SciFinder检索难点解析

----吉林大学　20161014

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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 Abstract Service

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

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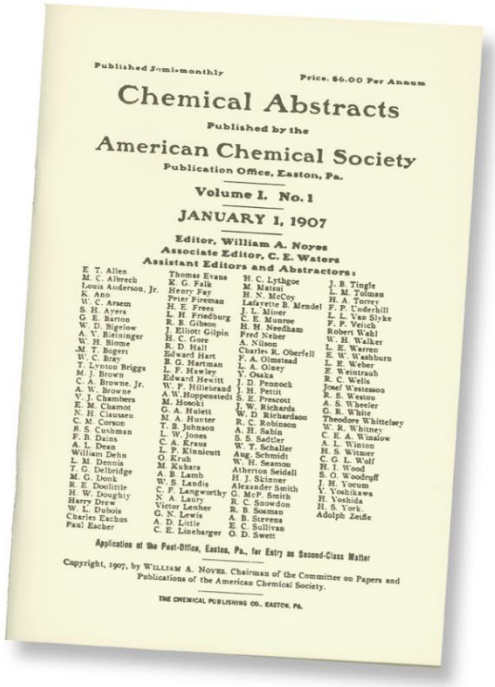
1907年，信息的汇集、管理发生了重大的变化

威廉•诺伊斯
(William A. Noyes)

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



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Application at the Post-Office, Easton, Pa., for Entry as Second-Class Matter

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Patents, journals, web, catalogs, etc.

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Aldrichimica ACTA

ACS chemical biology

Beilstein Journal of Organic Chemistry

division of polymer chemistry, inc American Chemical Society

JACS Journal of the American Chemical Society

ACS Chemical Neuroscience

The Journal of Physical Chemistry Letters

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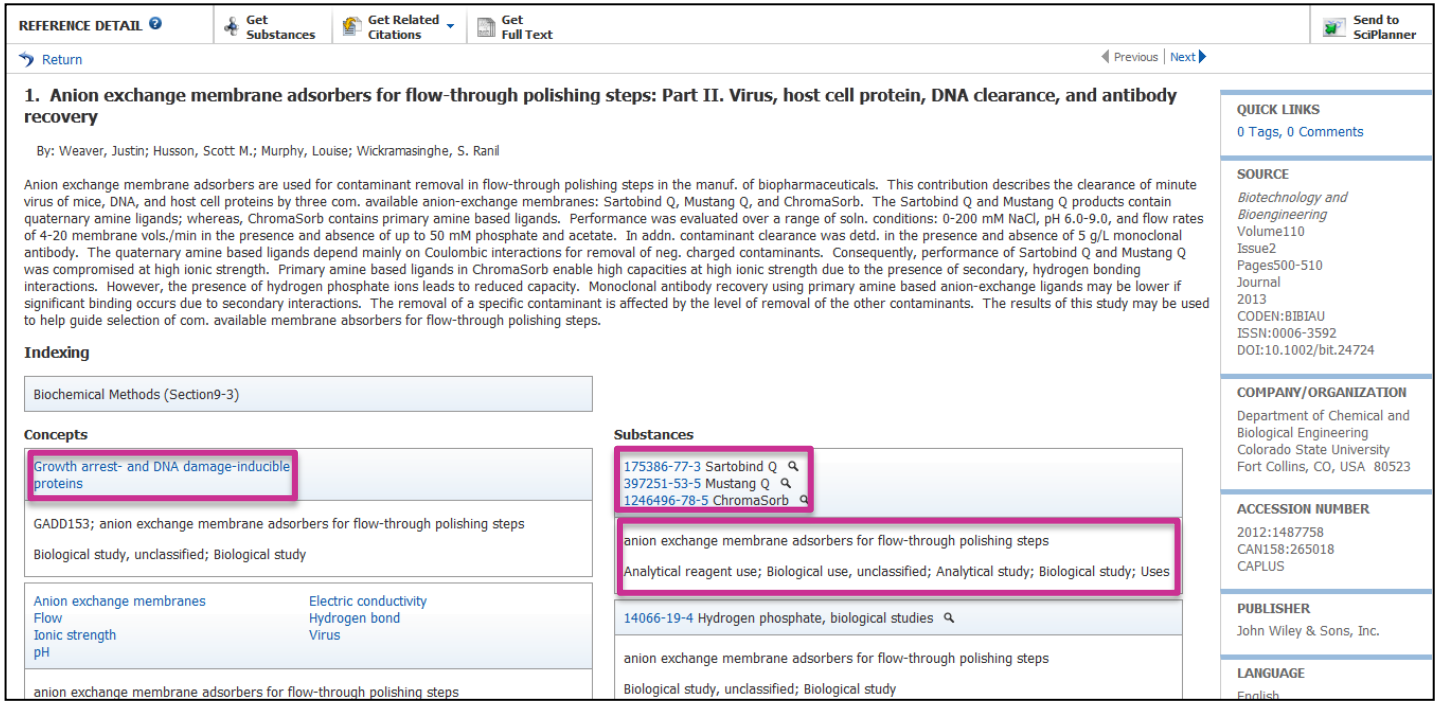
CAS数据最具价值的内容—人工标引



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

Return | Previous | Next

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

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

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

Indexing

Biochemical Methods (Section9-3)

Concepts

Growth arrest- and DNA damage-inducible proteins

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

Biological study, unclassified; Biological study

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

anion exchange membrane adsorbers for flow-through polishing steps

Substances

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

anion exchange membrane adsorbers for flow-through polishing steps

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

14066-19-4 Hydrogen phosphate, biological studies

anion exchange membrane adsorbers for flow-through polishing steps

Biological study, unclassified; Biological study

QUICK LINKS
0 Tags, 0 Comments

SOURCE
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Fort Collins, CO, USA 80523

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2012:1487758
CAN158:265018
CAPLUS

PUBLISHER
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LANGUAGE
English

Tips:

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

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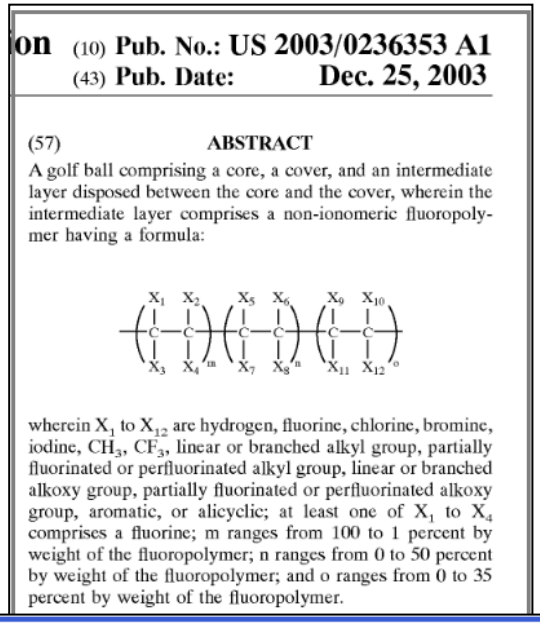
SciFinder对专利的加强



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	

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CAS最新动向—解决方案

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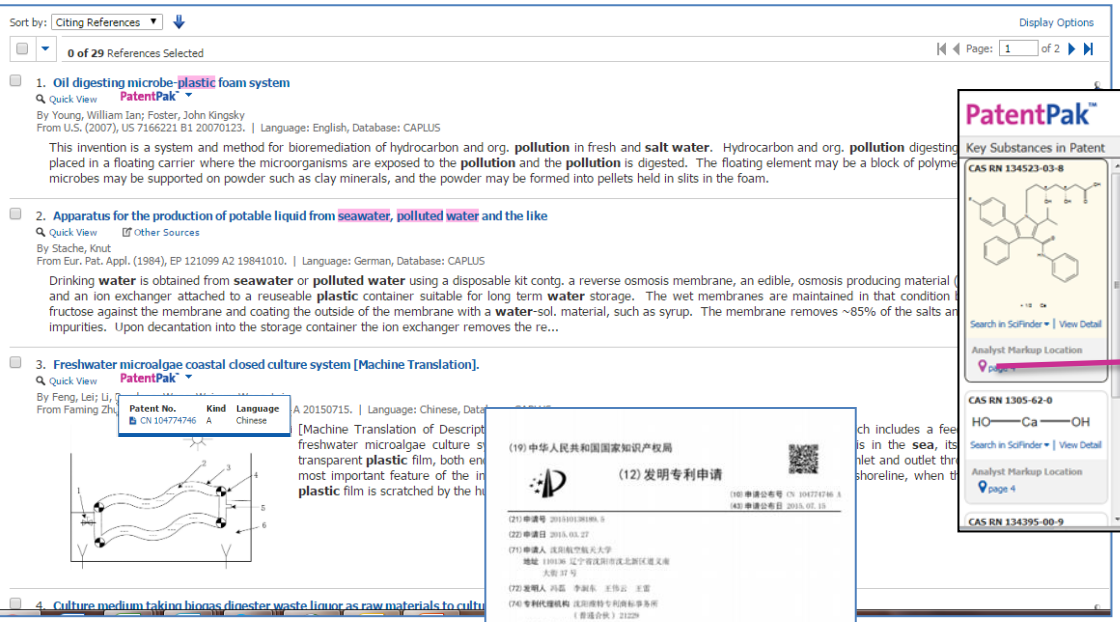
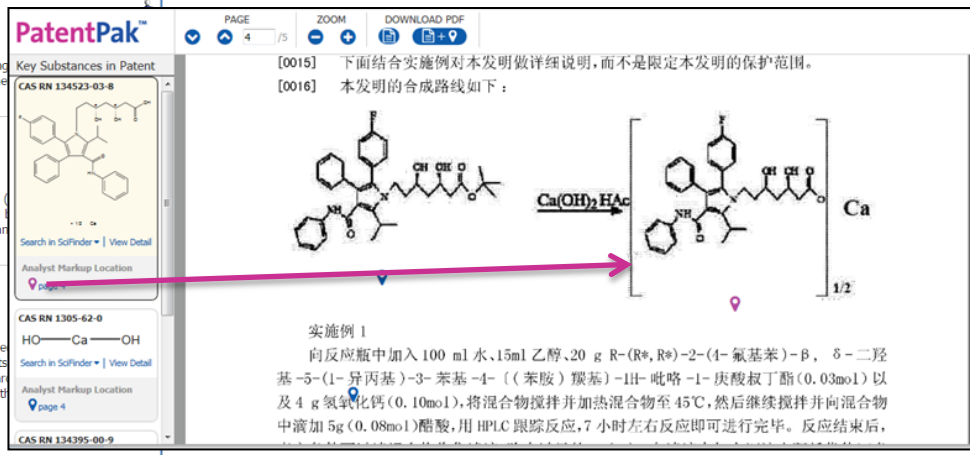
CAS最新动向—解决方案

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





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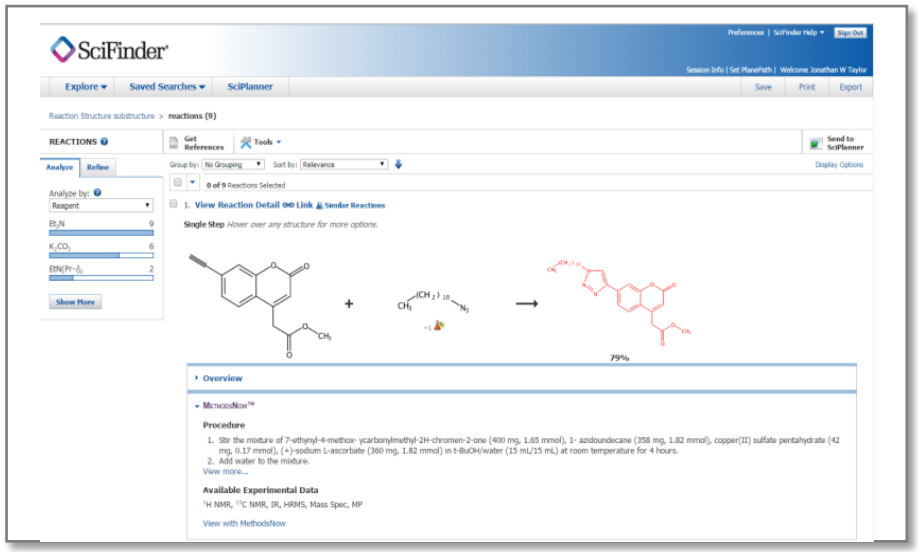
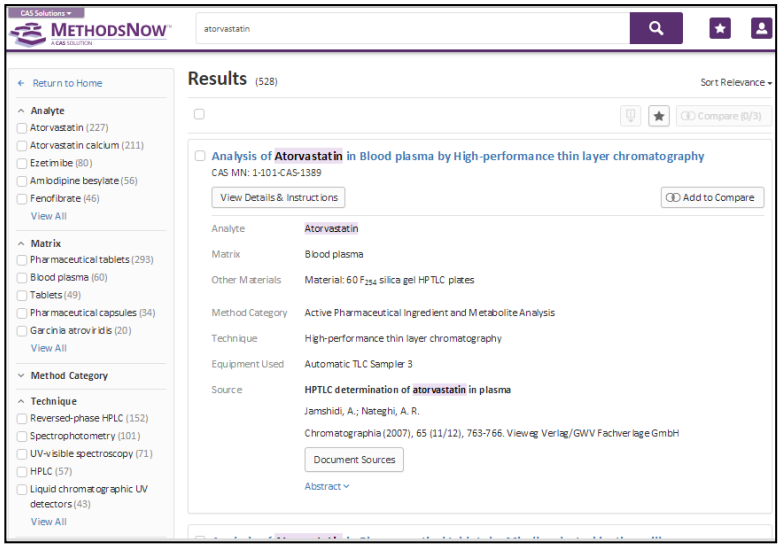
- CAS于2016年2月正式发布MethodsNow™
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求



嵌在SciFinder中的合成模块



单独的分析界面

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提 纲

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

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文献检索方法

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

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

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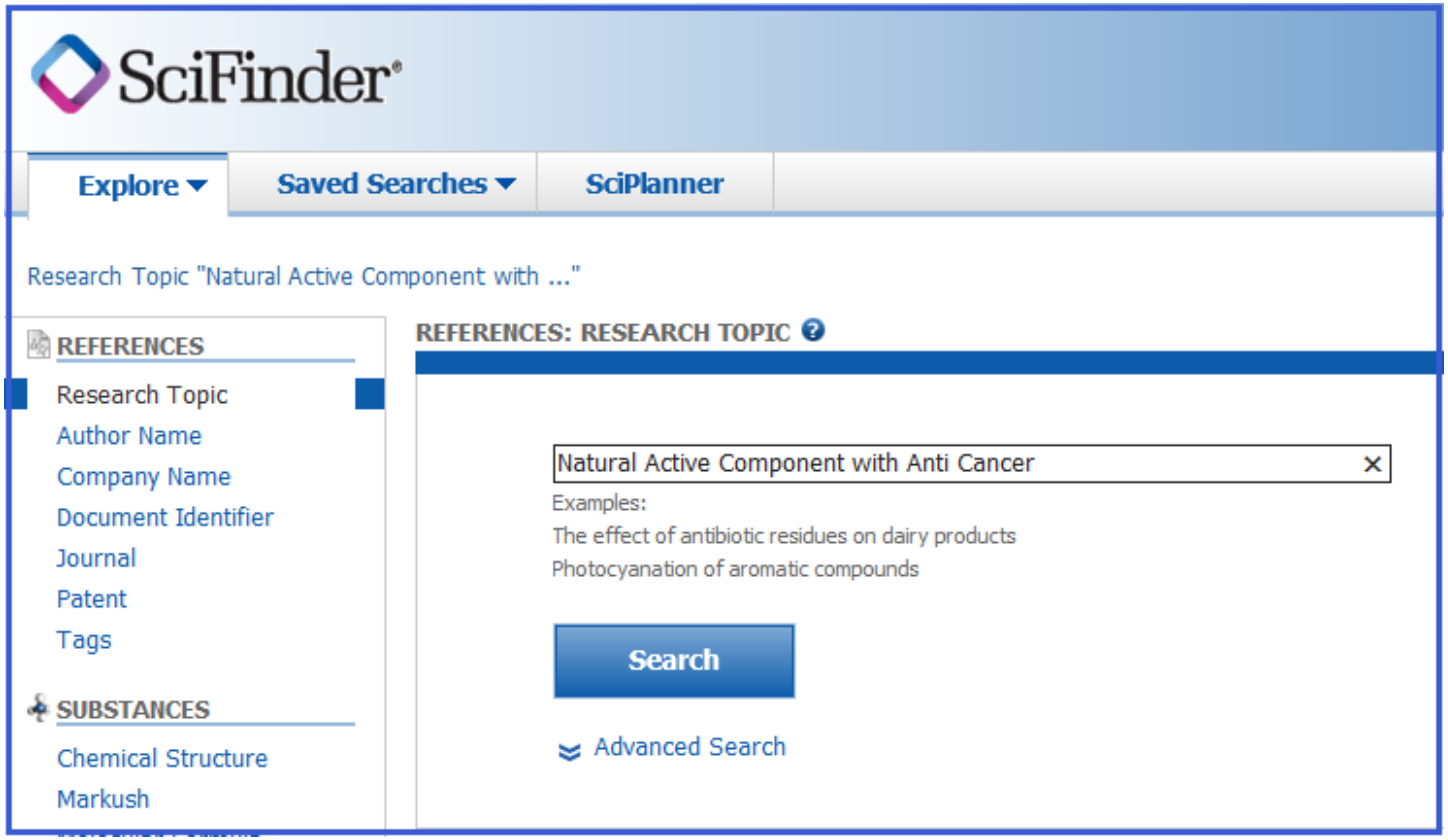
利用Index Term选词

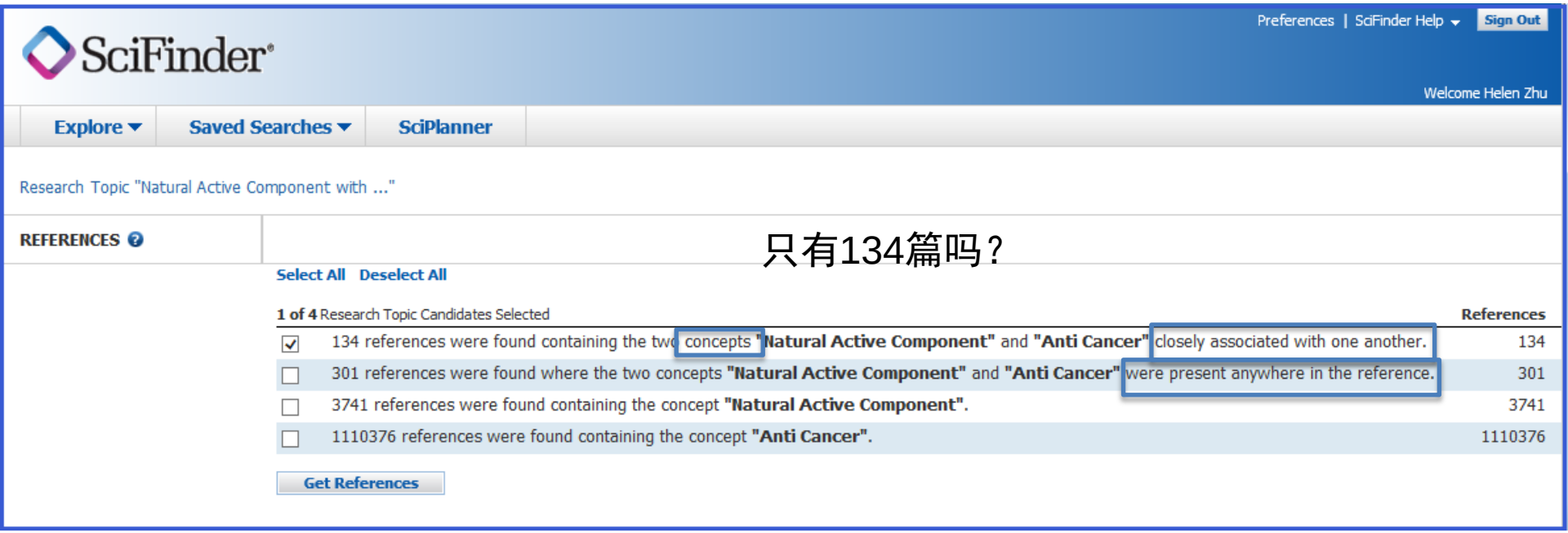
主题检索：植物中天然活性成分的抗癌研究

检索式： Natural Active Component with Anti Cancer



关键词之间用介词连接

利用Index Term选词



“Concept”表示做了同意词的扩展

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

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

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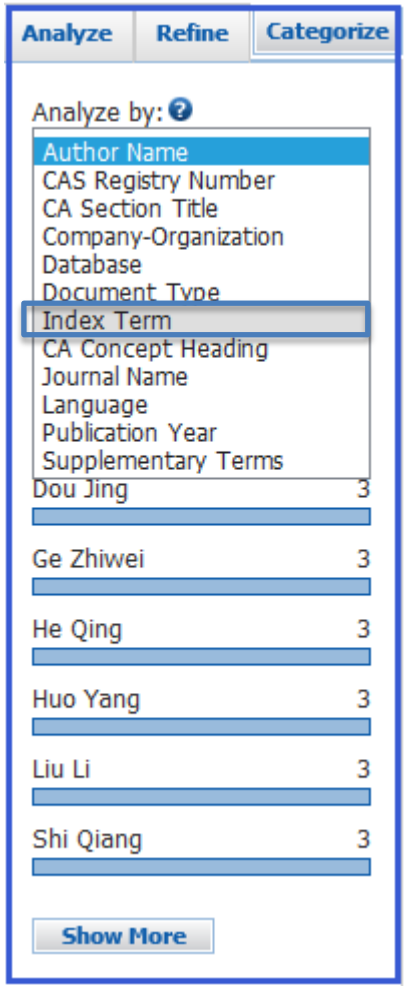
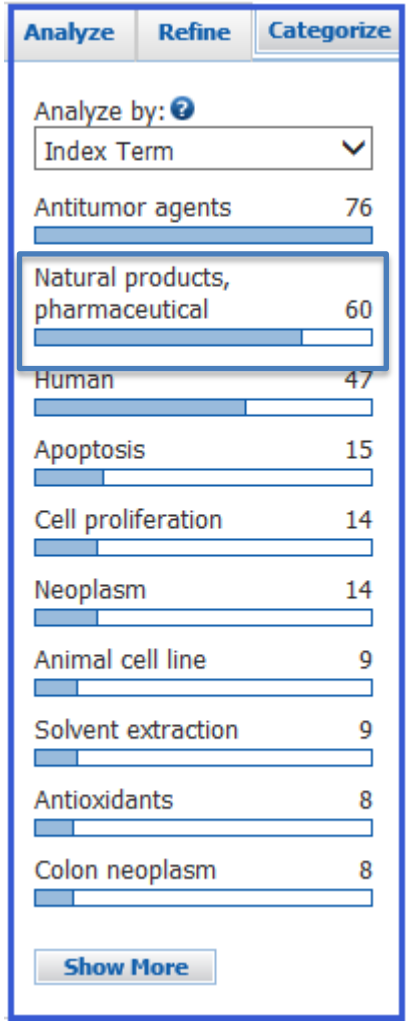
利用Index Term选词

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

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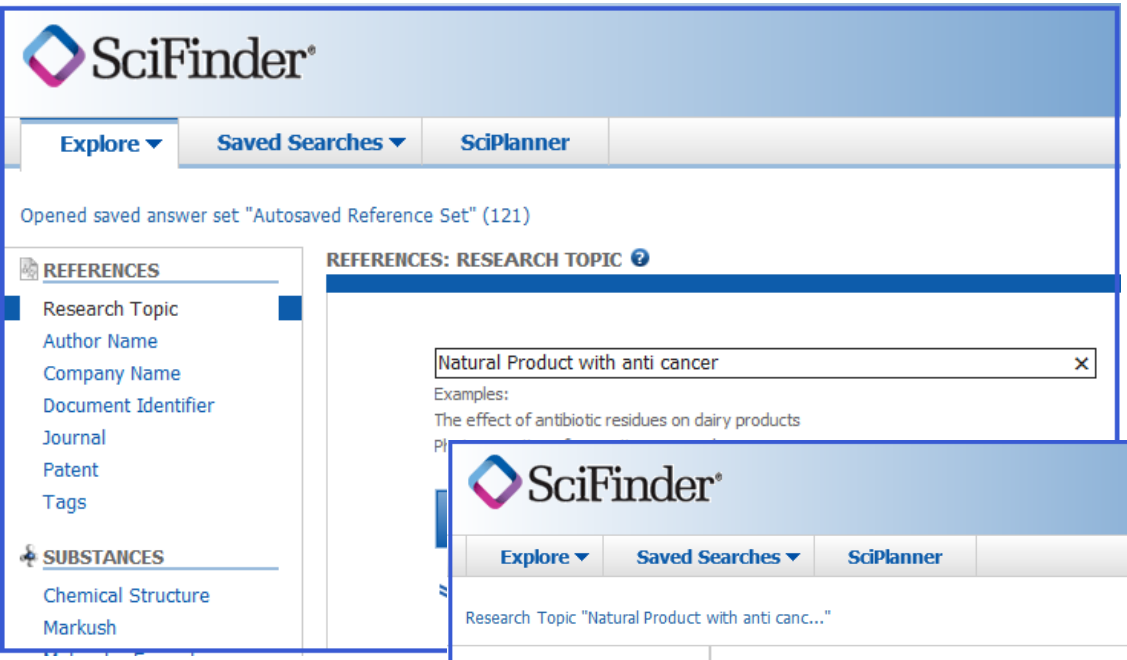
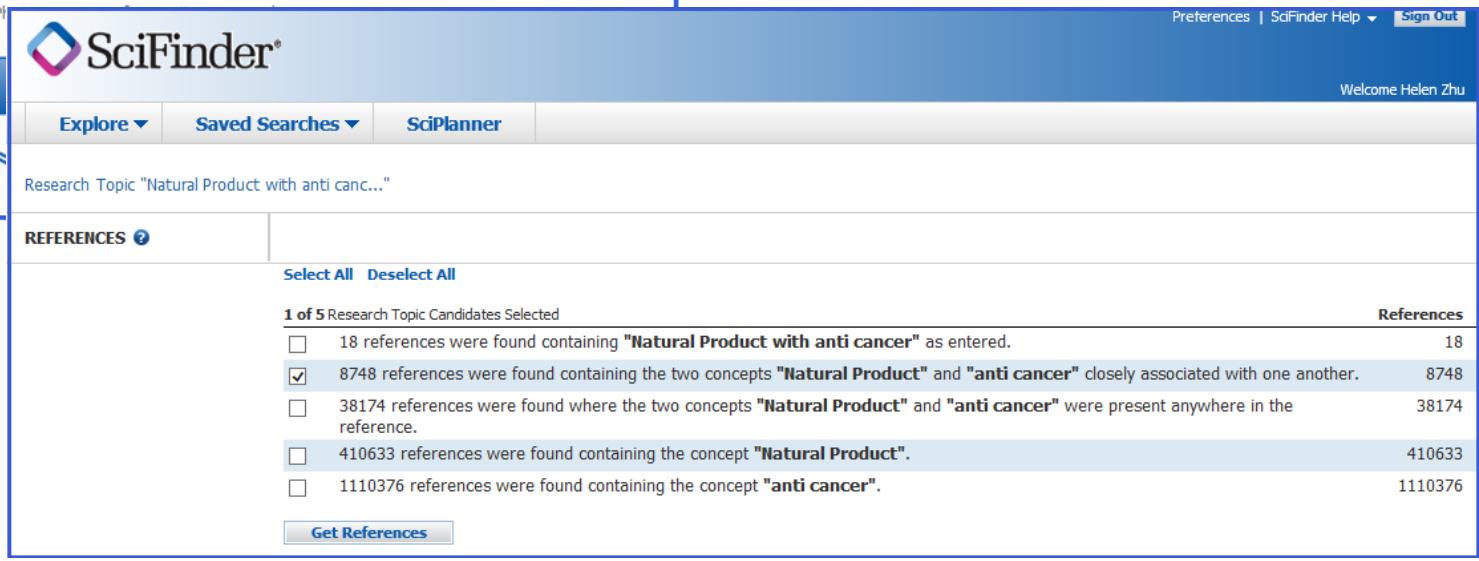
利用Index Term选词



新的检索式：

Natural Product with anti cancer



更换检索词后，结果放大了70倍

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STN中CAS Role

ANST Analytical Study

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

PREP Preparation

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

PROC Process

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

BIOL Biological Study

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

STN中CAS Role

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

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

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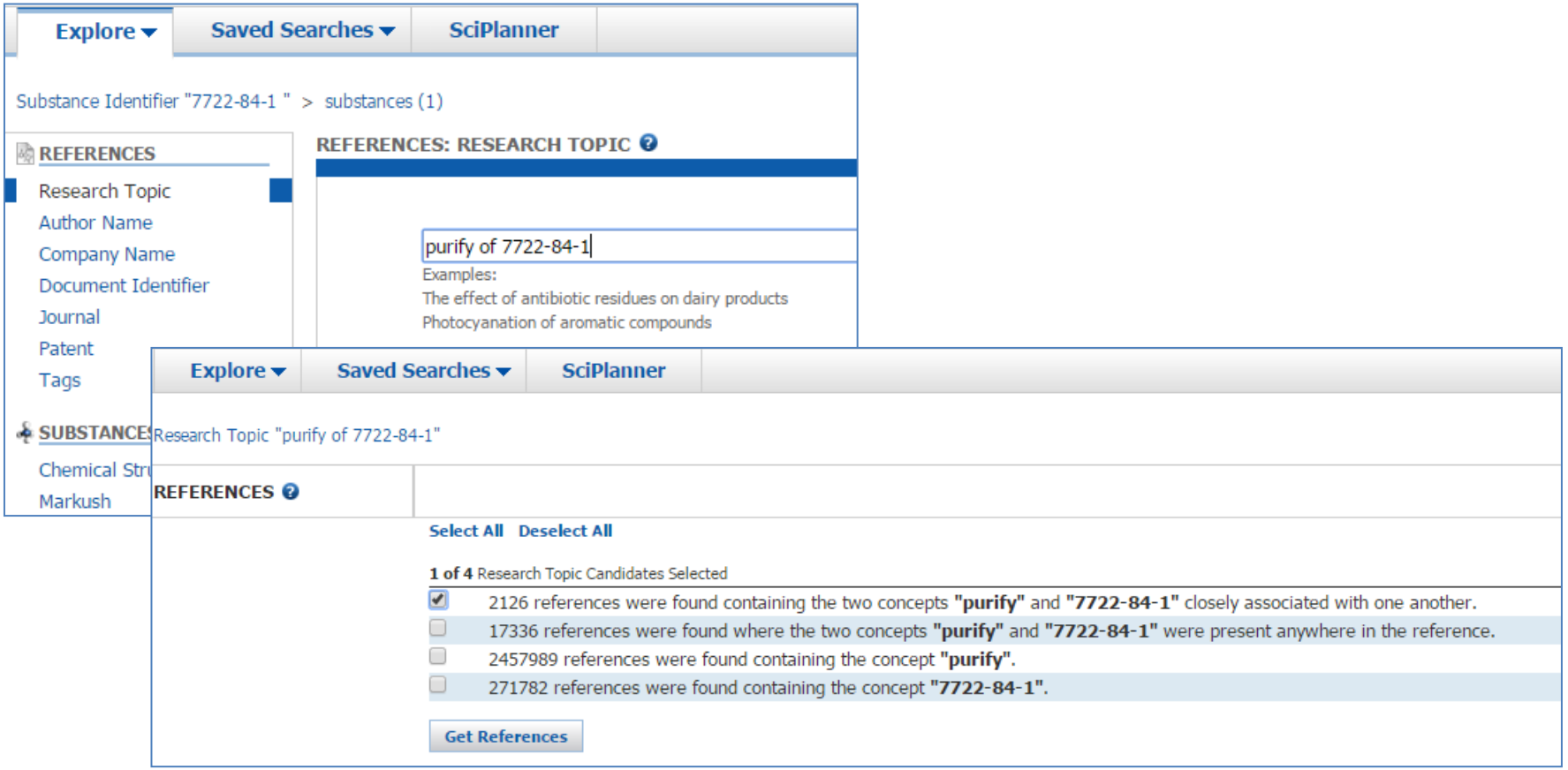
巧用CAS Role

查找纯化双氧水（7722-84-1）的文献



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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
Recycling
Sludges
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

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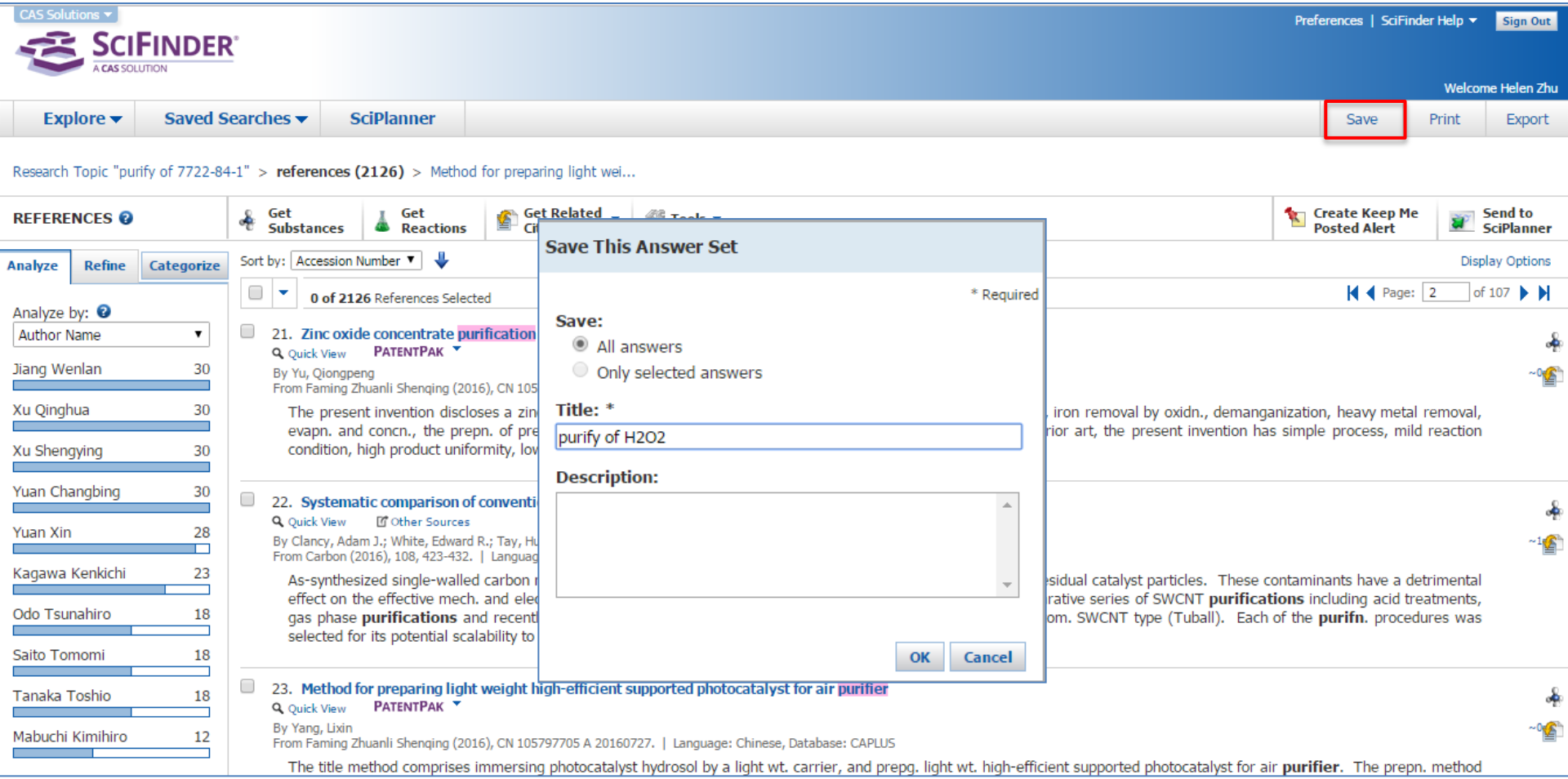
巧用CAS Role



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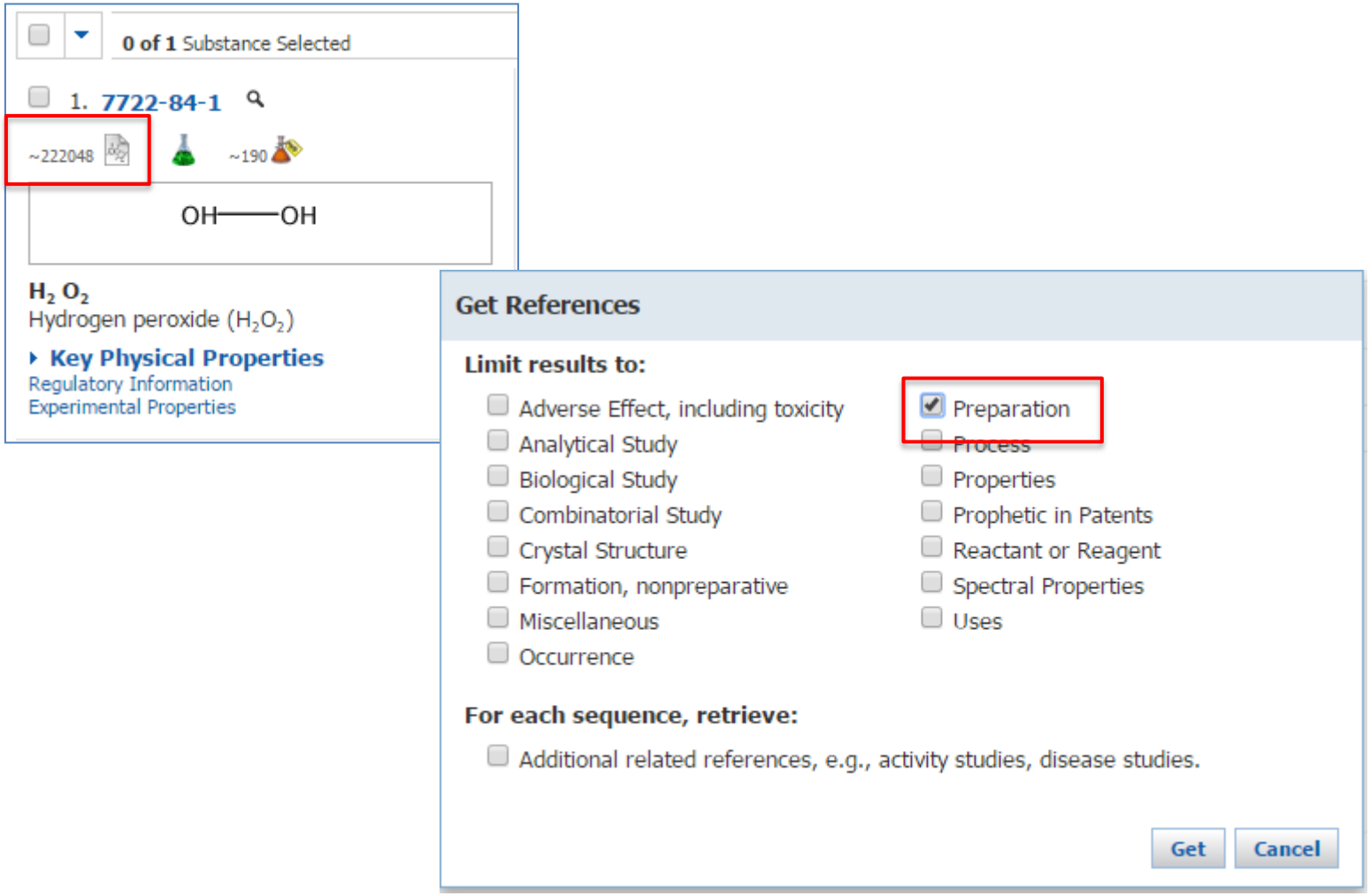
巧用CAS Role



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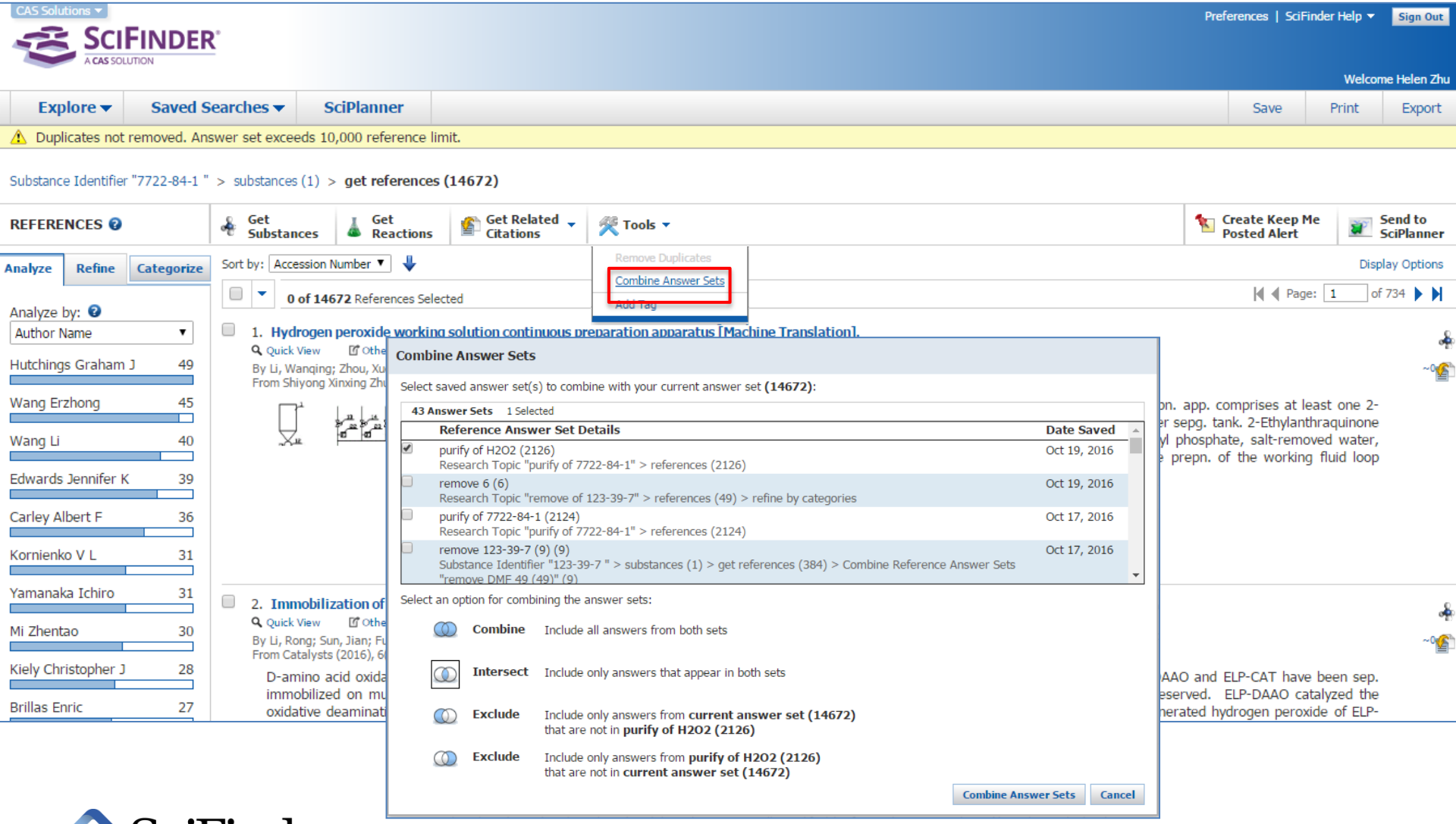

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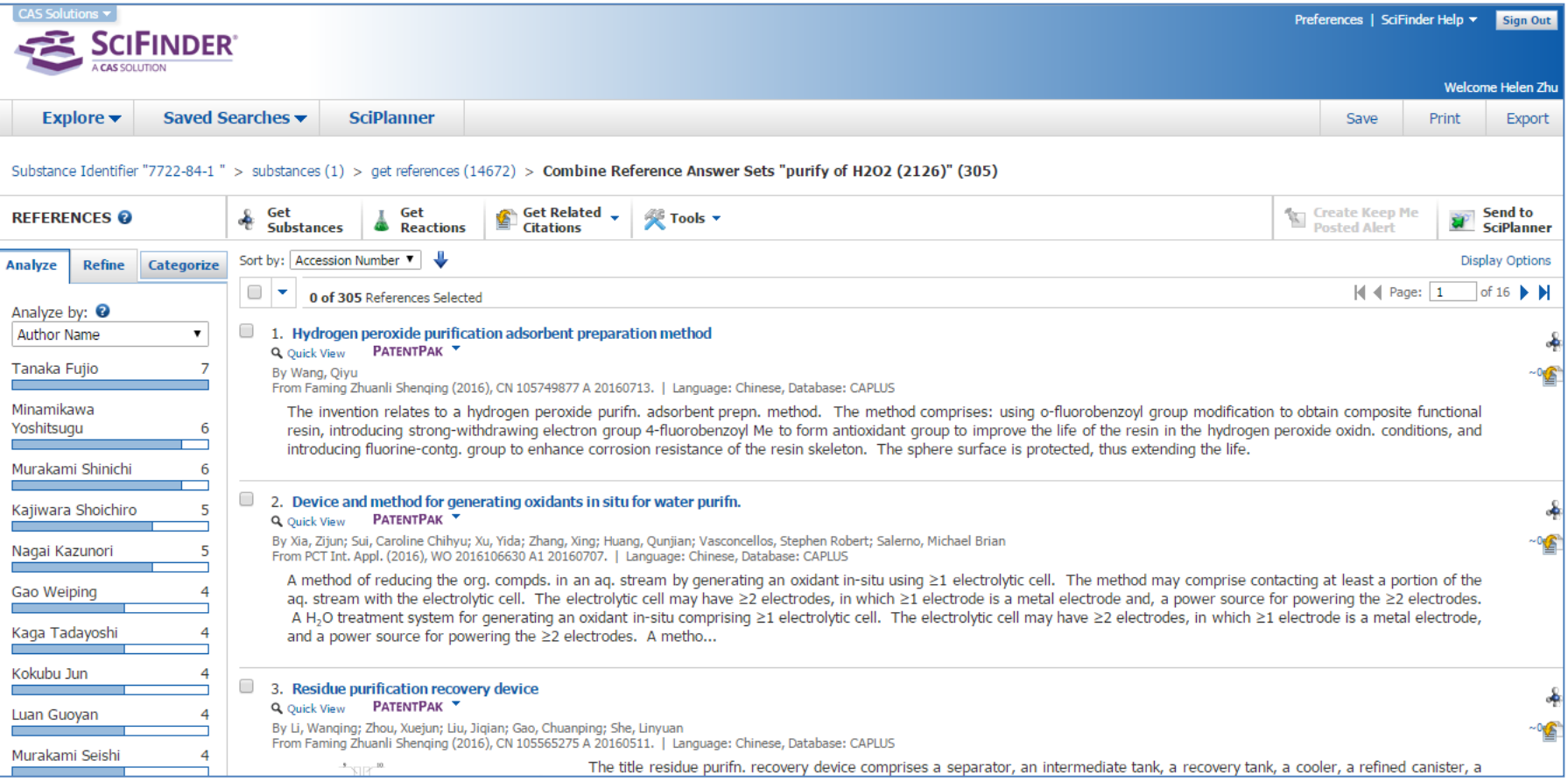
巧用CAS Role



浏览记录，判断是否符合要求

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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	A
CN 105749877 PATENTPAK	A		Jul 13, 2016	C

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

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善用Categorize去除噪音信息

检索文献：

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

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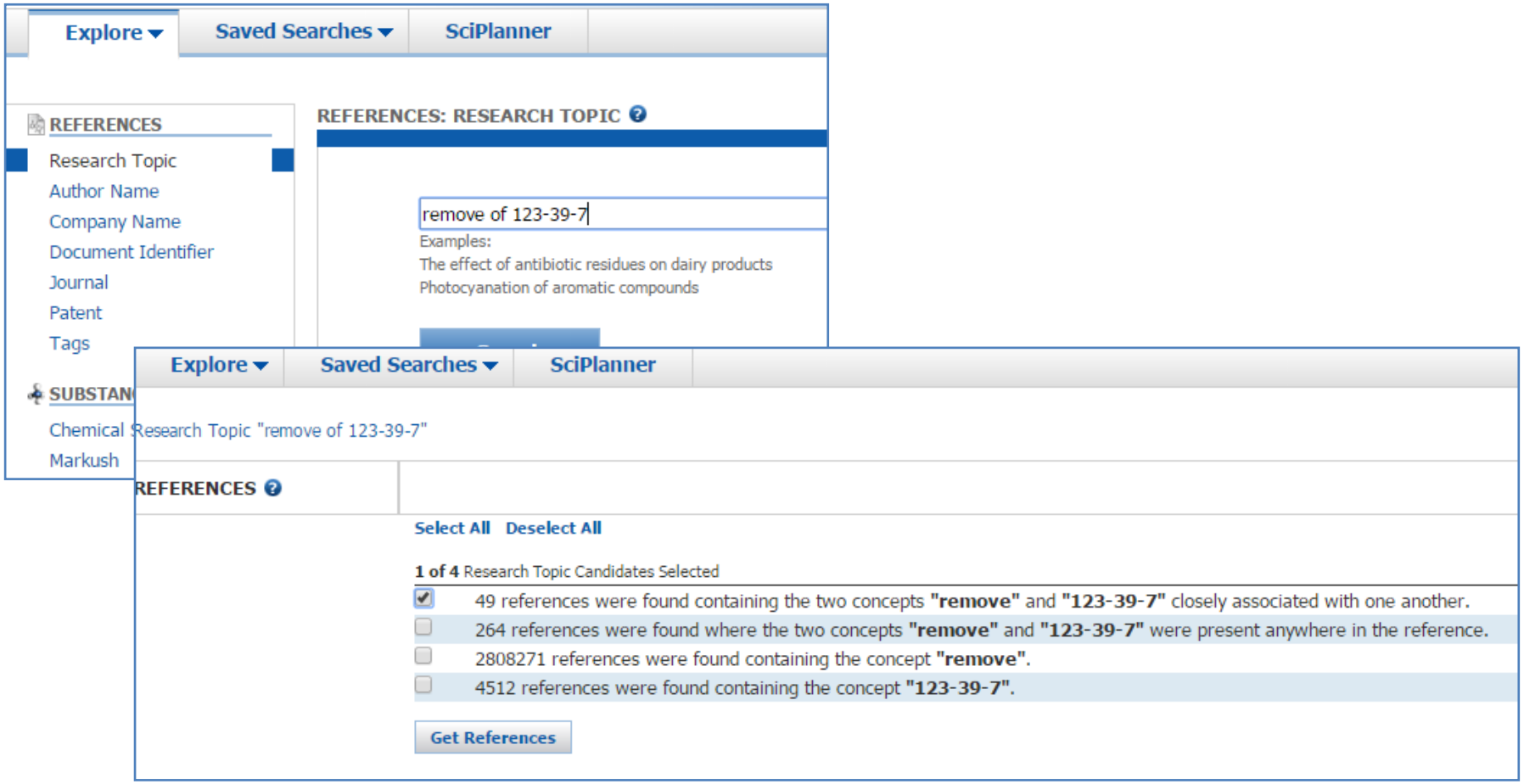
善用Categorize去除噪音信息

去除N-甲基甲酰胺（123-39-7）



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善用Categorize去除噪音信息

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

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

Dimethylamine (DMA) and N,N-dimethylformamide (DMF) are typical N-VOCs exhausted from manufg. factories. In the present study, the behavior of non-thermal plasma (NTP) was systematically investigated for removal of gas-phase DMA and DMF in a link tooth wheel-cylinder plasma reactor. Exptl. results show that DMA is much easier to be decompd. by NTP than DMF. Coexisting DMF has no effect on DMA conversion while DMF conversion is significantly promoted by the addn. of DMA. Regardless of initial gas compns. as well as DMA and DMF concn., CO_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

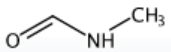
Volatile organic compounds

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

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善用Categorize去除噪音信息

3. Removing agent containing alkylamide mixture

By: Li, Bo; Yu, Ran

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

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

Patent Information

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

Priority Application

CN 2013-10646205	Dec 4, 2013

Indexing

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

Concepts

Coating removers — Photoresists

removing agent contg. alkylamide mixt.

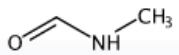
Amides

removing agent contg. alkylamide mixt.

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

Substances

123-39-7 N-Methylformamide



127-19-5 N, N-Dimethyl acetamide

removing agent contg. alkylamide mixt.

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

噪音信息更多，如何去除？

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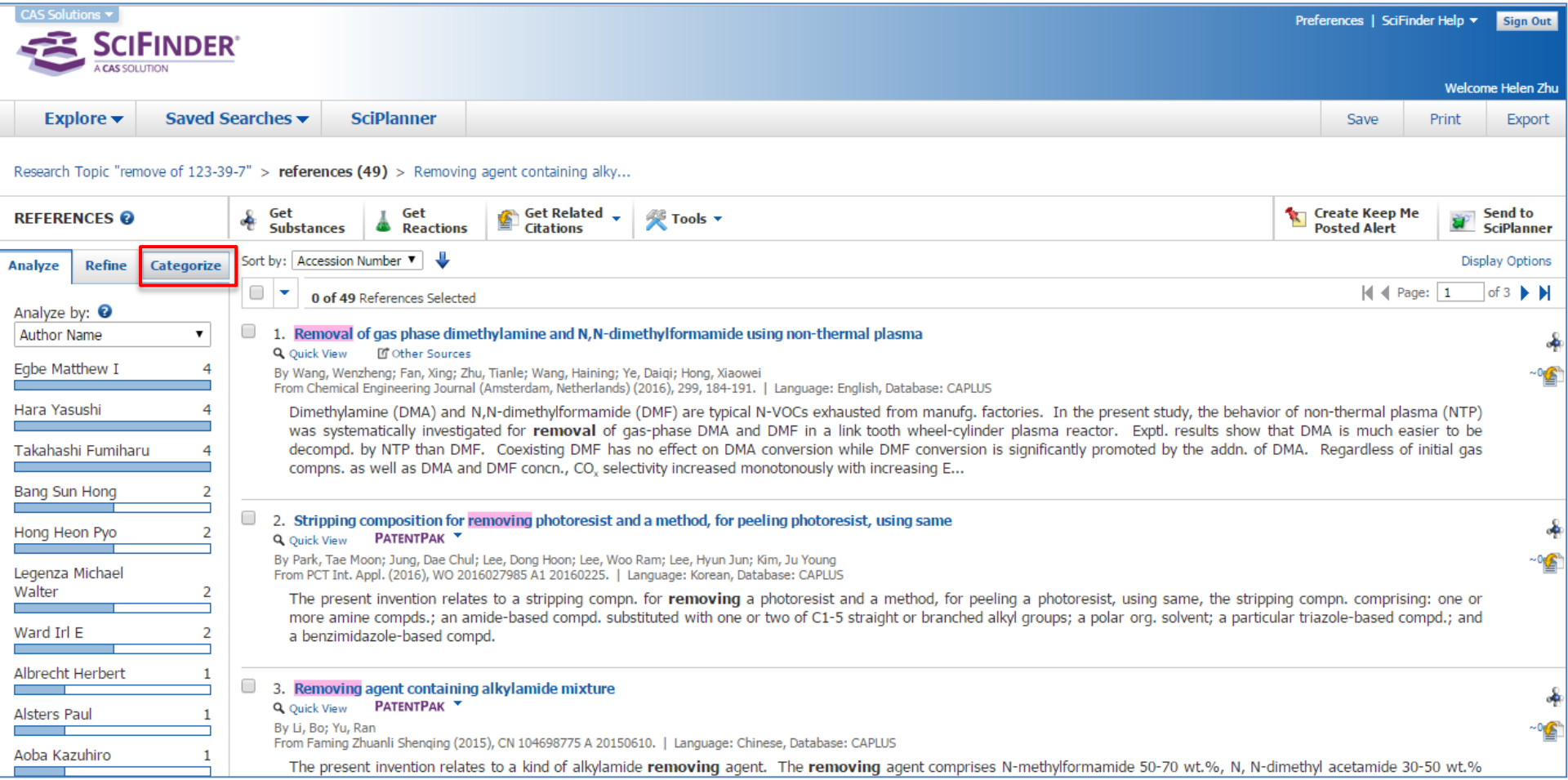
善用Categorize去除噪音信息



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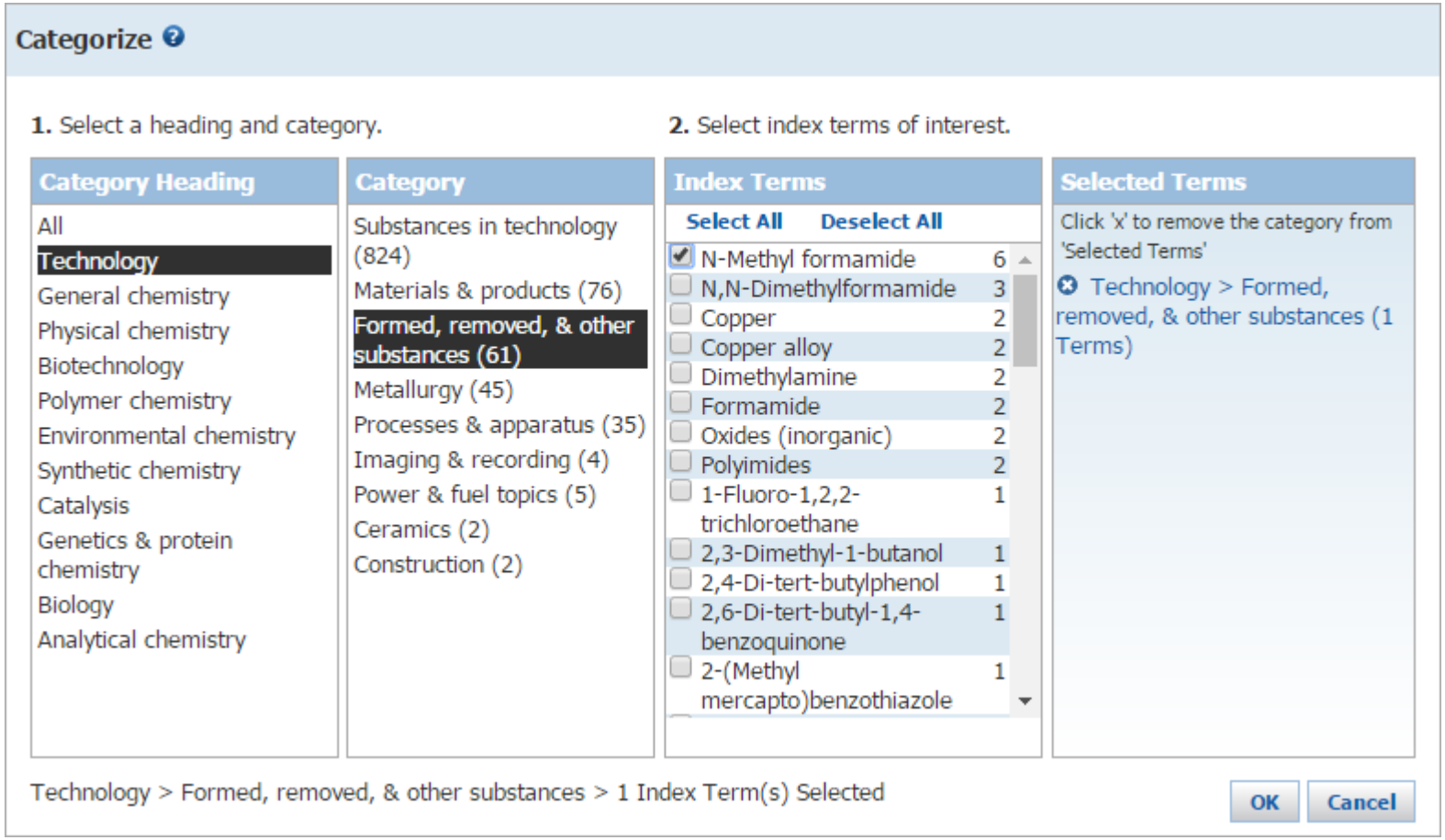
善用Categorize去除噪音信息



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提纲

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

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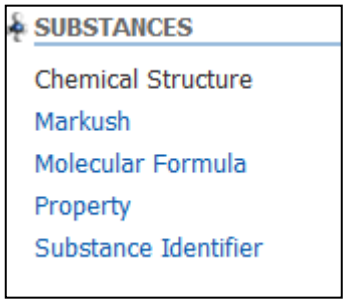
物质检索方法

- **功能方面**
  - 结构式
  - 分子式
  - 理化性质
  - 物质名称，CAS No



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

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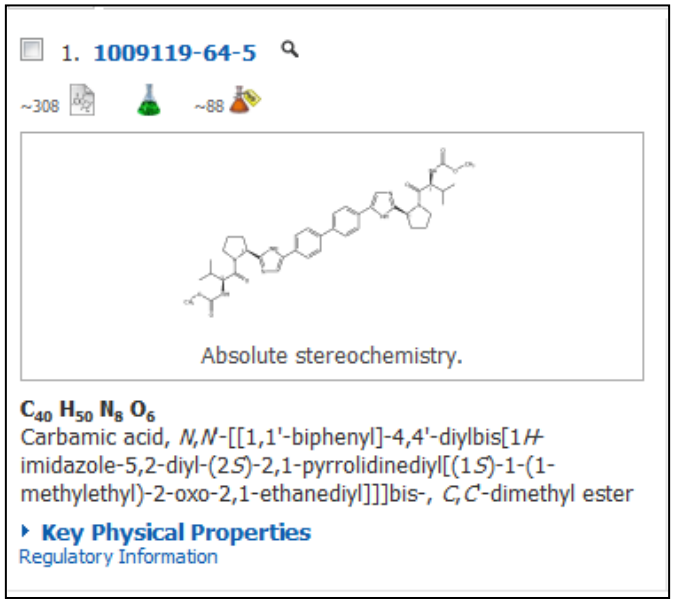
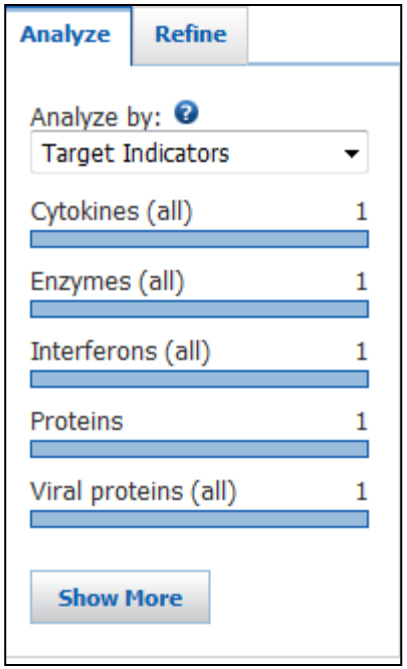
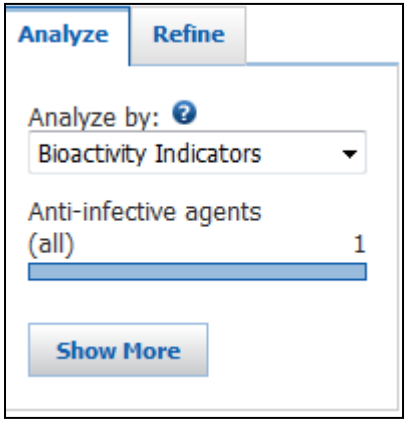
快速获得物质的生物活性及靶点信息





作用靶点



生物活性

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无机物及合金的检索

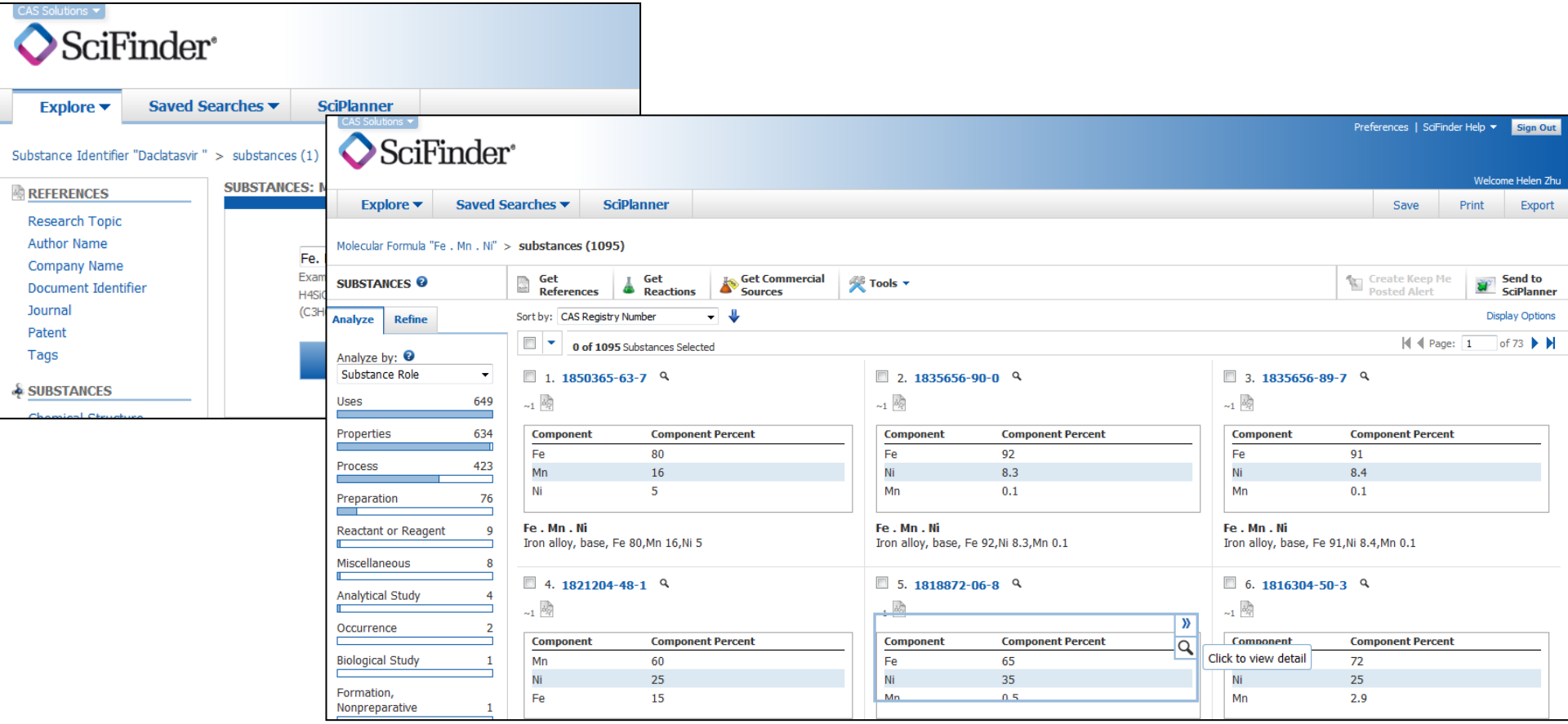
分子式书写规则—Hill 规则

- 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。

无机物及合金的检索

检索铁、锰、镍合金



合金物质以列表形式呈现

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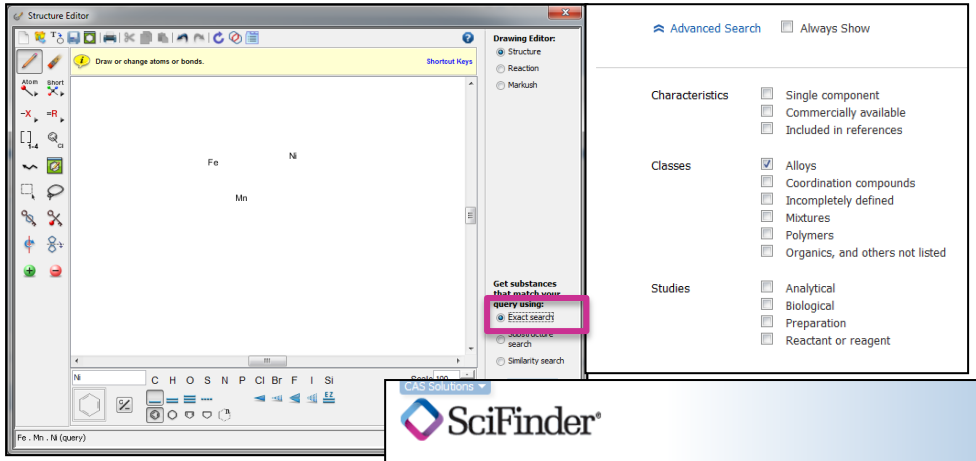
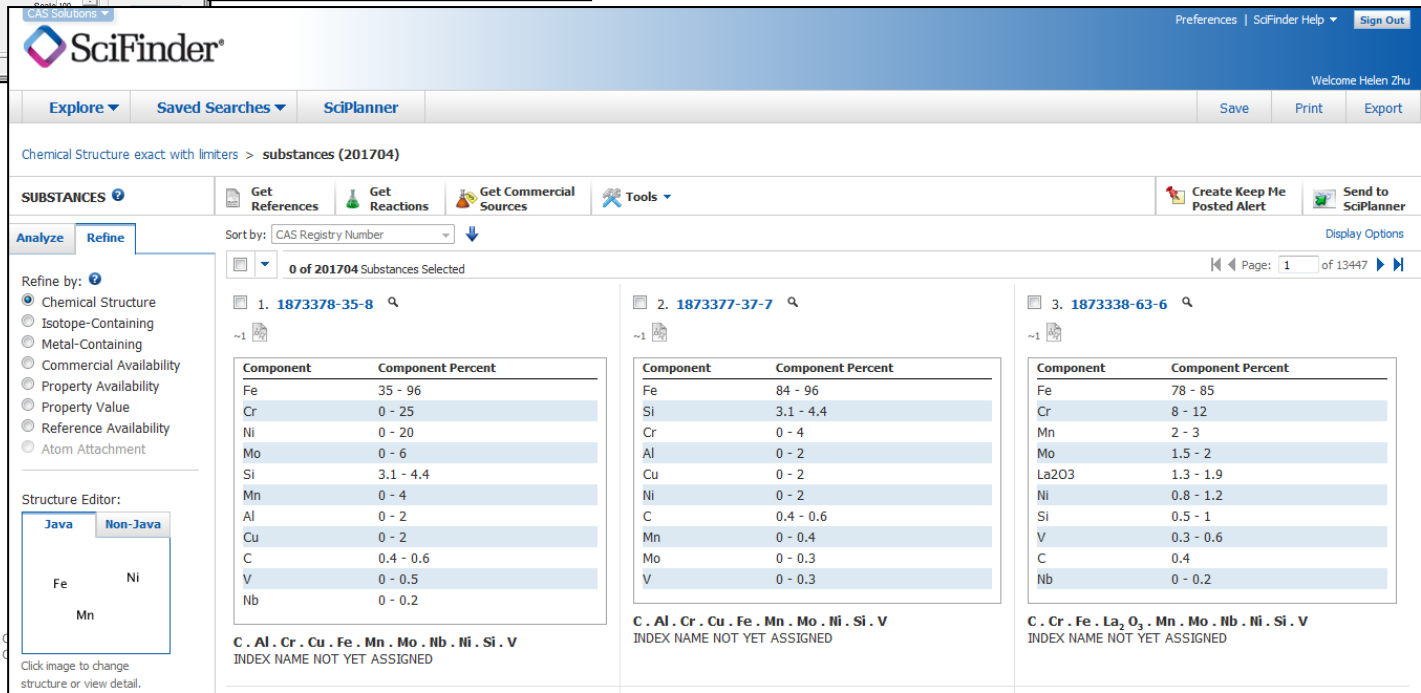
无机物及合金的检索

检索参杂铁、锰、镍原子的合金





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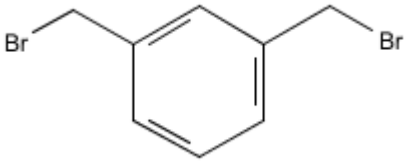
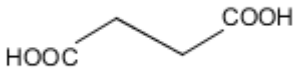
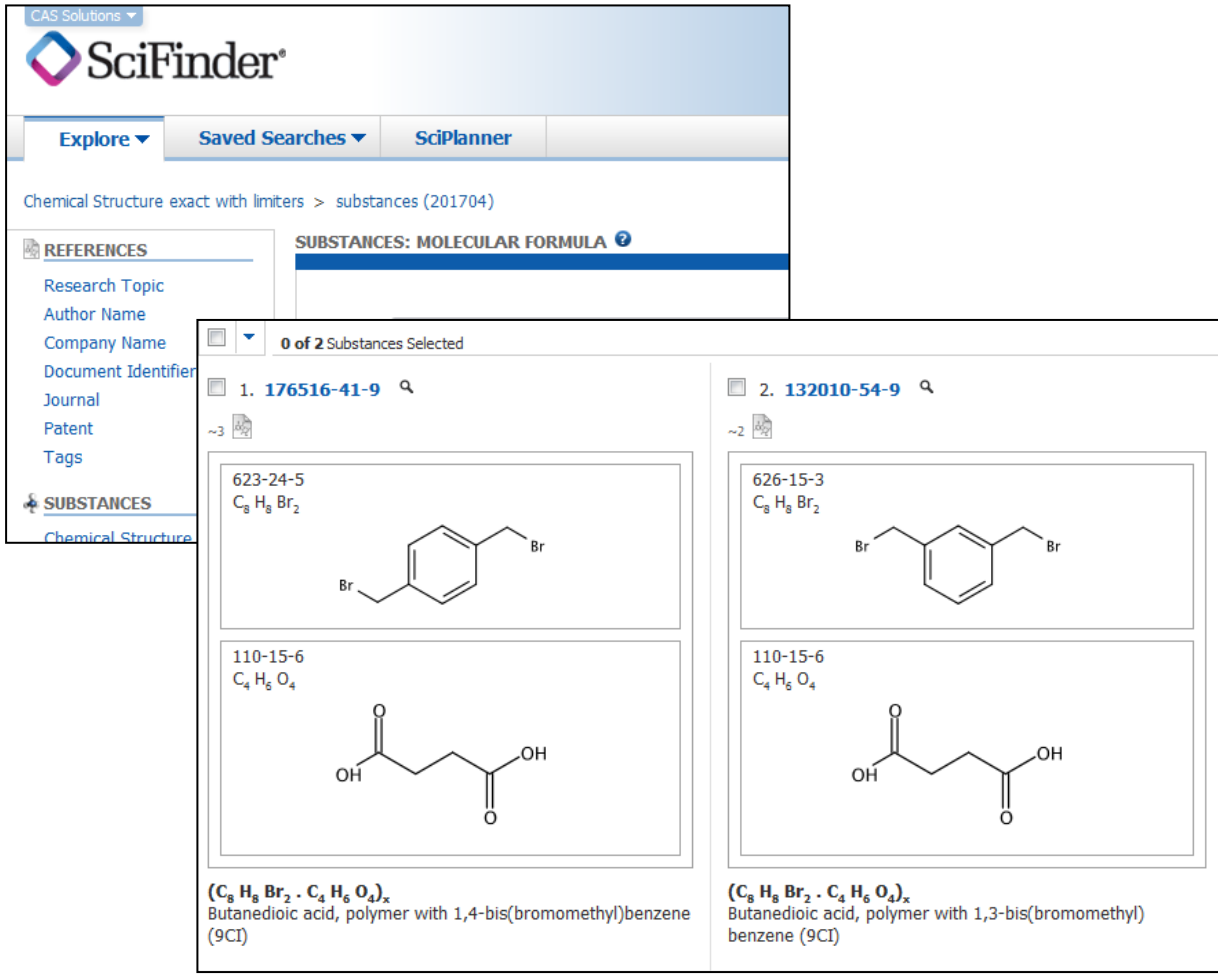
聚合物的检索

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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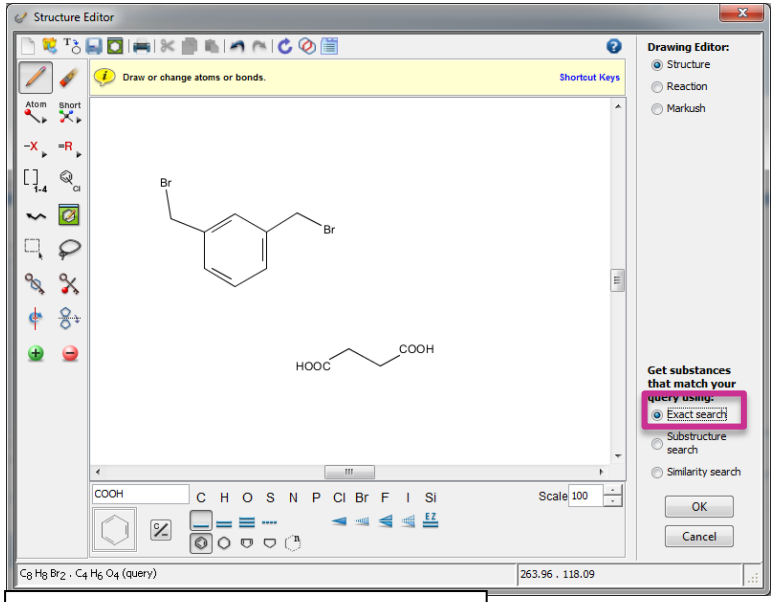
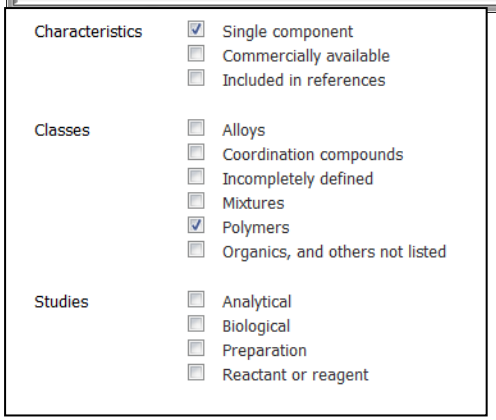
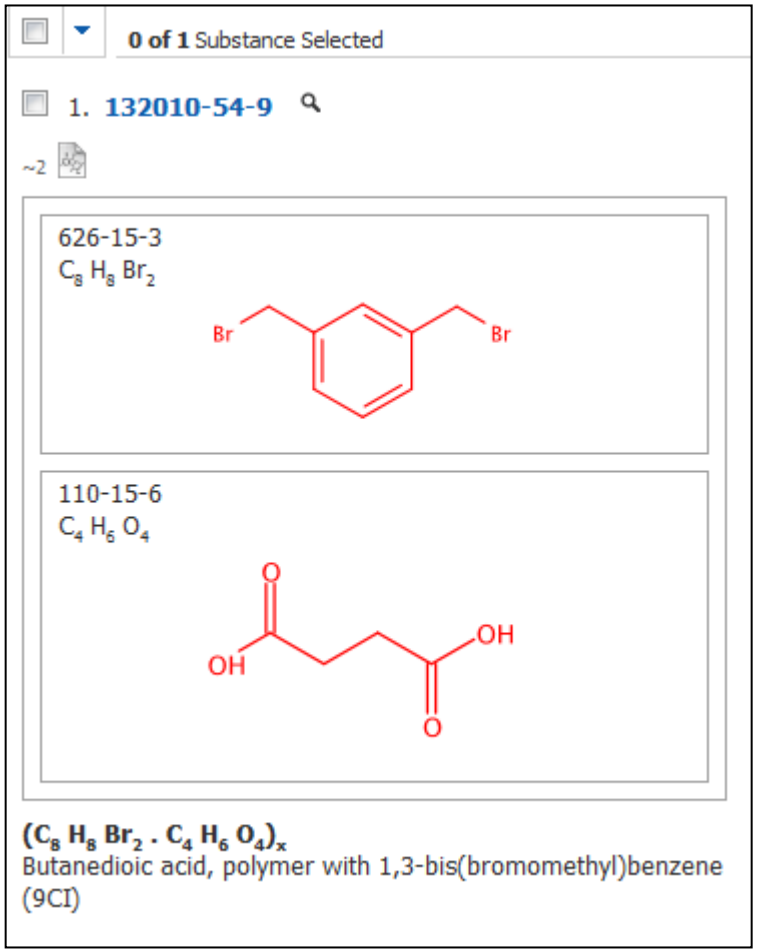
聚合物的检索





单一组分

聚合物



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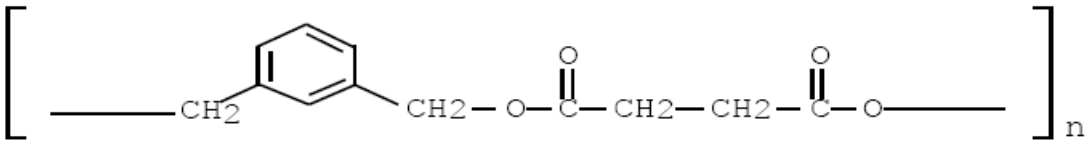
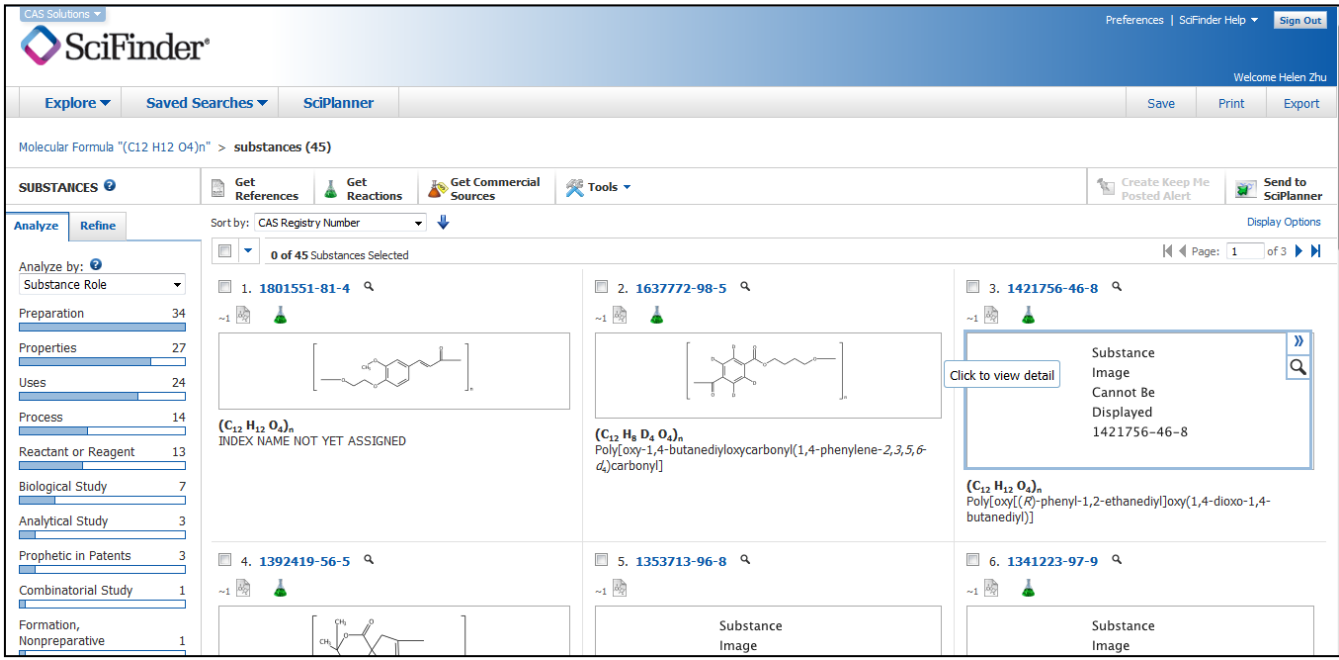
聚合物的检索

已知重复单元的聚合物



(C12 H12 O4)n



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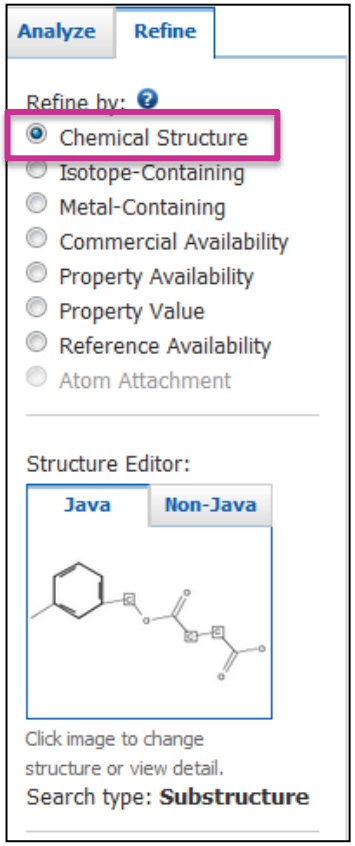
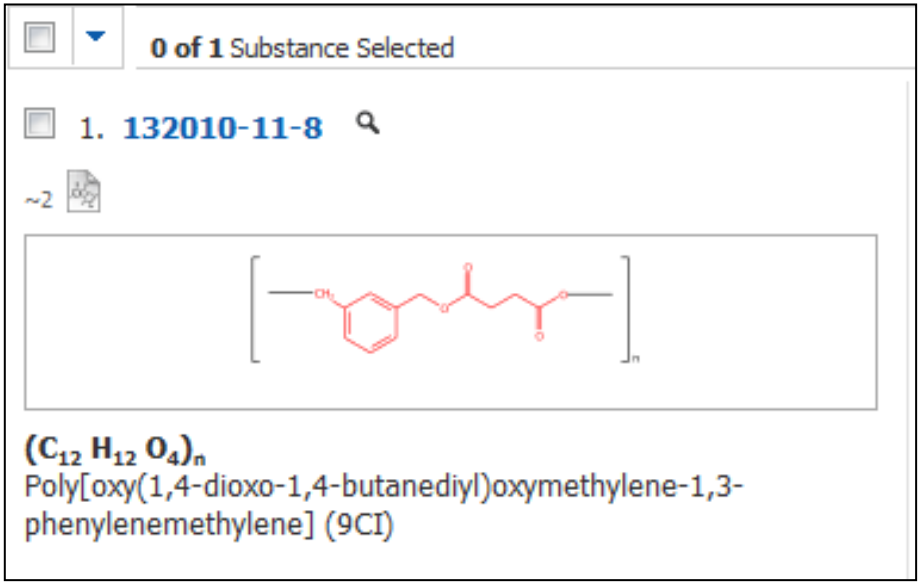
聚合物的检索





利用结构特征进行Refine，迅速查找需要的物质

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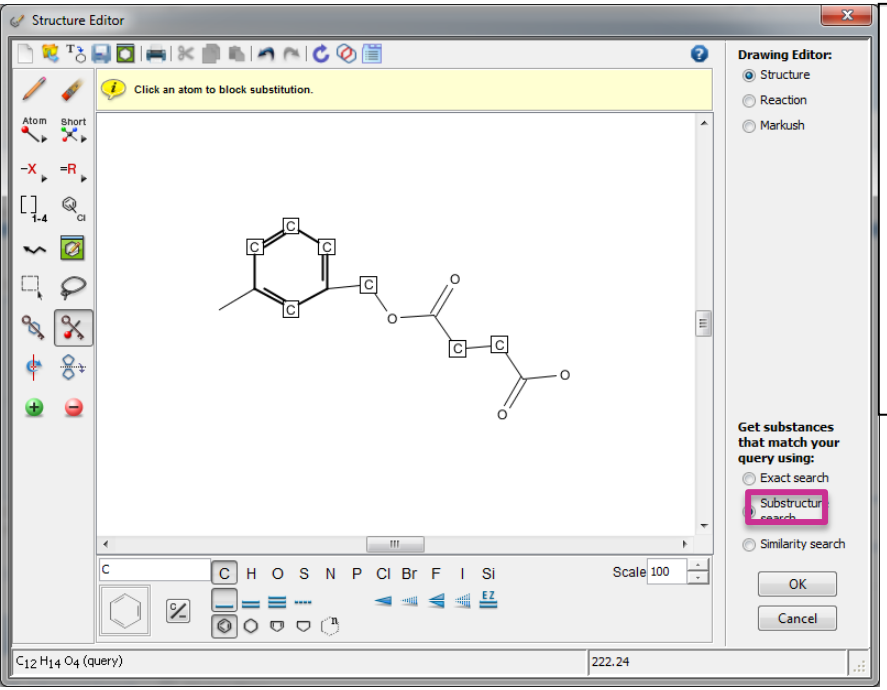
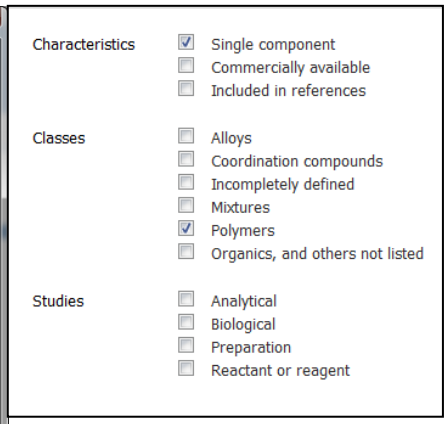
聚合物的检索



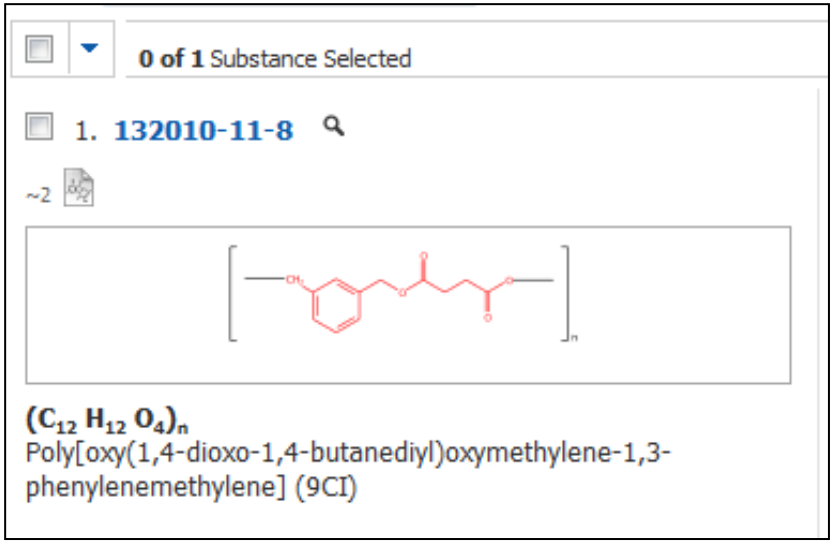
绘制好SRU后用亚结构检索

因为两段为开放状态



单一组分

聚合物



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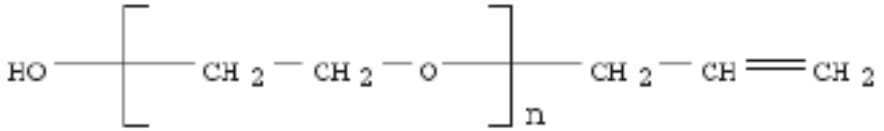
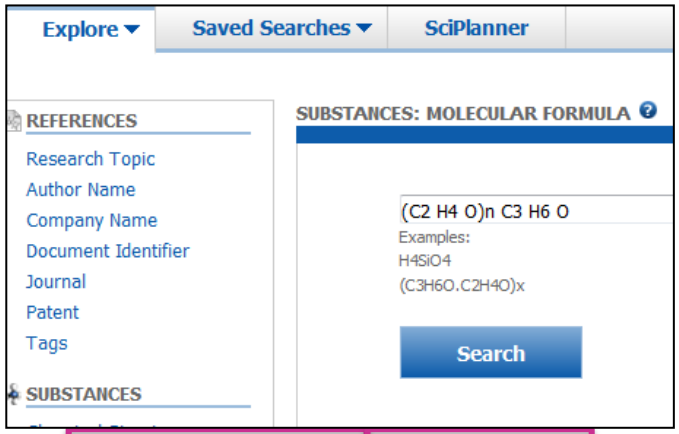
聚合物的检索

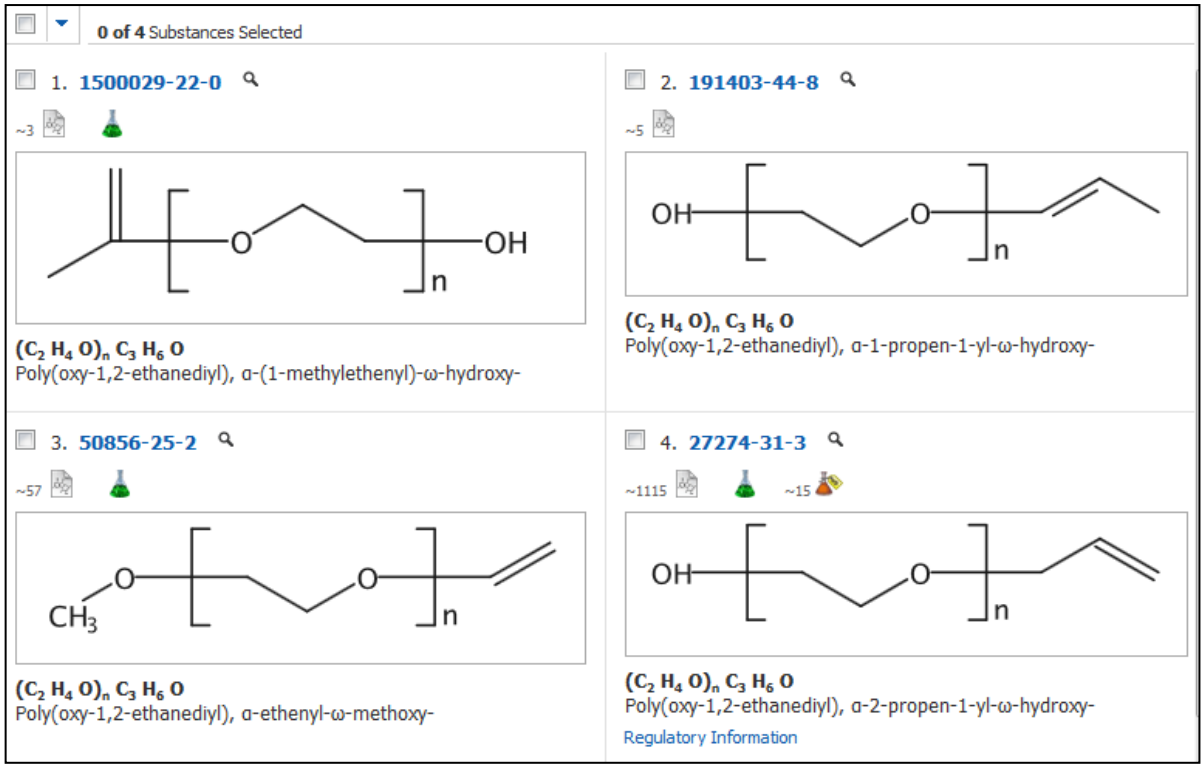
含端基和SRUs的聚合物





(C2 H4 O)n C3 H6 O

SRU部分　两端部分



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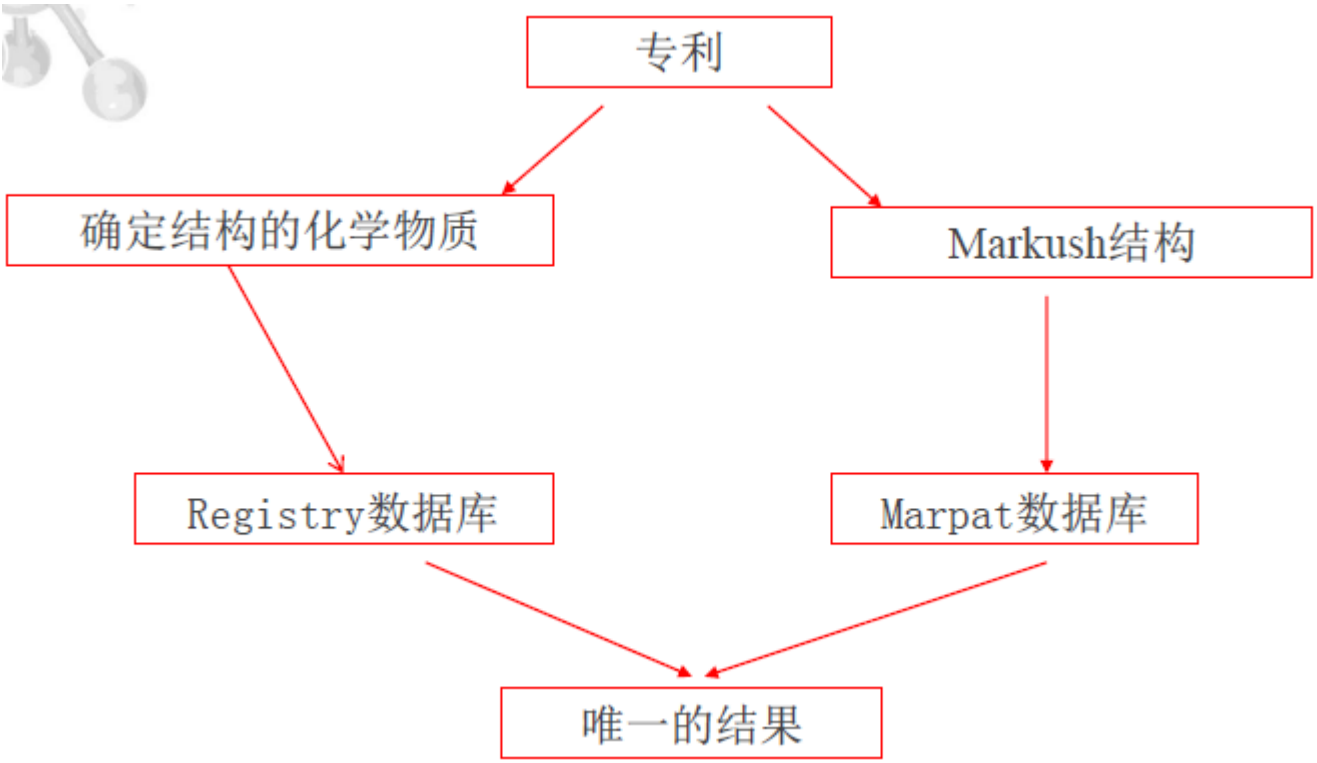
检索具有相同结构特征物质及专利文献



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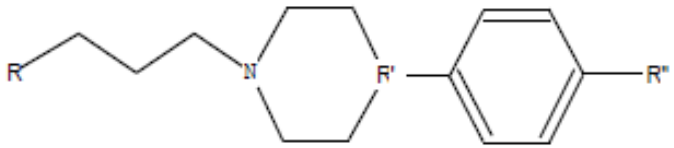
检索具有相同结构特征物质及专利文献

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

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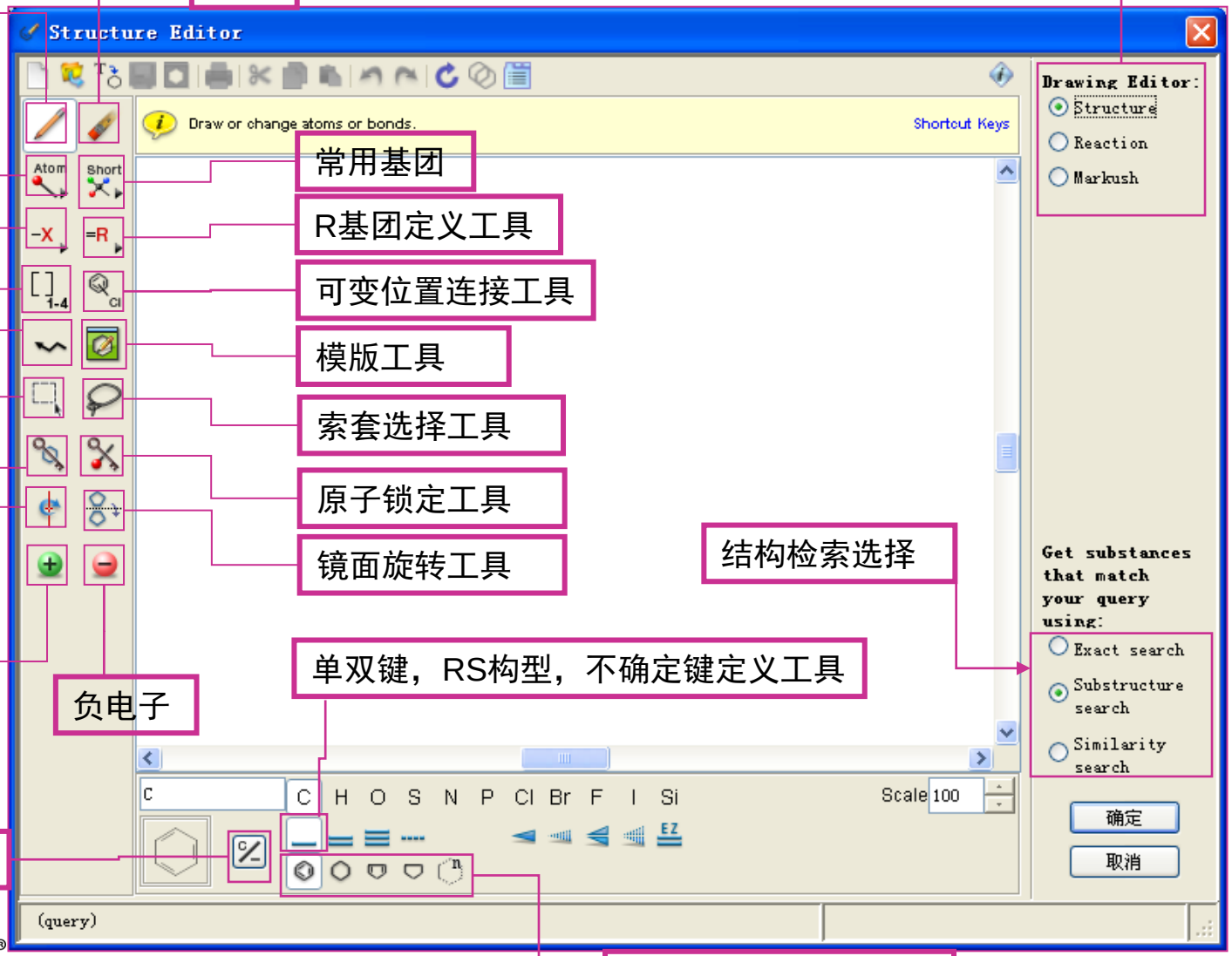
SciFinder结构编辑器



铅笔

橡皮

结构和反应切换功能

元素周期表

常用基团

可变基团

R基团定义工具

重复基团工具

可变位置连接工具

碳链工具

模版工具

选择工具

索套选择工具

环锁定工具

原子锁定工具

旋转工具

镜面旋转工具

结构检索选择

正电子

负电子

单双键，RS构型，不确定键定义工具

C原子和单键恢复工具

常见环，多元环工具

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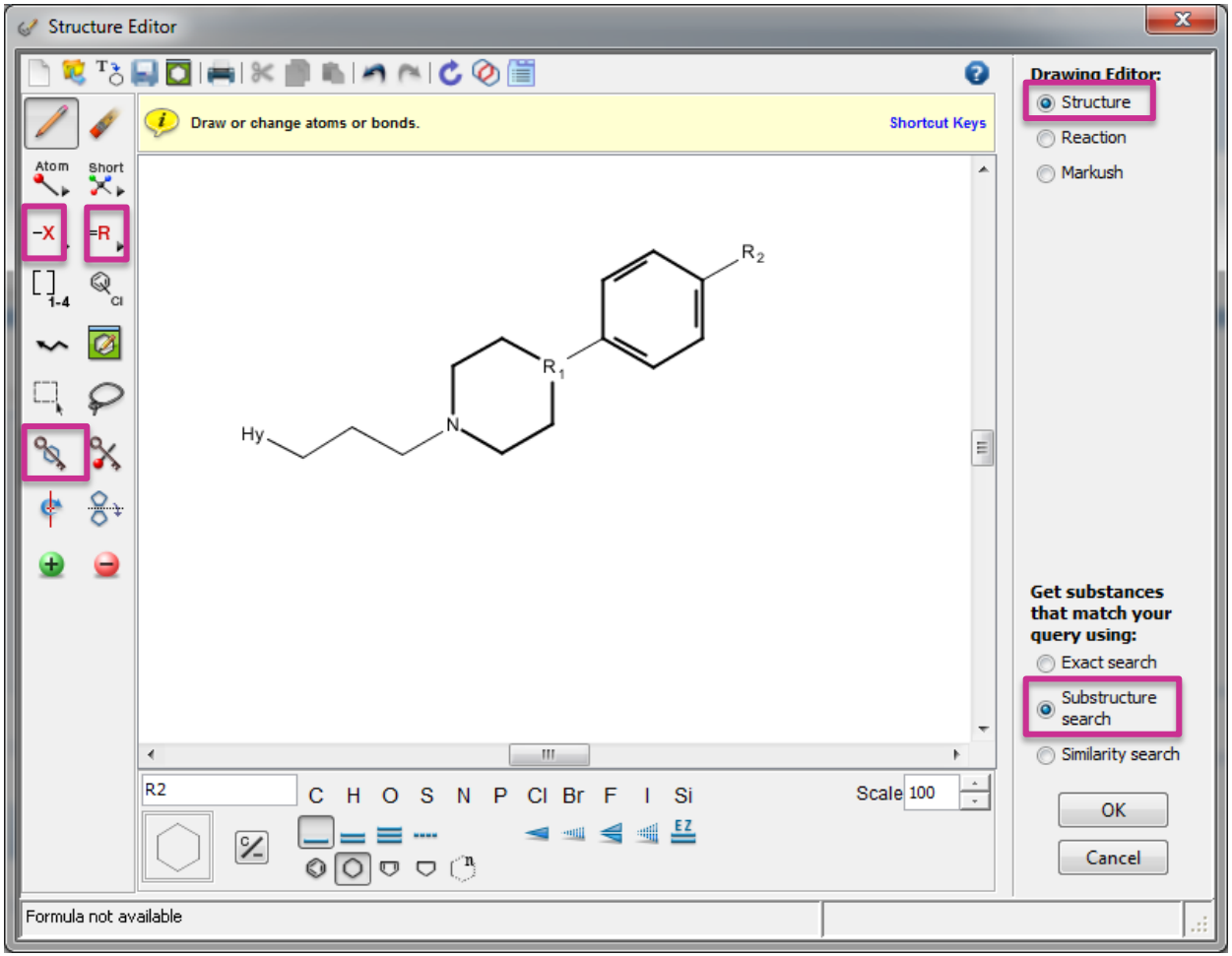
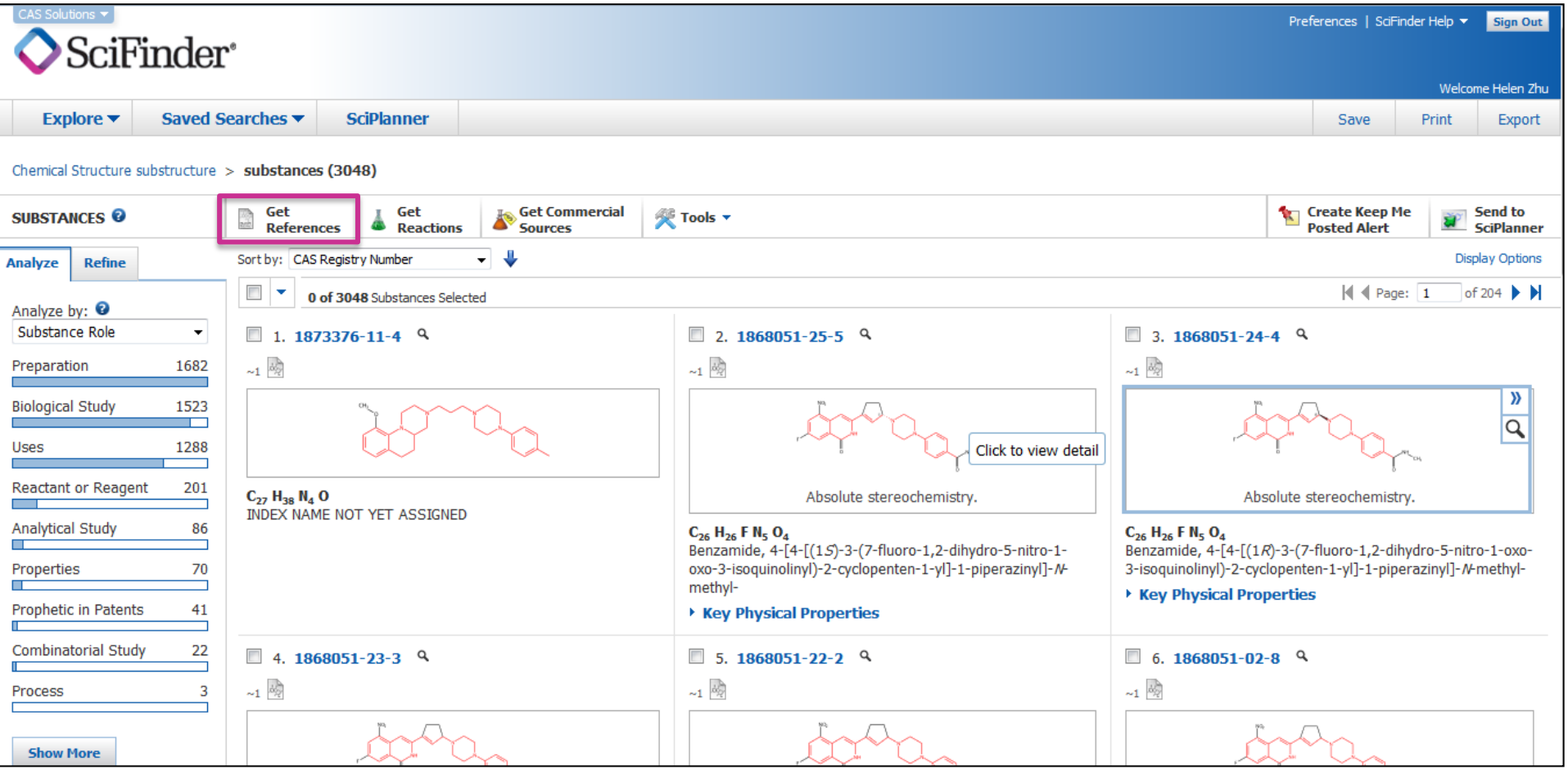
检索具有相同结构特征物质及专利文献



SciFinder®
A CAS Solution

检索具有相同结构特征物质及专利文献



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检索具有相同结构特征物质及专利文献

SciFinder

Welcome Helen Zhu

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

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0 of 408 References Selected | Page: 1 of 21

Refine by:
- Research Topic
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- Document Type
- Publication Year
- Language
- Database

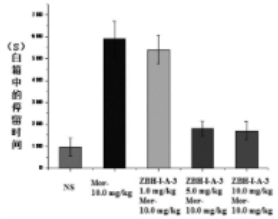
Document Type(s)
- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent

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



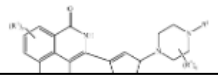
Title compds. I [wherein A = $(CH_2)_n$, n is 2 to 4; R = H, 4-Cl, 2,3-diCl, 4-CH_3, 2,3-diCH_3, 4-OCF_3, 4-OCH_3, 2-OCF_3, 2,6-diCH_3, 3,4-diCH_3, 3-CF_3, 4-Cl, 3-OCH_3, 2-C_2h_5, or 2-CH_3], and their pharmaceutically acceptable salts thereof, were prepd. as D3 acceptor ligands, which are used for 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

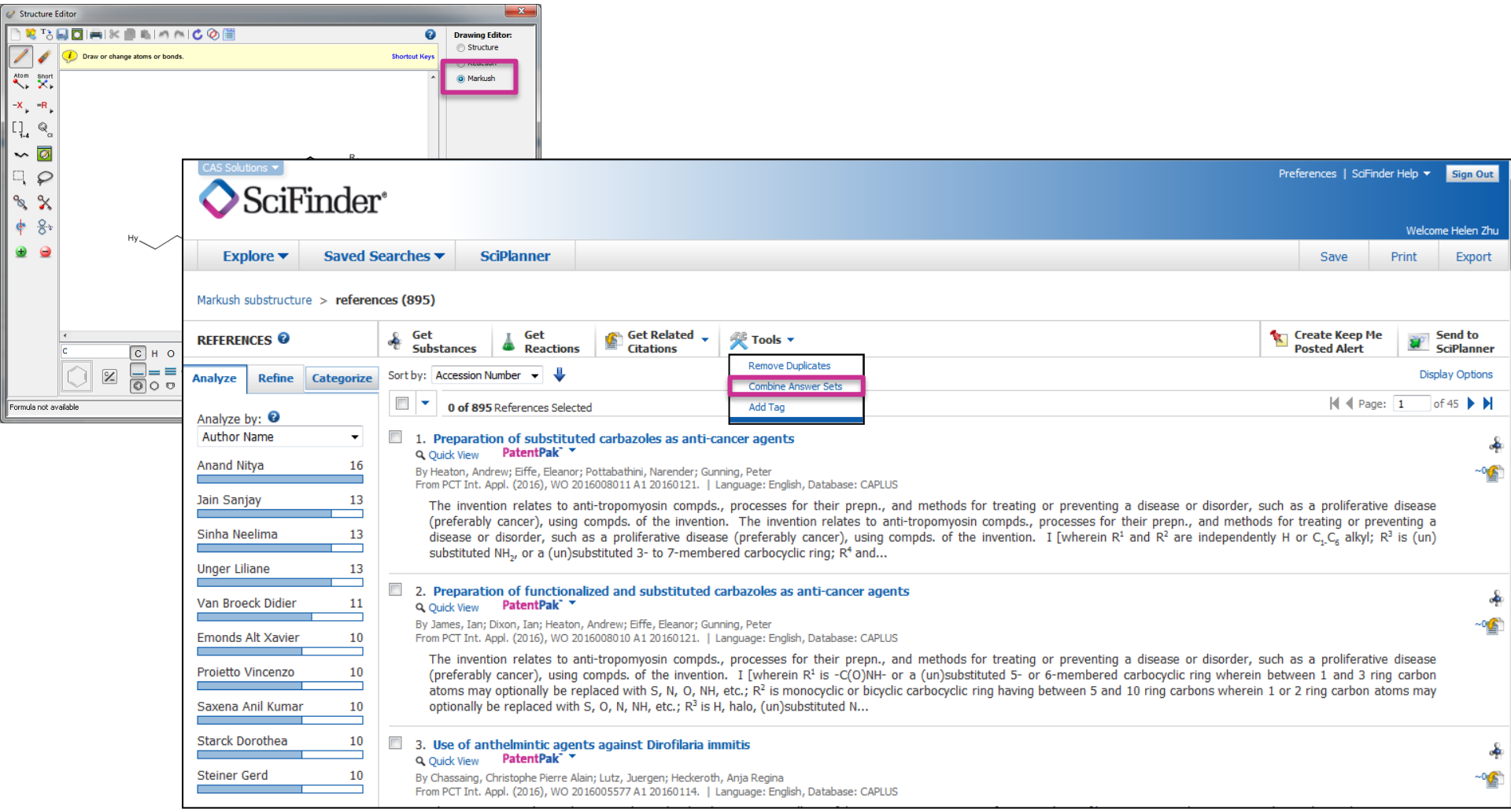
From PCT Int. Appl. (2016), WO 2016012956 A1 20160128. | Language: English, Database: CAPLUS



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

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

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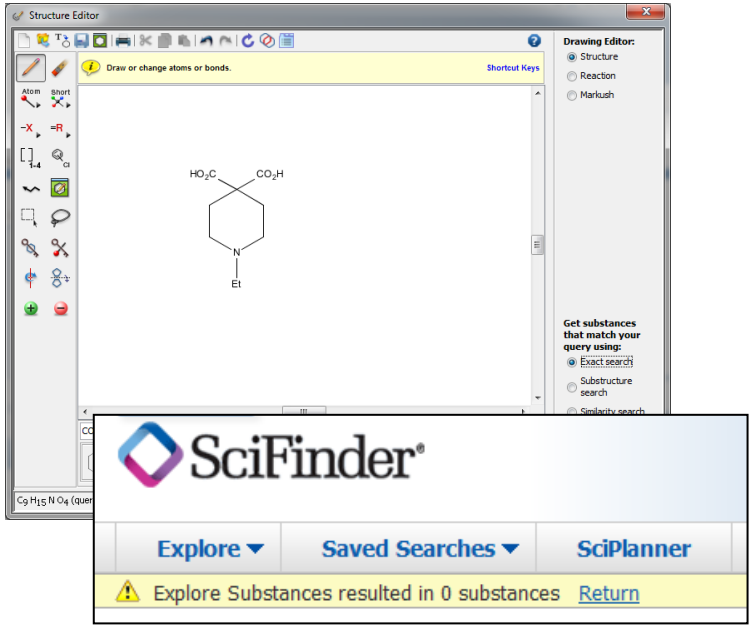
如何判断结构的新颖性

新颖性：是否存在？是否能申请专利？

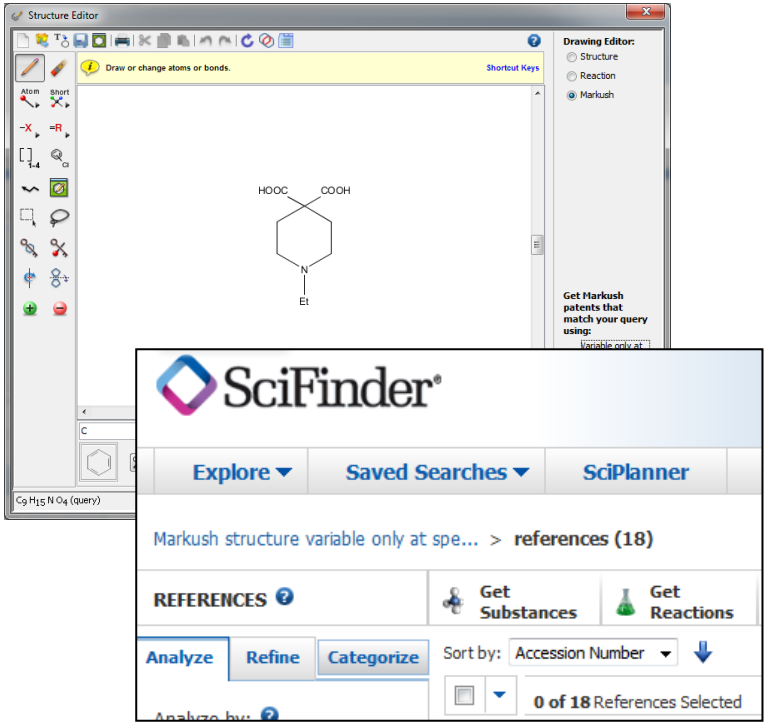
SciFinder相关物质库：Registry和Marpat

检索方法：物质检索？Markush检索？

Step1



Step1



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提纲

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

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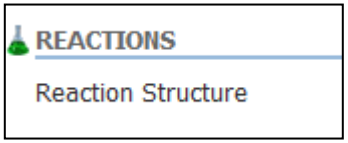
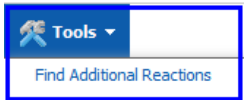
反应检索方法

- **功能方面**
  - 结构式



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



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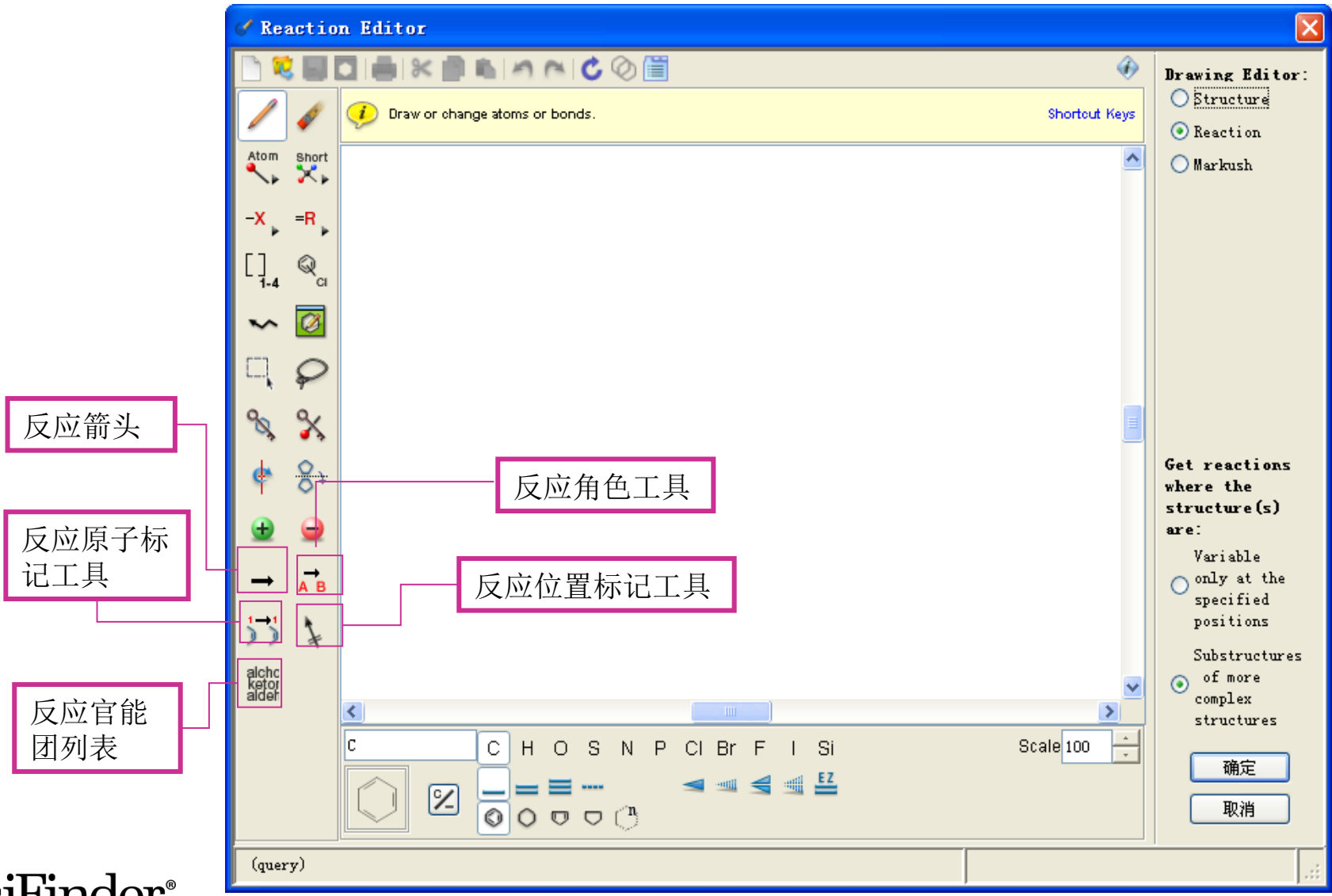
SciFinder中反应定义工具



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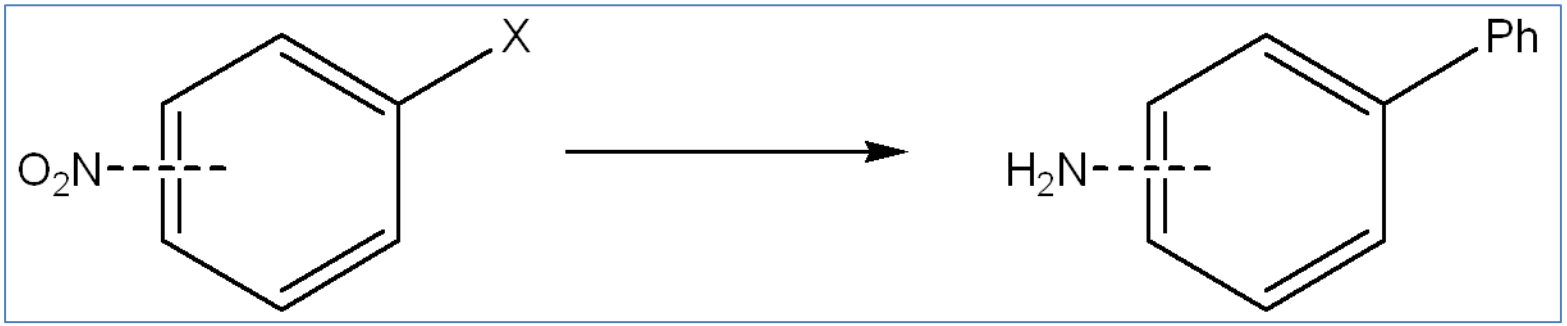
反应的精准定义

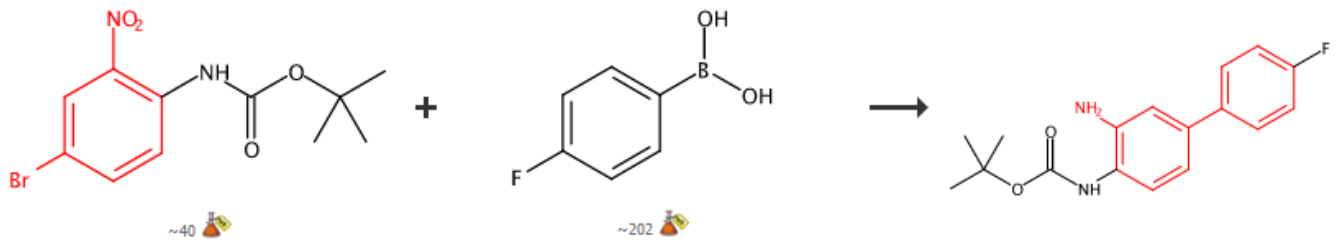
检索符合以下要求的反应，硝基还原的情况下，做**SUZUKI**偶联



反应的精准定义

2. **View Reaction Detail** Link

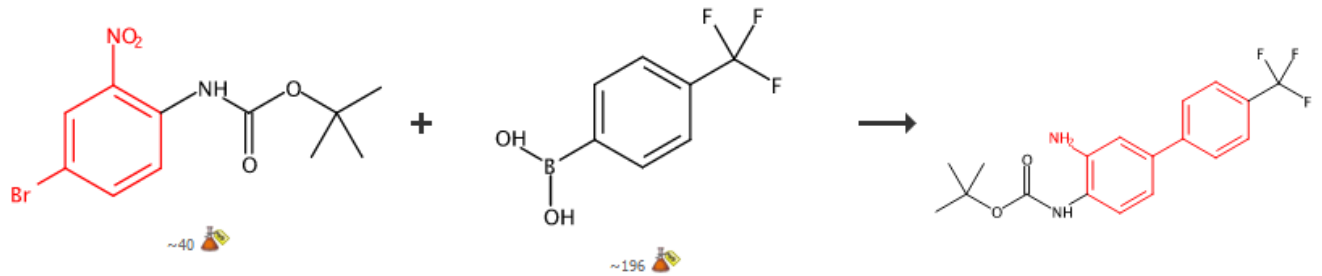
2 Steps *Hover over any structure for more options.*



符合要求的反应

7. **View Reaction Detail** Link **Similar Reactions**

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



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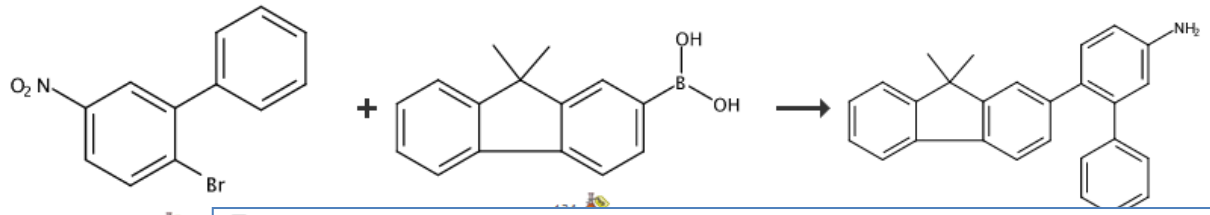
反应的精准定义

1. View Reaction Detail Link

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

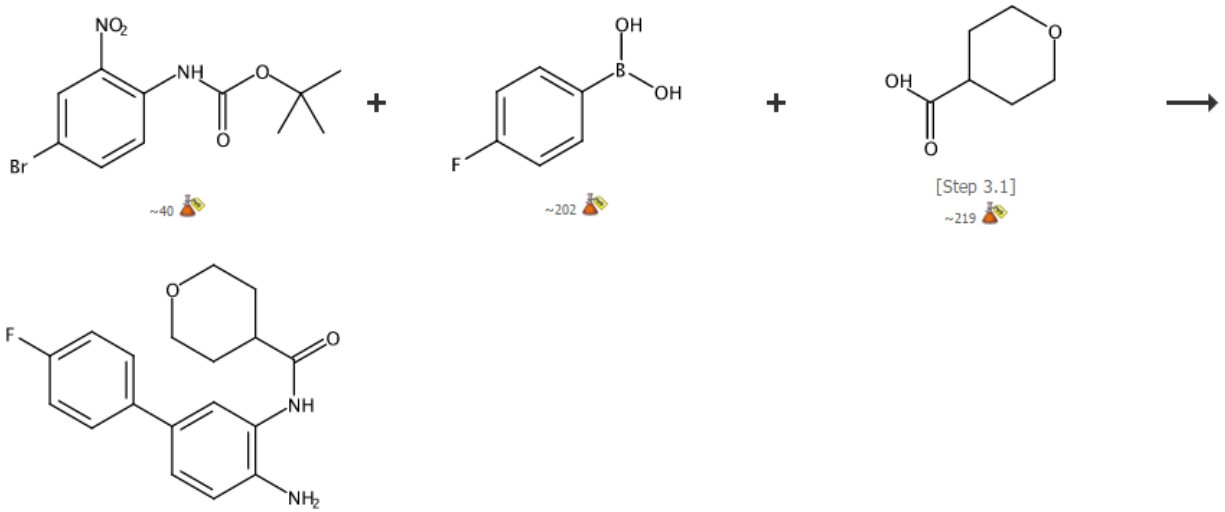


~14

不符合要求的反应

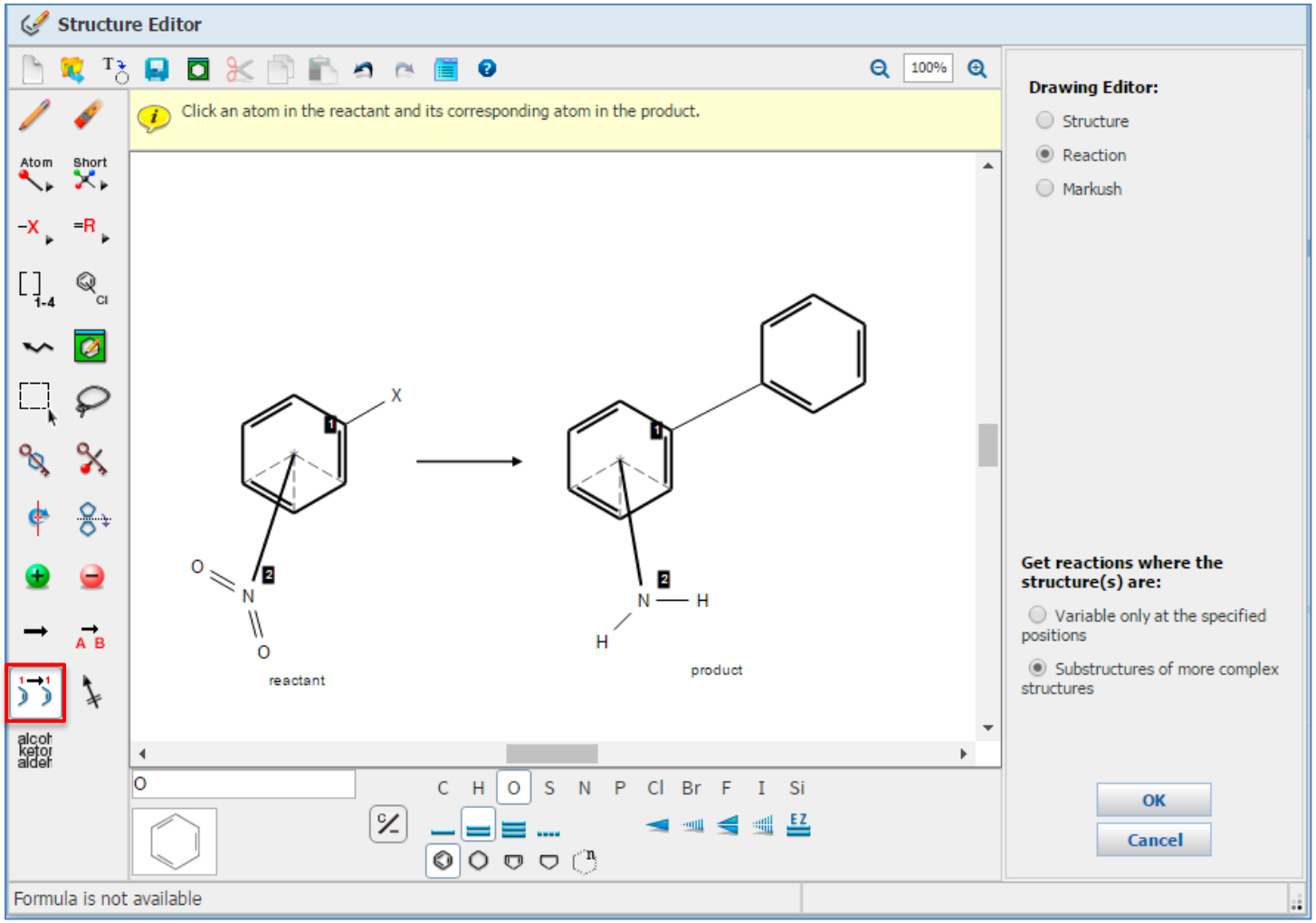
3. View Reaction Detail Link

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



~40 ~202 ~219

反应的精准定义



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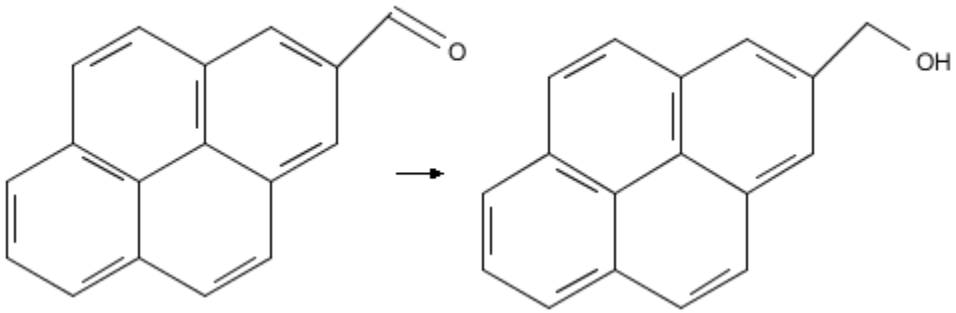
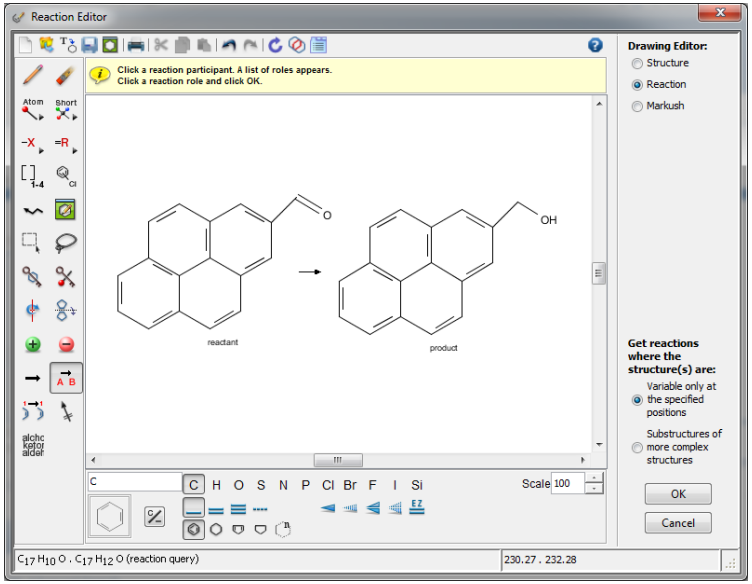
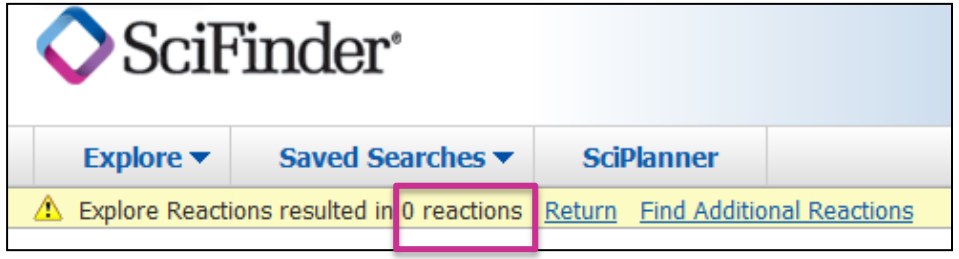
巧妙获得有实验步骤的相关反应

该还原反应如何操作？







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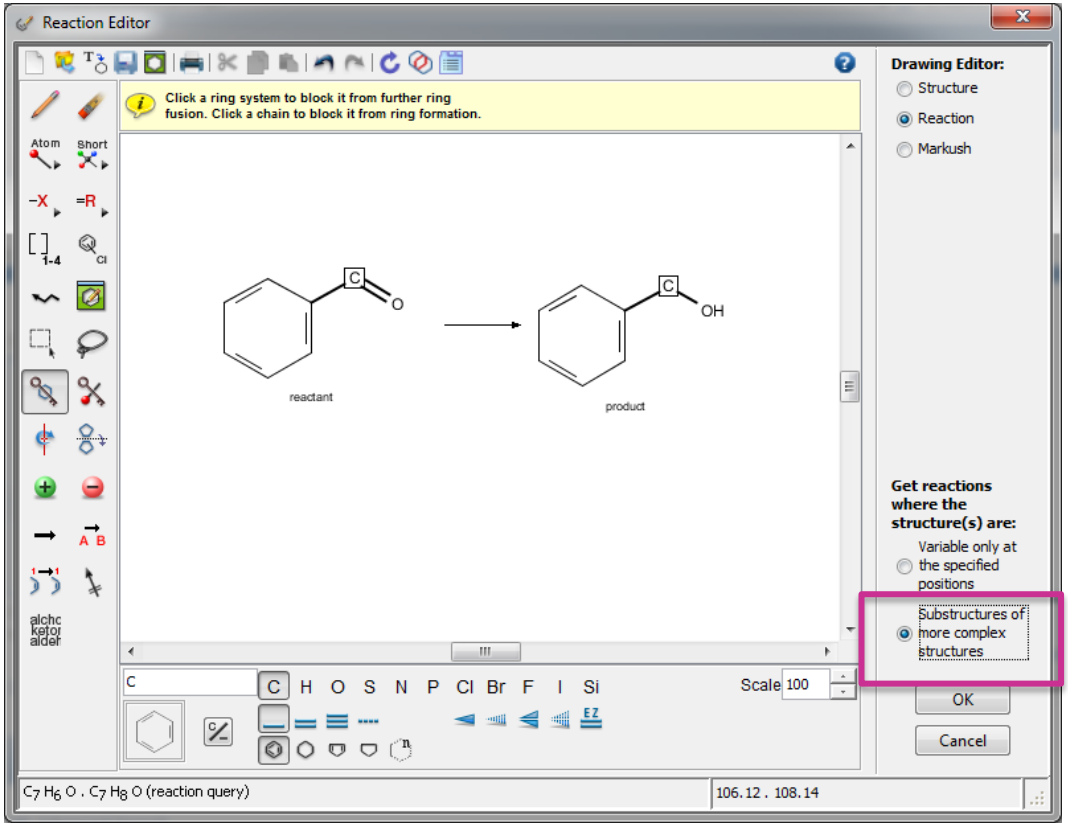
巧妙获得有实验步骤的相关反应



聚焦反应关键部位，查找相似反应

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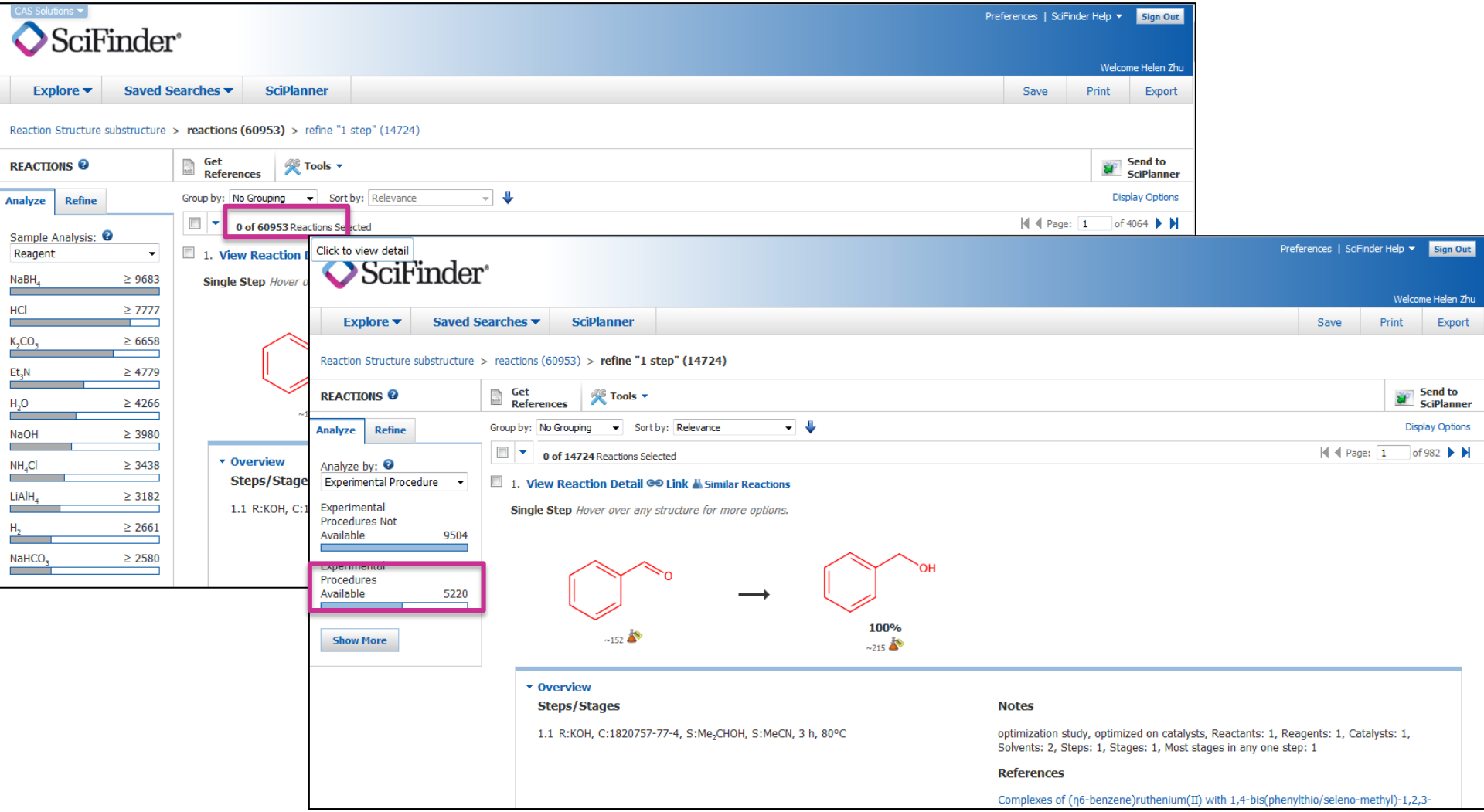
巧妙获得有实验步骤的相关反应



通过Refine获得单步反应后选取有实验步骤的反应

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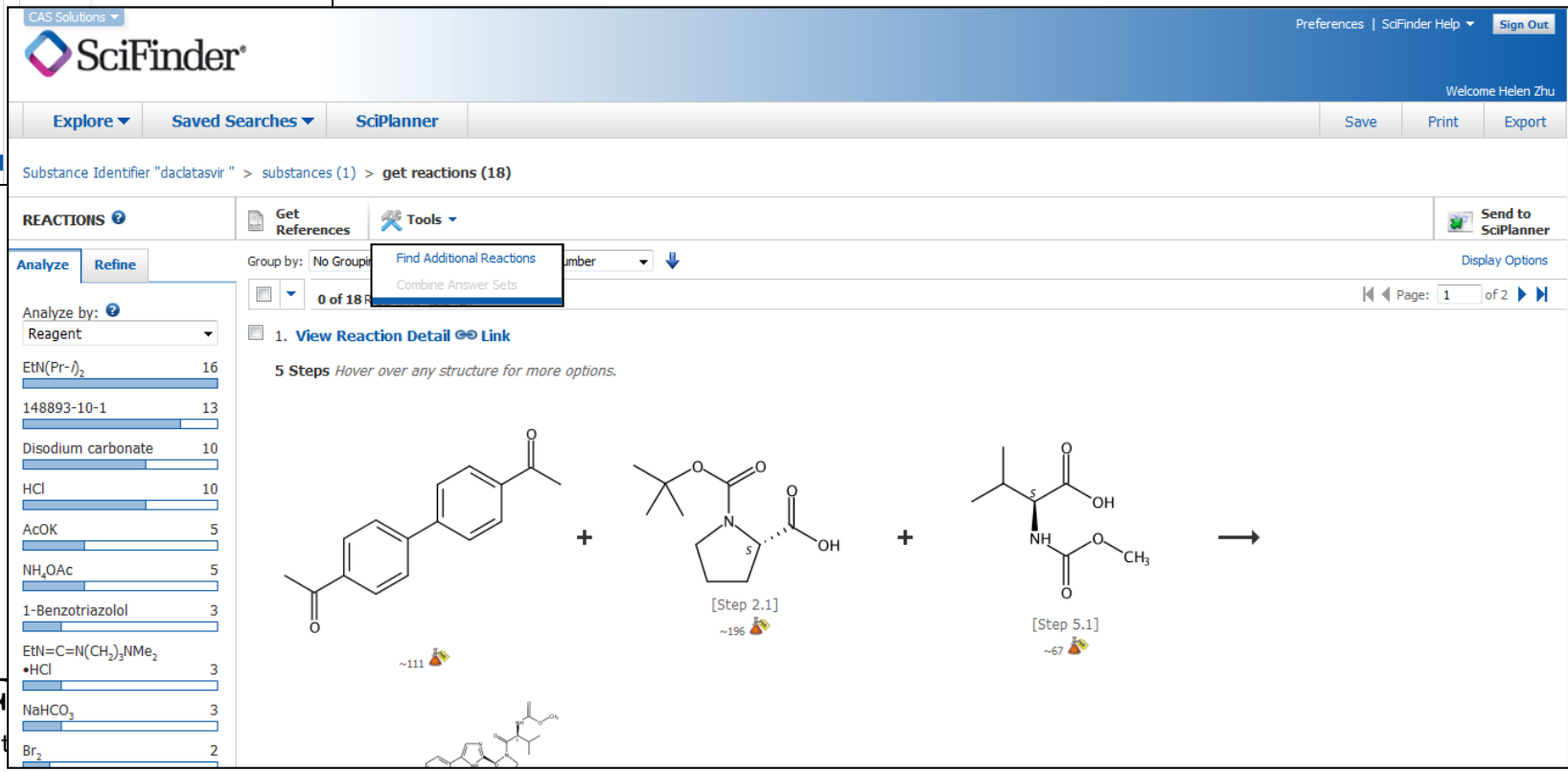
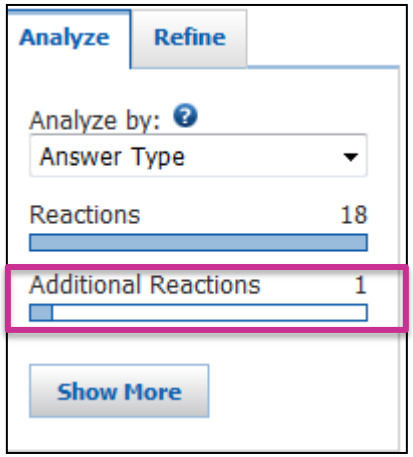
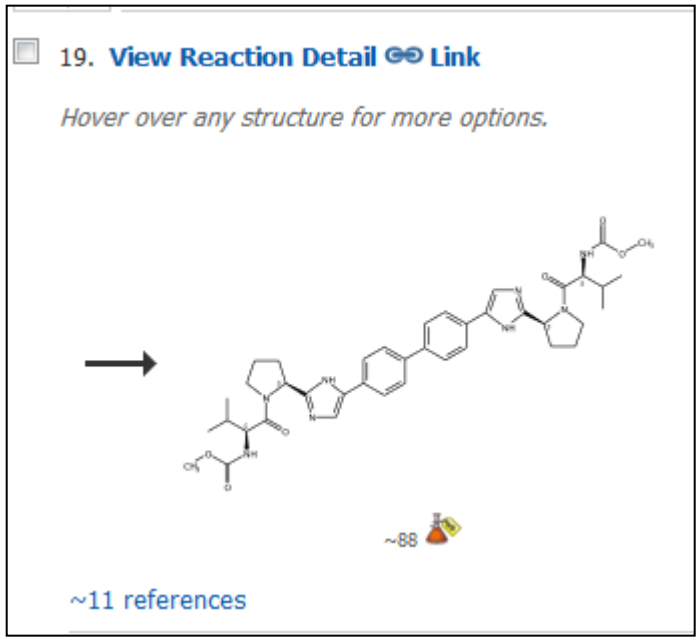
获得全面的反应信息

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

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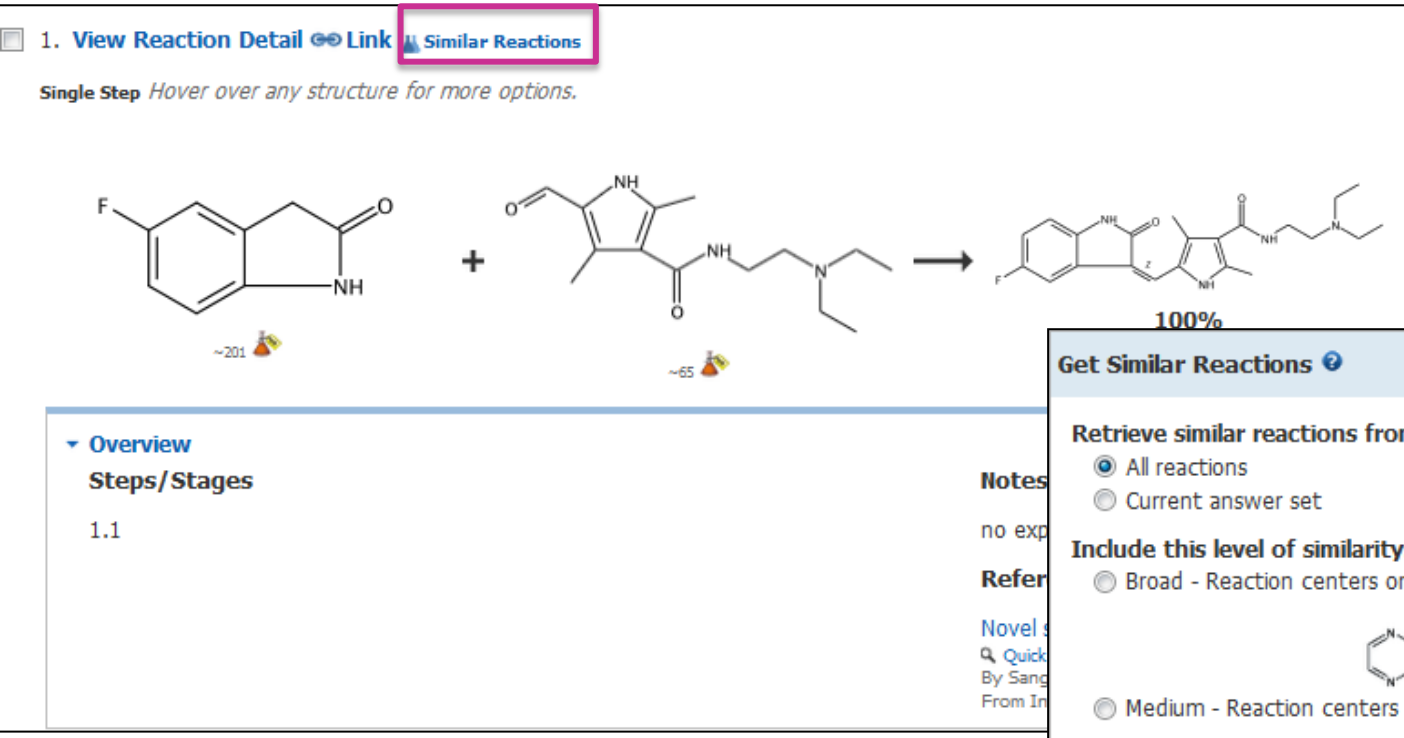
获得相关的反应信息



反应信息太少，通过Similar Reaction获得更多反应信息

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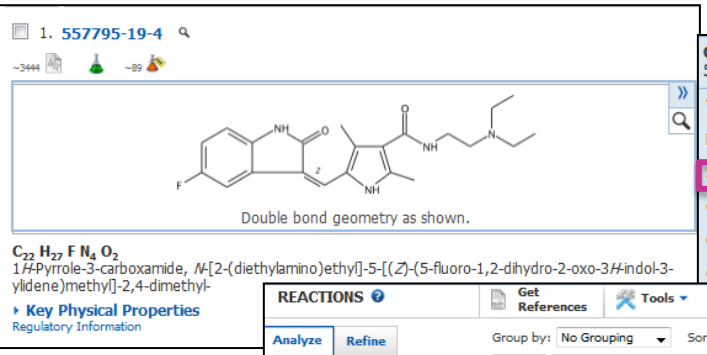
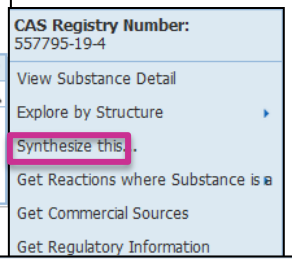
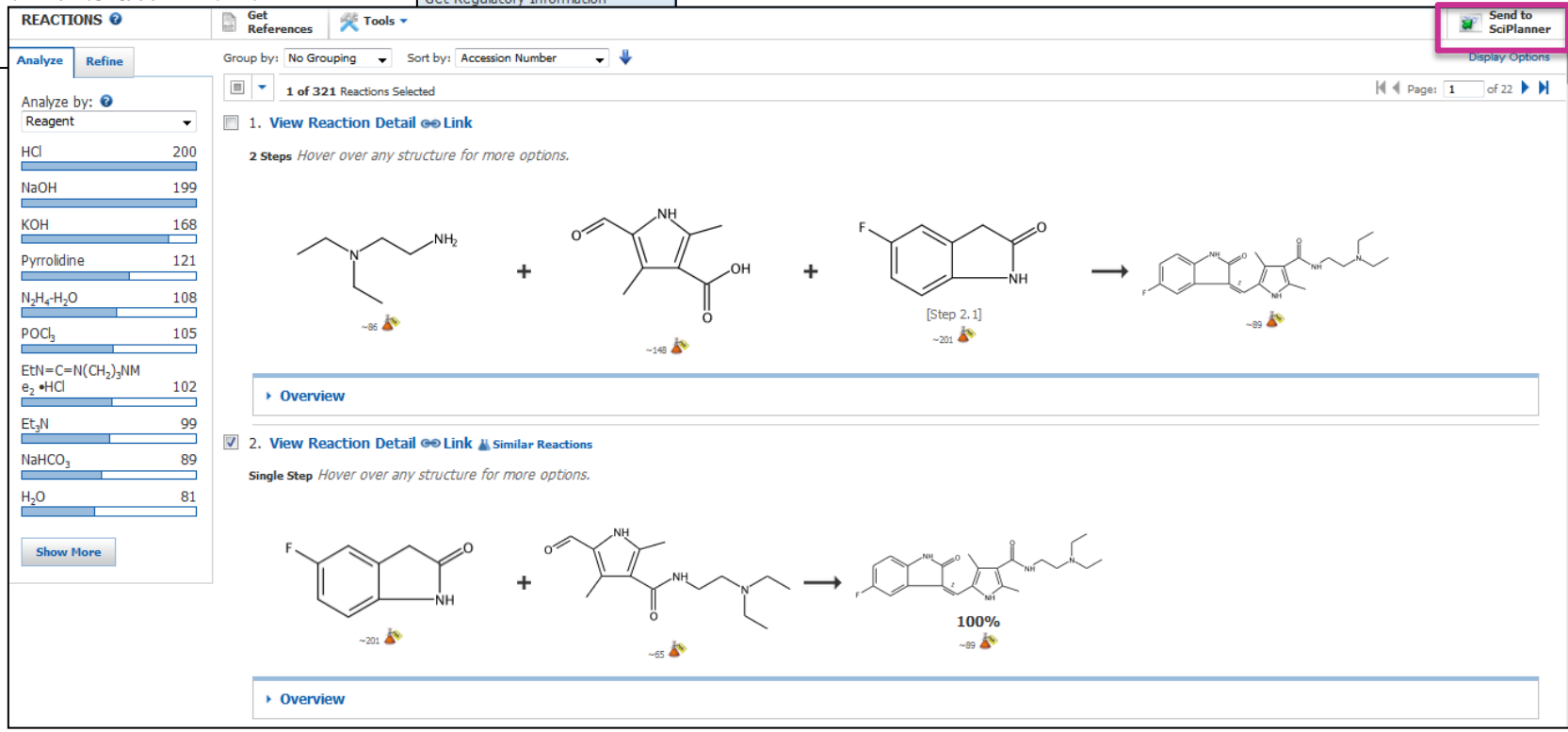
SciPlanner在逆合成反应分析中的应用





通过物质标准菜单获得合成反应



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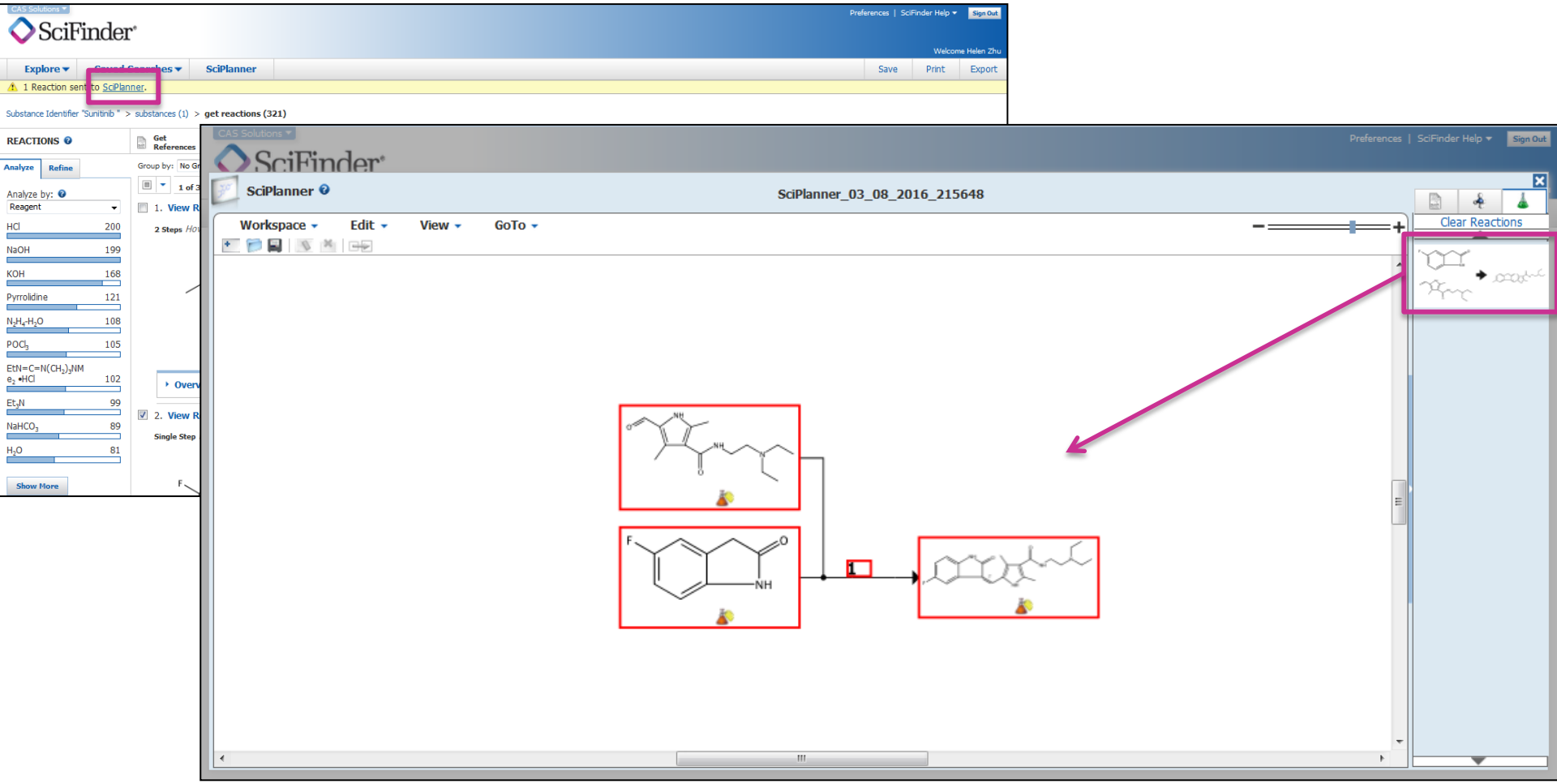
SciPlanner在逆合成反应分析中的应用



点击小图，按住鼠标左键拖入左侧编辑栏

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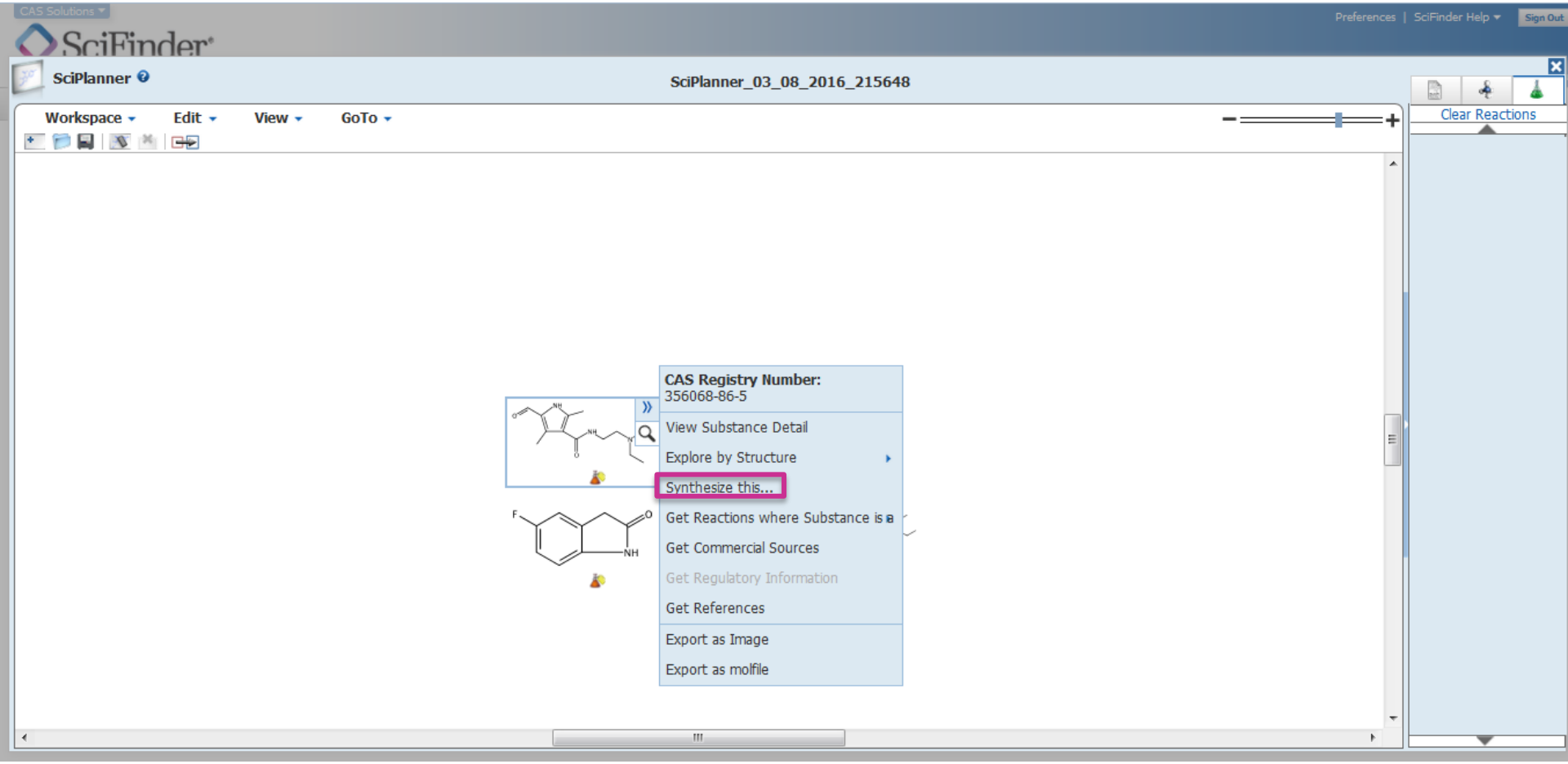
SciPlanner在逆合成反应分析中的应用



通过物质标准菜单获得中间体的合成反应

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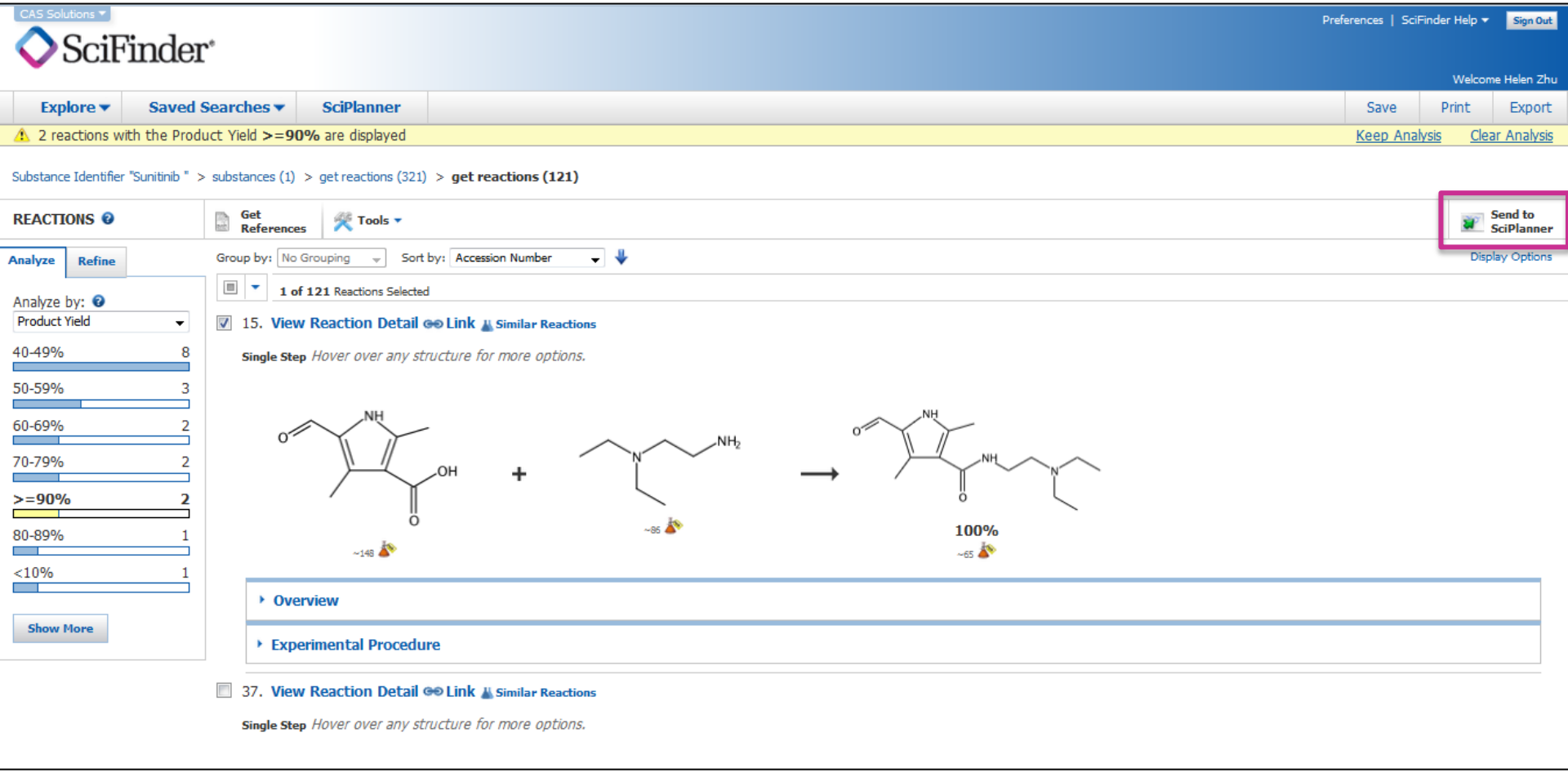

选择合适的反应，发送至SciPlanner

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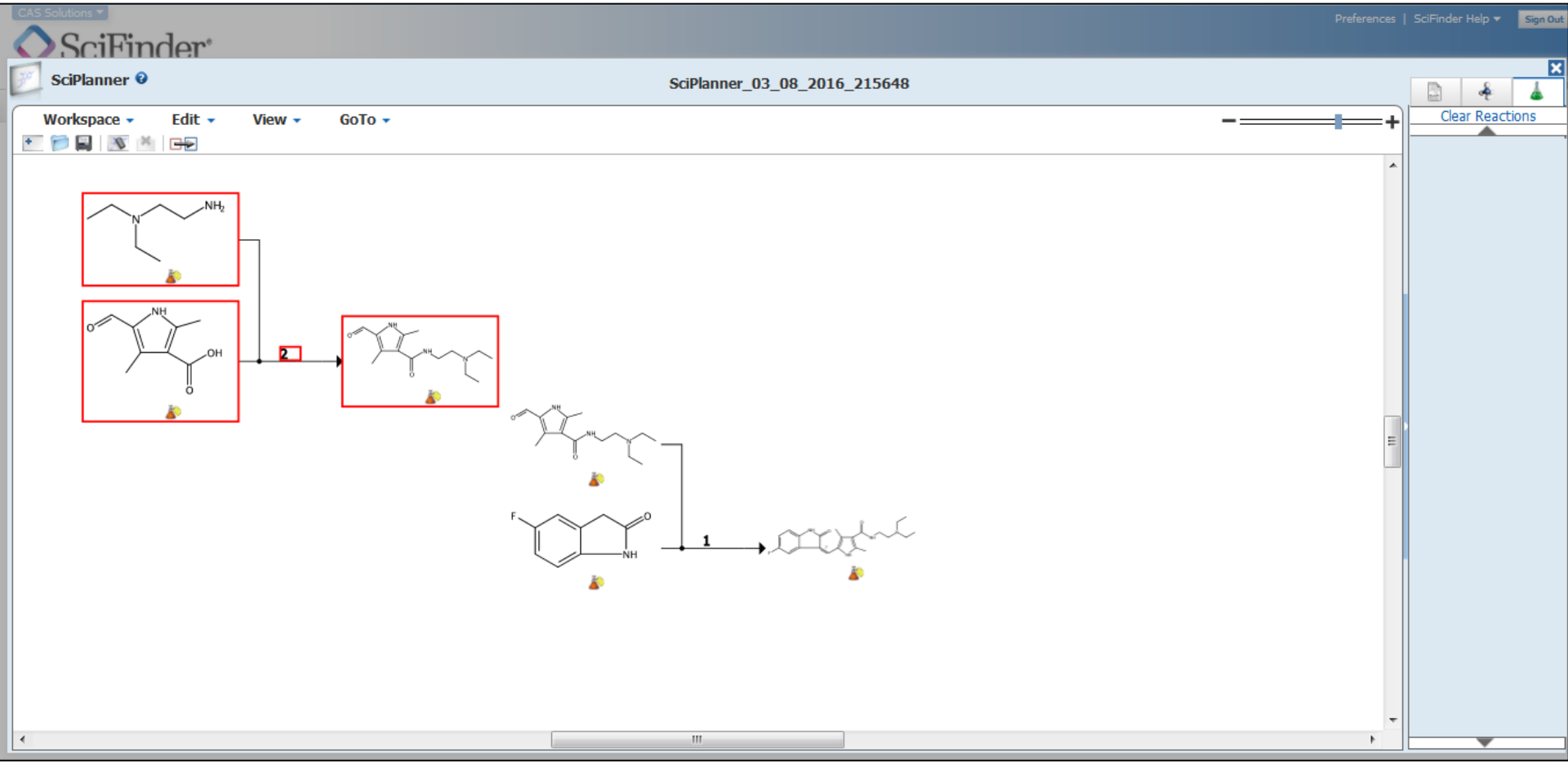
SciPlanner在逆合成反应分析中的应用



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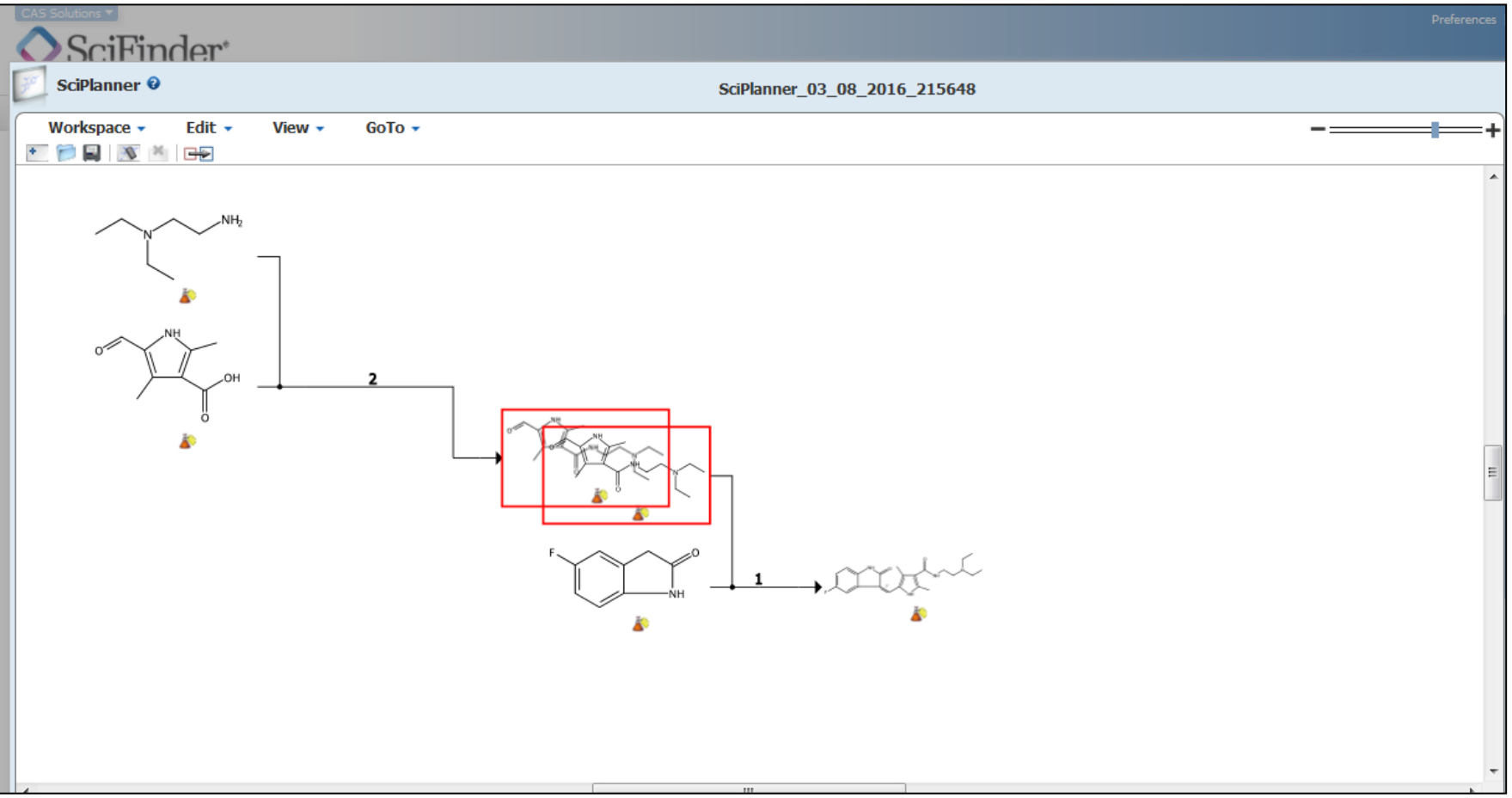
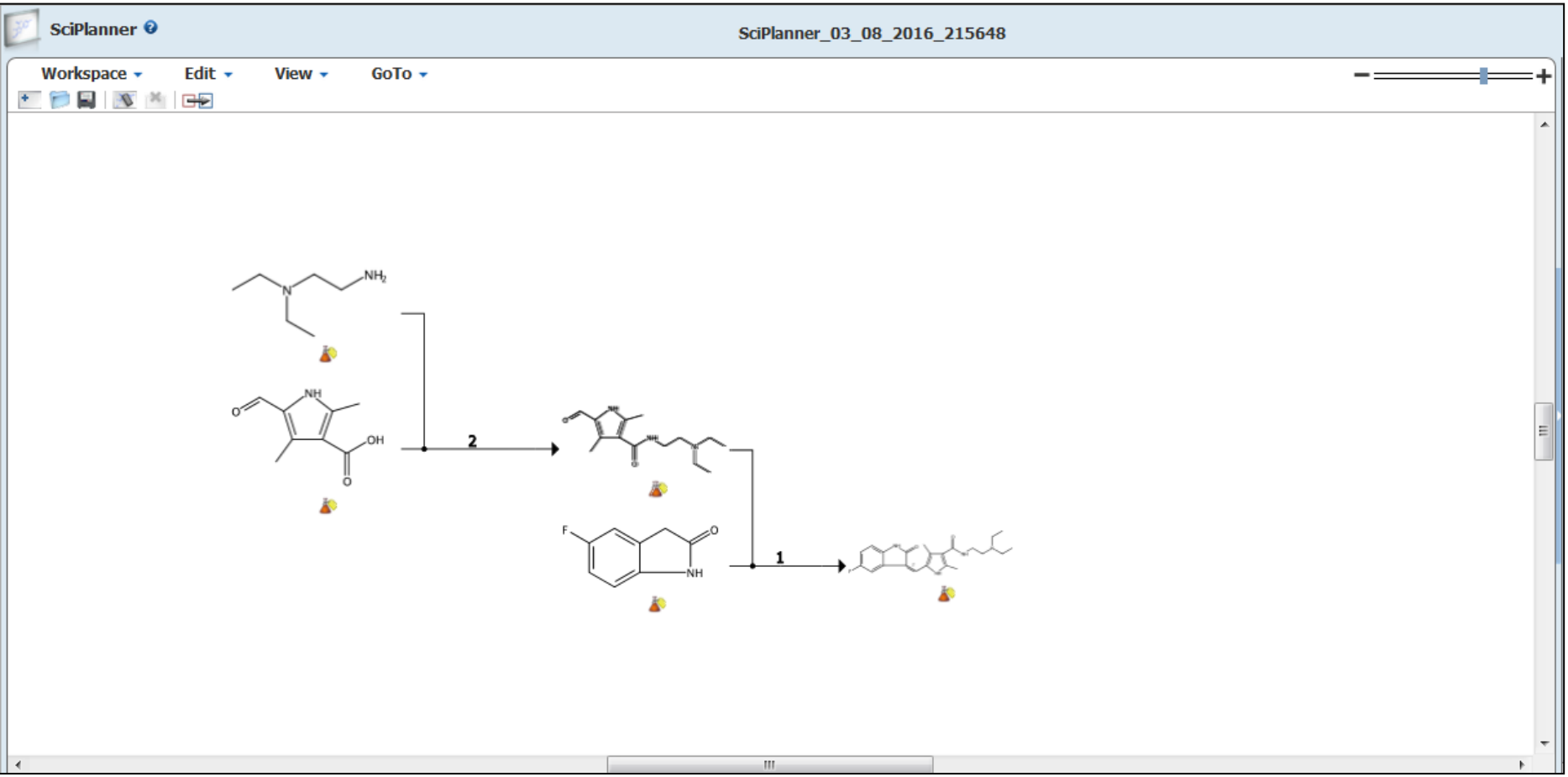
SciPlanner在逆合成反应分析中的应用



拖动相同物质之一直至两个红框重合

SciPlanner在逆合成反应分析中的应用



重复以上步骤直至原料易得

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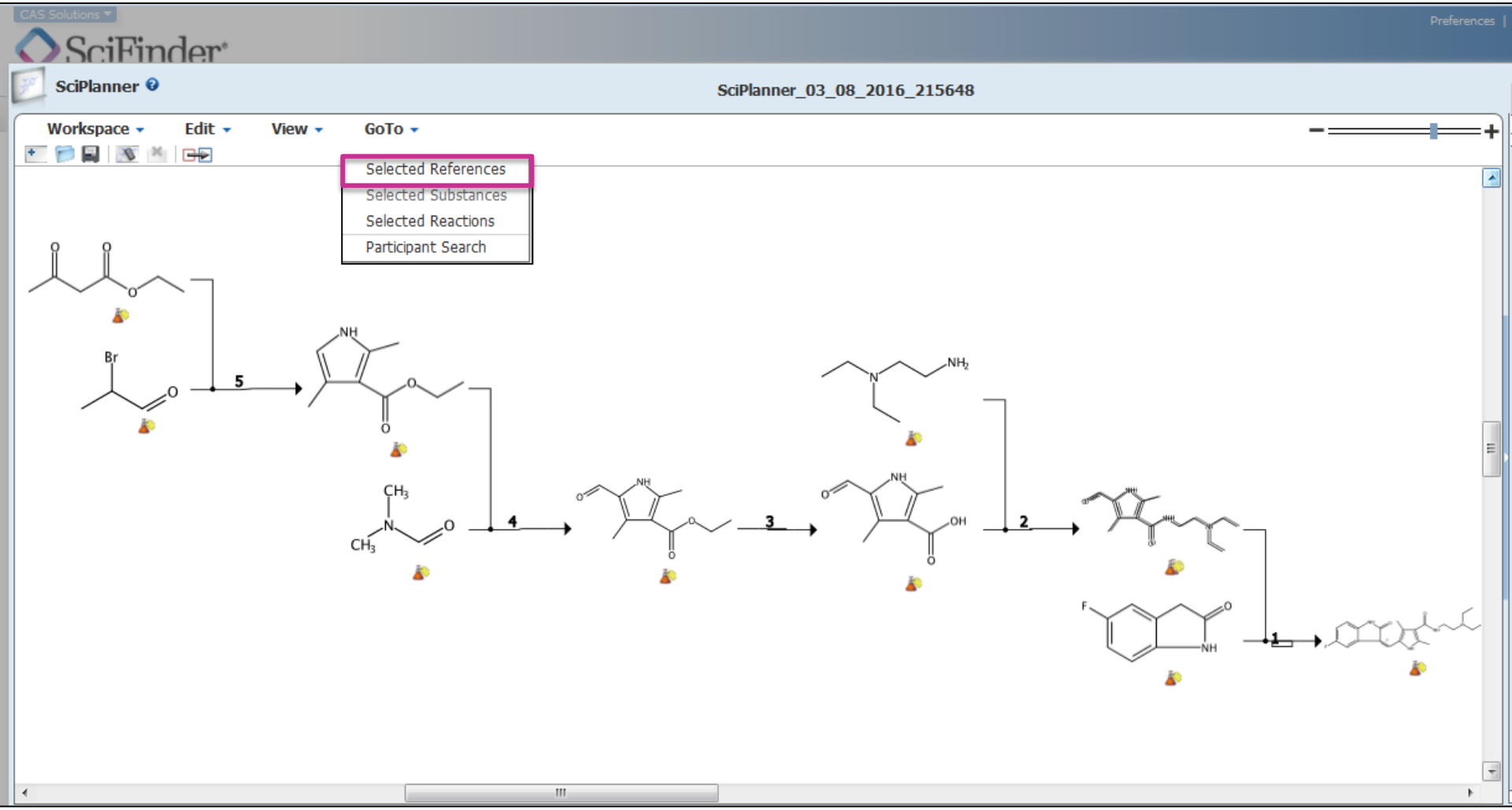

选中相应反应的编号，获得相应的文献

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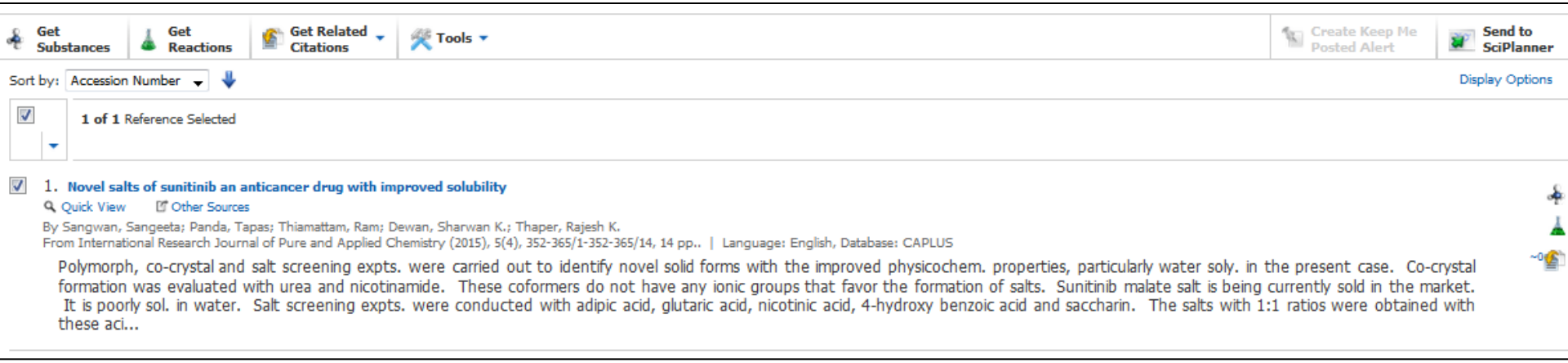

选中相应文献

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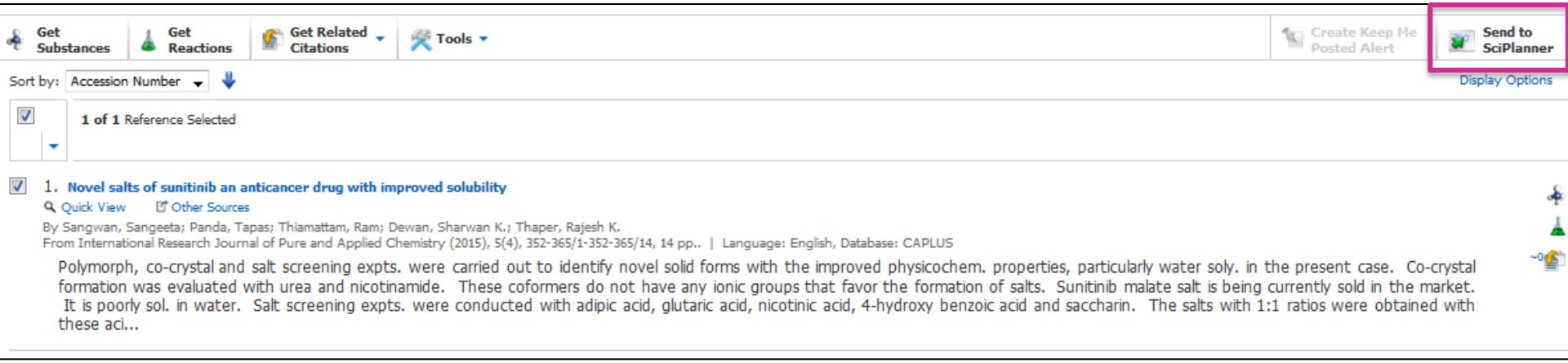

选中相应文献，发送至SciPlanner

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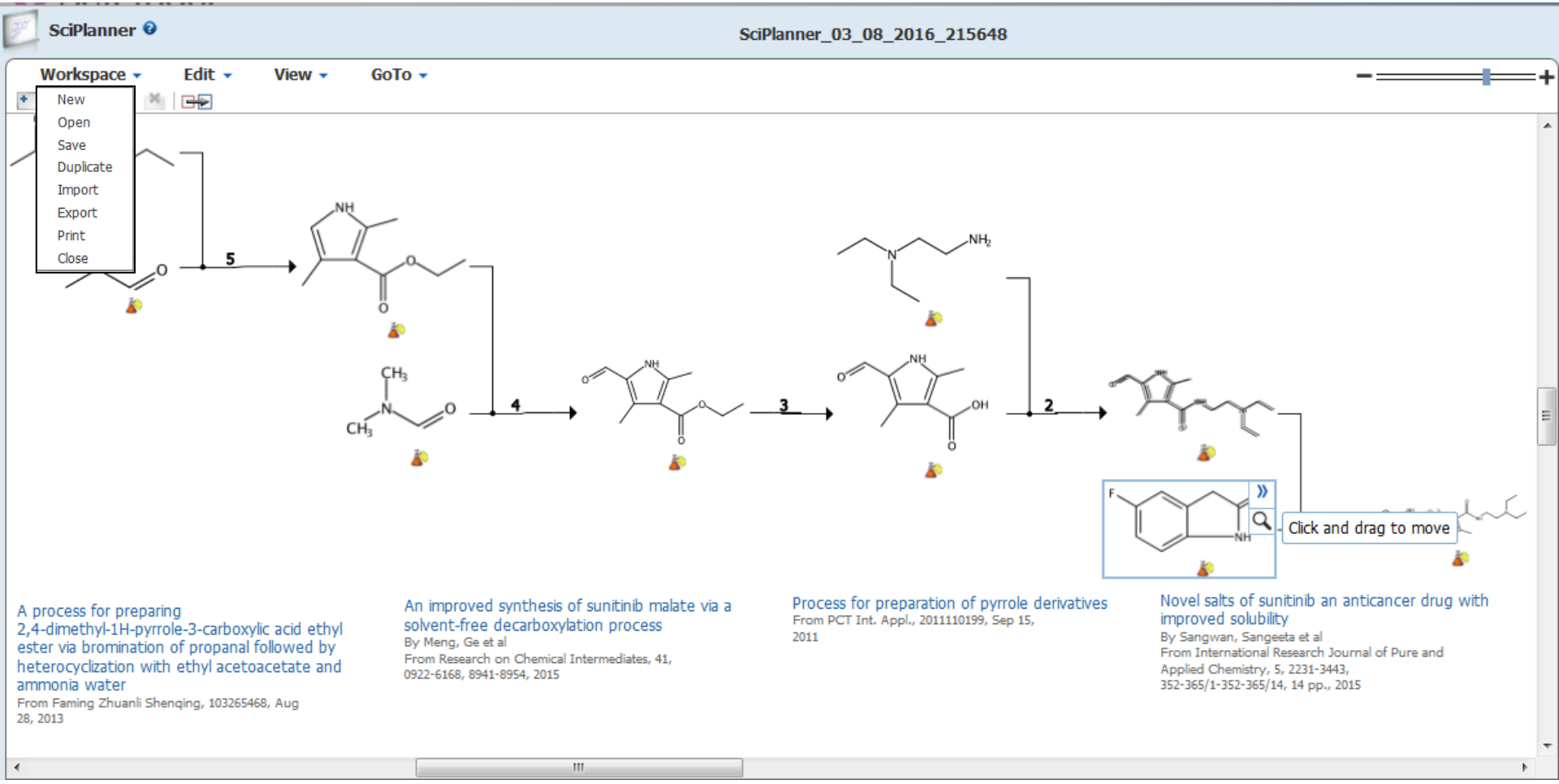
SciPlanner在逆合成反应分析中的应用



同法获得所有需要的文献，列在相应的反应下方

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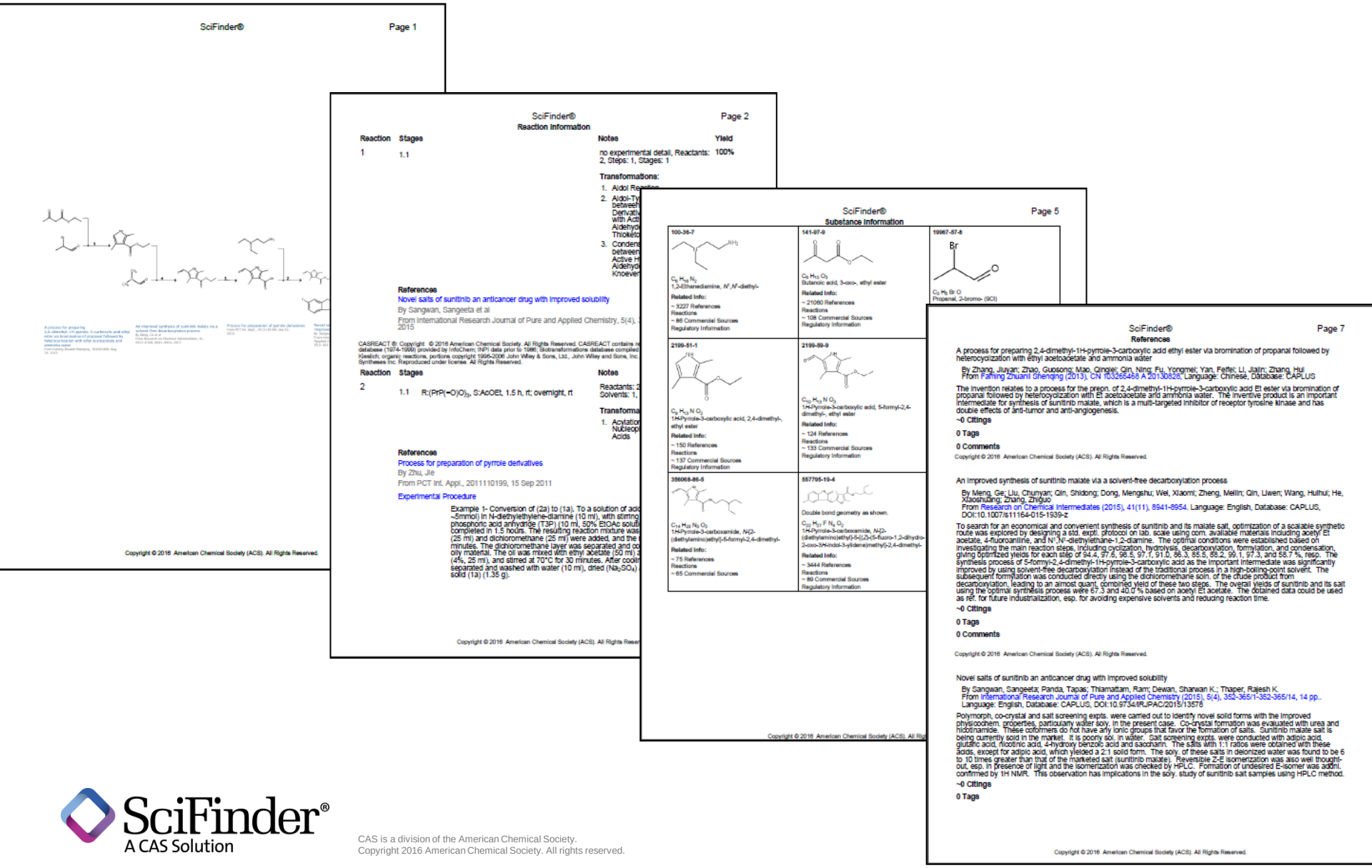
SciPlanner在逆合成反应分析中的应用



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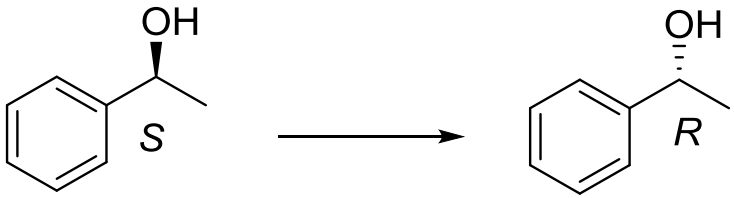
直接检索反应受限的处理

检索如下构型翻转的反应



案例分析

检索要求：

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

定义困难：

如何定义这个环系，杂环？C环？

Cbz和环的连接方法

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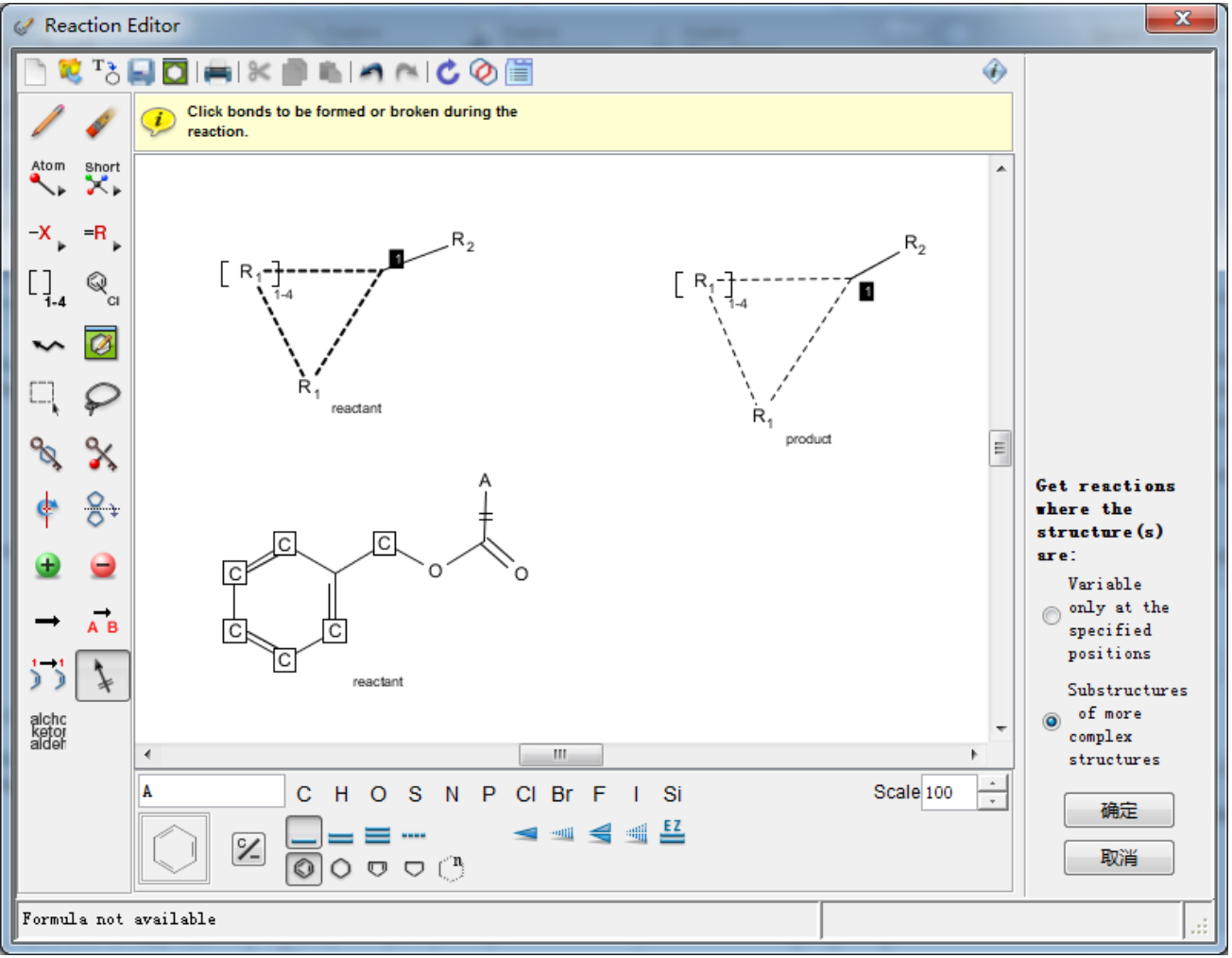
案例分析



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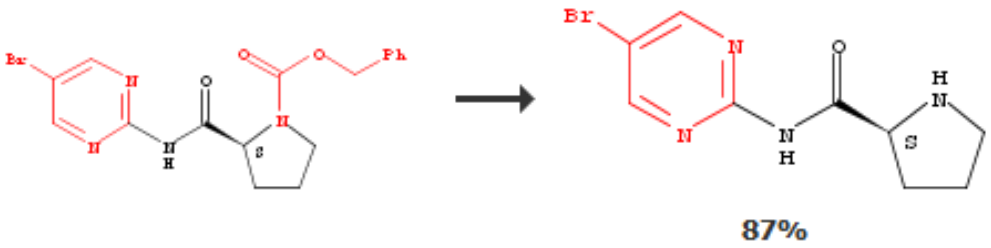
案例分析

32. **1 Hits in this Reference** **Similar Reactions**
Single Step *Hover over any structure for more options.*

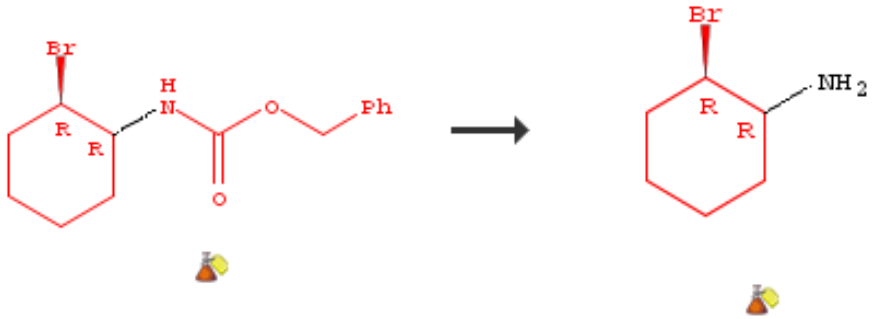


87%

- Overview
- Experimental Procedure

存在我们想要的结果集

33. **1 Hits in this Reference** **Similar Reactions**
Single Step *Hover over any structure for more options.*



- Overview
- Experimental Procedure

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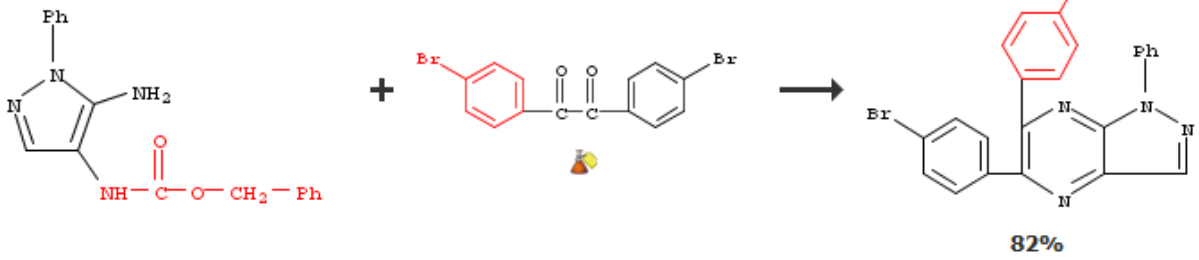
案例分析

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



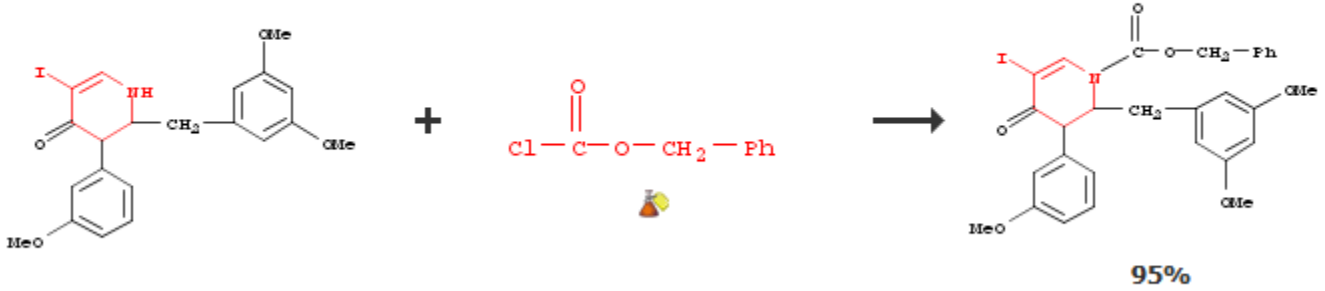
▸ Overview

▸ Experimental Procedure

存在大量的环与Cbz不在一个结构上的反应

如何去除？

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



▸ Overview

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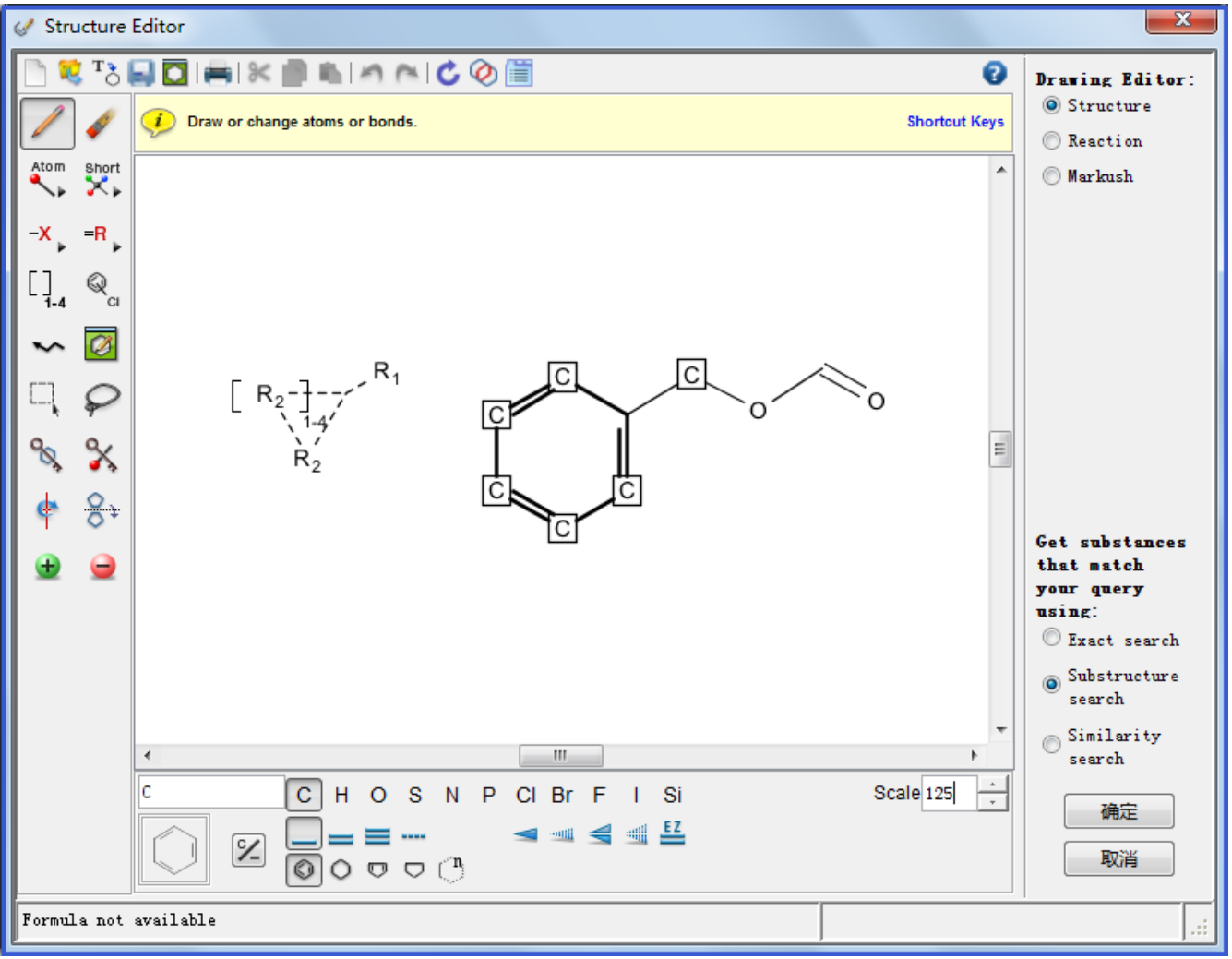
案例分析



这种类型的反应，需要先去检索和反应相关的物质

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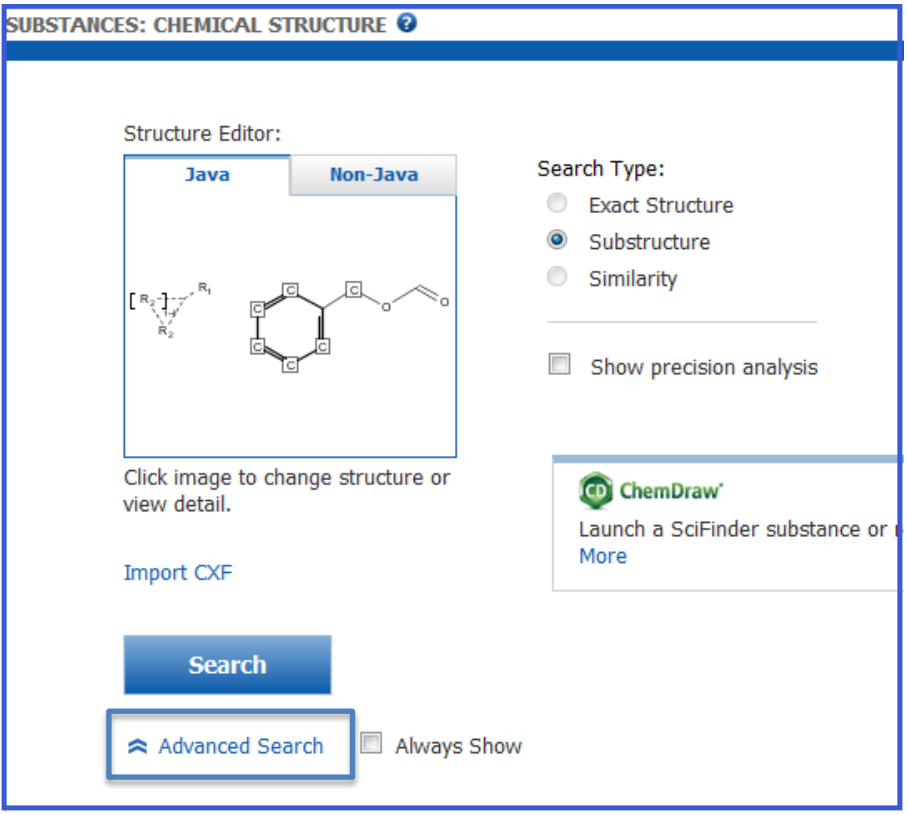
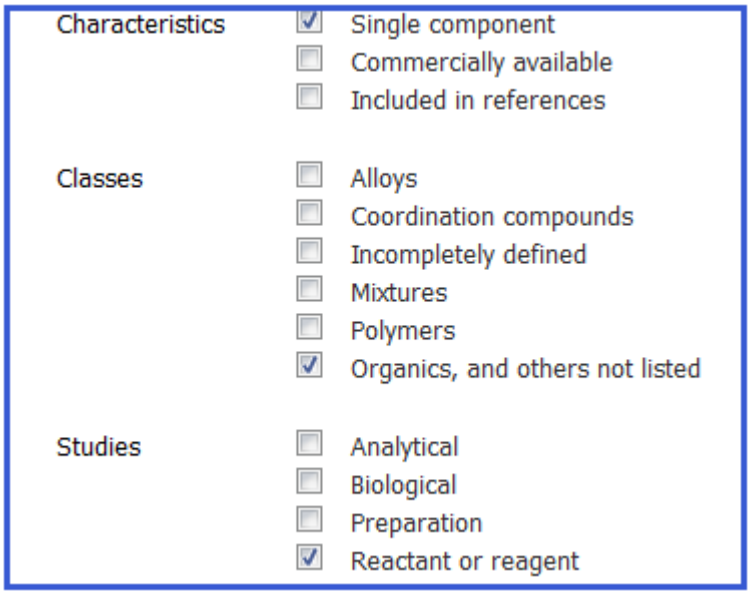
案例分析





需要定义为单一组分和具备反应物或试剂角色的物质

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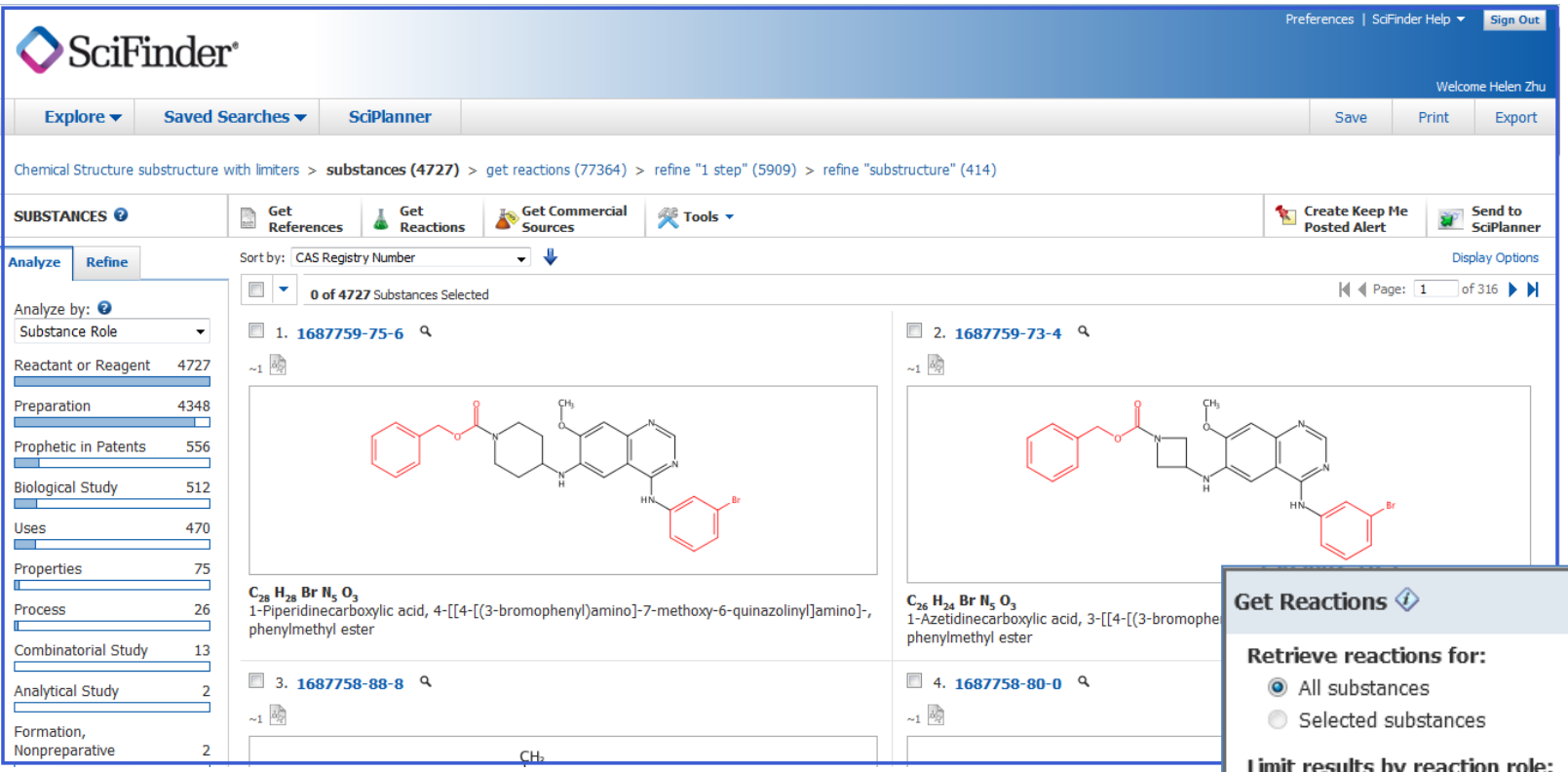
案例分析



获得所有的可能的反应物，并获得这些物质作为反应物的反应

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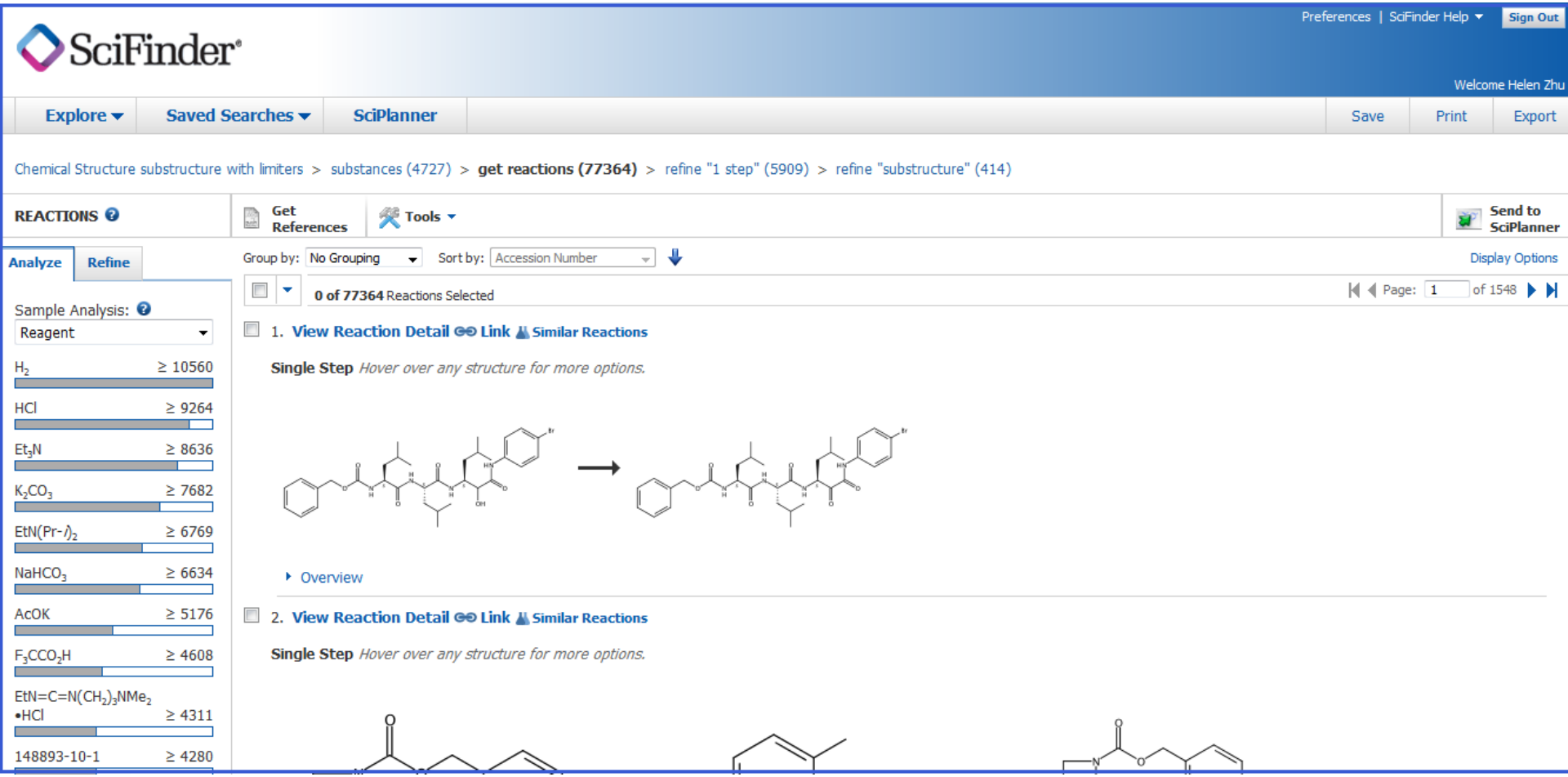
案例分析



这里的反应中的反应物都包含要求的结构，

这时需进一步把产物限定进去。

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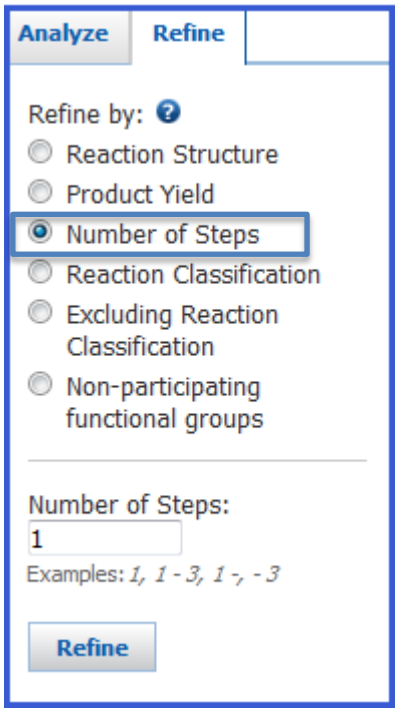
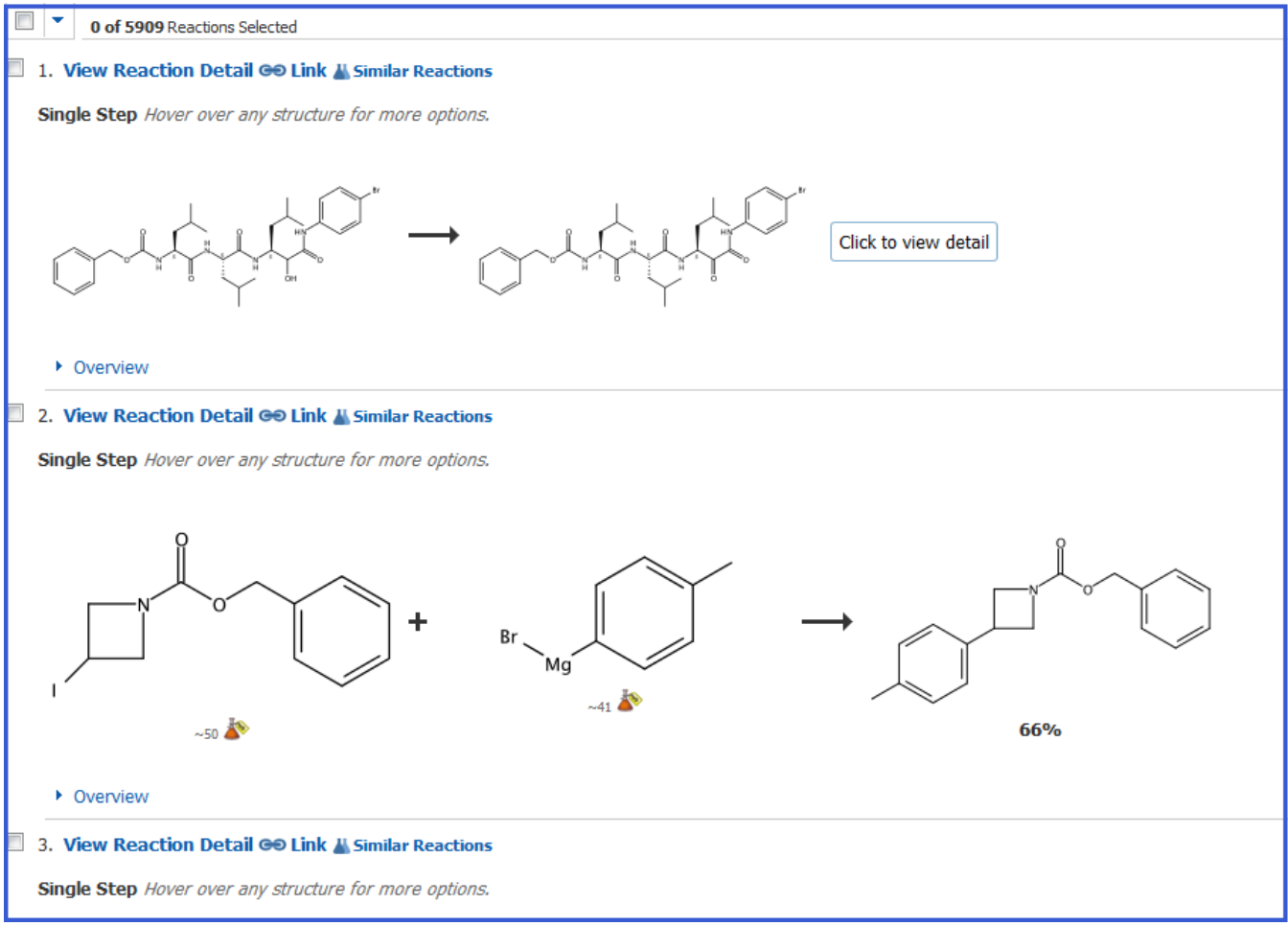
案例分析



先限定反应步数为一步反应



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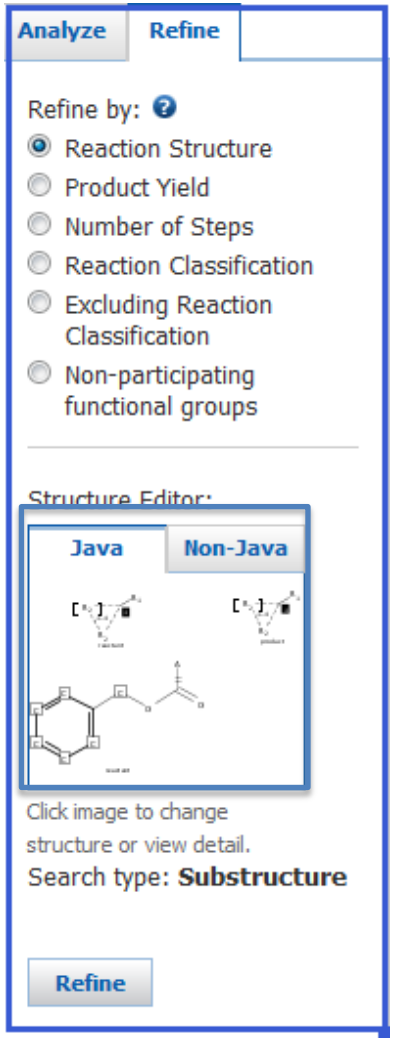
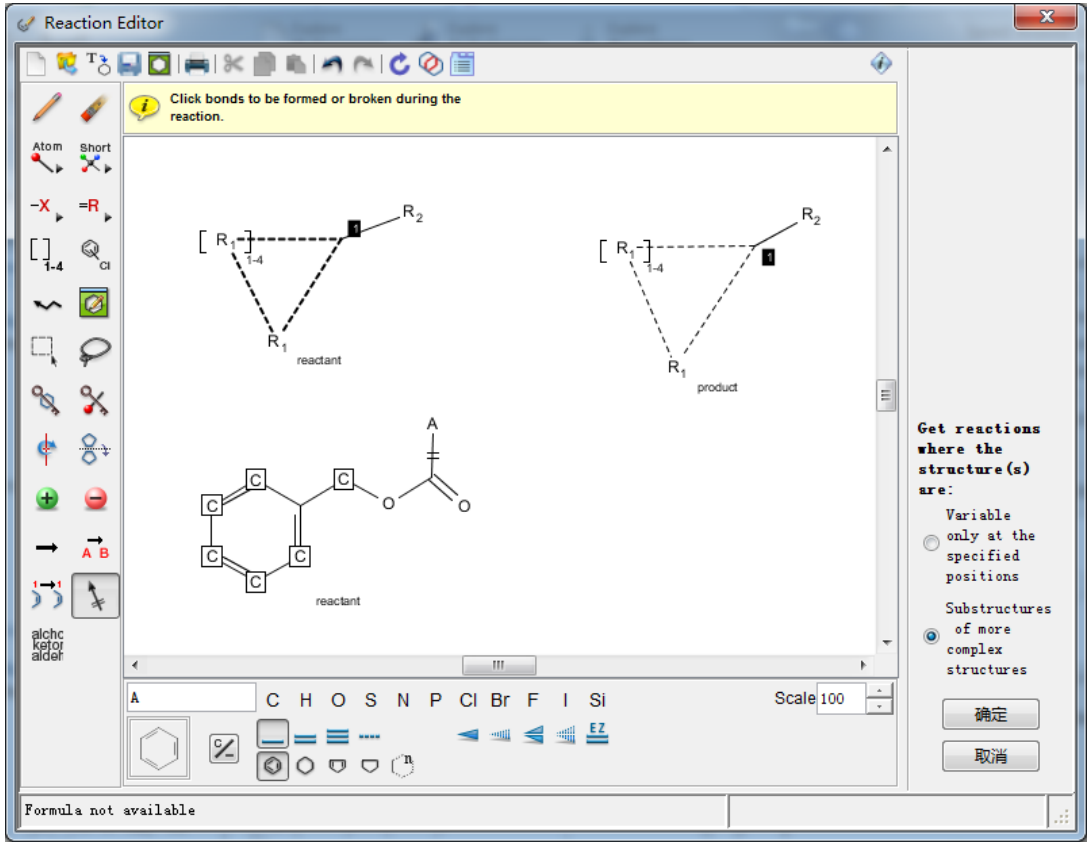
案例分析





再做反应中心限定，沿用之前的定义

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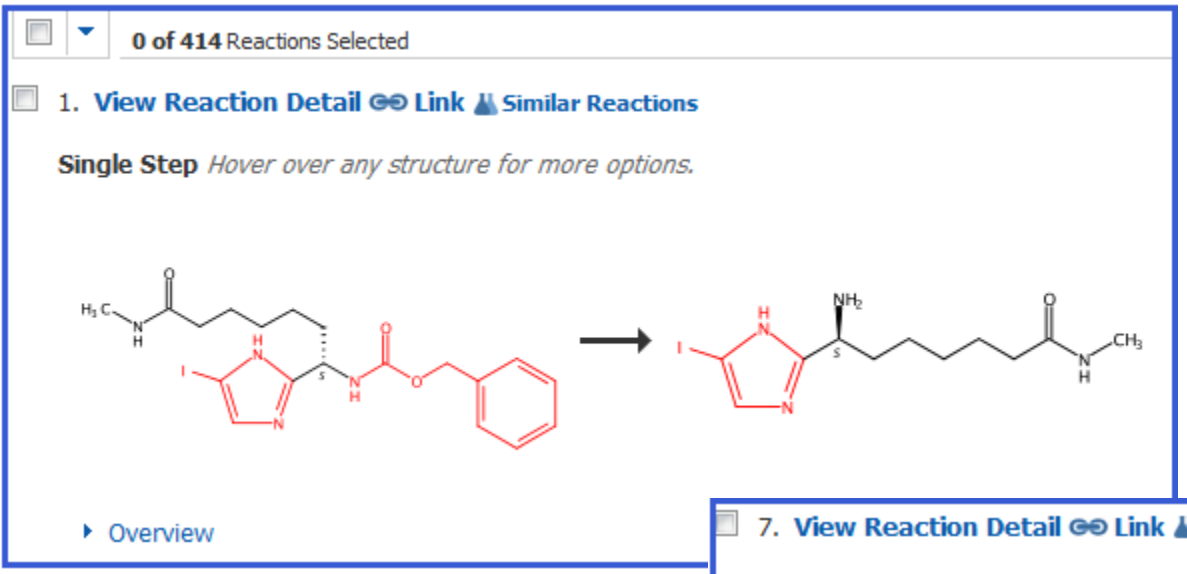
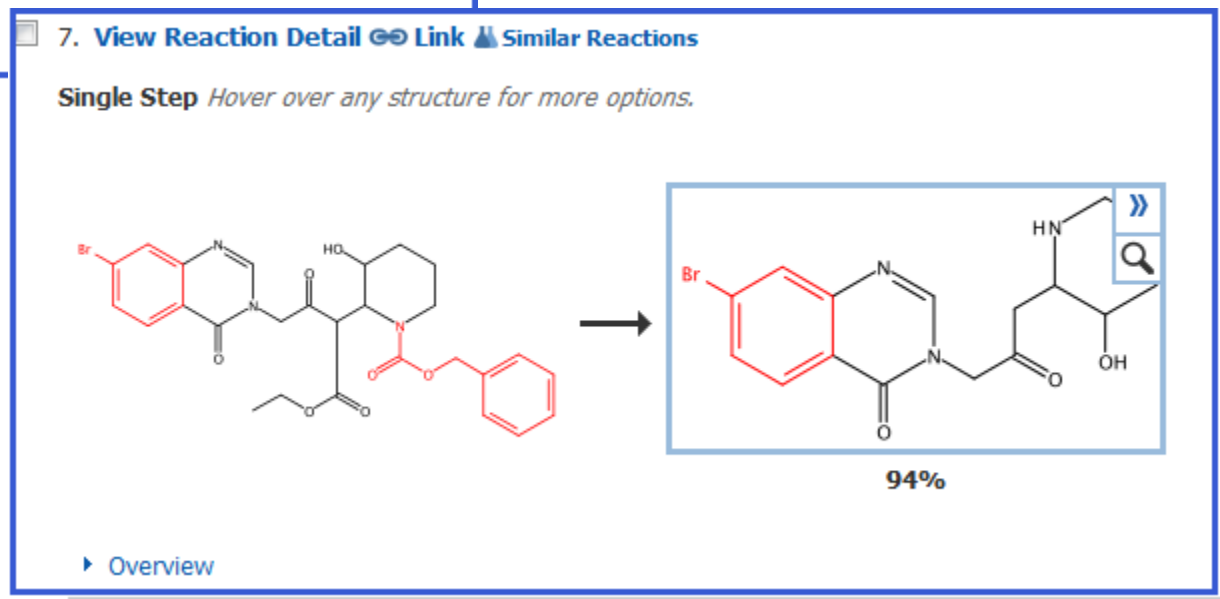
案例分析





都是我们想要的反应结果

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SciFinder中的检索思路

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

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谢 谢！

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