

朱传娴

客户顾问

hzhu@acsi.info

SciFinder检索难点解析

中国科技大学

2017.3.21



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 Abstracts Service

- ACS的分支机构
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市

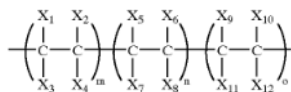


SciFinder对专利的加强

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_1 to X_{12} are hydrogen, fluorine, chlorine, bromine, iodine, CH_3 , CF_3 , 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_1 to X_4 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^1 to X^{12} are hydrogen, fluorine, chlorine, bromine, iodine, CH_3 , CF_3 , 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^1 to X^4 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	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	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		

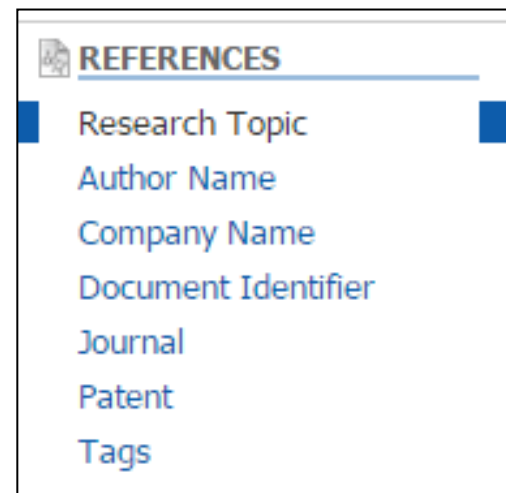
提纲

- 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
 - 避免标引时差引起的漏检

SciFinder检索——文献检索

■ 文献检索方法

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



■ 检索策略推荐

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

利用Inder 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 web interface. At the top, there is a navigation bar with 'CAS Solutions' and the SciFinder logo. Below this is a menu with 'Explore', 'Saved Searches', and 'SciPlanner'. The left sidebar contains two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there is a list of search criteria including 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. The 'Research Topic' option is selected. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field containing the text 'Natural Active Component with Anti Cancer'. Below the input field, there are examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the main content area, there is a link for 'Advanced Search'.

CAS Solutions

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Explore ▼ Saved Searches ▼ SciPlanner

REFERENCES

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

SUBSTANCES

- Chemical Structure
- Markush

REFERENCES: RESEARCH TOPIC ?

Natural Active Component with Anti Cancer

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

Search

Advanced Search

关键词之间用介词连接：in, with, of...

主题检索的候选项

CAS Solutions

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Preferences | SciFinder Help | Sign Out

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Explore | Saved Searches | SciPlanner

Research Topic "Natural Active Component with ..."

REFERENCES ⓘ

Select All Deselect All

1 of 4 Research Topic Candidates Selected

	References
<input checked="" type="checkbox"/> 153 references were found containing the two concepts "Natural Active Component" and "Anti Cancer" closely associated with one another.	153
<input type="checkbox"/> 349 references were found where the two concepts "Natural Active Component" and "Anti Cancer" were present anywhere in the reference.	349
<input type="checkbox"/> 4863 references were found containing the concept "Natural Active Component".	4863
<input type="checkbox"/> 1216569 references were found containing the concept "Anti Cancer".	1216569

Get References

只有153篇吗？

“Concepts”表示对主题词做了同义词的扩展；

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

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

利用Index Term选词

CAS Solutions

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Save | Print | Export

14 duplicates were automatically removed.

Research Topic "Natural Active Component with ..." > references (139)

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 139 References Selected

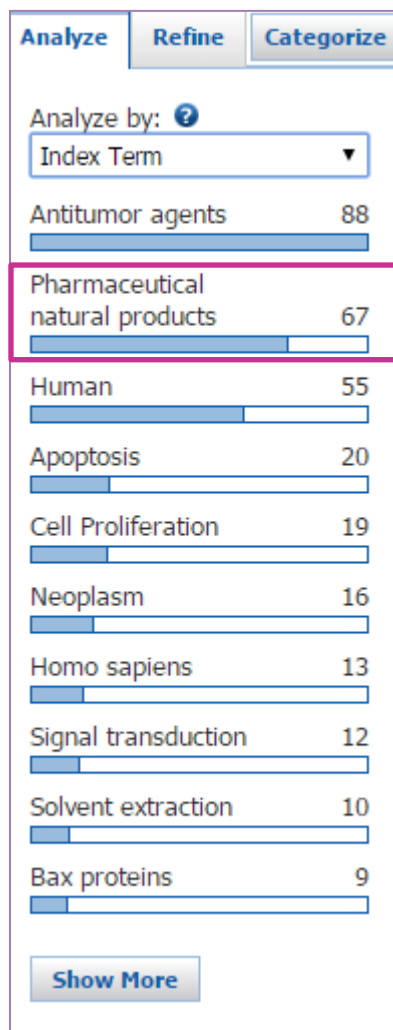
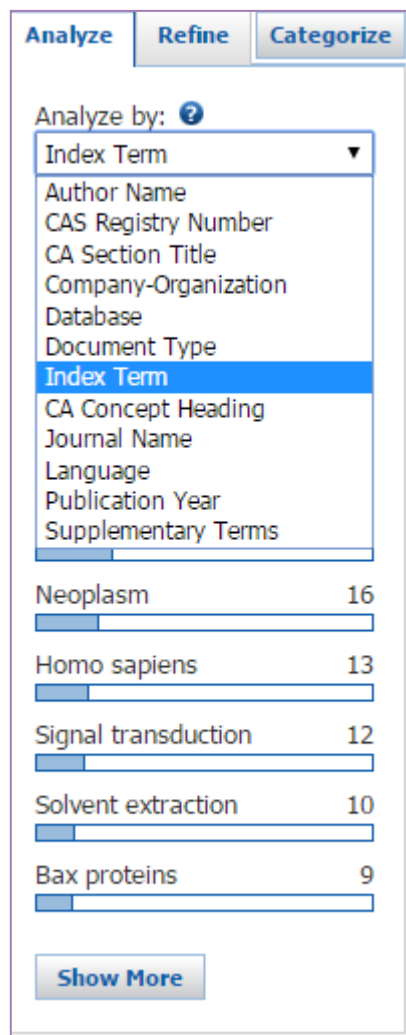
Page: 1 of 7

Analyze by: Author Name

Author	Count
Zhang Yaozhou	4
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. Preparation of staple food containing graviola extract**
PATENTPAK
By Jung, Chan Yeong
From Repub. Korean Kongkae Taeho Kongbo (2016), KR 2016117102 A 20161010. | Language: Korean, Database: CAPLUS
The authors describes an edible food contained graviola ext., which can increase the immune system in the human body and help to eliminate harmful toxic **components** in the human body by the **natural anti-cancer** agents, such as phytochems., acetylcholinesterase and acetogenin as **active** ingredient contained in graviola. Edible foods such as boiled rices, the mixed rice, the rice rolled in dried laver, noodles, Udong, knife-cut noodle, the clear soup with wheat flakes, instant noodle, rice-cake soup, cakes and breads are manufd. through mixing and kneading brown rice, flour, corn, soybean, potato,...
- 2. Effects of psoralen as an anti-tumor agent in human breast cancer MCF-7/ADR cells**
PATENTPAK
By Wang, Xiaohong; Cheng, Kai; Han, Yong; Zhang, Guoqiang; Dong, Jianli; Cui, Yuzhen; Yang, Zhenlin
From Biological & Pharmaceutical Bulletin (2016), 39(5), 815-822. | Language: English, Database: CAPLUS
Psoralen is a major **active component** of Psoralea corylifolia. In the present study, we analyzed psoralen-induced changes in human breast **cancer** MCF-7/ADR cells and investigated the underlying mechanisms of the **anticancer** effect on MCF-7/ADR cells. We measured cell viability by 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay to evaluate the cytotoxicity and multidrug resistance (MDR) reversal **activity** of psoralen. The cell cycle distribution and apoptosis, accumulation and efflux of rhodamine123 (Rh123), and P-glycoprotein (P-gp) expression levels of MCF-7/ADR cells ...
- 3. Skin care liquid containing snake and chinese medicine extract.**
PATENTPAK
By Cheng, Jinxue; Cheng, Gang; Zhu, Jieying

利用Index Term选词



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

是否用这个词去检索，效果会更好？

利用Index Term选词

Explore ▼ Saved Searches ▼ SciPlanner

Research Topic "Natural Active Component with ..." > references (139)

REFERENCES

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

SUBSTANCES

Chemical Name

Mar

REFERENCES: RESEARCH TOPIC ?

Natural Product with anti cancer

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

Search

Advanced Search

新的检索式:

Natural Product with anti cancer

REFERENCES ?

Select All Deselect All

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 19 references were found containing "Natural Product with anti cancer" as entered.	19
<input checked="" type="checkbox"/> 9987 references were found containing the two concepts "Natural Product" and "anti cancer" closely associated with one another.	9987
<input type="checkbox"/> 43362 references were found where the two concepts "Natural Product" and "anti cancer" were present anywhere in the reference.	43362
<input type="checkbox"/> 464095 references were found containing the concept "Natural Product".	464095
<input type="checkbox"/> 1216569 references were found containing the concept "anti cancer".	1216569

Get References

更换检索词后，结果放大近70倍

STN中的CAS Role

ANST Analytical Study

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

PREP Preparation

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

PROC Process

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

BIOL Biological Study

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

STN中的CAS Role

FORM Formation, Nonpreparative

Formation, Unclassified FMU

Geological or Astronomical Formation GFM

NANO Nanomaterial

OCCU Occurrence

Biological Occurrence BOC

Geological or Astronomical Occurrence GOC

Natural Product Occurrence NPO

Occurrence, Unclassified OCU

Pollutant POL

RACT Reactant or Reagent

Reactant RCT

Reagent RGT

USES Uses

Agricultural Use AGR

Analytical Reagent Use ARG

Biological Use, Unclassified BUU

Catalyst Use CAT

Cosmetic Use COS

Diagnostic Use DGN

Food or Feed Use FFD

Modifier or Additive Use MOA

Other Use, Unclassified NUU

Polymer in Formulation POF

Technical or Engineered Material Use TEM

Therapeutic Use THU

巧用CAS Role

查找纯化双氧水（7722-84-1）的文献

Explore ▼ Saved Searches ▼ SciPlanner

Substance Identifier "7722-84-1" > substances (1)

REFERENCES

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

REFERENCES: RESEARCH TOPIC ?

purify of 7722-84-1

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

Explore ▼ Saved Searches ▼ SciPlanner

SUBSTANCES Research Topic "purify of 7722-84-1"

- Chemical Structure
- Markush

REFERENCES ?

Select All Deselect All

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".

Get References

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

REFERENCES ?

Get Substances Get Reactions Get Related ▼ Tools

Display Options

Page: 2 of 107

REFERENCES ?

Analyze Refine Categorize

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

Sort by: Accession Number ▼

☐ 0 of 2126 References Selected

☐ 21. **Zinc oxide concentrate purification**
Quick View PATENTPAK ▼
By Yu, Qiongpeng
From Faming Zhuanli Shenqing (2016), CN 105...
The present invention discloses a zinc oxide concentrate purification method, comprising: evapn. and concn., the prepn. of pre... condition, high product uniformity, low...

☐ 22. **Systematic comparison of conventional and non-conventional purification methods for SWCNT**
Quick View Other Sources
By Clancy, Adam J.; White, Edward R.; Tay, Hu...
From Carbon (2016), 108, 423-432. | Language: English
As-synthesized single-walled carbon nanotubes (SWCNTs) are contaminated with residual catalyst particles. These contaminants have a detrimental effect on the effective mech. and elec. properties of SWCNTs. In this work, a systematic series of SWCNT purifications including acid treatments, oxidative treatments, and SWCNT type (Tuball). Each of the purification procedures was...

☐ 23. **Method for preparing light weight high-efficient supported photocatalyst for air purifier**
Quick View 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 wt. carrier, and prepg. light wt. high-efficient supported photocatalyst for air purifier. The prepn. method...

Save This Answer Set

* Required

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

H₂O₂
Hydrogen peroxide (H₂O₂)

► **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

SCI-FINDER
A CAS SOLUTION

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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

☐ **0 of 14672** References Selected

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

☐ **2. Immobilization of D-amino acid oxidase on mu...**
Quick View Other
By Li, Rong; Sun, Jian; Fu
From Catalysts (2016), 6

Combine Answer Sets

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

43 Answer Sets 1 Selected

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](#)

DER
A CAS SOLUTION

巧用CAS Role

CAS Solutions



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

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Analyze by: Author Name

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

Sort by: Accession Number

0 of 305 References Selected

Display Options

Page: 1 of 16

1. 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.

2. 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 ≥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 ≥2 electrodes, in which ≥1 electrode is a metal electrode and, a power source for powering the ≥2 electrodes. A H₂O treatment system for generating an oxidant in-situ comprising ≥1 electrolytic cell. The electrolytic cell may have ≥2 electrodes, in which ≥1 electrode is a metal electrode, and a power source for powering the ≥2 electrodes. A metho...

3. Residue purification recovery device

Quick View | PATENTPAK

By Li, Wanqing; Zhou, Xuejun; Liu, Jiqian; Gao, Chuanping; 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	Application No.	Date
CN 105749877	 PATENTPAK	A	Jul 13, 2016	7722-84-1P Hydrogen peroxide, preparation 	Page 2 in PATENTPAK
Priority Application				hydrogen peroxide purifn. adsorbent prepn. method	
CN 2015-10852280				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_2O_2 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_2O_2 characterized by passing H_2O_2 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_2O_2), preparation 	Page 2 in PATENTPAK
method of purifying hydrogen peroxide using reverse osmosis membrane and ion exchangers	
Purification or recovery; Preparation	

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REFERENCES: RESEARCH TOPIC ?

remove of 123-39-7

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Photocyanation of aromatic compounds

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SUBSTANCES

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- ☒ 49 references were found containing the two concepts "remove" and "123-39-7" closely associated with one another.
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- ☐ 2808271 references were found containing the concept "remove".
- ☐ 4512 references were found containing the concept "123-39-7".

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善用Categorize

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_x selectivity increased monotonously with increasing ED. But CO_x selectivity of 100% cannot be obtained even with ED higher than 70 J L⁻¹, 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 decompn. 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

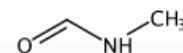
Volatile organic compounds


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

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
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Indexing

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

Concepts

Coating removers

Photoresists

removing agent contg. alkylamide mixt.

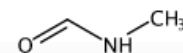
Amides

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

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

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Hong Heon Pyo 2
Legenza Michael Walter 2
Ward Irl E 2
Albrecht Herbert 1
Alsters Paul 1
Aoba Kazuhiro 1

☐ 1. **Removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma**
Quick View Other Sources
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 compns. as well as DMA and DMF concn., CO_x selectivity increased monotonously with increasing E...

☐ 2. **Stripping composition for removing photoresist and a method, for peeling photoresist, using same**
Quick View PATENTPAK
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.

☐ 3. **Removing agent containing alkylamide mixture**
Quick View PATENTPAK
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.%

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Category Heading	Category	Index Terms	Selected Terms
All	Substances in technology (824)	<div>Select All Deselect All</div> <div> <input checked="" type="checkbox"/> N-Methyl formamide 6 <input type="checkbox"/> N,N-Dimethylformamide 3 <input type="checkbox"/> Copper 2 <input type="checkbox"/> Copper alloy 2 <input type="checkbox"/> Dimethylamine 2 <input type="checkbox"/> Formamide 2 <input type="checkbox"/> Oxides (inorganic) 2 <input type="checkbox"/> Polyimides 2 <input type="checkbox"/> 1-Fluoro-1,2,2-trichloroethane 1 <input type="checkbox"/> 2,3-Dimethyl-1-butanol 1 <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 </div>	

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- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
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- Molecular Formula
- Property
- Substance Identifier

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Author Name	Count
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Fridell Robert A	18
Lemm Julie A	18
Sun Jin Hua	18
Wang Chunfu	17
Belema Makonen	16
O Boyle Donald R II	15
Hernandez Dennis	12

1. **Dacatasvir plus sofosbuvir for HCV in patients coinfecting with HIV-1**
Quick View | Other Sources
By Wyles, D. L.; Ruane, P. J.; Sulkowski, M. S.; Dieterich, D.; Luetkemeyer, A.; Morgan, T. R.; Sherman, K. E.; Dretter, R.; Fishbein, D.; Gathe, J. C., Jr.; et al
From New England Journal of Medicine (2015), 373(8), 714-725. | Language: English, Database: CAPLUS

Background: The combination of daclatasvir, a hepatitis C virus (HCV) NS5A inhibitor, and the NS5B inhibitor sofosbuvir has shown efficacy in patients with HCV mono-infection. Data are lacking on the efficacy and safety of this combination in patients coinfecting with human immunodeficiency virus type 1 (HIV-1). Methods: This was an open-label study involving 151 patients who had not received HCV treatment and 52 previously treated patients, all of whom were coinfecting with HIV-1. Previously untreated patients were randomly assigned in a 2:1 ratio to receive either 12 wk or 8 wk of daclatasvir...

2. **Consideration of viral resistance for optimization of direct antiviral therapy of hepatitis C virus genotype 1-infected patients**
Quick View | Other Sources
By Dietz, Julia; Susser, Simone; Berkowski, Caterina; Perner, Dany; Zeuzem, Stefan; Sarrazin, Christoph
From PLoS One (2015), 10(8), e0134395/1-e0134395/17. | Language: English, Database: CAPLUS

Different highly effective interferon-free treatment options for chronic hepatitis C virus (HCV) infection are currently available. Pre-existence of resistance associated variants (RAVs) to direct antiviral agents (DAAs) reduces sustained virologic response (SVR) rates by 3-53% in hepatitis C virus (HCV) genotype 1 infected patients depending on different predictors and the DAA regimen used. Frequencies of single and combined resistance to NS3, NS5A and NS5B inhibitors and consequences for the applicability of different treatment regimens are unknown. Parallel population based sequencing of HCV N...

3. **The novel cyclophilin inhibitor CPI-431-32 concurrently blocks HCV and HIV-1 infections via a similar mechanism of action**
Quick View | Other Sources
By Gallay, Philippe A.; Bobardt, Michael D.; Chatterji, Udayan; Trepanier, Daniel J.; Ure, Daren; Cosme, Foster, Robert
From PLoS One (2015), 10(8), e0134707/1-e0134707/18. | Language: English, Database: CAPLUS

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1. Safety and efficacy of dual direct-acting antiviral therapy (daclatasvir and asunaprevir) for chronic hepatitis C virus genotype 1 infection in patients on hemodialysis

Quick View Other Sources

By Toyoda, Hindeori; Kumada, Takashi; Tada, Toshifumi; Takaguchi, Koichi; Ishikawa, Toru; Tsuji, Kunihiro; Zeniya, Mikio; Iio, Etsuko; Tanaka, Yasuhito
From Journal of Gastroenterology (2016), Ahead of Print. | Language: English, Database: CAPLUS

Background: Hepatitis C virus (HCV) infection is a major comorbidity in patients receiving hemodialysis. Interferon-based antiviral therapy to eradicate HCV is less effective in patients receiving hemodialysis than patients without renal dysfunction. Recently reported combination therapy with two oral direct-acting antiviral drugs, **daclatasvir** and asunaprevir, both of which are metabolized in the liver and excreted into the bile ducts, reportedly showed a high rate of HCV eradication. We evaluated the safety and efficacy of this therapy in patients receiving hemodialysis. Methods: The safe...

2. Management of hepatitis C patients with decompensated liver disease

Quick View Other Sources

By Hsu, Ching-Sheng; Kao, Jia-Horng
From Expert Review of Gastroenterology & Hepatology (2016), Ahead of Print. | Language: English, Database: CAPLUS

Little is known about the tolerance and effectiveness of novel oral direct acting antivirals (DAA) in hepatitis C patients with decompensated cirrhosis. To examine the studies relevant to the treatment of hepatitis C virus(HCV)-related decompensated liver disease, we performed computer-based searches for English articles between 1947 and August 2015. Fourteen articles including HCV patients with decompensated cirrhosis were reviewed. The combinations of ledipasvir(LDV)/sofosbuvir(SOF)/ribavirin(RBV) for 12 wk, or **daclatasvir**/SOF/RBV for 12 wk are safe and effective for HCV genotype 1 or 4 i...

3. Khaya grandifoliola C.DC: a potential source of active ingredients against hepatitis C virus in vitro

Quick View Other Sources

By Galani, Boris Rosnay Tietcheu; Sahuc, Marie-Emmanuelle; Sass, Gabriele; Njayou, Frederic Nico; Loscher, Christine; Mkounga, Pierre; Deloison, Gaspard; Brodin, Priscille; Rouille, Yves; Tiegs, Gisa; et al
From Archives of Virology (2016), Ahead of Print. | Language: English, Database: CAPLUS

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1. Safety and efficacy of dual direct-acting antiviral therapy (daclatasvir and asunaprevir) for chronic hepatitis C virus genotype 1 infection in patients on hemodialysis

By: Toyoda, Hindeori; Kumada, Takashi; Tada, Toshifumi; Takaguchi, Koichi; Ishikawa, Toru; Tsuji, Kunihiko; Zeniya, Mikio; Iio, Etsuko; Tanaka, Yasuhito

Background: Hepatitis C virus (HCV) infection is a major comorbidity in patients receiving hemodialysis. Interferon-based antiviral therapy to eradicate HCV is less effective in patients receiving hemodialysis than patients without renal dysfunction. Recently reported combination therapy with two oral direct-acting antiviral drugs, **daclatasvir** and asunaprevir, both of which are metabolized in the liver and excreted into the bile ducts, reportedly showed a high rate of HCV eradication. We evaluated the safety and efficacy of this therapy in patients receiving hemodialysis. Methods: The safety and viral responses were compared among patients infected with HCV genotype 1, between 28 patients receiving hemodialysis, and propensity score-matched 56 patients without renal dysfunction. Results: The redn. in serum HCV RNA levels 1 day after the start of therapy was significantly larger ($p = 0.0329$) and the disappearance of serum HCV RNA occurred significantly earlier ($p = 0.0017$) in patients receiving hemodialysis than those without renal dysfunction. The rates of sustained viro. response, i.e., the eradication of HCV, were comparable between two groups; the rate of SVR12 was 100 % in patients receiving hemodialysis and 94.6 % in patients without renal dysfunction. No adverse constitutional events were obsd. in either of the groups. The elevation of serum alanine aminotransferase levels, a known adverse effect of these drugs, was obsd. in comparable rate of patients between the two groups. Conclusions: The therapy with **daclatasvir** and asunaprevir has high antiviral efficacy in patients receiving hemodialysis with

Indexing

Pharmacology (Section1)

Citations

Anon; Tada T, Kumada T, Toyoda H, et al Viral eradication reduces all-cause mortality in pat Berenguer, M; Hepatology, 10.1002/hep.22545 2008, 48, 1690
Chayama, K; Hepatology, 10.1002/hep.24724 2012, 55, 724
Deltene, P; Alim Pharmacol Ther, 10.1111/j.1365-2036.2011.04741.x 2011, 34, 454
Espinosa, M; Nephrol Dial Transplant, 10.1093/ndt/16.8.1669 2001, 16, 1669

17. The clinical features of patients with a Y93H variant of hepatitis C virus detected by a PCR invader assay

By: Kan, Toshi; Hashimoto, Senju; Kawabe, Naoto; Murao, Michihito; Nakano, Takuji; Shimazaki, Hiroaki; Nakaoka, Kazunori; Ohki, Masashi; Takagawa, Yuka; Kurashita, Takamitsu; Takamura, Tomoki; Yoshioka, Kentaro

Background: Resistance-assocd. variants (RAVs) reduce the efficacy of interferon (IFN)-free therapy with asunaprevir and **daclatasvir** for patients infected with hepatitis C virus (HCV) genotype 1b. The characteristics of patients with an L31 or a Y93 variant in the nonstructural 5A region detected by a polymerase chain reaction invader assay were investigated. Methods: In total, 201 patients with HCV genotype 1b were examd. for L31F/M/V variants or a Y93H variant by the polymerase chain reaction invader assay. Results: L31M and Y93H variants were detected in 4.6 and 21.4 % of patients, resp. Patients with an L31M variant had no significant characteristics. Patients with a Y93H variant had significantly higher HCV RNA levels (6.5 ± 0.5 log copies per mL vs 6.1 ± 0.7 log copies per mL, $p = 0.0002$), higher frequency of mutant type of the IFN-sensitivity-detg. region (88.4% vs 71.7% , $p = 0.0251$), and higher frequency of TT genotype at rs8099917 of IL28B (91.7% vs 54.3% , $p < 0.0001$) than those with Y93 wild-type strains. Multivariate anal. identified HCV RNA levels [odds ratio (OR) 3.72, 95 % confidence interval (CI) 1.71-8.06, $p = 0.0009$] and TT genotype at rs8099917 (OR 7.45, 95 % CI 2.11-26.4, $p = 0.0018$) as factors assocd. with the presence of a Y93H variant. Conclusion: The presence of a Y93H variant was assocd. with higher HCV RNA levels and TT genotype at rs8099917 of IL28B. Thus, patients with a Y93H variant may be ideal candidates for IFN-based therapy rather than IFN-free therapy, although the high viral load of these patients may reduce the response rate of IFN-based therapy.

Indexing

Immunochemistry (Section15-2)

Section cross-reference(s): 3

Concepts

Animal gene

IL28B; clin. features of patients with a Y93H variant of hepatitis C virus detected by a PCR invader assay

Biological study, unclassified; Properties; Biological study

Aging, animal
Genetic polymorphism
Hepatitis C
Homo sapiens
Immunotherapy
Sex

Blood platelet
Genotypes
Hepatitis C virus
Human
Leukocyte

Substances

57-88-5 Cholesterol, biological studies
60-27-5 Creatinine
635-65-4 Bilirubin, biological studies
9000-86-6 Alanine aminotransferase
9000-97-9 Aspartate aminotransferase
9001-26-7 Prothrombin
9004-61-9 Hyaluronic acid
9046-27-9 γ -GTP

clin. features of patients with a Y93H variant of hepatitis C virus detected by a PCR invader assay

Biological study, unclassified; Biological study

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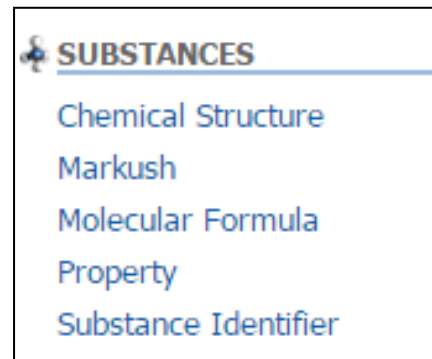
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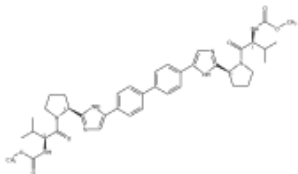
■ 物质检索策略推荐

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

快速获得物质的生物活性及靶点信息

1. 1009119-64-5

~308 ~88



Absolute stereochemistry.

C₄₀ H₅₀ N₈ O₆
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。

合金的检索

检索铁、锰、镍合金

CAS Solutions

SciFinder®

Explore Saved Searches SciPlanner

Substance Identifier "Daclatasvir" > substances (1)

REFERENCES

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

SUBSTANCES

Chemical Structure

SUBSTANCES: MOLECULAR FORMULA

Fe. Mn. Ni

Examples:

H4SiO4

(C3H7O2)

CAS Solutions

SciFinder®

Explore

Saved Searches

SciPlanner

Preferences | SciFinder Help

Sign Out

Welcome Helen Zhu

Save

Print

Export

Molecular Formula "Fe . Mn . Ni" > substances (1095)

SUBSTANCES

Get References

Get Reactions

Get Commercial Sources

Tools

Create Keep Me Posted Alert

Send to SciPlanner

Sort by: CAS Registry Number

0 of 1095 Substances Selected

Page: 1 of 73

Analyze Refine

Analyze by:

Substance Role

Uses 649

Properties 634

Process 423

Preparation 76

Reactant or Reagent 9

Miscellaneous 8

Analytical Study 4

Occurrence 2

Biological Study 1

Formation, Nonpreparative 1

1. 1850365-63-7

~1

Component	Component Percent
Fe	80
Mn	16
Ni	5

Fe . Mn . Ni
Iron alloy, base, Fe 80,Mn 16,Ni 5

4. 1821204-48-1

~1

Component	Component Percent
Mn	60
Ni	25
Fe	15

2. 1835656-90-0

~1

Component	Component Percent
Fe	92
Ni	8.3
Mn	0.1

Fe . Mn . Ni
Iron alloy, base, Fe 92,Ni 8.3,Mn 0.1

5. 1818872-06-8

~1

Component	Component Percent
Fe	65
Ni	35
Mn	0.5

3. 1835656-89-7

~1

Component	Component Percent
Fe	91
Ni	8.4
Mn	0.1

Fe . Mn . Ni
Iron alloy, base, Fe 91,Ni 8.4,Mn 0.1

6. 1816304-50-3

~1

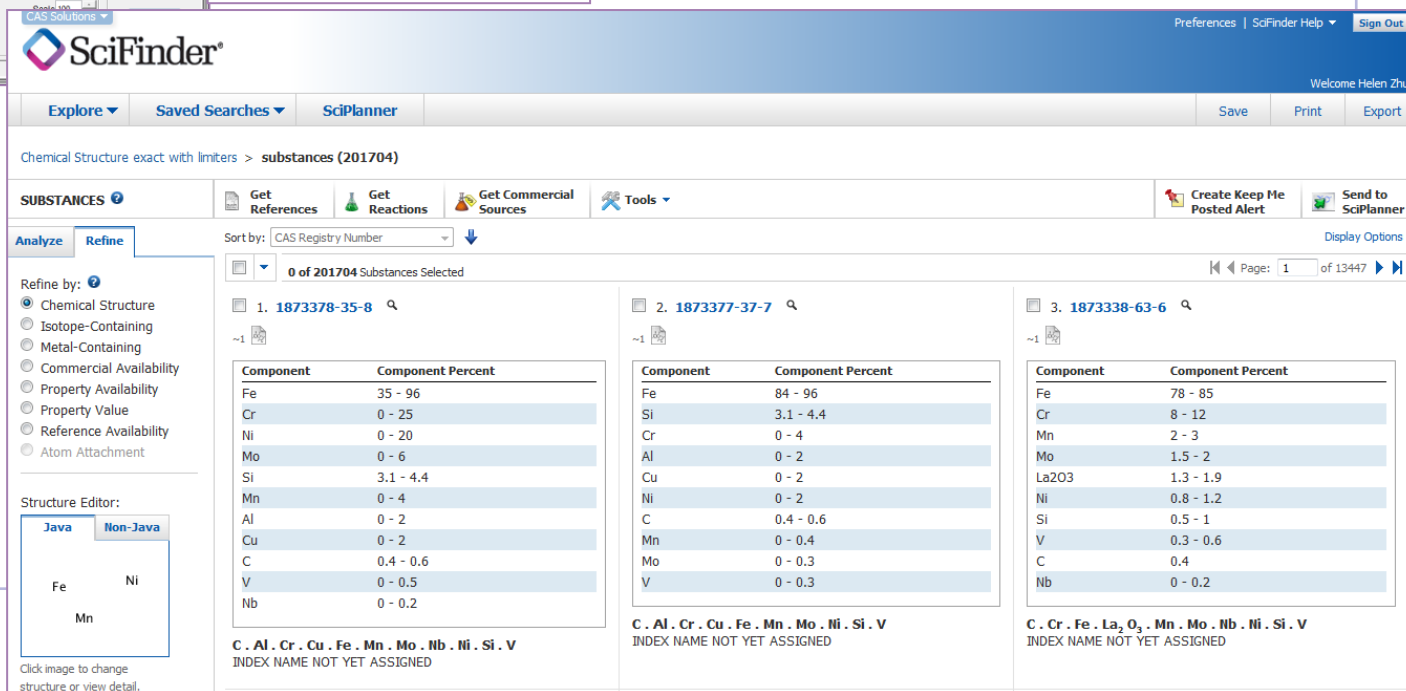
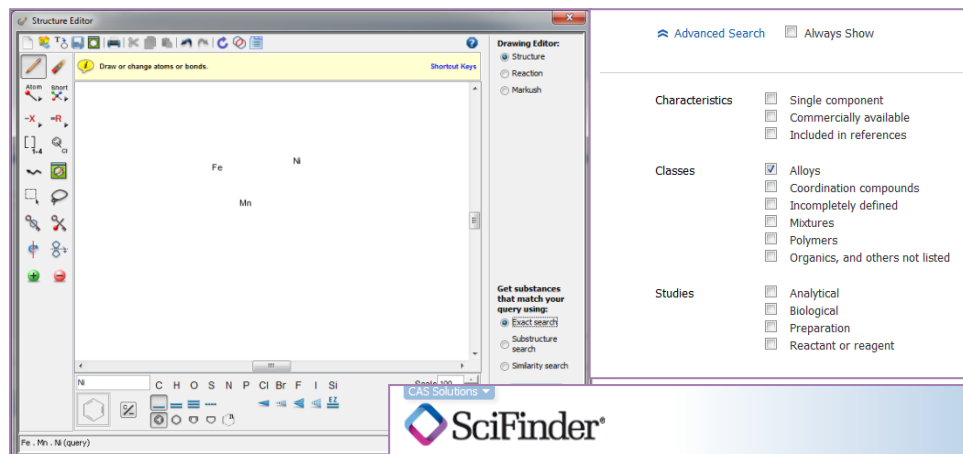
Component	Component Percent
Fe	72
Ni	25
Mn	2.9

Click to view detail

合金物质以列表形式呈现

合金的检索

检索参杂铁、锰、镍原子的合金



Chemical Structure exact with limiters > substances (201704)

Substances: 0 of 201704 Substances Selected

Sort by: CAS Registry Number

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 . La₂O₃ . Mn . Mo . Nb . Ni . Si . V
INDEX NAME NOT YET ASSIGNED

复杂无机物的检索

检索(N H₄) Sm (S O₄)₂ (H₂ O)₄, Ammonium Samarium Bis(sulfate(VI)) Tetrahydrate

CAS Solutions ▾
 **SCIFINDER**
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

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

SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

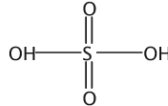
REACTIONS
Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

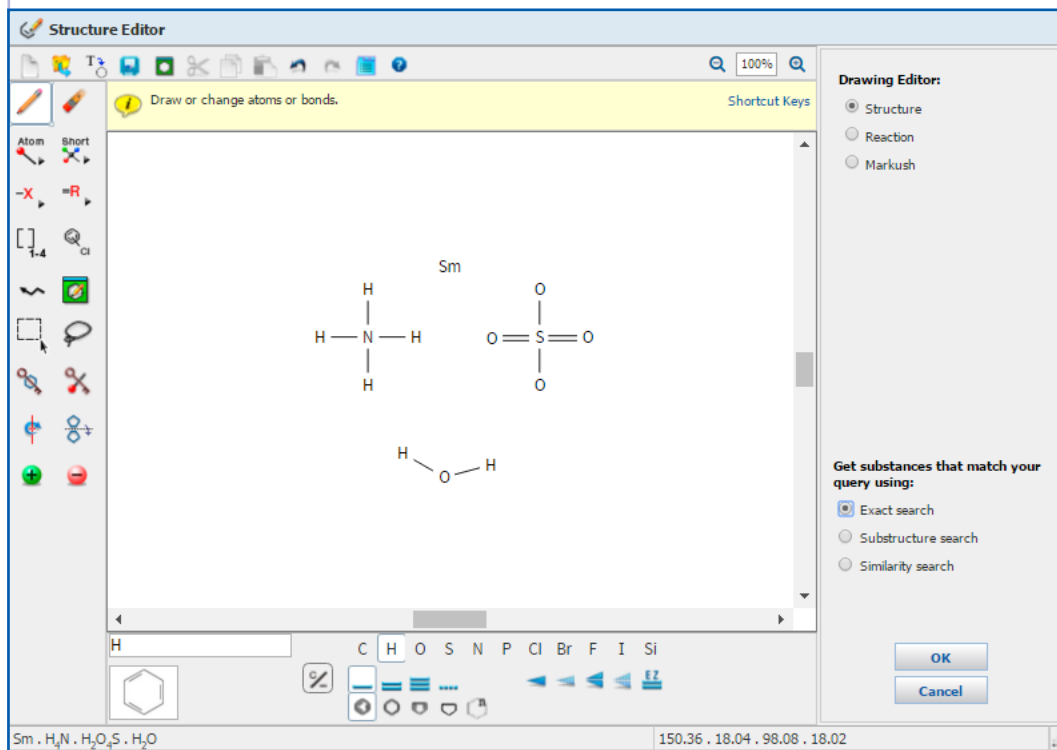
1. 34370-41-7
(Component: 7664-93-9)



- 1/2 NH₃
- 2 H₂O
- 1/2 Sm(III)

H₃N · 2 H₂O₄S · 4 H₂O · Sm
Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)

复杂无机物的检索



限定为单一组分




精确结构检索

复杂无机物的检索

Sort by: CAS Registry Number ↑

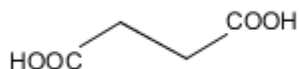
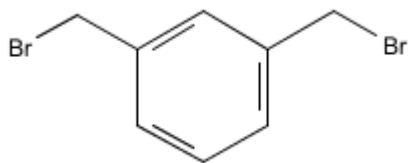
0 of 5 Substances Selected

倒序排列

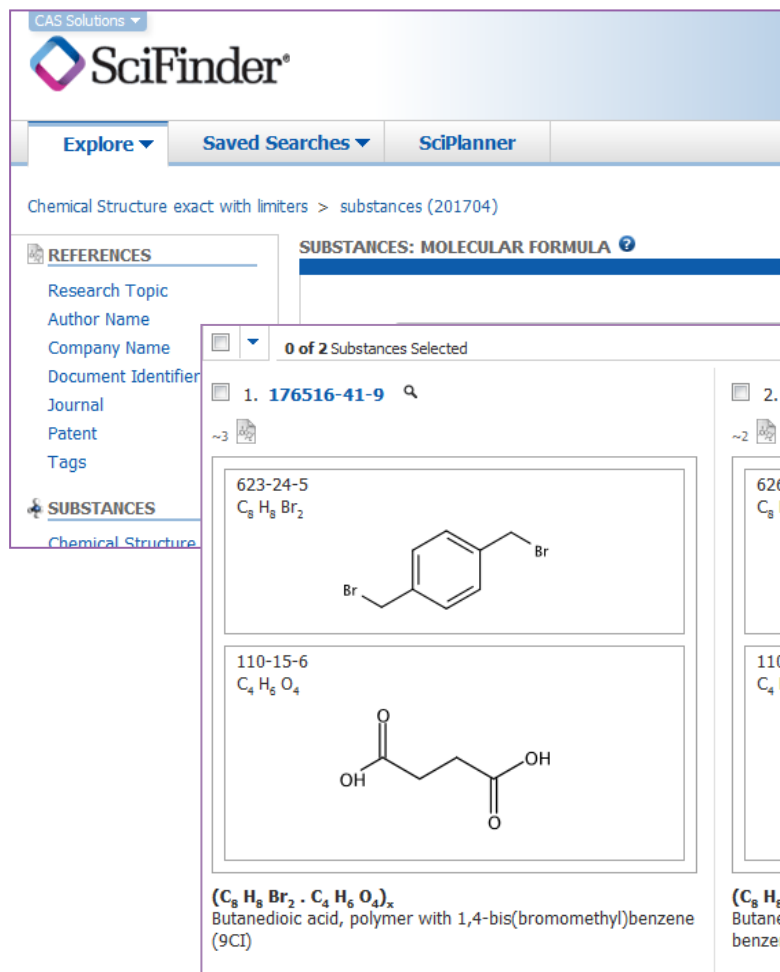
<p>1. 34370-41-7</p> <p>(Component: 7664-93-9)</p> <p>~12</p>  <ul style="list-style-type: none"> • 1/2 NH₄ • 2 H₂O • 1/2 Sm(III) <p>H₃N · 2 H₂O₄S · 4 H₂O · Sm Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)</p>	<p>2. 40148-71-8</p> <p>(Component: 7664-93-9)</p> <p>~1</p>  <ul style="list-style-type: none"> • NH₄ • 1/3 H₂O • 1/3 Sm(III) <p>H₃N · H₂O₄S · 1/3 H₂O · 1/3 Sm Sulfuric acid, ammonium samarium(3+) salt (3:3:1), monohydrate (9CI)</p>	<p>3. 40148-74-1</p> <p>(Component: 7664-93-9)</p> <p>~1</p>  <ul style="list-style-type: none"> • 1/2 NH₄ • H₂O • 1/2 Sm(III) <p>H₃N · 2 H₂O₄S · 2 H₂O · Sm Sulfuric acid, ammonium samarium(3+) salt (2:1:1), dihydrate (9CI)</p>	<p>4. 42949-48-4</p> <p>(Component: 736080-59-4)</p> <p>~1</p>  <ul style="list-style-type: none"> • NH₄⁺ • H₂O <p>(H₃O₁₁S₂Sm · H₄N · H₂O)_n Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium monohydrate, homopolymer (9CI)</p>
<p>5. 49856-58-8</p> <p>(Component: 736080-59-4)</p> <p>~0</p>  <ul style="list-style-type: none"> • NH₄⁺ • H₂O <p>H₈O₁₁S₂Sm · H₄N · H₂O Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium monohydrate (9CI)</p>			

聚合物的检索

已知起始原料的聚合物



$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$



CAS Solutions

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure exact with limiters > substances (201704)

REFERENCES

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

SUBSTANCES

Chemical Structure

0 of 2 Substances Selected

1. 176516-41-9

623-24-5
 $C_8H_8Br_2$

110-15-6
 $C_4H_6O_4$

$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$
Butanedioic acid, polymer with 1,4-bis(bromomethyl)benzene (9CI)

2. 132010-54-9

626-15-3
 $C_8H_8Br_2$

110-15-6
 $C_4H_6O_4$

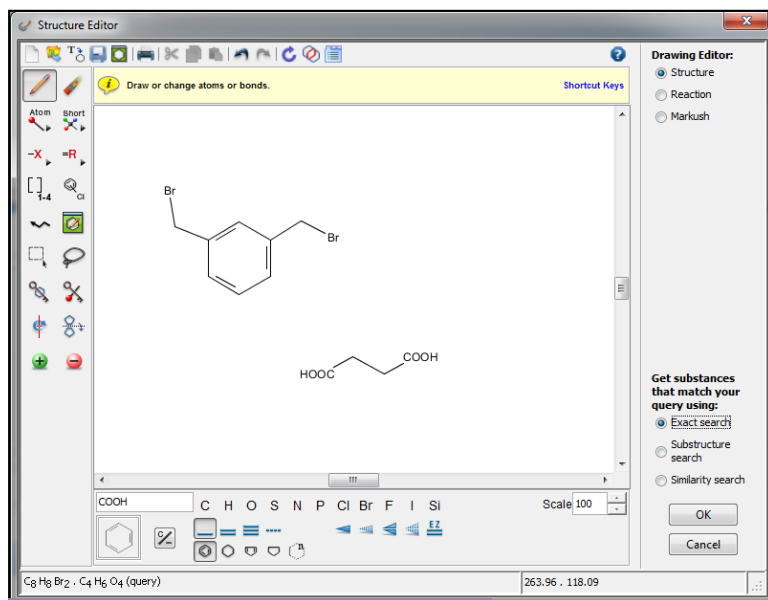
$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$
Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

分子式检索后会得到同分异构体



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A CAS SOLUTION

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

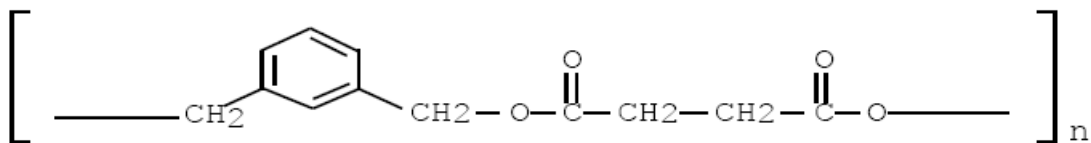
626-15-3
C₈ H₈ Br₂

110-15-6
C₄ H₆ O₄

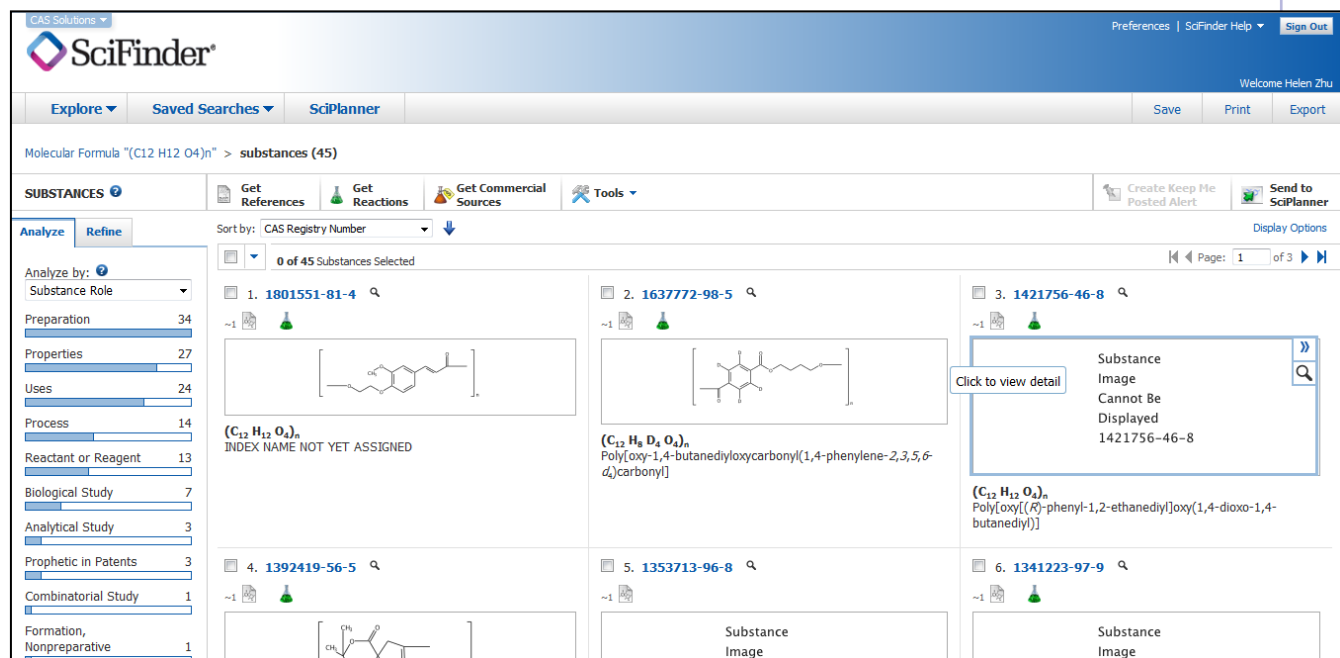
(C₈ H₈ Br₂ . C₄ H₆ O₄)_x
 Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

聚合物的检索

已知重复单元的聚合物



(C₁₂ H₁₂ O₄)_n



The screenshot displays the SciFinder web interface. The search criteria are set to "Molecular Formula (C₁₂ H₁₂ O₄)_n" and "substances (45)". The results are sorted by "CAS Registry Number". The interface shows a list of substances with their CAS numbers, chemical structures, and names. The first three results are highlighted:

- 1. 1801551-81-4: $(\text{C}_{12} \text{H}_{12} \text{O}_4)_n$, INDEX NAME NOT YET ASSIGNED
- 2. 1637772-98-5: $(\text{C}_{12} \text{H}_8 \text{O}_4)_n$, Poly[oxy-1,4-butanediylloxycarbonyl(1,4-phenylene-2,3,5,6-*q*)carbonyl]
- 3. 1421756-46-8: $(\text{C}_{12} \text{H}_{12} \text{O}_4)_n$, Poly[oxy[(*R*)-phenyl-1,2-ethanediyl]oxy(1,4-dioxo-1,4-butanediyl)]

The interface also includes a sidebar with "Analyze" and "Refine" options, and a "Substance Image" section for each result.

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

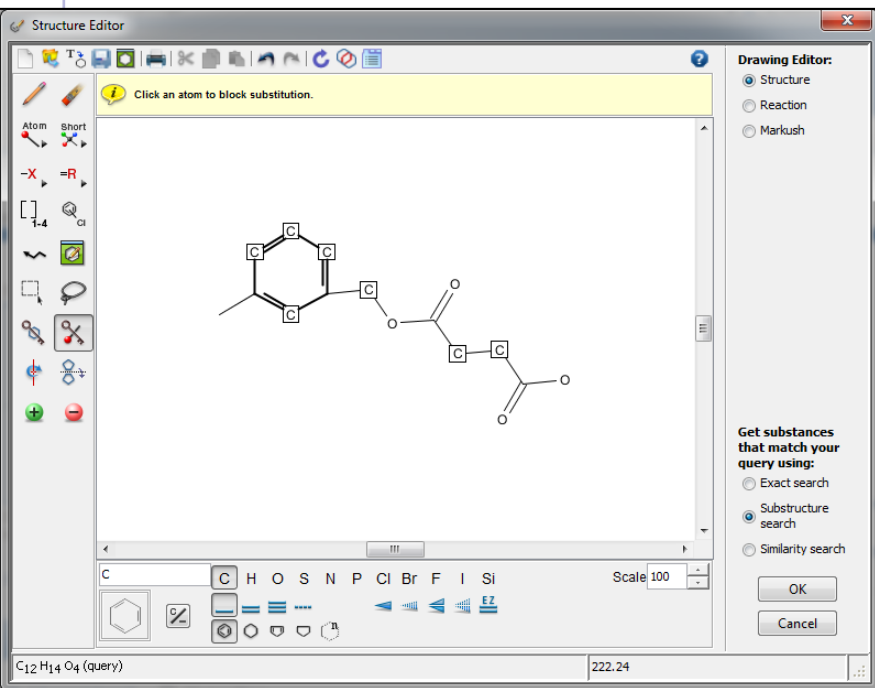
1. 132010-11-8

~2

(C₁₂ H₁₂ O₄)_n
Poly[oxy(1,4-dioxo-1,4-butanediyl)oxymethylene-1,3-phenylenemethylene] (9CI)

利用结构特征进行Refine，迅速查找需要的物质

聚合物的检索



- | | |
|-----------------|--|
| 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

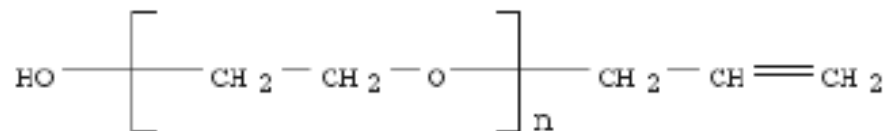
聚合物

绘制好SRU后用亚结构检索
因为两段为开放状态

(C₁₂H₁₂O₄)_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

SUBSTANCES: MOLECULAR FORMULA ?

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

Examples:
H₄SiO₄
(C₃H₆O.C₂H₄O)_x

Search



SRU部分

两端部分

0 of 4 Substances Selected

1. 1500029-22-0

~3

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

2. 191403-44-8

~5

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

3. 50856-25-2

~57

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

4. 27274-31-3

~1115

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

聚合物的检索

后处理聚合物的检索：

检索对由2, 5-呋喃二酮和苯乙烯聚合而成的物质进行结构修饰的聚合物

检索策略：

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

聚合物的检索

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Characteristics

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

Classes

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

Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

0 of 15 Substances Selected

1. **9011-13-6**

~10088 ~8

108-31-6
C₄ H₂ O₃

100-42-5
C₈ H₈

(C₈ H₈ · C₄ H₂ O₃)_x
2,5-Furandione, polymer with ethenylbenzene

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. **31075-11-3**

~1

100-42-5
C₈ H₈

24937-72-2
(C₄ H₂ O₃)_x

108-31-6
C₄ H₂ O₃

C₈ H₈ · (C₄ H₂ O₃)_x
Maleic anhydride, telomer with styrene (8CI)

3. **36512-28-4**

~3

108-31-6
C₄ H₂ O₃

9003-53-6
(C₈ H₈)_x

100-42-5
C₈ H₈

(C₈ H₈)_x · C₄ H₂ O₃
2,5-Furandione, telomer with ethenylbenzene (9CI)

4. **96411-80-2**

~1

19361-62-7
C₈ D₈

(C₈ D₈ · C₄ H₂ O₃)_x
2,5-Furandione, polymer with ethenyl-*d*₅-benzene-*d*₅ (9CI)

108-31-6
C₄ H₂ O₃

5. **106209-33-0**

~587

108-31-6
C₄ H₂ O₃

6. **112020-31-2**

~161

108-31-6
C₄ H₂ O₃

7. **128162-14-1**

~44

108-31-6
C₄ H₂ O₃

8. **145678-57-5**

~3

108-31-6
C₄ H₂ O₃

聚合物的检索

Explore ▾

Saved Searches ▾

SciPlanner

Chemical Structure exact with limiters > substances (15)

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

REFERENCES: RESEARCH TOPIC ?

9011-13-6D

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

REFERENCES ?

Get Substances

Get Reactions

Get Related Citations ▾

Tools ▾

Create Keep Me Posted Alert

Send to SciPlanner

Analyze Refine Categorize

Analyze by: ?

Author Name ▾

Konishi Kunihiro 24

Maeda Hiroshi 20

Yagi Norio 20

Chiba Takashi 19

Kitsunai Tomoyuki 18

Tong Wei 17

Kurokawa Kinya 16

Cao Min 15

Niimura Tetsuya 15

Sun Donghai 15

Show More

Sort by: Accession Number ▾

0 of 2013 References Selected

Page: 1 of 101

1. Lubricant composition comprising branched diesters and viscosity index improver

Quick View PATENTPAK ▾

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

From PCT Int. Appl. (2017), WO 2017021332 A1 20170209. | Language: English, Database: CAPLUS

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

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

Quick View PATENTPAK ▾

By Sakaguchi, Takeshi; Ogiwara, Naoto; Tosaki, Koichi; Kishi, Hiromasa; Kobayashi, Hidenobu

From Jpn. Tokkyo Koho (2017), JP 6074698 B1 20170208. | Language: Japanese, Database: CAPLUS

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

3. Lubricant composition comprising branched diesters and viscosity index improver

Quick View PATENTPAK ▾

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

From Eur. Pat. Appl. (2017), EP 3124579 A1 20170201. | Language: English, Database: CAPLUS

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

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

Quick View PATENTPAK ▾

By Yoshino, Hiroaki; Yanagida, Makoto

From Jpn. Kokai Tokkyo Koho (2017), JP 2017019906 A 20170126. | Language: Japanese, Database: CAPLUS

Title compn. comprises (A) a polyimide curing agent which is a polyimide compd. obtd. by reacting (a) a maleimide compd. having at least two N-substituted maleimide groups in one mol., (b) an aniline compd. having two arom. amino groups in one mol. and (c) an aminophenol compd. having one arom. amino group and at least one arom. hydroxyl group in one mol. in a mole ratio of [(a): (b): (c)] 4.0: 0.1-1.0: 0.1-1.0, and having bonding degree of 7 calcd. from the formula: bonding degree = wt. av. mol. wt./charged av. mol. wt.

聚合物的检索

1. Lubricant composition comprising branched diesters and viscosity index improver

By: Sanson, Julien; Champagne, Nicolas; Benard, Francois
Assignee: Total Marketing Services, Fr.

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

Patent Information

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

Priority Application

EP 2015-179371	A	Jul 31, 2015
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Indexing

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

Concepts

Base oils Crankcase oil
Lubricating oil additives Transesterification

lubricant compn. comprising branched diesters and viscosity index improver

Polyolefins

lubricant compn. comprising branched diesters and viscosity index improver

Modifier or additive use; Uses

Lubricating oil additives

viscosity improvers: lubricant compn. comprising branched diesters and viscosity index

Substances

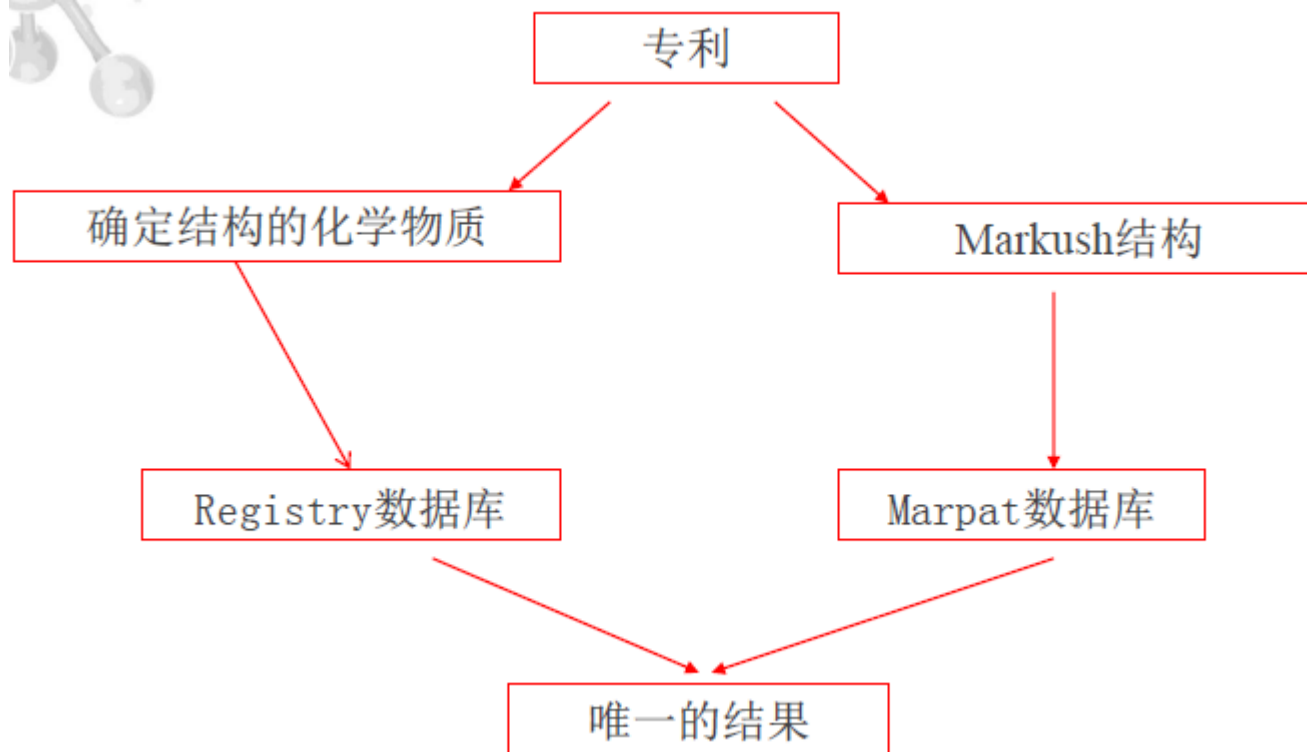
78-79-5D Isoprene, polymers
106-99-0D Butadiene, polymers
9003-31-0D Polyisoprene, hydrogenated
9011-13-6D Styrene-maleic anhydride copolymer, **esters**
25038-32-8D Isoprene-styrene copolymer, hydrogenated

lubricant compn. comprising branched diesters and viscosity index improver

Modifier or additive use; Uses

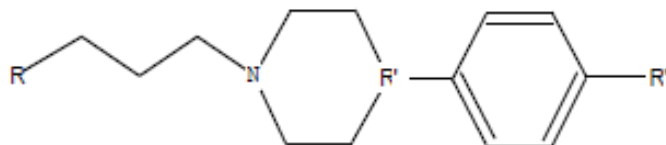
64-18-6 Formic acid
124-07-2 Octanoic acid
143-07-7 Dodecanoic acid
157336-71-5
1637033-75-4

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:

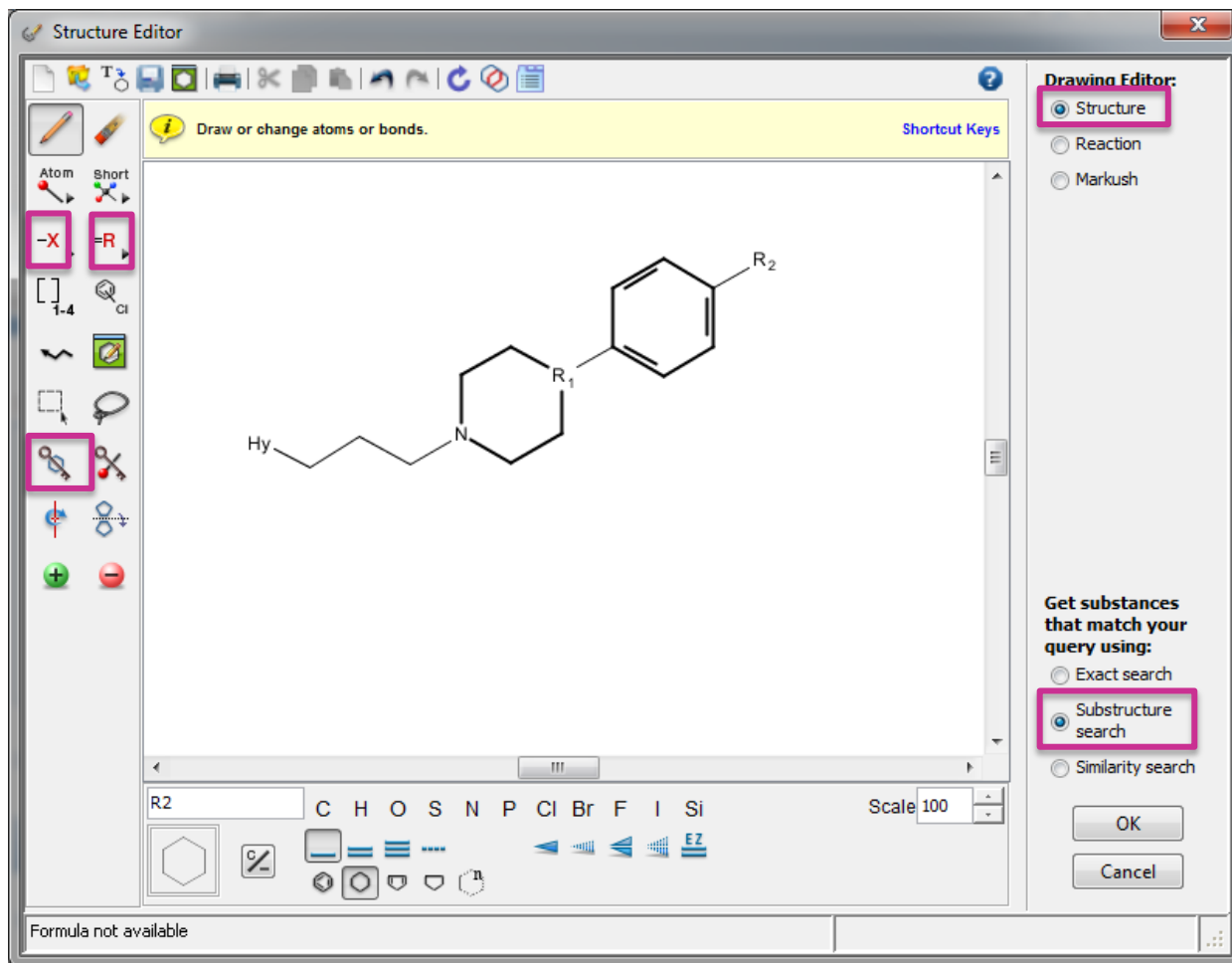
- R = 任意杂环
- R' = C, N, P
- R'' = C, N
- 6 圆环均为单环
- 价键不饱和的地方均允许有取代

SciFinder结构编辑器

The image shows the SciFinder Structure Editor interface with various tools labeled in Chinese. The labels are as follows:

- 橡皮 (Eraser)
- 结构 and 反应切换功能 (Structure and Reaction Switching Function)
- 铅笔 (Pencil)
- 元素周期表 (Periodic Table)
- 可变基团 (Variable Group)
- 重复基团工具 (Repeat Group Tool)
- 碳链工具 (Carbon Chain Tool)
- 选择工具 (Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 旋转工具 (Rotation Tool)
- 正电子 (Positron)
- C原子和单键恢复工具 (C Atom and Single Bond Recovery Tool)
- 常用基团 (Common Group)
- R基团定义工具 (R Group Definition Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 模版工具 (Template Tool)
- 索套选择工具 (Loop Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 负电子 (Electron)
- 常见环, 多元环工具 (Common Ring, Polycyclic Tool)
- 结构检索选择 (Structure Search Selection)

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

CAS Solutions

SciFinder®

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

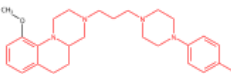
Prophetic in Patents 41

Combinatorial Study 22

Process 3

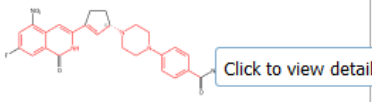
Show More

1. 1873376-11-4



$C_{27}H_{38}N_4O$
INDEX NAME NOT YET ASSIGNED

2. 1868051-25-5

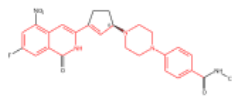


Absolute stereochemistry.

$C_{26}H_{26}F N_5 O_4$
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

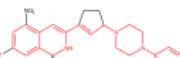


Absolute stereochemistry.

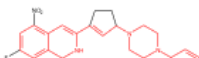
$C_{26}H_{26}F N_5 O_4$
Benzamide, 4-[4-[(1*R*)-3-(7-fluoro-1,2-dihydro-5-nitro-1-oxo-3-isoquinolinyl)-2-cyclopenten-1-yl]-1-piperazinyl]-*N*-methyl-

Key Physical Properties

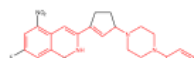
4. 1868051-23-3



5. 1868051-22-2



6. 1868051-02-8



检索具有相同结构特征物质及专利文献



Welcome Helen Zhu

Explore ▾

Saved Searches ▾

SciPlanner

Save

Print

Export

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

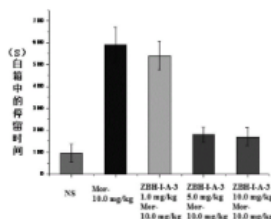
Patent

1. Hexahydro-pyrazino quinolines D3 acceptor 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



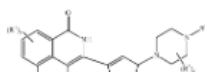
Title compds. I [wherein A = (CH₂)_n, n is 2 to 4; R = H, 4-Cl, 2,3-diCl, 4-CH₃, 2,3-diCH₃, 4-OCF₃, 4-OCH₃, 2-OCF₃, 2,6-diCH₃, 3,4-diCH₃, 3-CF₃, 4-Cl, 3-OCH₃, 2-C₂H₅, or 2-CH₃], and their pharmaceutically acceptable salts thereof, were prepd. as D3 acceptor ligands, which are used for treating nervous centralis mental disorder such as Parkinson's disease, schizophrenia, drug dependence and etc. effectively. Thus, the invention compd. I [A = (CH₂)₂; R = H] was prepd. and gave a D3 acceptor K_i 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

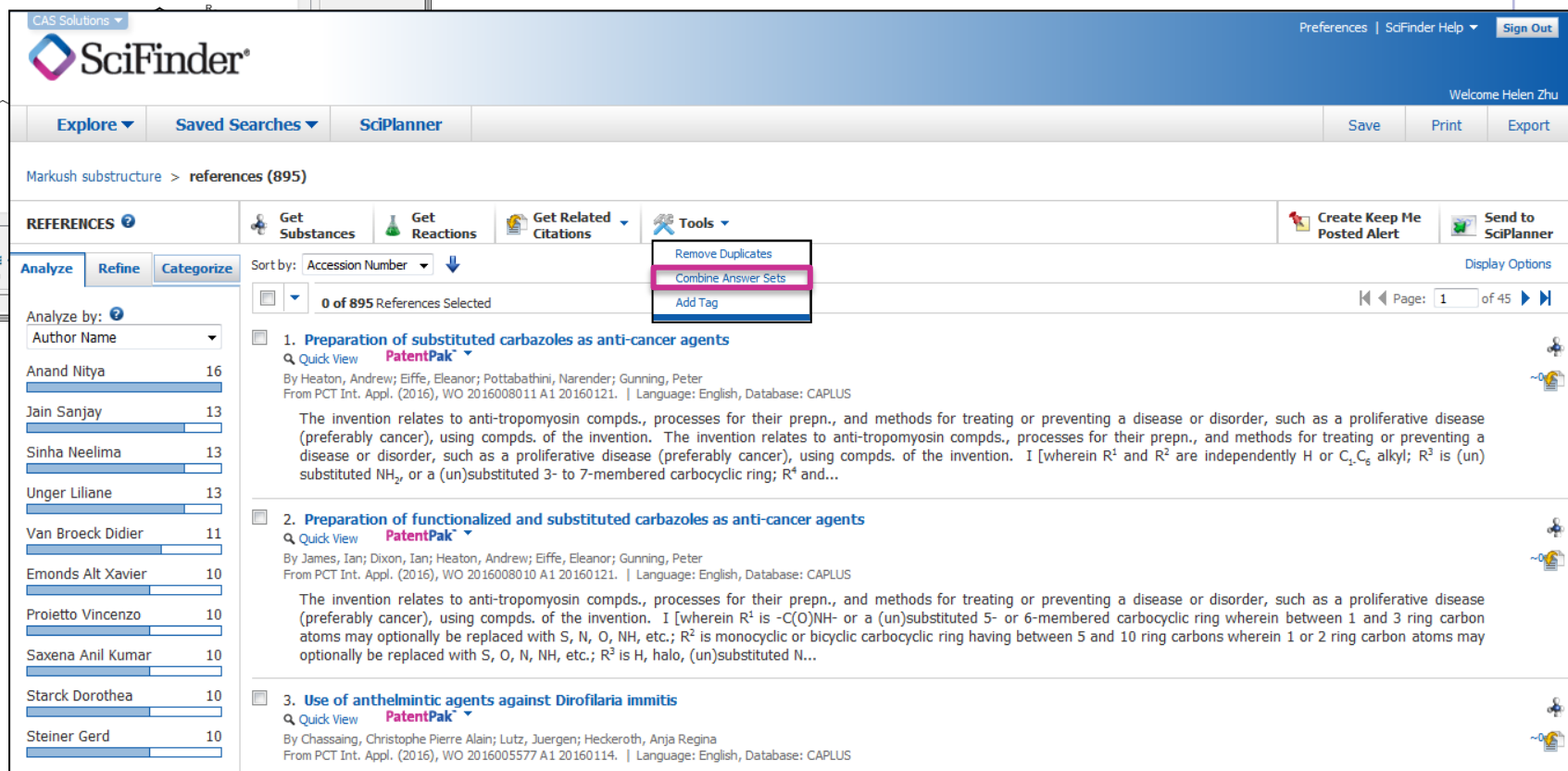
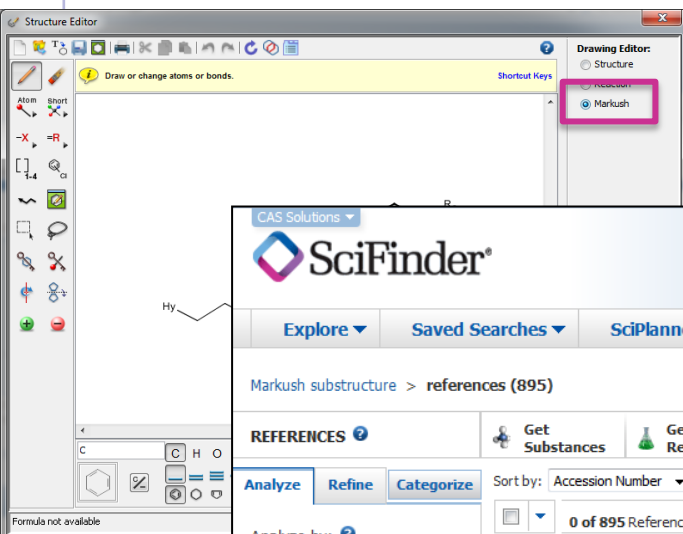


Disclosed are compds. of formula I, their tautomeric forms, stereoisomers, and pharmaceutically acceptable salts thereof, pharmaceutical compns. including a compd., tautomer, stereoisomer, or salt thereof, and methods of treating or preventing diseases or disorders, for example, cancer, that are amenable 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 R¹ is independently halo, CN, NO₂, perfluoroalkyl, acyl, etc.; R²

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



SciFinder®

Markush substructure > references (895)

REFERENCES

Analyze Refine Categorize

Analyze by: Author Name

Author	Count
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

1. Preparation of substituted carbazoles as anti-cancer agents

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

From PCT Int. Appl. (2016), WO 2016008011 A1 20160121. | Language: English, Database: CAPLUS

The invention relates to anti-tropomyosin compds., processes for their prep., and methods for treating or preventing a disease or disorder, such as a proliferative disease (preferably cancer), using compds. of the invention. The invention relates to anti-tropomyosin compds., processes for their prep., and methods for treating or preventing a disease or disorder, such as a proliferative disease (preferably cancer), using compds. of the invention. I [wherein R¹ and R² are independently H or C₁-C₆ alkyl; R³ is (un)substituted NH₂, or a (un)substituted 3- to 7-membered carbocyclic ring; R⁴ and...

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

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

From PCT Int. Appl. (2016), WO 2016008010 A1 20160121. | Language: English, Database: CAPLUS

The invention relates to anti-tropomyosin compds., processes for their prep., and methods for treating or preventing a disease or disorder, such as a proliferative disease (preferably cancer), using compds. of the invention. I [wherein R¹ 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.; R² 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.; R³ is H, halo, (un)substituted N...

3. Use of anthelmintic agents against *Dirofilaria immitis*

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

From PCT Int. Appl. (2016), WO 2016005577 A1 20160114. | Language: English, Database: CAPLUS

与前一个结果集合并，得到完整的结果集

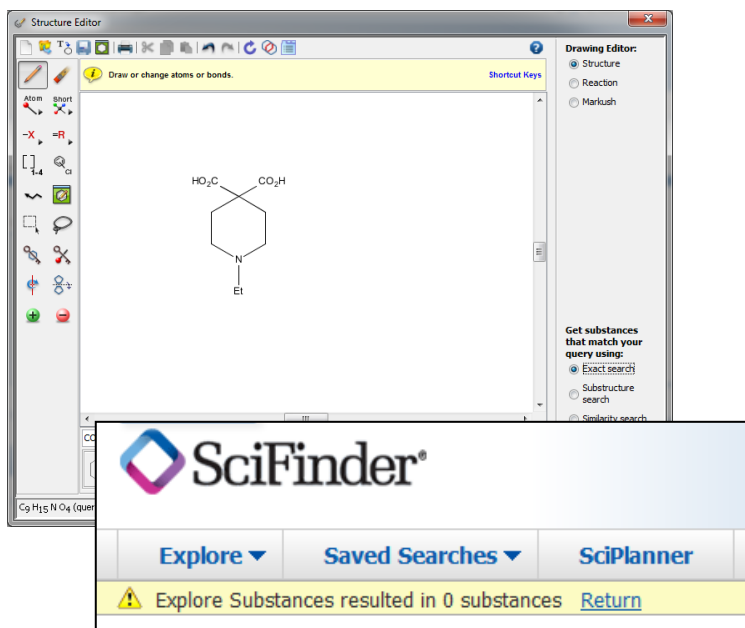
如何判断结构的新颖性

新颖性：是否存在？是否能申请专利？

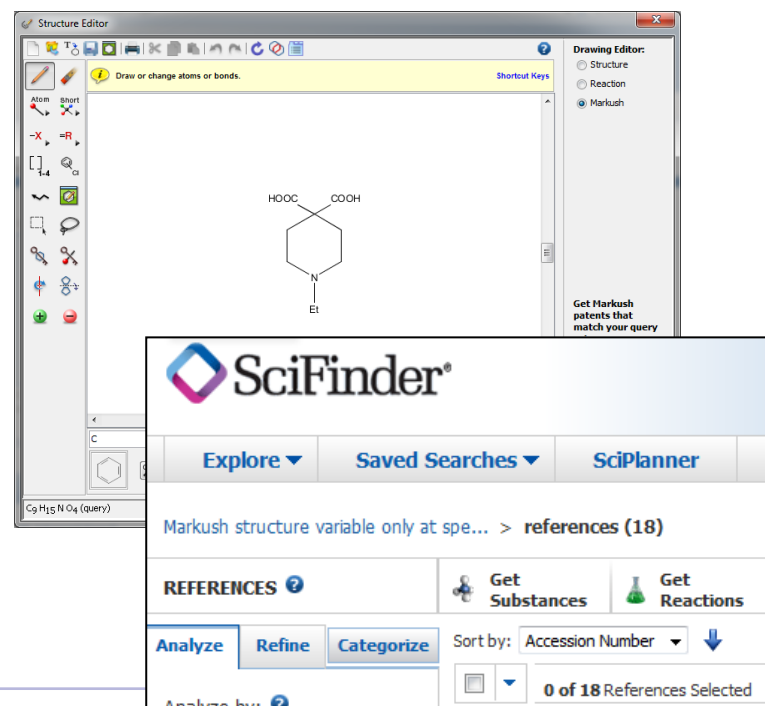
SciFinder相关物质库：Registry和Marpat

检索方法：物质检索？Markush检索？

Step1



Step1



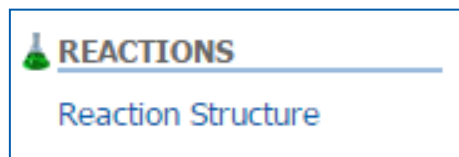
提纲

- 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
 - 直接检索反应受限时如何处理
 - 案例分析

SciFinder检索选项——反应检索

- 反应检索方法

结构式



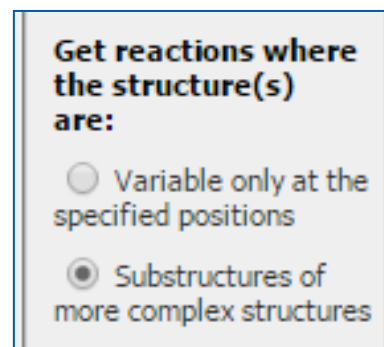
- 常用获取方法

已知物质：由物质获取反应

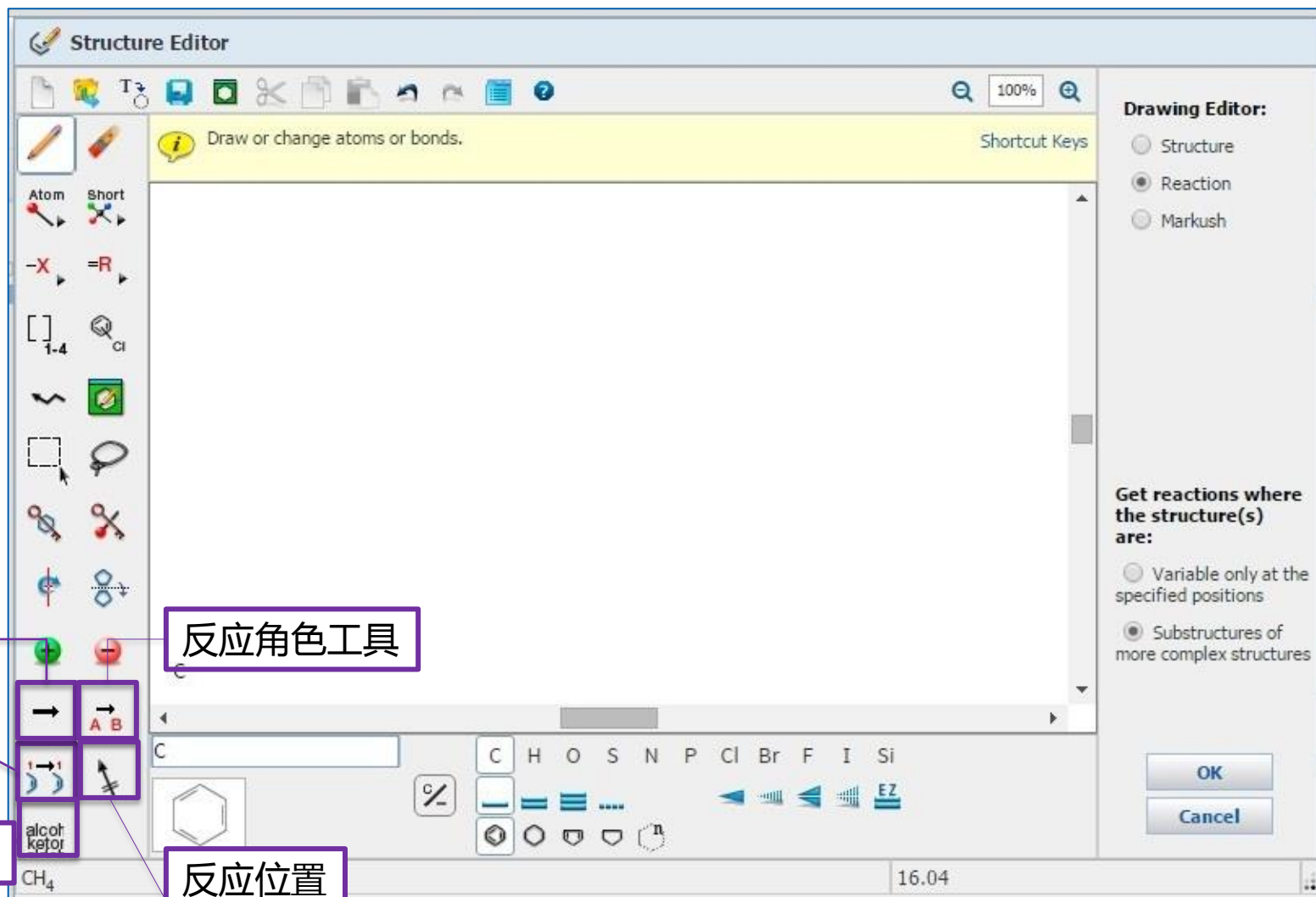
已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索

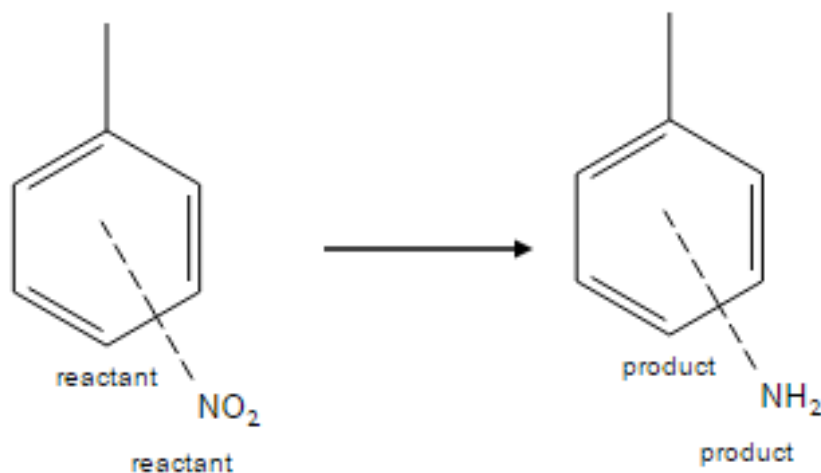


反应绘制工具



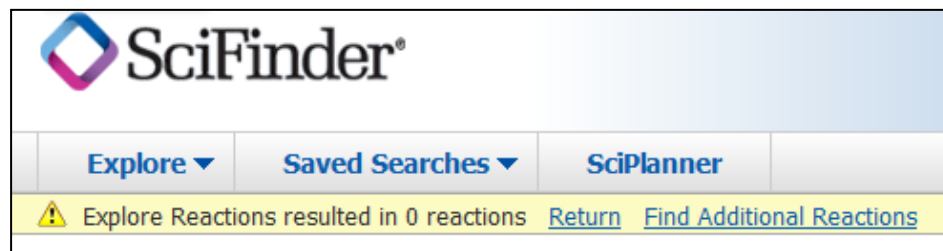
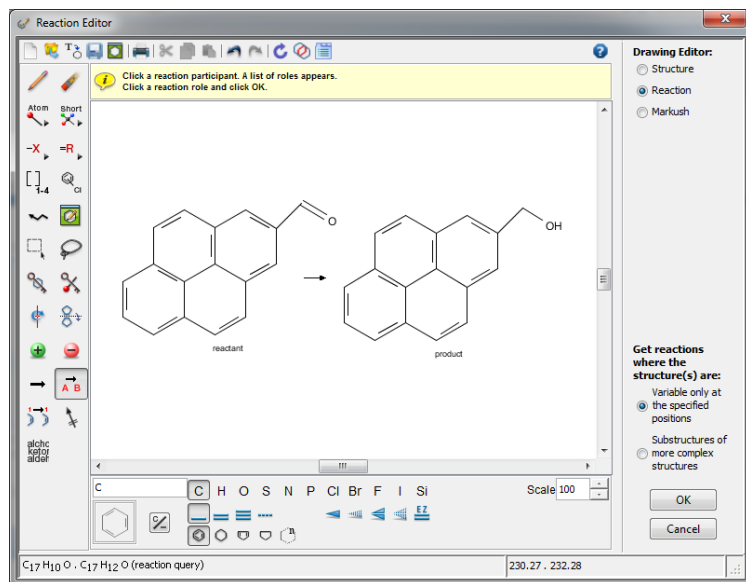
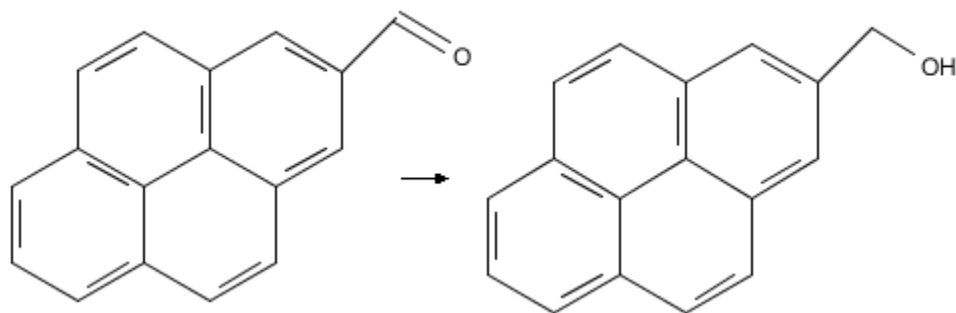
反应的精准定义

检索符合以下要求的反应，硝基还原

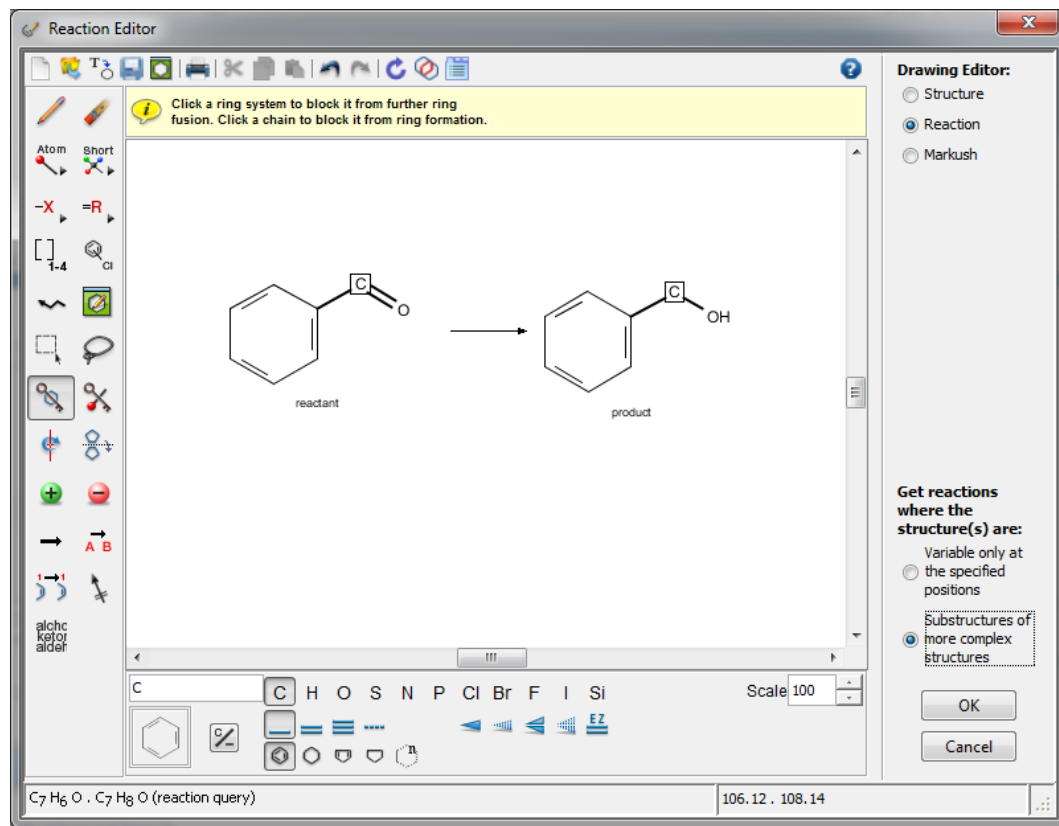


巧妙获得有实验步骤的相关反应

该还原反应如何操作？



巧妙获得有反应步骤的相关反应



聚焦反应关键部位，查找相似反应

巧妙获得有反应步骤的相关反应

The screenshot displays the SciFinder web interface. At the top, the navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main search path is 'Reaction Structure substructure > reactions (60953) > refine "1 step" (14724)'. The left sidebar shows a 'Sample Analysis' section with a list of reagents and their counts: NaBH₄ (≥ 9683), HCl (≥ 7777), K₂CO₃ (≥ 6658), Et₃N (≥ 4779), H₂O (≥ 4266), NaOH (≥ 3980), NH₄Cl (≥ 3438), LiAlH₄ (≥ 3182), H₂ (≥ 2661), and NaHCO₃ (≥ 2580). The 'Analyze' tab is active, showing a 'Refine' section with 'Experimental Procedure' selected. The 'Overview Steps/Stages' section lists '1.1 R:KOH, C:1'. The main reaction list shows '0 of 14724 Reactions Selected'. The 'Single Step' section displays a reaction scheme: benzaldehyde (C₆H₅CHO) reacting to form benzyl alcohol (C₆H₅CH₂OH) with a 100% yield. The reaction conditions are '1.1 R:KOH, C:1820757-77-4, S:Me₂CHOH, S:MeCN, 3 h, 80°C'. The 'Notes' section mentions 'optimization study, optimized on catalysts, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1'. The 'References' section lists 'Complexes of (η⁶-benzene)ruthenium(II) with 1,4-bis(phenylthio/seleno-methyl)-1,2,3-

通过Refine获得单步反应后选取有实验步骤的反应

获得全面的反应信息

查找合成Dacatasvir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

CAS Solutions

SciFinder®

Preferences | SciFinder Help ▾ Sign Out

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner

Save Print Export

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

REACTIIONS ⓘ

Get References Tools ▾

Analyze Refine

Analyze by: ⓘ

Reagent

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

Group by: No Grouping Sort by: Accession Number ▾

0 of 18 Reactions Selected

1. View Reaction Detail ⓘ Link

5 Steps Hover over any structure for more options.

~111

[Step 2.1]
~196

[Step 5.1]
~67

获得全面的反应信息

Analyze Refine

Analyze by: ?

Answer Type

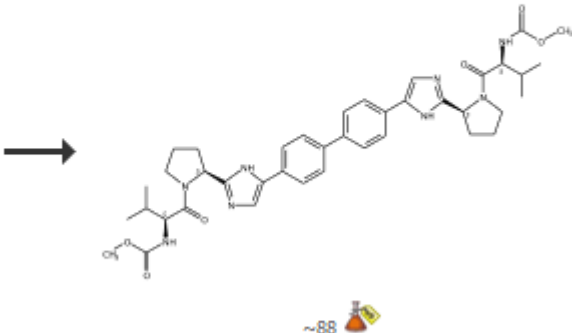
Reactions 18

Additional Reactions 1

Show More

19. View Reaction Detail [Link](#)

Hover over any structure for more options.



~88

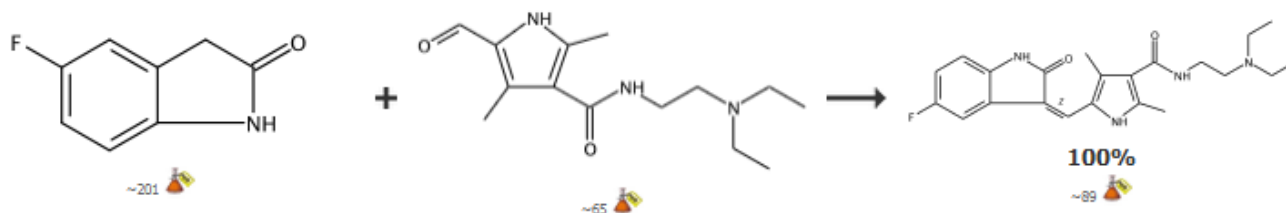
~11 references

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

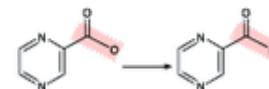
Get Similar Reactions ?

Retrieve similar reactions from:

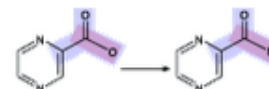
- ☒ All reactions
- ☐ Current answer set

Include this level of similarity:

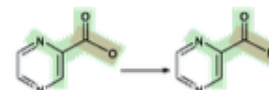
- ☐ Broad - Reaction centers only (157156)



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



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



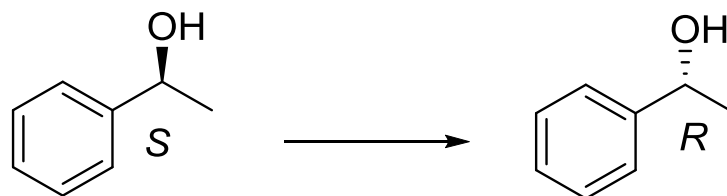
Get Reactions

Cancel

反应信息太少，通过Similar Reaction
获得更多反应信息

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

检索硅羟基酯化的反应，找出其中的聚合物反应？

案例分析

The screenshot displays the SciFinder Structure Editor interface. On the left, a 'Variables' panel lists search criteria: X (Any halogen), M (Any metal), A (Any atom except H), Q (Any atom except C or H), Ak (Any carbon chain), Cy (Any cycle), Cb (Any carbocycle), and Hy (Any heterocycle). The main 'Structure Editor' window shows a chemical reaction: a reactant (Si-O-H) reacting to form a product (Si-O-C(=O)-Ak). The 'Drawing Editor' on the right has 'Reaction' selected. Below it, the search criteria 'Get reactions where the structure(s) are:' are set to 'Substructures of more complex structures'. A search filter panel on the far right shows 'Number of Steps' set to 1, with examples 1, 1-3, 1-, -3. Other filters include Solvents, Non-participating Functional Groups, Classifications (Biotransformation, Catalyzed, Chemoselective, Combinatorial, Electrochemical, Gas-phase, Non-catalyzed, Photochemical, Radiochemical, Regioselective, Stereoselective), and Sources (Any source, Patents only, Sources other than patents).

Variables

- X Any halogen
- M Any metal
- A Any atom except H
- Q Any atom except C or H
- Ak Any carbon chain
- Cy Any cycle
- Cb Any carbocycle
- Hy Any heterocycle

Structure Editor

Click and drag to select objects. Ctrl-click to select or deselect individual objects.

reactant: OSi → product: OSiC(=O)Ak

Drawing Editor:

- ☐ Structure
- ☒ Reaction
- ☐ Markush

Get reactions where the structure(s) are:

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

Search Filter Panel:

- Solvents: ☒ Select Solvents
- Non-participating Functional Groups: ☒ Select Groups
- Number of Steps: (Examples: 1, 1-3, 1-, -3)
- Classifications:
 - ☐ Biotransformation
 - ☐ Catalyzed
 - ☐ Chemoselective
 - ☐ Combinatorial
 - ☐ Electrochemical
 - ☐ Gas-phase
 - ☐ Non-catalyzed
 - ☐ Photochemical
 - ☐ Radiochemical
 - ☐ Regioselective
 - ☐ Stereoselective
- Sources:
 - ☒ Any source
 - ☐ Patents only
 - ☐ Sources other than patents

Formula is not available

案例分析

REACTIONS

Get References Tools Send to SciFinder

Analyze **Refine**

Analyze by:
 Reagent

BuLi	7
Et ₃ N	7
KOH	4
2-MeC ₅ H ₄ N	3
(AcO) ₂ SnBu ₂	2
31900-57-9	2
4-DMAP	2
808384-16-9	2
AcOH	2
AIBN	2

[Show More](#)

Group by: No Grouping Sort by: Relevance

0 of 105 Reactions Selected Page: 1 of 3

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

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

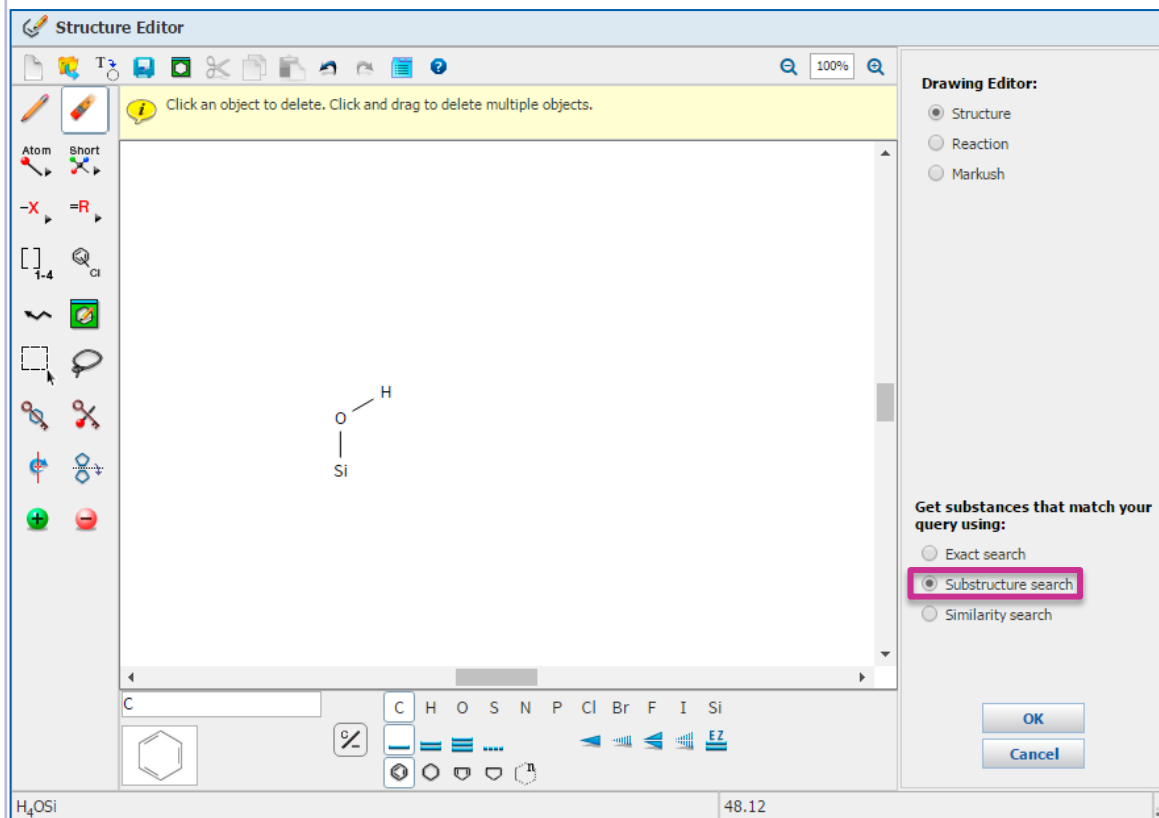
[Overview](#)

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

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

问题：如何找到含Si的聚合物上的羟基酯化反应？

案例分析



Characteristics

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

Classes

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

Studies

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

聚合物

案例分析

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Chemical Structure substructure with limiters > substances (17460)

SUBSTANCES ⓘ

Get References **Get Reactions** Get Commercial Sources Tools ▾

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: Relevance

0 of 17460 Substances Selected

Analyze by: Substance Role

Preparation 12398

Uses 11376

Properties 6534

Biological Study 2138

Reactant or Reagent 1847

Process 1444

Analytical Study 291

Prophetic in Patents 84

Formation, Nonpreparative 38

Combinatorial Study 27

1. 165754-29-0

14475-38-8
H₄ O Si

OH—SiH₃

(H₄ O Si)₂
Silanol, dimer (9CI)

2. 182320-10-1

83892-34-6
H₂ O Si

OH—SiH

(H₂ O Si)₂
Silylene, hydroxy-, dimer (9CI)

3. 119758-01-9

14475-38-8
H₄ O Si

OH—SiH₃

9005-32-7
Unspecified

Substance
Image
Cannot Be
Displayed
9005-32-7

4. 91029-76-4

14475-38-8
H₄ O Si

OH—SiH₃

1067-57-8
C₇ H₁₈ O₃ Si

(C₇ H₁₈ O₃ Si)
Silanol, poly (9CI)

Click to view details

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

案例分析

REACTIONS

Get References **Tools** Select to view available menu items.

Analyze Refine

Analyze by: Reagent

Et₃N 859

HCl 507

F₃CCO₂H 357

K₂CO₃ 301

p-MeC₆H₄SO₂NHNH₂ 244

1-Benzotriazolol 236

EtN=C=N(CH₂)₃NMe •HCl 234

KOH 231

NaHCO₃ 223

H₂O 222

Show More

Group by: No Group **Combine Answer Sets** Number

0 of 3966 Reactions Selected

Display Options

Page: 1 of 80

1. [View Reaction Detail](#)

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

Overview

2. [View Reaction Detail](#)

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

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (3966):

19 Answer Sets 1 Selected

Reaction Answer Set Details	Date Saved
<input checked="" type="checkbox"/> Si-OH酯化 (105)	Apr 27, 2016
Reaction structure substructure with limiters > reactions (105)	Apr 27, 2016
<input type="checkbox"/> Si-OH 酯化 (42)	Apr 27, 2016
Reaction structure substructure with limiters > reactions (42)	Apr 27, 2016
<input type="checkbox"/> 1-1 (7476)	Apr 26, 2016
Chemical structure exact with limiters > substances (11) > get reactions (7476)	Apr 26, 2016
<input type="checkbox"/> guangxue 1 (7476)	Apr 19, 2016
Chemical structure exact with limiters > substances (11) > get reactions (7476)	Apr 19, 2016
<input type="checkbox"/> 1-1 (72863)	Apr 13, 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 (3966)** that are not in **Si-OH酯化 (105)**

☐ **Exclude** Include only answers from **Si-OH酯化 (105)** that are not in **current answer set (3966)**

Combine Answer Sets Cancel

案例分析

REACTIONS

Get References Tools

Analyze

Analyze by: Reagent

Et₃N 5
KOH 4
(AcO)₂SnBu₂ 2
31900-57-9 2
808384-16-9 2
AIBN 2
NaOH 2
SiO₂ 2
1332-29-2 1
2530-83-8 1

Show More

Group by: No Grouping Sort by: Accession Number

0 of 32 Reactions Selected

1. View Reaction Detail

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

Overview

2. View Reaction Detail

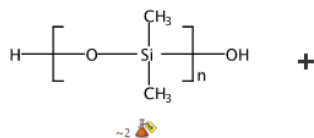
Single Step *Hover over any structure for more options.*

Waiting for scifinder.cas.org...

案例分析

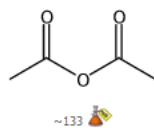
3. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.

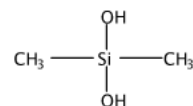


4. View Reaction Detail [Link](#)

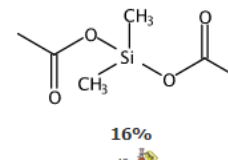
Single Step Hover over any structure for more options.



+

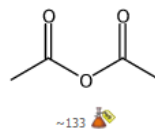


→

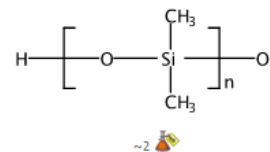


6. View Reaction Detail [Link](#)

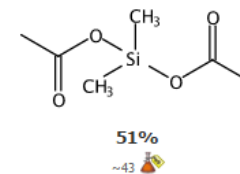
Single Step Hover over any structure for more options.



+



→

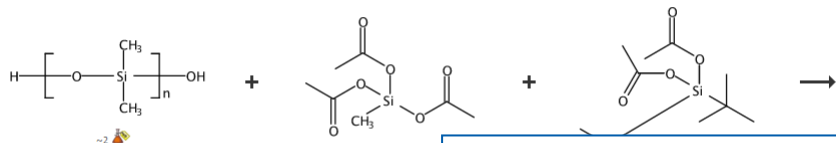


符合要求的反应

案例分析

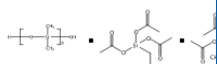
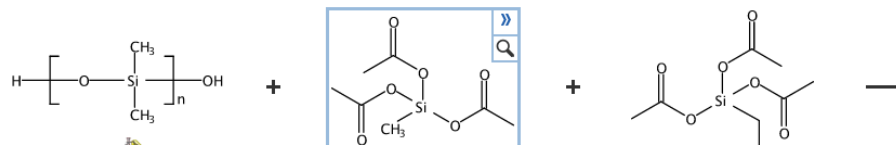
1. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



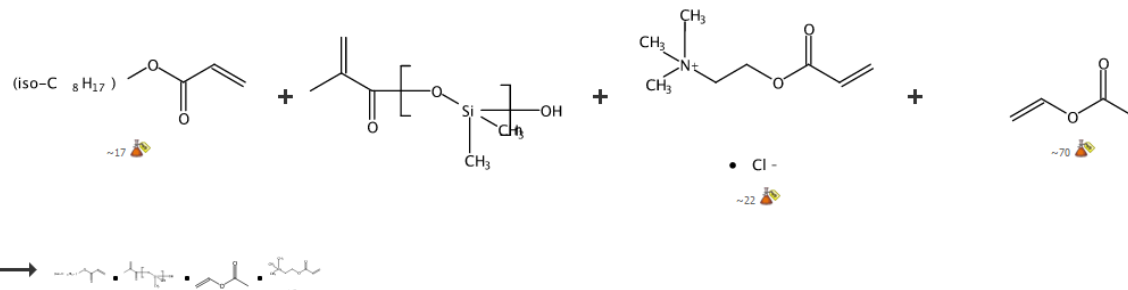
2. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



8. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



不符合要求的反应

如何去除？

案例分析

思路一：筛出原料中已经包含酯化物的反应

Analyze Refine

Refine by: ?

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

Structure Editor:

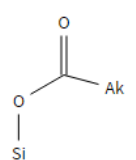
Java Non-Java

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

Refine

Structure Editor

Click a reaction participant. A list of roles appears.
Click a reaction role and click OK.



reactant

Get reactions where the structure(s) are:

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

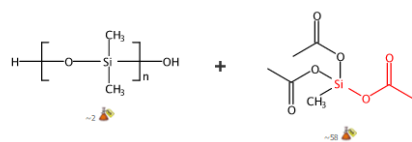
OK Cancel

Formula is not available

案例分析

1. View Reaction Detail [Link](#)

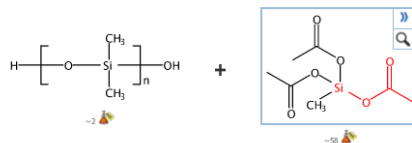
Single Step Hover over any structure for more options.



Overview

2. View Reaction Detail [Link](#)

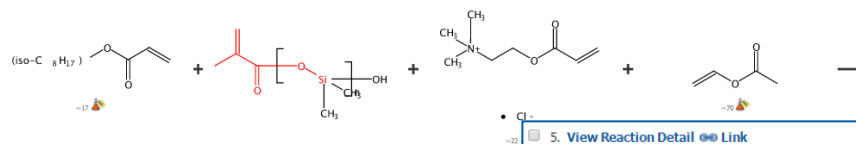
Single Step Hover over any structure for more options.



希望筛选的反应

3. View Reaction Detail [Link](#)

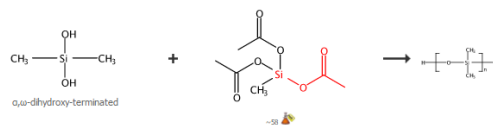
Single Step Hover over any structure for more options.



Overview

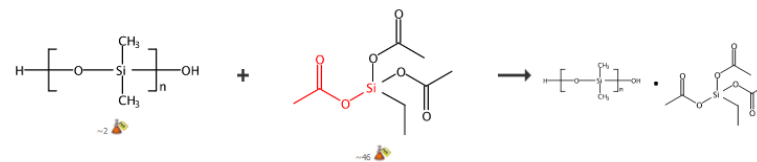
4. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



5. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.

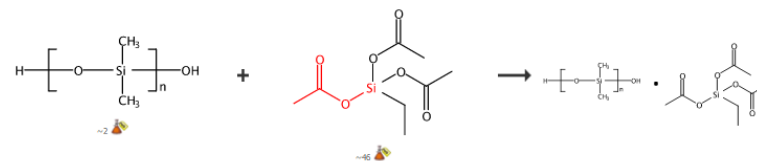


Overview

Experimental Procedure

6. View Reaction Detail [Link](#)

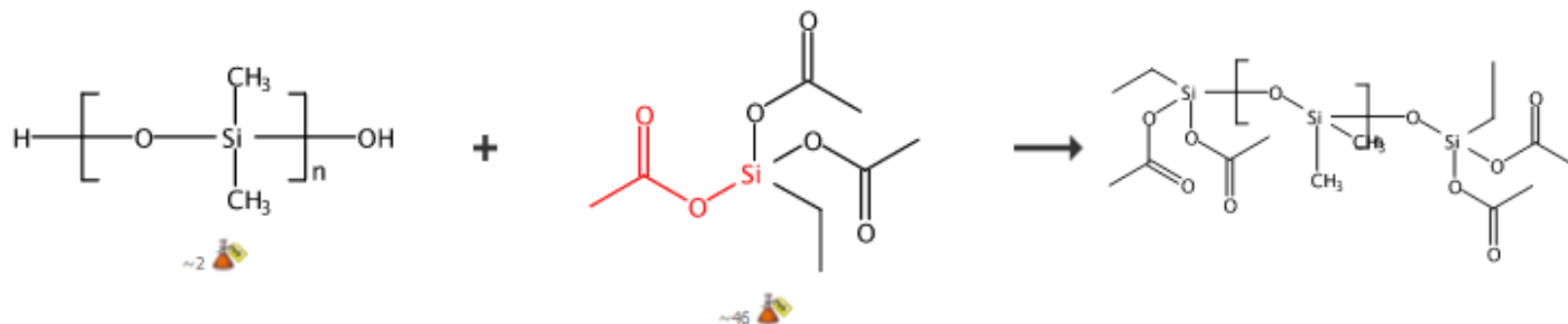
Single Step Hover over any structure for more options.



案例分析

8. View Reaction Detail [Link](#)

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

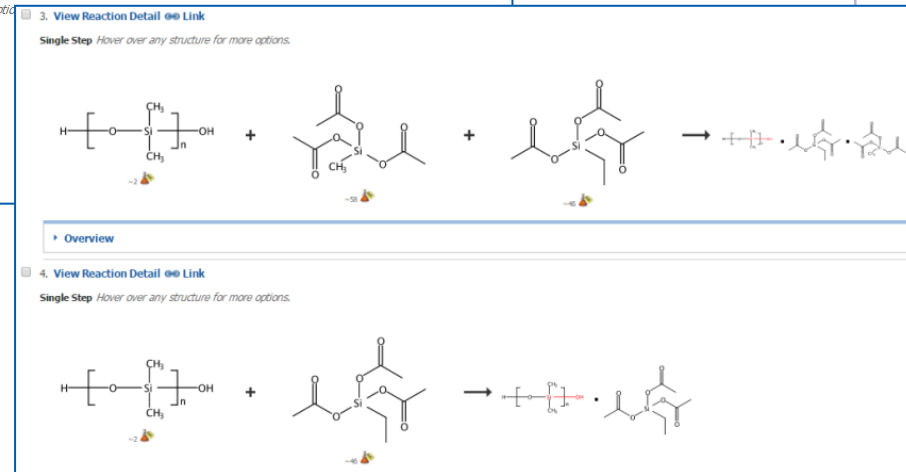
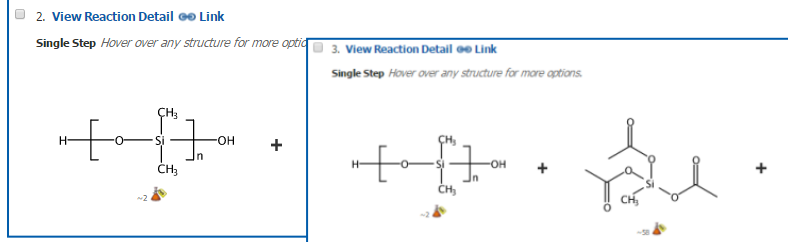
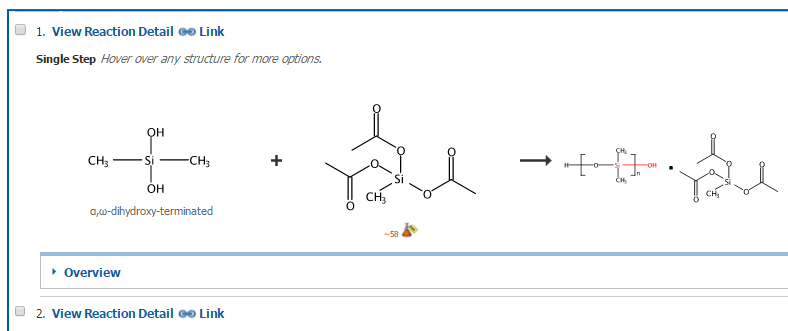
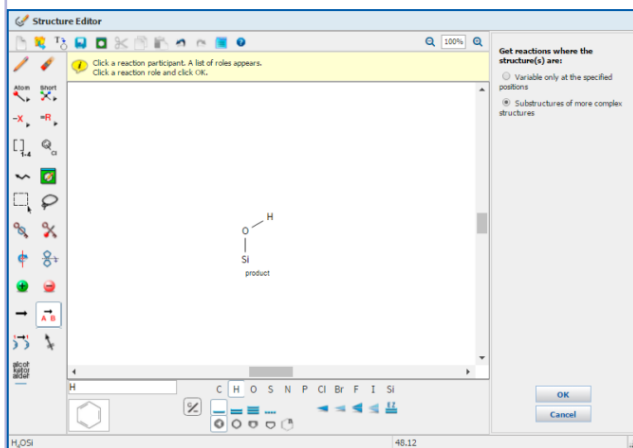


不希望筛除的反应

思路一不可行！

案例分析

思路二：筛出产物中仍然包含原料的反应



都是希望筛选的反应

案例分析

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (20):

Reaction Answer Set Details	Date Saved
32 (32)	Apr 27, 2016
3966 (3966)	Apr 27, 2016
Opened saved answer set "Si-OH[1]" (105) > Combine Reaction Answer Sets "3966 (3966)" (32)	
Chemical Structure substructure with limiters > substances (17460) > get reactions (3966)	Apr 27, 2016
Si-OH[1] (105)	Apr 27, 2016
Reaction Structure substructure with limiters > reactions (105)	Apr 27, 2016
Si-OH[1] (42)	Apr 27, 2016
Reaction Structure substructure with limiters > reactions (42)	Apr 27, 2016
1:1 (7476)	Apr 26, 2016

Select an option for combining the answer sets:

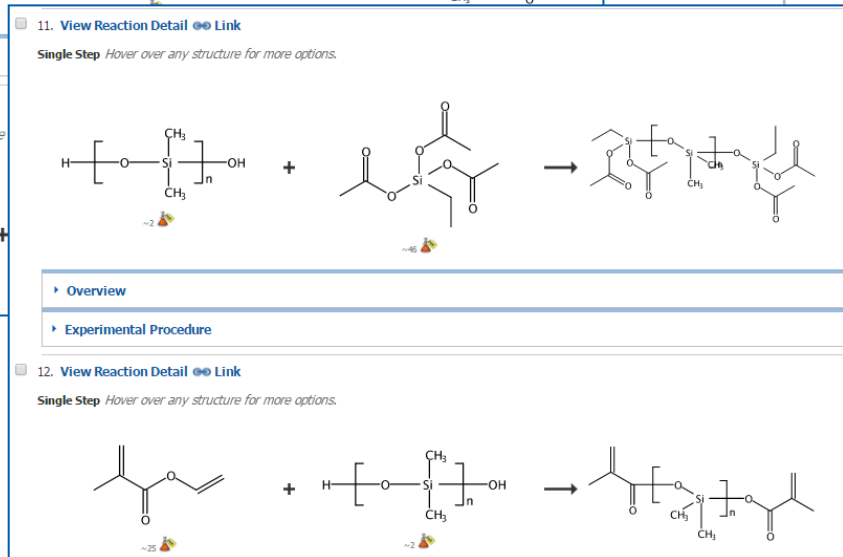
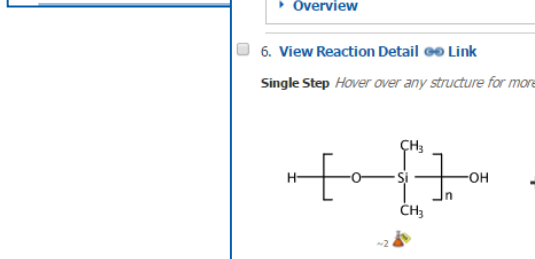
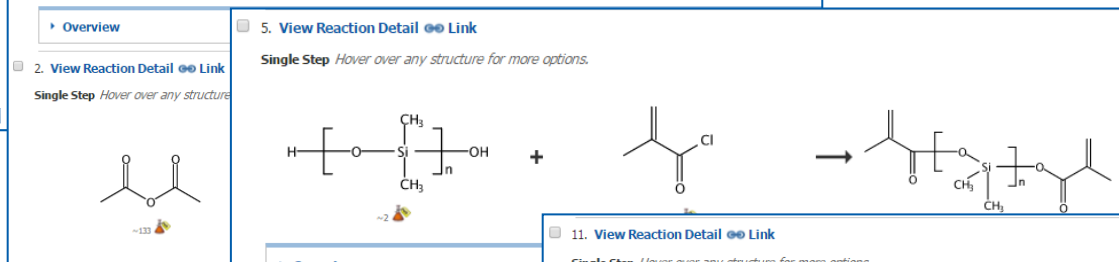
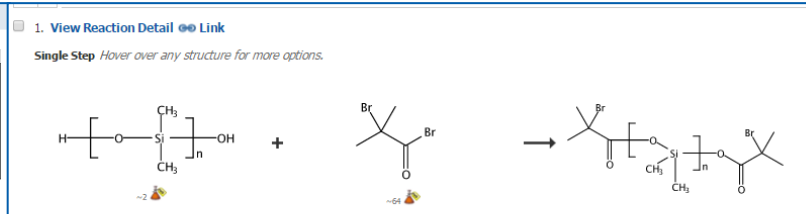
☒ **Combine** Include all answers from both sets

☐ **Intersect** Include only answers that appear in both sets

☐ **Exclude** Include only answers from **current answer set (20)** that are not in **32 (32)**

☒ **Exclude** Include only answers from **32 (32)** that are not in **current answer set (20)**

[Combine Answer Sets](#) [Cancel](#)



都是符合要求的反应

SciFinder中的检索思路

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

更多培训资料请访问

www.cas-china.org

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