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SciFinder检索难点解析

中国科技大学

2017.3.21

SCIFINDER®
A CAS SOLUTION

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

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提纲

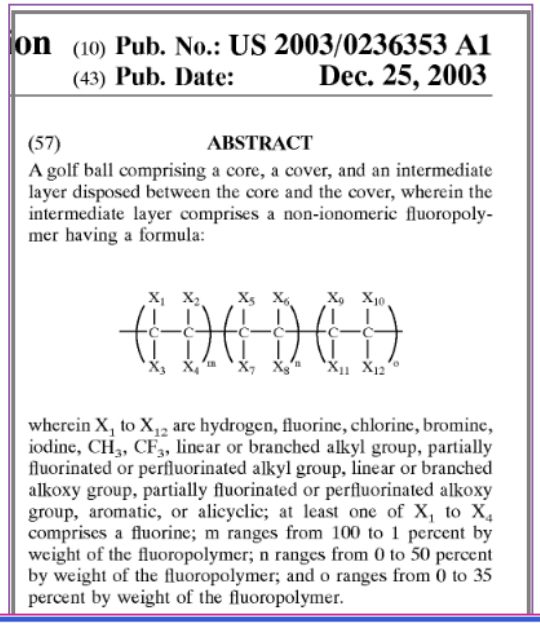
- SciFinder介绍
  - 索引的价值
  - 增值的专利信息
  - CAS最新动向

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® A CAS SOLUTION

SciFinder对专利的加强



ion (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 0f 0.795, and water absorption <0.05%.

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SciFinder中的专利族信息的价值

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

Patent Information

Patent No.		Kind	Language	Date	Application No.	Date
US 20030236353		A1		Dec 25, 2003	US 2002-171355	Jun 13, 2002
US 6747110		B2		Jun 8, 2004		
JP 2004041721		A		Feb 12, 2004	JP 2003-166490	Jun 11, 2003
US 20040192833	PatentPak	A1	English	Sep 30, 2004	US 2004-817366	Apr 2, 2004
US 7083856		B2		Aug 1, 2006		
US 20040210017		A1		Oct 21, 2004	US 2004-842607	May 10, 2004
US 7101944		B2		Sep 5, 2006		
US 20040236018	PatentPak	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	

SciFinder® A CAS SOLUTION

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

SCIFINDER® A CAS SOLUTION

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

关键词之间用介词连接：in, with, of...

SciFinder
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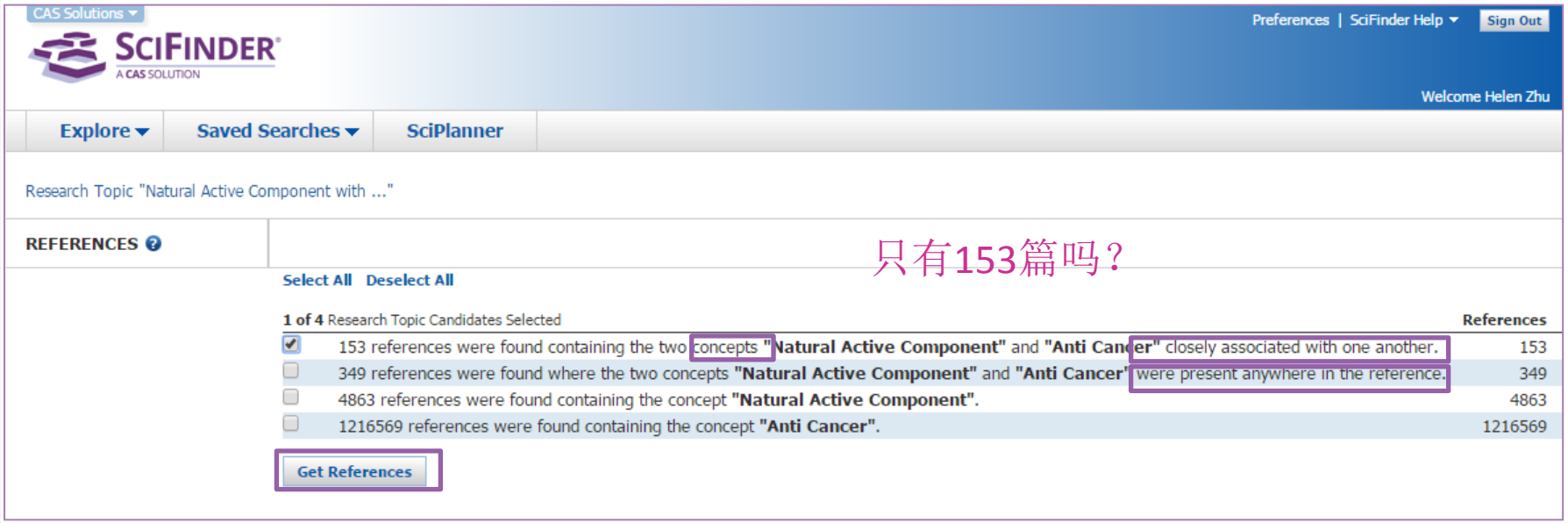
主题检索的候选项



"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；

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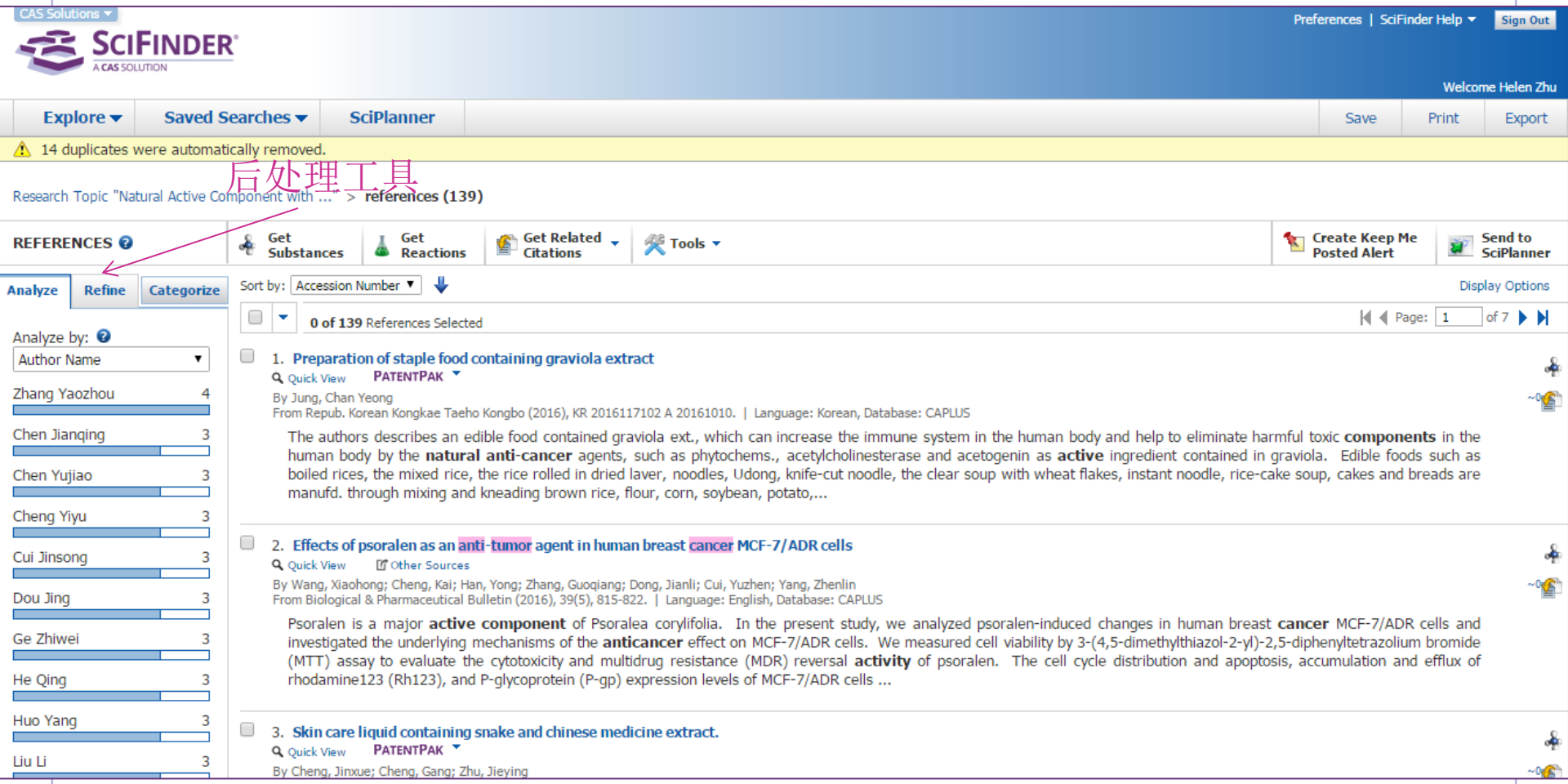
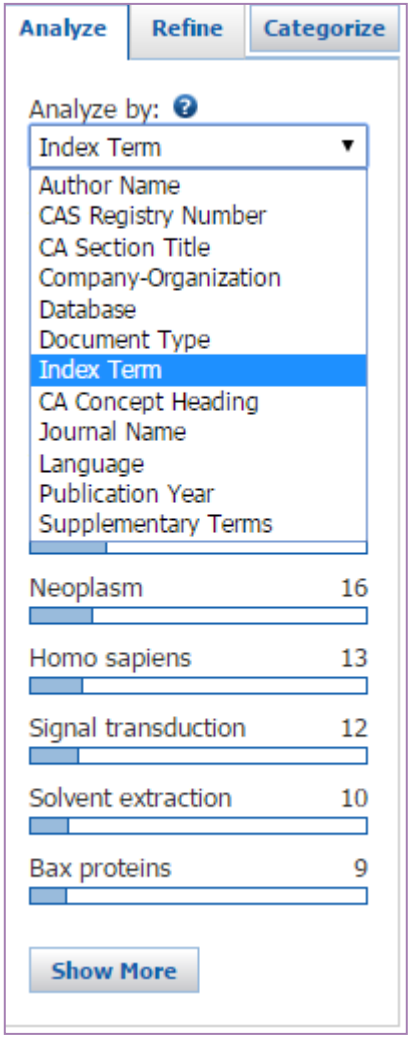
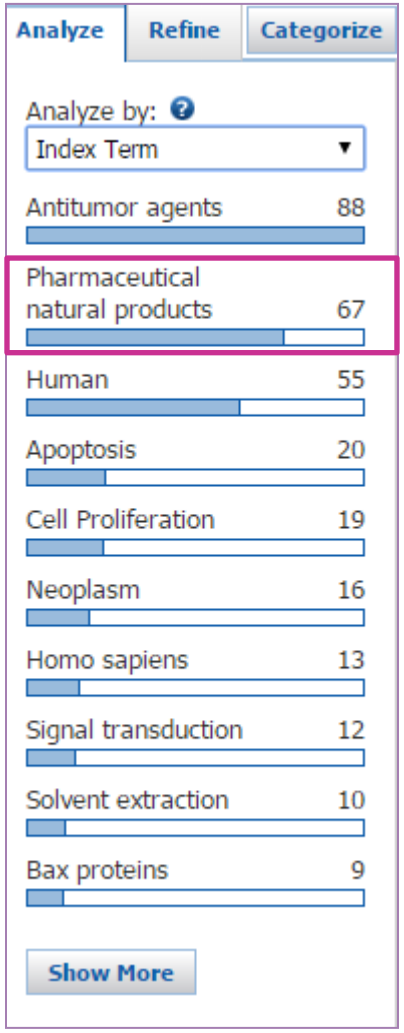
利用Index Term选词



利用Index Term选词



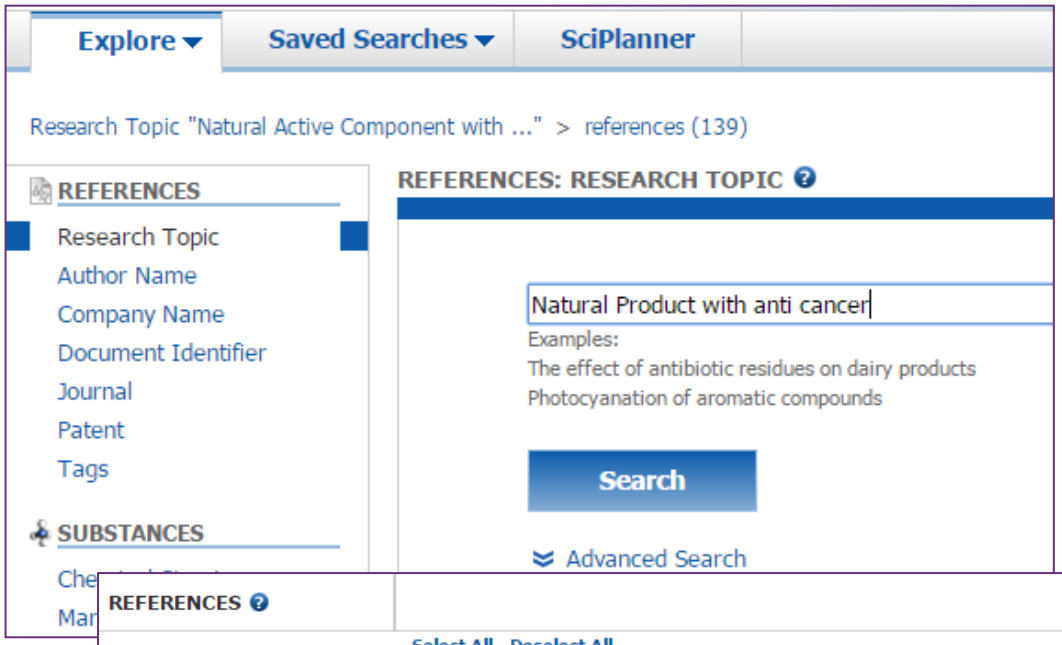


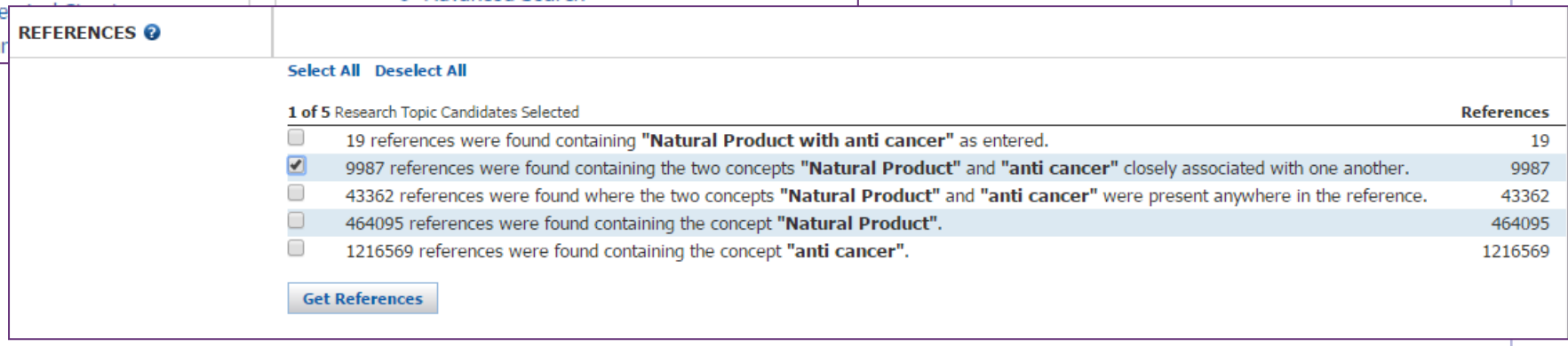
Index Term基于内容的分析工具，发现natural products, Pharmaceutical 这个和天然活性成分很相关的词

是否用这个词去检索，效果会更好？

SciFinder® A CAS SOLUTION

利用Index Term选词





新的检索式：

Natural Product with anti cancer

更换检索词后，结果放大近70倍

SciFinder® A CAS SOLUTION

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

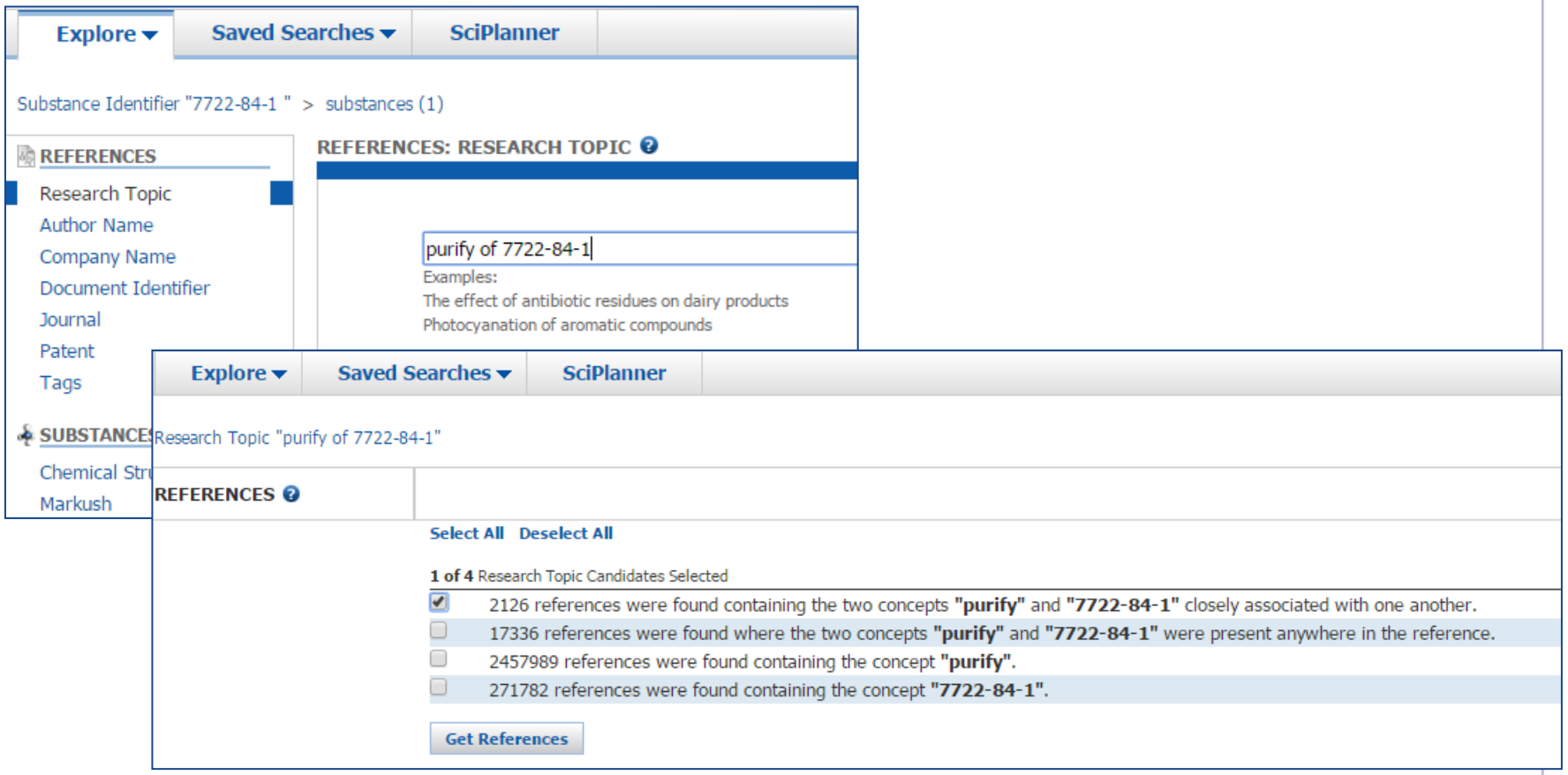
FORM	**Formation, Nonpreparative**	
	Formation, Unclassified	FMU
	Geological or Astronomical Formation	GFM
NANO	**Nanomaterial**	
OCCU	**Occurrence**	
	Biological Occurrence	BOC
	Geological or Astronomical Occurrence	GOC
	Natural Product Occurrence	NPO
	Occurrence, Unclassified	OCU
	Pollutant	POL

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

SciFinder® A CAS SOLUTION

巧用CAS Role

查找纯化双氧水（7722-84-1）的文献



SciFinder® A CAS SOLUTION

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

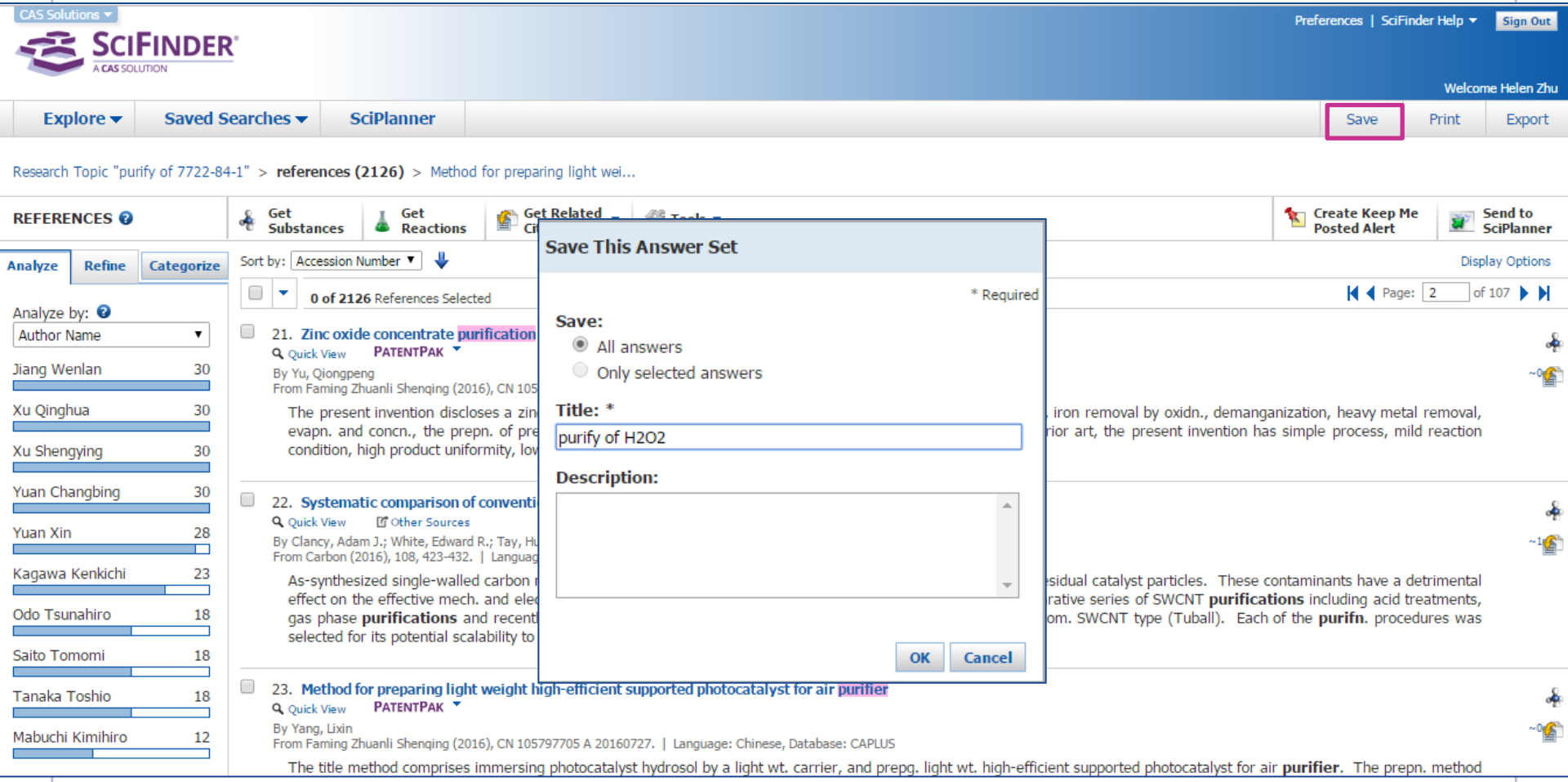
a method for a kind of tailwater cascade oxidn. depth purifn. [Machine Translation].

Pollutant; Removal or disposal; Occurrence; Process

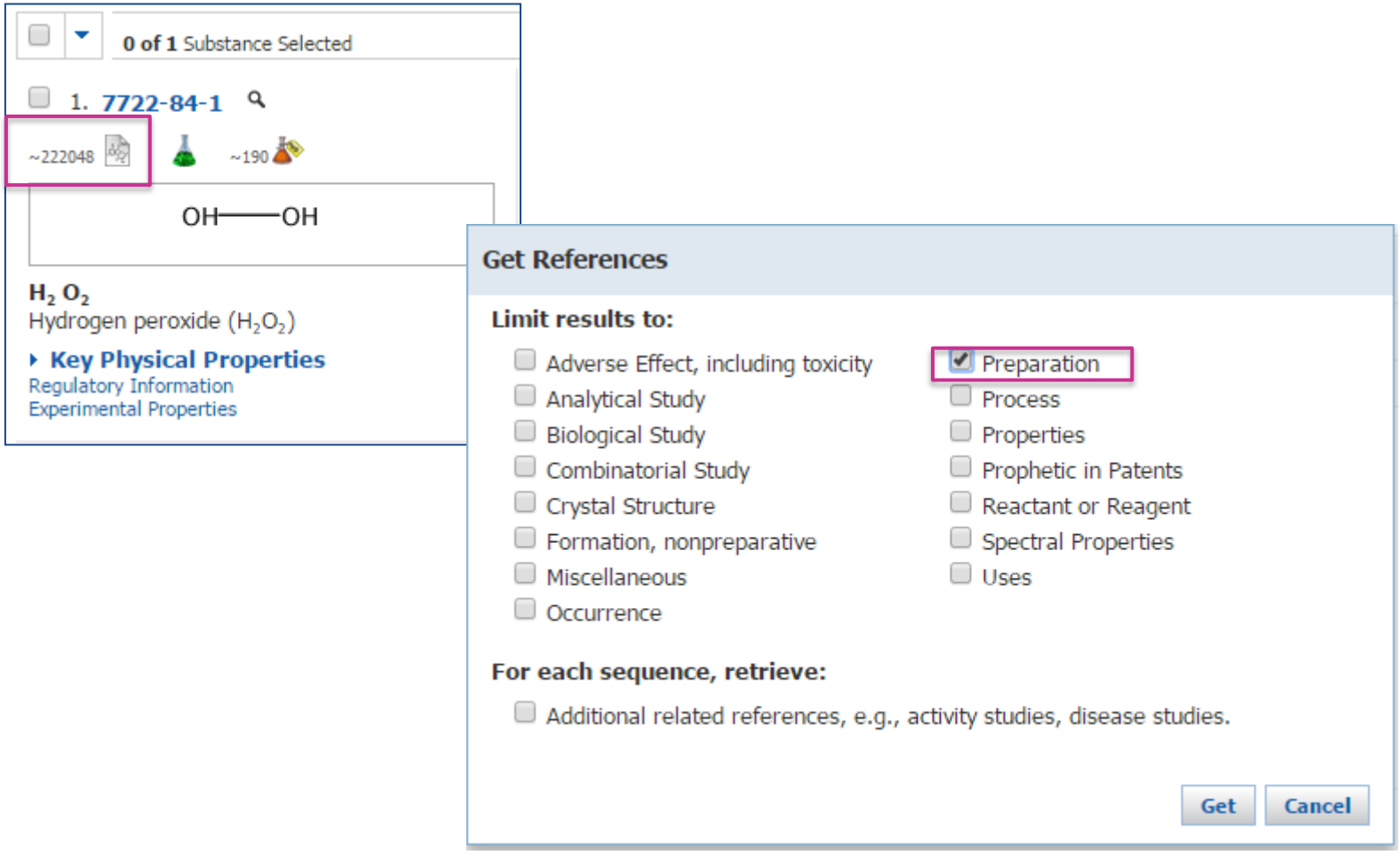
噪音信息

SciFinder® A CAS SOLUTION

巧用CAS Role

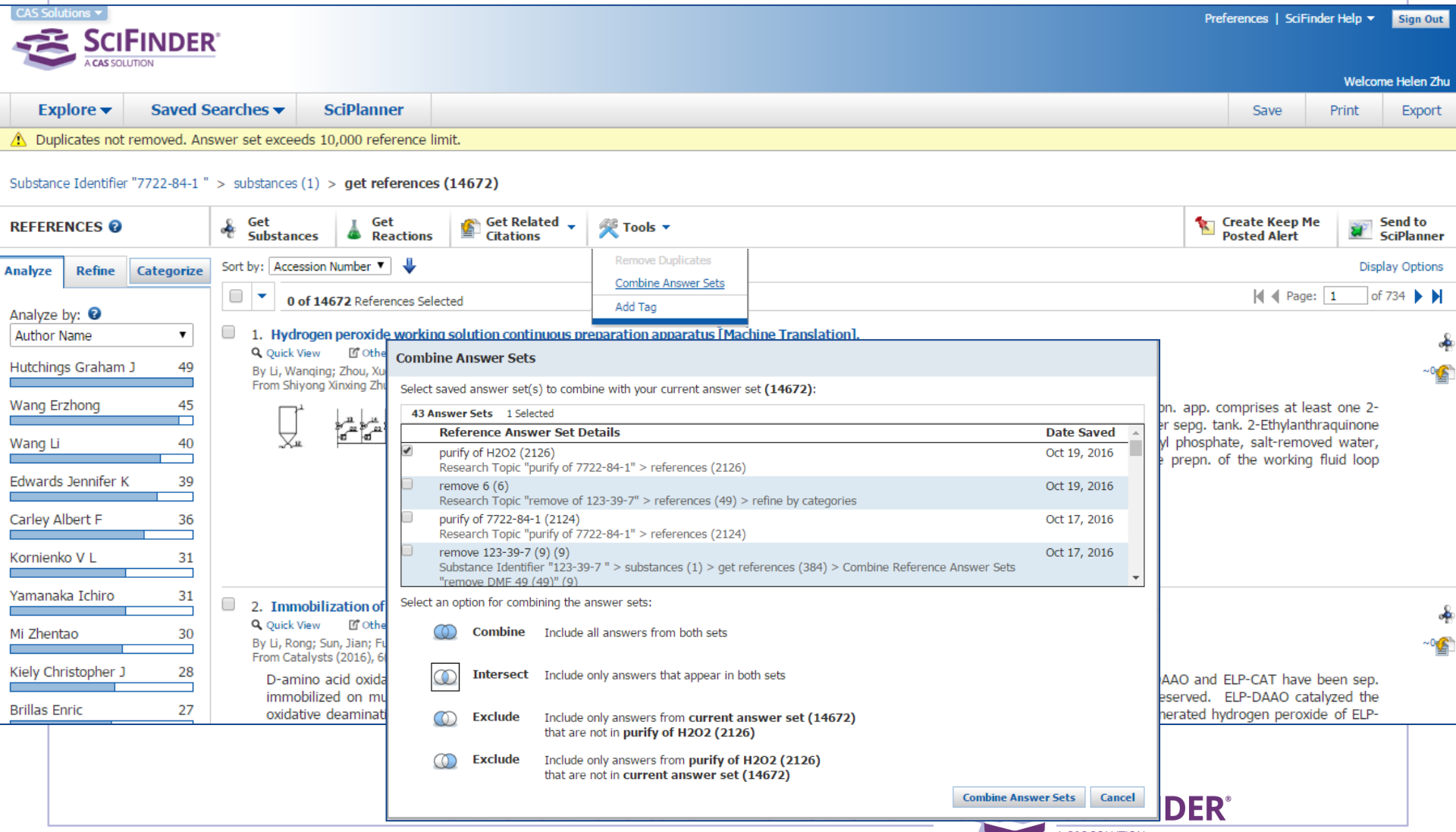

CAS Solutions
SciFinder
A CAS SOLUTION
Preferences | SciFinder Help
Sign Out
Welcome Helen Zhu
Explore
Saved Searches
SciPlanner
Save
Print
Export
Research Topic "purify of 7722-84-1" > references (2126) > Method for preparing light wei...
REFERENCES
Get Substances
Get Reactions
Get Related
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Categorize
Sort by: Accession Number
Display Options
0 of 2126 References Selected
Page: 2 of 107
Analyze by:
Author Name
Jiang Wenlan 30
Xu Qinghua 30
Xu Shengying 30
Yuan Changbing 30
Yuan Xin 28
Kagawa Kenkichi 23
Odo Tsunahiro 18
Saito Tomomi 18
Tanaka Toshio 18
Mabuchi Kimihiro 12
21. Zinc oxide concentrate purification
Quick View
PATENTPAK
By Yu, Qiongpeng
From Faming Zhuanli Shenqing (2016), CN 105
The present invention discloses a zin
evapn. and concn., the prepn. of pre
condition, high product uniformity, lov
iron removal by oxidn., demanganization, heavy metal removal,
rior art, the present invention has simple process, mild reaction
22. Systematic comparison of conventi
Quick View
Other Sources
By Clancy, Adam J.; White, Edward R.; Tay, Hu
From Carbon (2016), 108, 423-432. | Languag
As-synthesized single-walled carbon
effect on the effective mech. and ele
gas phase purifications and recenti
selected for its potential scalability to
sidual catalyst particles. These contaminants have a detrimental
rative series of SWCNT purifications including acid treatments,
om. SWCNT type (Tuball). Each of the purifn. 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

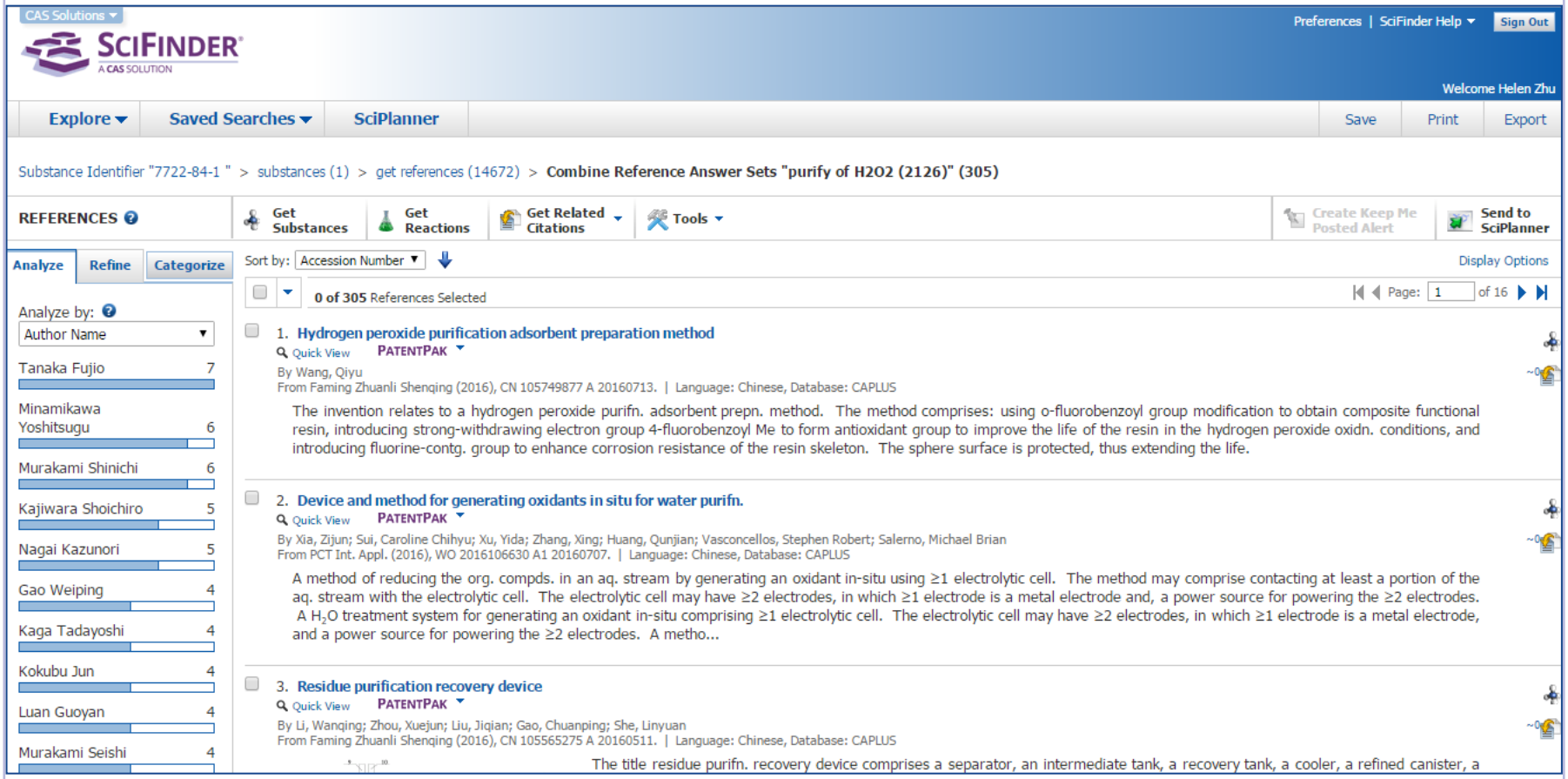


SciFinder® A CAS SOLUTION

巧用CAS Role


CAS Solutions
SciFinder
A CAS SOLUTION
Preferences | SciFinder Help
Sign Out
Welcome Helen Zhu
Explore
Saved Searches
SciPlanner
Save
Print
Export
Duplicates not removed. Answer set exceeds 10,000 reference limit.
Substance Identifier "7722-84-1 " > substances (1) > get references (14672)
REFERENCES
Get Substances
Get Reactions
Get Related Citations
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Categorize
Sort by: Accession Number
Remove Duplicates
Combine Answer Sets
Add Tag
Display Options
0 of 14672 References Selected
Page: 1 of 734
Analyze by:
Author Name
Hutchings Graham J 49
Wang Erzhong 45
Wang Li 40
Edwards Jennifer K 39
Carley Albert F 36
Kornienko V L 31
Yamanaka Ichiro 31
Mi Zhentao 30
Kiely Christopher J 28
Brillas Enric 27
1. Hydrogen peroxide working solution continuous preparation apparatus [Machine Translation].
Quick View
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
purify of H2O2 (2126)
Research Topic "purify of 7722-84-1" > references (2126)
Oct 19, 2016
remove 6 (6)
Research Topic "remove of 123-39-7" > references (49) > refine by categories
Oct 19, 2016
purify of 7722-84-1 (2124)
Research Topic "purify of 7722-84-1" > references (2124)
Oct 17, 2016
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
2. Immobilization of
Quick View
D-amino acid oxida
immobilized on mu
oxidative deaminat
AAO and ELP-CAT have been sep.
eserved. ELP-DAAO catalyzed the
herated hydrogen peroxide of ELP-

巧用CAS Role



浏览记录，判断是否符合要求

SciFinder
A CAS SOLUTION

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		

Priority Application

CN 2015-10852280	Nov 26, 2015

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

hydrogen peroxide purifn. adsorbent prepn. method

Purification or recovery; Preparation

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

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

The invention relates to a method of purifying H_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 (H2O2), preparation Page 2 in PATENTPAK

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

Purification or recovery; Preparation

都是需要的文献

SCIFINDER® A CAS SOLUTION

善用Categorize

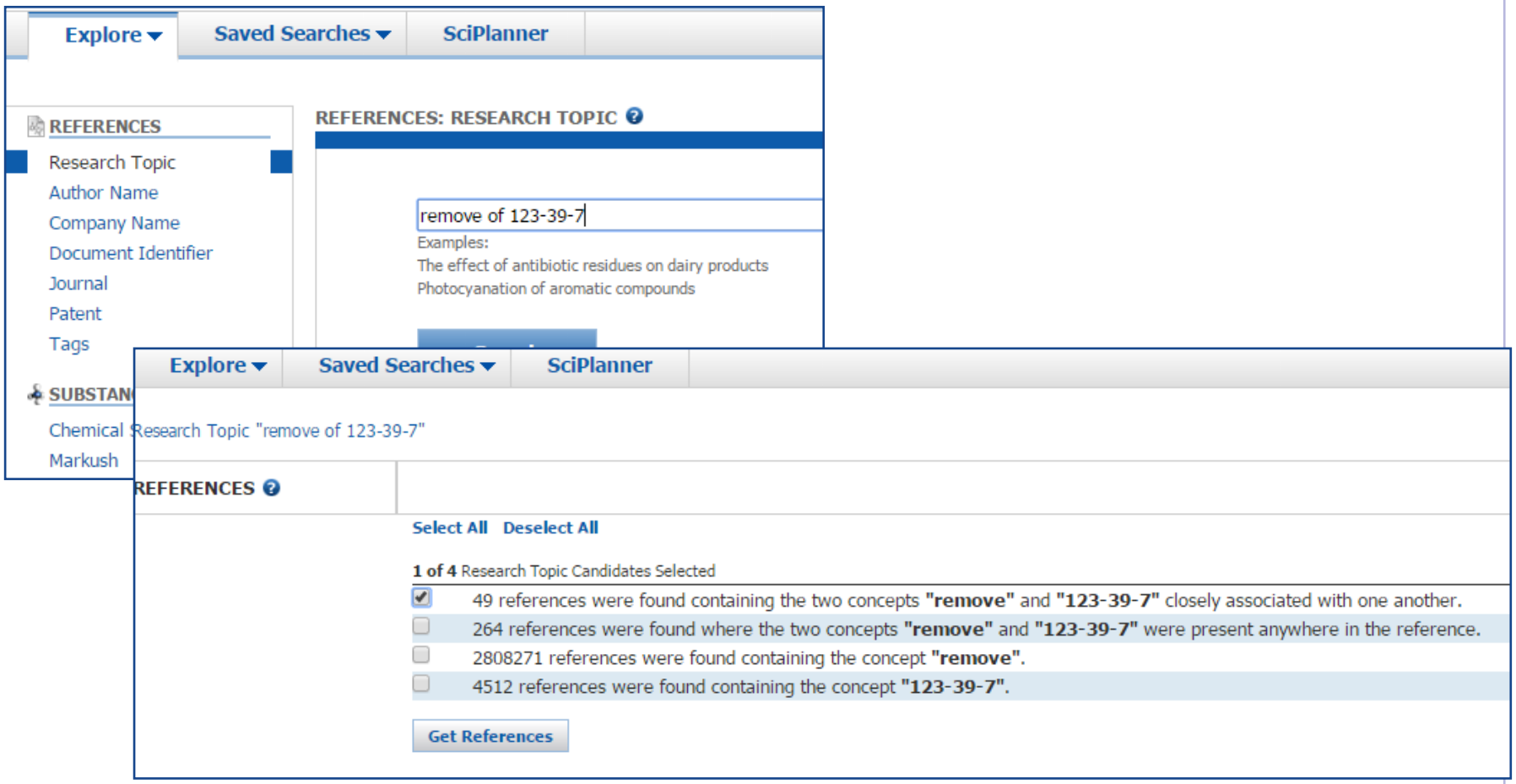
检索文献：

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

SciFinder® A CAS SOLUTION

善用Categorize

去除N-甲基甲酰胺（123-39-7）



SciFinder®
A CAS SOLUTION

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 degrdn. were proposed. The org. products from DMA and DMF decompn. by NTP were found to have great soly. and high biodegradability. Thus, NTP enhanced absorption/biol. method is suggested for complete removal of DMA and DMF.

Indexing

Air Pollution and Industrial Hygiene (Section59-4)

Concepts

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

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

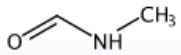
Volatile organic compounds

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

Removal or disposal; Process

Substances

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



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

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

Formation, unclassified; Formation, nonpreparative

需要的文献

SciFinder® A CAS SOLUTION

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

Indexing

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

Concepts

Coating removers — Photoresists

removing agent contg. alkylamide mixt.

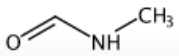
Amides

removing agent contg. alkylamide mixt.

Other use, unclassified; Physical, engineering or chemical process; Process; Uses

Substances

123-39-7 N-Methylformamide



127-19-5 N, N-Dimethyl acetamide

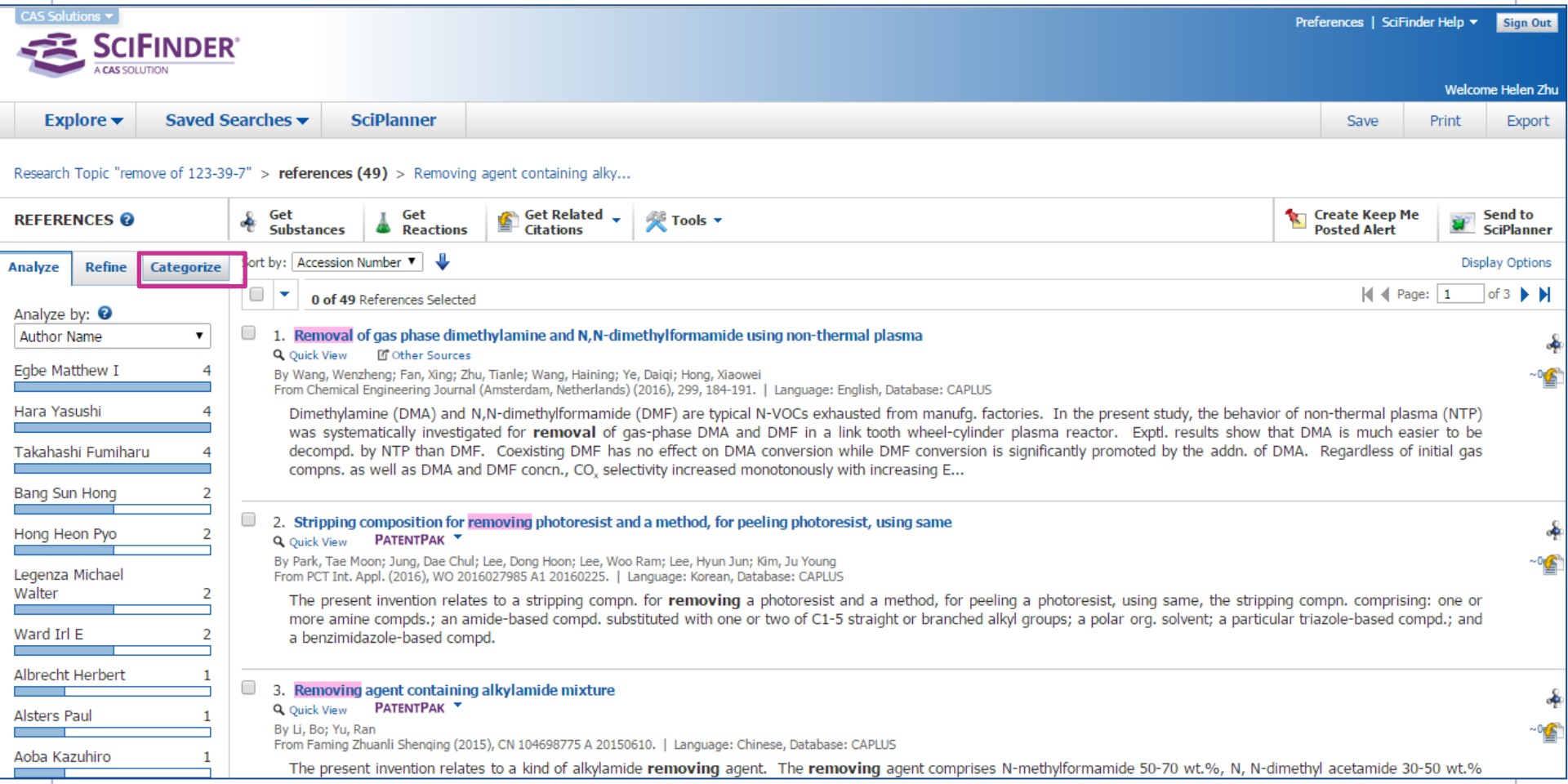
removing agent contg. alkylamide mixt.

Other use, unclassified; Physical, engineering or chemical process; Process; Uses

噪音信息更多，如何去除？

SciFinder® A CAS SOLUTION

善用Categorize



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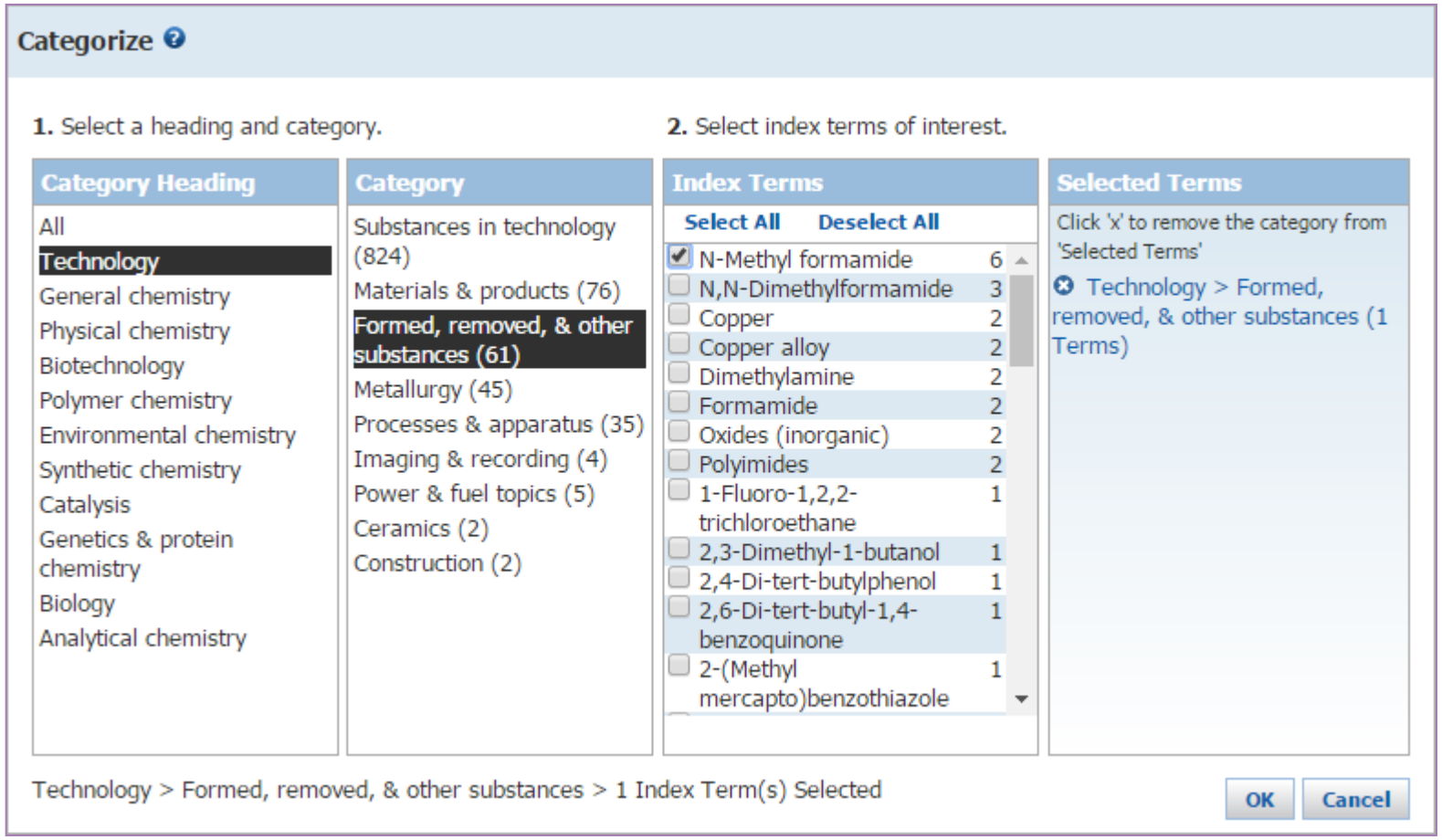
善用Categorize



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避免标引时差引起的漏检

Update frequency

- Updated daily
- Patent references from nine major issuing authorities available within two days from the time the patent was issued

9大核心专利机构发布的专利2日内收录进SciFinder

Bibliographic information and abstracts for all articles in more than 1,500 key scientific journals are added to CAplus[SM] within 7 days. The list below is sorted alphabetically by the full journal title and also includes the journal abbreviation and CODEN. This is not the full list of publications covered by CAS, and the list is subject to change.

核心期刊的文献7日内收录进SciFinder

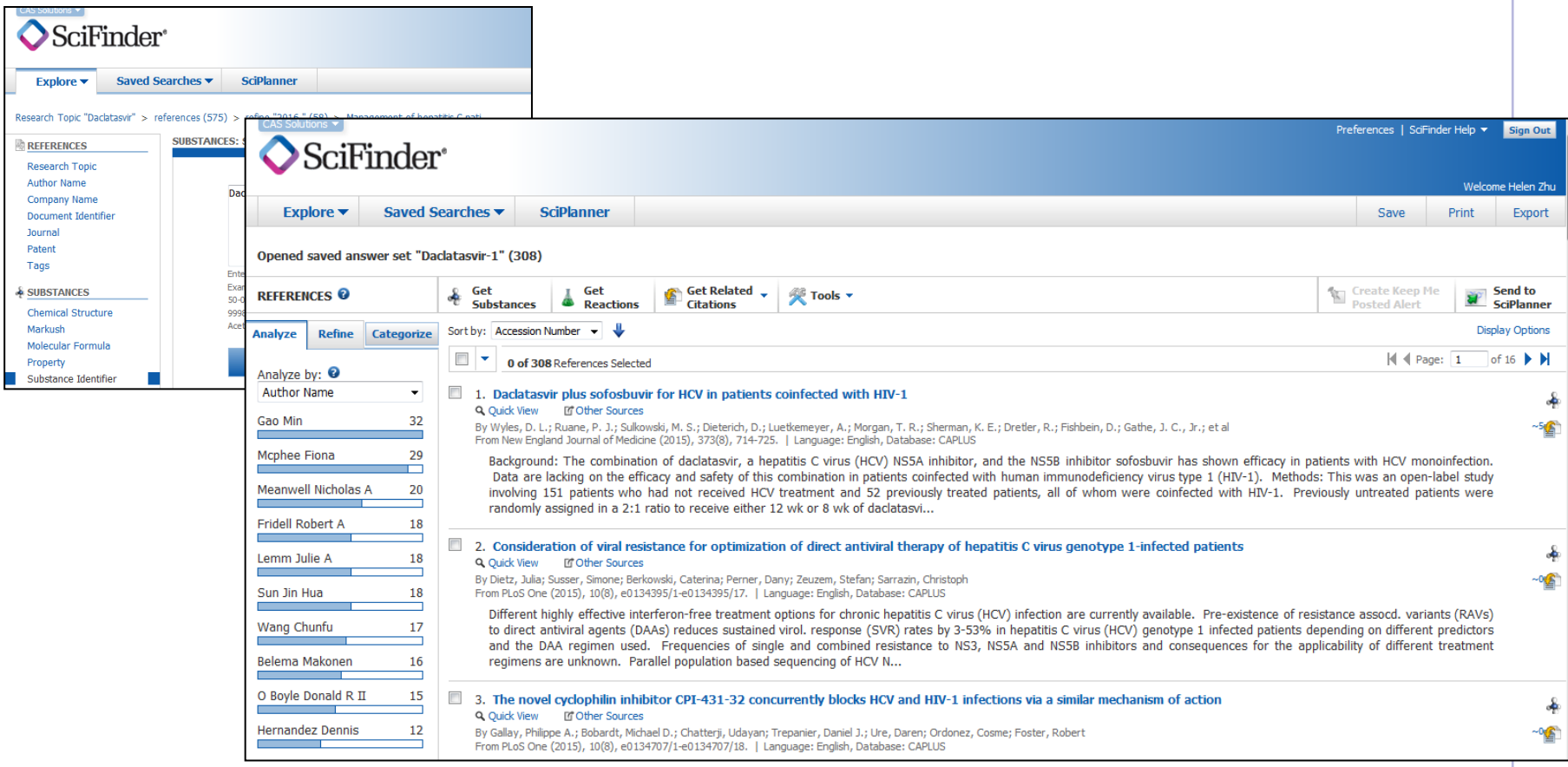
对核心期刊及核心专利机构发布的专利的标引在2-3周内完成

在收录至标引期间的文献可能会漏检！

SciFinder® A CAS SOLUTION

避免标引时差引起的漏检

检索治疗肝病的药物Daclatasvir的相关文献



通过检索物质获得文献准确，但是不够新

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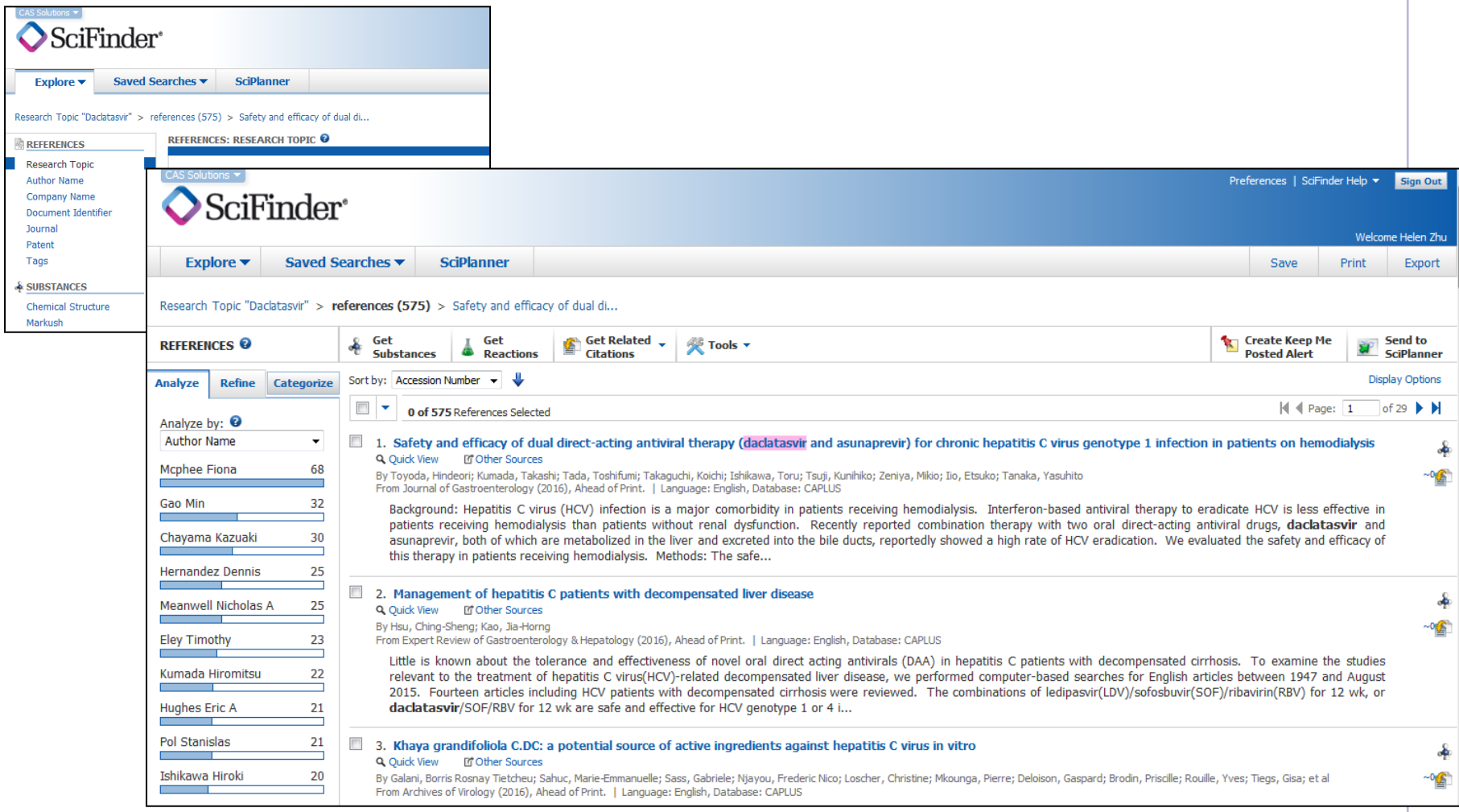
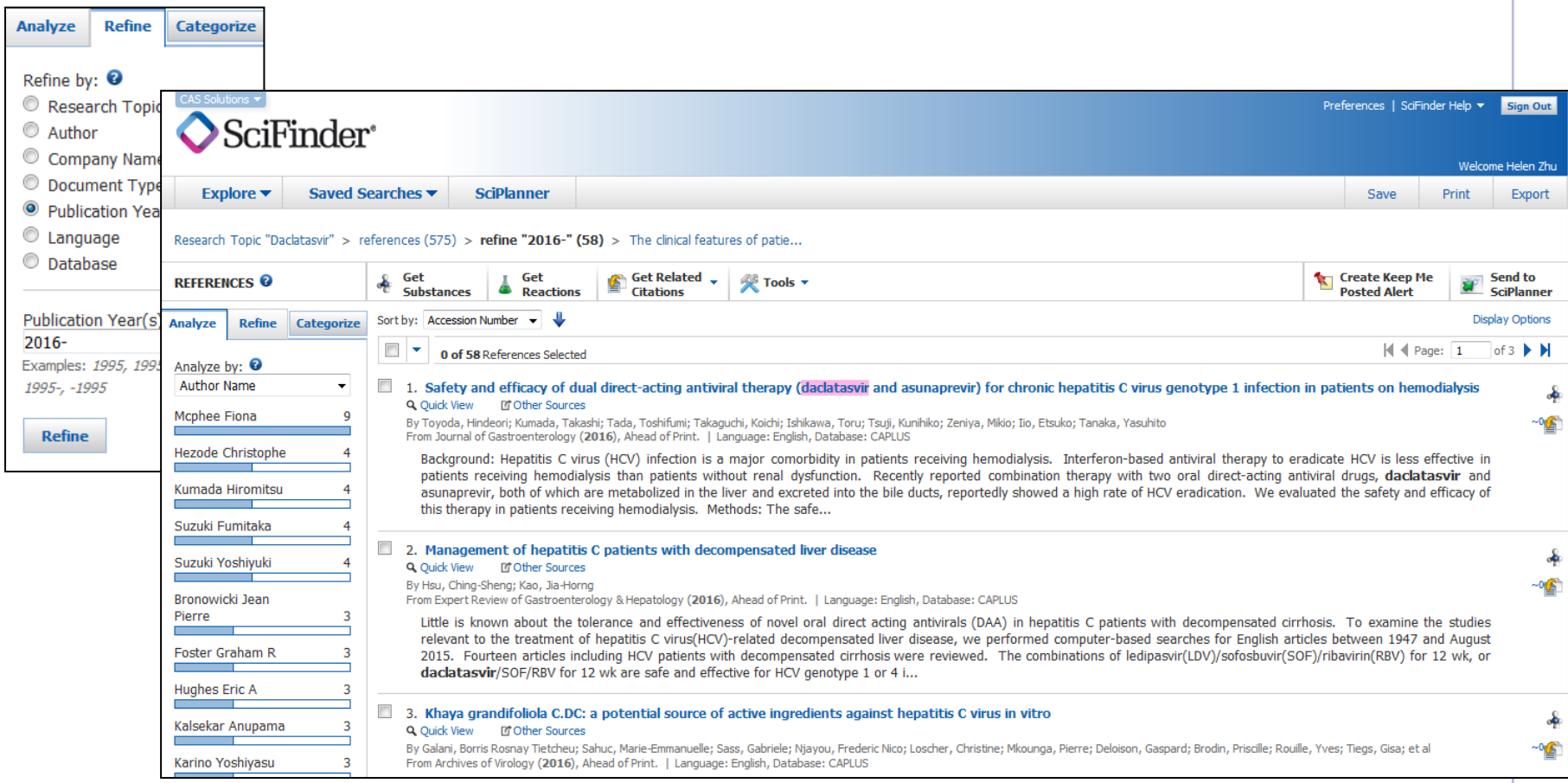
避免标引时差引起的漏检



通过主题直接检索物质名称，发现最新的文献

SCIFINDER® A CAS SOLUTION

避免标引时差引起的漏检



通过PY限定最新的文献，与通过物质检索获得的结果集合并

SciFinder® A CAS SOLUTION

避免标引时差引起的漏检

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 virol. 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
Deltenre, 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

标引未完成

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

By: Kan, Toshiki; 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
Blood platelet
Genetic polymorphism
Genotypes
Hepatitis C
Hepatitis C virus
Homo sapiens
Human
Immunotherapy
Leukocyte
Sex

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

目标物质未做重点研究

SciFinder® A CAS SOLUTION

提纲

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

SCIFINDER® A CAS SOLUTION

SciFinder检索选项——物质检索

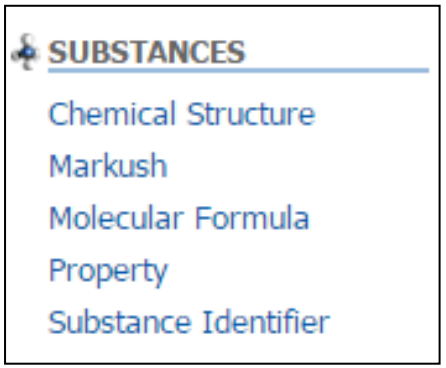
- 物质检索方法

  —结构式检索

  —分子式检索

  —理化性质检索

  —物质标识符检索：化学名称，CAS RN



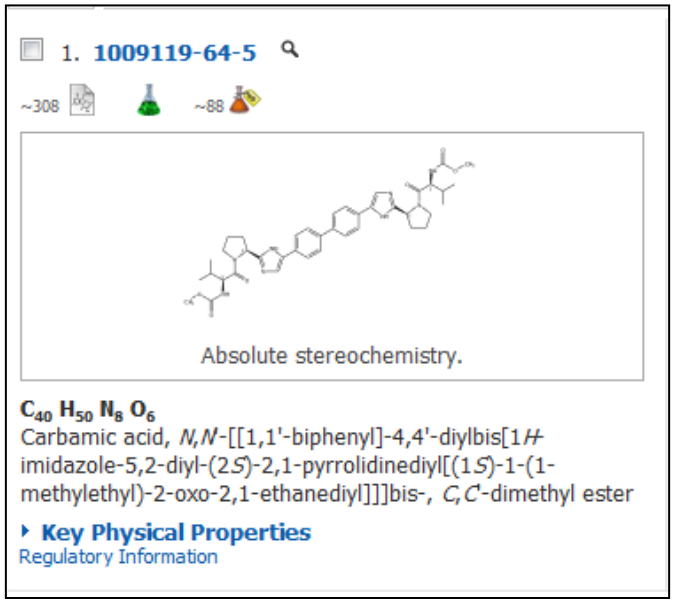
- 物质检索策略推荐

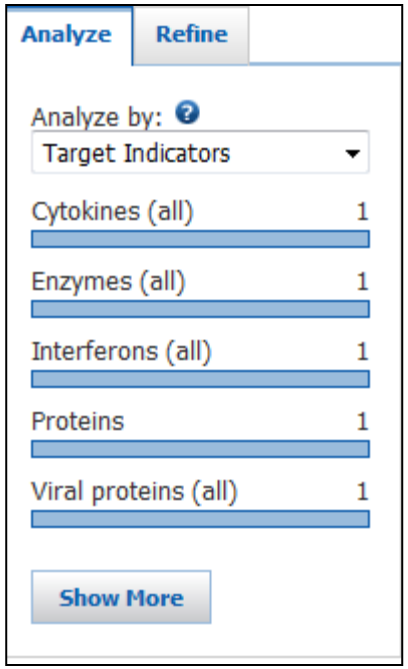
  —有机化合物，天然产物：结构检索

  —无机物，合金：分子式检索

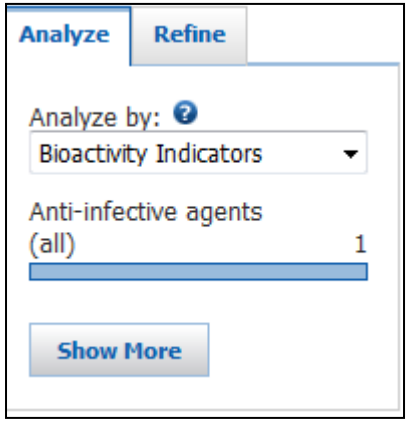
  —高分子化合物：分子式检索和结构检索

快速获得物质的生物活性及靶点信息





作用靶点



生物活性

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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。

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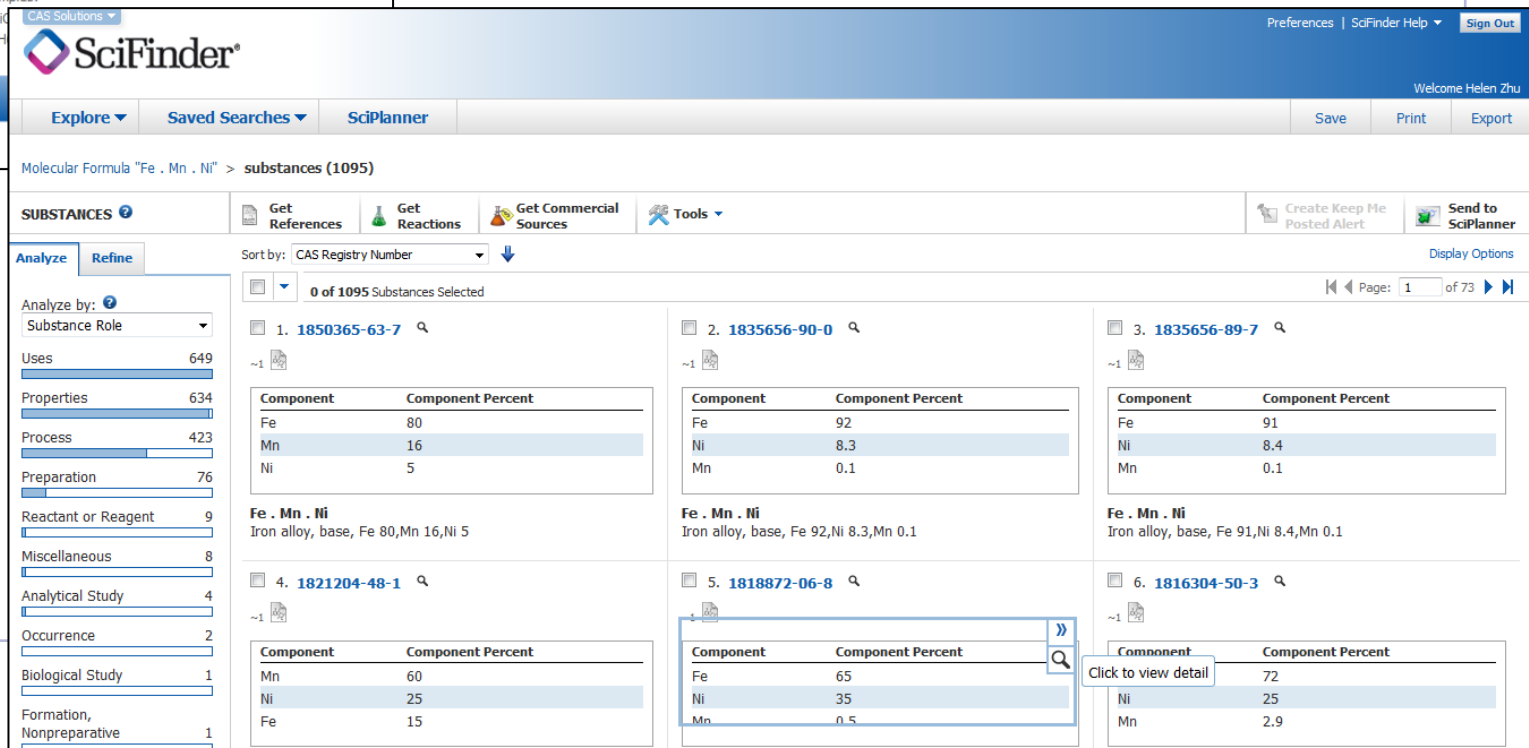
合金的检索

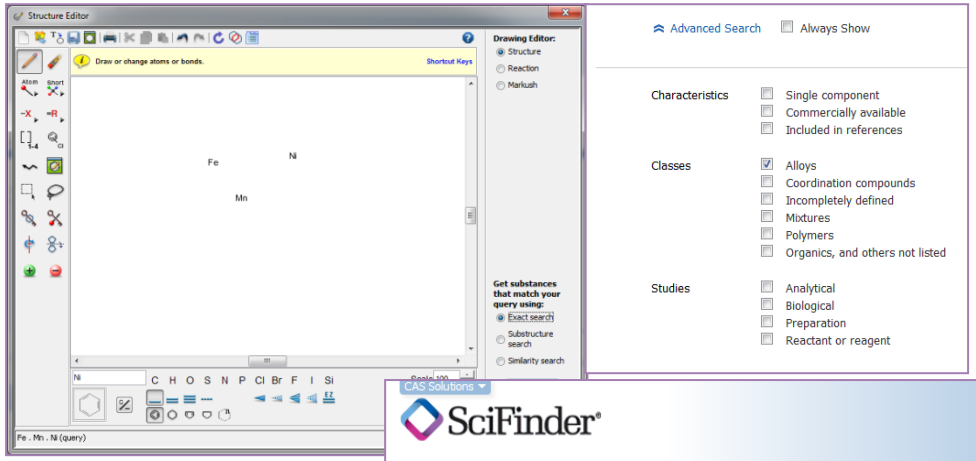
检索铁、锰、镍合金

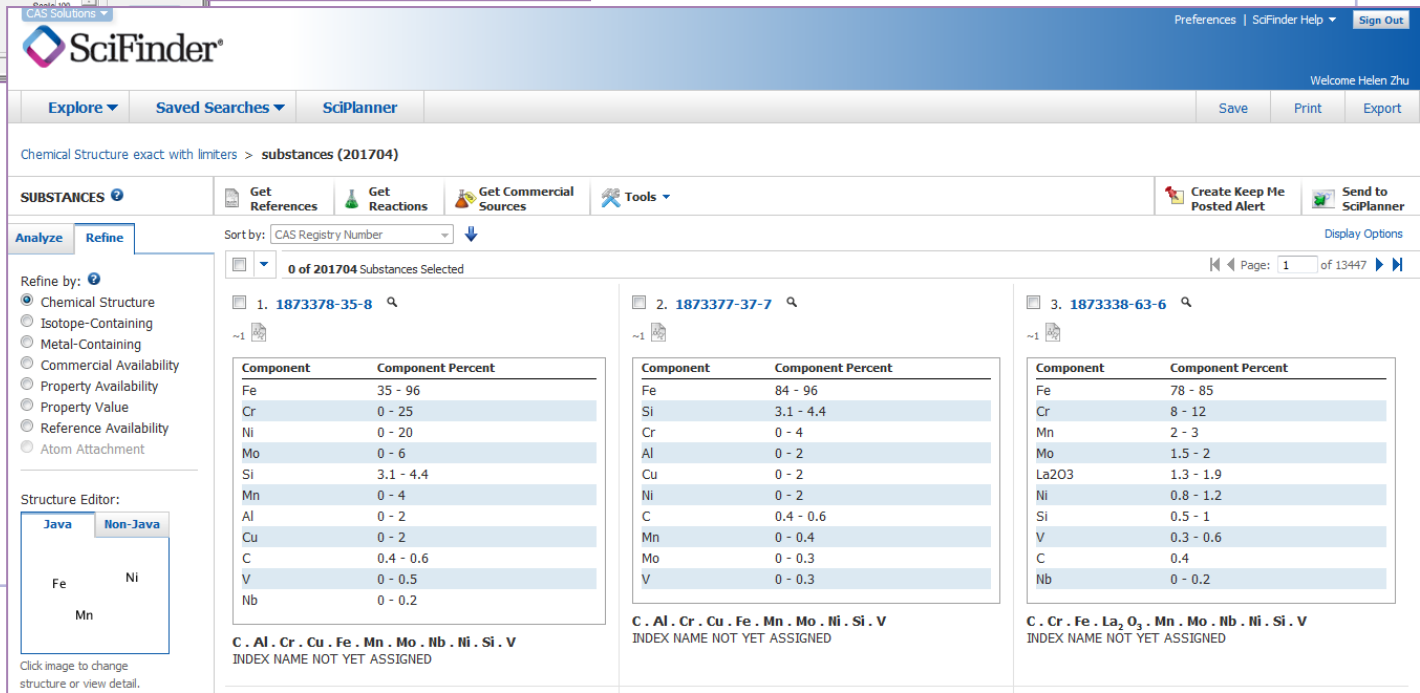
合金物质以列表形式呈现



合金的检索

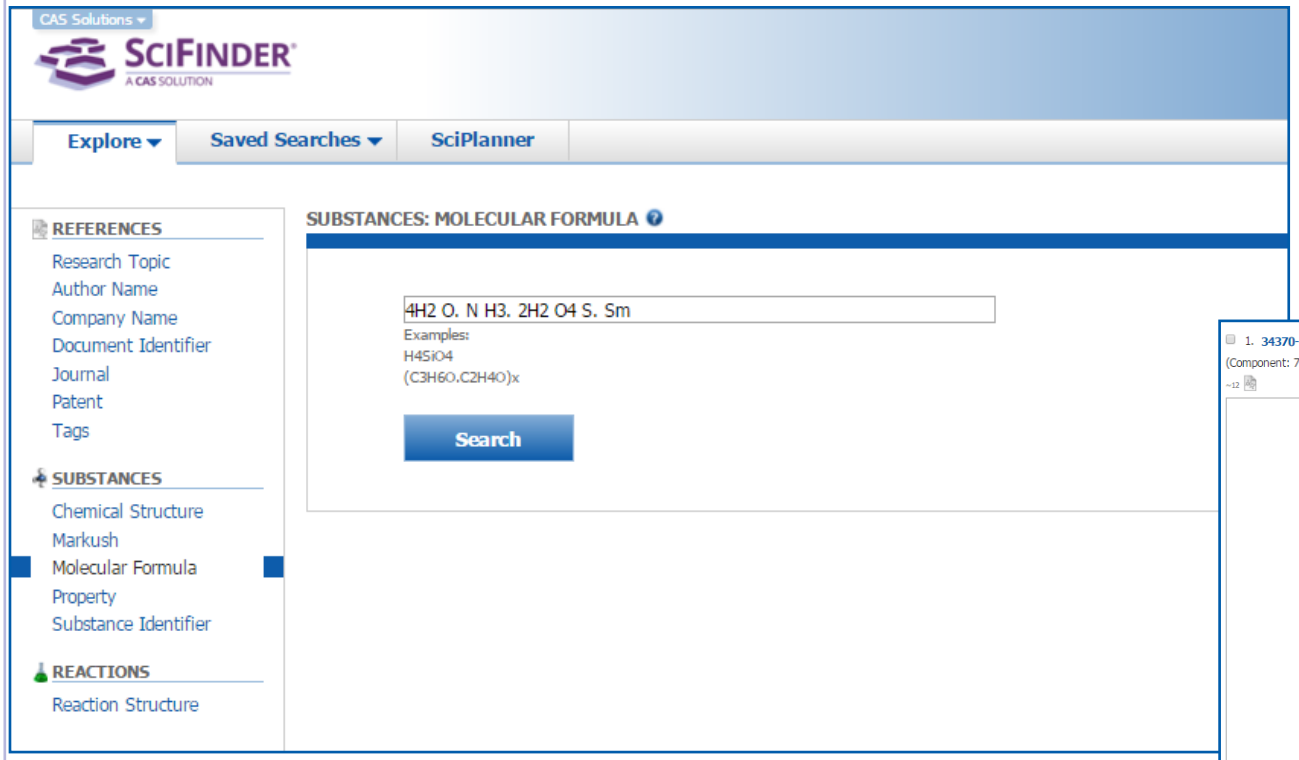
检索参杂铁、锰、镍原子的合金

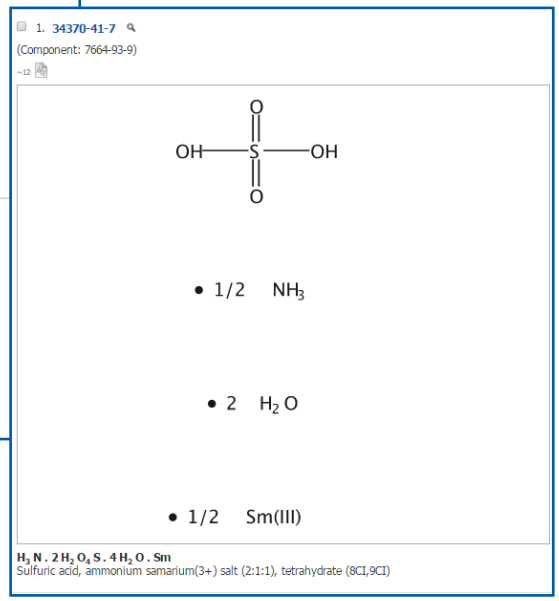




复杂无机物的检索

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





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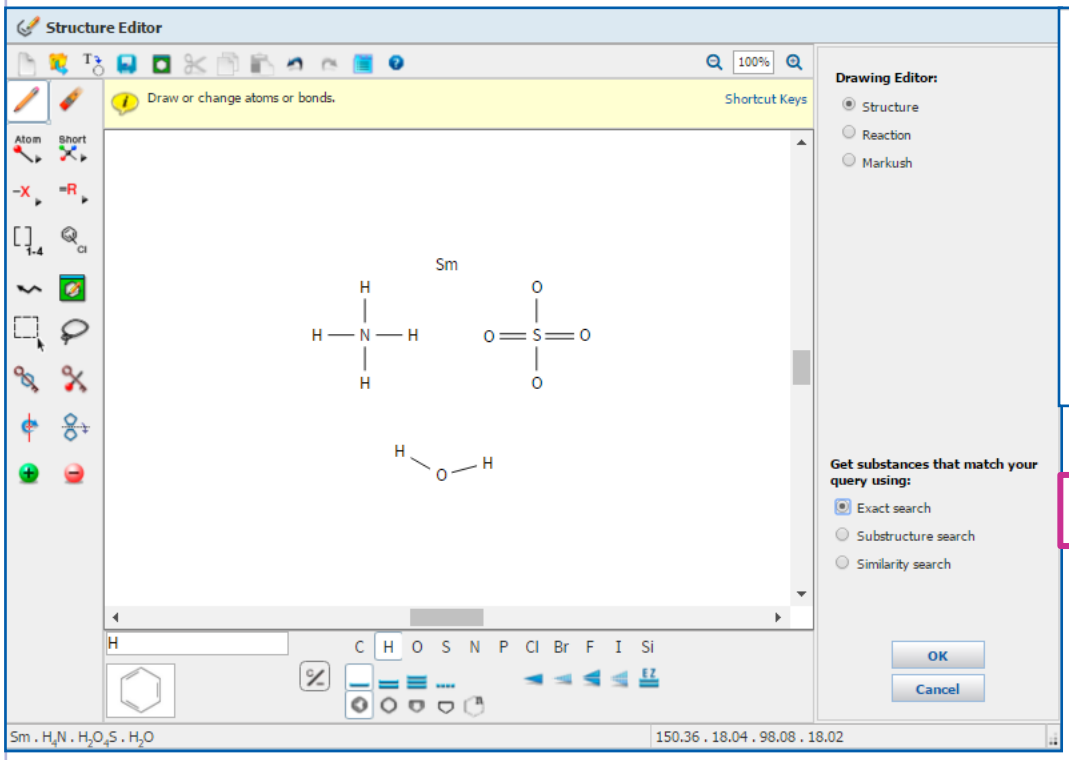
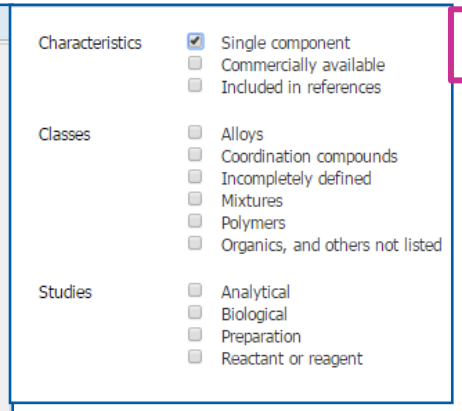
复杂无机物的检索

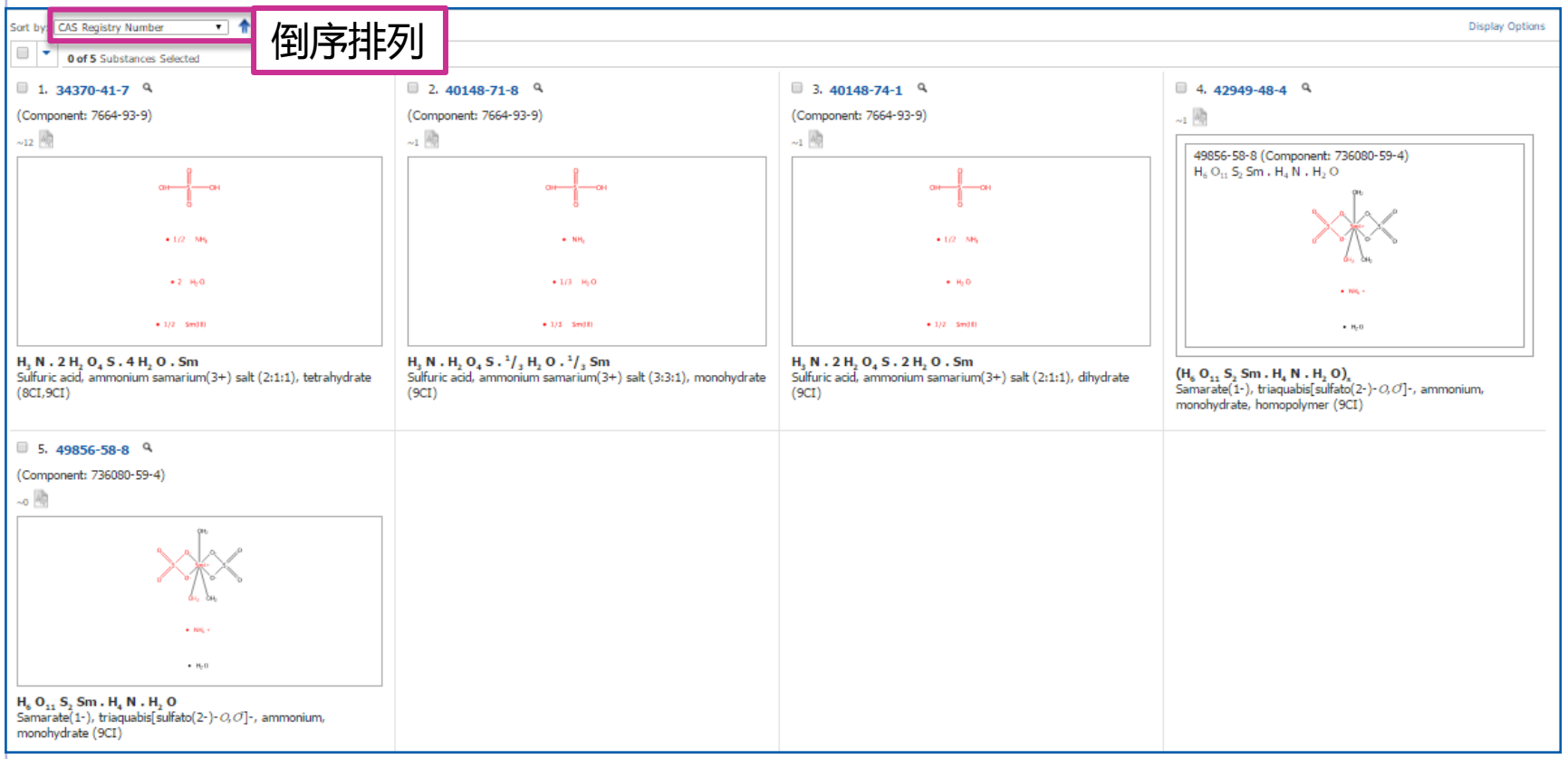




限定为单一组分

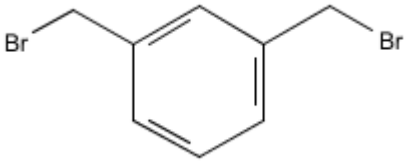
精确结构检索

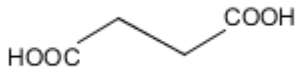
复杂无机物的检索


Sort by: CAS Registry Number
倒序排列
Display Options
0 of 5 Substances Selected
1. 34370-41-7
(Component: 7664-93-9)
~12
H2 N . 2 H2 O4 S . 4 H2 O . Sm
Sulfuric acid, ammonium samarium(3+) salt (2:1:1), tetrahydrate (8CI,9CI)
2. 40148-71-8
(Component: 7664-93-9)
~1
H3 N . H2 O4 S . 1/3 H2 O . 1/3 Sm
Sulfuric acid, ammonium samarium(3+) salt (3:3:1), monohydrate (9CI)
3. 40148-74-1
(Component: 7664-93-9)
~1
H3 N . 2 H2 O4 S . 2 H2 O . Sm
Sulfuric acid, ammonium samarium(3+) salt (2:1:1), dihydrate (9CI)
4. 42949-48-4
~1
49856-58-8 (Component: 736080-59-4)
H6 O11 S2 Sm . H4 N . H2 O
(H6 O11 S2 Sm . H4 N . H2 O)x
Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium, monohydrate, homopolymer (9CI)
5. 49856-58-8
(Component: 736080-59-4)
~0
H6 O11 S2 Sm . H4 N . H2 O
Samarate(1-), triaquabis[sulfato(2-)-O,O']-, ammonium, monohydrate (9CI)

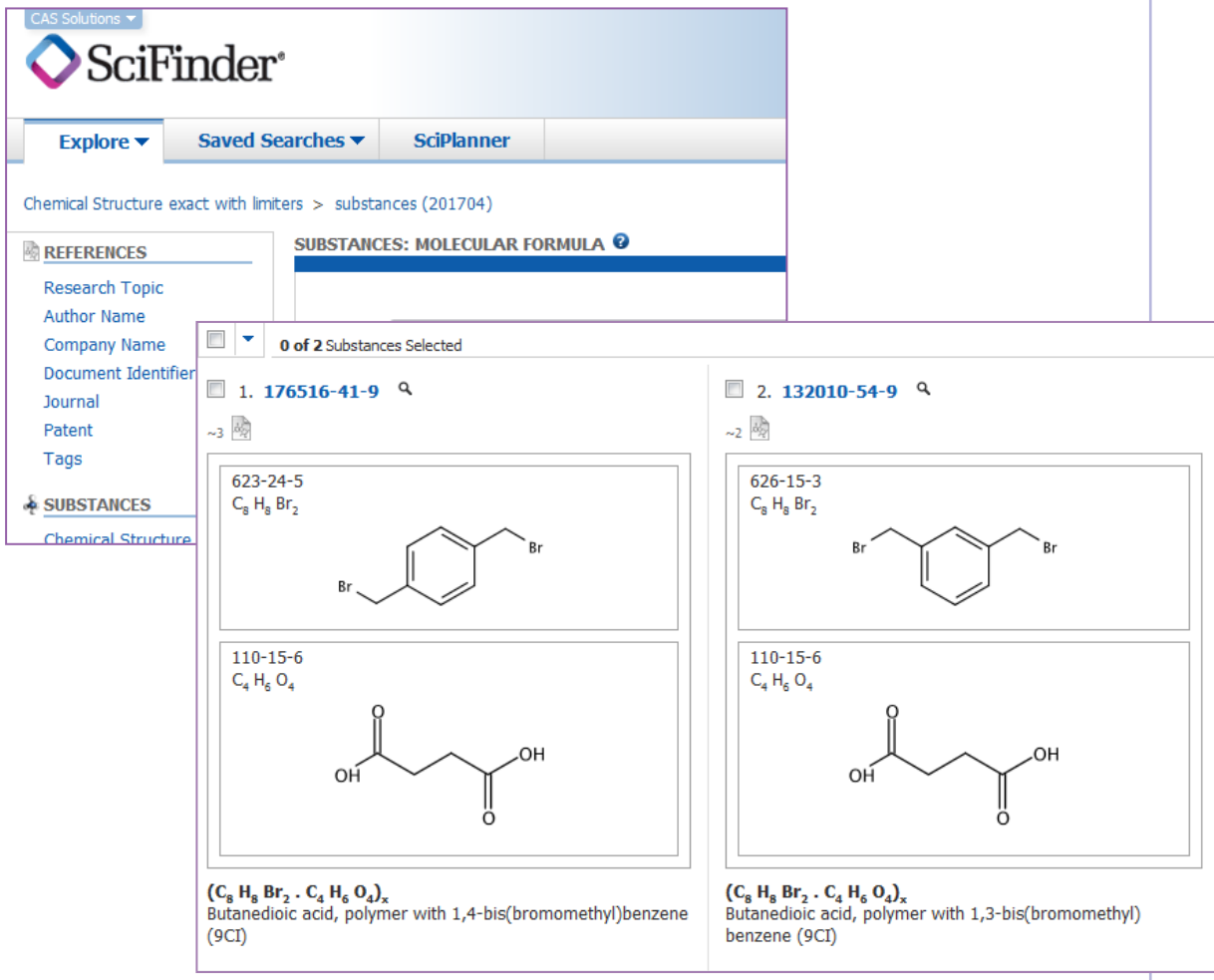
聚合物的检索

已知起始原料的聚合物





（C8 H8 Br2 . C4 H6 O4）x



分子式检索后会得到同分异构体

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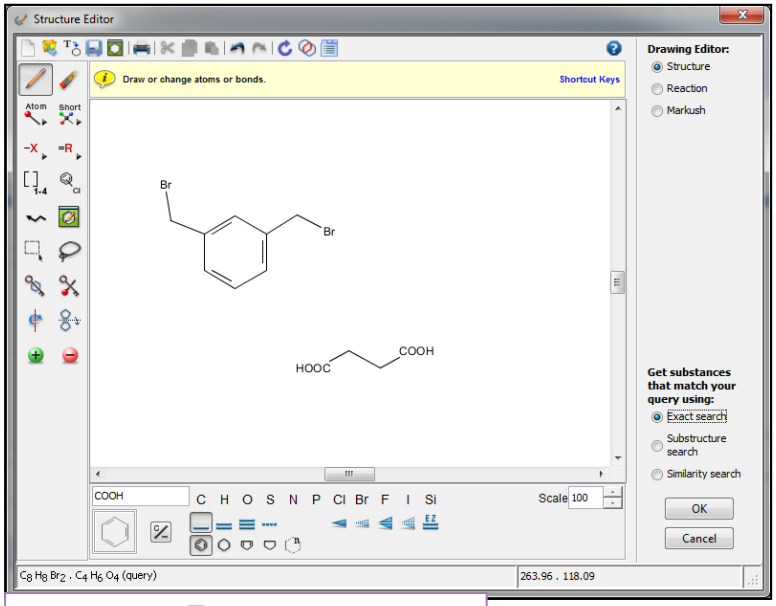
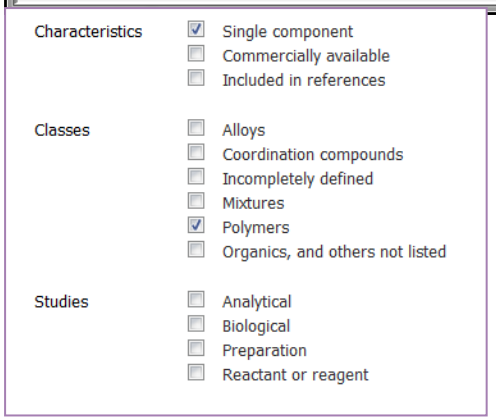
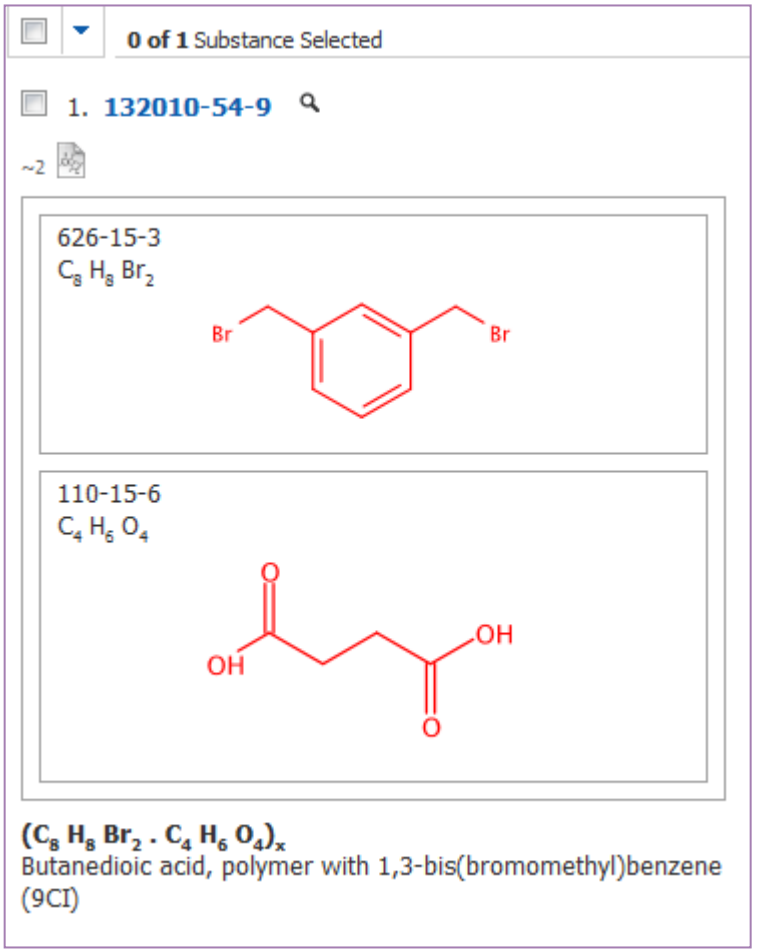
聚合物的检索





单一组分

聚合物



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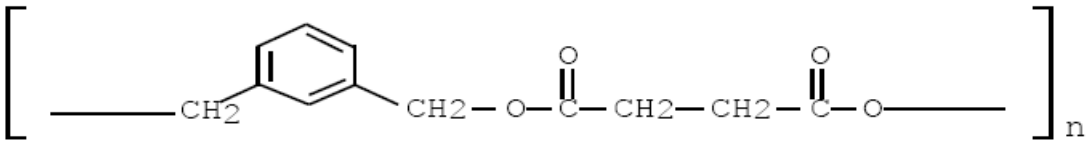
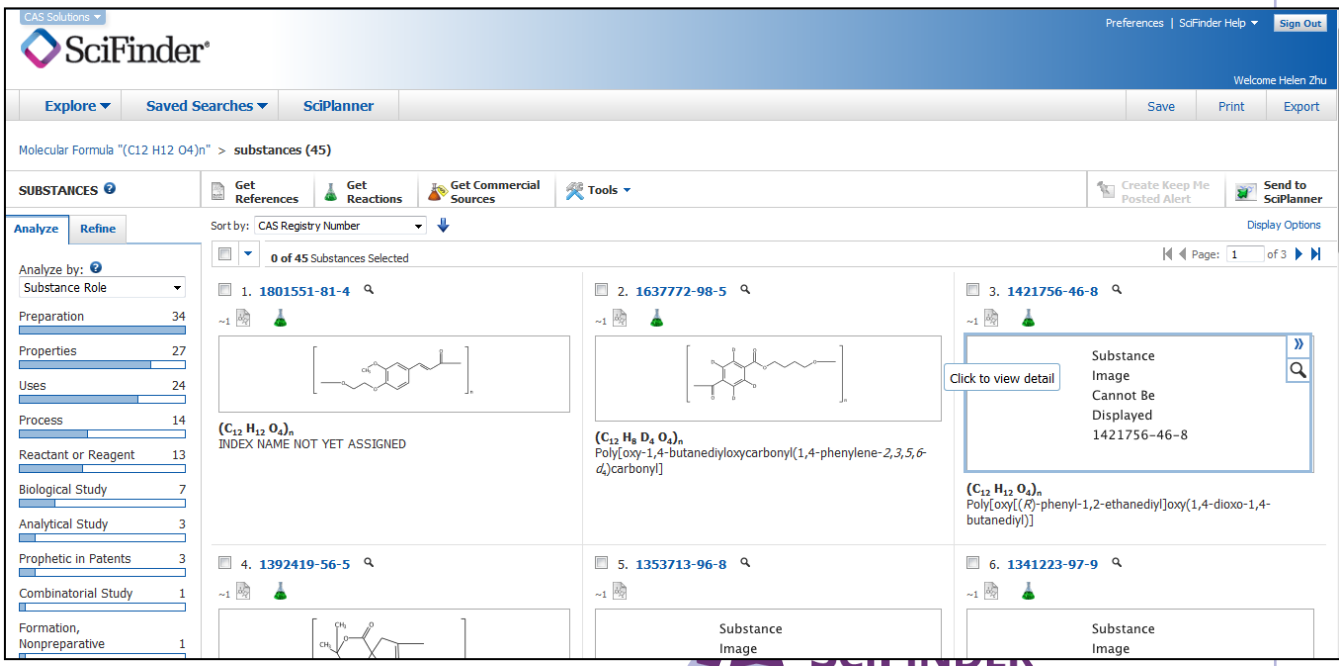
聚合物的检索

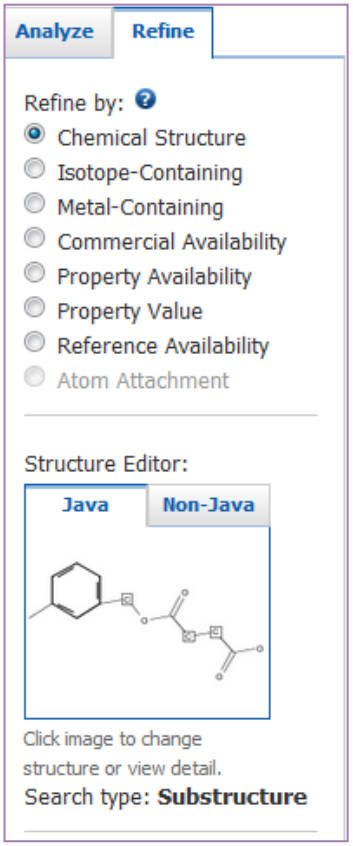
已知重复单元的聚合物

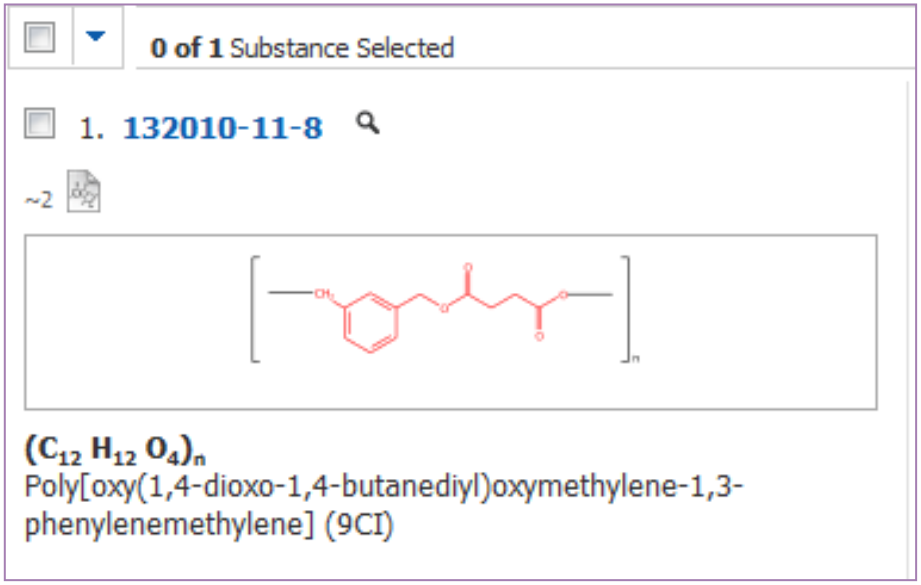


(C12 H12 O4)n



聚合物的检索

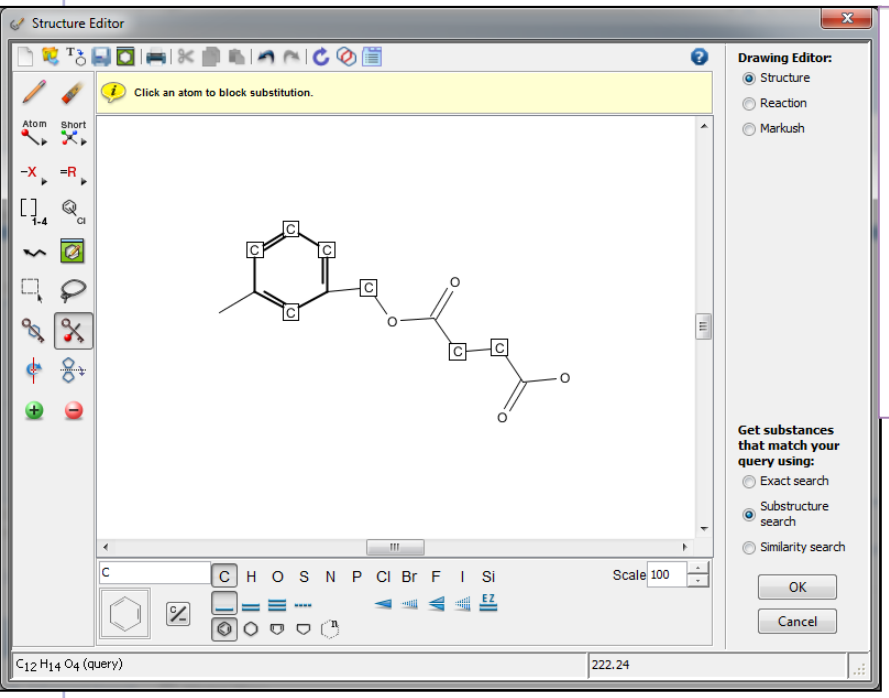




利用结构特征进行Refine，迅速查找需要的物质

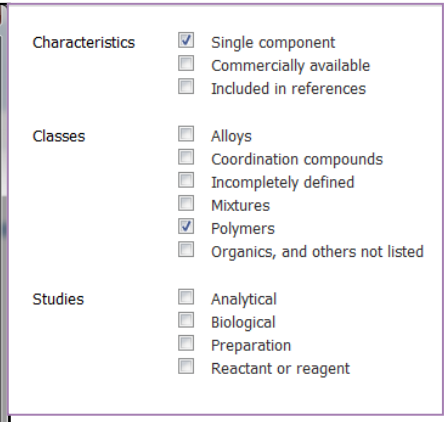
SciFinder® A CAS SOLUTION

聚合物的检索



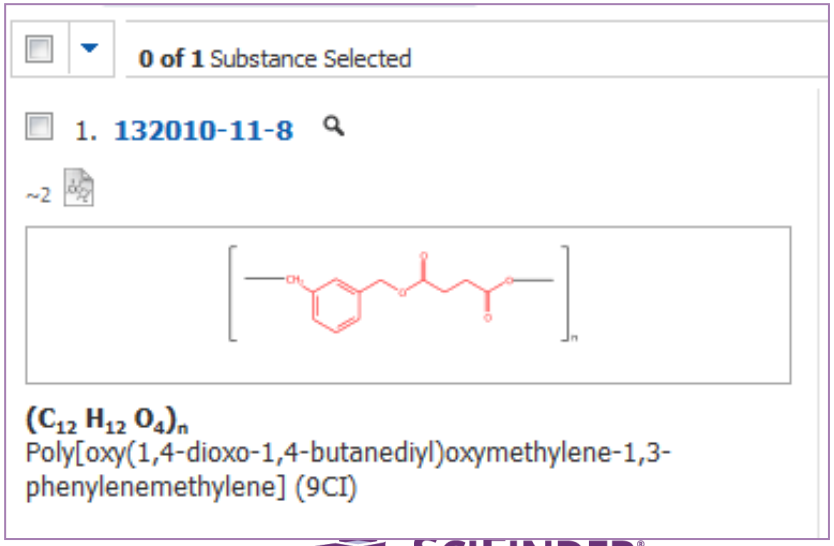
绘制好SRU后用亚结构检索

因为两段为开放状态



单一组分

聚合物



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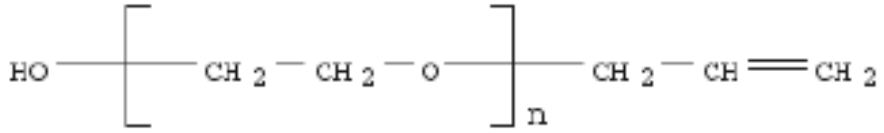
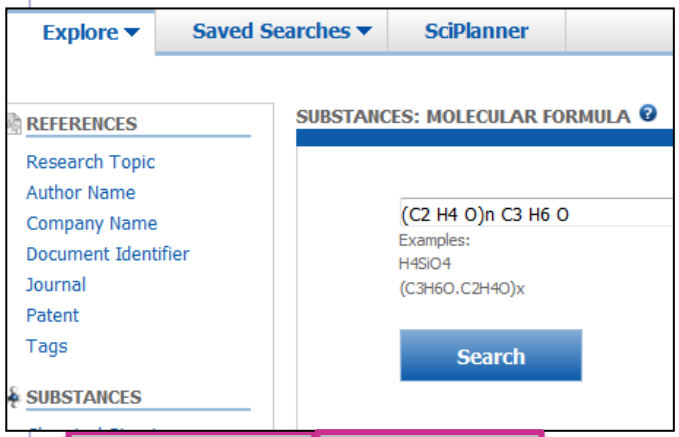
聚合物的检索

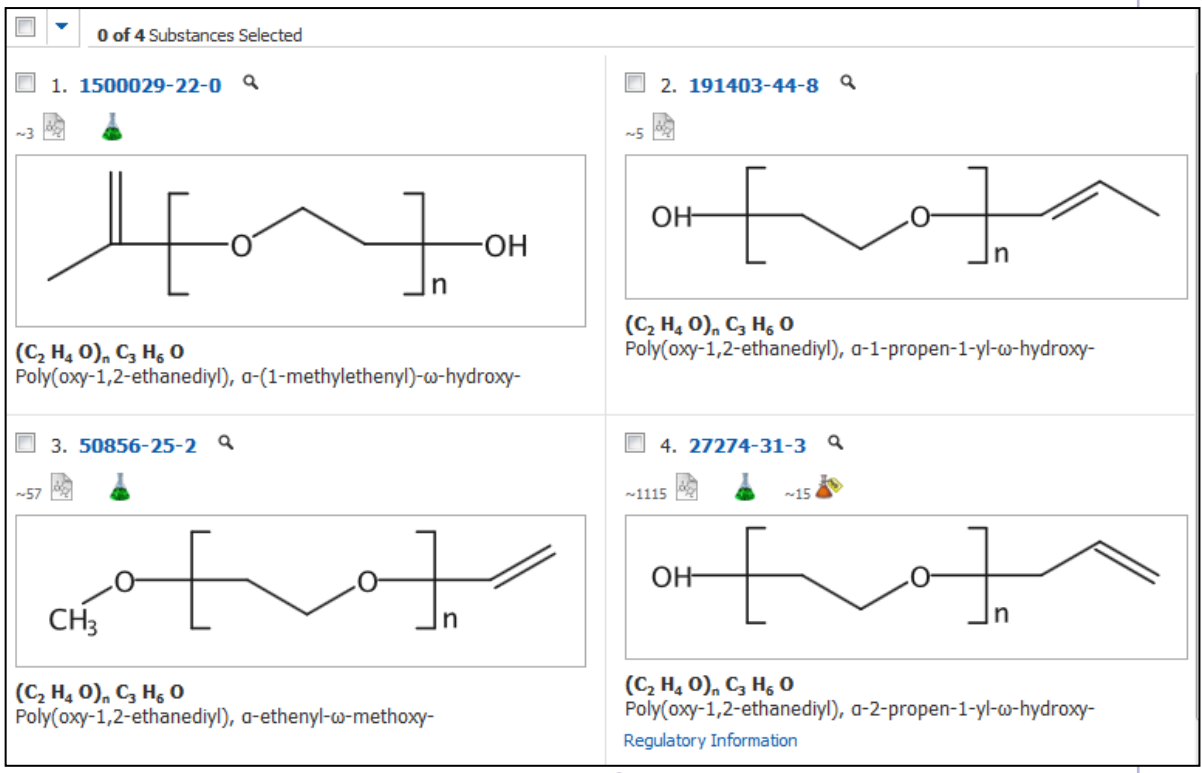
含端基和SRUs的聚合物





(C2 H4 O)n C3 H6 O

SRU部分　　两端部分



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聚合物的检索

后处理聚合物的检索：

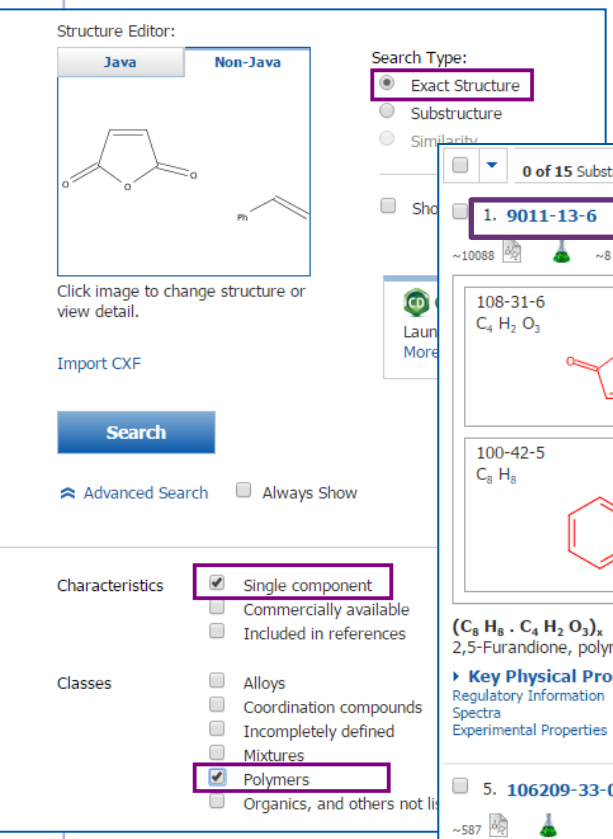
检索对由2, 5-呋喃二酮和苯乙烯聚合而成的物质进行结构修饰的聚合物

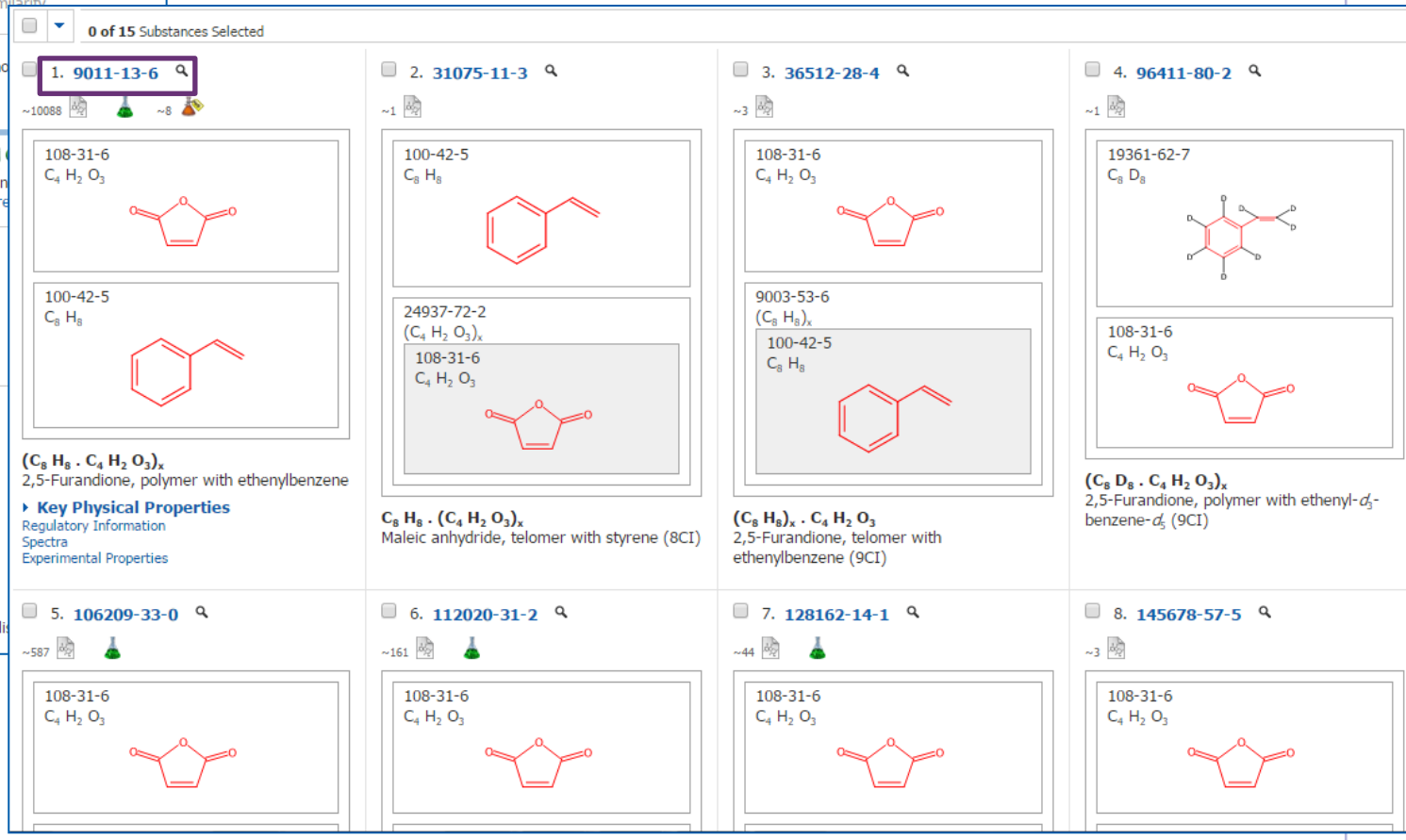
检索策略：

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





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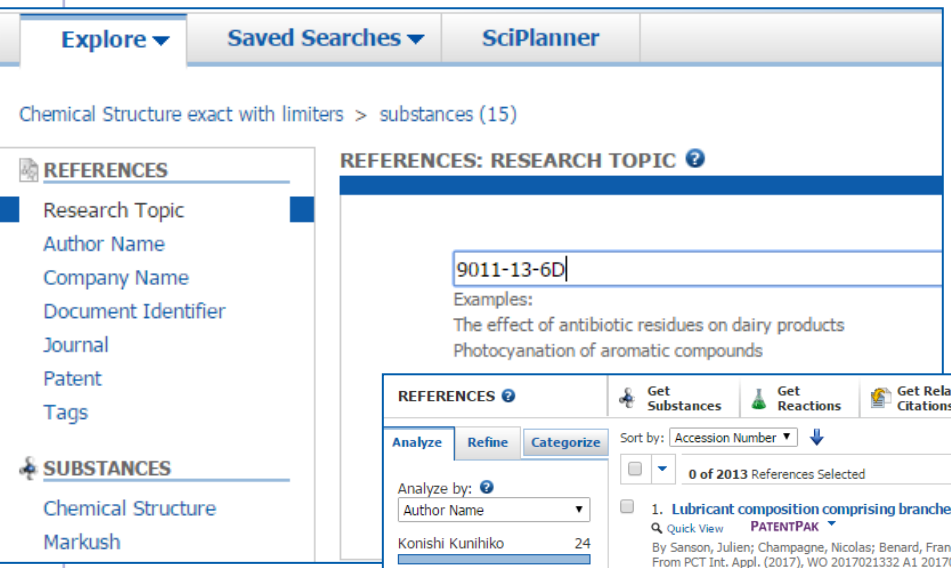
聚合物的检索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Chemical Structure exact with limiters > substances (15)
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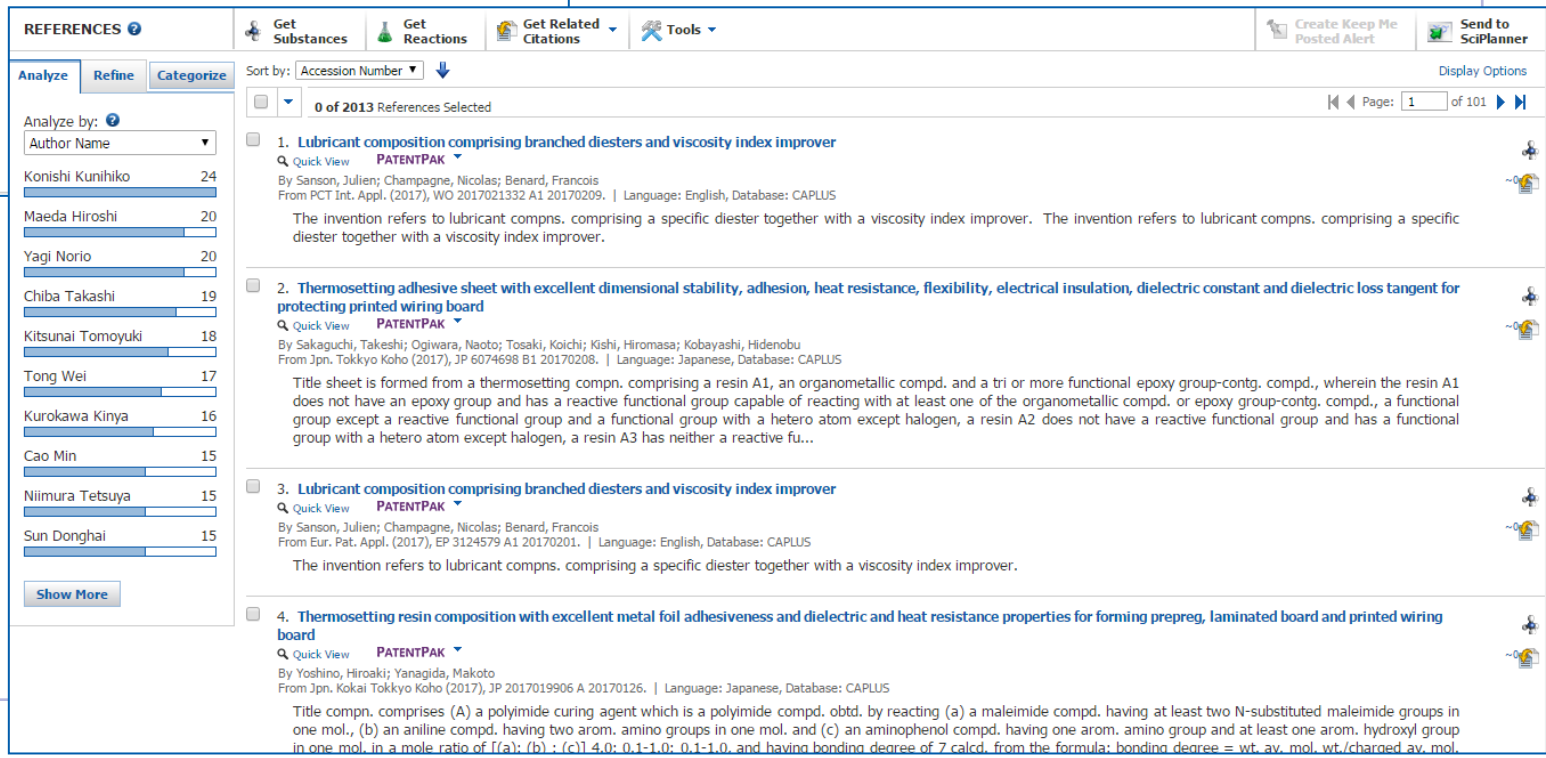
SUBSTANCES
Chemical Structure
Markush
REFERENCES: RESEARCH TOPIC
9011-13-6D
Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds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Page: 1 of 101
Analyze by:
Author Name
Konishi Kunihiko 24
Maeda Hiroshi 20
Yagi Norio 20
Chiba Takashi 19
Kitsunai Tomoyuki 18
Tong Wei 17
Kurokawa Kinya 16
Cao Min 15
Niimura Tetsuya 15
Sun Donghai 15
Show More
1. Lubricant composition comprising branched diesters and viscosity index improver
Quick View PATENTPAK
By Sanson, Julien; Champagne, Nicolas; Benard, Francois
From PCT Int. Appl. (2017), WO 2017021332 A1 20170209. | Language: English, Database: CAPLUS
The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver. The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.
2. Thermosetting adhesive sheet with excellent dimensional stability, adhesion, heat resistance, flexibility, electrical insulation, dielectric constant and dielectric loss tangent for protecting printed wiring board
Quick View PATENTPAK
By Sakaguchi, Takeshi; Ogiwara, Naoto; Tosaki, Koichi; Kishi, Hiromasa; Kobayashi, Hidenobu
From Jpn. Tokkyo Koho (2017), JP 6074698 B1 20170208. | Language: Japanese, Database: CAPLUS
Title sheet is formed from a thermosetting compn. comprising a resin A1, an organometallic compd. and a tri or more functional epoxy group-contg. compd., wherein the resin A1 does not have an epoxy group and has a reactive functional group capable of reacting with at least one of the organometallic compd. or epoxy group-contg. compd., a functional group except a reactive functional group and a functional group with a hetero atom except halogen, a resin A2 does not have a reactive functional group and has a functional group with a hetero atom except halogen, a resin A3 has neither a reactive fu...
3. Lubricant composition comprising branched diesters and viscosity index improver
Quick View PATENTPAK
By Sanson, Julien; Champagne, Nicolas; Benard, Francois
From Eur. Pat. Appl. (2017), EP 3124579 A1 20170201. | Language: English, Database: CAPLUS
The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.
4. Thermosetting resin composition with excellent metal foil adhesiveness and dielectric and heat resistance properties for forming prepreg, laminated board and printed wiring board
Quick View PATENTPAK
By Yoshino, Hiroaki; Yanagida, Makoto
From Jpn. Kokai Tokkyo Koho (2017), JP 2017019906 A 20170126. | Language: Japanese, Database: CAPLUS
Title compn. comprises (A) a polyimide curing agent which is a polyimide compd. obtd. by reacting (a) a maleimide compd. having at least two N-substituted maleimide groups in one mol., (b) an aniline compd. having two arom. amino groups in one mol. and (c) an aminophenol compd. having one arom. amino group and at least one arom. hydroxyl group in one mol. in a mole ratio of [(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.

聚合物的检索

1. Lubricant composition comprising branched diesters and viscosity index improver

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

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

Patent Information

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

Priority Application

EP 2015-179371	A	Jul 31, 2015

Indexing

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

Concepts

Base oils
Crankcase oil
Lubricating oil additives
Transesterification

lubricant compn. comprising branched diesters and viscosity index improver

Polyolefins

lubricant compn. comprising branched diesters and viscosity index improver

Modifier or additive use; Uses

Lubricating oil additives

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

Substances

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

lubricant compn. comprising branched diesters and viscosity index improver

Modifier or additive use; Uses

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

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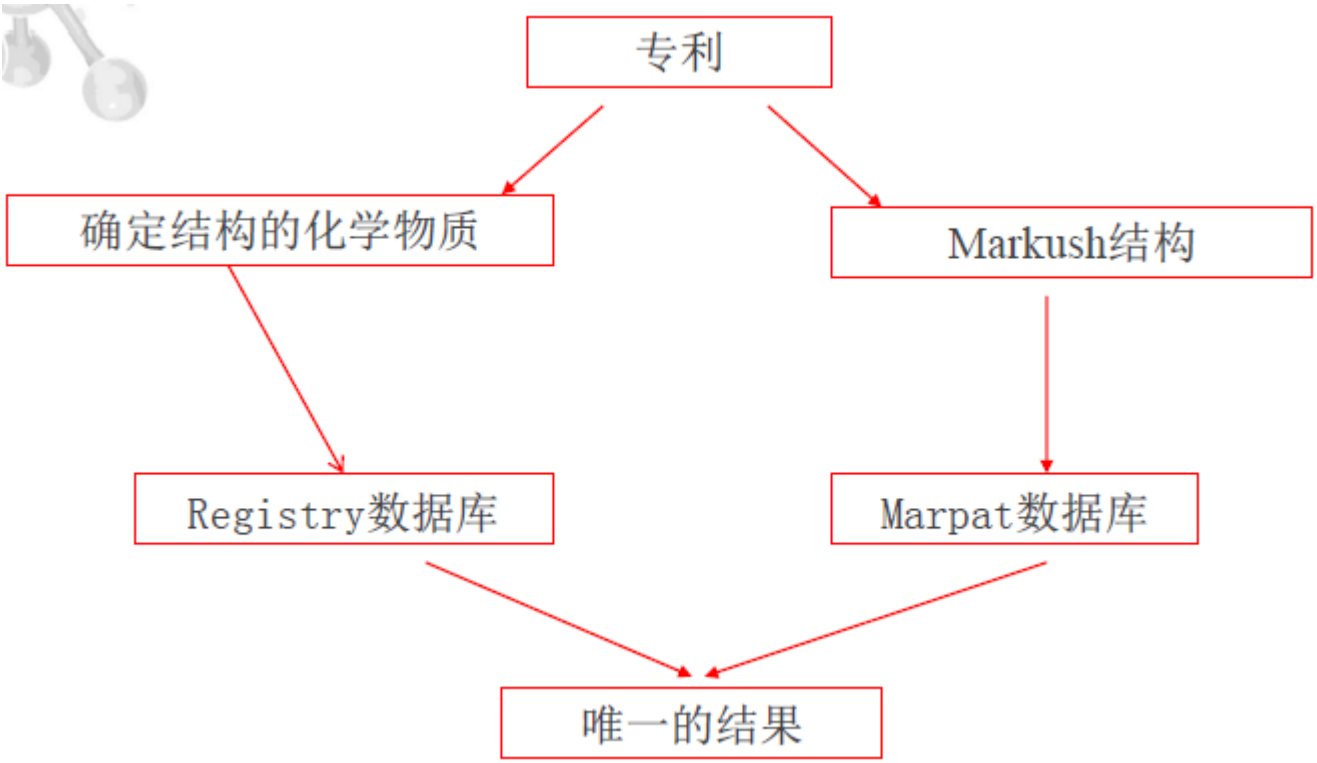
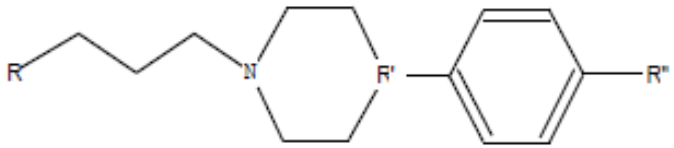
检索具有相同结构特征物质及专利文献



检索具有相同结构特征物质及专利文献

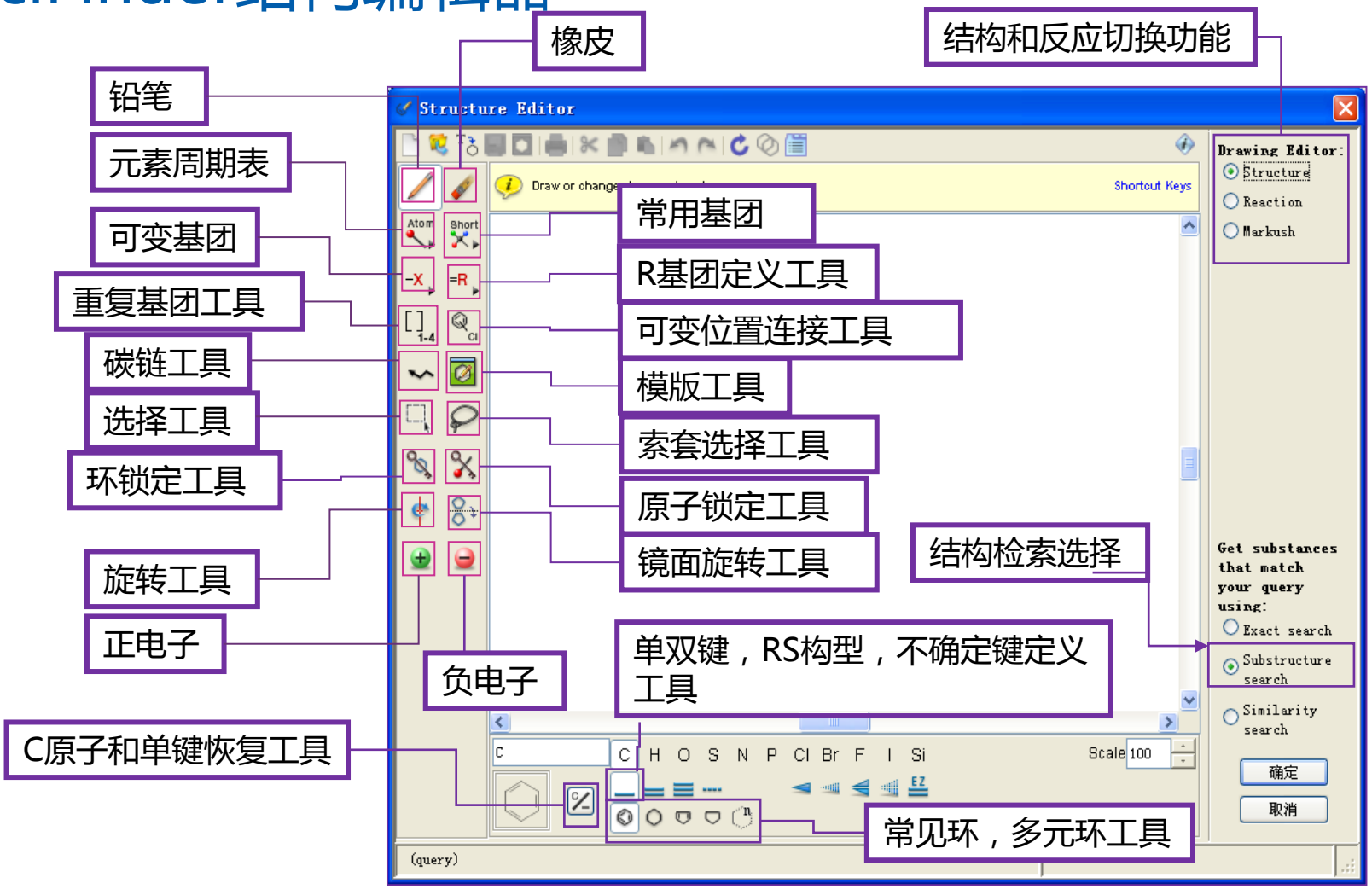
查询报道具有如下结构特征专利文献:



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



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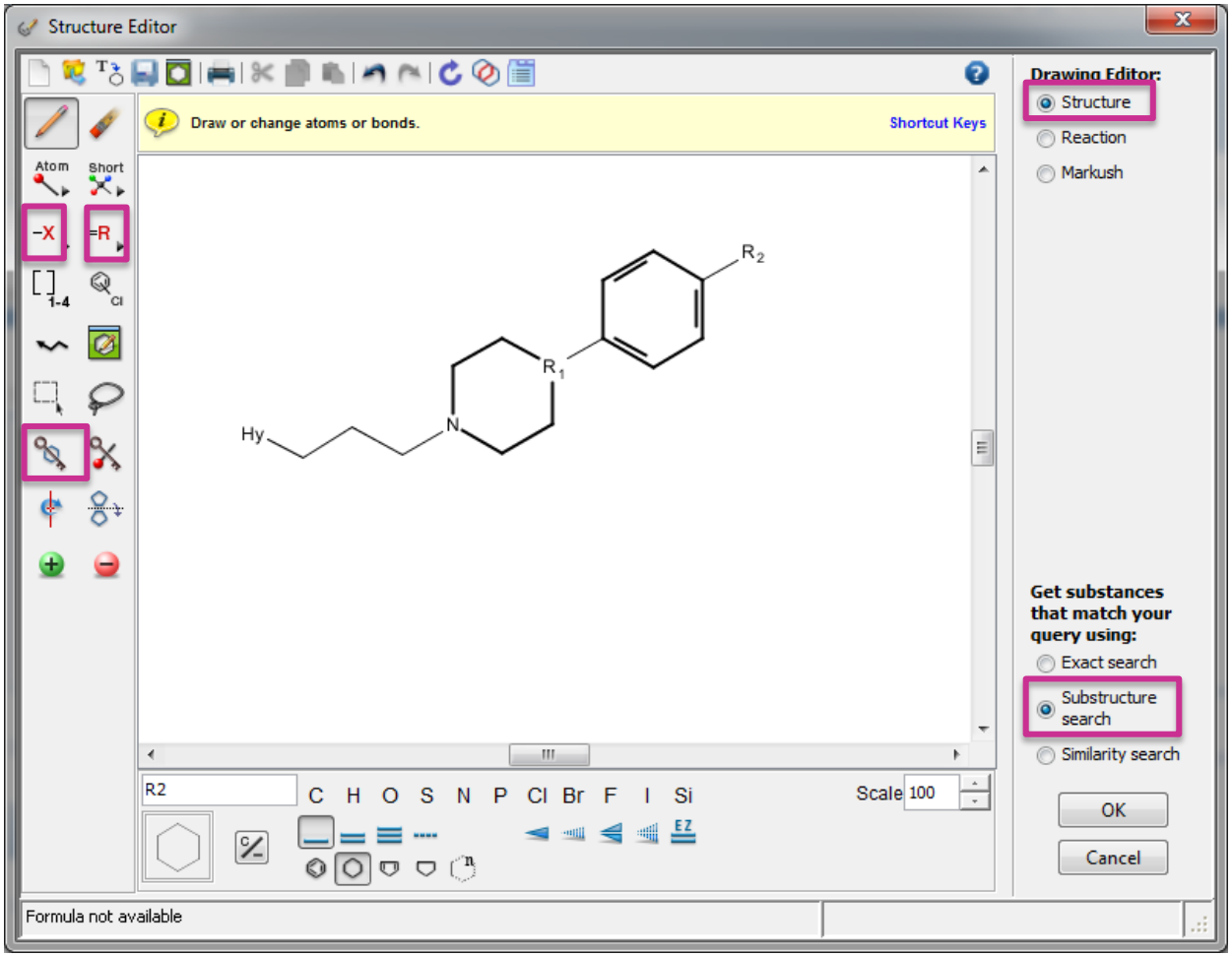

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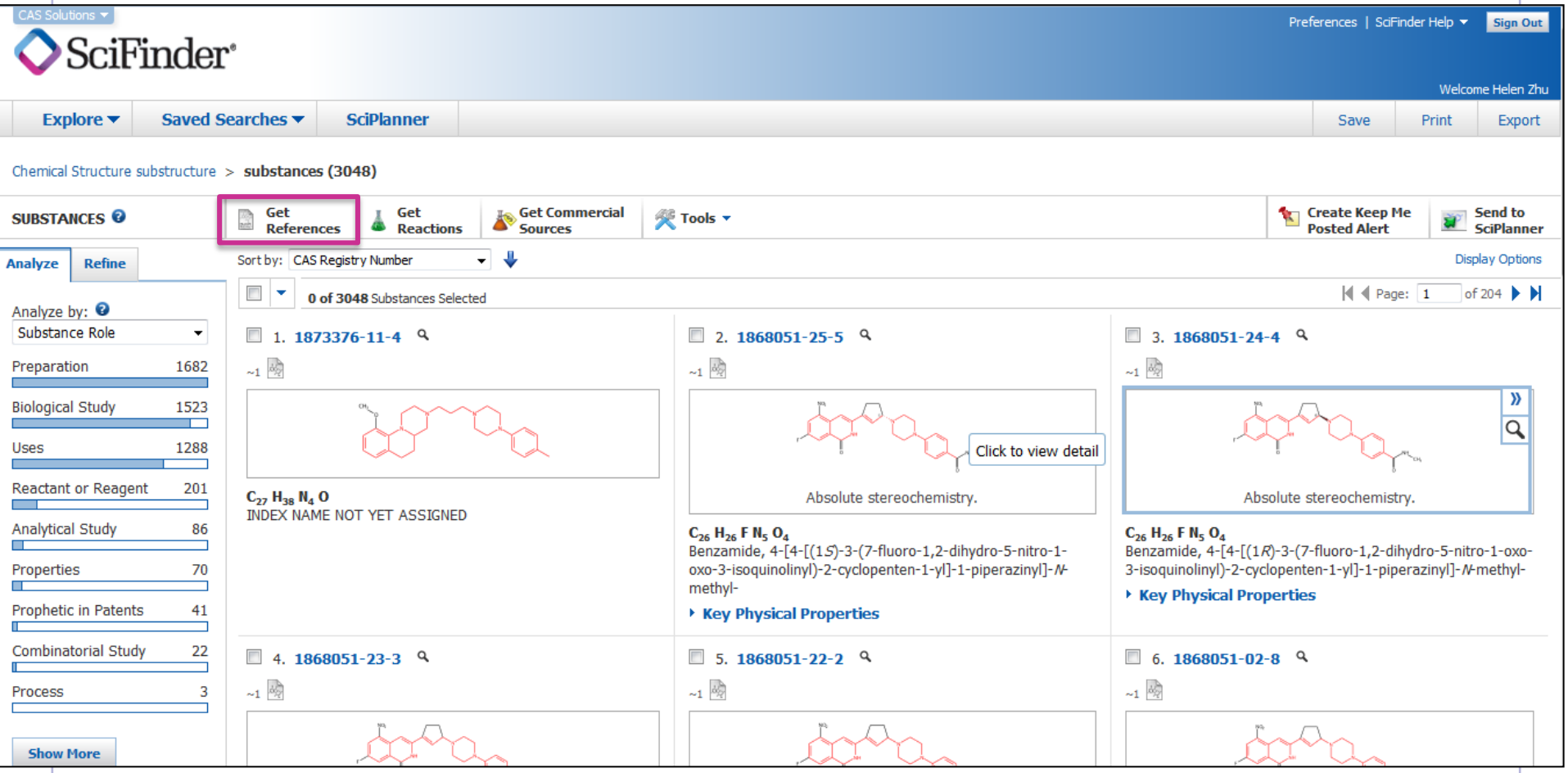

检索具有相同结构特征物质及专利文献

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

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- Document Type
- Publication Year
- Language
- Database

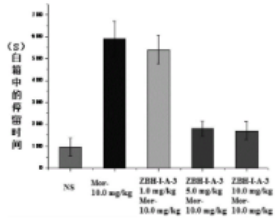
Document Type(s)
- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent

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



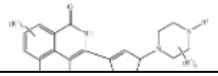
Title compds. I [wherein A = $(CH_2)_n$, n is 2 to 4; R = H, 4-Cl, 2,3-diCl, 4-CH_3, 2,3-diCH_3, 4-OCF_3, 4-OCH_3, 2-OCF_3, 2,6-diCH_3, 3,4-diCH_3, 3-CF_3, 4-Cl, 3-OCH_3, 2-C_2h_5, or 2-CH_3], and their pharmaceutically acceptable salts thereof, were prepd. as D3 acceptor ligands, which are used for treating nervous centralis mental disorder such as Parkinson's disease, schizophrenia, drug dependence and etc. effectively. Thus, the invention compd. I [A = $(CH_2)_3$; 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 R^1 is independently halo, CN, NO_2, perfluoroalkyl, acyl,e tc.; R^2

通过DT限定获得专利文献，保存

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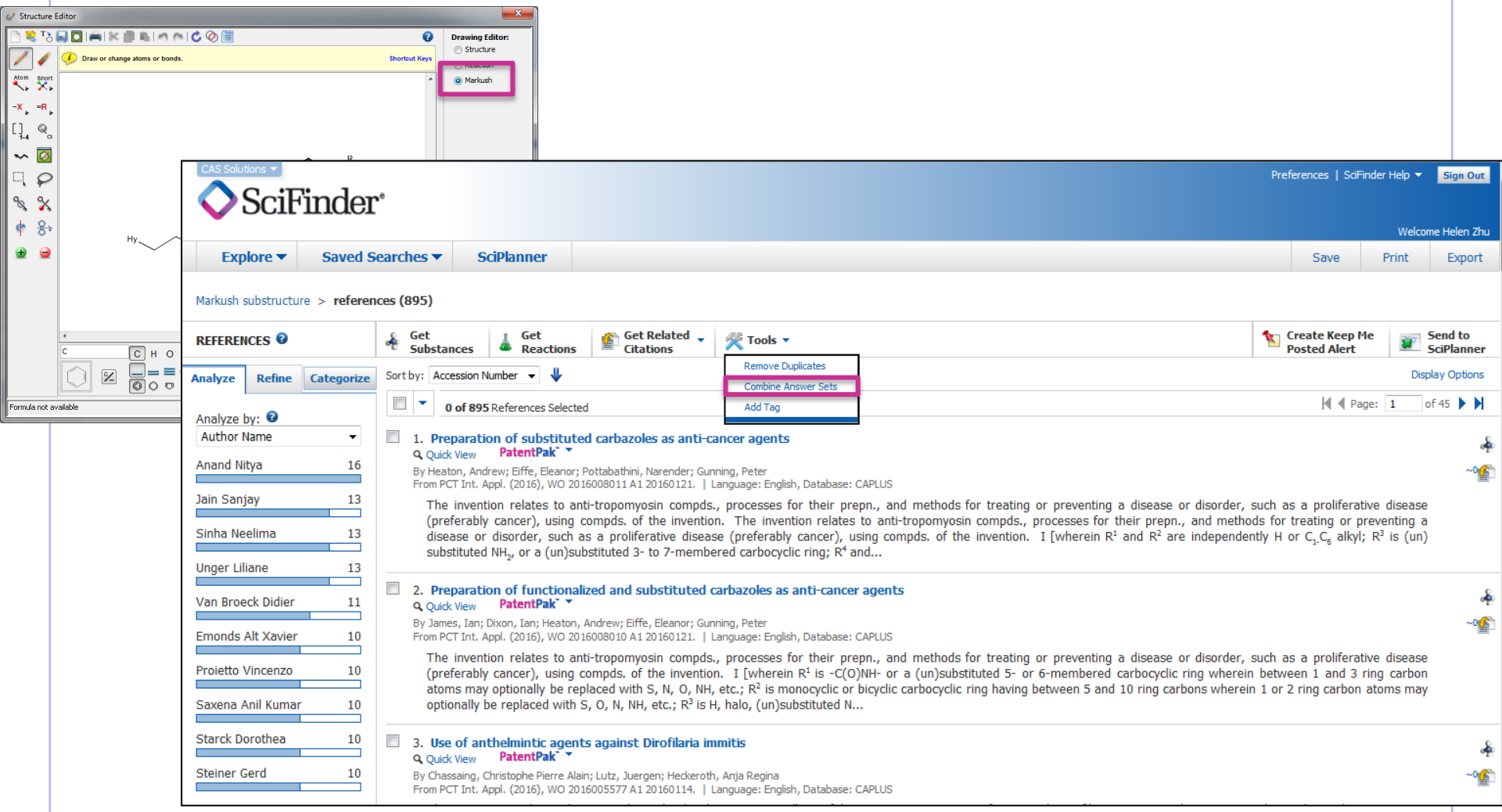
检索具有相同结构特征物质及专利文献



与前一个结果集合并，得到完整的结果集

SciFinder® A CAS SOLUTION

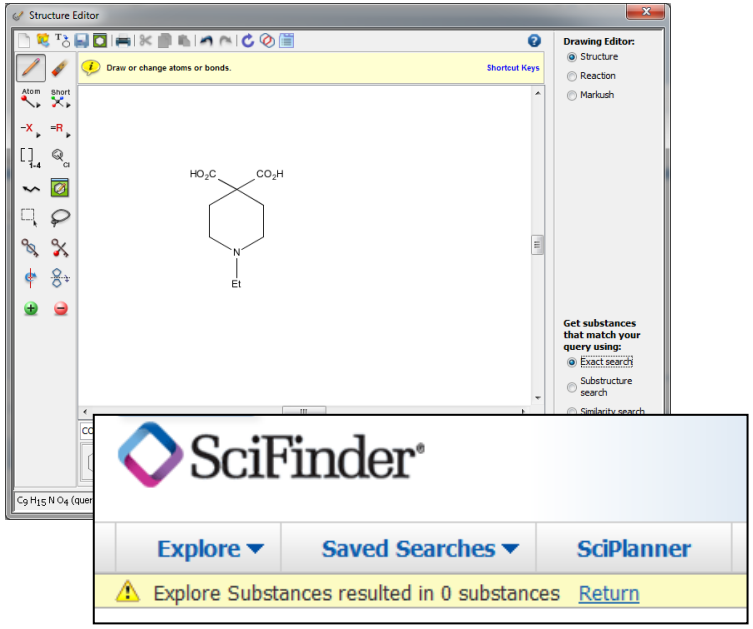
如何判断结构的新颖性

新颖性：是否存在？是否能申请专利？

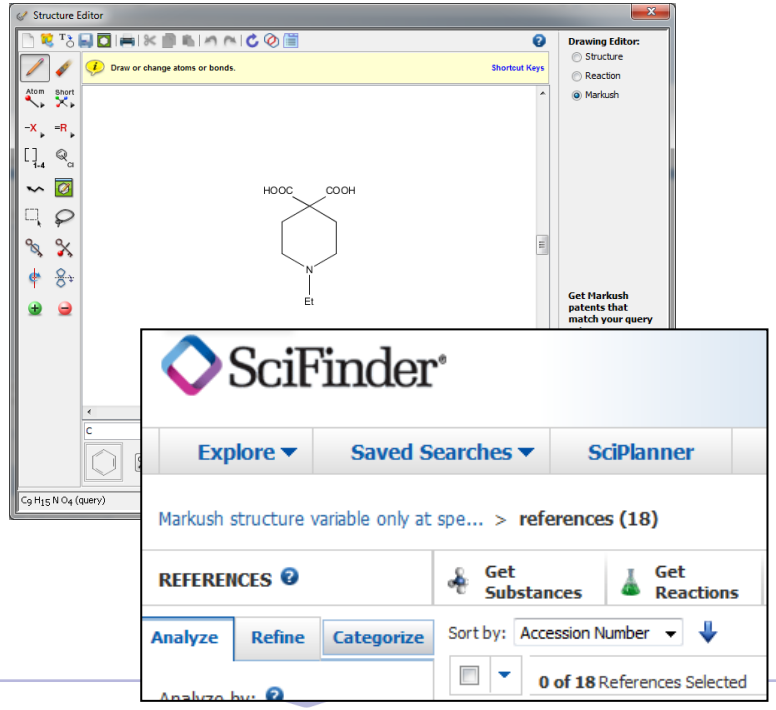
SciFinder相关物质库：Registry和Marpat

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

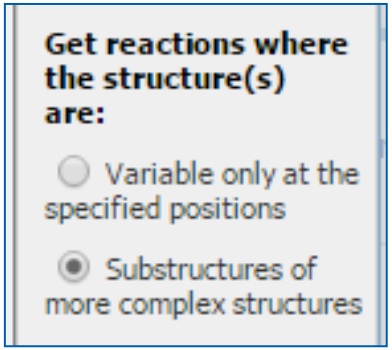
- 常用获取方法

  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



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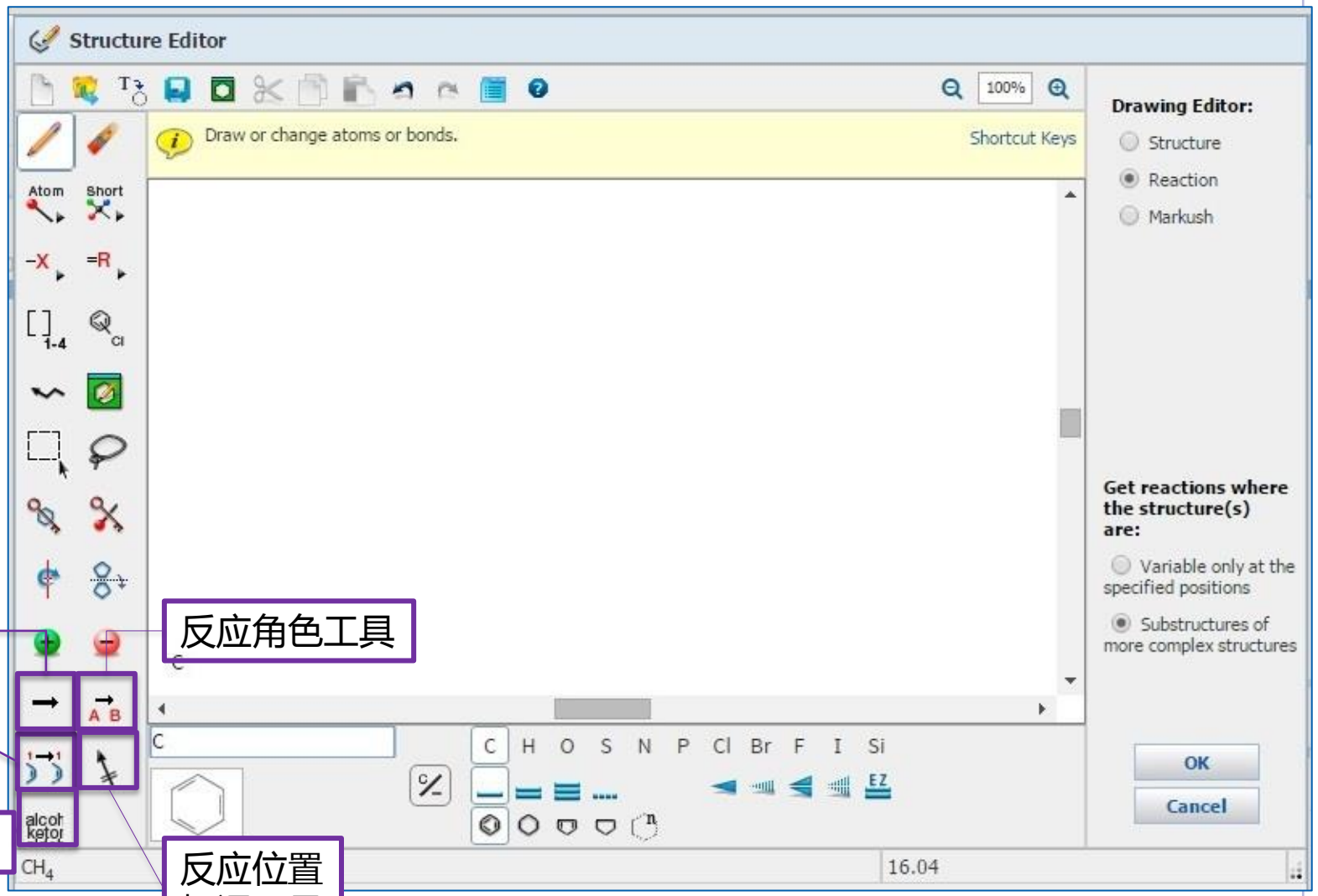
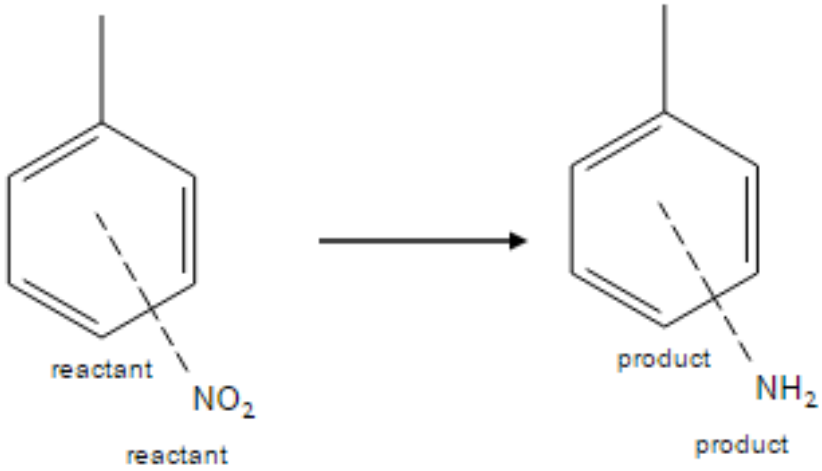
反应绘制工具


Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
C H O S N P Cl Br F I Si
CH4
16.04
反应箭头
反应角色工具
反应原子标记工具
官能团列表
反应位置标记工具

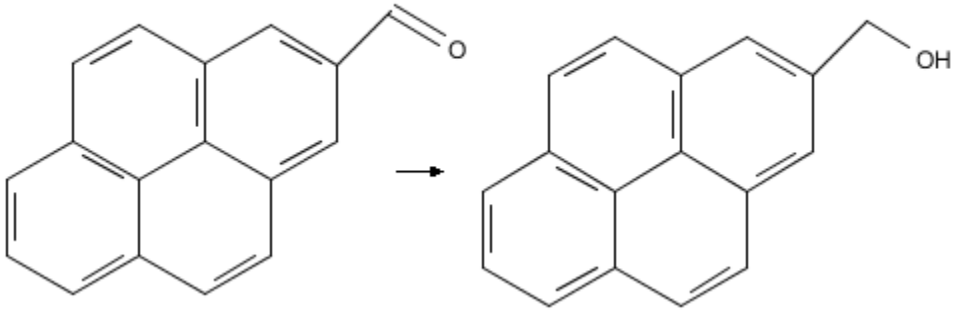
反应的精准定义

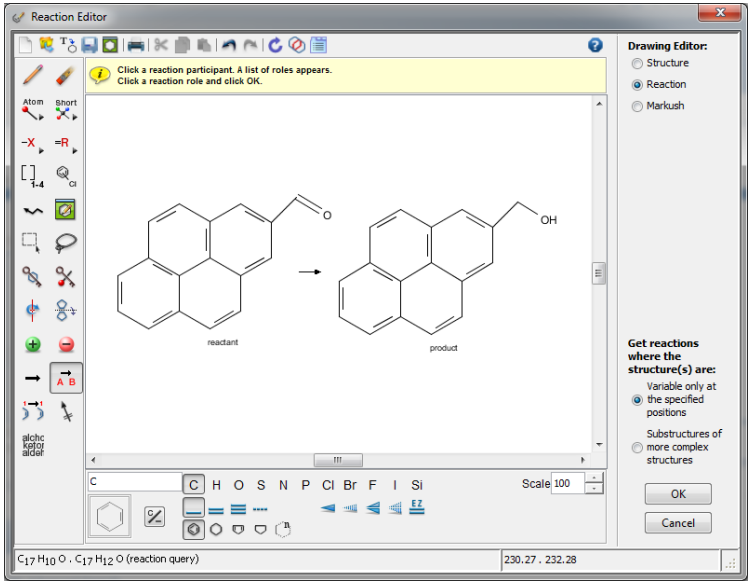
检索符合以下要求的反应，硝基还原

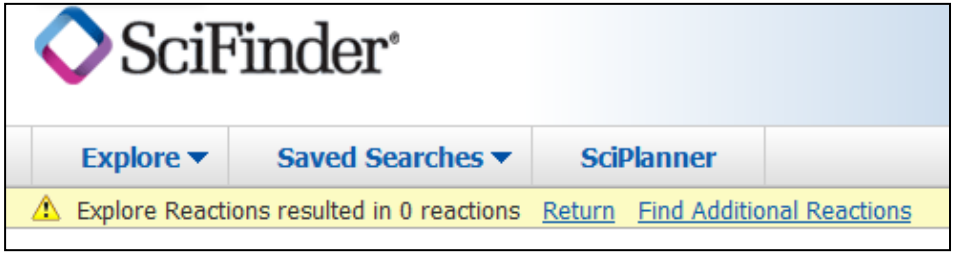


巧妙获得有实验步骤的相关反应

该还原反应如何操作？







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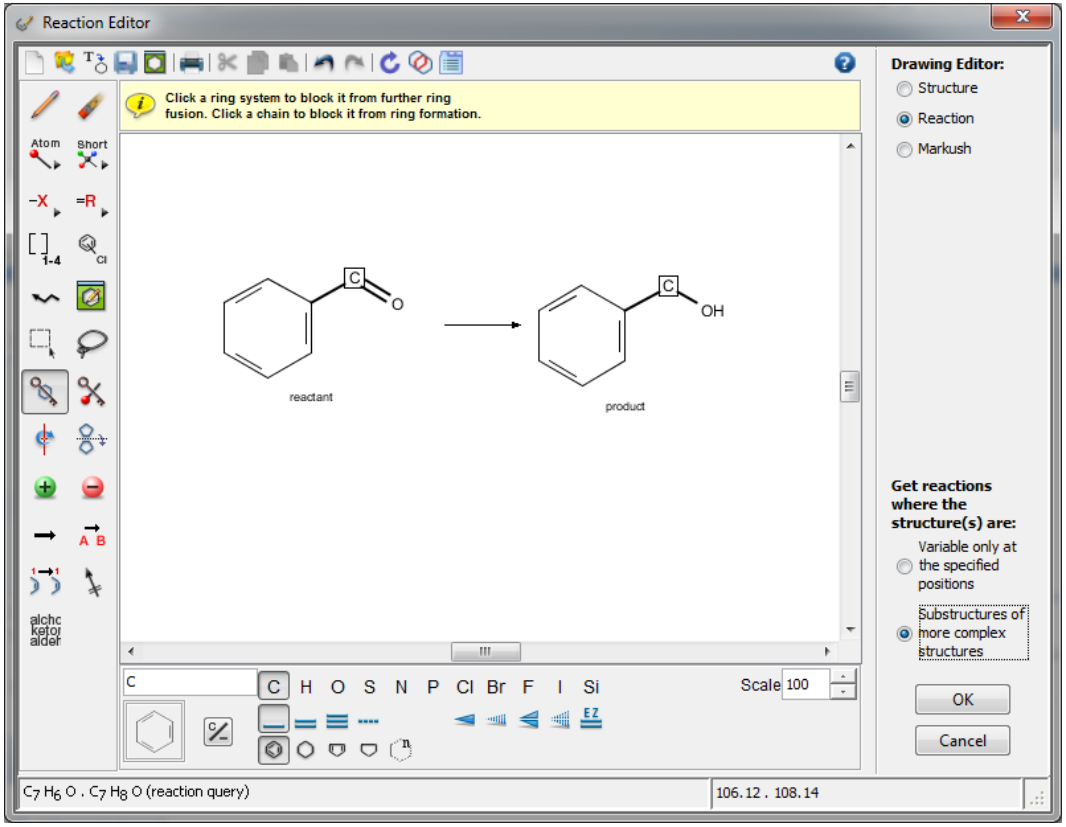
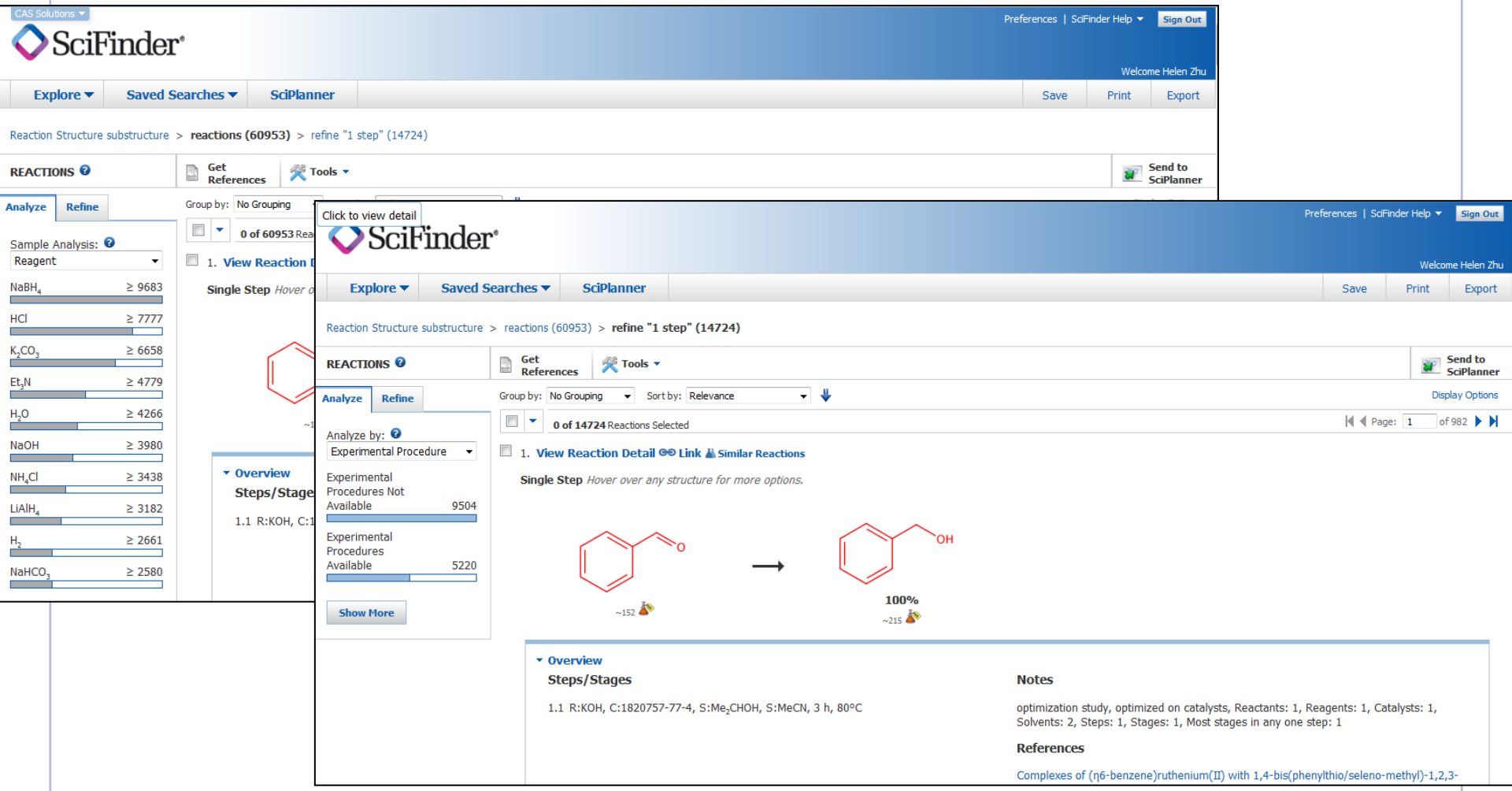
巧妙获得有反应步骤的相关反应



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

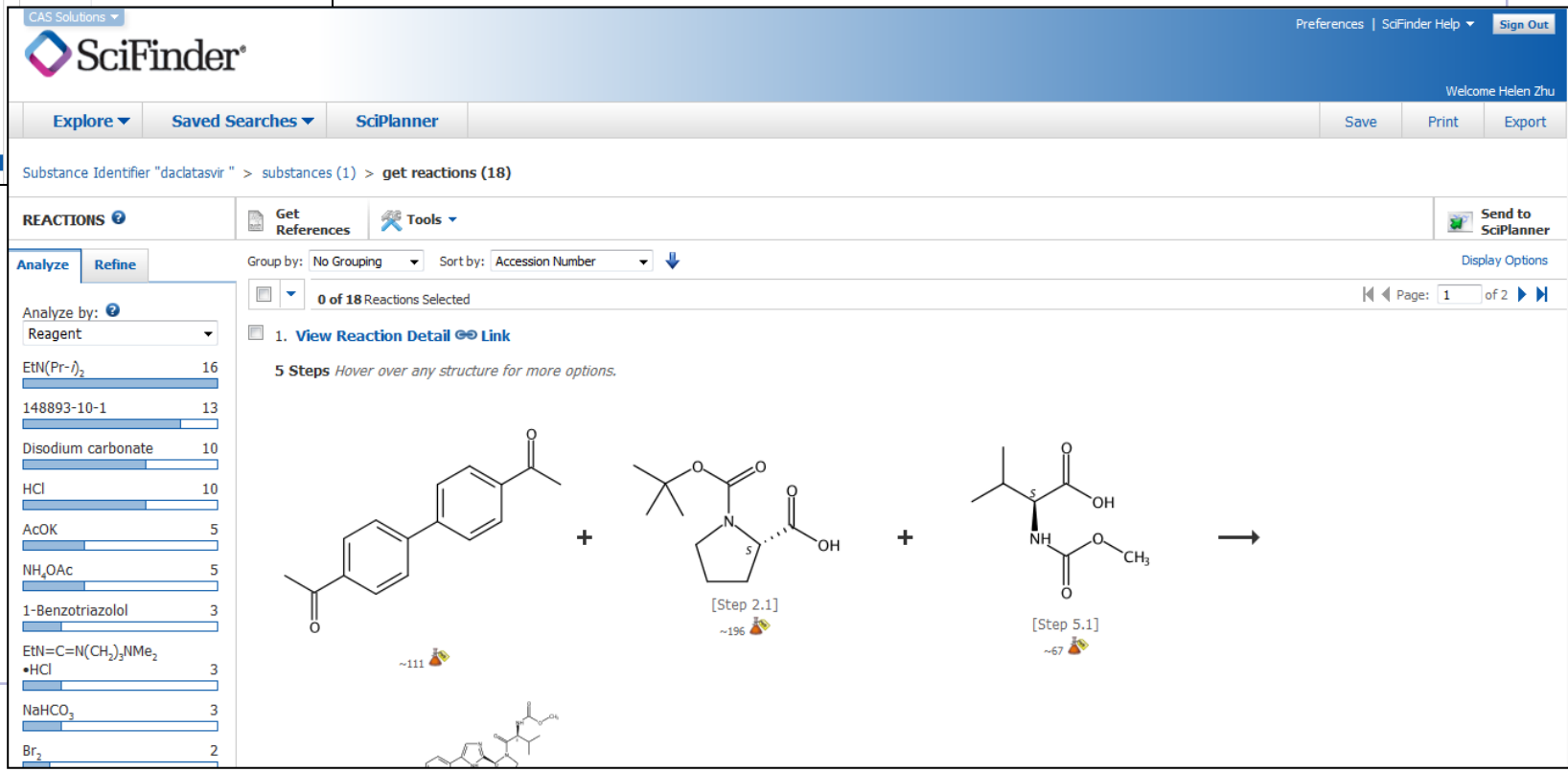


通过Refine获得单步反应后选取有实验步骤的反应

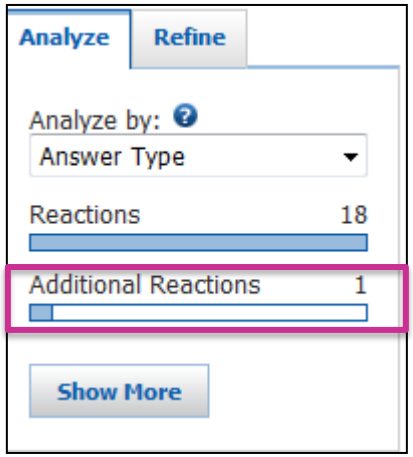
SCIFINDER® A CAS SOLUTION

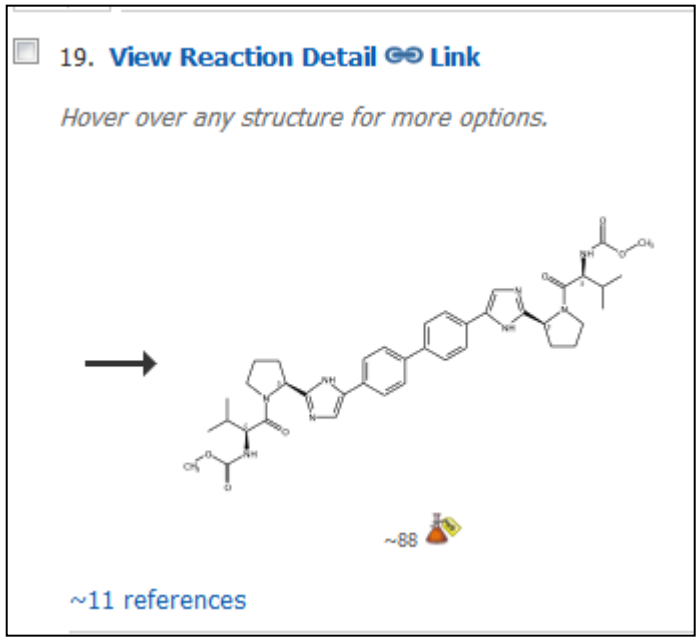
获得全面的反应信息

查找合成Daclatasvir的反应



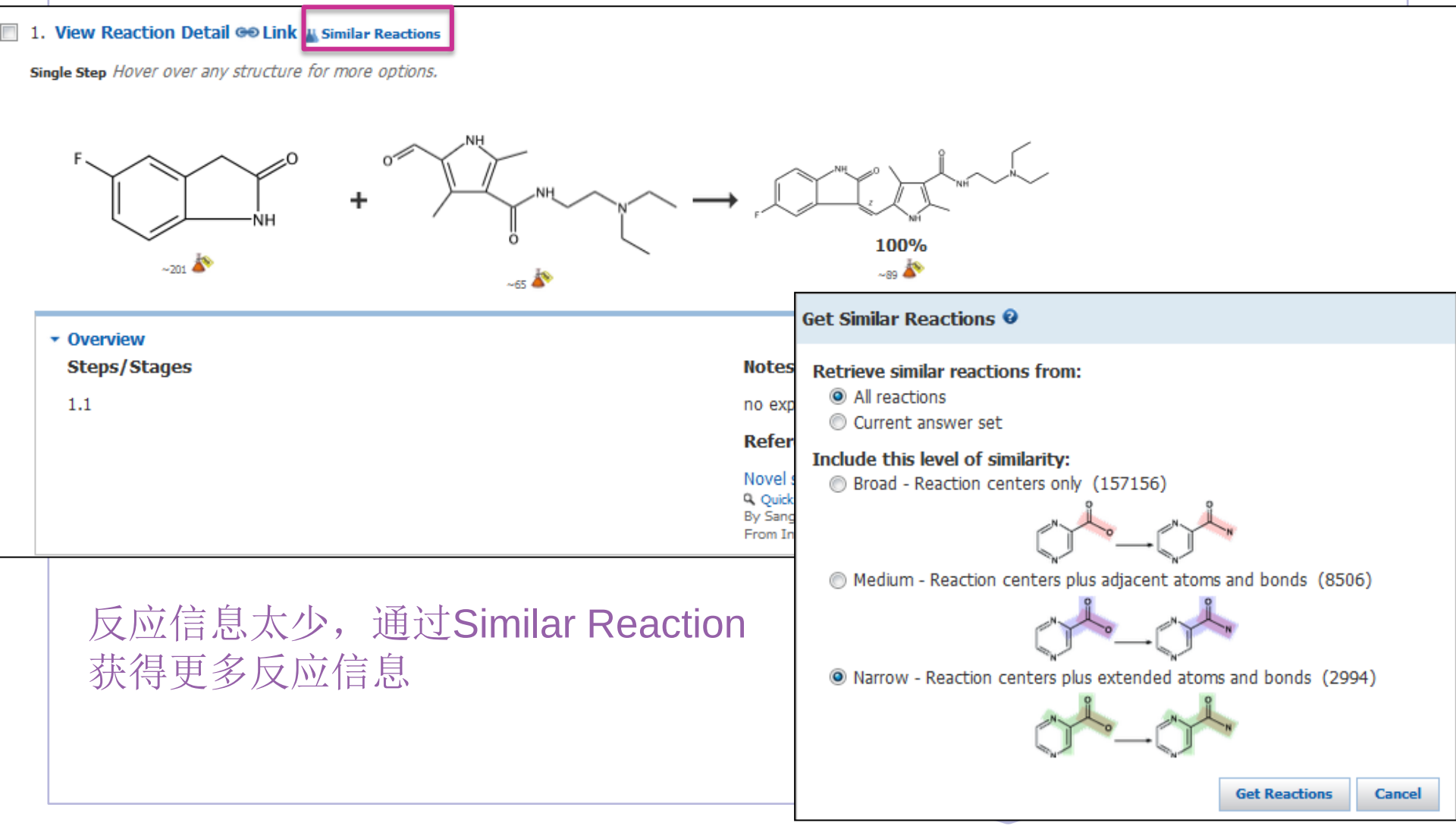
获得全面的反应信息





获得的附加反应不是完整反应

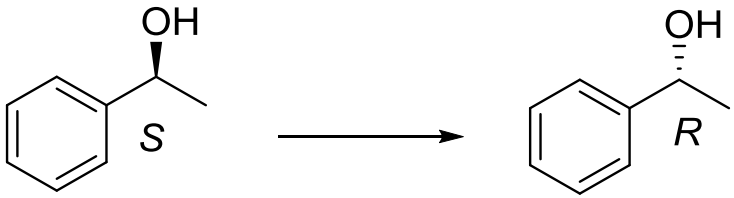
获得相关的反应信息



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

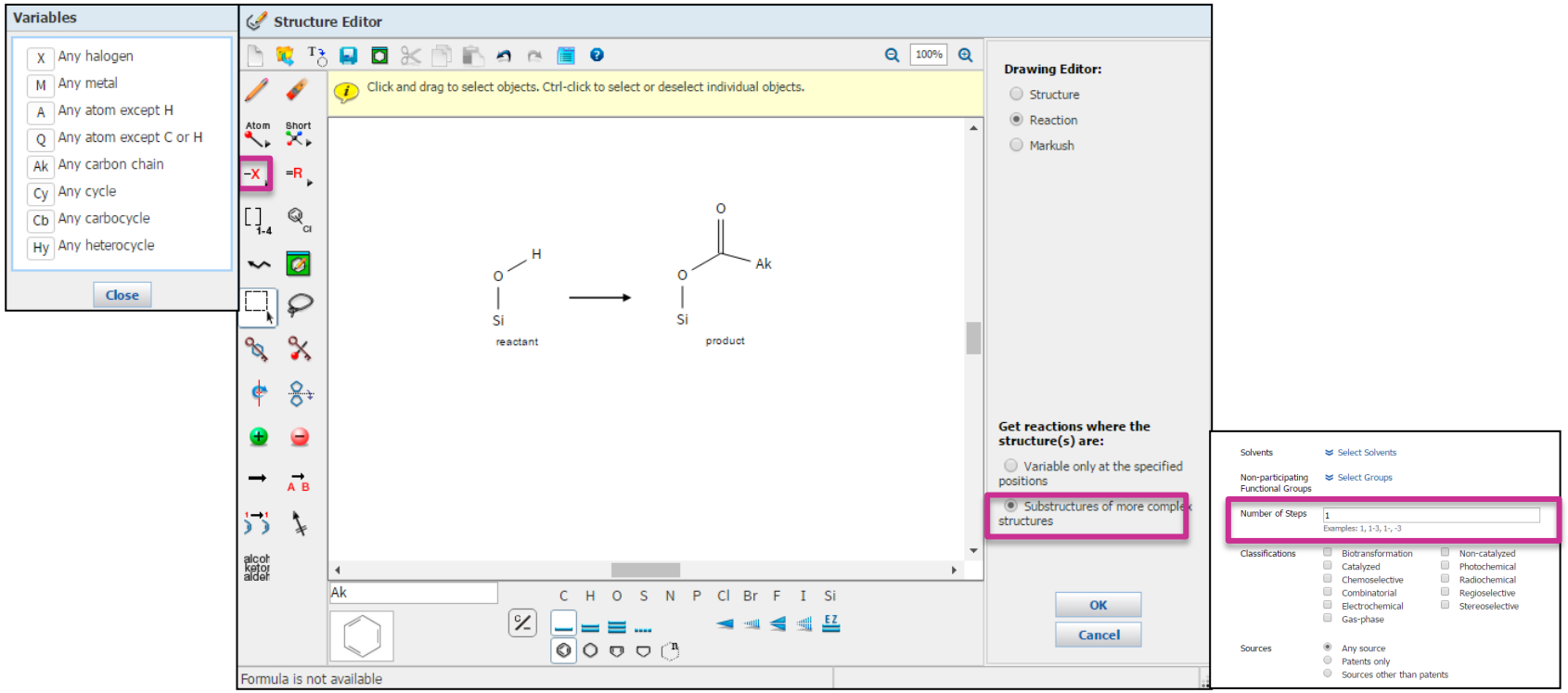
检索如下构型翻转的反应



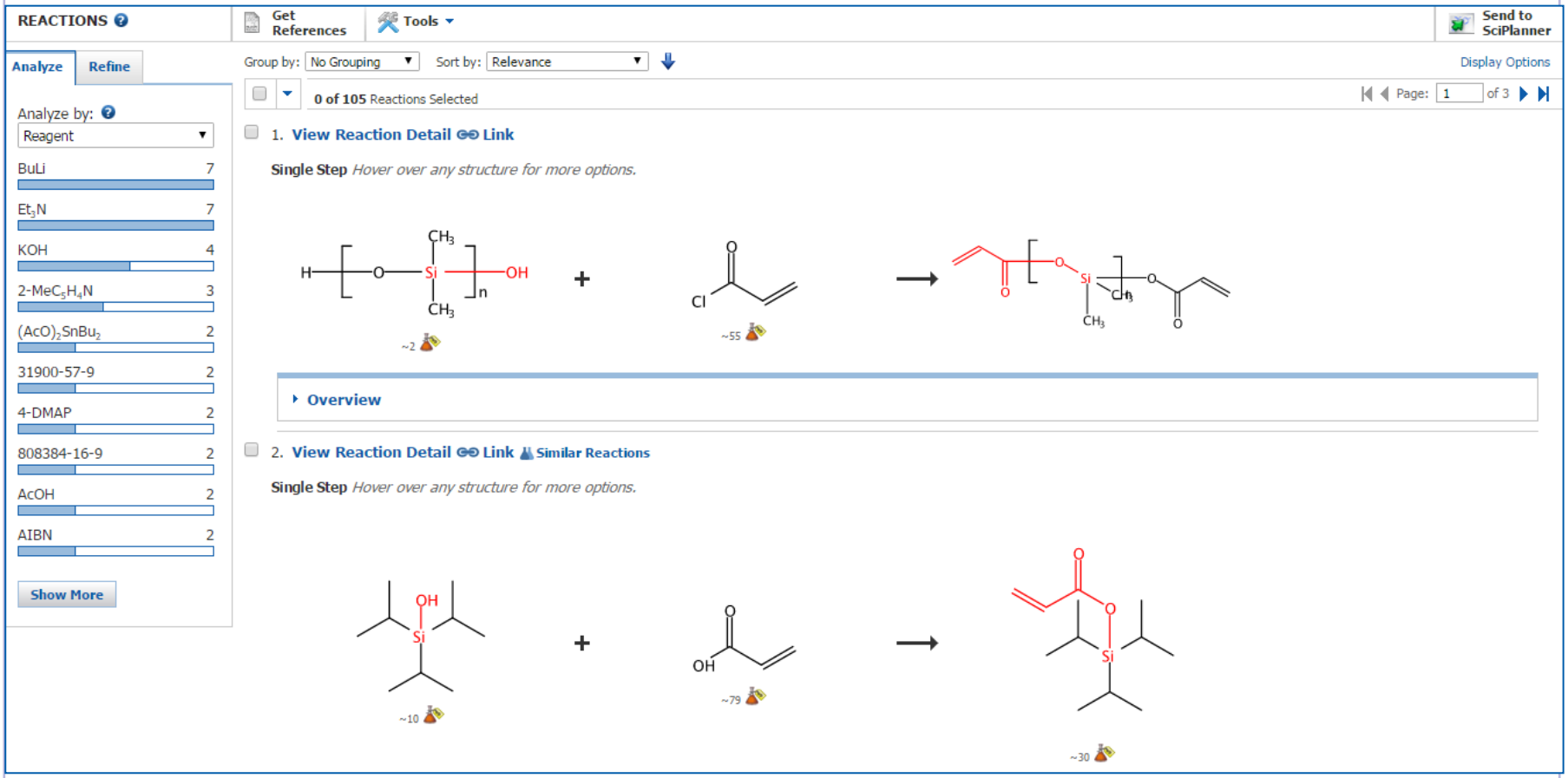
案例分析

检索硅羟基酯化的反应，找出其中的聚合物反应？

案例分析

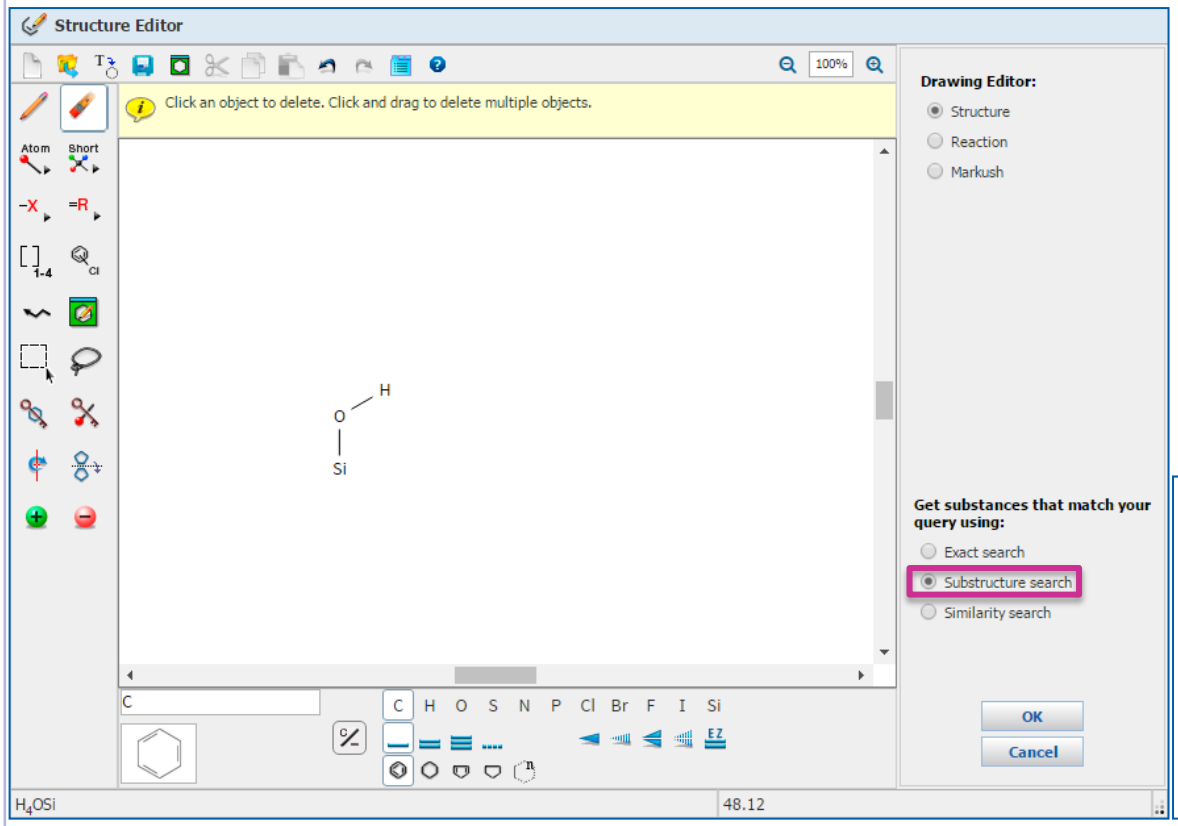

Variables
X Any halogen
M Any metal
A Any atom except H
Q Any atom except C or H
Ak Any carbon chain
Cy Any cycle
Cb Any carbocycle
Hy Any heterocycle
Close
Structure Editor
Click and drag to select objects. Ctrl-click to select or deselect individual objects.
reactant
product
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
Formula is not available
Solvents
Select Solvents
Non-participating Functional Groups
Select Groups
Number of Steps
Classifications
Biotransformation
Catalyzed
Chemoselective
Combinatorial
Electrochemical
Gas-phase
Non-catalyzed
Photochemical
Radiochemical
Regioselective
Stereoselective
Sources
Any source
Patents only
Sources other than patents

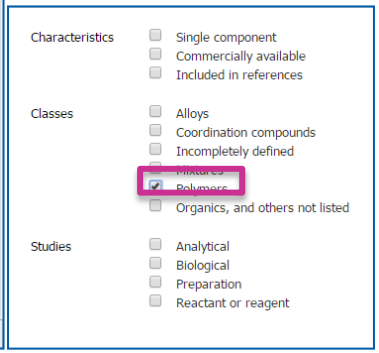
案例分析



问题：如何找到含Si的聚合物上的羟基酯化反应？

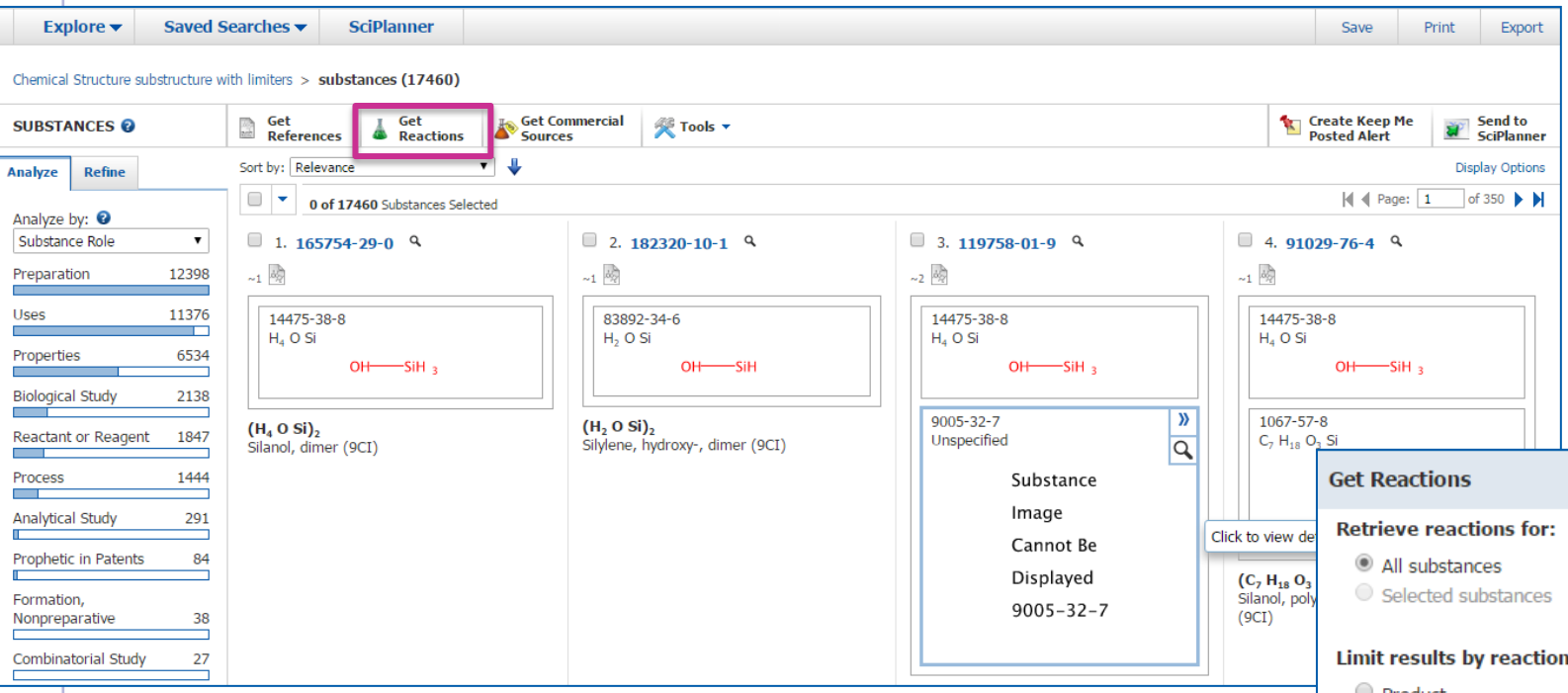
案例分析

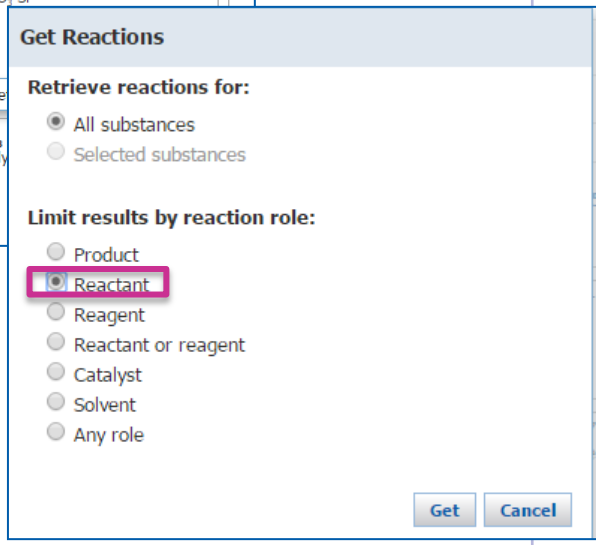

Structure Editor
100%
Click an object to delete. Click and drag to delete multiple objects.
Atom
Bhort
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search
OK
Cancel
C H O S N P Cl Br F I Si
H4OSi
48.12


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





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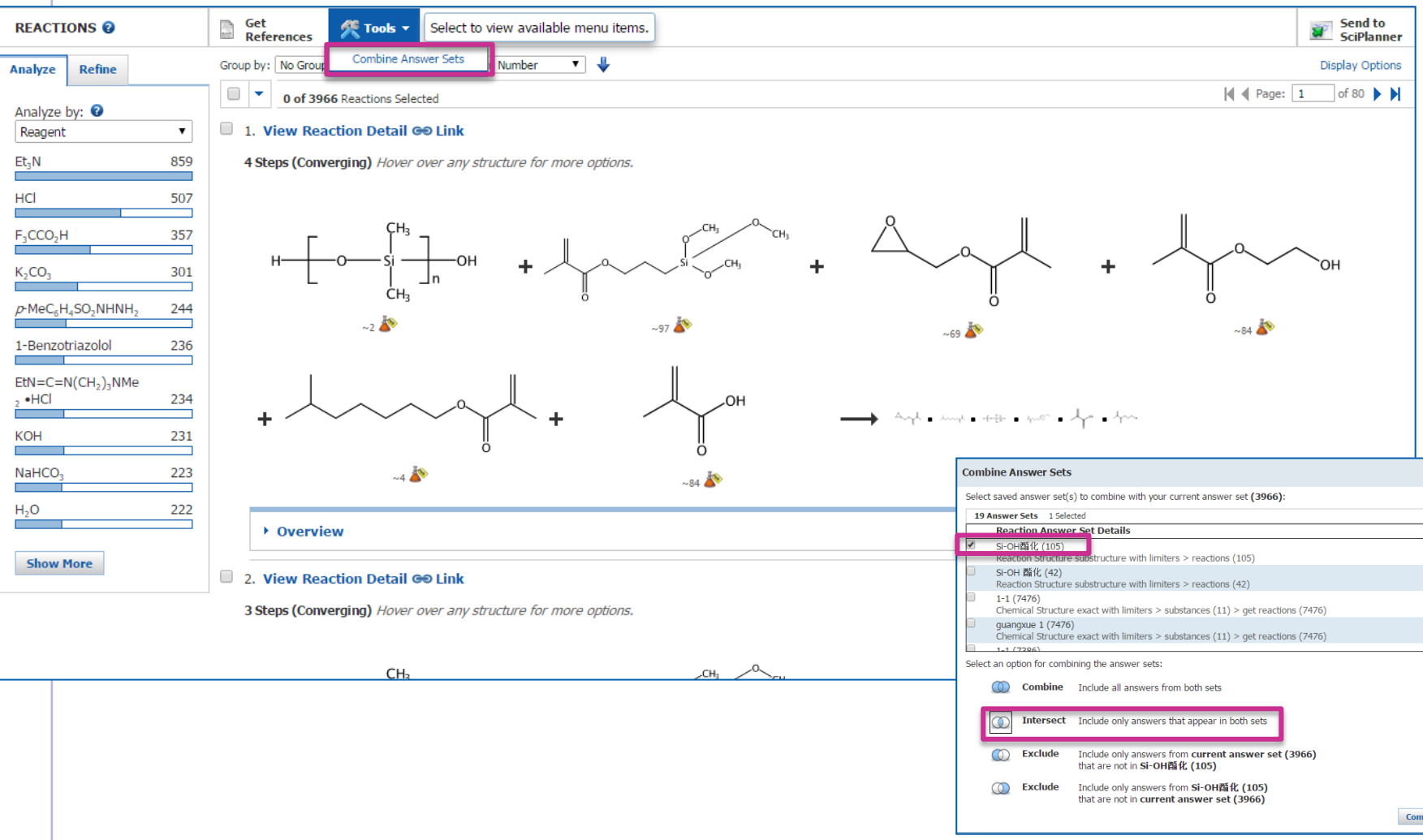
案例分析



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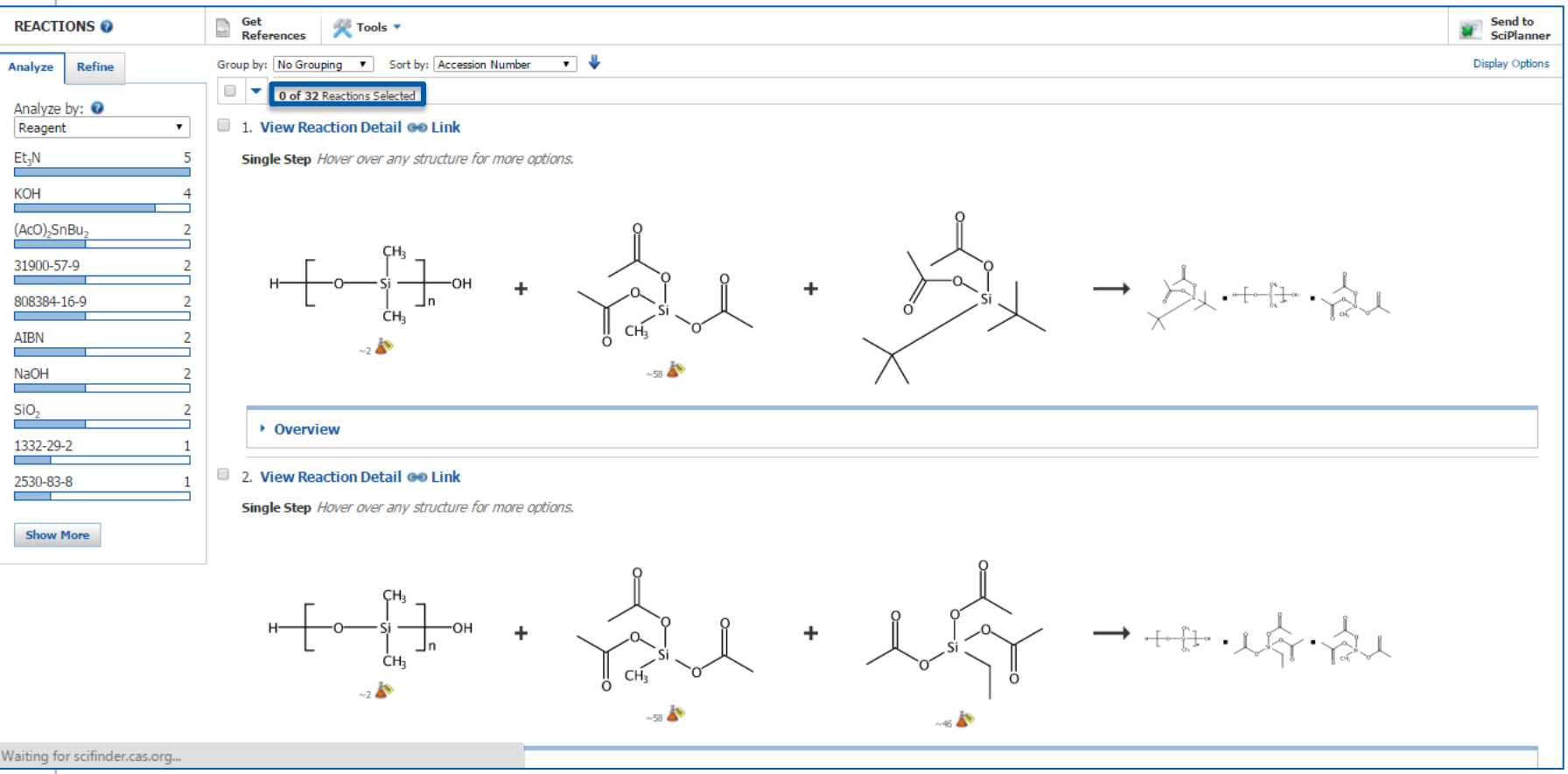
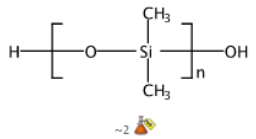
案例分析


REACTIONS
Get References
Tools
Send to SciPlanner
Analyze
Refine
Group by: No Grouping
Sort by: Accession Number
Display Options
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
0 of 32 Reactions Selected
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.
Waiting for scifinder.cas.org...

案例分析

3. View Reaction Detail Link

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



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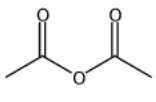
+

4. View Reaction Detail Link

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



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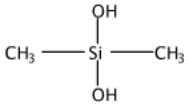
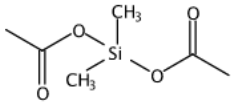


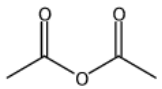
hydroxy and alkyl terminated or copolymer



16%

6. View Reaction Detail Link

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



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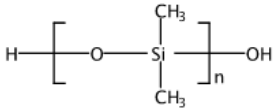

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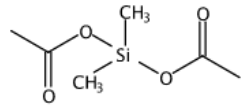

51%

~43

符合要求的反应

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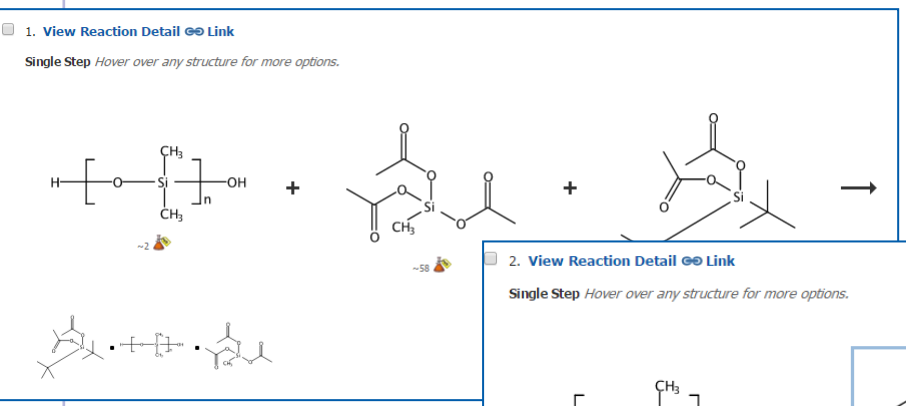
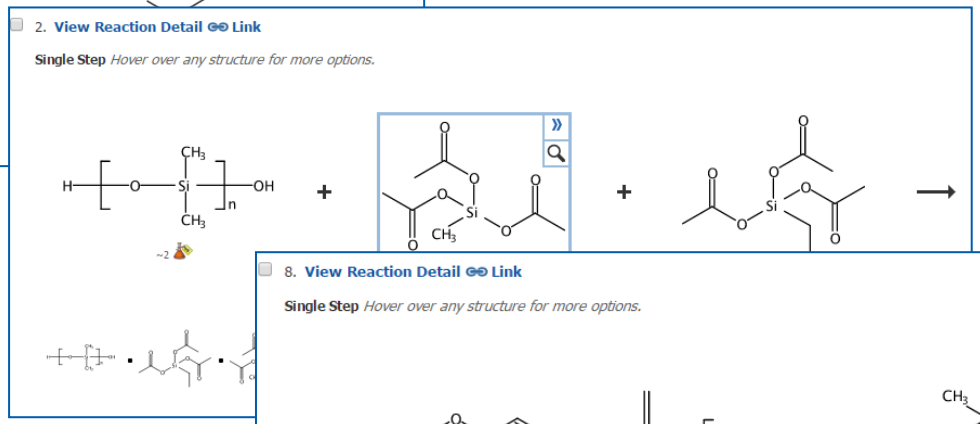
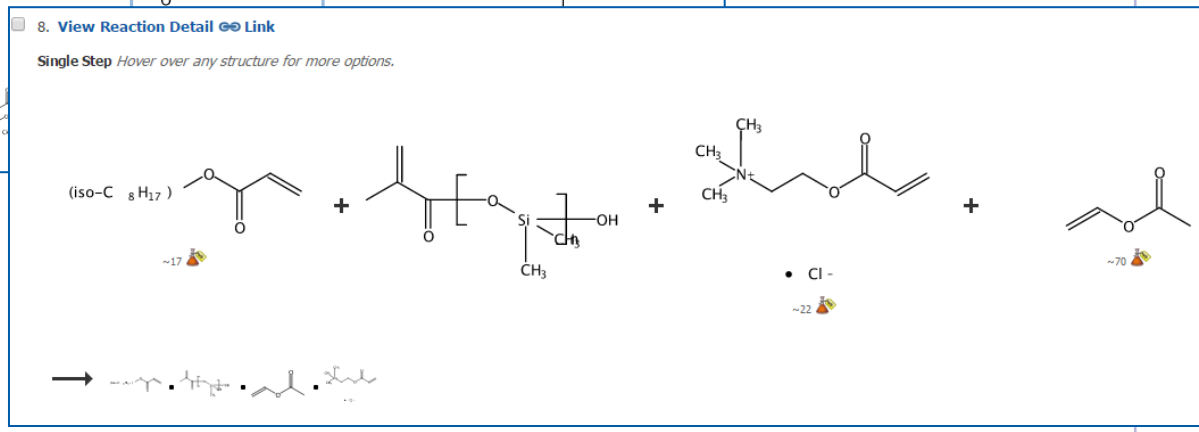
案例分析





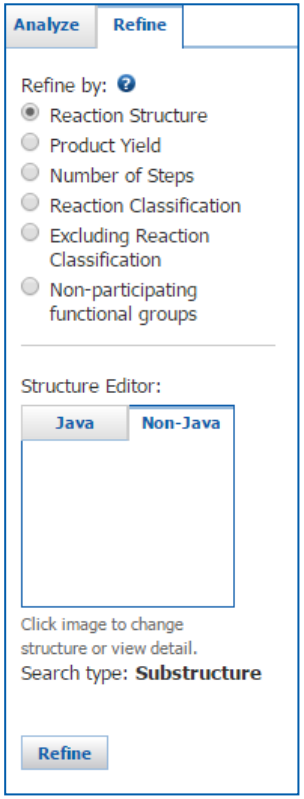


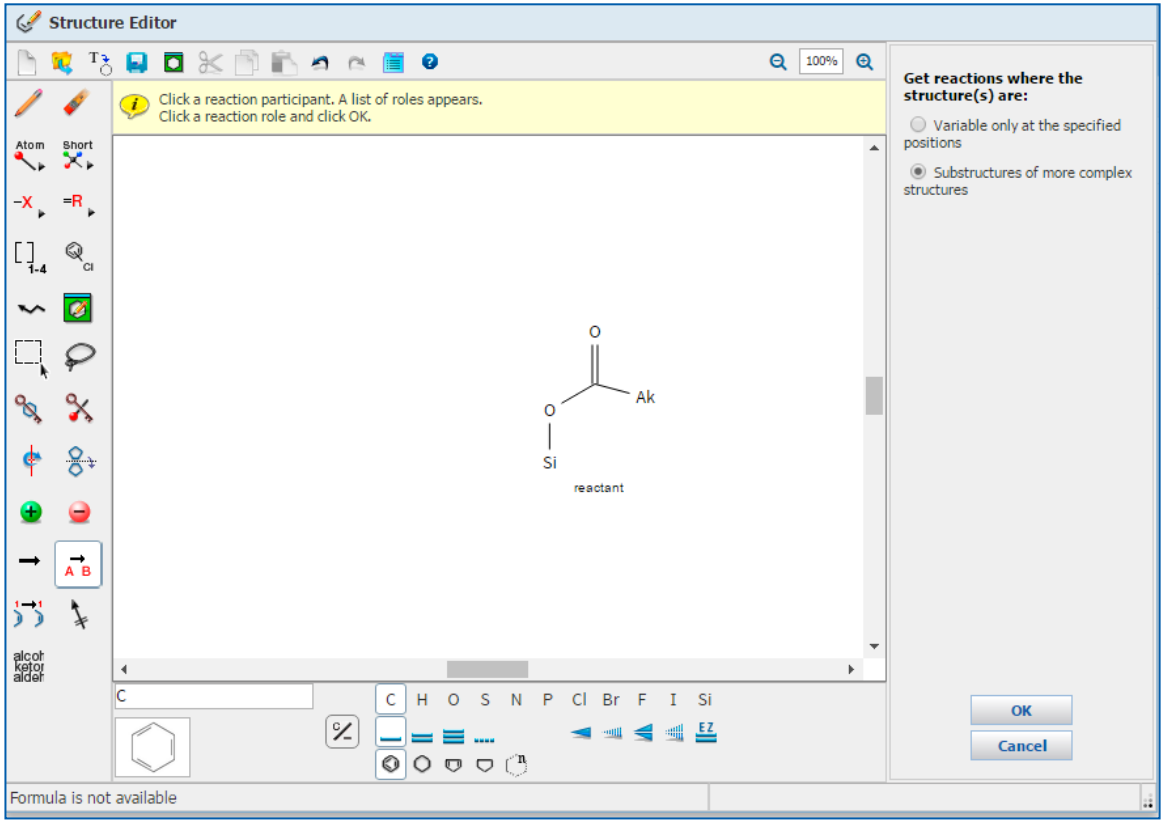
不符合要求的反应

如何去除？

案例分析

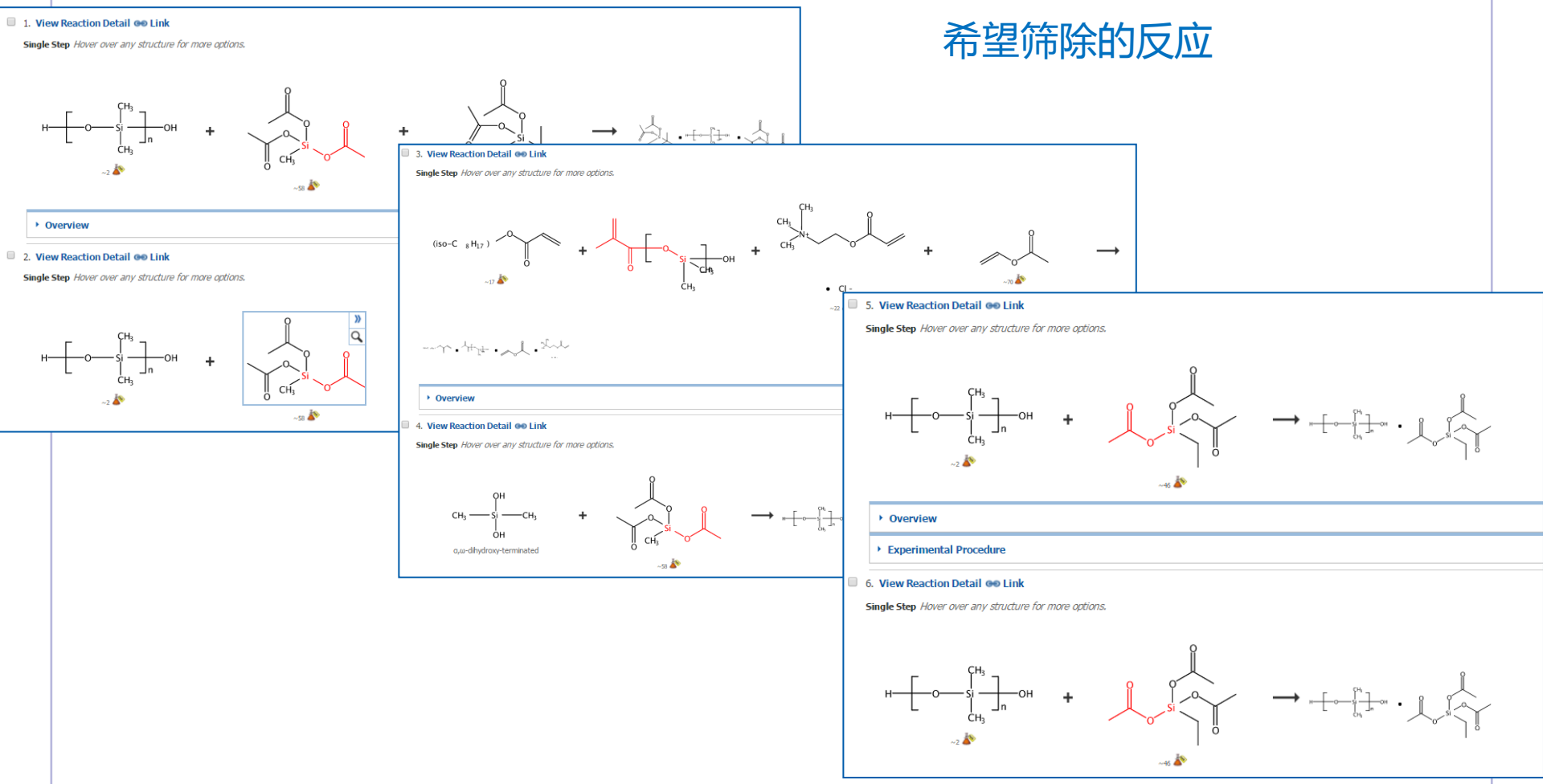
思路一：筛出原料中已经包含酯化物的反应





案例分析

希望筛除的反应



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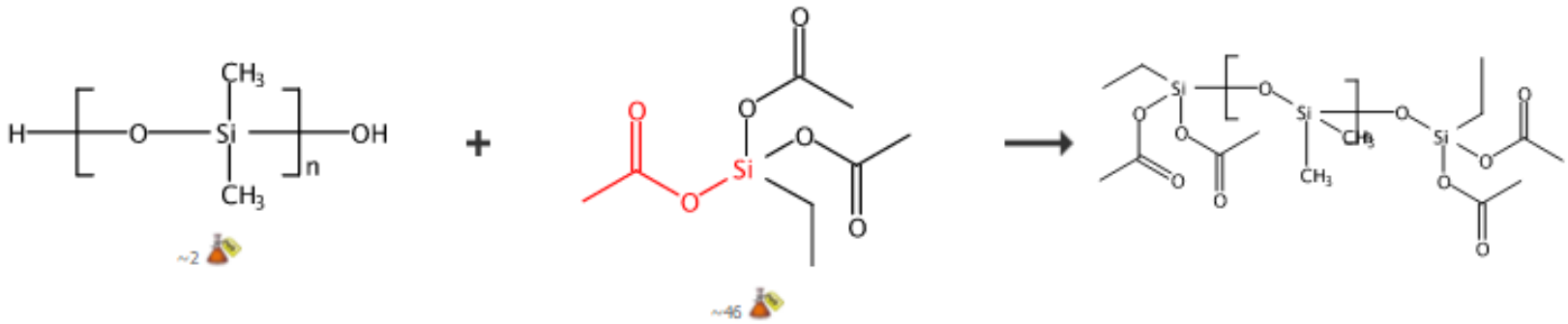
案例分析

8. **View Reaction Detail** **Link**

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

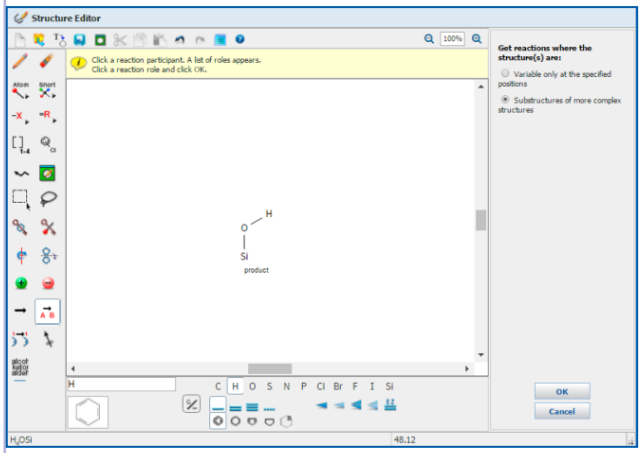


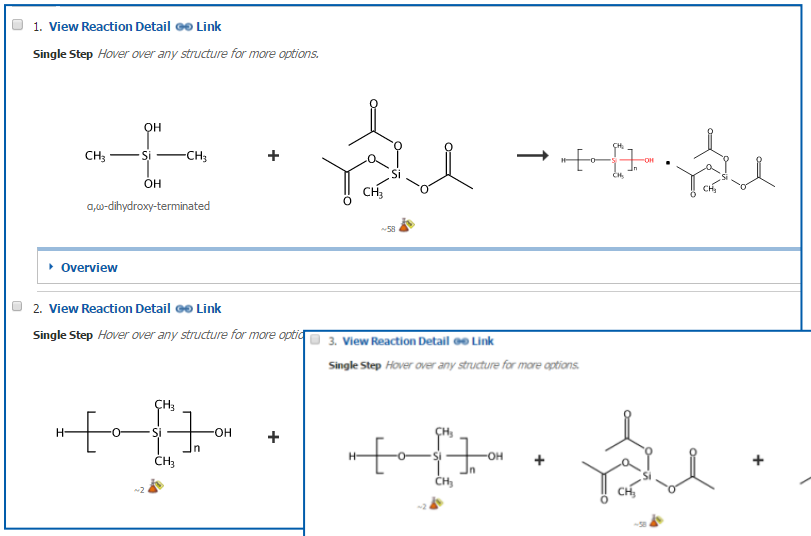
不希望筛除的反应

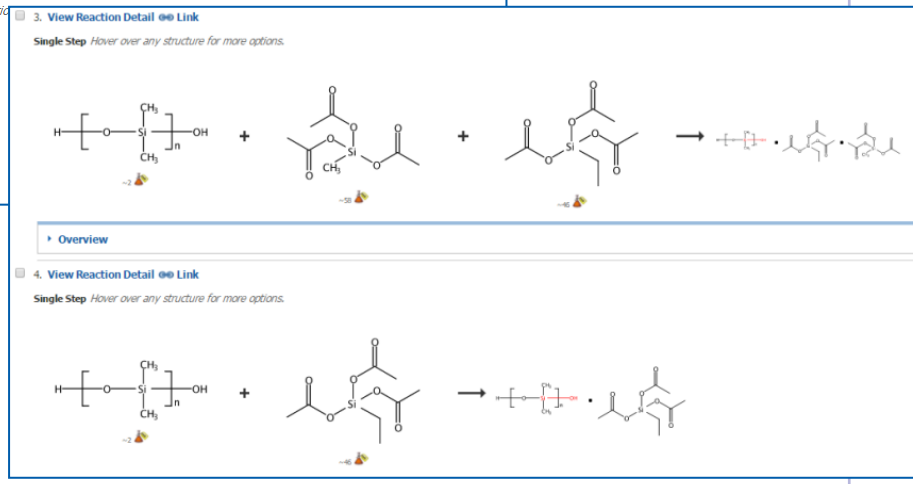
思路一不可行！

案例分析

思路二：筛出产物中仍然包含原料的反应

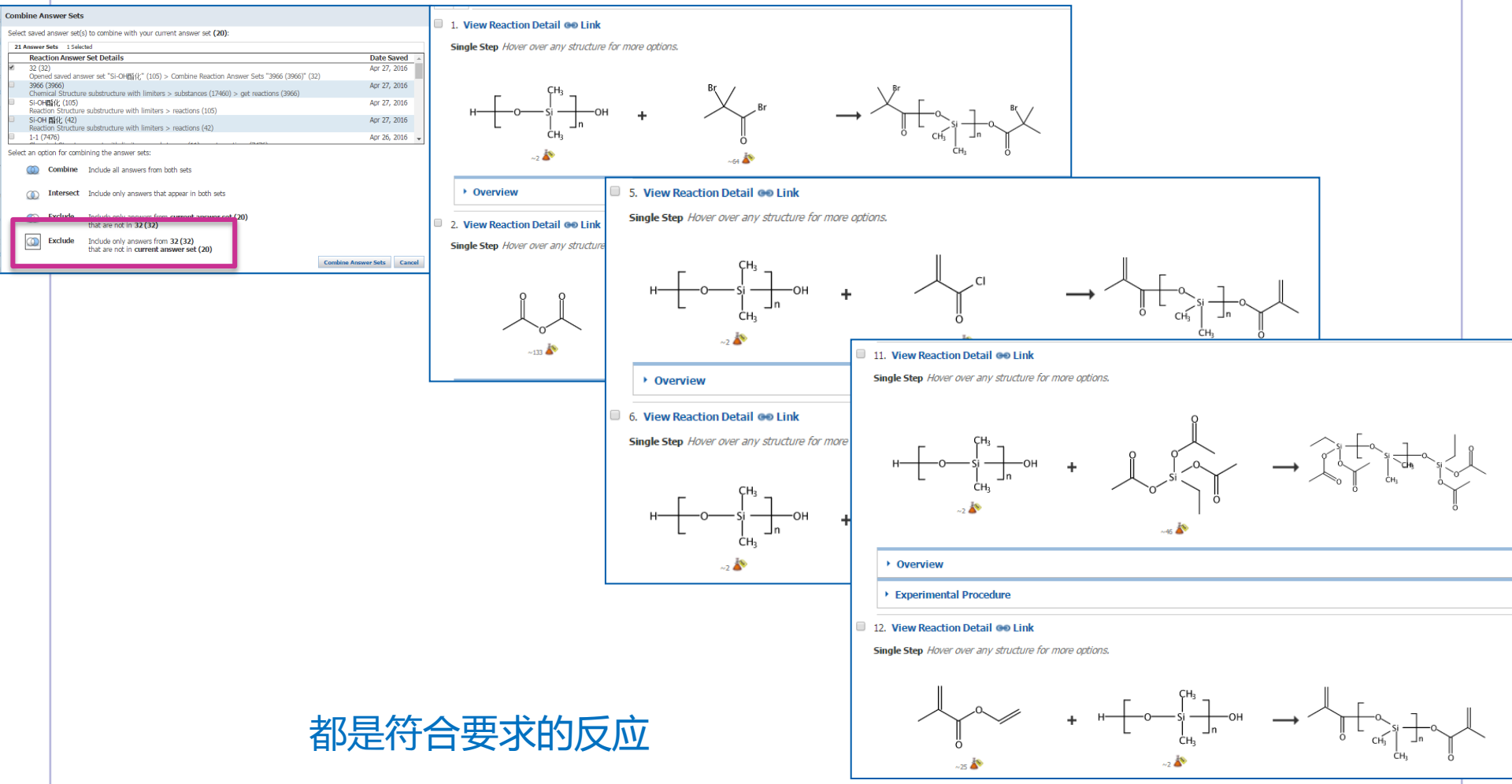






都是希望筛除的反应

案例分析



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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010-62508026

china@acsi.info