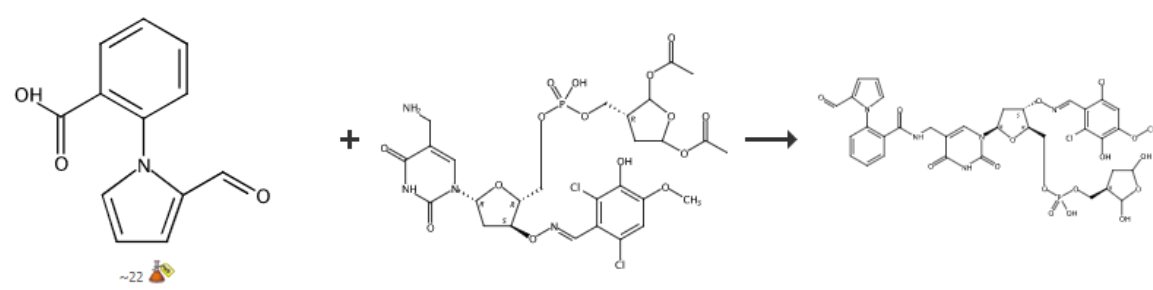
Group by: No Grouping Sort by: Accession Number

Display Options

0 of 66 Reactions Selected

1. View Reaction Detail Link

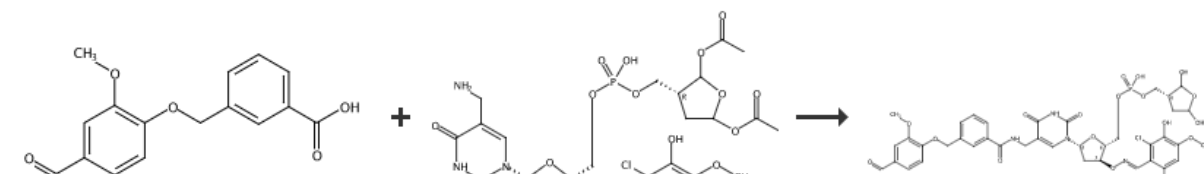
2 Steps Hover over any structure for more options.



~22

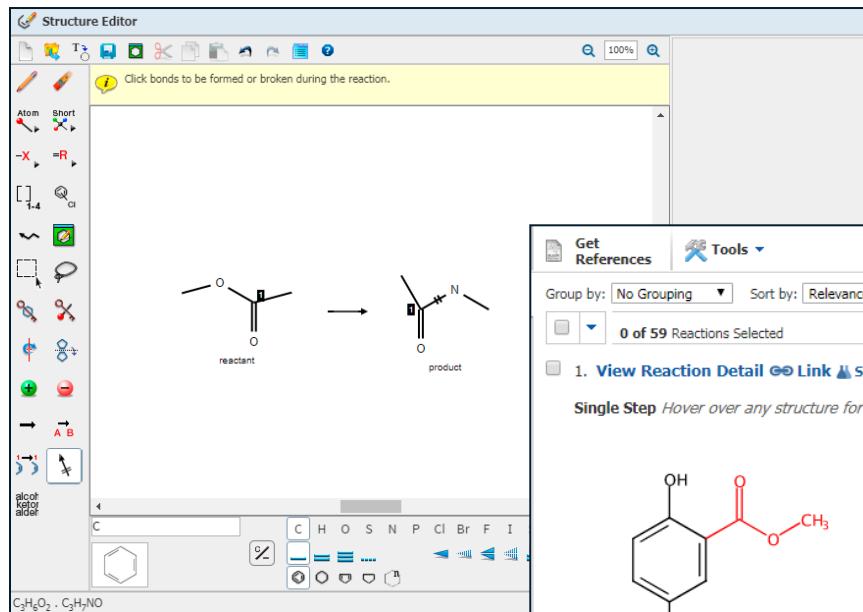
2. View Reaction Detail Link

2 Steps Hover over any structure for more options.



酰化剂为羧酸，不符合要求

# 新化合物合成路线设计



进一步限定用酯做酰化剂的反应

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Relevance

0 of 59 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~74

~120

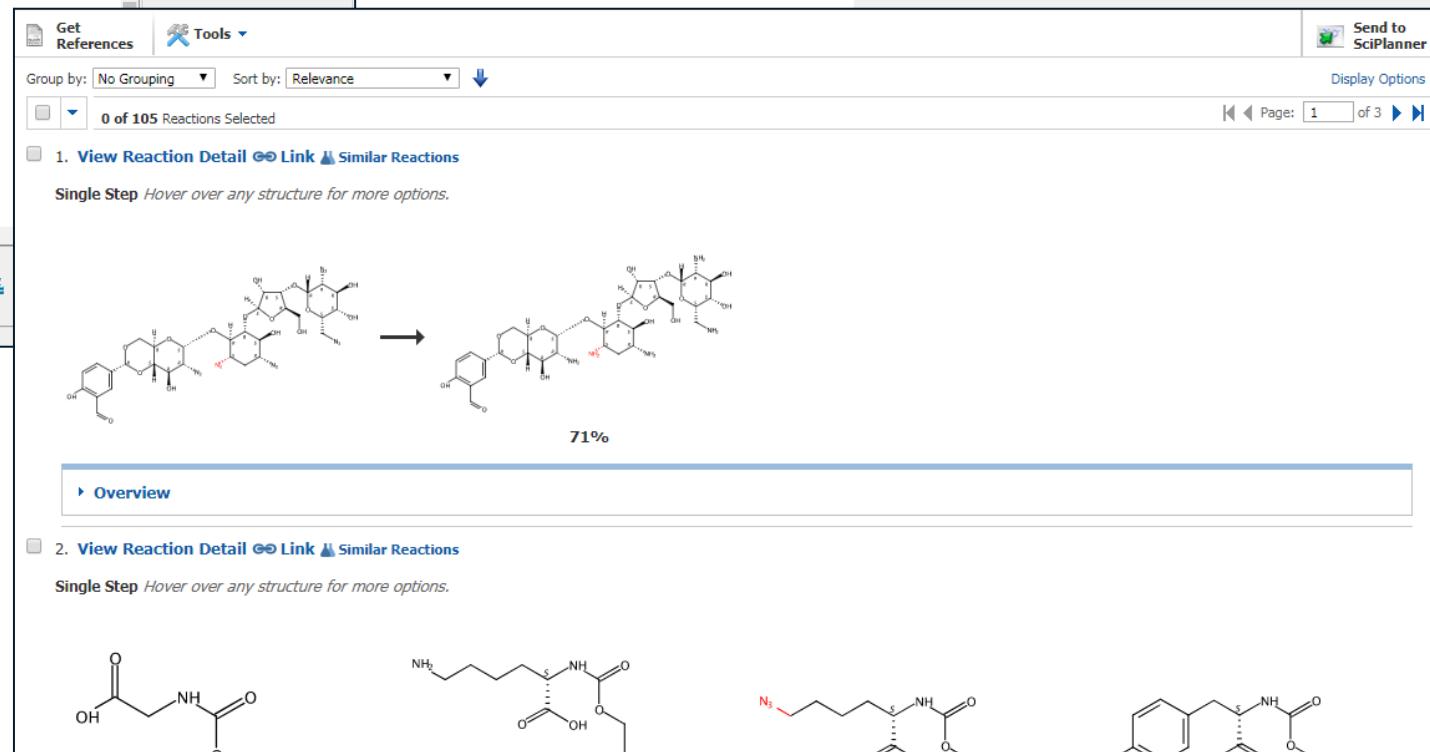
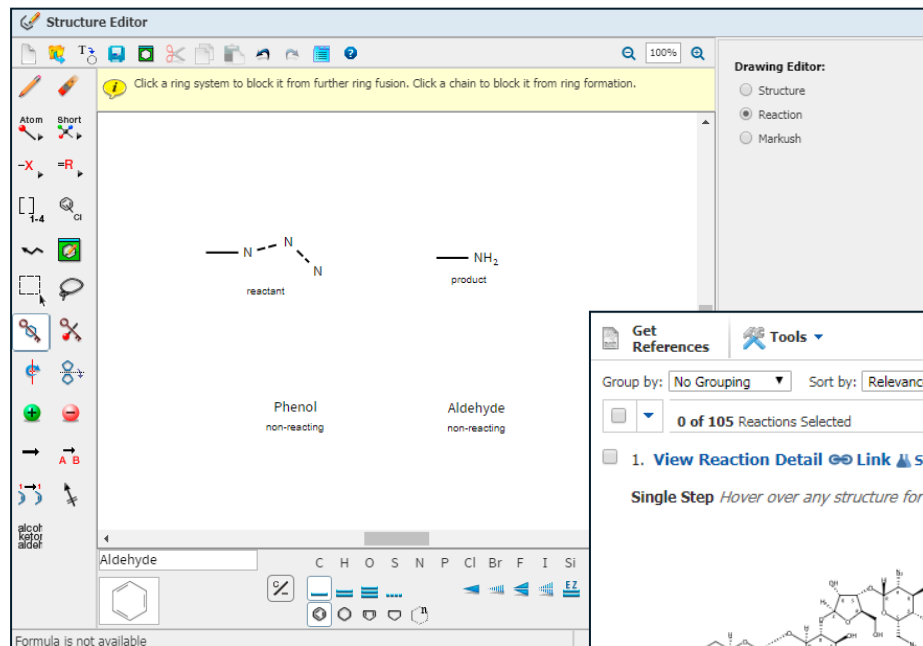
Overview

2. View Reaction Detail Link

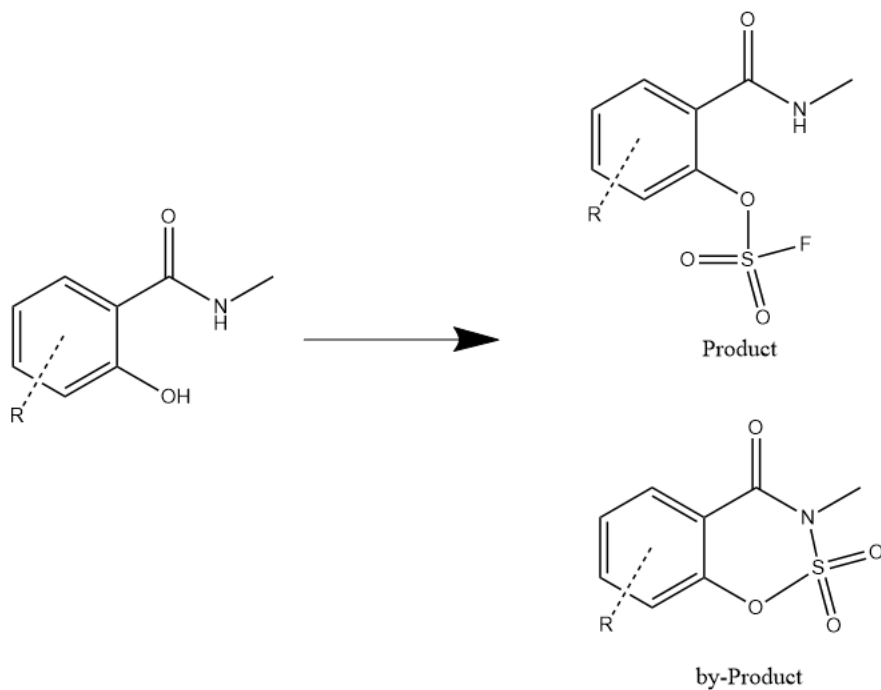
2 Steps Hover over any structure for more options.

# 新化合物合成路线设计

## 反应2



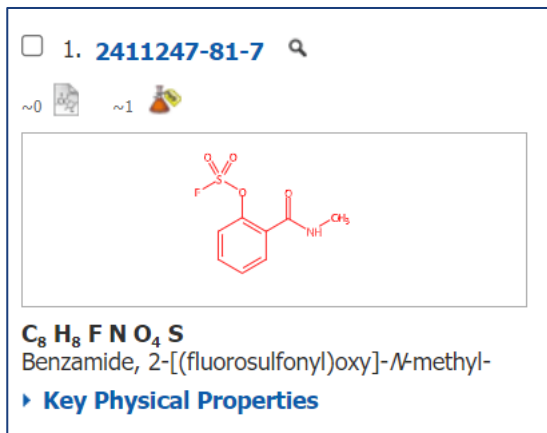
# 案例分析



如何提高主产物的收率？

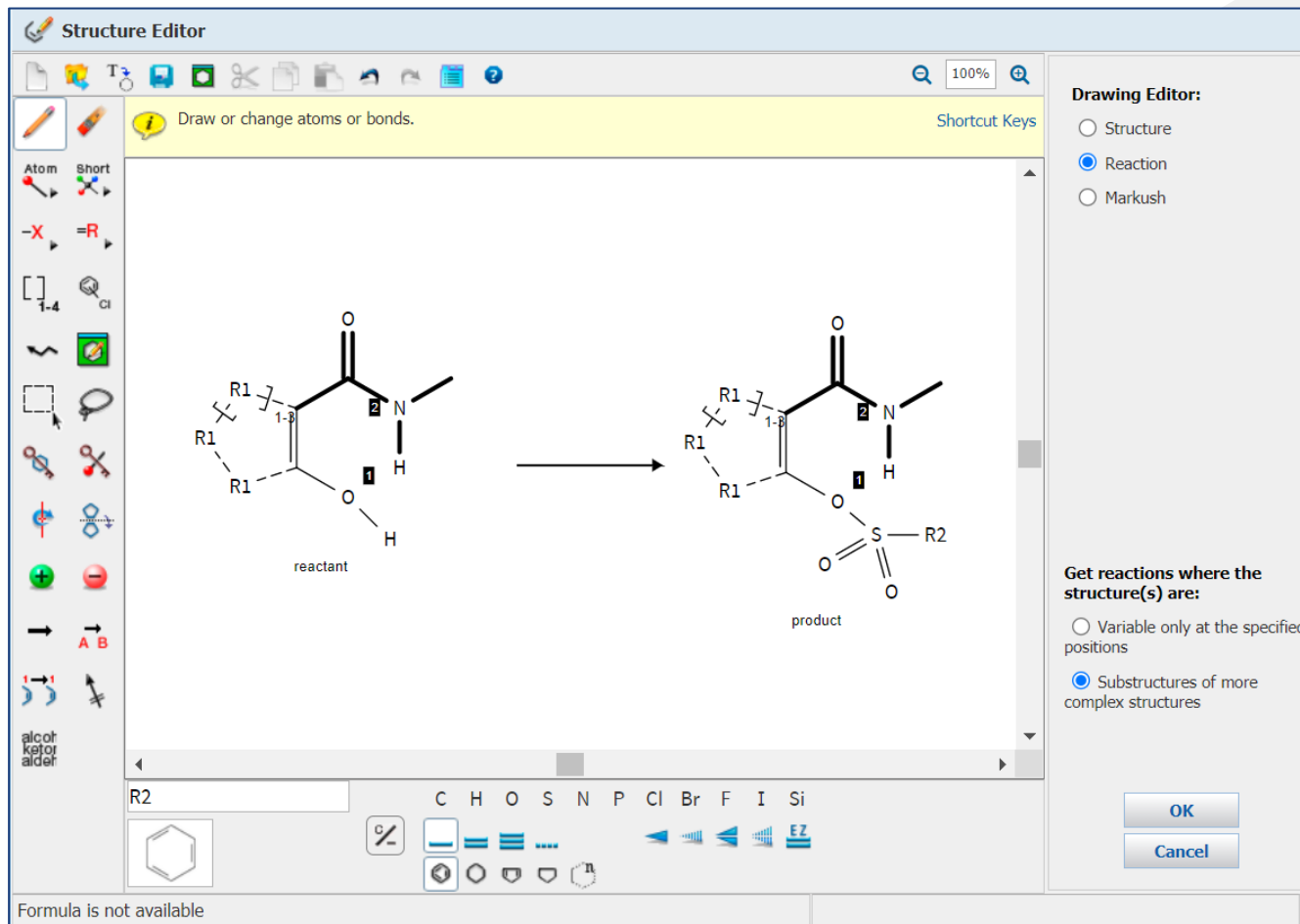
# 案例分析

## 1. 检索主产物



没有相关反应!

## 2. 扩大范围进行检索



R1=C、N、O; R2=X、OH

# 案例分析

**REACTIONS** ?

Get References Tools

Analyze Refine

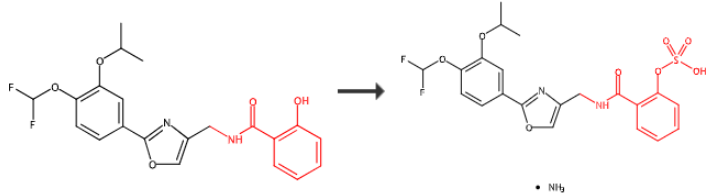
Analyze by: ?  
 Reagent  
 2699-79-8 1  
 ClSO<sub>3</sub>H 1  
 Show More

Group by: No Grouping Sort by: Accession Number

0 of 2 Reactions Selected

☐ 1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

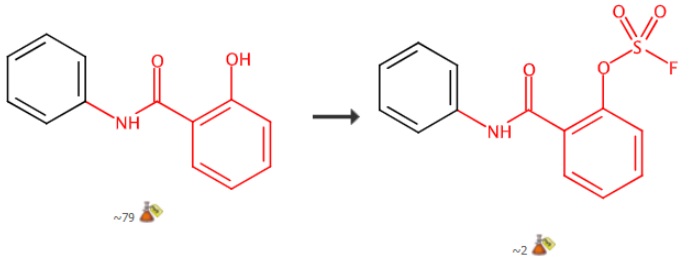


• NH<sub>2</sub>

Overview

☐ 2. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



~79 ~2

Overview

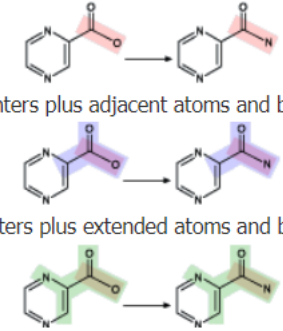
**Get Similar Reactions** ?

Retrieve similar reactions from:

- ☒ All reactions
- ☐ Current answer set

Include this level of similarity:

- ☐ Broad - Reaction centers only (99265)
- ☐ Medium - Reaction centers plus adjacent atoms and bonds (237)
- ☒ Narrow - Reaction centers plus extended atoms and bonds (221)



Get Reactions Cancel

Similar Reaction: 获得更多相关反应信息



# 案例分析

Group by: **No Grouping** Sort by: **Similarity**

☐ 0 of 221 Reactions Selected

☐ 1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

**Single Step** *Hover over any structure for more options.*

[Overview](#)

☐ 2. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

**Single Step** *Hover over any structure for more options.*

[Overview](#)

☐ 3. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

**Single Step** *Hover over any structure for more options.*

如何获得相关度更大的反应信息？

## 案例分析

Analyze

Refine

Refine by: ?

☐ Reaction Structure

☐ Product Yield

☐ Number of Steps

☐ Reaction Classification

☐ Excluding Reaction Classification

☒ Non-participating functional groups

Non-participating Functional Group(s)

View: 

All217

1 Selected

Clear Selections

☐ pi-Allyl

☐ Allyl Alcohol

☐ Allyl Halide

☒ Amide

☐ Amidine

☐ Amine Oxide

☐ AMINES

☐ Anhydride

Reactions must have

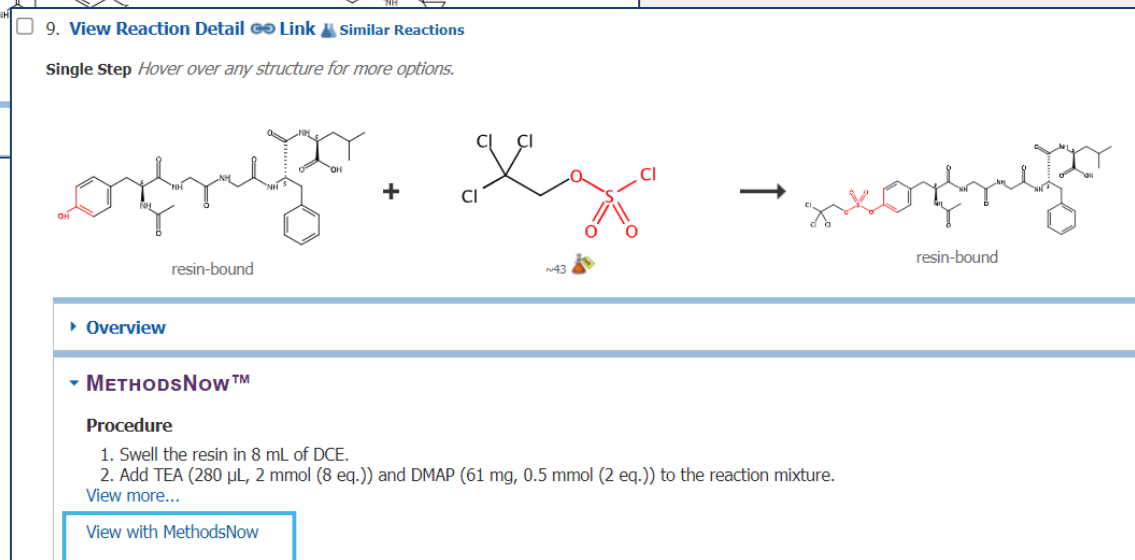
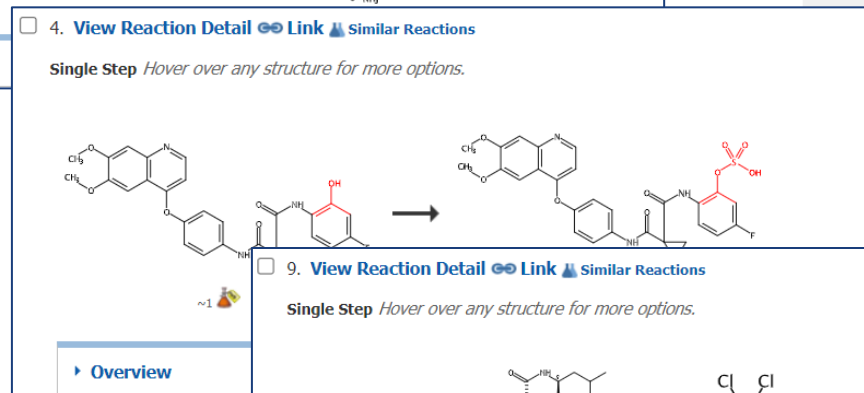
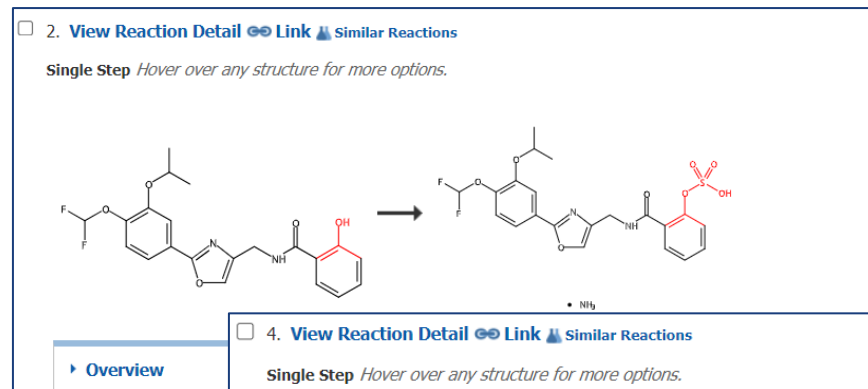
☒ all selections

☐ any selection

Refine

## Refine—Non-participating Function Group

## 进一步筛选选择性反应



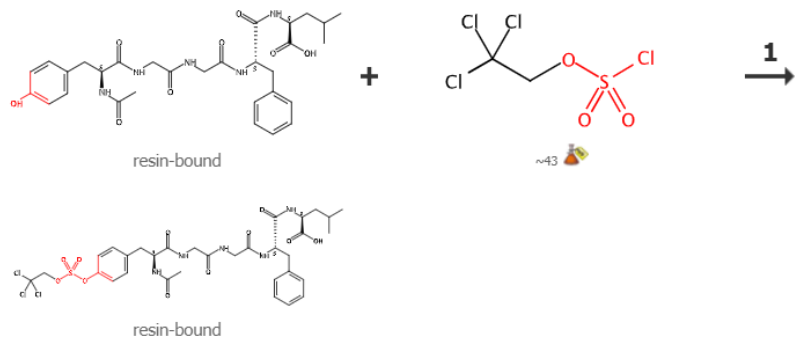
# 高效获取反应详情--MethodsNow

A general sequence independent solid phase method for the site specific synthesis of multiple sulfated-tyrosine containing peptides

By Bunschoten, Anton; Kruijtz, John A. W.; Ippel, Johannes H.; de Haas, Carla J. C.; van Strijp, Jos A. G.; Kemmink, Johan; Liskamp, Rob M. J.

From Chemical Communications (Cambridge, United Kingdom), (21), 2999-3001; 2009

Published by Royal Society of Chemistry



Products	<i>N</i> -Acetyl- <i>O</i> -[(2,2,2-trichloroethoxy)sulfonyl]-L-tyrosylglycylglycyl-L-phenylalanyl-L-leucine, resin-bound, CAS RN: 1173091-38-7
Reactants	<i>N</i> -Acetyl-L-tyrosylglycylglycyl-L-phenylalanyl-L-leucine, resin-bound, CAS RN: 78922-82-4 Chlorosulfuric acid, 2,2,2-trichloroethyl ester, CAS RN: 764-09-0
Reagents	Triethylamine, CAS RN: 121-44-8 4-(Dimethylamino)pyridine, CAS RN: 1122-58-3
Solvents	1,2-Dichloroethane, CAS RN: 107-06-2
Procedure	<ol style="list-style-type: none"><li>1. Swell the resin in 8 mL of DCE.</li><li>2. Add TEA (280 <math>\mu</math>L, 2 mmol (8 eq.)) and DMAP (61 mg, 0.5 mmol (2 eq.)) to the reaction mixture.</li><li>3. Shake the mixture until complete dissolution.</li><li>4. Add 2,2,2-trichloroethyl chlorosulfate (265 <math>\mu</math>L, 2 mmol (8 eq.)) to the mixture.</li><li>5. Shake the reaction mixture overnight.</li><li>6. Wash the resin with DCE (3x), and ether (3x).</li><li>7. Dry the resin in vacuo over <math>P_2O_5</math> to obtain the product.</li></ol>
Transformation	Preparation of Inorganic Esters from Alcohols
CAS Method Number	3-022-CAS-6472590

物质信息  
名称  
角色

实验过程

反应类型

MethodsNow中的实验详情不仅包含原文中描述的实验内容，还包括supporting information中涉及的实验内容

# 反应检索小结

1. 反应检索方法汇总与区分
2. 反应绘制工具的灵活使用
3. 反应结果排序: Group by Transformation/Document
4. 反应结果的快速纵览及筛选, 例如non-participating functional group;
5. 相似反应的获取获得更多启发
6. MethodsNow获取反应详情
7. SciPlanner工具助于自定义设计拟合成反应路线

# 大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的检索策略
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize
  - 如何高效阅读专利文献详情(CAS PatentPak)
- 物质相关信息的检索策略
  - 检索具有相同结构特征的物质
  - Markush检索
  - 如何筛选天然产物
  - 无机复合物、聚合物的检索
- 反应相关信息的检索策略
  - 如何检索化学选择性反应
  - 直接检索反应受限时如何处理
  - 新化合物的合成路线设计
  - 案例分析
  - 如何高效获取反应详情
- 获取分析方法的策略 (CAS Analytical Methods)



# 高效获取分析方法详情

## CAS Analytical Methods

- CAS Analytical Methods介绍
- 关键词检索
- 检索结果的分析、精炼与详情
- 多个分析方法的对照



# CAS Analytical Methods分析方法类别

目前有13个大类，45个小类；某些子类属于多种方法分类：

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

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

**Pharmacology / Toxicology:** 成瘾药物检测，有毒物检测...

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

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

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

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

**Agricultural Applications / Analysis:** 除草剂分析...

**Food Analysis:** 脂肪酸分析，脂肪酸酯分析，蛋白质分析...

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

**Miscellaneous:** 化妆品分析，爆炸物分析，纳米材料分析...

**Water:** 阴阳离子分析、环境分析、废水分析、微量元素分析...


**Polymer:** 聚合物分析...





# 简洁易用的检索界面

CAS Analytical Methods 登陆网址 [www.methodsnow.com](http://www.methodsnow.com)

CAS Solutions


 Analytical Methods

 Saved

 Account

## Search

Enter keyword, matrix, analyte, etc.



Advanced Search

### Browse Method Categories

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

### Recent Searches

Browse: Chiral Separation



# 关键词检索分析方法

CAS Solutions ▾

CAS Analytical Methods ★ Saved Account

## Search

Enter keyword, matrix, analyte, etc.

taxol

- taxol c
- taxol d
- taxoleic acid

CAS Solutions ▾

CAS Analytical Methods ★ Saved Account

[← Return to Home](#)

## Advanced Search

Keyword ▾ taxol

AND ▾ Technique ▾ HPLC

Add Search Criteria

Q Clear

# 检索结果分析与精炼

分析物

基质

方法分类

技术&仪器

年份

CAS Solutions

CAS Analytical Methods

boron nitride

Q

☆

👤

Return to Home

^ Analyte

☐ Chromium (20)

☐ Titanium (17)

☐ Molybdenum (14)

☐ 2,2-Bis(4-hydroxyphenyl)propane (13)

☐ 1,1-Bis(4-hydroxyphenyl)cyclohexane (12)

View All

▼ Matrix

^ Method Category

☐ Element Detection (47)

☐ Biomolecule Isolation Assay (30)

☐ Water / Wastewater / Sludge Analysis (30)

☐ Suboptimal Analysis (28)

☐ Toxin Assay (16)

View All

^ Technique

☐ Electrothermal atomic absorption spectroscopy (20)

Results (192)

Sort Relevance ▼

☐

📄

☆

Compare (0/3)

☐ Analysis of Atomic nitrogen in Boron nitride by Chemical digestion

CAS MN: 1-119-CAS-264573

View Details & Instructions


Add to Compare


Analyte	Atomic nitrogen
Matrix	Boron nitride
Other Materials	Reagent: Hydrofluoric acid; Methyl red; Sodium hydroxide; Ethanol; Methylene blue; Sulfuric acid Material: PTFE-container; Volumetric flask (100 mL); Erlenmeyer flask
Method Category	Element Detection
Technique	Acid-base titration; Chemical digestion
Equipment Used	High pressure decomposition device; Distillation device
Source	<b>The precise determination of nitrogen in boron nitride</b> Gruner, W.; Hassler, J.; Barth, P.; Behm, J.; Sunderkoetter, J. Journal of the European Ceramic Society (2009), 29 (10), 2029-2035. Elsevier Ltd.

Full Text ▼

Abstract ▼

© 2021 American Chemical Society. All rights reserved.

ACS  
International

CAS  
A division of the  
American Chemical Society

# 分析方法详情

Method Detail

1 of 192

← Prev

Next →

📄

★

Analysis of Atomic nitrogen in Boron nitride by Chemical digestion

CAS MN: 1-119-CAS-264573

Method Category:Element Detection

Technique:Acid-base titration; Chemical digestion

Materials	Role	Image	CAS RN
Atomic nitrogen	analyte	<a href="#">View Structure</a>	17778-88-0
Boron nitride	matrix	<a href="#">View Structure</a>	10043-11-5
PTFE-container	material		
Volumetric flask (100 mL)	material		
Erlenmeyer flask	material		
Hydrofluoric acid	reagent	<a href="#">View Structure</a>	7664-39-3
Methyl red	reagent	<a href="#">View Structure</a>	493-52-7
Sodium hydroxide	reagent	<a href="#">View Structure</a>	1310-73-2
Ethanol	reagent	<a href="#">View Structure</a>	64-17-5
Methylene blue	reagent	<a href="#">View Structure</a>	61-73-4
Sulfuric acid	reagent	<a href="#">View Structure</a>	7664-93-9

Source

The precise determination of nitrogen in boron nitride

Gruner, W.; Hassler, J.; Barth, P.; Behm, J.; Sunderkoetter, J.

Journal of the European Ceramic Society (2009), 29 (10), 2029 - 2035. Elsevier Ltd.

CODEN: JECSER | ISSN: 09552219 | DOI: 10.1016/j.jeurceramsoc.2008.12.021

Full Text ▾

Abstract ^

To further improve the high performance ceramic material BN it is necessary to advance its analytics. The quant. determination of the nitrogen content as main component is compared by three methods: the carrier gas hot extraction, the LIOH fusion, and the Kjeldahl method. Thereby specific methodical aspects are critically highlighted with respect to the trueness and precision of the nitrogen anal. The "chem." plays a fundamental role in all methods. In the case of the instrumental anal. by CGHE important critical aspects are the calibration of CGHE measurements and the improvement of reproducibility which needs a much better understanding of the chem. reactions in the crucible. In case of the Kjeldahl method it is of decisive importance to apply an adequate high temperature of 260° for decomposition, whereas the melt-decomposition with LIOH is affected by melt additions

Equipment Used

High pressure decomposition device, Berghof Products and Instruments GmbH, Germany

Distillation device, Vapodest 3, erhardt Laboratory Systems, Germany

所用材料、标题摘要、著录信息、仪器

# 分析方法详情

## Instructions

### Boron nitride sample

1. Collect boron nitride sample containing 0.1% soluble boric oxide, 0.7% oxygen for analysis.

### Digestion

1. Weigh 0.2 g of the BN sample in a PTFE-container with 10 mL of HF-acid (40%).
2. Decompose the sample for 20 h at a temperature of 260 °C in a high pressure decomposition device (Berghof Products and Instruments GmbH, Germany).
3. Cool the solution and transfer into a volumetric flask (100 mL).

### Acid-base titration using Kjeldahl method

1. Measure 20 - 30 mL of the solution in a sample cup and transfer into the Kjeldahl container built into the distillation device (Vapodest 3, erhardt Laboratory Systems, Germany).
2. Titrate 30 mL sulfuric acid (0.05 mol/L) into an Erlenmeyer flask and dilute with approximately 120 mL of water.
3. Add 2 - 3 mL of indicator solution (0.2% methyl red + 0.1% methylene blue in ethanol p.a.).
4. Apply the solution of sodium hydroxide (40%) to the sample and distill with steam into the Erlenmeyer flask.
5. Titrate excessive sulfuric acid with sodium hydroxide solution (0.1 mol/L).
6. Calculate the nitrogen content as wt.% using the following equation:  $N_{\text{total}}\% = (V_{\text{H}_2\text{SO}_4}f_{\text{H}_2\text{SO}_4} - V_{\text{NaOH}}f_{\text{NaOH}})F/ms$ ;  $V_{\text{acid}}$ : consumption of 0.1 M H<sub>2</sub>SO<sub>4</sub> [mL]; F: 70945 (titrimetric factor with 0.2 g solid sample);  $f_{\text{H}_2\text{SO}_4}$ : titration correction factor of H<sub>2</sub>SO<sub>4</sub> solution;  $f_{\text{NaOH}}$ : titration correction factor of NaOH solution; ms: sample mass of taken liquid [mg].

## Validation

Precision	0.20% (RSD)
Concentration	55.76 ± 0.11% wt

## 操作步骤和数据有效性验证



# 浏览方法分类

## Browse Method Categories

Agricultural Applications / Analysis

Bioassays

Biomolecule Isolation

Environmental Analysis

Food Analysis

Fuels / Geology / Biofuels

Historical Analysis / Dating

Miscellaneous

Organic Compound Analysis

Organometallics / Inorganics

Pharmacology / Toxicology

Polymer Analysis

Water Analysis

## [Browse Method Categories](#) > Organic Compound Analysis

Active Pharmaceutical Ingredient and Metabolite Analysis

Chiral Separation

Natural Product Isolation Analysis

Organic Compound Analysis

# 对照多个感兴趣的分析方法详情

CAS Solutions Analytical Methods

Browse: Organic Compound Analysis

Results (33850) Sort Relevance

☐   Compare (0/3)

☐ **Analysis of Sulfitocobalamin by Reversed-phase HPLC**  
CAS MN: 1-132-CAS-468124

[View Details & Instructions](#) [Add to Compare](#)

Analyte	Sulfitocobalamin
Other Materials	Reagent: Hypochlorous acid; Ethanol Material: Sep-Pak Vac (5 g) C <sub>18</sub> cartridge; Reversed-phase HPLC column (Wakosil-II 5C18RS $\Phi$ 4.6 $\times$ 150 mm <sup>2</sup> ; particle size 5 $\mu$ m) <a href="#">View All</a>
Method Category	Organic Compound Analysis
Technique	UV-visible spectroscopy; Reversed-phase HPLC; Solid phase extraction
Equipment Used	High-performance liquid chromatographic system; UV-Visible detector; System controller; Degasser; HPLC pumps; Column oven; Chromatodata processing system
Source	<b>Food Additives (Hypochlorous Acid Water, Sodium Metabisulfite, and Sodium Sulfite) Strongly Affect the Chemical and Biological Properties of Vitamin B<sub>12</sub> in Aqueous Solution</b> Okamoto, Naho; Bito, Tomohiro; Hiura, Nanami; Yamamoto, Ayaka; Iida, Mayu; Baba, Yasuhiro; Fujita, Tomoyuki; Ishihara, Atsushi; Yabuta, Yukinori; Watanabe, Fumio ACS Omega (2020), 5 (11), 6207-6214. American Chemical Society <a href="#">Full Text</a>

Results (33850) Sort Relevance

☐   Compare (3/3)

☐ **Analysis of Sulfitocobalamin by Reversed-phase HPLC**  
CAS MN: 1-132-CAS-468124

[View Details & Instructions](#) [Remove from Compare](#)

Analyte	Sulfitocobalamin
Other Materials	Reagent: Hypochlorous acid; Ethanol Material: Sep-Pak Vac (5 g) C <sub>18</sub> cartridge; Reversed-phase HPLC column (Wakosil-II 5C18RS $\Phi$ 4.6 $\times$ 150 mm <sup>2</sup> ; particle size 5 $\mu$ m) <a href="#">View All</a>
Method Category	Organic Compound Analysis
Technique	UV-visible spectroscopy; Reversed-phase HPLC; Solid phase extraction
Equipment Used	High-performance liquid chromatographic system; UV-Visible detector; System controller; Degasser; HPLC pumps; Column oven; Chromatodata processing system
Source	<b>Food Additives (Hypochlorous Acid Water, Sodium Metabisulfite, and Sodium Sulfite) Strongly Affect the Chemical and Biological Properties of Vitamin B<sub>12</sub> in Aqueous Solution</b>

# 对照多个感兴趣的分析方法详情

Compare Methods			
<div>Expand All   Collapse All</div>			
	1	2	3
Title	Analysis of Sulfitecobalamin by Reversed-phase HPLC	Analysis of Phenol by Spectrophotometry	Analysis of 2-Chlorophenol in Irrigation waters by Solid phase extraction
CAS Method Number	1-132-CAS-468124	1-132-CAS-467381	1-132-CAS-466437
Method Category	Organic Compound Analysis	Organic Compound Analysis	Organic Compound Analysis
Technique	UV-visible spectroscopy; Reversed-phase HPLC; Solid phase extraction	Spectrophotometry	Liquid chromatography; UV-Visible detectors; Reverse phase extraction
Analyte	Sulfitecobalamin	Phenol	2-Chlorophenol; 2,3-Dichlorophenol; 2,4-Dichlorophenol
Matrix			Irrigation waters
Other Materials	Hypochlorous acid; Ethanol; Sep-Pak Vac (5 g) C <sub>18</sub> cartridge; Reversed-phase HPLC column (Wakosil-II 5C18RS Φ 4.6 × 150 mm)	3-Methyl-2-benzothiazolinone hydrazone; Phosphate; Glutaraldehyde; Reed	Hydrochloric acid; Triphenylbenzene chloride (FeCl <sub>3</sub> ); Nitrogen
Equipment Used	High-performance liquid chromatographic system, Shimadzu; UV-Visible detector, SPD-10AV, Shimadzu; System controller, SCL-10A		
Source	Food Additives (Hypochlorous Acid Water, Sodium Metabisulfite, and Sodium Sulfite) Strongly Affect the Chemical and Biological Properties of Reed Membranes		
Preparation	Fabrication of the reed biosensor		
Method	Treatment cyanocobalamin (CN-B <sub>12</sub> )		
Retention Time	27.171 min		
Linearity Range	5 - 100 μM		
Limit of Detection	2.5 μM		
Recovery	30% in 80.0 ng/mL added concentration (read from figure), 2-chlorophenol, 39% in 80.0 ng/mL added concentration (read from figure)		

# CAS Analytical Methods使用方法小结:

1. CAS Analytical Methods目前有13个大类， 45个小类； 某些子类属于多种方法分类；
2. 可通过关键词检索， 或者浏览方法分类来获取分析方法结果；
3. 检索结果可通过分析物、基质、方法分类、技术&仪器， 以及年份来纵览或精炼；
4. 所有的分析方法都可获取详情， 包括所用材料、标题摘要、著录信息、仪器、实验条件、操作步骤和数据有效性验证等信息；
5. 支持三种不同的分析方法之间的对照， 以表格的形式清晰对比呈现所有的实验详情。



# 浏览器选择建议

- Windows 7以上用户建议升级IE到10以上，不支持IE7、IE8
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

# 如何获取CAS SciFinder账号

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username:  Tips

Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer:  Why?

请注意:

1.必须输入真实姓名和邮箱。  
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。

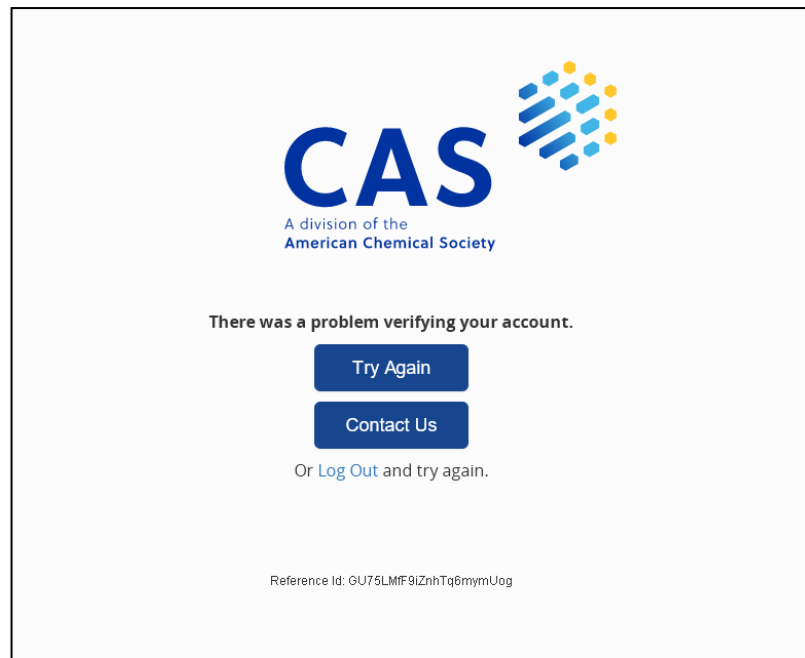
单击 Register (注册)。

登录学校图书馆网站找到CAS SciFinder数据库说明页, 按照提示进行注册

# 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（以电子形式存储不超过5,000条记录）
- 不得账号分享
- 不得将账号用于非学术研究

# 常见问题



- 确认账号密码是否正确

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

# 谢谢！

关注我们



**ACS**  
Chemistry for Life®

运用化学的力量改善人们的生活

[china@acs-i.org](mailto:china@acs-i.org)

+86-10-62508026/27

[www.cas.org](http://www.cas.org)

美国化学文摘社北京代表处