



# SciFinder检索难点解析

——吉林大学 20161014

# 提纲

- SciFinder介绍
- SciFinder 文献检索难点解析
- SciFinder 物质检索难点解析
- SciFinder 反应检索难点解析

# 提纲

- **SciFinder**介绍
  - 索引的价值
  - 增值的专利信息
  - **CAS**最新动向

# 美国化学文摘社—Chemical Abstract Service

- 创建于1907年，简称“CAS”
- 美国化学会（ACS）的分支机构
- 密切关注、标引和提炼全球化学相关的科技文献
- 最早创立了《化学文摘》
- 总部位于美国俄亥俄州的哥伦布市

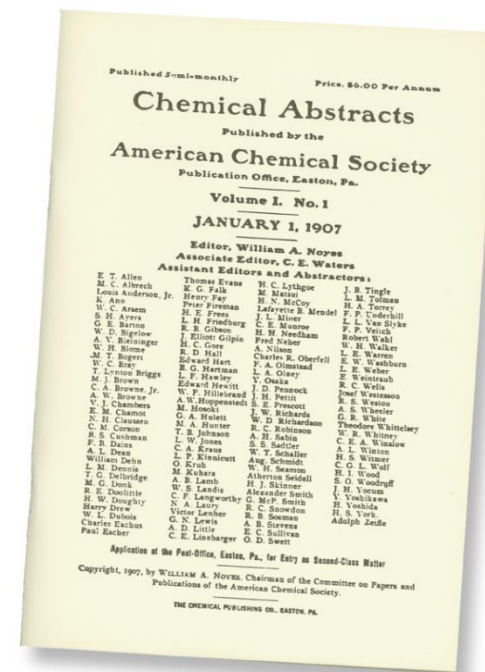


# 1907年，信息的汇集、管理发生了重大的变化



威廉·诺伊斯  
(William A. Noyes)

- “化学文摘” 创刊
- 当年编制近12,000条文摘
- 今天，CAS每年收录、创建来自期刊、专利和其他已公开信息的文摘达到了100余万条



# CAS构建最高质量的化学数据库

Patents,  
journals, web,  
catalogs, etc.

CAS<sup>®</sup>

A division of the American Chemical Society

CAS  
Scientists



arXiv.org

Aldrichimica ACTA  
VOL. 40, NO. 1 • 2007

ACS  
chemical  
biology

Beilstein Journal of  
Organic Chemistry

division of polymer chemistry, inc  
American Chemical Society

J | A | C | S  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical  
Neuroscience

THE JOURNAL OF  
PHYSICAL CHEMISTRY  
Letters

Cornell University  
Library



U.S. Patent  
Office

SciFinder<sup>®</sup>  
A CAS Solution

CAS is a division of the American Chemical Society.  
Copyright 2016 American Chemical Society. All rights reserved.

# CAS数据最具价值的内容—人工标引

**REFERENCE DETAIL** | Get Substances | Get Related Citations | Get Full Text | Send to SciPlanner

Return | Previous | Next

## 1. Anion exchange membrane adsorbers for flow-through polishing steps: Part II. Virus, host cell protein, DNA clearance, and antibody recovery

By: Weaver, Justin; Husson, Scott M.; Murphy, Louise; Wickramasinghe, S. Ranil

Anion exchange membrane adsorbers are used for contaminant removal in flow-through polishing steps in the manuf. of biopharmaceuticals. This contribution describes the clearance of minute virus of mice, DNA, and host cell proteins by three com. available anion-exchange membranes: Sartobind Q, Mustang Q, and ChromaSorb. The Sartobind Q and Mustang Q products contain quaternary amine ligands; whereas, ChromaSorb contains primary amine based ligands. Performance was evaluated over a range of soln. conditions: 0-200 mM NaCl, pH 6.0-9.0, and flow rates of 4-20 membrane vols./min in the presence and absence of up to 50 mM phosphate and acetate. In addn. contaminant clearance was detd. in the presence and absence of 5 g/L monoclonal antibody. The quaternary amine based ligands depend mainly on Coulombic interactions for removal of neg. charged contaminants. Consequently, performance of Sartobind Q and Mustang Q was compromised at high ionic strength. Primary amine based ligands in ChromaSorb enable high capacities at high ionic strength due to the presence of secondary, hydrogen bonding interactions. However, the presence of hydrogen phosphate ions leads to reduced capacity. Monoclonal antibody recovery using primary amine based anion-exchange ligands may be lower if significant binding occurs due to secondary interactions. The removal of a specific contaminant is affected by the level of removal of the other contaminants. The results of this study may be used to help guide selection of com. available membrane adsorbers for flow-through polishing steps.

**Indexing**

Biochemical Methods (Section9-3)

**Concepts**

Growth arrest- and DNA damage-inducible proteins

GADD153; anion exchange membrane adsorbers for flow-through polishing steps

Biological study, unclassified; Biological study

Anion exchange membranes | Electric conductivity  
Flow | Hydrogen bond  
Ionic strength | Virus  
pH

anion exchange membrane adsorbers for flow-through polishing steps

**Substances**

175386-77-3 Sartobind Q  
397251-53-5 Mustang Q  
1246496-78-5 ChromaSorb

anion exchange membrane adsorbers for flow-through polishing steps

Analytical reagent use; Biological use, unclassified; Analytical study; Biological study; Uses

14066-19-4 Hydrogen phosphate, biological studies

anion exchange membrane adsorbers for flow-through polishing steps

Biological study, unclassified; Biological study

**QUICK LINKS**

0 Tags, 0 Comments

**SOURCE**

Biotechnology and Bioengineering  
Volume110  
Issue2  
Pages500-510  
Journal  
2013  
CODEN:BIIBIAU  
ISSN:0006-3592  
DOI:10.1002/bit.24724

**COMPANY/ORGANIZATION**

Department of Chemical and Biological Engineering  
Colorado State University  
Fort Collins, CO, USA 80523

**ACCESSION NUMBER**

2012:1487758  
CAN158:265018  
CAPLUS

**PUBLISHER**

John Wiley & Sons, Inc.

**LANGUAGE**

English

## Tips:

1. 98%以上的文献，都经过人工标引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS Registry Number®标引文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域



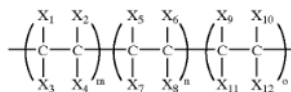
# SciFinder对专利的加强

**on** (10) **Pub. No.:** US 2003/0236353 A1

(43) **Pub. Date:** Dec. 25, 2003

(57) **ABSTRACT**

A golf ball comprising a core, a cover, and an intermediate layer disposed between the core and the cover, wherein the intermediate layer comprises a non-ionomeric fluoropolymer having a formula:



wherein X<sub>1</sub> to X<sub>12</sub> are hydrogen, fluorine, chlorine, bromine, iodine, CH<sub>3</sub>, CF<sub>3</sub>, linear or branched alkyl group, partially fluorinated or perfluorinated alkyl group, linear or branched alkoxy group, partially fluorinated or perfluorinated alkoxy group, aromatic, or alicyclic; at least one of X<sub>1</sub> to X<sub>4</sub> comprises a fluorine; m ranges from 100 to 1 percent by weight of the fluoropolymer; n ranges from 0 to 50 percent by weight of the fluoropolymer; and o ranges from 0 to 35 percent by weight of the fluoropolymer.

改写的标题和摘要:

1. 更真实反映原文内容
2. 明确指出专利的科技要点
3. 翻译50多种语言的专利

## 3. Golf balls comprising non-ionomeric fluoropolymer

By: Rajagopalan, Murali  
Assignee: Acushnet Co., USA

A golf ball comprises a core, a cover, and an intermediate layer disposed between the core and the cover, wherein the intermediate layer comprises a non-ionomeric fluoropolymer having a formula  $-[CX^1(X^3)CX^2(X^4)]-[CX^5(X^7)CX^6(X^8)]-[CX^9(X^{11})CX^{10}(X^{12})]-$ ; wherein X<sup>1</sup> to X<sup>12</sup> are hydrogen, fluorine, chlorine, bromine, iodine, CH<sub>3</sub>, CF<sub>3</sub>, linear or branched alkyl group, partially fluorinated or perfluorinated alkyl group, linear or branched alkoxy group, partially fluorinated or perfluorinated alkoxy group, arom., or alicyclic; at least one of X<sup>1</sup> to X<sup>4</sup> comprises a fluorine; m ranges from 100 to 1 percent by wt. of the fluoropolymer; n ranges from 0 to 50 percent by wt. of the fluoropolymer; and o ranges from 0 to 35 percent by wt. of the fluoropolymer. Thus, a compn. of the an intermediate layer of a golf ball contains Kynar Flex 2900-04 (hexafluoropropylene-vinylidene fluoride copolymer). The intermediate layer was molded over a polybutadiene core to give a golf ball with an ATTI compression of 80, and a COR at 125 ft/s of 0.795, and water absorption <0.05%.



# SciFinder中的专利族信息的价值

- 多种语言等同件（用户可以选择阅读自己母语的专利）
- 查看专利保护国家及未保护的国家市场
- 通过专利分类代码判断专利公开状态
- 发明专利保护的范围和规模
- 基本专利（被数据库索引的第一篇专利）及化学索引等同件
- 判断专利申请及是否需要申请专利的市场相关信息

Patent Information					
Patent No.	Kind	Language	Date	Application No.	Date
US 20030236353	A1		Dec 25, 2003	US 2002-171355	Jun 13, 2002
US 6747110	B2		Jun 8, 2004		
JP 2004041721	A		Feb 12, 2004	JP 2003-166490	Jun 11, 2003
US 20040192833	PatentPak <sup>™</sup> A1	English	Sep 30, 2004	US 2004-817366	Apr 2, 2004
US 7083856	B2		Aug 1, 2006		
US 20040210017	A1		Oct 21, 2004	US 2004-842607	May 10, 2004
US 7101944	B2		Sep 5, 2006		
US 20040236018	PatentPak <sup>™</sup> A1	English	Nov 25, 2004	US 2004-867073	Jun 14, 2004
US 7009002	B2		Mar 7, 2006		
Priority Application					
US 2002-171355	A		Jun 13, 2002		
US 2004-842607	A2		May 10, 2004		

# CAS最新动向—解决方案

## PatentPak™

 **NCI™ Global**  
*A Solution Powered by CAS*

 **METHODSNOW™**  
A CAS SOLUTION

 **CHEMZENT™**  
A CAS SOLUTION

 **SciFinder®**  
A CAS Solution

CAS is a division of the American Chemical Society.  
Copyright 2016 American Chemical Society. All rights reserved.

# CAS最新动向—解决方案

- CAS于2015年2月正式发布PatentPak™
- 专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息

Sort by: Citing References | Display Options

0 of 29 References Selected | Page: 1 of 2

1. Oil digesting microbe-plastic foam system  
 PatentPak™  
 By Young, William Ian; Foster, John Kingsley  
 From U.S. (2007), US 7166221 B1 20070123. | Language: English, Database: CAPLUS

This invention is a system and method for bioremediation of hydrocarbon and org. pollution in fresh and salt water. Hydrocarbon and org. pollution digesting is placed in a floating carrier where the microorganisms are exposed to the pollution and the pollution is digested. The floating element may be a block of polymer microbes may be supported on powder such as clay minerals, and the powder may be formed into pellets held in slits in the foam.

2. Apparatus for the production of potable liquid from seawater, polluted water and the like  
 PatentPak™  
 By Stache, Knut  
 From Eur. Pat. Appl. (1984), EP 121099 A2 19841010. | Language: German, Database: CAPLUS

Drinking water is obtained from seawater or polluted water using a disposable kit contg. a reverse osmosis membrane, an edible, osmosis producing material and an ion exchanger attached to a reusable plastic container suitable for long term water storage. The wet membranes are maintained in that condition fructose against the membrane and coating the outside of the membrane with a water-sol. material, such as syrup. The membrane removes >85% of the salts and impurities. Upon decantation into the storage container the ion exchanger removes the re...

3. Freshwater microalgae coastal closed culture system [Machine Translation].  
 PatentPak™  
 By Feng, Lei; Li, J.  
 From Faming Zh...

Patent No. CN 104774746 A  
 Kind A  
 Language Chinese  
 A 20150715. | Language: Chinese, Database: CAPLUS

[Machine Translation of Description] freshwater microalgae culture system transparent plastic film, both entry and outlet of the plastic film is scratched by the h...

4. Culture medium taking biomass filterster waste liquor as raw materials to culture

(19) 中华人民共和国国家知识产权局  
 (12) 发明专利申请  
 (51) Int. Cl. C12P 1/00 (2006.01)  
 (52) CIP 1/00 (2006.01)  
 (71) 申请人 沈阳航空航天大学  
 地址 110136 辽宁省沈阳市沈北新区道义大街10号  
 (72) 发明人 尹强 李强 王得云 王雷  
 (74) 专利代理机构 沈阳国特专利商标事务所 (普通合伙) 21229  
 代理人 李强

PatentPak™

Key Substances in Patent  
 CAS RN 134523-03-8  
 Search in SciFinder | View Detail  
 Analyst Markup Location  
 page 4

CAS RN 1305-62-0  
 HO—Ca—OH  
 Search in SciFinder | View Detail  
 Analyst Markup Location  
 page 4

CAS RN 134395-00-9

[0015] 下面结合实施例对本发明做详细说明,而不是限定本发明的保护范围。  
 [0016] 本发明的合成路线如下:

实例例 1  
 向反应瓶中加入 100 ml 水、15ml 乙醇、20 g R-(R\*,R\*)-2-(4-氟基苯)-β, δ-二羟基-5-(1-异丙基)-3-苯基-4-((苯胺)羧基)-1H-吡咯-1-庚酸叔丁酯(0.03mol)以及 4 g 氢氧化钙(0.10mol),将混合物搅拌并加热混合物至 45°C,然后继续搅拌并向混合物中滴加 5g (0.08mol)醋酸,用 HPLC 跟踪反应,7 小时左右反应即可进行完毕。反应结束后,

Ca(OH)<sub>2</sub>·HAc

Ca

# CAS最新动向—解决方案

- CAS于2016年2月正式发布MethodsNow™
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求

SciFinder interface showing a chemical reaction. The reaction involves a substituted benzimidazole derivative reacting with a methylamine derivative to form a product in 79% yield. The interface includes search filters, a procedure section, and experimental data.

嵌在SciFinder中的合成模块

MethodsNow interface showing search results for 'atorvastatin'. The results list various methods for the analysis of atorvastatin in blood plasma, including thin layer chromatography and HPLC. The interface includes filters for analyte, matrix, and method category.

单独的分析界面

# 提 纲

- **SciFinder** 文献检索难点解析
  - 利用Index Term修正检索词
  - 巧用CAS Role
  - 善用Categorize去除噪音信息

# 文献检索方法

## ■ 功能方面

- 主题检索
- 作者名检索
- 机构名检索
- 文献标示符检索
- 期刊和专利名称
- 从物质，反应获得文献



## ■ 检索方法推荐

- 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：植物中天然活性成分的抗癌研究

检索式： Natural Active Component with Anti Cancer

The screenshot displays the SciFinder search interface. At the top, the SciFinder logo is visible. Below it, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. The main search area shows the research topic 'Natural Active Component with ...'. On the left, there are two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are options like 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Under 'SUBSTANCES', there are options like 'Chemical Structure' and 'Markush'. The main search area contains a search box with the text 'Natural Active Component with Anti Cancer'. Below the search box, there are examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is located below the examples. At the bottom of the search area, there is a link for 'Advanced Search'.

关键词之间用介词连接

# 利用Index Term选词

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

Research Topic "Natural Active Component with ..."

REFERENCES ?

只有134篇吗?

Select All Deselect All

1 of 4 Research Topic Candidates Selected

	References
<input checked="" type="checkbox"/> 134 references were found containing the two concepts "Natural Active Component" and "Anti Cancer" closely associated with one another.	134
<input type="checkbox"/> 301 references were found where the two concepts "Natural Active Component" and "Anti Cancer" were present anywhere in the reference.	301
<input type="checkbox"/> 3741 references were found containing the concept "Natural Active Component".	3741
<input type="checkbox"/> 1110376 references were found containing the concept "Anti Cancer".	1110376

Get References

“Concept”表示做了同意词的扩展

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

“were present anywhere in the reference”表示同时出现在一段话中

# 利用Index Term选词

SciFinder® 后处理工具

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

13 duplicates were automatically removed.

Research Topic "Natural Active Component with ..." > references (121)

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 121 References Selected

Analyze by: Author Name

Chen Jianqing	3
Chen Yujiao	3
Cheng Yiyu	3
Cui Jinsong	3
Dou Jing	3
Ge Zhiwei	3
He Qing	3
Huo Yang	3
Liu Li	3

1. Construction of 2-deoxy thioglycoside donors using S-methyl and S-ethyl cyclopropenium iodide salts

Quick View | Other Sources

By Bylsma, Marissa; Bennett, Clay

From Abstracts of Papers, 250th ACS National Meeting & Exposition, Boston, MA, United States, August 16-20, 2015 (2015), CARB-92. | Language: English, Database: CAPLUS

2-deoxy-sugars are a crit. **component** of many **natural** products with antibiotic and/or **anti-cancer activity**. The use of glycorandomization to improve the **activity** of these compds. has been relatively underexplored, due in part to the difficulties assocd. with deoxy-sugar oligosaccharide synthesis. Among the challenges assocd. with the construction of these mols. is the instability of many deoxy-sugar donors. One way to overcome these challenges is by using stable sugar donors, such as thioglycosides. The construction of thioglycosides frequently requires the use of harsh conditions, however,...

2. Separation of the active components from nereis virens and the mechanism of action against a375 cell

Quick View | Other Sources

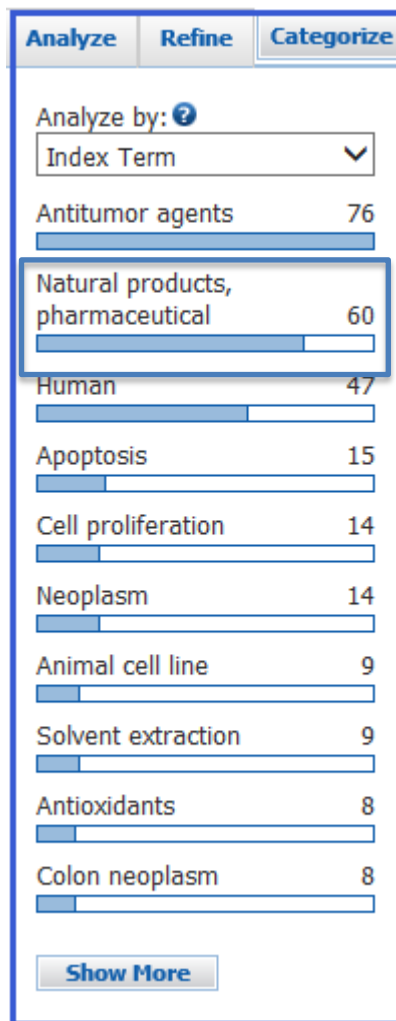
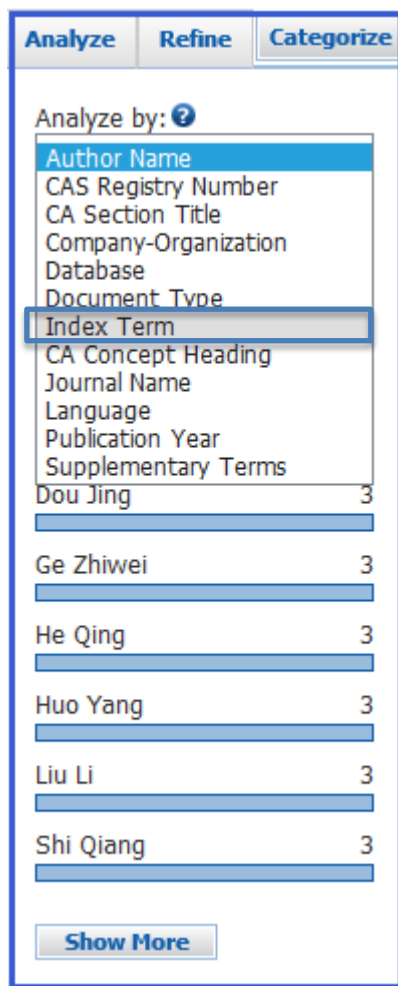
By Zhang, Rong-sheng; Li, Feng; Li, Yun-lei; Zheng, Yun-quan; Guo, Yang-hao

From Yaowu Shengwu Jishu (2014), 21(5), 402-405. | Language: Chinese, Database: CAPLUS

For the research of the vitro **antitumor activity** and mechanism of Nereis virens exts., the freeze-dried powder of Nereis virens, a kind of marine annelid, was leached with ethanol and extd. with Et acetate, and finally the ext. A<sub>1</sub> was obtained. B<sub>1</sub> was sepd. by silica gel column by segmented gradient elution, among which B<sub>4</sub> that was eluted with petroleum ether/ethyl acetate(V/V 3:7) had a good **anti-tumor activity**. By using preparative HPLC, B<sub>4</sub> underwent a further gradient elution and five **components** of C<sub>4</sub> were obtained. By MTT assay, **component** C<sub>4</sub> had a significant effect to impede A375 cell ...

3. Screening method and application of multi-target anti-tumor traditional chinese medicine active ingredient [Machine Translation]

# 利用Index Term选词



Index Term基于内容的分析工具，发现natural products, Pharmaceutical这个词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

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Opened saved answer set "Autosaved Reference Set" (121)

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

新的检索式：  
Natural Product with anti cancer

SciFinder®

Preferences | SciFinder Help ▾ Sign Out

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner

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

REFERENCES ⓘ

Select All Deselect All

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 18 references were found containing "Natural Product with anti cancer" as entered.	18
<input checked="" type="checkbox"/> 8748 references were found containing the two concepts "Natural Product" and "anti cancer" closely associated with one another.	8748
<input type="checkbox"/> 38174 references were found where the two concepts "Natural Product" and "anti cancer" were present anywhere in the reference.	38174
<input type="checkbox"/> 410633 references were found containing the concept "Natural Product".	410633
<input type="checkbox"/> 1110376 references were found containing the concept "anti cancer".	1110376

Get References

更换检索词后，结果放大了70倍

# STN中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



# STN中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

The screenshot displays the SciFinder interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, the breadcrumb path reads 'Substance Identifier "7722-84-1" > substances (1)'. A left sidebar contains a 'REFERENCES' section with a search dropdown menu. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and shows a search input field containing 'purify of 7722-84-1'. Below the input field, there are 'Examples:' listed as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A second screenshot is overlaid on the bottom right, showing a 'SUBSTANCES' section with a search for 'Research Topic "purify of 7722-84-1"'. This overlay shows a 'REFERENCES' section with a 'Select All Deselect All' button and a list of '1 of 4 Research Topic Candidates Selected':

- 2126 references were found containing the two concepts "purify" and "7722-84-1" closely associated with one another.
- 17336 references were found where the two concepts "purify" and "7722-84-1" were present anywhere in the reference.
- 2457989 references were found containing the concept "purify".
- 271782 references were found containing the concept "7722-84-1".

A 'Get References' button is located at the bottom of the overlay.

# 巧用CAS Role

## 1. A method for a kind of tailwater cascade oxidation depth purification [Machine Translation].

By: Liu, Fuqiang; Luo, Kun; Shuang, Chendong; Hu, Dabo; Zhao, Wei; Jiang, Bicun; Yan, Tingting; Li, Jianhua; Li, Aimin  
Assignee: Nanjing University, Peop. Rep. China

[Machine Translation of Descriptors]. The invention discloses a kind of biochem. oxidn. cascade tail water depth purifn. method, belongs to biochem. tail water depth treatment tech. field. The present invention firstly adopts ferrous and hydrogen peroxide to carry out oxidn. to participate in the pre-oxidn., then using subsequent preliminary sedimentation stage when pH is 2.5~ 6 formed on iron mud waste water adsorption and flocculation, remove part of org. and inorg. phosphorus, Reduce photocatalytic oxidn. strengthen weakened section of org. and inorg. phosphorus load impact; further use of catalytic oxidn. depth to remove orgs., strengthen the subsequent secondary sedimentation stage pH as 6-9, the formation of iron mud back to pre-oxidn. section, as a catalyst recycling, reduce medicine consumption and low sludge amt. The present invention also play the pre-oxidn. zone hydroxyl free radical reaction is quick and has broad-spectrum resistance characteristics, and effectively utilizes neutralization pptn. when different pH scope formed iron mud adsorption characteristics and catalytic activity, significantly improves the reaction efficiency, low reagent consumption, and effectively realize the recycling of iron mud.

### Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 106007080	A		Oct 12, 2016	CN 2016-10521105	Jul 1, 2016

### Priority Application

CN 2016-10521105	Jul 1, 2016
------------------	-------------

### Indexing

Waste Treatment and Disposal (Section60)

### Concepts

Adsorption  
Sludges

Recycling  
pH

a method for a kind of tailwater cascade oxidn. depth purifn. [Machine Translation].

### Substances

1333-74-0 Hydrogen 🔍

7439-89-6 Iron 🔍

7722-84-1 Hydrogen peroxide (H2O2) 🔍



7723-14-0 Phosphorus 🔍

a method for a kind of tailwater cascade oxidn. depth purifn. [Machine Translation].

Pollutant; Removal or disposal; Occurrence; Process

## 噪音信息

# 巧用CAS Role

CAS Solutions ▼ Preferences | SciFinder Help ▼ Sign Out

**SCIFINDER**  
A CAS SOLUTION

Welcome Helen Zhu

Explore ▼ | Saved Searches ▼ | SciPlanner | Save | Print | Export

Research Topic "purify of 7722-84-1" > **references (2126)** > Method for preparing light wei...

REFERENCES ?

Get Substances | Get Reactions | Get Related | Task

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Accession Number ▼ ↓

0 of 2126 References Selected \* Required

Analyze by: ?

Author Name ▼

Jiang Wenlan	30
Xu Qinghua	30
Xu Shengying	30
Yuan Changbing	30
Yuan Xin	28
Kagawa Kenkichi	23
Odo Tsunahiro	18
Saito Tomomi	18
Tanaka Toshio	18
Mabuchi Kimihiro	12

21. **Zinc oxide concentrate purification**  
PATENTPAK ▼  
By Yu, Qiongpeng  
From Faming Zhuanli Shenqing (2016), CN 105...  
The present invention discloses a zinc oxide concentrate purification method, comprising: evaporation and concentration, the preparation of pre-precipitation solution, the precipitation, the filtration, the washing, the drying, the calcination, the grinding, the sieving, the packaging, the storage, the transportation, the use, the iron removal by oxidation, demanganization, heavy metal removal, and the like. The present invention has a simple process, mild reaction conditions, and high product uniformity, low energy consumption, and low cost.

22. **Systematic comparison of conventional and novel purification methods for single-walled carbon nanotubes**  
By Clancy, Adam J.; White, Edward R.; Tay, Hu  
From Carbon (2016), 108, 423-432. | Language: English  
As-synthesized single-walled carbon nanotubes (SWCNTs) contain various impurities, including residual catalyst particles. These contaminants have a detrimental effect on the effective mechanism and electrical properties of SWCNTs. This paper reports a systematic comparison of SWCNT purifications including acid treatments, oxidative treatments, and other methods. The results show that the oxidative treatment is the most effective method for SWCNT purification. Each of the purification procedures was evaluated based on the yield, purity, and the effect on the properties of SWCNTs.

23. **Method for preparing light weight high-efficient supported photocatalyst for air purifier**  
PATENTPAK ▼  
By Yang, Lixin  
From Faming Zhuanli Shenqing (2016), CN 105797705 A 20160727. | Language: Chinese, Database: CAPLUS  
The title method comprises immersing photocatalyst hydrosol by a light weight carrier, and preparing light weight high-efficient supported photocatalyst for air purifier. The preparation method comprises: preparing photocatalyst hydrosol, preparing light weight carrier, immersing photocatalyst hydrosol by light weight carrier, and preparing light weight high-efficient supported photocatalyst for air purifier.

### Save This Answer Set

**Save:**

All answers

Only selected answers

**Title: \***

purify of H2O2




**Description:**

OK Cancel

# 巧用CAS Role

0 of 1 Substance Selected

1. 7722-84-1

~222048   ~190 

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:

- |   |   |
|---|---|
| <input type="checkbox"/> Adverse Effect, including toxicity | <input checked="" 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 type="checkbox"/> Uses                   |
| <input type="checkbox"/> Occurrence                         |   |

### 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

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 (14672)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools

Analyze | Refine | Categorize | Sort by: Accession Number | Remove Duplicates | Combine Answer Sets | Add Tag | Display Options

0 of 14672 References Selected

Analyze by: Author Name

Hutchings Graham J 49  
Wang Erzhong 45  
Wang Li 40  
Edwards Jennifer K 39  
Carley Albert F 36  
Kornienko V L 31  
Yamanaka Ichiro 31  
Mi Zhentao 30  
Kiely Christopher J 28  
Brillas Enric 27

1. Hydrogen peroxide working solution continuous preparation apparatus [Machine Translation].  
By Li, Wanqing; Zhou, Xu  
From Shiyong Xinxing Zh...

2. Immobilization of D-amino acid oxidase immobilized on mu... oxidative deaminat...

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (14672):

Reference Answer Set Details	Date Saved
<input checked="" type="checkbox"/> purify of H2O2 (2126) Research Topic "purify of 7722-84-1" > references (2126)	Oct 19, 2016
<input type="checkbox"/> remove 6 (6) Research Topic "remove of 123-39-7" > references (49) > refine by categories	Oct 19, 2016
<input type="checkbox"/> purify of 7722-84-1 (2124) Research Topic "purify of 7722-84-1" > references (2124)	Oct 17, 2016
<input type="checkbox"/> remove 123-39-7 (9) (9) Substance Identifier "123-39-7" > substances (1) > get references (384) > Combine Reference Answer Sets "remove DMF 49 (49)" (9)	Oct 17, 2016

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 (14672)** that are not in **purify of H2O2 (2126)**
- Exclude** Include only answers from **purify of H2O2 (2126)** that are not in **current answer set (14672)**

Combine Answer Sets | Cancel

on. app. comprises at least one 2-  
er sepg. tank. 2-Ethylanthraquinone  
yl phosphate, salt-removed water,  
e prepn. of the working fluid loop

AAO and ELP-CAT have been sep.  
reserved. ELP-DAAO catalyzed the  
nerated hydrogen peroxide of ELP-



# 巧用CAS Role

CAS Solutions Preferences | SciFinder Help | Sign Out

**SciFinder**  
A CAS SOLUTION

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Substance Identifier "7722-84-1" > substances (1) > get references (14672) > Combine Reference Answer Sets "purify of H2O2 (2126)" (305)

REFERENCES Create Keep Me Posted Alert | Send to SciPlanner

Get Substances | Get Reactions | Get Related Citations | Tools

Analyze | Refine | Categorize | Sort by: Accession Number | Display Options

0 of 305 References Selected | Page: 1 of 16

Analyze by: Author Name

Tanaka Fujio	7
Minamikawa Yoshitsugu	6
Murakami Shinichi	6
Kajiwara Shoichiro	5
Nagai Kazunori	5
Gao Weiping	4
Kaga Tadayoshi	4
Kokubu Jun	4
Luan Guoyan	4
Murakami Seishi	4

- Hydrogen peroxide purification adsorbent preparation method**  
Quick View PATENTPAK  
By Wang, Qiyu  
From Faming Zhuanli Shenqing (2016), CN 105749877 A 20160713. | Language: Chinese, Database: CAPLUS  
The invention relates to a hydrogen peroxide purifn. adsorbent prepn. method. The method comprises: using o-fluorobenzoyl group modification to obtain composite functional resin, introducing strong-withdrawing electron group 4-fluorobenzoyl Me to form antioxidant group to improve the life of the resin in the hydrogen peroxide oxidn. conditions, and introducing fluorine-contg. group to enhance corrosion resistance of the resin skeleton. The sphere surface is protected, thus extending the life.
- Device and method for generating oxidants in situ for water purifn.**  
Quick View PATENTPAK  
By Xia, Zijun; Sui, Caroline Chihyu; Xu, Yida; Zhang, Xing; Huang, Qunjian; Vasconcellos, Stephen Robert; Salerno, Michael Brian  
From PCT Int. Appl. (2016), WO 2016106630 A1 20160707. | Language: Chinese, Database: CAPLUS  
A method of reducing the org. compds. in an aq. stream by generating an oxidant in-situ using  $\geq 1$  electrolytic cell. The method may comprise contacting at least a portion of the aq. stream with the electrolytic cell. The electrolytic cell may have  $\geq 2$  electrodes, in which  $\geq 1$  electrode is a metal electrode and, a power source for powering the  $\geq 2$  electrodes. A H<sub>2</sub>O treatment system for generating an oxidant in-situ comprising  $\geq 1$  electrolytic cell. The electrolytic cell may have  $\geq 2$  electrodes, in which  $\geq 1$  electrode is a metal electrode, and a power source for powering the  $\geq 2$  electrodes. A metho...
- Residue purification recovery device**  
Quick View PATENTPAK  
By Li, Wanqing; Zhou, Xuejun; Liu, Jiqian; Gao, Chuanning; She, Linyuan  
From Faming Zhuanli Shenqing (2016), CN 105565275 A 20160511. | Language: Chinese, Database: CAPLUS  
The title residue purifn. recovery device comprises a separator, an intermediate tank, a recovery tank, a cooler, a refined canister, a

浏览记录，判断是否符合要求

# 巧用CAS Role


## 1. Hydrogen peroxide purification adsorbent preparation method

By: Wang, Qiyu  
Assignee: Wang, Jinming, Peop. Rep. China

The invention relates to a hydrogen peroxide purifn. adsorbent prepn. method. The method comprises: using o-fluorobenzoyl group modification to obtain composite functional resin, introducing strong-withdrawing electron group 4-fluorobenzoyl Me to form antioxidant group to improve the life of the resin in the hydrogen peroxide oxidn. conditions, and introducing fluorine-contg. group to enhance corrosion resistance of the resin skeleton. The sphere surface is protected, thus extending the life.

### Patent Information

Patent No.	Kind	Language	Date
CN 105749877	A		Jul 13, 2016
<b>Priority Application</b>			
CN 2015-10852280			Nov 26, 2015

7722-84-1P Hydrogen peroxide, preparation  Page 2 in **PATENTPAK**

hydrogen peroxide purifn. adsorbent prepn. method


Purification or recovery; Preparation

## 8. Method of purifying hydrogen peroxide using reverse osmosis membrane and ion exchangers

By: Myung, Jung Jae  
Assignee: Dongwoo Fine-Chem Co., Ltd., S. Korea

The invention relates to a method of purifying H<sub>2</sub>O<sub>2</sub> by using a reverse osmosis membrane which is a C nanomaterial-coated porous polymer scaffolds, an anion exchange resin and a cation exchange resin. More specifically, the invention relates to a method of purifying H<sub>2</sub>O<sub>2</sub> characterized by passing H<sub>2</sub>O<sub>2</sub> through a cation exchange resin and an anion exchange resin after passing through a reverse osmosis membrane coated with C nanomaterials over porous polymer scaffolds.



7722-84-1P Hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>), preparation  Page 2 in **PATENTPAK**

method of purifying hydrogen peroxide using reverse osmosis membrane and ion exchangers

Purification or recovery; Preparation

都是需要的文献

# 善用Categorize去除噪音信息

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去除噪音信息

去除N-甲基甲酰胺（123-39-7）

The screenshot displays the SciFinder interface. At the top, there are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". On the left, a sidebar menu is open, showing "REFERENCES" and "SUBSTAN" categories. Under "REFERENCES", options include "Research Topic", "Author Name", "Company Name", "Document Identifier", "Journal", "Patent", and "Tags".

The main content area is titled "REFERENCES: RESEARCH TOPIC". A search input field contains the text "remove of 123-39-7". Below the input field, there are "Examples:" listed as "The effect of antibiotic residues on dairy products" and "Photocyanation of aromatic compounds".

A second window or overlay is shown in the foreground, also with the same navigation tabs. It displays the search results for the query "Research Topic 'remove of 123-39-7'". The results are categorized under "REFERENCES". There are "Select All" and "Deselect All" buttons. Below these, it states "1 of 4 Research Topic Candidates Selected". A list of four candidates is shown, each with a checkbox:

- 49 references were found containing the two concepts "remove" and "123-39-7" closely associated with one another.
- 264 references were found where the two concepts "remove" and "123-39-7" were present anywhere in the reference.
- 2808271 references were found containing the concept "remove".
- 4512 references were found containing the concept "123-39-7".

At the bottom of this overlay, there is a "Get References" button.

# 善用Categorize去除噪音信息

## 1. Removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

By: Wang, Wenzheng; Fan, Xing; Zhu, Tianle; Wang, Haining; Ye, Daiqi; Hong, Xiaowei

Dimethylamine (DMA) and N,N-dimethylformamide (DMF) are typical N-VOCs exhausted from manufg. factories. In the present study, the behavior of non-thermal plasma (NTP) was systematically investigated for removal of gas-phase DMA and DMF in a link tooth wheel-cylinder plasma reactor. Exptl. results show that DMA is much easier to be decompd. by NTP than DMF. Coexisting DMF has no effect on DMA conversion while DMF conversion is significantly promoted by the addn. of DMA. Regardless of initial gas compns. as well as DMA and DMF concn., CO<sub>x</sub> selectivity increased monotonously with increasing ED. But CO<sub>x</sub> selectivity of 100% cannot be obtained even with ED higher than 70 J L<sup>-1</sup>, indicating the formation of org. intermediates during DMA and DMF decompn. Based on org. products anal. with GC-MS and mol. optimization results with d. functional theory calcn., possible mechanisms on DMA and DMF degrdn. were proposed. The org. products from DMA and DMF decompn. by NTP were found to have great soly. and high biodegradability. Thus, NTP enhanced absorption/biol. method is suggested for complete removal of DMA and DMF.

### Indexing

Air Pollution and Industrial Hygiene (Section59-4)

### Concepts

Absorption	Air pollution control
Bond energy	Bond length
Decomposition	Decomposition catalysts
Plasma	Waste gas treatment

removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

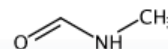
Volatile organic compounds

removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

Removal or disposal; Process

### Substances

56-40-6 Glycine, formation (nonpreparative) 🔍  
64-18-6 Formic acid, formation (nonpreparative) 🔍  
75-12-7 Formamide, formation (nonpreparative) 🔍  
79-20-9 Methyl acetate 🔍  
105-37-3 Ethyl propionate 🔍  
107-31-3 Methyl formate 🔍  
123-39-7 N-Methyl formamide 🔍



144-62-7 Oxalic acid, formation (nonpreparative) 🔍

removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

Formation, unclassified; Formation, nonpreparative

需要的文献

# 善用Categorize去除噪音信息

## 3. Removing agent containing alkylamide mixture

By: Li, Bo; Yu, Ran

Assignee: Qingdao Hui Cheng Petrochemical Technology Co., Ltd., Peop. Rep. China

The present invention relates to a kind of alkylamide removing agent. The removing agent comprises N-methylformamide 50-70 wt.%, N, N-dimethyl acetamide 30-50 wt.% and water as balance. The alkylamide removing agent of the present invention has water compatibility, and has no corrosivity for copper or copper alloy, and is generally nontoxic to mankind and environment. Because the constituent of alkylamide removing agent only comprises two main constituents, the removing agent after use can be easily by fractionation and recombine to original formula, and can be recycled to apply in the prepn. process to achieve the effect of reducing cost and environmental protection. The present invention also provides a method of using the removing agent of the present invention to remove photoresist.

### Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 104698775	PATENTPAK	A	Jun 10, 2015	CN 2013-10646205	Dec 4, 2013

### Priority Application

CN 2013-10646205	Dec 4, 2013
------------------	-------------

### Indexing

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (Section74-5)

### Concepts

Coating removers	Photoresists
removing agent contg. alkylamide mixt.	
Amides	
removing agent contg. alkylamide mixt.	
Other use, unclassified; Physical, engineering or chemical process; Process; Uses	

### Substances

123-39-7 N-Methylformamide	
127-19-5 N, N-Dimethyl acetamide	
removing agent contg. alkylamide mixt.	
Other use, unclassified; Physical, engineering or chemical process; Process; Uses	

噪音信息更多，如何去除？

# 善用Categorize去除噪音信息

CAS Solutions Preferences | SciFinder Help | Sign Out

**SCIFINDER**  
A CAS SOLUTION

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner Save | Print | Export

Research Topic "remove of 123-39-7" > **references (49)** > Removing agent containing alky...

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 49 References Selected

Analyze by: Author Name

Author Name	
Egbe Matthew I	4
Hara Yasushi	4
Takahashi Fumiharu	4
Bang Sun Hong	2
Hong Heon Pyo	2
Legenza Michael Walter	2
Ward Irl E	2
Albrecht Herbert	1
Alsters Paul	1
Aoba Kazuhiro	1

- Removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma**  
By Wang, Wenzheng; Fan, Xing; Zhu, Tianle; Wang, Haining; Ye, Daiqi; Hong, Xiaowei  
From Chemical Engineering Journal (Amsterdam, Netherlands) (2016), 299, 184-191. | Language: English, Database: CAPLUS  
Dimethylamine (DMA) and N,N-dimethylformamide (DMF) are typical N-VOCs exhausted from manufg. factories. In the present study, the behavior of non-thermal plasma (NTP) was systematically investigated for **removal** of gas-phase DMA and DMF in a link tooth wheel-cylinder plasma reactor. Exptl. results show that DMA is much easier to be decompd. by NTP than DMF. Coexisting DMF has no effect on DMA conversion while DMF conversion is significantly promoted by the addn. of DMA. Regardless of initial gas compons. as well as DMA and DMF concn., CO<sub>2</sub> selectivity increased monotonously with increasing E...
- Stripping composition for removing photoresist and a method, for peeling photoresist, using same**  
By Park, Tae Moon; Jung, Dae Chul; Lee, Dong Hoon; Lee, Woo Ram; Lee, Hyun Jun; Kim, Ju Young  
From PCT Int. Appl. (2016), WO 2016027985 A1 20160225. | Language: Korean, Database: CAPLUS  
The present invention relates to a stripping compn. for **removing** a photoresist and a method, for peeling a photoresist, using same, the stripping compn. comprising: one or more amine compds.; an amide-based compd. substituted with one or two of C1-5 straight or branched alkyl groups; a polar org. solvent; a particular triazole-based compd.; and a benzimidazole-based compd.
- Removing agent containing alkylamide mixture**  
By Li, Bo; Yu, Ran  
From Faming Zhuanli Shenqing (2015), CN 104698775 A 20150610. | Language: Chinese, Database: CAPLUS  
The present invention relates to a kind of alkylamide **removing** agent. The **removing** agent comprises N-methylformamide 50-70 wt.%, N, N-dimethyl acetamide 30-50 wt.%

# 善用Categorize去除噪音信息

**Categorize** ⓘ

1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in technology (824)	<b>Select All</b> <b>Deselect All</b>	Click 'x' to remove the category from 'Selected Terms'
<b>Technology</b>	<b>Formed, removed, &amp; other substances (61)</b>	<input checked="" type="checkbox"/> N-Methyl formamide   6	<input checked="" type="checkbox"/> Technology > Formed, removed, & other substances (1 Terms)
General chemistry	Materials & products (76)	<input type="checkbox"/> N,N-Dimethylformamide   3	
Physical chemistry	Metallurgy (45)	<input type="checkbox"/> Copper   2	
Biotechnology	Processes & apparatus (35)	<input type="checkbox"/> Copper alloy   2	
Polymer chemistry	Imaging & recording (4)	<input type="checkbox"/> Dimethylamine   2	
Environmental chemistry	Power & fuel topics (5)	<input type="checkbox"/> Formamide   2	
Synthetic chemistry	Ceramics (2)	<input type="checkbox"/> Oxides (inorganic)   2	
Catalysis	Construction (2)	<input type="checkbox"/> Polyimides   2	
Genetics & protein chemistry		<input type="checkbox"/> 1-Fluoro-1,2,2-trichloroethane   1	
Biology		<input type="checkbox"/> 2,3-Dimethyl-1-butanol   1	
Analytical chemistry		<input type="checkbox"/> 2,4-Di-tert-butylphenol   1	
		<input type="checkbox"/> 2,6-Di-tert-butyl-1,4-benzoquinone   1	
		<input type="checkbox"/> 2-(Methyl mercapto)benzothiazole   1	

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

OK   Cancel



# 提纲

- SciFinder物质检索难点解析
  - 快速获得物质的生物活性及靶点信息
  - 无机物及合金的检索
  - 聚合物的检索
  - 检索具有相同结构特征物质及专利文献
  - 如何判断结构的新颖性

# 物质检索方法

- 功能方面

- 结构式
- 分子式
- 理化性质
- 物质名称, CAS No

SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

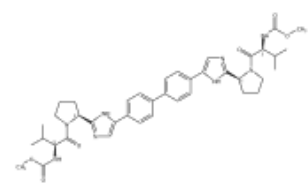
- 推荐的物质检索功能

- 有机物、天然产物及衍生物: 结构检索比较方便
- 无机物、合金: 分子式检索比较方便
- 高分子化合物: 优先分子式检索, 其次结构检索

# 快速获得物质的生物活性及靶点信息

1. 1009119-64-5

~308 ~88



Absolute stereochemistry.

**C<sub>40</sub> H<sub>50</sub> N<sub>8</sub> O<sub>6</sub>**  
Carbamic acid, *N,N*-[[[1,1'-biphenyl]-4,4'-diylbis[1*H*-imidazole-5,2-diyl-(2*S*)-2,1-pyrrolidinediyl][(1*S*)-1-(1-methylethyl)-2-oxo-2,1-ethanediy]]]bis-, *C,C'*-dimethyl ester

► **Key Physical Properties**  
Regulatory Information

Analyze Refine

Analyze by:   
Target Indicators

Cytokines (all)	1
Enzymes (all)	1
Interferons (all)	1
Proteins	1
Viral proteins (all)	1

Show More

作用靶点

Analyze Refine

Analyze by:   
Bioactivity Indicators

Anti-infective agents (all)	1
-----------------------------	---

Show More

生物活性

# 无机物及合金的检索

## 分子式书写规则—Hill 规则

### ■ 单一组分物质：

- 对于不含C的物质，按照字母顺序排序
- 对于含C的物质，C、H写在前面，其他的按照字母顺序排列
- 相邻的两个元素之间必须有区分号，即数字或者空格，倘若数字为1，那么可以用空格来区分
- 区分大小写

### ■ 多组分物质：

- 每一组分必须遵照单一组分物质的分子式来书写。
- 不同组分之间的排序按照各组分的首元素的字母顺序排序，但是含C组分的一定排在不含C的组分前面。**用点将不同的组分分开**
- 倘若不同组分的首元素相同，则看元素数量多少，数量多的排在前面，若元素数量一样，则按次元素的顺序排列。

# 无机物及合金的检索

## 检索铁、锰、镍合金

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' options. The main search area shows the molecular formula 'Fe . Mn . Ni' and a search for 'substances (1095)'. The results are sorted by 'CAS Registry Number' and show 0 of 1095 substances selected. A left sidebar contains a 'REFERENCES' section with various filters and a 'SUBSTANCES' section with a bar chart showing the distribution of substances across different categories.

The search results are presented in a grid format, with each entry showing the CAS Registry Number and a table of components and their percentages. For example, entry 1 (CAS 1850365-63-7) shows Fe at 80%, Mn at 16%, and Ni at 5%. Entry 2 (CAS 1835656-90-0) shows Fe at 92%, Ni at 8.3%, and Mn at 0.1%. Entry 3 (CAS 1835656-89-7) shows Fe at 91%, Ni at 8.4%, and Mn at 0.1%. Entry 4 (CAS 1821204-48-1) shows Mn at 60%, Ni at 25%, and Fe at 15%. Entry 5 (CAS 1818872-06-8) shows Fe at 65%, Ni at 35%, and Mn at 0.5%. Entry 6 (CAS 1816304-50-3) shows Ni at 72%, Mn at 25%, and Mn at 2.9%.

合金物质以列表形式呈现

# 无机物及合金的检索

检索参杂铁、锰、镍原子的合金

Structure Editor: Draw or change atoms or bonds. Shortcuts Keys

Drawing Editor:  
● Structure  
○ Reaction  
○ Markup

Get substances that match your query using:  
● Exact search  
○ Substructure search  
○ Similarity 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

SciFinder®  
Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Chemical Structure exact with limiters > substances (201704)

STANCES  Get References  Get Reactions  Get Commercial Sources  Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine

Sort by: CAS Registry Number

0 of 201704 Substances Selected

Page: 1 of 13447

1. 1873378-35-8

Component	Component Percent
Fe	35 - 96
Cr	0 - 25
Ni	0 - 20
Mo	0 - 6
Si	3.1 - 4.4
Mn	0 - 4
Al	0 - 2
Cu	0 - 2
C	0.4 - 0.6
V	0 - 0.5
Nb	0 - 0.2

C . Al . Cr . Cu . Fe . Mn . Mo . Ni . Si . V  
INDEX NAME NOT YET ASSIGNED

2. 1873377-37-7

Component	Component Percent
Fe	84 - 96
Si	3.1 - 4.4
Cr	0 - 4
Al	0 - 2
Cu	0 - 2
Ni	0 - 2
C	0.4 - 0.6
Mn	0 - 0.4
Mo	0 - 0.3
V	0 - 0.3

C . Al . Cr . Cu . Fe . Mn . Mo . Ni . Si . V  
INDEX NAME NOT YET ASSIGNED

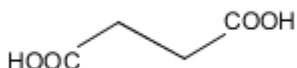
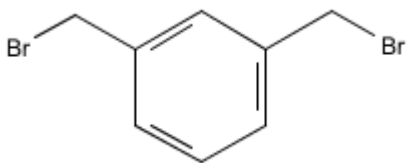
3. 1873338-63-6

Component	Component Percent
Fe	78 - 85
Cr	8 - 12
Mn	2 - 3
Mo	1.5 - 2
La2O3	1.3 - 1.9
Ni	0.8 - 1.2
Si	0.5 - 1
V	0.3 - 0.6
C	0.4
Nb	0 - 0.2

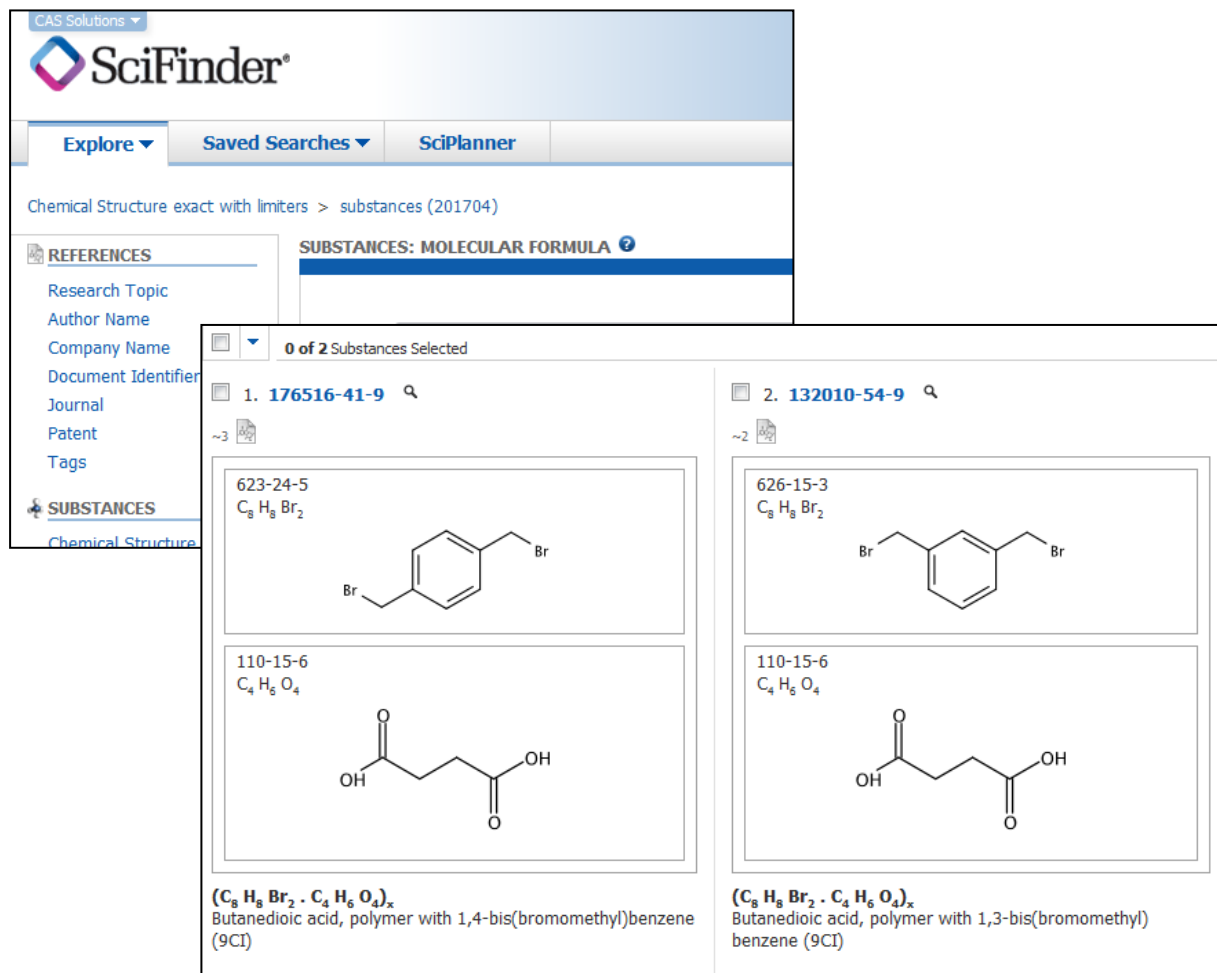
C . Cr . Fe . La<sub>2</sub>O<sub>3</sub> . Mn . Mo . Nb . Ni . Si . V  
INDEX NAME NOT YET ASSIGNED

# 聚合物的检索

已知起始原料的聚合物



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

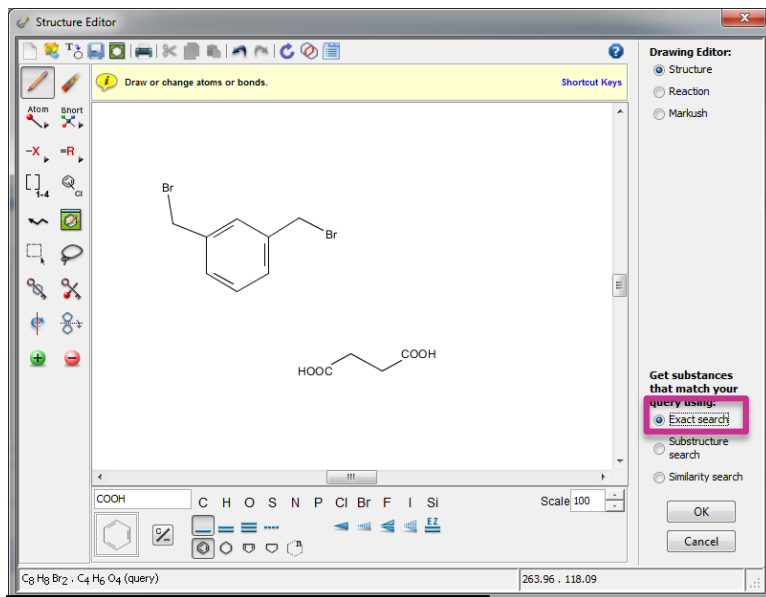


The screenshot displays the SciFinder interface. The search criteria are "Chemical Structure exact with limiters" and "substances (201704)". The search results are categorized under "SUBSTANCES: MOLECULAR FORMULA". Two results are shown:

- Result 1: 176516-41-9. Molecular formula:  $C_8 H_8 Br_2$ . Structure: 1,4-bis(bromomethyl)benzene. Polymer description:  $(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$  Butanedioic acid, polymer with 1,4-bis(bromomethyl)benzene (9CI).
- Result 2: 132010-54-9. Molecular formula:  $C_8 H_8 Br_2$ . Structure: 1,3-bis(bromomethyl)benzene. Polymer description:  $(C_8 H_8 Br_2 \cdot C_4 H_6 O_4)_x$  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



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

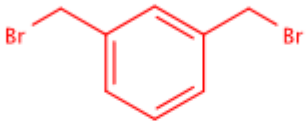
聚合物

0 of 1 Substance Selected

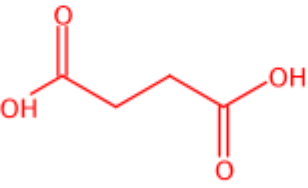
1. **132010-54-9** 🔍

~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>

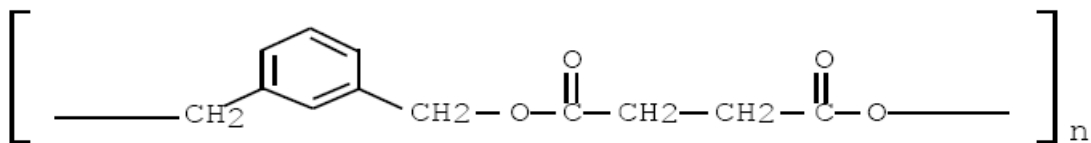


**(C<sub>8</sub>H<sub>8</sub>Br<sub>2</sub> · C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>)<sub>x</sub>**  
 Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene  
 (9CI)



# 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>

SciFinder®  
Molecular Formula "(C<sub>12</sub> H<sub>12</sub> O<sub>4</sub>)<sub>n</sub>" > substances (45)

Sort by: CAS Registry Number

0 of 45 Substances Selected

Index	CAS Registry Number	Chemical Name	Molecular Formula
1	1801551-81-4	[Structure]	(C <sub>12</sub> H <sub>12</sub> O <sub>4</sub> ) <sub>n</sub> INDEX NAME NOT YET ASSIGNED
2	1637772-98-5	Poly[oxy-1,4-butanediolyloxycarbonyl(1,4-phenylene-2,3,5,6- <i>d</i> )carbonyl]	(C <sub>12</sub> H <sub>8</sub> D <sub>4</sub> O <sub>4</sub> ) <sub>n</sub>
3	1421756-46-8	Poly[oxy[( <i>R</i> )-phenyl-1,2-ethanediy]oxy(1,4-dioxo-1,4-butanediyl)]	(C <sub>12</sub> H <sub>12</sub> O <sub>4</sub> ) <sub>n</sub>
4	1392419-56-5	[Structure]	
5	1353713-96-8	Substance Image	
6	1341223-97-9	Substance Image	

# 聚合物的检索

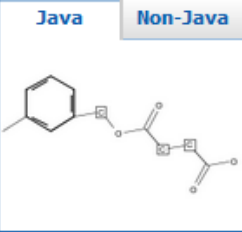
Analyze Refine

Refine by: ?

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

Structure Editor:


Java Non-Java

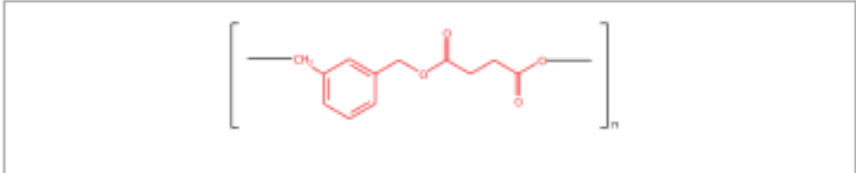


Click image to change structure or view detail.  
Search type: **Substructure**

0 of 1 Substance Selected

1. **132010-11-8** 🔍

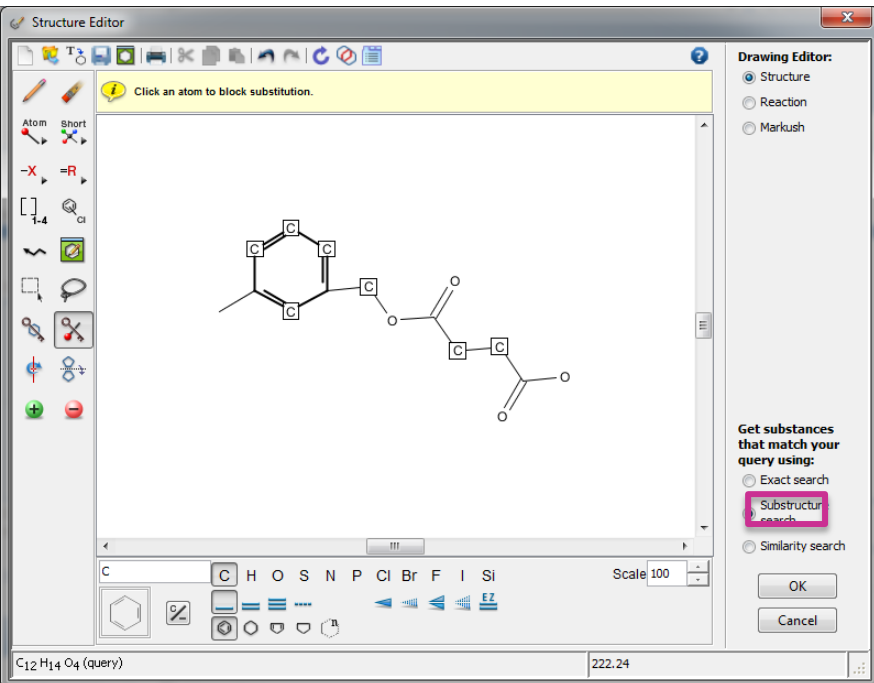
~2 



**(C<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)

利用结构特征进行Refine，迅速查找需要的物质

# 聚合物的检索



单一组分

聚合物

绘制好SRU后用亚结构检索  
因为两段为开放状态

0 of 1 Substance Selected

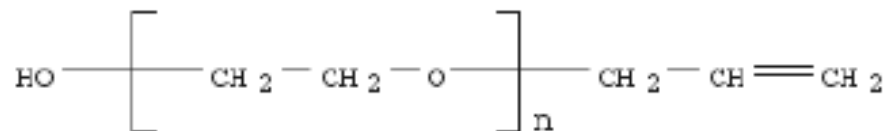
1. 132010-11-8

~2

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

# 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

$(\text{C}_2 \text{H}_4 \text{O})_n \text{C}_3 \text{H}_6 \text{O}$

Examples:  
H4SiO4  
 $(\text{C}_3\text{H}_6\text{O} \cdot \text{C}_2\text{H}_4\text{O})_x$

Search

$(\text{C}_2 \text{H}_4 \text{O})_n \text{C}_3 \text{H}_6 \text{O}$

SRU部分 两端部分

0 of 4 Substances Selected

1. 1500029-22-0

$(\text{C}_2 \text{H}_4 \text{O})_n \text{C}_3 \text{H}_6 \text{O}$   
Poly(oxy-1,2-ethanediyl),  $\alpha$ -(1-methylethenyl)- $\omega$ -hydroxy-

2. 191403-44-8

$(\text{C}_2 \text{H}_4 \text{O})_n \text{C}_3 \text{H}_6 \text{O}$   
Poly(oxy-1,2-ethanediyl),  $\alpha$ -1-propen-1-yl- $\omega$ -hydroxy-

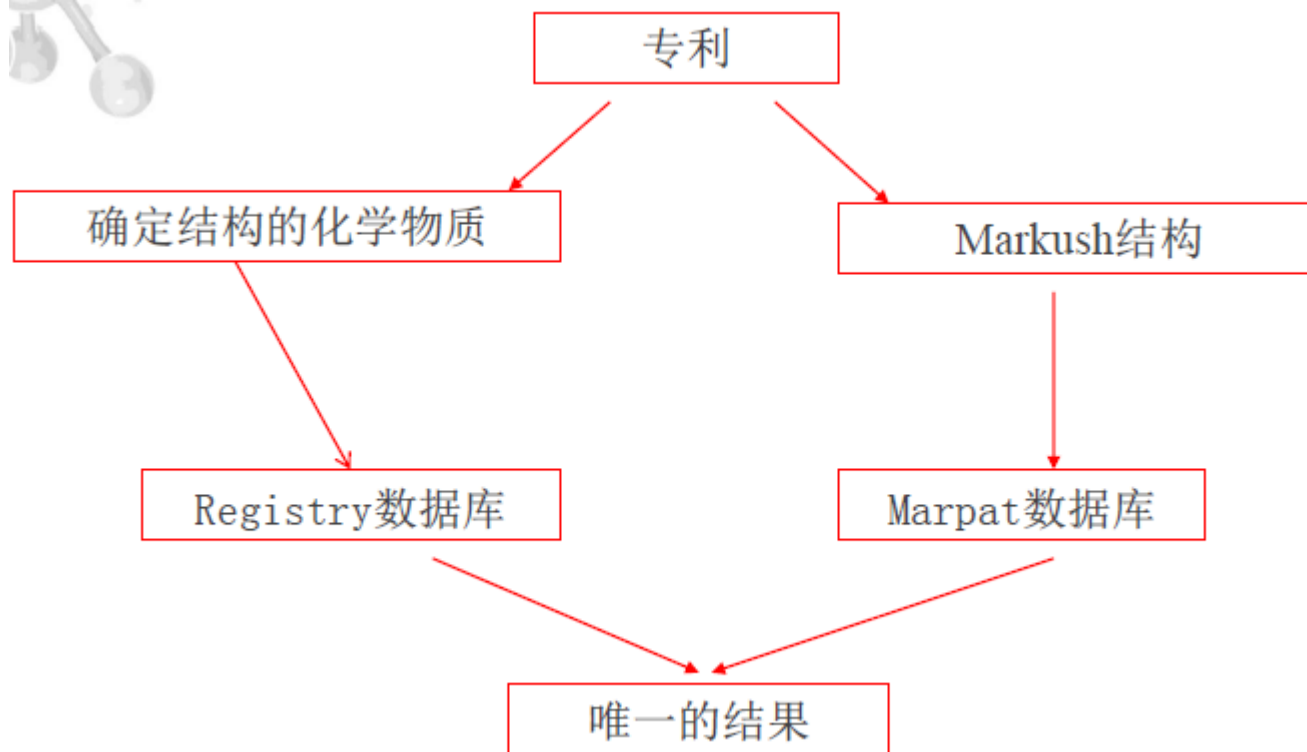
3. 50856-25-2

$(\text{C}_2 \text{H}_4 \text{O})_n \text{C}_3 \text{H}_6 \text{O}$   
Poly(oxy-1,2-ethanediyl),  $\alpha$ -ethenyl- $\omega$ -methoxy-

4. 27274-31-3

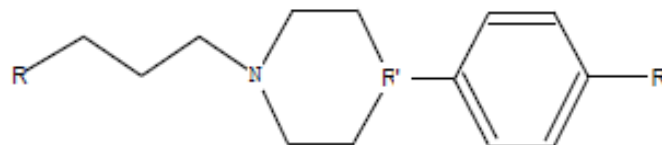
$(\text{C}_2 \text{H}_4 \text{O})_n \text{C}_3 \text{H}_6 \text{O}$   
Poly(oxy-1,2-ethanediyl),  $\alpha$ -2-propen-1-yl- $\omega$ -hydroxy-  
Regulatory Information

# 检索具有相同结构特征物质及专利文献



# 检索具有相同结构特征物质及专利文献

查询报道具有如下结构特征专利文献:



要求:

- R = 任意杂环
- R' = C, N, P
- R'' = C, N
- 6 圆环均为单环
- 价键不饱和的地方均允许有取代

# SciFinder结构编辑器

Structure Editor

橡皮

铅笔

元素周期表

可变基团

重复基团工具

碳链工具

选择工具

环锁定工具

旋转工具

正电子

负电子

常用基团

R基团定义工具

可变位置连接工具

模版工具

索套选择工具

原子锁定工具

镜面旋转工具

单双键, RS构型, 不确定键定义工具

结构检索选择

结构 and 反应切换功能

Drawing Editor:  
 Structure  
 Reaction  
 Markush

Get substances that match your query using:  
 Exact search  
 Substructure search  
 Similarity search

确定  
取消

C原子和单键恢复工具

常见环, 多元环工具

Scale 100

(query)

C H O S N P Cl Br F I Si

SciFinder®  
A CAS Solution

CAS is a division of the American Chemical Society.  
Copyright 2016 American Chemical Society. All rights reserved.

# 检索具有相同结构特征物质及专利文献

The screenshot displays the SciFinder Structure Editor window. The main canvas shows a chemical structure consisting of a piperidine ring substituted with a propyl group (labeled 'Hy') and a phenyl ring (labeled 'R<sub>2</sub>'). The piperidine ring is also labeled with 'R<sub>1</sub>' at the point of attachment to the phenyl ring. The interface includes a toolbar on the left with various drawing tools, a top menu bar, and a right-hand panel with search options. The 'Drawing Editor' panel has 'Structure' selected. The 'Get substances that match your query using:' panel has 'Substructure search' selected. The bottom status bar indicates 'Formula not available'.

Structure Editor

Draw or change atoms or bonds. [Shortcut Keys](#)

Atom Short

-X =R

[ ] 1-4 Cl

Hy R<sub>1</sub> R<sub>2</sub>

Structure Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK

Cancel

Formula not available



# 检索具有相同结构特征物质及专利文献

CAS Solutions

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Chemical Structure substructure > substances (3048)

SUBSTANCES **Get References** Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Sort by: CAS Registry Number

0 of 3048 Substances Selected Page: 1 of 204

Analyze by: Substance Role

Preparation 1682  
Biological Study 1523  
Uses 1288  
Reactant or Reagent 201  
Analytical Study 86  
Properties 70  
Prophetic in Patents 41  
Combinatorial Study 22  
Process 3

Show More

1. **1873376-11-4**  
~1  
  
**C<sub>27</sub>H<sub>38</sub>N<sub>4</sub>O**  
INDEX NAME NOT YET ASSIGNED

2. **1868051-25-5**  
~1  
  
Absolute stereochemistry.  
**C<sub>26</sub>H<sub>26</sub>FN<sub>5</sub>O<sub>4</sub>**  
Benzamide, 4-[4-[(1*S*)-3-(7-fluoro-1,2-dihydro-5-nitro-1-oxo-3-isoquinolinyl)-2-cyclopenten-1-yl]-1-piperazinyl]-*N*-methyl-  
▶ **Key Physical Properties**

3. **1868051-24-4**  
~1  
  
Absolute stereochemistry.  
**C<sub>26</sub>H<sub>26</sub>FN<sub>5</sub>O<sub>4</sub>**  
Benzamide, 4-[4-[(1*R*)-3-(7-fluoro-1,2-dihydro-5-nitro-1-oxo-3-isoquinolinyl)-2-cyclopenten-1-yl]-1-piperazinyl]-*N*-methyl-  
▶ **Key Physical Properties**

4. **1868051-23-3**  
~1

5. **1868051-22-2**  
~1

6. **1868051-02-8**  
~1

# 检索具有相同结构特征物质及专利文献

Chemical Structure substructure > substances (3048) > get references (408)

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 408 References Selected

Page: 1 of 21

Refine by: ⓘ

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

Document Type(s)

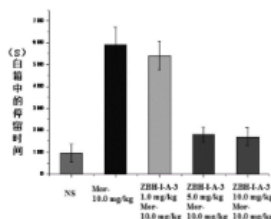
- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent

1. Hexahydro-pyrazino quinolines D3 receptor ligand, preparation method and application thereof

Quick View PatentPak ▾

By Cai, Jin; Ji, Min; Zhou, Benhua

From Faming Zhuanli Shenqing (2016), CN 105294685 A 20160203. | Language: Chinese, Database: CAPLUS



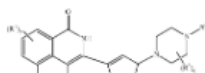
Title compds. I [wherein A = (CH<sub>2</sub>)<sub>n</sub>, n is 2 to 4; R = H, 4-Cl, 2,3-diCl, 4-CH<sub>3</sub>, 2,3-diCH<sub>3</sub>, 4-OCF<sub>3</sub>, 4-OCH<sub>3</sub>, 2-OCF<sub>3</sub>, 2,6-diCH<sub>3</sub>, 3,4-diCH<sub>3</sub>, 3-CF<sub>3</sub>, 4-Cl, 3-OCH<sub>3</sub>, 2-C<sub>2</sub>H<sub>5</sub>, or 2-CH<sub>3</sub>], and their pharmaceutically acceptable salts thereof, were prepd. as D3 receptor ligands, which are used for treating nervous centralis mental disorder such as Parkinson's disease, schizophrenia, drug dependence and etc. effectively. Thus, the invention compd. I [A = (CH<sub>2</sub>)<sub>2</sub>; R = H] was prepd. and gave a D3 receptor K<sub>i</sub> value of 11.7±1.8nM.

2. Isoquinolinone derivatives as PARP inhibitors and their preparation

Quick View PatentPak ▾

By Jana, Gourhari; Sinha, Neelima; Karche, Navnath Popat; Kurhade, Sanjay Pralhad; Tilekar, Ajay Ramchandra; Gupta, Nishant Ramniwasji; Irlapati, Nageswara Rao; Kukreja, Gagan; Palle, Venkata P.; Kamboj, Rajender Kumar

From PCT Int. Appl. (2016), WO 2016012956 A1 20160128. | Language: English, Database: CAPLUS



Disclosed are compds. of formula I, their tautomeric forms, stereoisomers, and pharmaceutically acceptable salts thereof, pharmaceutical compns. including a compd., tautomer, stereoisomer, or salt thereof, and methods of treating or preventing diseases or disorders, for example, cancer, that are amenable to treatment or prevention by inhibiting the PARP enzyme of a subject. Compds. of formula I wherein p is 0, 1 and 2; q is 0, 1, 2, an 3; each R<sup>1</sup> is independently halo, CN, NO<sub>2</sub>, perfluoroalkyl, acyl, e tc.; R<sup>2</sup>

通过DT限定获得专利文献，保存

# 检索具有相同结构特征物质及专利文献

The screenshot displays the SciFinder web interface. At the top, there's a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows search results for 'Markush substructure' with 895 references. A 'Tools' dropdown menu is open, highlighting 'Combine Answer Sets'. On the left, a 'REFERENCES' sidebar lists authors and their counts. Below the search results, three patent entries are visible, each with a brief description of the invention.

Structure Editor

Draw or change atoms or bonds.

Drawing Editor:  
Structure  
Markush

SciFinder®

Explore Saved Searches SciPlanner

Markush substructure > references (895)

REFERENCES

Analyze Refine Categorize

Analyze by: Author Name

Anand Nitya 16

Jain Sanjay 13

Sinha Neelima 13

Unger Liliane 13

Van Broeck Didier 11

Emonds Alt Xavier 10

Proietto Vincenzo 10

Saxena Anil Kumar 10

Starck Dorothea 10

Steiner Gerd 10

Sort by: Accession Number

0 of 895 References Selected

Remove Duplicates

Combine Answer Sets

Add Tag

1. Preparation of substituted carbazoles as anti-cancer agents

By Heaton, Andrew; Eiffe, Eleanor; Pottabathini, Narendar; Gunning, Peter

The invention relates to anti-tropomyosin compds., processes for their prepn., and methods for treating or preventing a disease or disorder, such as a proliferative disease (preferably cancer), using compds. of the invention. I [wherein R<sup>1</sup> and R<sup>2</sup> are independently H or C<sub>1-6</sub> alkyl; R<sup>3</sup> is (un)substituted NH<sub>2</sub>, or a (un)substituted 3- to 7-membered carbocyclic ring; R<sup>4</sup> and...

2. Preparation of functionalized and substituted carbazoles as anti-cancer agents

By James, Ian; Dixon, Ian; Heaton, Andrew; Eiffe, Eleanor; Gunning, Peter

The invention relates to anti-tropomyosin compds., processes for their prepn., and methods for treating or preventing a disease or disorder, such as a proliferative disease (preferably cancer), using compds. of the invention. I [wherein R<sup>1</sup> is -C(O)NH- or a (un)substituted 5- or 6-membered carbocyclic ring wherein between 1 and 3 ring carbon atoms may optionally be replaced with S, N, O, NH, etc.; R<sup>2</sup> is monocyclic or bicyclic carbocyclic ring having between 5 and 10 ring carbons wherein 1 or 2 ring carbon atoms may optionally be replaced with S, O, N, NH, etc.; R<sup>3</sup> is H, halo, (un)substituted N...

3. Use of anthelmintic agents against *Dirofilaria immitis*

By Chassaing, Christophe Pierre Alain; Lutz, Juergen; Heckerroth, Anja Regina

与前一个结果集合并，得到完整的结果集

# 如何判断结构的新颖性

**新颖性：** 是否存在？ 是否能申请专利？

**SciFinder相关物质库：** Registry和Marpat

**检索方法：** 物质检索？ Markush检索？

Step1

Structure Editor

Draw or change atoms or bonds.

Atom Short

HO<sub>2</sub>C CO<sub>2</sub>H

Et

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

SciFinder®

Explore Saved Searches SciPlanner

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

Step1

Structure Editor

Draw or change atoms or bonds.

Atom Short

HOOC COOH

Et

Drawing Editor:

- Structure
- Reaction
- Markush

Get Markush patents that match your query using:

Variable only at

SciFinder®

Explore Saved Searches SciPlanner

Markush structure variable only at spe... > references (18)

REFERENCES

Analyze Refine Categorize

Sort by: Accession Number

0 of 18 References Selected

# 提纲

- **SciFinder**反应检索难点解析
  - 反应的精准定义
  - 巧妙获得有实验步骤的相关反应
  - 反应信息太少时如何获得更多的反应信息
  - 利用**SciPlanner**做逆合成反应分析
  - 直接检索反应受限时如何处理
  - 案例分析

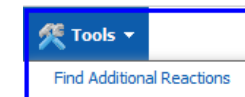
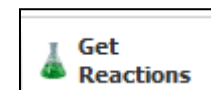
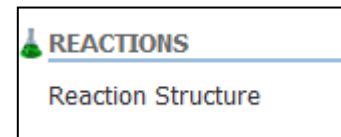
# 反应检索方法

- 功能方面

- 结构式

- 检索方法推荐

- 已知物质：先查找物质，通过标准菜单获得相应反应
  - 已知文献：链接至文献中的反应
  - 扩展检索：对单步反应获得相似反应
  - 扩展检索：对已知反应获得更多反应



# SciFinder中反应定义工具

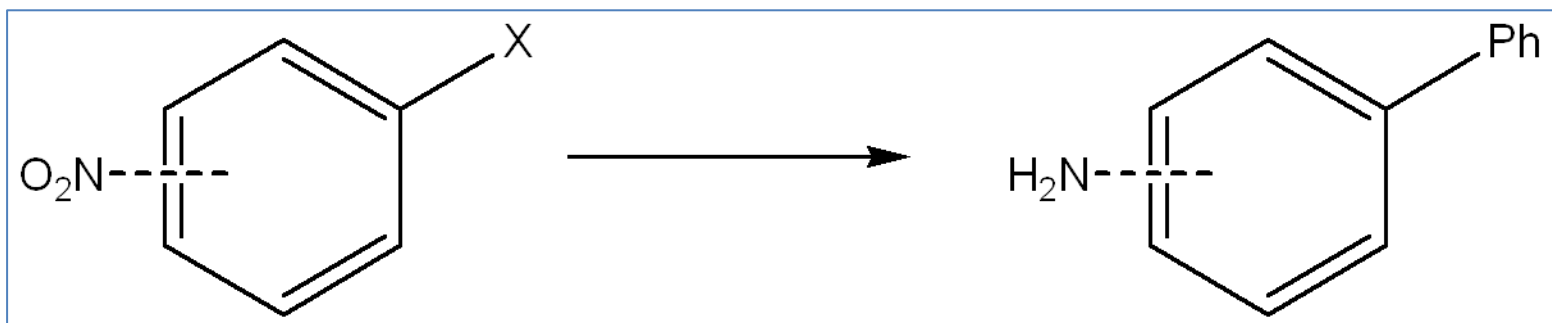
The image shows the SciFinder Reaction Editor interface. On the left, there is a vertical toolbar with various icons. Four callout boxes with pink borders and lines pointing to specific icons contain the following Chinese text:

- 反应箭头 (Reaction Arrow)
- 反应原子标记工具 (Reaction Atom Marking Tool)
- 反应官能团列表 (Reaction Functional Group List)
- 反应角色工具 (Reaction Role Tool)
- 反应位置标记工具 (Reaction Position Marking Tool)

The main window of the Reaction Editor is titled "Reaction Editor" and contains a large central canvas. Below the canvas is a horizontal toolbar with chemical symbols (C, H, O, S, N, P, Cl, Br, F, I, Si) and other drawing tools. On the right side, there is a "Drawing Editor" panel with radio buttons for "Structure", "Reaction", and "Markush". Below this panel, there is a section titled "Get reactions where the structure(s) are:" with radio buttons for "only at the specified positions" and "of more complex structures". At the bottom right of the panel are "确定" (OK) and "取消" (Cancel) buttons. The bottom status bar of the window shows "(query)".

# 反应的精准定义

检索符合以下要求的反应，硝基还原的情况下，做**SUZUKI**偶联

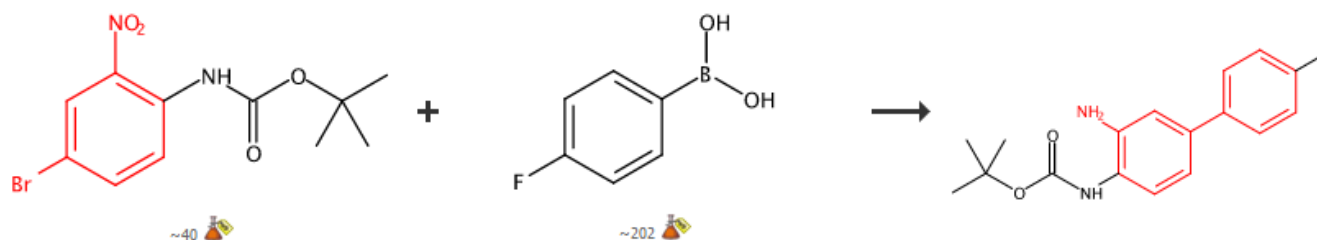




# 反应的精准定义

## 2. View Reaction Detail [Link](#)

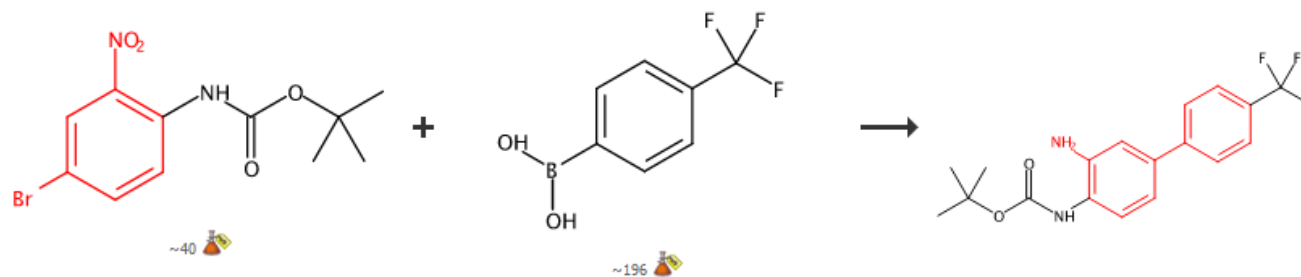
2 Steps *Hover over any structure for more options.*



符合要求的反应

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

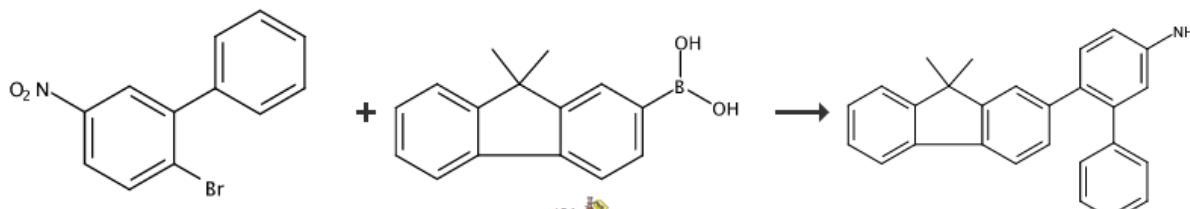
Single Step *Hover over any structure for more options.*



# 反应的精准定义

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

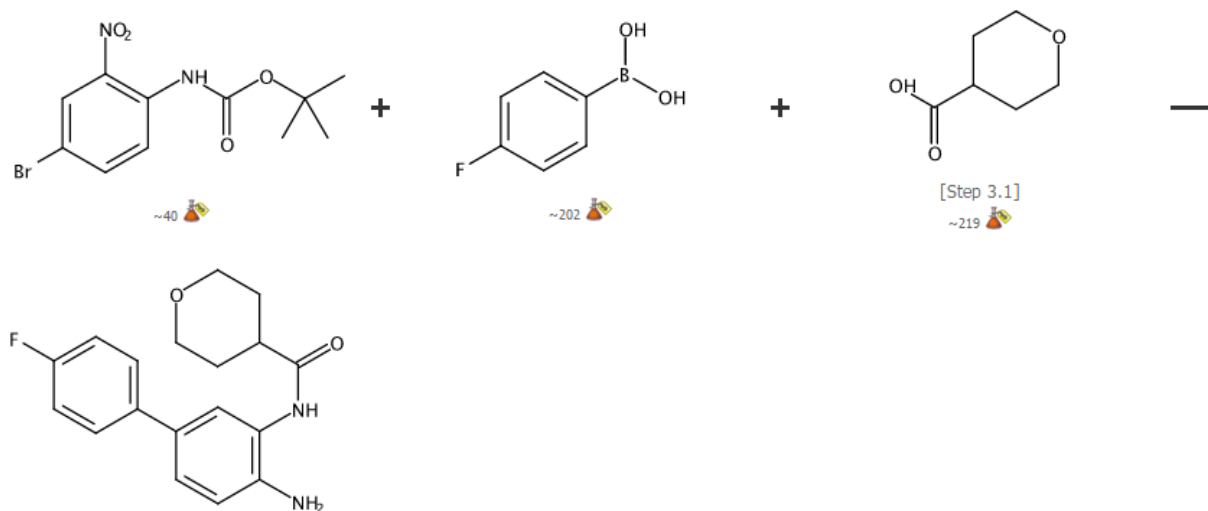
2 Steps Hover over any structure for more options.



不符合要求的反应

## 3. View Reaction Detail [Link](#)

4 Steps Hover over any structure for more options.

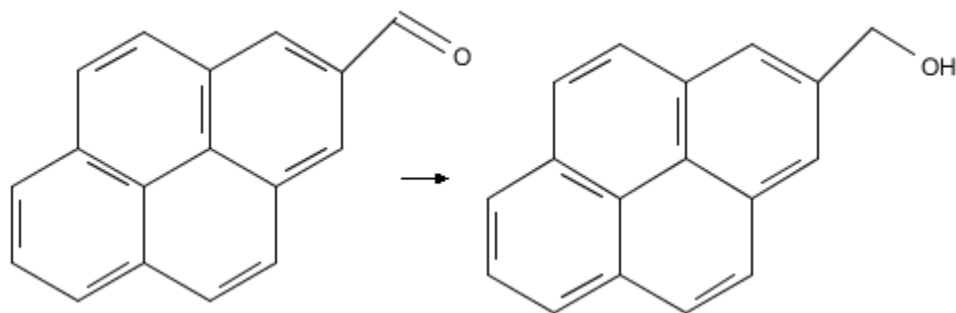


# 反应的精准定义

The screenshot displays the 'Structure Editor' software interface. The main workspace shows a chemical reaction: a benzene ring with a nitro group (NO<sub>2</sub>) and a substituent 'X' at the para position (labeled '1') reacts to form a benzene ring with a primary amine group (NH<sub>2</sub>) and the same substituent 'X' at the para position (labeled '1'). The nitro group is labeled '2' and the amine group is labeled '2'. A yellow banner at the top of the workspace contains the instruction: 'Click an atom in the reactant and its corresponding atom in the product.' The left sidebar contains various drawing tools, with the 'Reaction' tool (two curved arrows) highlighted in a red box. The right sidebar, titled 'Drawing Editor:', has three radio buttons: 'Structure', 'Reaction' (which is selected), and 'Markush'. Below this, a section titled 'Get reactions where the structure(s) are:' has two radio buttons: 'Variable only at the specified positions' and 'Substructures of more complex structures' (which is selected). At the bottom right of the right sidebar are 'OK' and 'Cancel' buttons. The bottom status bar shows 'Formula is not available' and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si.

# 巧妙获得有实验步骤的相关反应

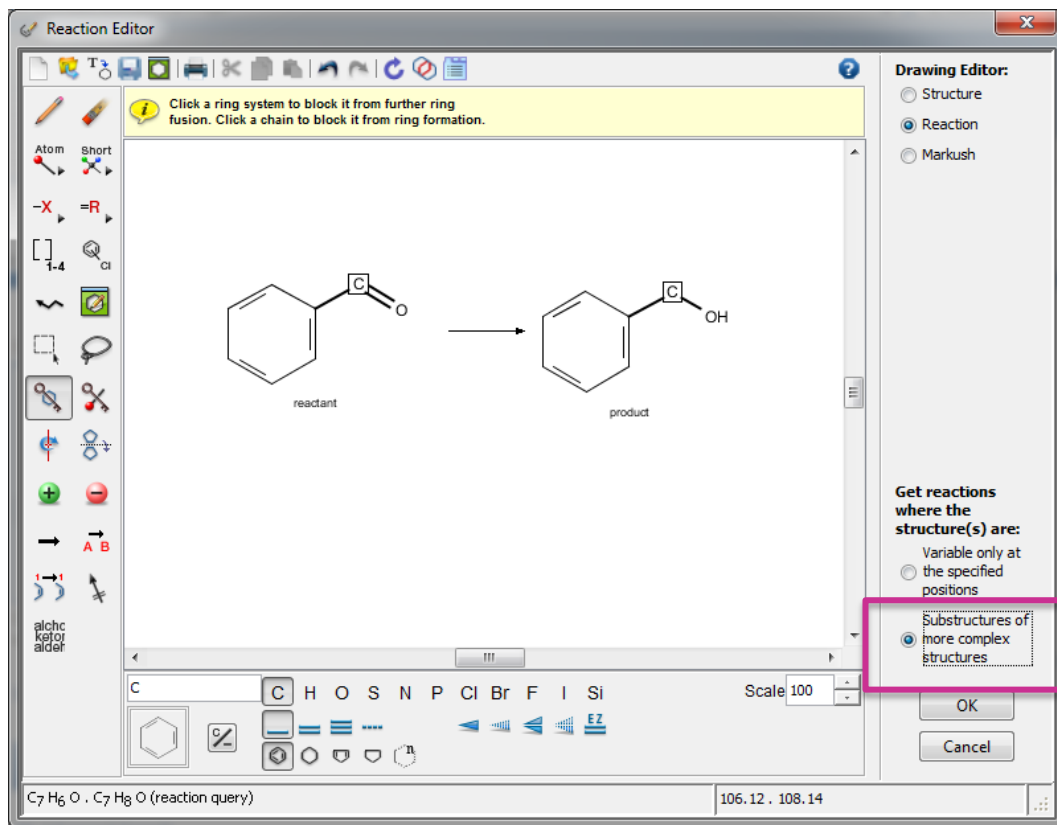
该还原反应如何操作？



The screenshot shows the Reaction Editor window. The main area displays the reaction between the aldehyde and the alcohol. The left sidebar contains drawing tools, and the right sidebar has a 'Drawing Editor' section with radio buttons for 'Structure', 'Reaction', and 'Markush'. Below that, there are options to 'Get reactions where the structure(s) are:' with radio buttons for 'Variable only at the specified positions' and 'Substructures of more complex structures'. At the bottom, there is a chemical formula input field showing 'C<sub>17</sub>H<sub>10</sub>O · C<sub>17</sub>H<sub>12</sub>O (reaction query)' and a 'Scale' of 100.

The screenshot shows the SciFinder search results page. The SciFinder logo is at the top left. Below it are navigation buttons for 'Explore', 'Saved Searches', and 'SciPlanner'. A yellow warning banner at the bottom states 'Explore Reactions resulted in 0 reactions' with a red box around the number '0'. To the right of the banner are links for 'Return' and 'Find Additional Reactions'.

# 巧妙获得有实验步骤的相关反应



聚焦反应关键部位，查找相似反应

# 巧妙获得有实验步骤的相关反应

Reaction Structure substructure > reactions (60953) > refine "1 step" (14724)

REACTIIONS **?** Get References Tools Send to SciPlanner

Analyze Refine Group by: No Grouping Sort by: Relevance Display Options

0 of 60953 Reactions Selected Page: 1 of 4064

Sample Analysis: Reagent

NaBH <sub>4</sub>	≥ 9683
HCl	≥ 7777
K <sub>2</sub> CO <sub>3</sub>	≥ 6658
Et <sub>3</sub> N	≥ 4779
H <sub>2</sub> O	≥ 4266
NaOH	≥ 3980
NH <sub>4</sub> Cl	≥ 3438
LiAlH <sub>4</sub>	≥ 3182
H <sub>2</sub>	≥ 2661
NaHCO <sub>3</sub>	≥ 2580

Overview Steps/Stages

1.1 R:KOH, C:1

Analyze by: Experimental Procedure

Experimental Procedures Not Available	9504
Experimental Procedures Available	5220

Show More

1. View Reaction Detail [Click to view detail](#)

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

Reaction Structure substructure > reactions (60953) > refine "1 step" (14724)

REACTIIONS **?** Get References Tools Send to SciPlanner

Analyze Refine Group by: No Grouping Sort by: Relevance Display Options

0 of 14724 Reactions Selected Page: 1 of 982

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

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

Reaction scheme: Benzaldehyde (C<sub>6</sub>H<sub>5</sub>CHO) → Benzyl alcohol (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>OH) with 100% yield.

~152 → ~215

Overview Steps/Stages

1.1 R:KOH, C:1820757-77-4, S:Me<sub>2</sub>CHOH, S:MeCN, 3 h, 80°C

Notes

optimization study, optimized on catalysts, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Complexes of (η<sup>6</sup>-benzene)ruthenium(II) with 1,4-bis(phenylthio/seleno-methyl)-1,2,3-

# 获得全面的反应信息

查找合成Daclatasvir的反应

CAS Solutions  
SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Reaction Structure substructure > reactions (60953) > refine "1 step" (14724)

REFERENCES

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

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

SUBSTANCES: SUBSTANCE IDENTIFIER

daclatasvir

CAS Solutions  
SciFinder®

Preferences | SciFinder Help ▾ Sign Out

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner

Save Print Export

Substance Identifier "daclatasvir" > substances (1) > get reactions (18)

REACTIONS

Get References Tools ▾

Analyze Refine

Group by: No Grouping Number ▾

0 of 18

Find Additional Reactions  
Combine Answer Sets

1. View Reaction Detail Link

5 Steps Hover over any structure for more options.

Analyze by: Reagent

ETN(Pr- <i>i</i> ) <sub>2</sub>	16
148893-10-1	13
Disodium carbonate	10
HCl	10
AcOK	5
NH <sub>4</sub> OAc	5
1-Benzotriazolol	3
ETN=C=N(CH <sub>2</sub> ) <sub>3</sub> NMe <sub>2</sub>	3
+HCl	3
NaHCO <sub>3</sub>	3
Br <sub>2</sub>	2

Chemical reaction scheme showing the synthesis of Daclatasvir. The reaction involves the coupling of a substituted benzamide derivative (with a 4-acetylphenyl group) and a chiral auxiliary (a pyrrolidine derivative with a tert-butyl ester and a hydroxyl group) with a chiral auxiliary (a chiral auxiliary with a hydroxyl group and a methyl ester group). The reaction is shown in two steps: [Step 2.1] and [Step 5.1].

Chemical structures shown in the reaction scheme:

- 4-acetylphenyl group
- tert-butyl ester
- pyrrolidine ring
- hydroxyl group
- chiral auxiliary (with hydroxyl and methyl ester)

Page: 1 of 2

# 获得全面的反应信息

Analyze Refine

Analyze by: ?  
Answer Type

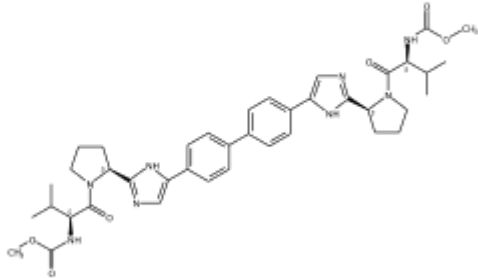
Reactions 18

Additional Reactions 1

Show More

19. View Reaction Detail [Link](#)

Hover over any structure for more options.



~88

~11 references

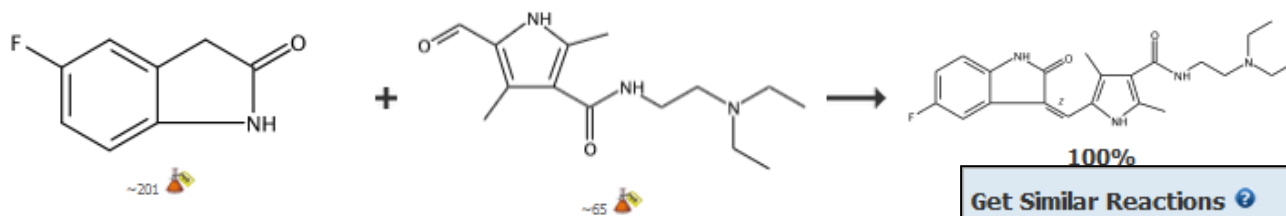
获得的附加反应不是完整反应



# 获得相关的反应信息

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

Single Step Hover over any structure for more options.



## Overview

### Steps/Stages

1.1

## Notes

no exp

## Refer

Novel s

Quick

By Sang

From In

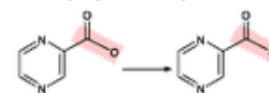
## Get Similar Reactions

### Retrieve similar reactions from:

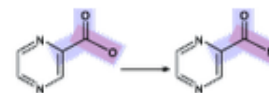
- All reactions
- Current answer set

### Include this level of similarity:

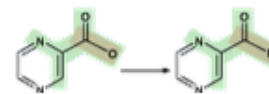
- Broad - Reaction centers only (157156)



- Medium - Reaction centers plus adjacent atoms and bonds (8506)



- Narrow - Reaction centers plus extended atoms and bonds (2994)



Get Reactions

Cancel

反应信息太少，通过Similar Reaction  
获得更多反应信息

# SciPlanner在逆合成反应分析中的应用

1. 557795-19-4

Double bond geometry as shown.

C<sub>22</sub> H<sub>27</sub> F N<sub>4</sub> O<sub>2</sub>  
1H-Pyrrole-3-carboxamide, N-[2-(diethylamino)ethyl]-5-[(Z)-(5-fluoro-1,2-dihydro-2-oxo-3H-indol-3-ylidene)methyl]-2,4-dimethyl-

**CAS Registry Number:**  
557795-19-4

- View Substance Detail
- Explore by Structure
- Synthesize this**
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information

通过物质标准菜单获得合成反应

REACTIONS

Analyze Refine

Analyze by: Reagent

HCl	200
NaOH	199
KOH	168
Pyrrolidine	121
N <sub>2</sub> H <sub>4</sub> ·H <sub>2</sub> O	108
POCl <sub>3</sub>	105
EtN=C=N(CH <sub>2</sub> ) <sub>3</sub> NM e <sub>2</sub> ·HCl	102
Et <sub>3</sub> N	99
NaHCO <sub>3</sub>	89
H <sub>2</sub> O	81

Show More

Get References Tools

Group by: No Grouping Sort by: Accession Number

1 of 321 Reactions Selected

1. View Reaction Detail Link

2 Steps 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

Send to SciPlanner

# SciPlanner在逆合成反应分析中的应用

SciFinder®  
Welcome Helen Zhu

Explore | **Guided Searches** | SciPlanner | Save | Print | Export

⚠ 1 Reaction sent to SciPlanner.

Substance Identifier "Sunbnb" > substances (1) > get reactions (321)

REACTIONS

Analyze | Refine

Analyze by: Reagent

HCl	200
NaOH	199
KOH	168
Pyrrolidine	121
N <sub>2</sub> H <sub>4</sub> ·H <sub>2</sub> O	108
POCl <sub>3</sub>	105
EtN=C=N(CH <sub>2</sub> ) <sub>2</sub> NM e <sub>2</sub> ·HCl	102
Et <sub>3</sub> N	99
NaHCO <sub>3</sub>	89
H <sub>2</sub> O	81

Show More

SciPlanner\_03\_08\_2016\_215648

Workspace | Edit | View | GoTo

Clear Reactions

Click the small reaction arrow icon in the workspace and drag it into the left sidebar editor.

点击小图，按住鼠标左键拖入左侧编辑栏

# SciPlanner在逆合成反应分析中的应用

The screenshot displays the SciFinder SciPlanner software interface. The main workspace shows two chemical structures. The top structure is a complex heterocyclic compound with a methyl group, a carbonyl group, and a side chain. A context menu is open over this structure, listing several actions. The 'Synthesize this...' option is highlighted with a red box. Below it, another chemical structure is visible, which is a benzimidazole derivative with a fluorine substituent. The interface includes a top navigation bar with 'Workspace', 'Edit', 'View', and 'GoTo' menus, and a right-hand panel with a 'Clear Reactions' button. The title bar indicates the session ID 'SciPlanner\_03\_08\_2016\_215648'.

CAS Registry Number:  
356068-86-5

- 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
- Export as molfile

通过物质标准菜单获得中间体的合成反应

# SciPlanner在逆合成反应分析中的应用

CAS Solutions

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

Save | Print | Export

2 reactions with the Product Yield  $\geq 90\%$  are displayed

Keep Analysis | Clear Analysis

Substance Identifier "Sunitinib" > substances (1) > get reactions (321) > get reactions (121)

REACTIONS

Get References | Tools

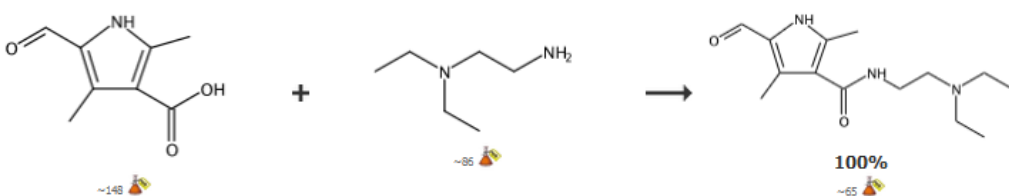
Analyze | Refine

Group by: No Grouping | Sort by: Accession Number

1 of 121 Reactions Selected

15. View Reaction Detail | Link | Similar Reactions

Single Step Hover over any structure for more options.



Overview

Experimental Procedure

37. View Reaction Detail | Link | Similar Reactions

Single Step Hover over any structure for more options.

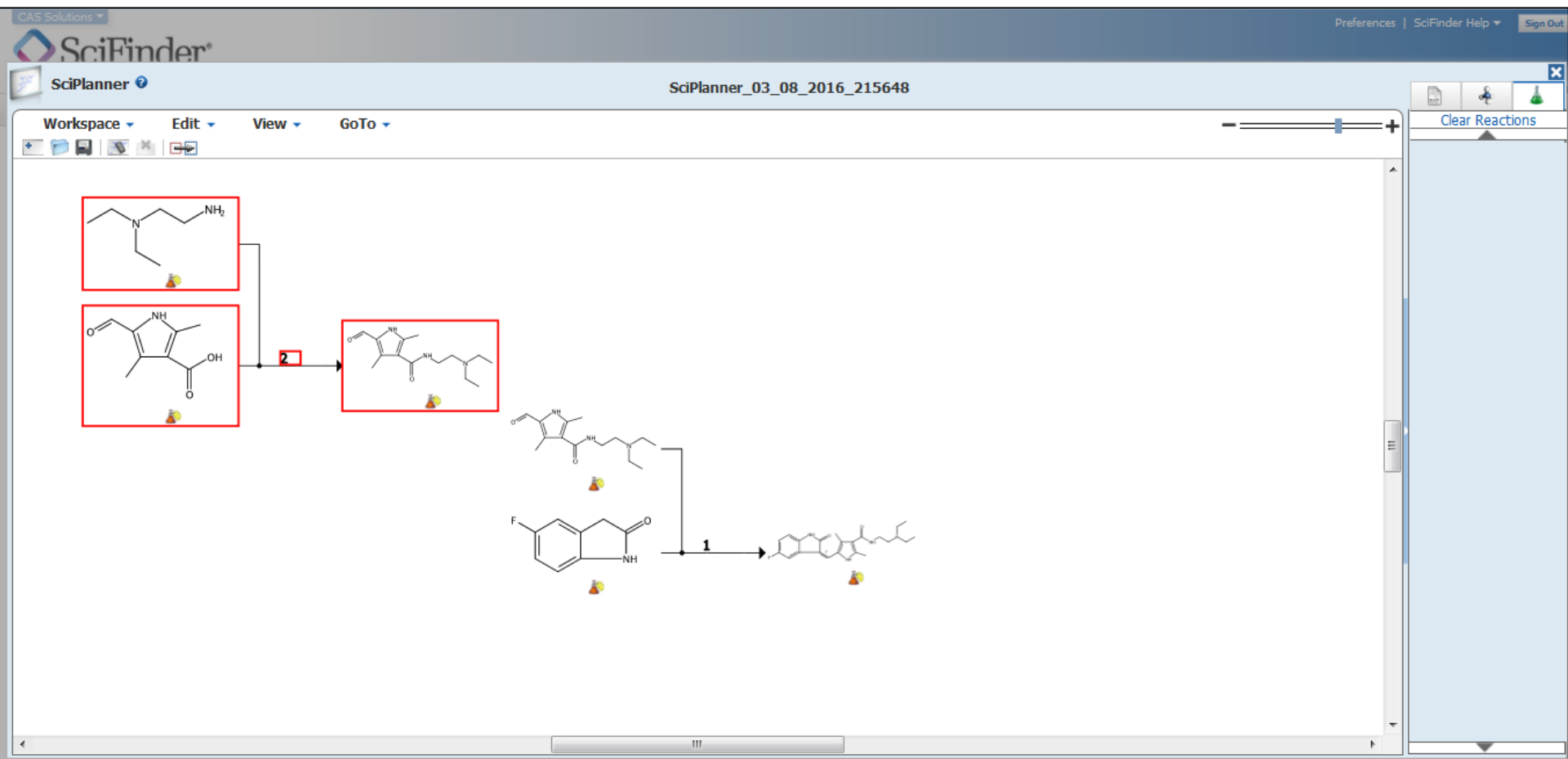
Send to SciPlanner

Display Options

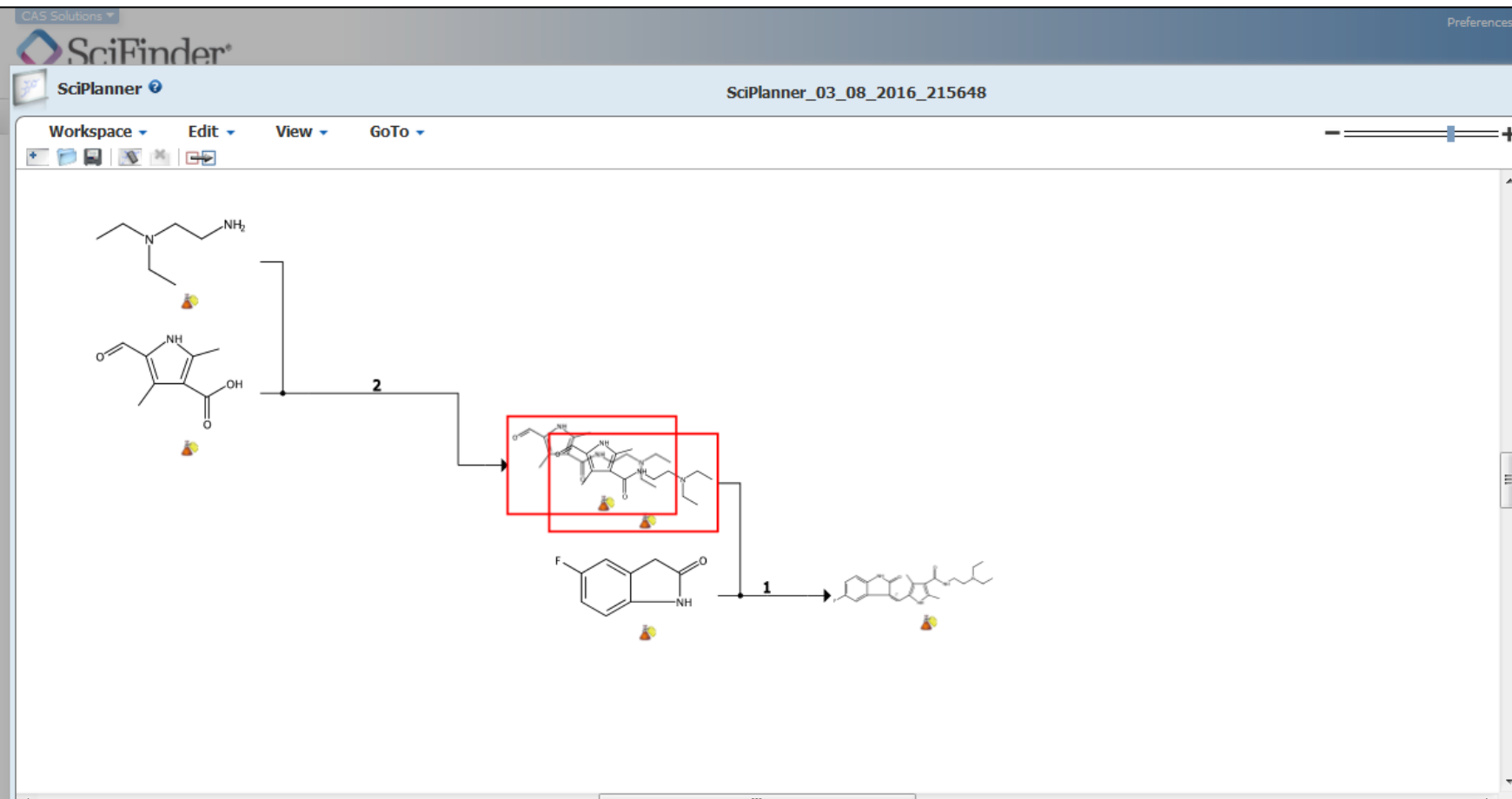
Analyze by:	Count
Product Yield	
40-49%	8
50-59%	3
60-69%	2
70-79%	2
$\geq 90\%$	2
80-89%	1
<10%	1

选择合适的反应，发送至SciPlanner

# SciPlanner在逆合成反应分析中的应用

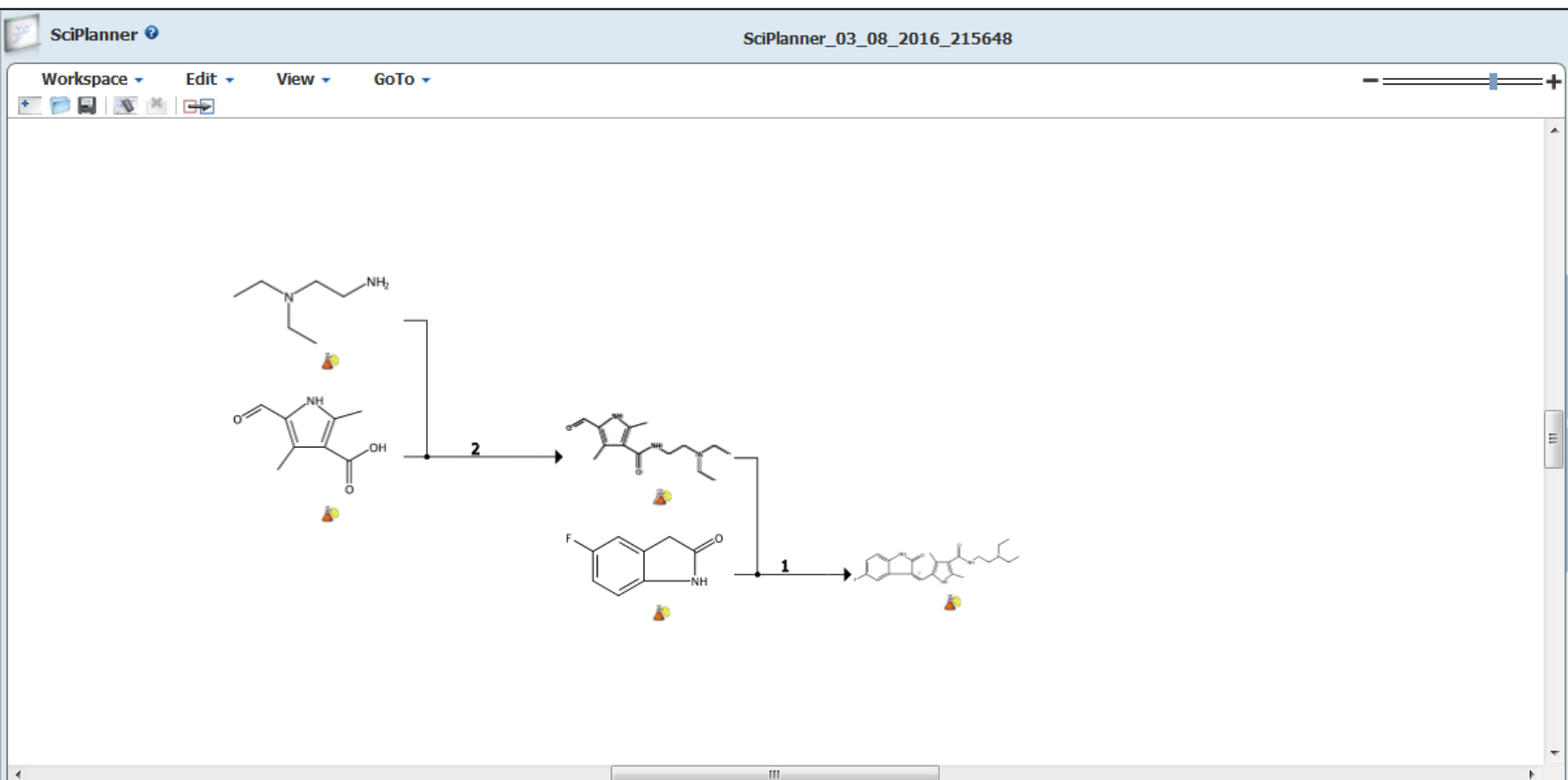


# SciPlanner在逆合成反应分析中的应用



拖动相同物质之一直至两个红框重合

# SciPlanner在逆合成反应分析中的应用



重复以上步骤直至原料易得



# SciPlanner在逆合成反应分析中的应用

The screenshot displays the SciPlanner interface within the SciFinder environment. The main workspace shows a retrosynthetic analysis of a target molecule, with disconnections numbered 1 through 5. A dropdown menu is open, showing options: Selected References (highlighted), Selected Substances, Selected Reactions, and Participant Search. The reaction scheme includes various chemical structures such as aldehydes, ketones, and heterocyclic compounds.

选中相应反应的编号，获得相应的文献

# SciPlanner在逆合成反应分析中的应用

The screenshot displays the SciPlanner web interface. At the top, there are navigation buttons: 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. On the right, there are buttons for 'Create Keep Me Posted Alert' and 'Send to SciPlanner'. Below the navigation bar, a 'Sort by:' dropdown menu is set to 'Accession Number'. A selection box shows '1 of 1 Reference Selected'. The first reference is selected and displayed:

**1. Novel salts of sunitinib an anticancer drug with improved solubility**  
Quick View Other Sources

By Sangwan, Sangeeta; Panda, Tapas; Thiamattam, Ram; Dewan, Sharwan K.; Thaper, Rajesh K.  
From International Research Journal of Pure and Applied Chemistry (2015), 5(4), 352-365/1-352-365/14, 14 pp.. | Language: English, Database: CAPLUS

Polymorph, co-crystal and salt screening expts. were carried out to identify novel solid forms with the improved physicochem. properties, particularly water soly. in the present case. Co-crystal formation was evaluated with urea and nicotinamide. These cofomers do not have any ionic groups that favor the formation of salts. Sunitinib malate salt is being currently sold in the market. It is poorly sol. in water. Salt screening expts. were conducted with adipic acid, glutaric acid, nicotinic acid, 4-hydroxy benzoic acid and saccharin. The salts with 1:1 ratios were obtained with these aci...

选中相应文献

# SciPlanner在逆合成反应分析中的应用

The screenshot shows the SciFinder search results page. At the top, there are navigation buttons: 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. On the right, there are buttons for 'Create Keep Me Posted Alert' and 'Send to SciPlanner', which is highlighted with a red box. Below the navigation bar, there is a 'Sort by: Accession Number' dropdown menu. A selection box shows '1 of 1 Reference Selected'. The first reference is listed as '1. Novel salts of sunitinib an anticancer drug with improved solubility'. Below the title, there are links for 'Quick View' and 'Other Sources'. The author information is 'By Sangwan, Sangeeta; Panda, Tapas; Thiamattam, Ram; Dewan, Sharwan K.; Thaper, Rajesh K.'. The source is 'From International Research Journal of Pure and Applied Chemistry (2015), 5(4), 352-365/1-352-365/14, 14 pp.. | Language: English, Database: CAPLUS'. The abstract text is: 'Polymorph, co-crystal and salt screening expts. were carried out to identify novel solid forms with the improved physicochem. properties, particularly water soly. in the present case. Co-crystal formation was evaluated with urea and nicotinamide. These cofomers do not have any ionic groups that favor the formation of salts. Sunitinib malate salt is being currently sold in the market. It is poorly sol. in water. Salt screening expts. were conducted with adipic acid, glutaric acid, nicotinic acid, 4-hydroxy benzoic acid and saccharin. The salts with 1:1 ratios were obtained with these aci...'. On the right side of the abstract, there are icons for 'Send to SciPlanner', 'Print', and 'Download'.

选中相应文献，发送至SciPlanner

# SciPlanner在逆合成反应分析中的应用

Workspace Edit View GoTo

New  
Open  
Save  
Duplicate  
Import  
Export  
Print  
Close

5

4

3

2

Click and drag to move

A process for preparing 2,4-dimethyl-1H-pyrrole-3-carboxylic acid ethyl ester via bromination of propanal followed by heterocyclization with ethyl acetoacetate and ammonia water  
From Faming Zhuanli Shenqing, 103265468, Aug 28, 2013

An improved synthesis of sunitinib malate via a solvent-free decarboxylation process  
By Meng, Ge et al  
From Research on Chemical Intermediates, 41, 0922-6168, 8941-8954, 2015

Process for preparation of pyrrole derivatives  
From PCT Int. Appl., 2011110199, Sep 15, 2011

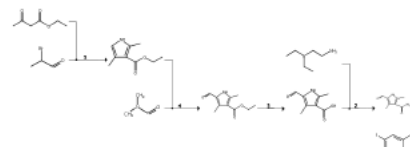
Novel salts of sunitinib an anticancer drug with improved solubility  
By Sangwan, Sangeeta et al  
From International Research Journal of Pure and Applied Chemistry, 5, 2231-3443, 352-365/1-352-365/14, 14 pp., 2015

同法获得所有需要的文献，列在相应的反应下方

# SciPlanner在逆合成反应分析中的应用

SciFinder®

Page 1



A process for preparing novel salts of sunitinib...  
An improved synthesis of sunitinib malate...  
Process for preparation of pyrolo derivatives...

Copyright © 2016 American Chemical Society (ACS). All Rights Reserved.

SciFinder®  
Reaction Information

Page 2

Reaction Stages

1 1.1

Notes

no experimental detail, Reactants: 100%  
2, Steps: 1, Stages: 1

Yield

Transformations:

1. Aldol Reaction
2. Aldol-Ty between Derivat with Acti Aldetyl Thioleto
3. Condens between Active H Aldetyl Knoever

References

Novel salts of sunitinib an anticancer drug with improved solubility  
By Sangwan, Sangeeta et al  
From International Research Journal of Pure and Applied Chemistry, 5(4), 2015

CASREACT® Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains a database (1974-1999) provided by InfoChem. RFP data prior to 1980. Subtransformations database compiled Kluwer, organic reactions, performs copyright 1999-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc. Synthesys Inc. Reproduced under license. All Rights Reserved.

Reaction Stages

2 1.1

R<sub>1</sub>(PPi(O)O)<sub>2</sub>, SAcOEt, 1.5 h, rt, overnight, rt

Notes

Reactants: 2  
Solvents: 1,

Transforma

1. Acylation Nucleop ACIDS

References

Process for preparation of pyrolo derivatives  
By Zhu, Jie  
From PCT Int. Appl., 2011110199, 15 Sep 2011  
Experimental Procedure

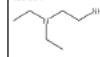
Example 1- Conversion of (2a) to (1a). To a solution of acid (~5mmol) in N-diethylethylene-diamine (10 ml), with stirring phosphoric acid anhydride (P<sub>2</sub>O<sub>5</sub>) (10 ml, 50% EtOAc solid) completed in 1.5 hours. The resulting reaction mixture was (25 ml) and dichloromethane (25 ml) were added, and the minutes. The dichloromethane layer was separated and oily material. The oil was mixed with ethyl acetate (50 ml) (4%, 25 ml), and stirred at 70°C for 30 minutes. After cooled separated and washed with water (10 ml), dried (Na<sub>2</sub>SO<sub>4</sub>) solid (1a) (1.35 g).

Copyright © 2016 American Chemical Society (ACS). All Rights Reserved.

SciFinder®  
Substance Information

Page 5

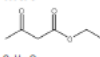
100-36-7



C<sub>8</sub>H<sub>16</sub>N<sub>2</sub>  
1,2-Ethanediamine, N,N'-diethyl-

Related Info:  
~ 3227 References  
Reactions  
~ 85 Commercial Sources  
Regulatory Information

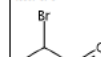
14147-0



C<sub>8</sub>H<sub>14</sub>O<sub>2</sub>  
Butanoic acid, 3-oxo-, ethyl ester

Related Info:  
~ 21060 References  
Reactions  
~ 158 Commercial Sources  
Regulatory Information

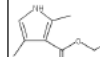
19967-07-8



C<sub>3</sub>H<sub>4</sub>BrO  
Propenal, 2-oxo- (E)

Related Info:  
~ 124 References  
Reactions  
~ 133 Commercial Sources  
Regulatory Information

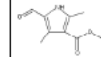
2190-51-1



C<sub>12</sub>H<sub>20</sub>N O<sub>2</sub>  
14-Methyl-3-carboxylic acid, 2,4-dimethyl-, ethyl ester

Related Info:  
~ 150 References  
Reactions  
~ 137 Commercial Sources  
Regulatory Information

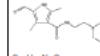
2190-50-9



C<sub>12</sub>H<sub>18</sub>N O<sub>2</sub>  
14-Methyl-3-carboxylic acid, 5-formyl-2,4-dimethyl-, ethyl ester

Related Info:  
~ 124 References  
Reactions  
~ 133 Commercial Sources  
Regulatory Information

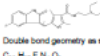
35608-95-5



C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>  
14-Pyridin-3-carboxamide, N2-(diethylamino)ethyl-5-formyl-2,4-dimethyl-

Related Info:  
~ 75 References  
Reactions  
~ 65 Commercial Sources

587765-19-4



C<sub>12</sub>H<sub>17</sub>F N<sub>2</sub>O<sub>2</sub>  
14-Pyridin-3-carboxamide, N2-(diethylamino)ethyl-5-(2-(5-fluoro-1,2-dihydro-2-oxo-3-methyl-5-oxo-1H-pyridin-2-yl)-2,4-dimethyl-

Related Info:  
~ 3444 References  
Reactions  
~ 65 Commercial Sources  
Regulatory Information

SciFinder®  
Reference

Page 7

A process for preparing 2,4-dimethyl-1H-pyridine-3-carboxylic acid ethyl ester via bromination of propanal followed by heterocyclization with ethyl acetoacetate and ammonia water

By Zhang, Juyun; Zhao, Guosong; Mao, Qingli; Qin, Ning; Fu, Yongmei; Yan, Fafei; Li, Jialin; Zhang, Hui  
From *Fahing Zhuanji Shengqi* (2013), CN 103265458 A 20130326; Language: Chinese, Database: CAPLUS

The invention relates to a process for the prepn. of 2,4-dimethyl-1H-pyridine-3-carboxylic acid Et ester via bromination of propanal followed by heterocyclization with Et acetoacetate and ammonia water. The inventive product is an important intermediate for synthesis of sunitinib malate, which is a multi-targeted inhibitor of receptor tyrosine kinase and has double effects of anti-tumor and anti-angiogenesis.

~0 Citings

0 Tags

0 Comments

Copyright © 2016 American Chemical Society (ACS). All Rights Reserved.

An improved synthesis of sunitinib malate via a solvent-free decarboxylation process

By Meng, Ge; Liu, Chunyan; Qin, Shidong; Dong, Mengshu; Wei, Xiaoni; Zheng, Meilin; Qin, Luwen; Wang, Huihui; He, Xiaosheng; Zhang, Zhiguo  
From *Research on Chemical Intermediates* (2015), 41(11), 8941-8954. Language: English, Database: CAPLUS, DOI:10.1007/s11164-015-1539-2

To search for an economical and convenient synthesis of sunitinib and its malate salt, optimization of a scalable synthetic route was explored by designing a salt-extract protocol on lab. scale using com. available materials including acetyl Et acetoate, 4-fluoropyridine, and N,N'-diethylethylene-1,2-diamine. The optimal conditions were established based on investigating the main reaction steps, including cyclization, hydrolysis, decarboxylation, formylation, and condensation, giving optimized yields for each step of 84.4, 71.2, 85.8, 97.1, 91.0, 86.3, 85.5, 69.2, 95.1, 97.3, and 58.7%, resp. The synthesis process of 5-formyl-2,4-dimethyl-1H-pyridine-3-carboxylic acid as the important intermediate was significantly improved by using solvent-free decarboxylation instead of the traditional process in a high-boiling-point solvent. The subsequent formylation was conducted directly using the dichloromethane soln. of the crude product from decarboxylation, leading to an almost quant. combined yield of these two steps. The overall yields of sunitinib and its salt using the optimal synthesis process were 67.3 and 40.7%, based on acetyl Et acetoate. The obtained data could be used as ref. for future industrialization, esp. for avoiding expensive solvents and reducing reaction time.

~0 Citings

0 Tags

0 Comments

Copyright © 2016 American Chemical Society (ACS). All Rights Reserved.

Novel salts of sunitinib an anticancer drug with improved solubility

By Sangwan, Sangeeta; Panda, Tapas; Thiamattam, Ram; Dewan, Sharwan K.; Thapper, Rajesh K.  
From *International Research Journal of Pure and Applied Chemistry* (2015), 5(4), 352-365/1-352-365/14, 14 pp. Language: English, Database: CAPLUS, DOI:10.5491/IRJPC201513571

Poly-morph, co-crystal and salt screening expts. were carried out to identify novel solid forms with the improved physicochem. properties, particularly water soly. In the present case, Co-crystal formation was evaluated with urea and nicotinamide. These co-formers do not have any ionic groups that favor the formation of salts. Sunitinib malate salt is being currently sold in the market. It is poorly sol. in water. Salt screening expts. were conducted with acetic acid, glutaric acid, furoic acid, 4-hydroxy benzoic acid and saccharin. The salts with 1:1 ratios were obtained with these acids, except for adipic acid which yielded a 2:1 solid form. The soly. of these salts in deionized water was found to be 6 to 10 times greater than that of the marketed salt (sunitinib malate). Reversible Z:E isomerization was also well thought-out, esp. in presence of light and the isomerization was checked by HPLC. Formation of undesired E-isomer was added, confirmed by 1H NMR. This observation has implications in the soly. study of sunitinib salt samples using HPLC method.

~0 Citings

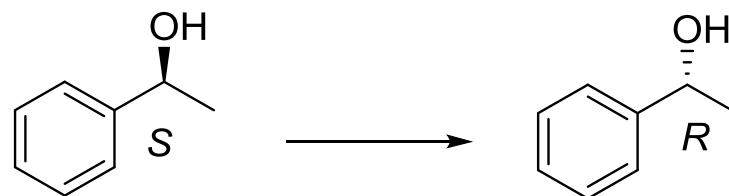
0 Tags

0 Comments

Copyright © 2016 American Chemical Society (ACS). All Rights Reserved.

# 直接检索反应受限的处理

检索如下构型翻转的反应



# 案例分析

## 检索要求:

- 某个结构中包含环和**Cbz**，环上存在**Br**或者**I**
- 寻找脱**Cbz**的一步反应，而环上卤素不脱掉

## 定义困难:

如何定义这个环系，杂环？C环？

Cbz和环的连接方法

# 案例分析

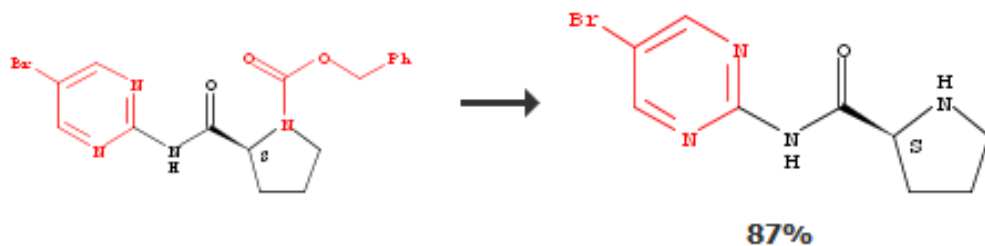
The screenshot displays the Reaction Editor interface. At the top, a yellow banner reads "Click bonds to be formed or broken during the reaction." The main workspace shows three chemical structures: a reactant with a dashed triangle labeled  $[R_1]_{1-4}$  and  $R_2$ , a product with a dashed triangle labeled  $[R_1]_{1-4}$  and  $R_2$ , and a full chemical structure of a cyclic molecule with a side chain labeled "reactant". The left sidebar contains various tool icons for atom selection, bond editing, and reaction types. The bottom toolbar includes a formula input field (containing "A"), a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), a scale slider (set to 100), and a list of stereochemical options (E, Z). On the right side, a panel titled "Get reactions where the structure(s) are:" offers two radio button options: "Variable only at the specified positions" and "Substructures of more complex structures". At the bottom right of this panel are buttons for "确定" (OK) and "取消" (Cancel). A status bar at the bottom left indicates "Formula not available".



# 案例分析

32. 1 Hits in this Reference Similar Reactions

Single Step Hover over any structure for more options.



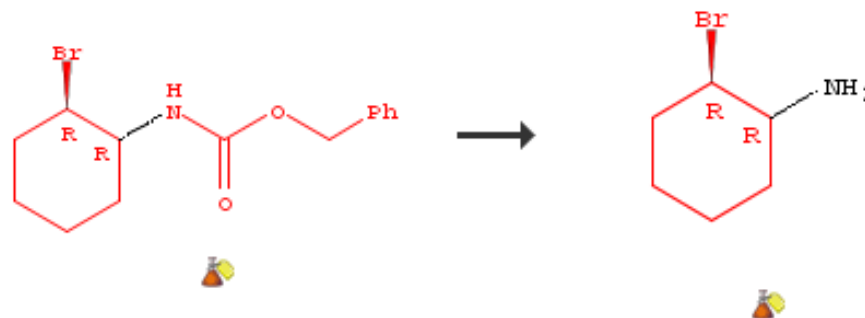
Overview

Experimental Procedure

存在我们想要的结果集

33. 1 Hits in this Reference Similar Reactions

Single Step Hover over any structure for more options.

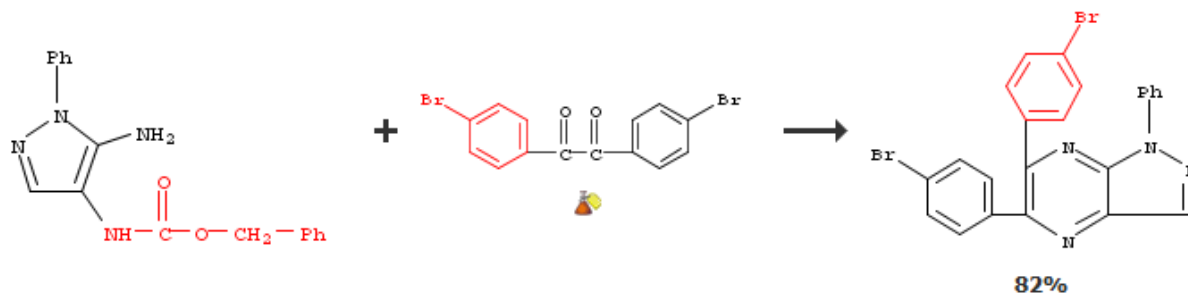


Overview

Experimental Procedure

# 案例分析

36. 1 Hits in this Reference Similar Reactions  
Single Step Hover over any structure for more options.

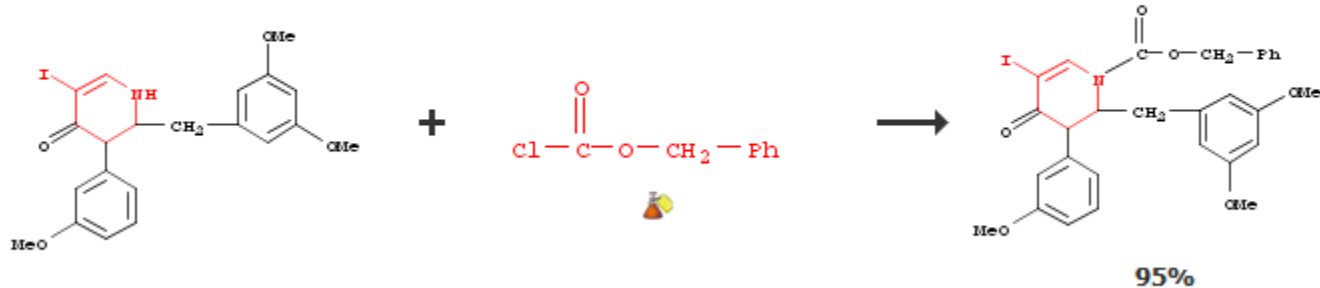


- ▶ Overview
- ▶ Experimental Procedure

存在大量的环与Cbz不在一个结构上的反应

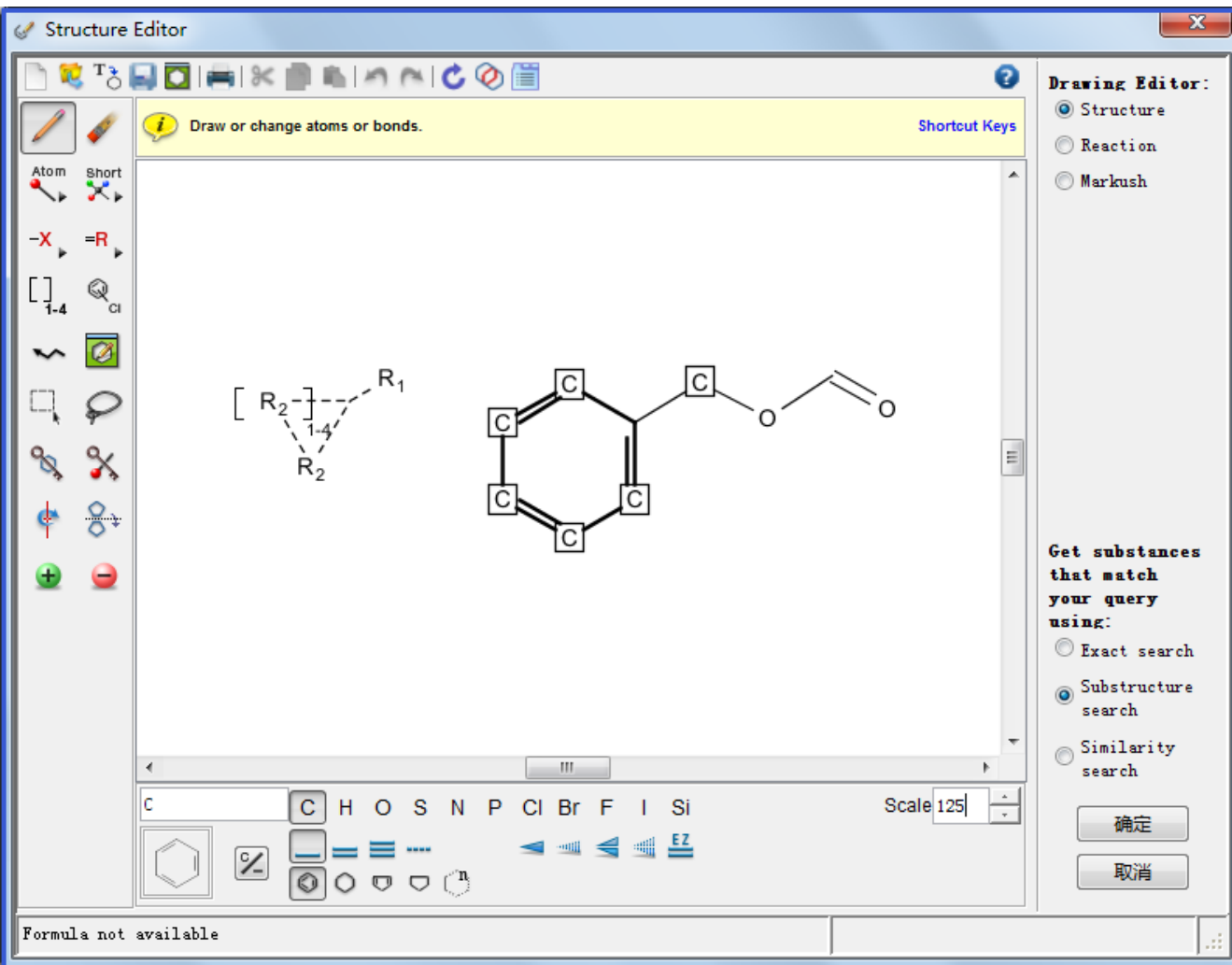
如何去除？

38. 1 Hits in this Reference Similar Reactions  
Single Step Hover over any structure for more options.



- ▶ Overview

# 案例分析



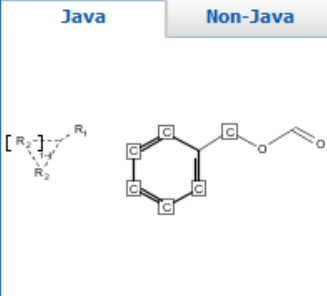
这种类型的反应，  
需要先去检索和反  
应相关的物质

# 案例分析

SUBSTANCES: CHEMICAL STRUCTURE ?

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

Show precision analysis

 ChemDraw

Launch a SciFinder substance or [More](#)

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 type="checkbox"/> Biological
	<input type="checkbox"/> Preparation
	<input checked="" type="checkbox"/> Reactant or reagent

需要定义为单一组分和具备  
反应物或试剂角色的物质

# 案例分析

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Chemical Structure substructure with limiters > substances (4727) > get reactions (77364) > refine "1 step" (5909) > refine "substructure" (414)

SUBSTANCES ⓘ Get References Get Reactions Get Commercial Sources Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Sort by: CAS Registry Number Display Options

0 of 4727 Substances Selected Page: 1 of 316

Analyze by: Substance Role

Reactant or Reagent 4727

Preparation 4348

Prophetic in Patents 556

Biological Study 512

Uses 470

Properties 75

Process 26

Combinatorial Study 13

Analytical Study 2

Formation, Nonpreparative 2

1. 1687759-75-6  
~1  
Cc1nc2c(ncn2C(=O)OCc3ccccc3)c4ccc(N)cc4

$C_{28}H_{28}BrN_5O_3$   
1-Piperidinecarboxylic acid, 4-[[4-[(3-bromophenyl)amino]-7-methoxy-6-quinazoliny]amino]-, phenylmethyl ester

2. 1687759-73-4  
~1  
Cc1nc2c(ncn2C(=O)OCc3ccccc3)c4ccc(N)cc4

$C_{26}H_{24}BrN_5O_3$   
1-Azetidinecarboxylic acid, 3-[[4-[(3-bromophenyl)amino]-7-methoxy-6-quinazoliny]amino]-, phenylmethyl ester

3. 1687758-88-8  
~1  
CH3

4. 1687758-80-0  
~1  
CH3

**Get Reactions ⓘ**

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

- Product
- Reactant
- Reagent
- Reactant or reagent
- Catalyst
- Solvent
- Any role

Get Cancel

获得所有的可能的反应物，并获得  
这些物质作为反应物的反应

# 案例分析

SciFinder® Preferences | SciFinder Help Sign Out

Welcome Helen Zhu

Explore Saved Searches SciPlanner Save Print Export

Chemical Structure substructure with limiters > substances (4727) > get reactions (77364) > refine "1 step" (5909) > refine "substructure" (414)

REACTIONS Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Accession Number

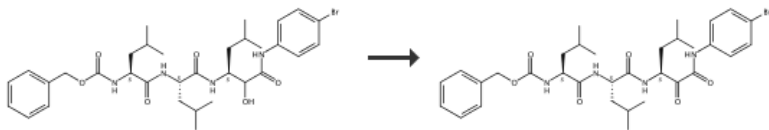
0 of 77364 Reactions Selected

Sample Analysis: Reagent

H <sub>2</sub>	≥ 10560
HCl	≥ 9264
Et <sub>3</sub> N	≥ 8636
K <sub>2</sub> CO <sub>3</sub>	≥ 7682
EtN(Pr- <i>i</i> ) <sub>2</sub>	≥ 6769
NaHCO <sub>3</sub>	≥ 6634
AcOK	≥ 5176
F <sub>3</sub> CCO <sub>2</sub> H	≥ 4608
EtN=C=N(CH <sub>2</sub> ) <sub>3</sub> NMe <sub>2</sub>	≥ 4311
•HCl	≥ 4311
148893-10-1	≥ 4280

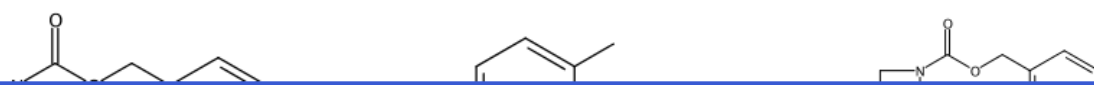
1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



2. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



这里的反应中的反应物都包含要求的结构，  
这时需进一步把产物限定进去。

# 案例分析

Analyze Refine

Refine by: ?

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

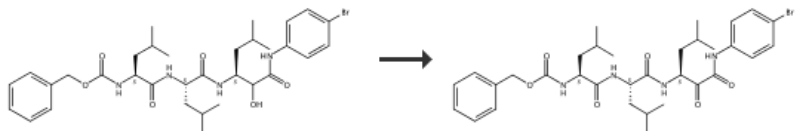
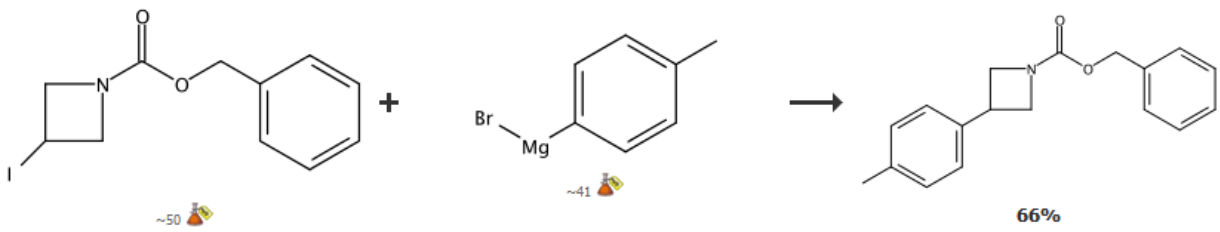
Number of Steps:

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

Refine

先限定反应步数为一步反应

0 of 5909 Reactions Selected

- 1. View Reaction Detail** [Link](#) [Similar Reactions](#)  
**Single Step** *Hover over any structure for more options.*  
  
[Click to view detail](#)  
[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.*

# 案例分析

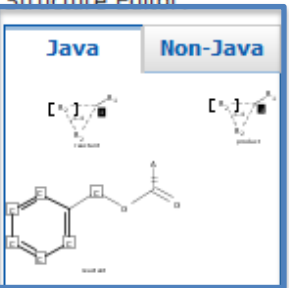
Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

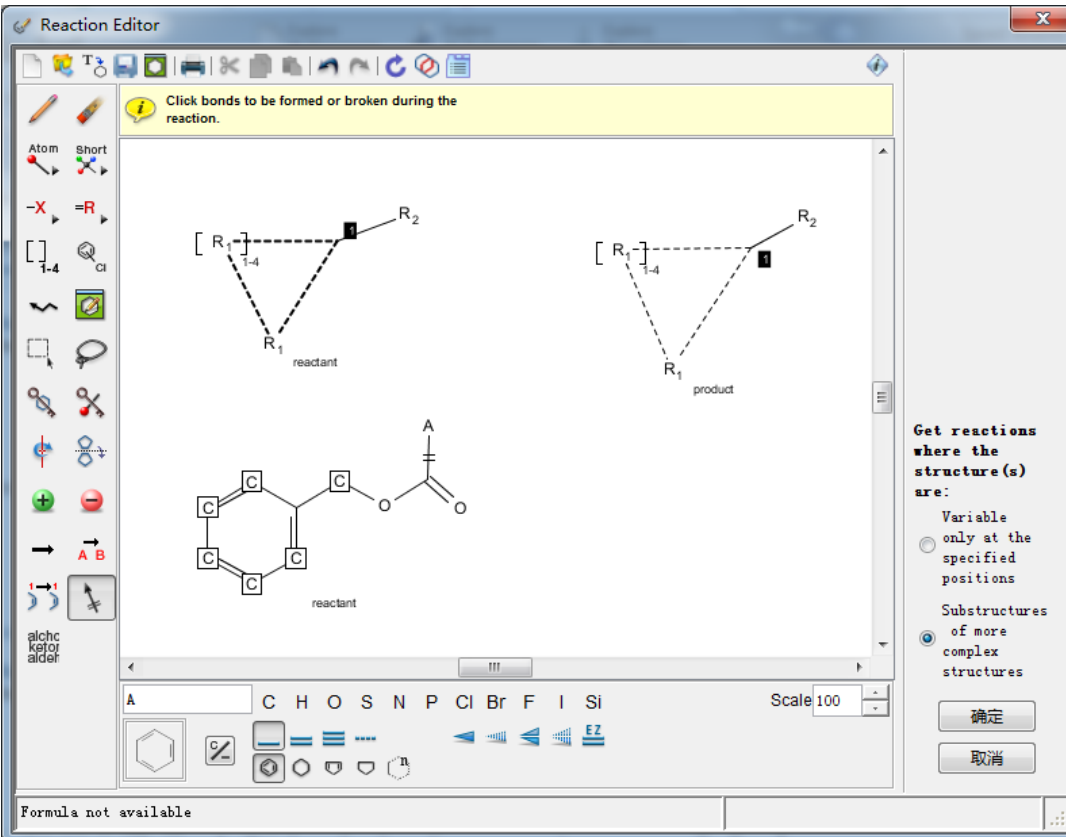


Click image to change structure or view detail.  
Search type: **Substructure**

Refine

Reaction Editor

Click bonds to be formed or broken during the reaction.



reactant

product

reactant

Get reactions where the structure(s) are:

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

确定

取消

Formula not available

再做反应中心限定，沿用之前的定义

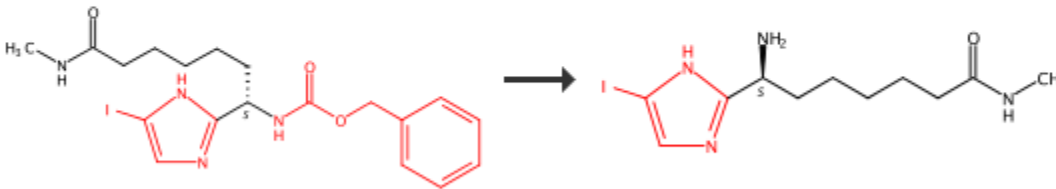


# 案例分析

0 of 414 Reactions Selected

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

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

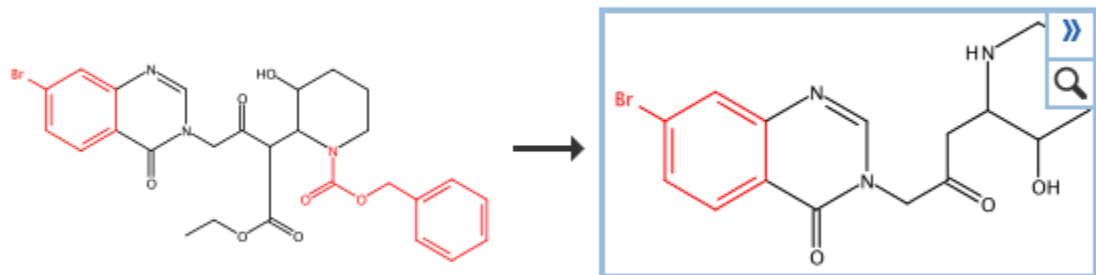


► Overview

都是我们想要的反应结果

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

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



94%

► Overview

# SciFinder中的检索思路

1. 初步检索
2. 浏览结果集，判断是否符合要求，利用系统工具限定结果
3. **修正检索式**，再次检索
4. 浏览结果集，判断



美国化学文摘社北京代表处

010-62508026

china@acsi.info



谢谢！

朱传娴  
高校客户顾问  
hzhu@acsi.info