SciFinder Web使用介绍

四川大学图书馆　　胡静
Tel：85402225
Email：hu.jing@scu.edu.cn

内容

1. 概述
2. 检索方式
3. 补充问题

概述

涵盖世界范围98%以上的相关文献（期刊、会议论文、报告、专利等）

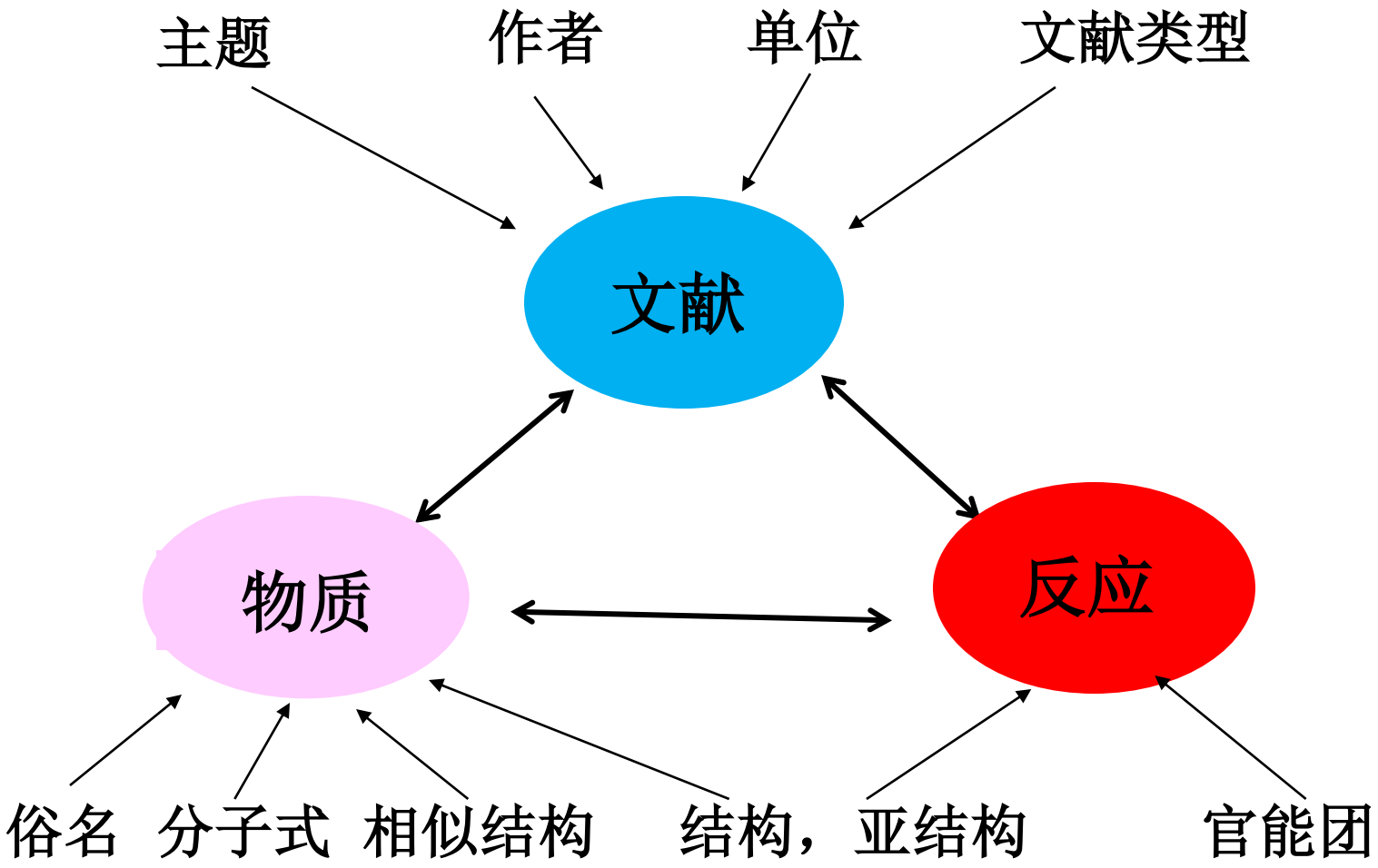
检索方式多样化

为什么推荐！！！

检索技巧简单

强大的分析功能

概述-多样化的检索方式



概述-多样化的检索方式

CAS REGISTRY℠

>6600万有机无机物质

>6300生物序列

每天更新约12000新物质

物质报道文献，回溯到1802年

物质信息包含了大量的实验数据，预测数据，以及物质标签和谱图

CASREACT®

>4170万单步和多步反应

>1400万物质合成制备信息

源自专利和期刊文献

每首更新3-5万条单步多步反应

反应回溯到1840年

CAS Databases

CAplus℠

>3500万专利和期刊信息

>10000种期刊的覆盖

62个专利发行机构

每天更新3000条记录

文献回溯到19世纪初

引文信息回溯到1997年之前，超过3亿条引文信息

MARPART®

>92.7万专利中的有机，有机金属结构

回溯至1961年

每天更新（60-75篇专利引文，以及150-200个Markush结构）

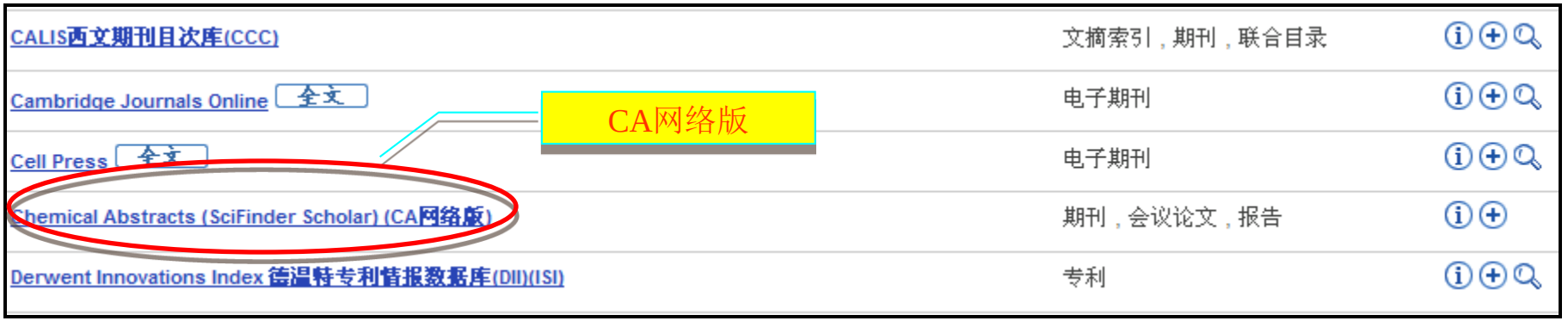
概述-简单的检索技巧

使用介词（如 at、by、in、of 、for、to等 ）或冠词连接检索词，组成短语。

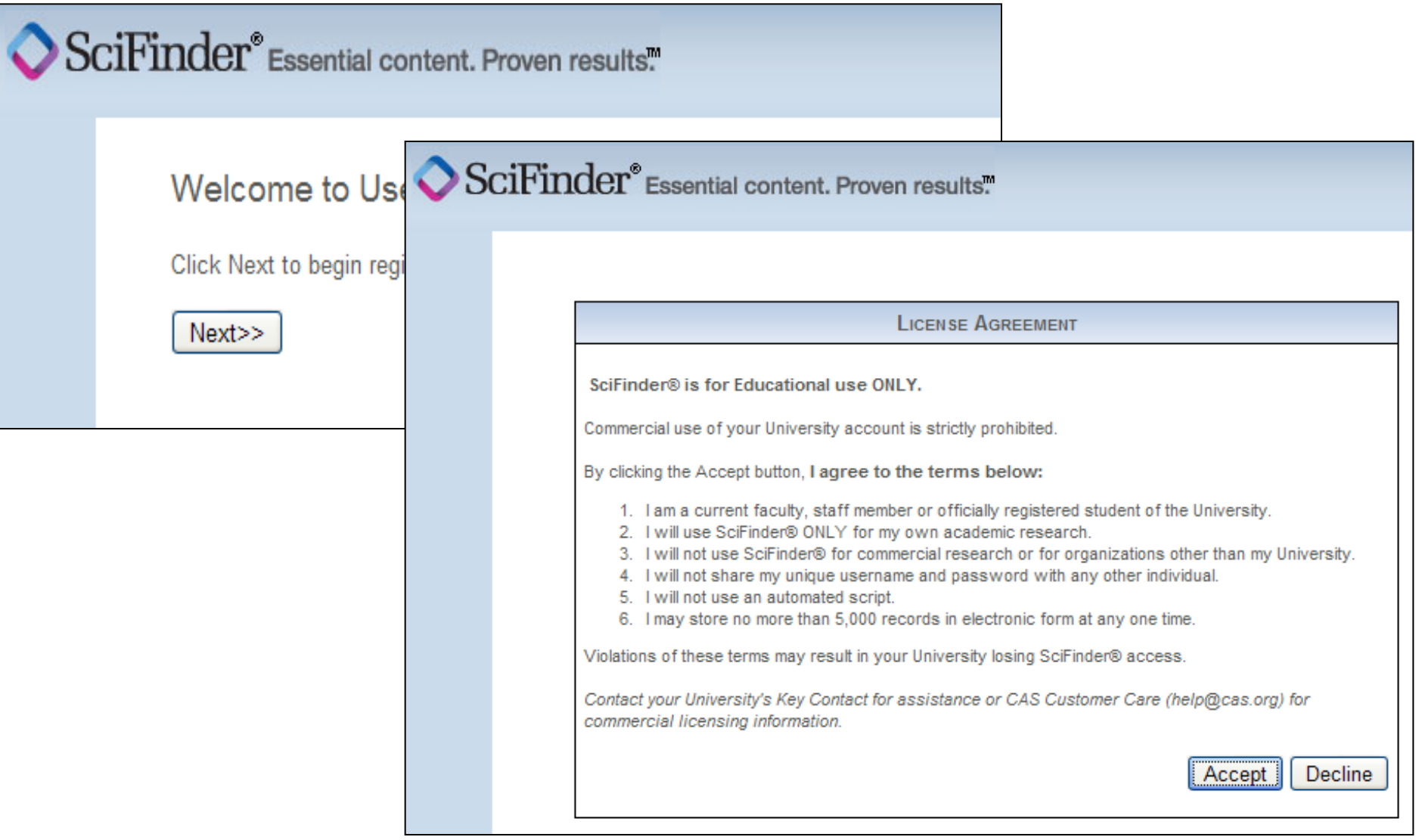
系统能自动识别全名和缩写、名词的单复数、动词的不同时态，自动进行截词处理，不需人工截词。

系统能对输入的检索词自动进行同义词、近义词的扩展检索。

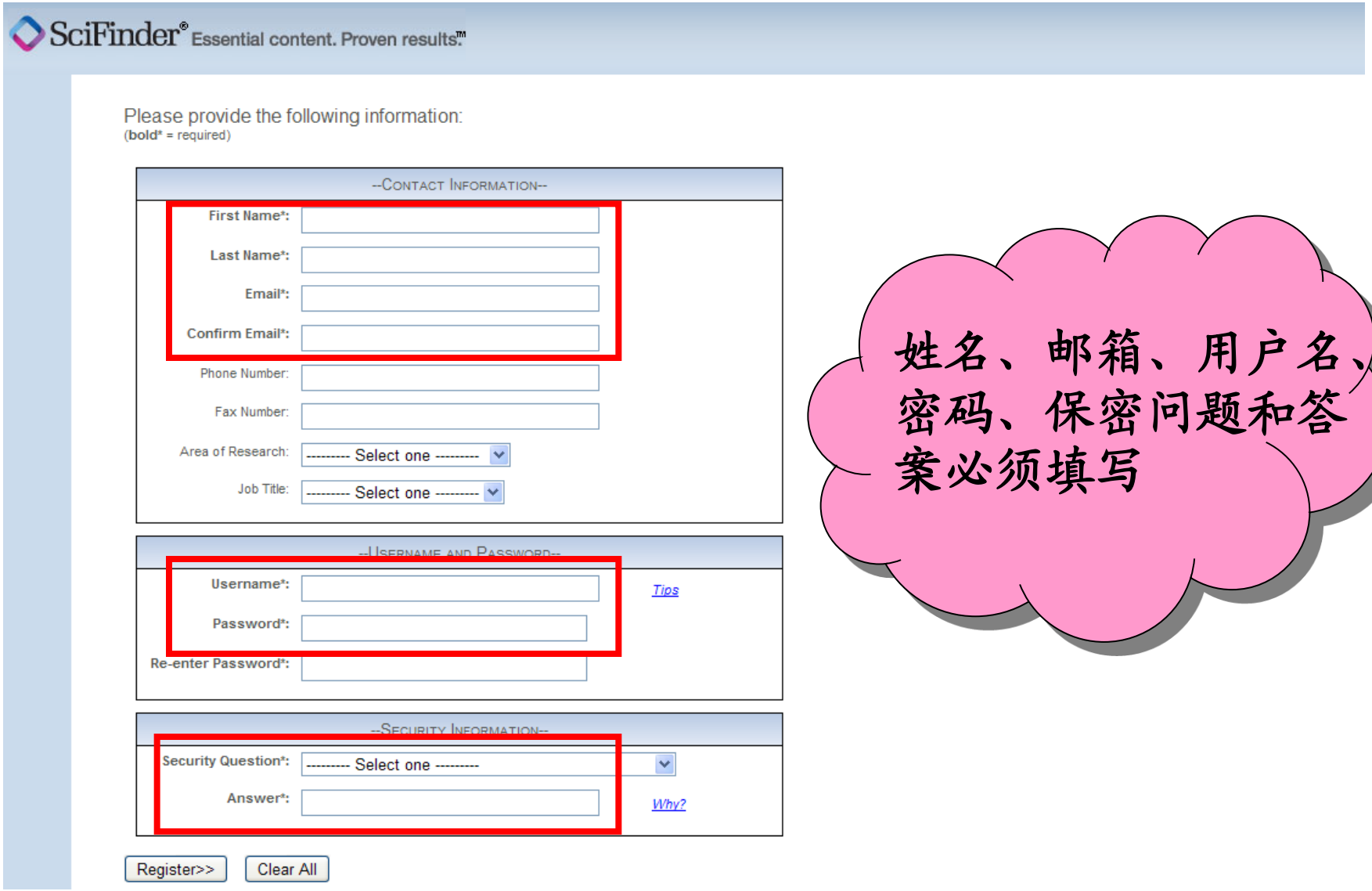
概述-SciFinder的注册和登陆



概述-SciFinder的注册和登陆



每个用户必须输入各自信息



姓名、邮箱、用户名、密码、保密问题和答案必须填写

设置用户名及密码注意事项

用户名：必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- -（破折号）
- _（下划线）
- .（句点）
- @（表示“at”的符号）

密码：必须包含 7-15 个字符，并且至少包含三个以下字符：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

对新ID的Email确认

SciFinder® ...Part of the process™

Almost Finished

Thank you for completing the initial step in registering to use SciFinder®!

You will receive an e-mail message from CAS that includes a link and instructions for completing the registration process. ***You must click the link within 48 hours***. If not, you will need to begin the registration process again.

From: CAS

Dear user,

To complete your SciFinder registration, you must click the link provided below. By clicking the link, you agree to all of the following terms and conditions:

- I will not share my username and password with any other person.
- I will search only for myself and not for others or other organizations.
- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
- I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.
- My organization's SciFinder License and the CAS Information Use Policies (http://www.cas.org/legal/infopolicy.html) apply to my use of SciFinder.
- I will contact my SciFinder Key Contact if I have questions.

If you do not accept these terms and conditions, do not click the link and delete this e-mail message.

https://scifinder.cas.org/registration/completeRegistration.html?regKey=B8CB6727-86F3-F014-11E6-D312D80AC094

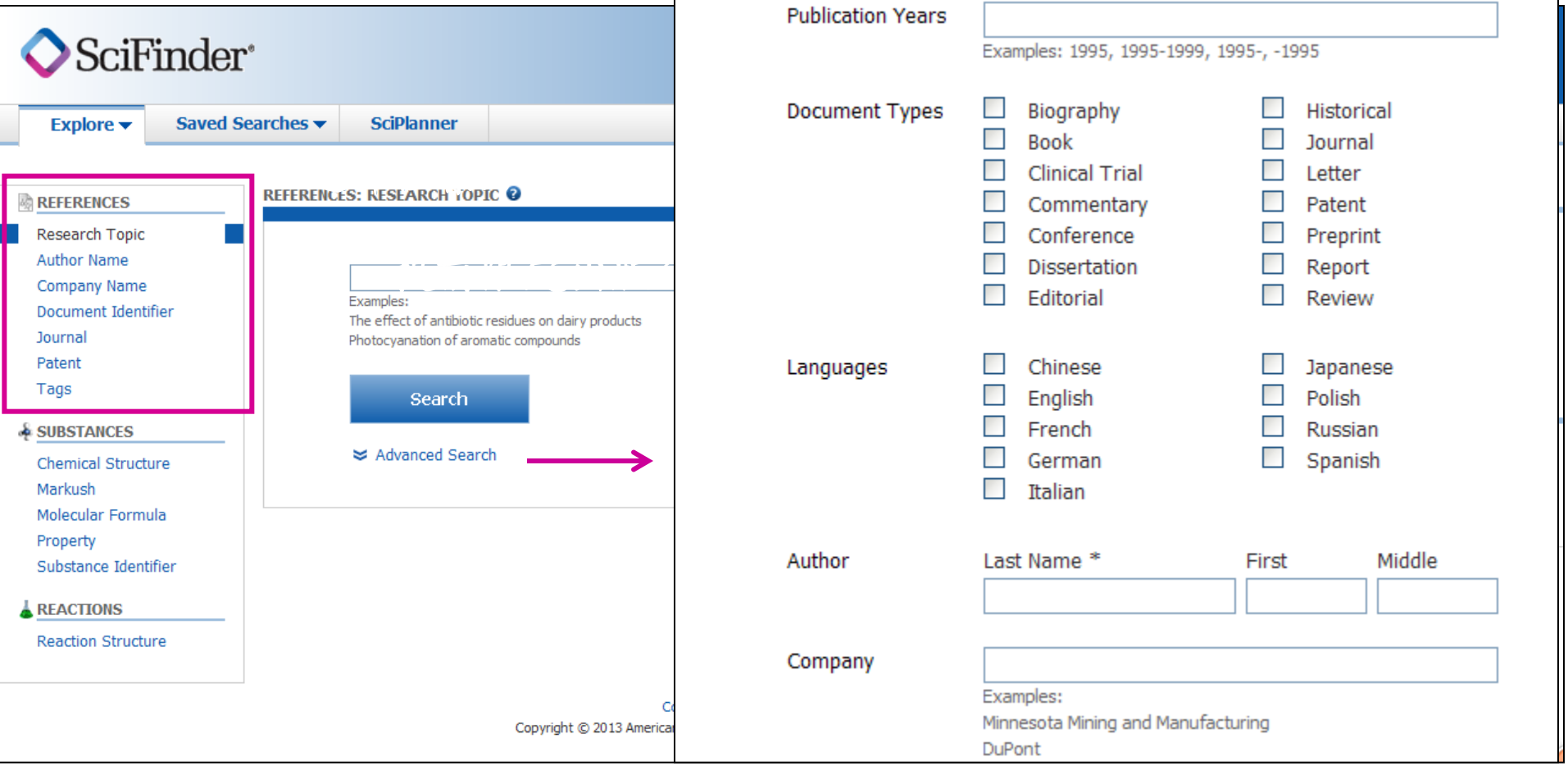
This link is valid for only one use and will expire within 48 hours.

If you need assistance at any time, consult the key contact at your organization.

48小时内打开并阅读 CAS 的电子邮件激活链接

检索方式

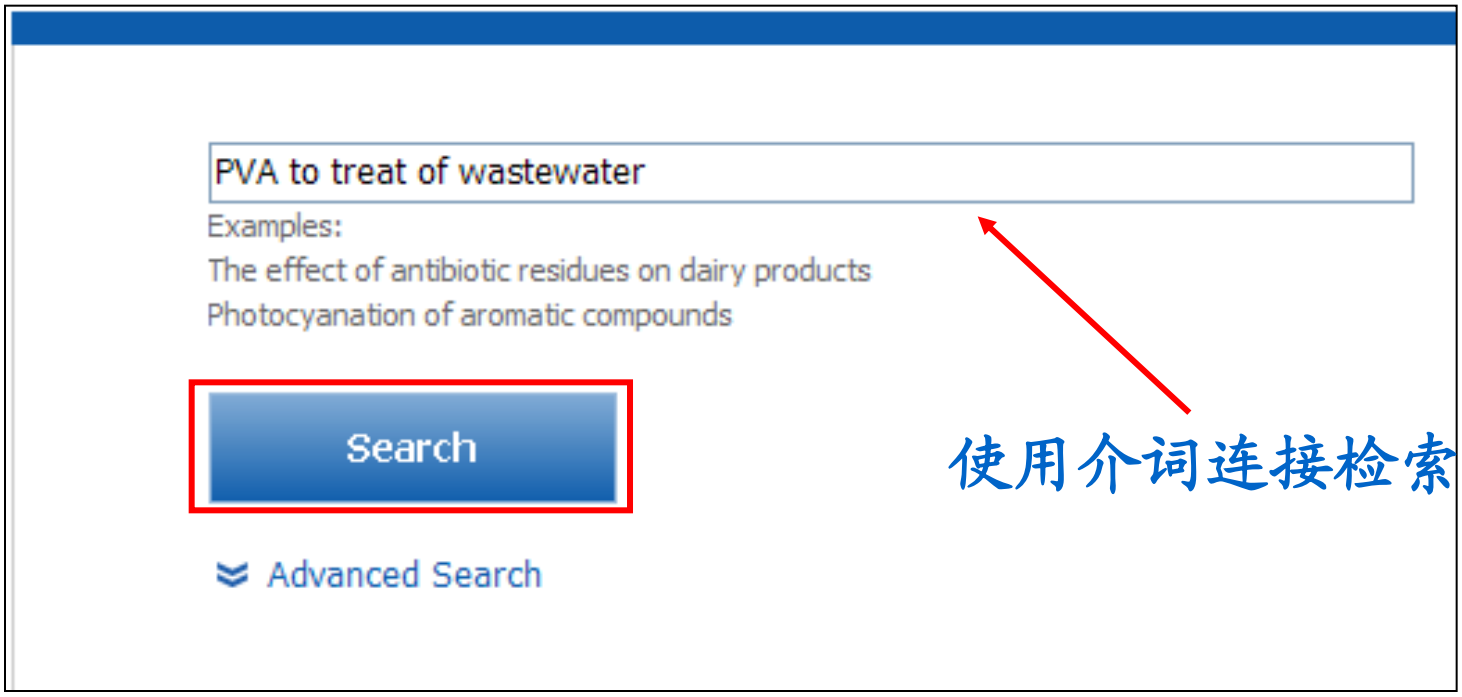
文献　　物质　　反应


SciFinder
Explore
Saved Searches
SciPlanner
REFERENCES
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier
REACTIONS
Reaction Structure
REFERENCES: RESEARCH TOPIC
Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Search
Advanced Search
Copyright © 2013 America
Publication Years
Examples: 1995, 1995-1999, 1995-, -1995
Document Types
Biography
Book
Clinical Trial
Commentary
Conference
Dissertation
Editorial
Historical
Journal
Letter
Patent
Preprint
Report
Review
Languages
Chinese
English
French
German
Italian
Japanese
Polish
Russian
Spanish
Author
Last Name *
First
Middle
Company
Examples:
Minnesota Mining and Manufacturing
DuPont

检索实例：

搜索主题：印染废水中聚乙烯醇的处理技术

关键词：	聚乙烯醇	PVA
	处理	treat
	废水	wastewater


PVA to treat of wastewater
Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Search
Advanced Search
使用介词连接检索

Select All Deselect All

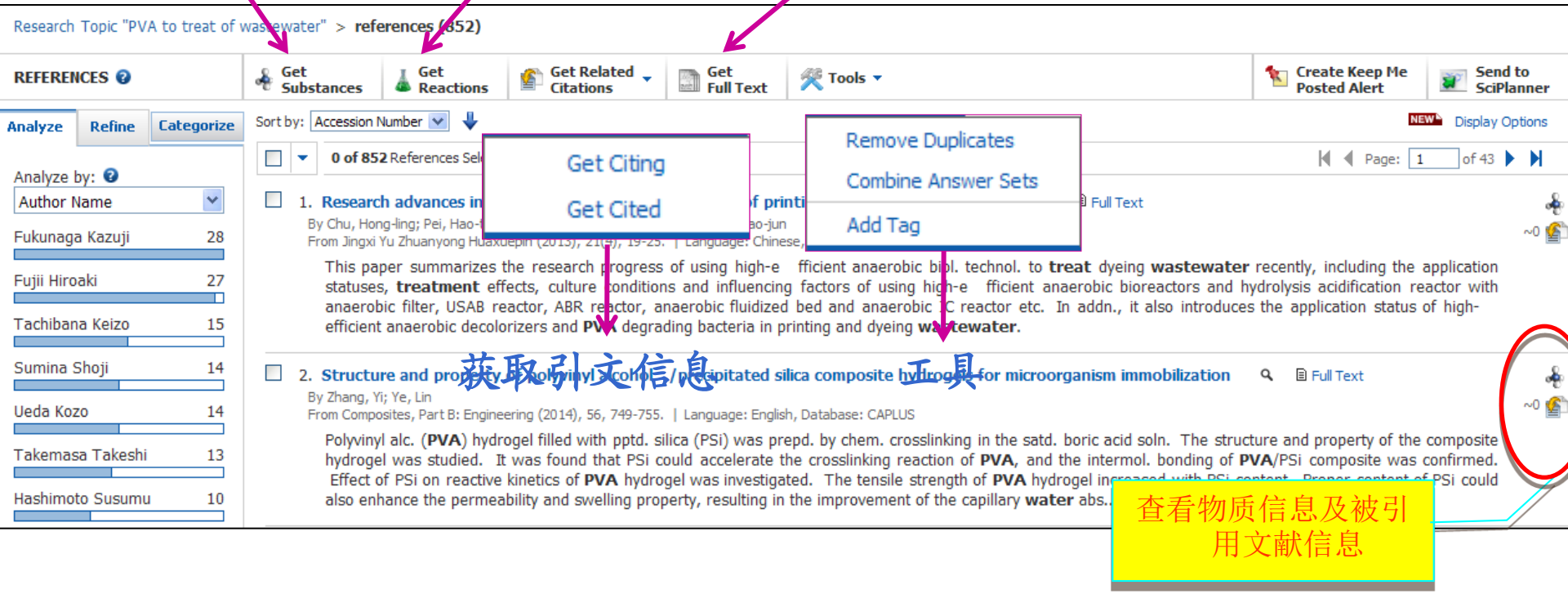
1 of 12 Research Topic Candidates Selected

- [ ] 1 reference was found containing **"PVA to treat of wastewater"** as entered.
- [x] 852 references were found containing all of the concepts **"PVA"**, **"treat"** and **"wastewater"** closely associated with one another
- [ ] 2493 references were found where all of the concepts **"PVA"**, **"treat"** and **"wastewater"** were present anywhere in the reference.
- [ ] 7427 references were found containing the two concepts **"PVA"** and **"treat"** closely associated with one another.
- [ ] 25379 references were found where the two concepts **"PVA"** and **"treat"** were present anywhere in the reference.
- [ ] 1438 references were found containing the two concepts **"PVA"** and **"wastewater"** closely associated with one another.
- [ ] 2843 references were found where the two concepts **"PVA"** and **"wastewater"** were present anywhere in the reference.
- [ ] 394252 references were found containing the two concepts **"treat"** and **"wastewater"** closely associated with one another.
- [ ] 408749 references were found where the two concepts **"treat"** and **"wastewater"** were present anywhere in the reference.
- [ ] 157404 references were found containing the concept **"PVA"**.
- [ ] 9077577 references were found containing the concept **"treat"**.
- [ ] 490642 references were found containing the concept **"wastewater"**.

Get References

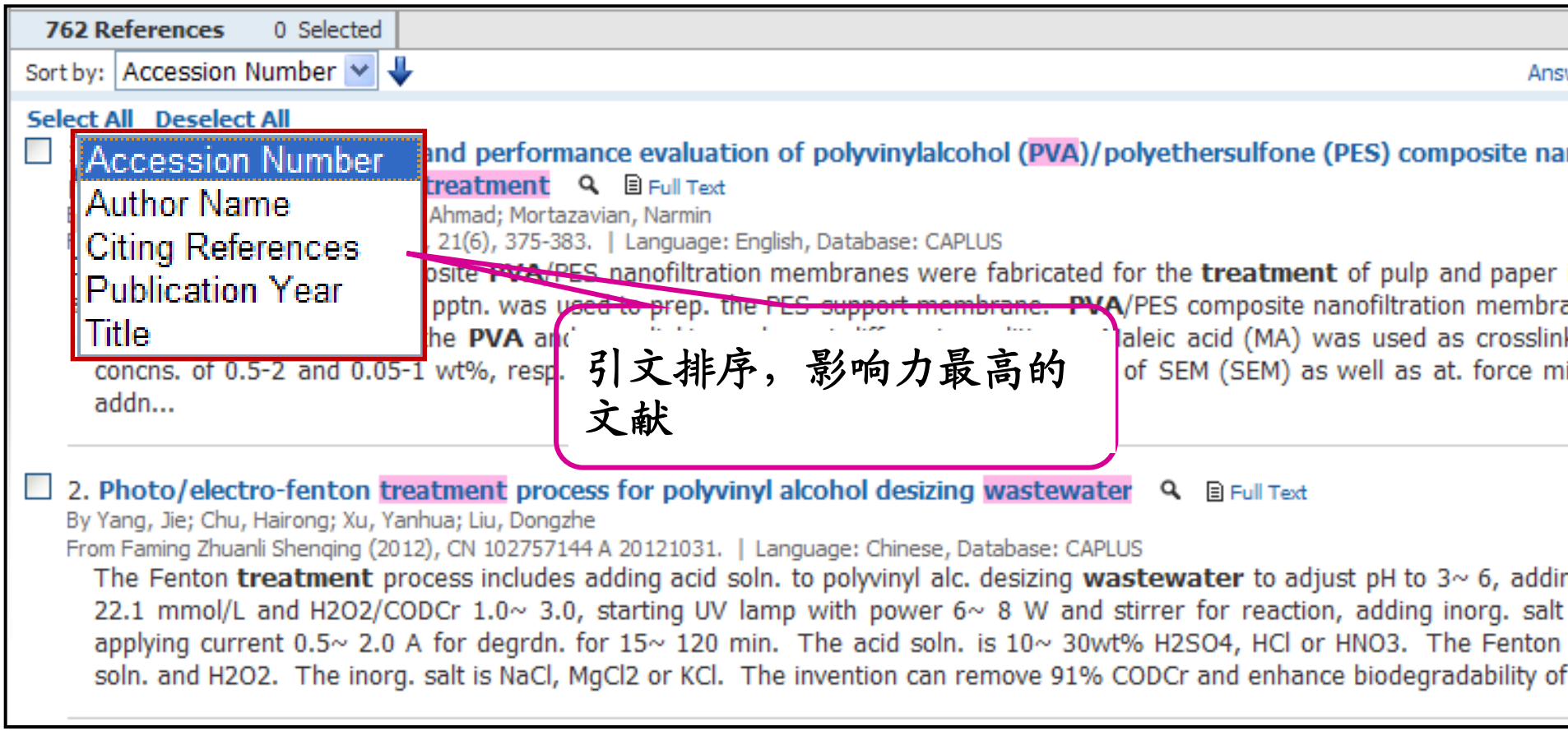
1. “concept”表示：SciFinder 检索系统自动把检索词的名词单复数、英美文法上的差异、该词的动词、形容词、副词、名词形式等进行扩展。
2. “closely associated with one another”表示检索词同时出现在一句话中。
3. “present anywhere in the reference”表示检索词同时出现在一段话当中。

获取物质信息　　获取结构信息　　获取全文



获取引文信息　　工具

查看物质信息及被引用文献信息


762 References
0 Selected
Sort by:
Accession Number
Select All
Deselect All
Accession Number
Author Name
Citing References
Publication Year
Title
and performance evaluation of polyvinylalcohol (PVA)/polyethersulfone (PES) composite na
treatment
Full Text
Ahmad; Mortazavian, Narmin
21(6), 375-383. | Language: English, Database: CAPLUS
nanofiltration membranes were fabricated for the treatment of pulp and paper
pptn. was used to prep. the PES support membrane. PVA/PES composite nanofiltration membra
the PVA
maleic acid (MA) was used as crosslink
concns. of 0.5-2 and 0.05-1 wt%, resp.
of SEM (SEM) as well as at. force mi
addn...
引文排序，影响力最高的文献
2. Photo/electro-fenton treatment process for polyvinyl alcohol desizing wastewater
Full Text
By Yang, Jie; Chu, Hairong; Xu, Yanhua; Liu, Dongzhe
From Faming Zhuanli Shenqing (2012), CN 102757144 A 20121031. | Language: Chinese, Database: CAPLUS
The Fenton treatment process includes adding acid soln. to polyvinyl alc. desizing wastewater to adjust pH to 3~ 6, addir
22.1 mmol/L and H2O2/CODCr 1.0~ 3.0, starting UV lamp with power 6~ 8 W and stirrer for reaction, adding inorg. salt
applying current 0.5~ 2.0 A for degrdn. for 15~ 120 min. The acid soln. is 10~ 30wt% H2SO4, HCl or HNO3. The Fenton
soln. and H2O2. The inorg. salt is NaCl, MgCl2 or KCl. The invention can remove 91% CODCr and enhance biodegradability of

点击文献标题，阅读单篇文献详细信息

文献详细著录信息

文献摘要信息

重要概念索引

1. Polymeric flocculants

By: Guillet, James Edwin; Heskins, Michael; Murray, D. Gary

Assignee: Can.

Wastewaters contg. aq. suspensions of clay fines are flocculated rapidly using high mol. wt. (visc
55-3] and copolymers with I contg. ≥50% of polymd. N-isopropylacrylamide units. The floc has
also used in the manuf. of paper. Thus, aq. suspensions were prepd. from mixts. of sand and cl
isopropylacrylamide to give a homogeneous floc contg. ≤66.3% of solids.

专利信息

Patent Information

Patent No.	Kind	Date	Applica
CA 1180827	A1	Jan 8, 1985	CA 1982
US 4536294	A	Aug 20, 1985	US 1983

Priority Application

CA 1982-399215	A	Mar 23, 1982

Indexing

Waste Treatment and Disposal (Section 60-3)

Substances

25189-55-3
28500-83-6
81565-38-0
97366-13-7
97366-15-9
97366-16-0

flocculant, in treatment of wastewater contg. clay suspensions

Process

28377-46-0
31261-19-5
97366-18-2
97366-19-3
97381-57-2

flocculant, in treatment of wastewaters contg. clay suspensions

Process

9003-05-8
9003-06-9
25085-02-3
65324-25-6

flocculants contg., in treatment of wastewaters contg. clay suspensions

Process

Patent Information

Jan 8, 1985
CA 1180827
A1

Application

Mar 23, 1982
CA 1982-399215

Priority

Mar 23, 1982
CA 1982-399215

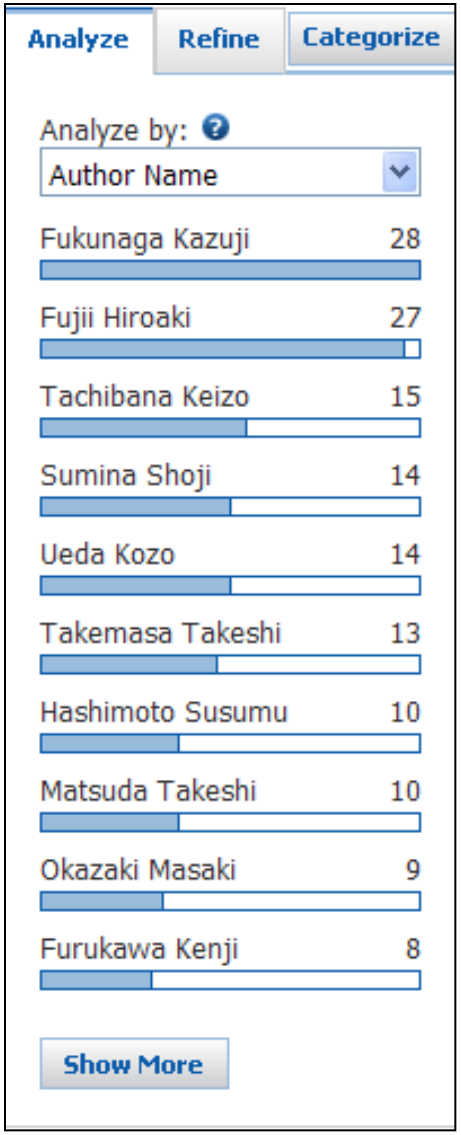
Source

Can.
38 pp.
Patent
1985
CODEN: CAXXA4

Classifications

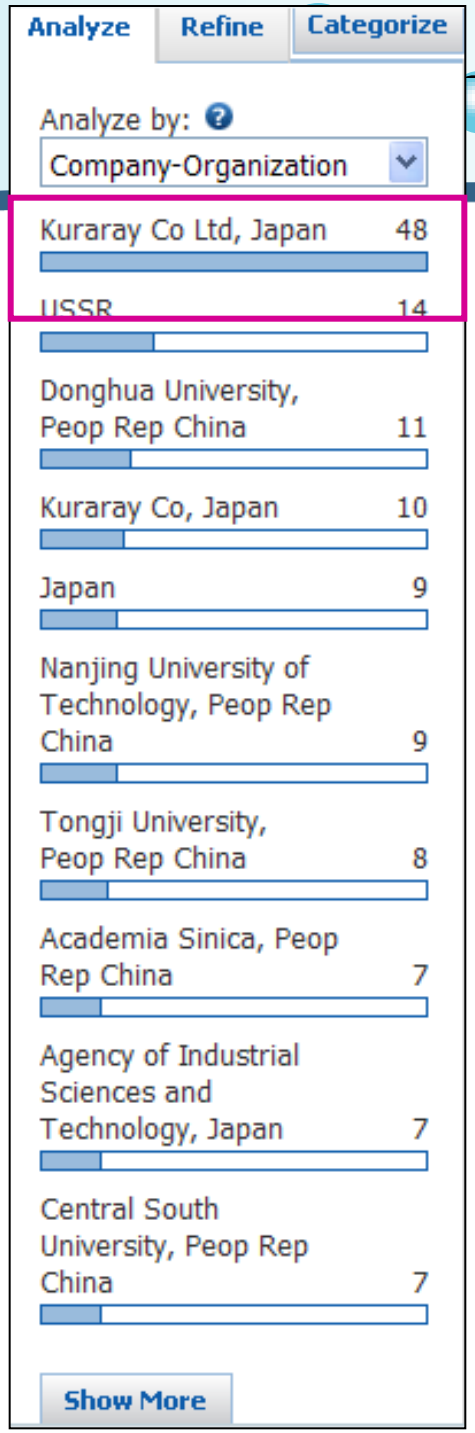
Main IPC C02F001-56

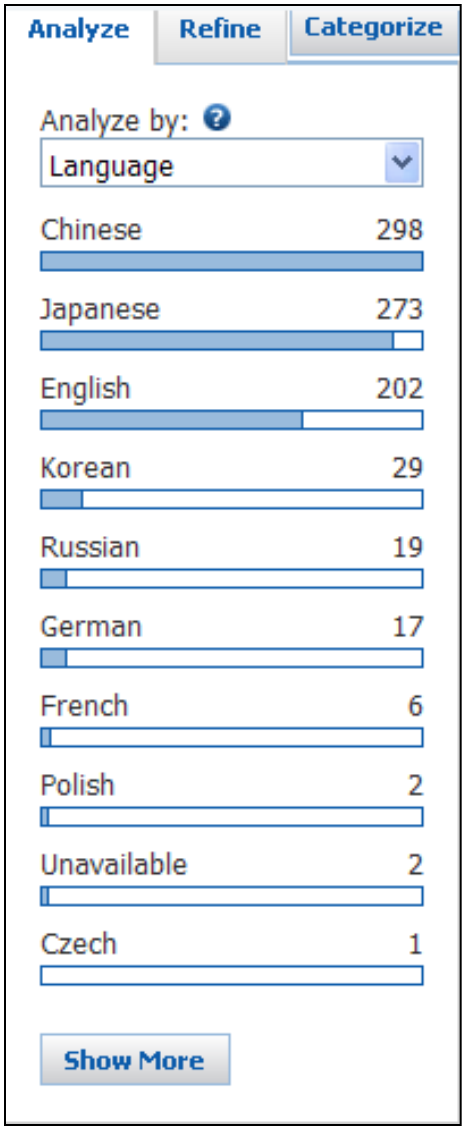

Research Topic "PVA to treat of wastewater" > references (852)
REFERENCES
Get Full Text
Tools
系统分析功能
Analyze
Refine
Categorize
0 of 852 References
Analyze by:
Author Name
Fukunaga Kazuji 28
Fujii Hiroaki 27
Tachibana Keizo 15
Sumina Shoji 14
Ueda Kozo 14
Takemasa Takeshi 13
Hashimoto Susumu 10
Author Name
CAS Registry Number
CA Section Title
Company-Organization
Database
Document Type
Index Term
CA Concept Heading
Journal Name
Language
Publication Year
Supplementary Terms
biochemical treatment of printing and dyeing wastewater
Full Text
Wei-zhong; Meng, Rui; Zhang, Bao-jun
13), 21(4), 19-25. | Language: Chinese, Database: CAPLUS
earch progress of using high-e fficient anaerobic biol. technol. to treat dyeing wa
ulture conditions and influencing factors of using high-e fficient anaerobic biorea
ABR reactor, anaerobic fluidized bed and anaerobic IC reactor etc. In addn., it als
nd PVA degrading bacteria in printing and dyeing wastewater.
vinyl alcohol /precipitated silica composite hydrogels for microorganism immob
14), 56, 749-755. | Language: English, Database: CAPLUS
ed with pptd. silica (PSi) was prepd. by chem. crosslinking in the satd. boric acid soln
ound that PSi could accelerate the crosslinking reaction of PVA, and the intermol. b
s of PVA hydrogel was investigated. The tensile strength of PVA hydrogel increased
d swelling property, resulting in the improvement of the capillary water abs...



作者分析，了解本领域，本课题的主要研究人员。

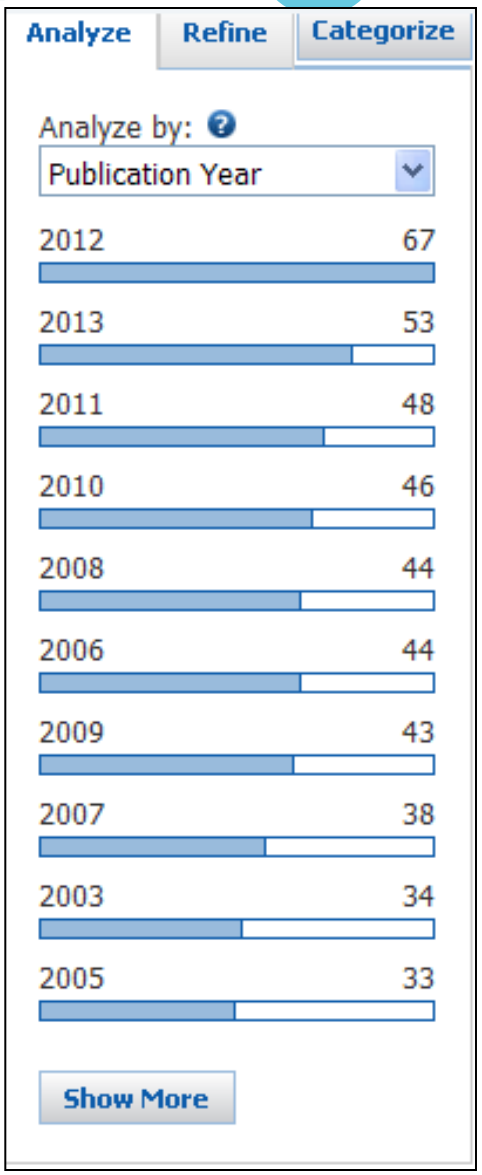
组织机构分析，了解本领域的核心研究机构

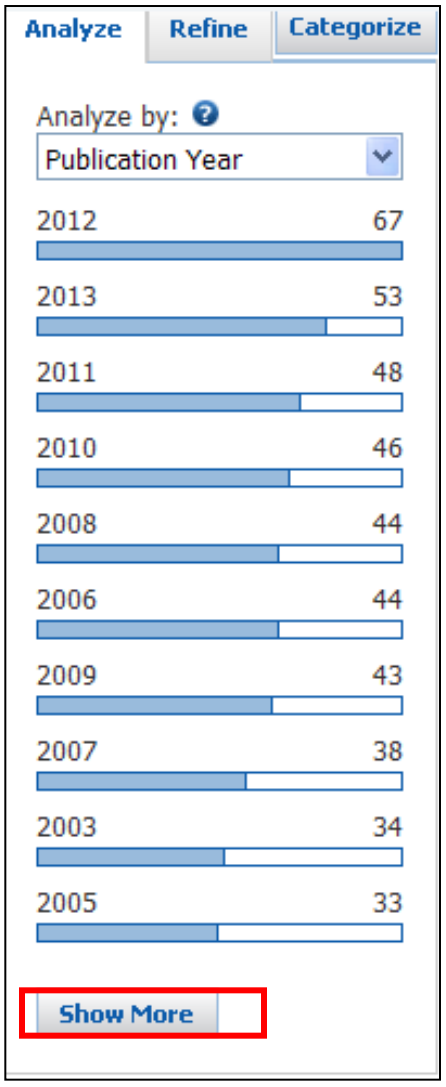


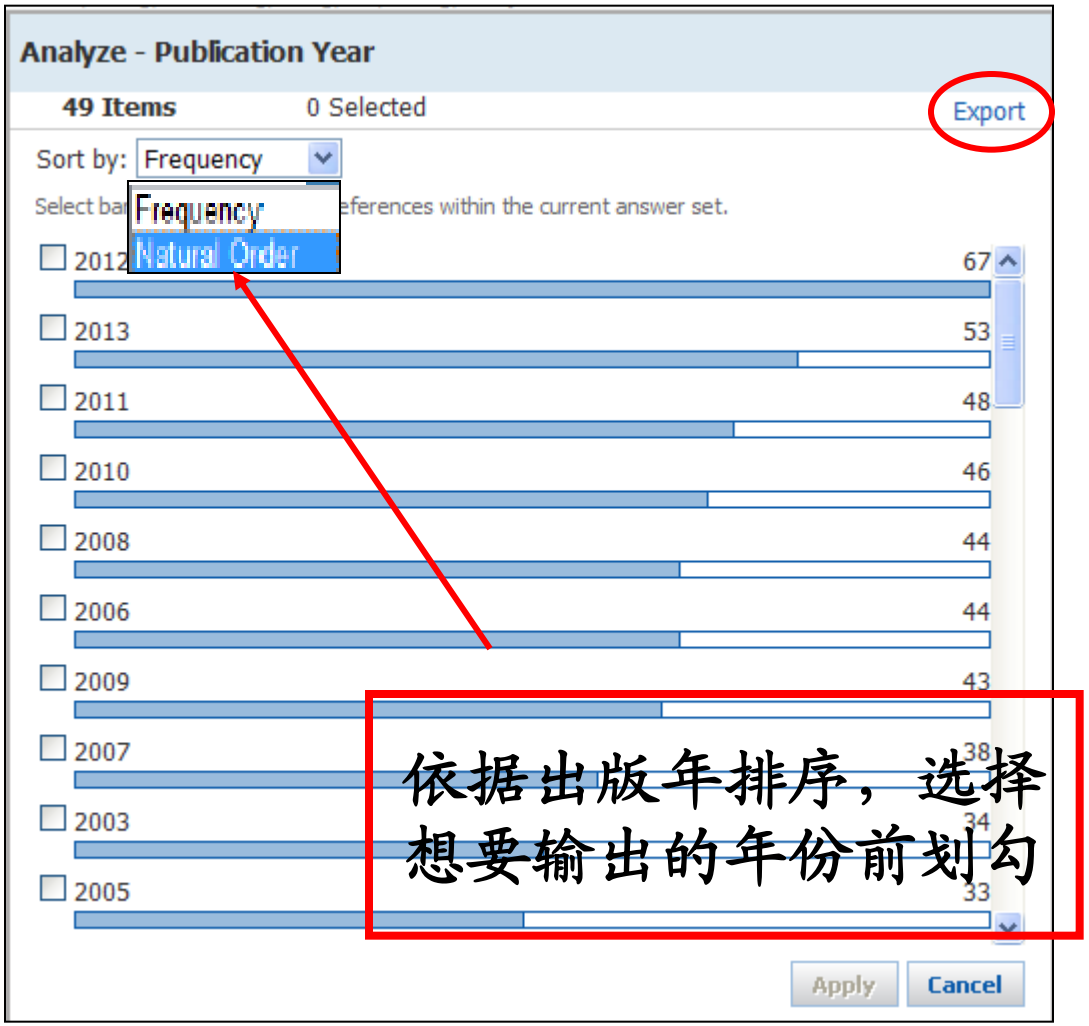


语言分析，了解该课题主要研究地区

出版年份分析，了解该课题主要研究时期。







依据出版年排序，选择想要输出的年份前划勾

Export Analysis - Publication Year

Export:

- (•) All
- ( ) Selected
- ( ) Range

Example: *2-20*

For:

Offline review

- (•) Portable Document Format (*.pdf)
- ( ) Microsoft Excel Worksheet (*.xls)

以PDF格式输出

hofiltration/membrane sepn. method to **treat** and reuse tannin- and NaCl-contg. food processing **wastewater** consists of: adjusting
o 4.0-7.0 using NaOH or 30% HCl, filtering to remove insol. solid particles to yield a filtrate, then filtrating the filtrate through a microfiltration
l permeate liq. I and retention liq. I; sepg. permeate and retention liqs. I through a nanofiltration membrane to yield permeate liq. II and
king retention liqs. I and II, performing vacuum evapn. and salt crystn. to yield condensed **water**, NaCl crystal...

actions ~0 Citings Full Text Link 0 Comments 0 Tags

aring high-density porous carrier for biological fluidized-bed wastewater treatment

Yangyang; Lu, Beibei; Chen, Yingwen; Zhu, Shemin; Wa
qing (2011), CN 102211807 A 20111012. Language: C
orous carrier is prepd. from (by wt.%) fly ash
od comprises the steps of: (1) mixing fly ashe
days, (2) tableting, drying at 80-100° for 4-
pores with an inorg. acid or base, drying, impr

esive 2-10, and **water** 15-
r and the adhesive, stirring,
ith a sieve (20-40 meshes),

actions ~0 Citings Full Text Link

nti-fouling coating matrix for waste and

ehui
qing (2011), CN 102199392 A 20110928. Language: C
ises dispersing nano cuprous oxide in solvent
kly, adding the oil-sol. nano cuprous oxide,
l, Na dodecyl benzenesulfonate, dodecyltrime
yester coating matrix soln. is toluene, xylene,

trix(alkyd resin) soln. at 60-
de is C12-C18 alkanoic acid,
nyl pyrrolidone and/or **PVA**.

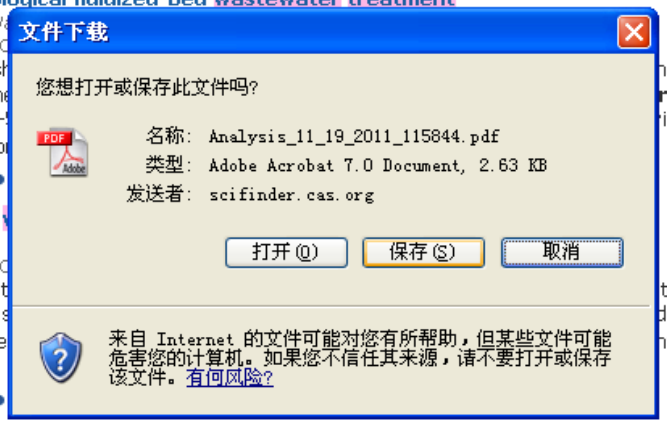
actions ~0 Citings Full Text Link

ucing cuprous oxide nanoparticle-loaded filter screen used in wastewater treatment

qing (2011), CN 102198349 A 20110928. Language: Chinese, Database: CAPLUS
oses method for producing cuprous oxide nanoparticle-loaded filter screen used in **wastewater treatment**. The method comprises adding
protector into **water**, and ultrasonically stirring to completely dissolve the copper salt and protector; soaking fabric in the soln., adding a
n., heating to 60-80° under normal pressure or high pressure, and keeping the temp. for 30-60 min; and dewatering the fabric through rolling,
gh the method, cuprous oxide nanoparticle is well dispersed in the fabric. The inventive filter screen has go...

actions ~0 Citings Full Text Link 0 Comments 0 Tags

vell on-line profile control agent prepared by using waste residue from oilfield wastewater treatment



Export Analysis - Publication Year

Export:

- (•) All
- ( ) Selected
- ( ) Range

Example: *2-20*

For:

Offline review

- ( ) Portable Document Format (*.pdf)
- (•) Microsoft Excel Worksheet (*.xls)

以Excel格式输出

. Language: French, Database: CAPLUS

treating wastewater resulting from the synthesis of a halogenated vinyl polymer, such as PVC or P

en 6 and 8, by flo … d process com

h at least one tar … °C. The halo

ated homopolyme…

Text Link

g from the synt…

guage: French, Datab…

treating waste… h as PVC or P

en 6 and 8, by flo … d process com

h at least one tar … °C. The halo

ated homopolyme…

Text Link

stewater contai… eparation

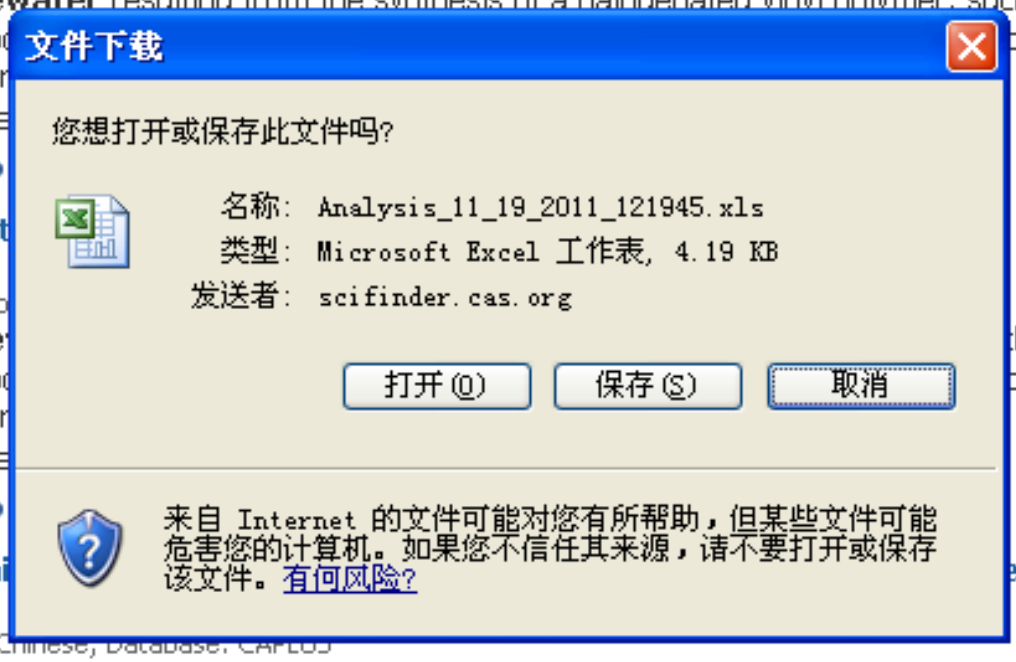
qing

111026. Language: Chinese, Database: CAPLUS

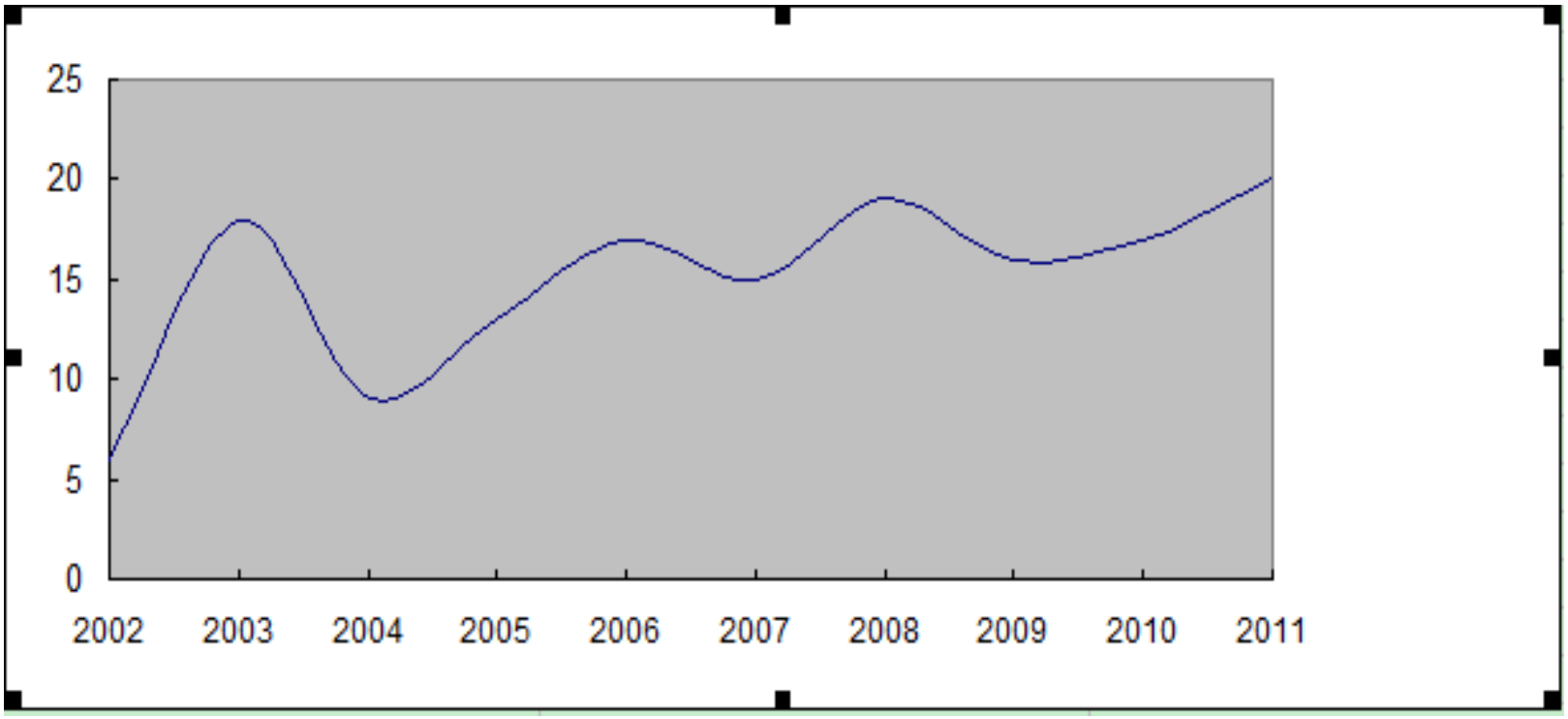
. method to **treat** and reuse tannin- and NaCl-contg. food processing **wastewater** consists

% HCl, filtering to remove insol. solid particles to yield a filtrate, then filtrating the filtrate through a

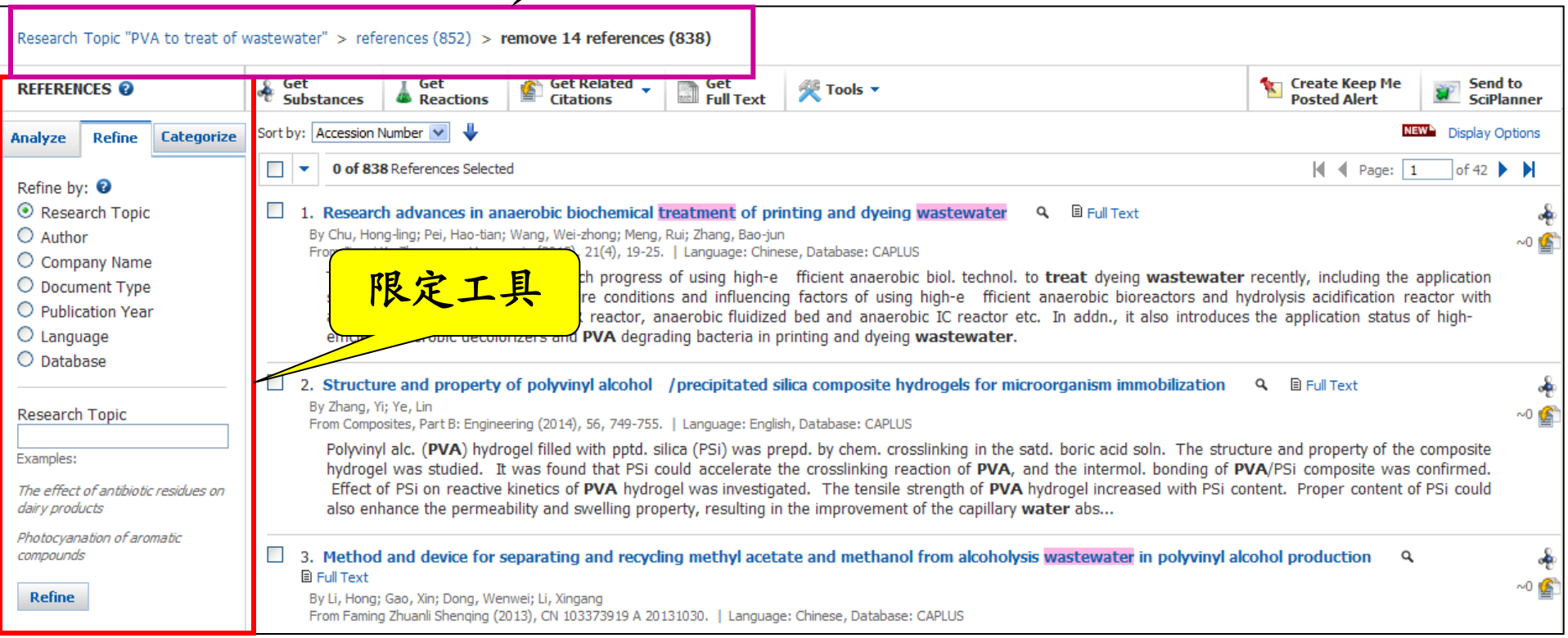
tion liq. I; sepg. permeate and retention liqs. I through a nanofiltration membrane to yield permea

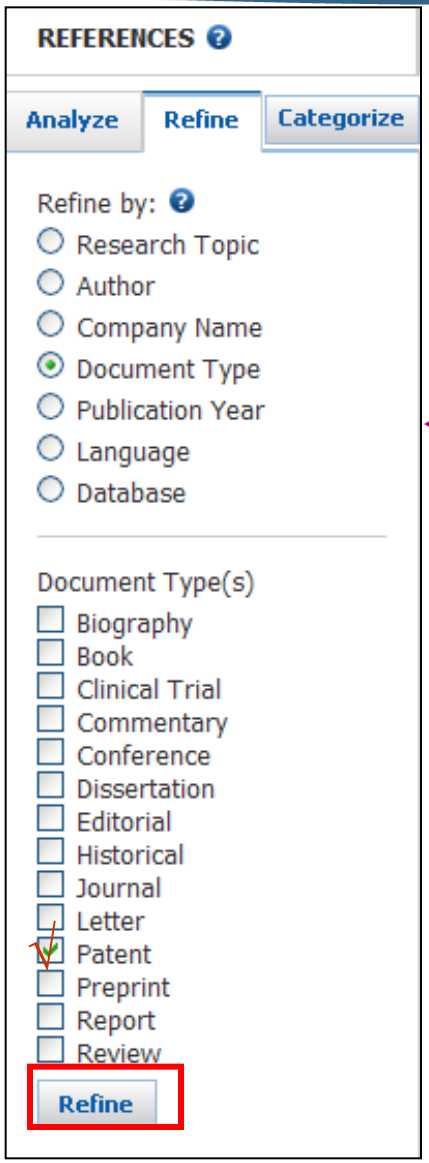


Excel导出数据做图

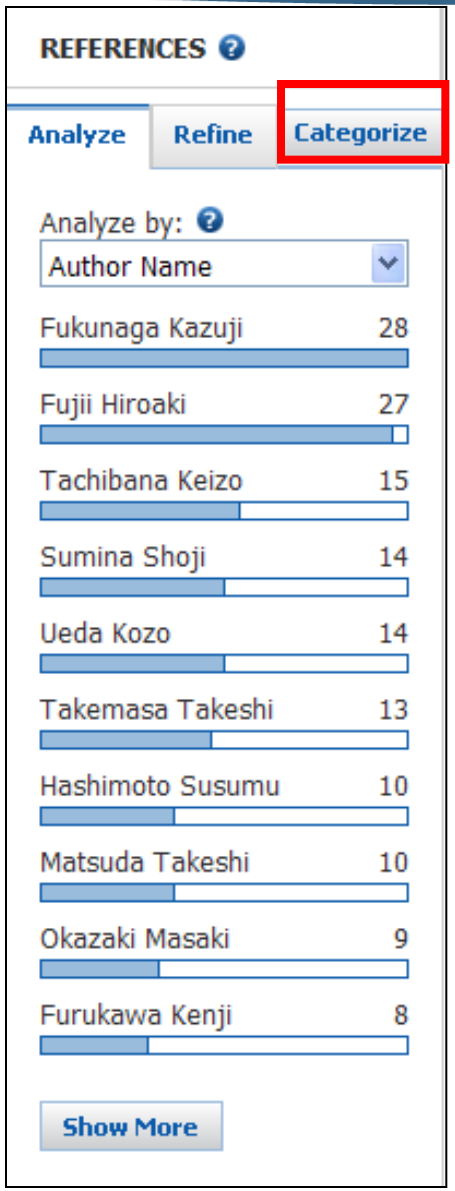


返回之前的检索结果


Research Topic "PVA to treat of wastewater" > references (852) > remove 14 references (838)
REFERENCES
Get Substances
Get Reactions
Get Related Citations
Get Full Text
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Categorize
Sort by: Accession Number
Display Options
0 of 838 References Selected
Page: 1 of 42
Refine by:
Research Topic
Author
Company Name
Document Type
Publication Year
Language
Database
限定工具
1. Research advances in anaerobic biochemical treatment of printing and dyeing wastewater
Full Text
By Chu, Hong-ling; Pei, Hao-tian; Wang, Wei-zhong; Meng, Rui; Zhang, Bao-jun
21(4), 19-25. | Language: Chinese, Database: CAPLUS
ch progress of using high-e fficient anaerobic biol. technol. to treat dyeing wastewater recently, including the application re conditions and influencing factors of using high-e fficient anaerobic bioreactors and hydrolysis acidification reactor with reactor, anaerobic fluidized bed and anaerobic IC reactor etc. In addn., it also introduces the application status of high-
PVA degrading bacteria in printing and dyeing wastewater.
2. Structure and property of polyvinyl alcohol /precipitated silica composite hydrogels for microorganism immobilization
Full Text
By Zhang, Yi; Ye, Lin
From Composites, Part B: Engineering (2014), 56, 749-755. | Language: English, Database: CAPLUS
Polyvinyl alc. (PVA) hydrogel filled with pptd. silica (PSi) was prepd. by chem. crosslinking in the satd. boric acid soln. The structure and property of the composite hydrogel was studied. It was found that PSi could accelerate the crosslinking reaction of PVA, and the intermol. bonding of PVA/PSi composite was confirmed. Effect of PSi on reactive kinetics of PVA hydrogel was investigated. The tensile strength of PVA hydrogel increased with PSi content. Proper content of PSi could also enhance the permeability and swelling property, resulting in the improvement of the capillary water abs...
3. Method and device for separating and recycling methyl acetate and methanol from alcoholysis wastewater in polyvinyl alcohol production
Full Text
By Li, Hong; Gao, Xin; Dong, Wenwei; Li, Xingang
From Faming Zhuanli Shenqing (2013), CN 103373919 A 20131030. | Language: Chinese, Database: CAPLUS
Research Topic
Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Refine



文献类型分析，快速获得专利、会议、报告、综述等特定类型的文献



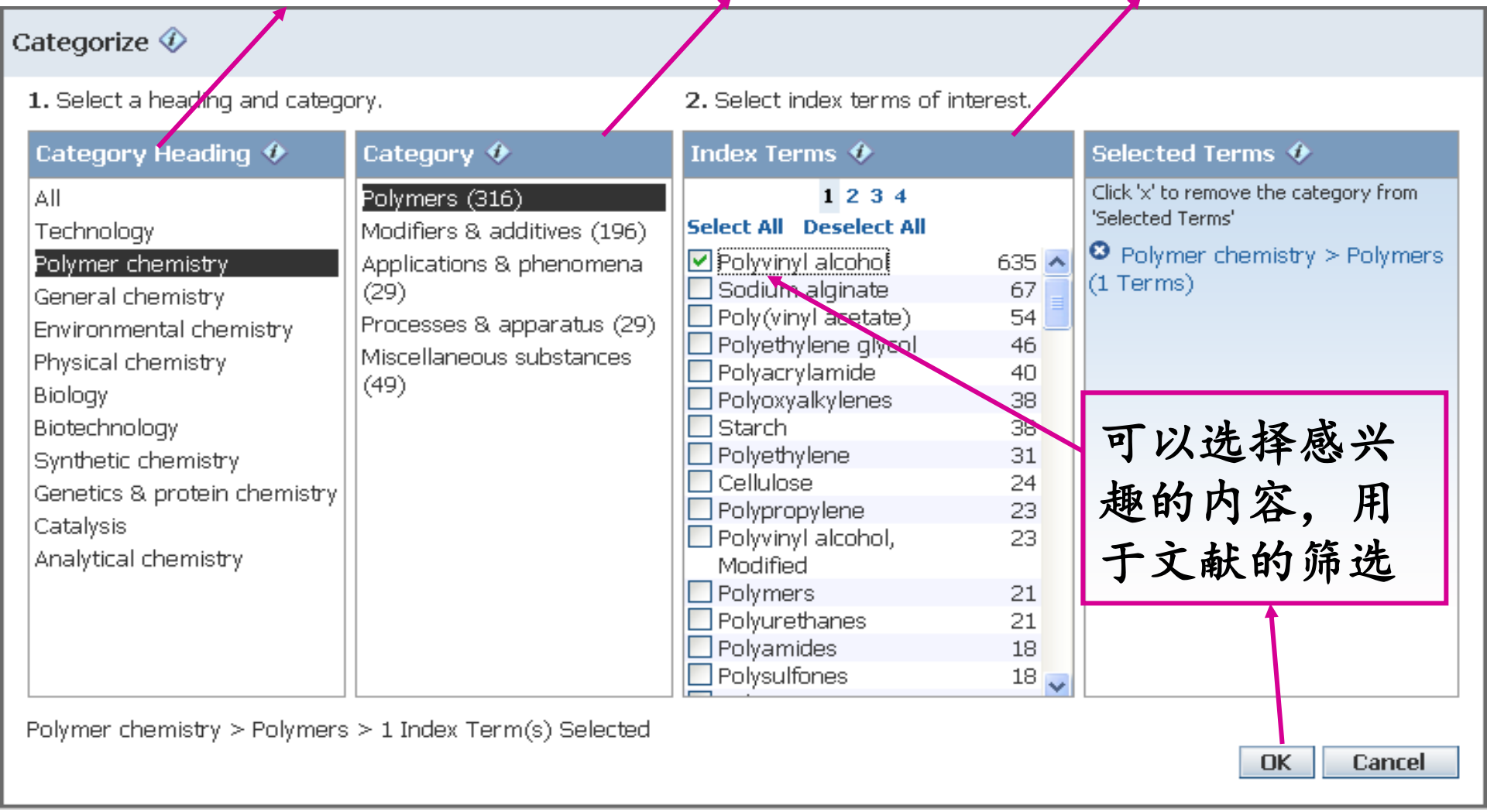
Categorize系统分类分析工具

Categorize系统分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

一级目录

二级目录

三级目录

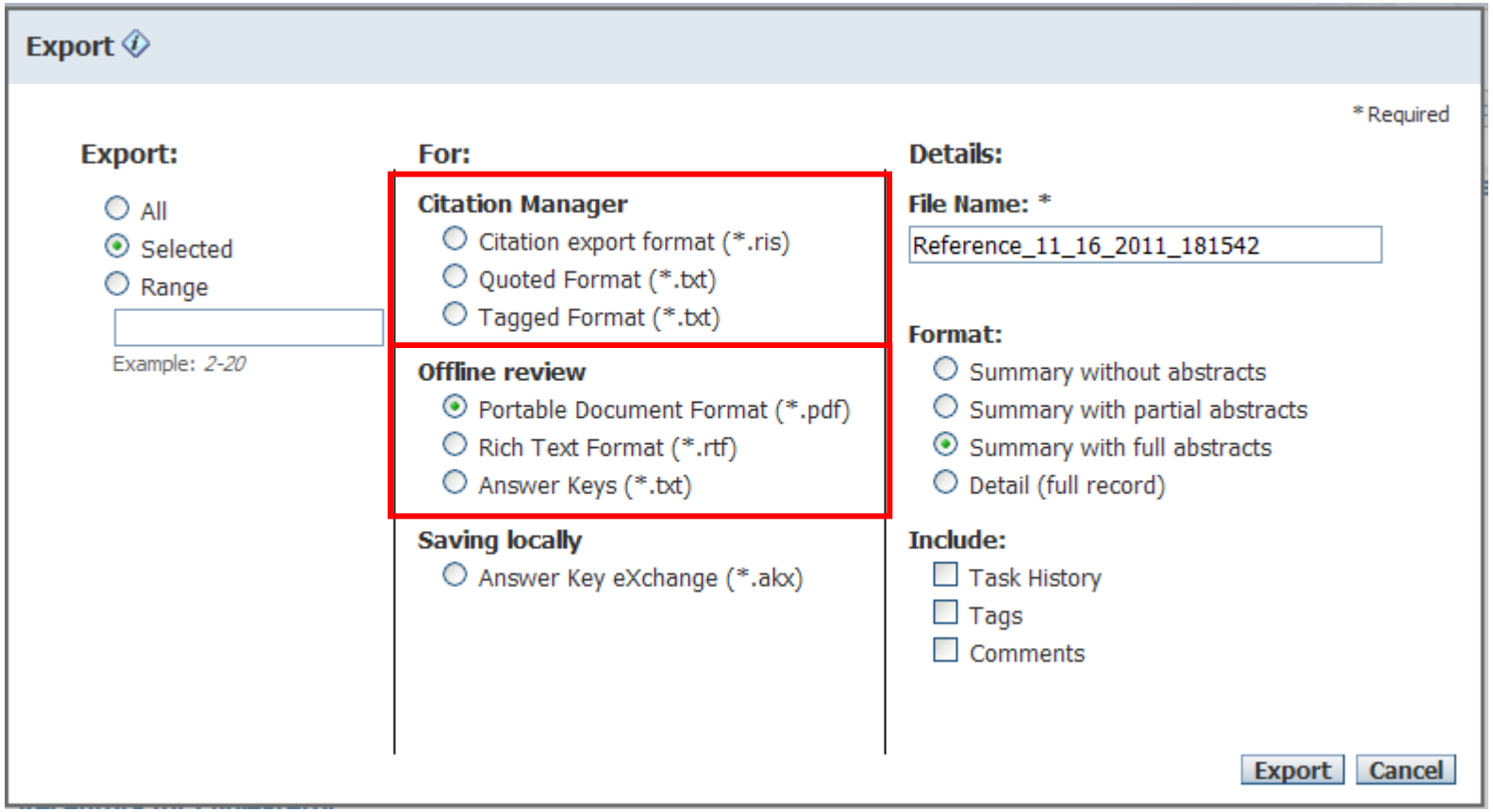


可以选择感兴趣的内容，用于文献的筛选

结果保存

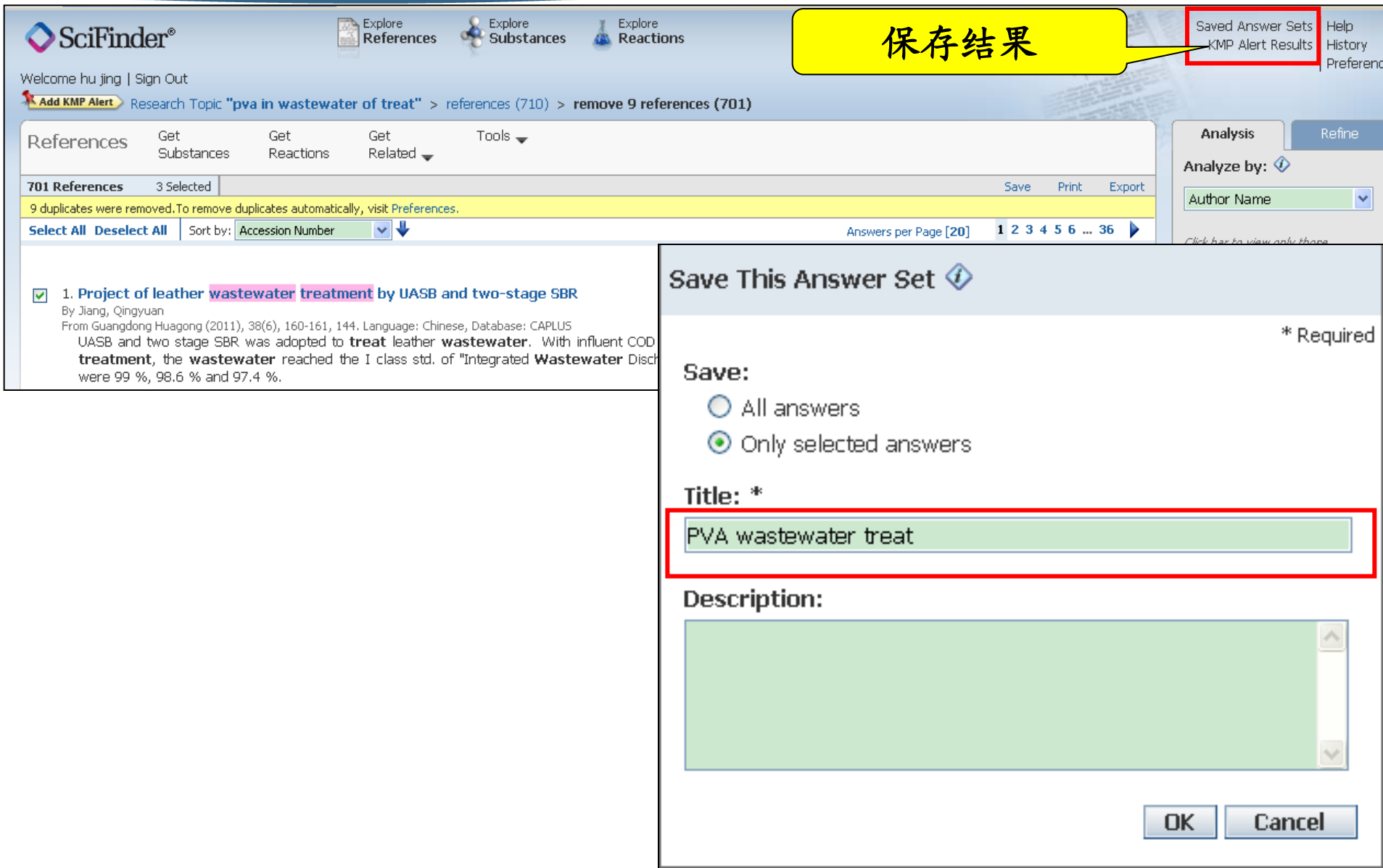
Save：将检索结果保存到SFS系统内部

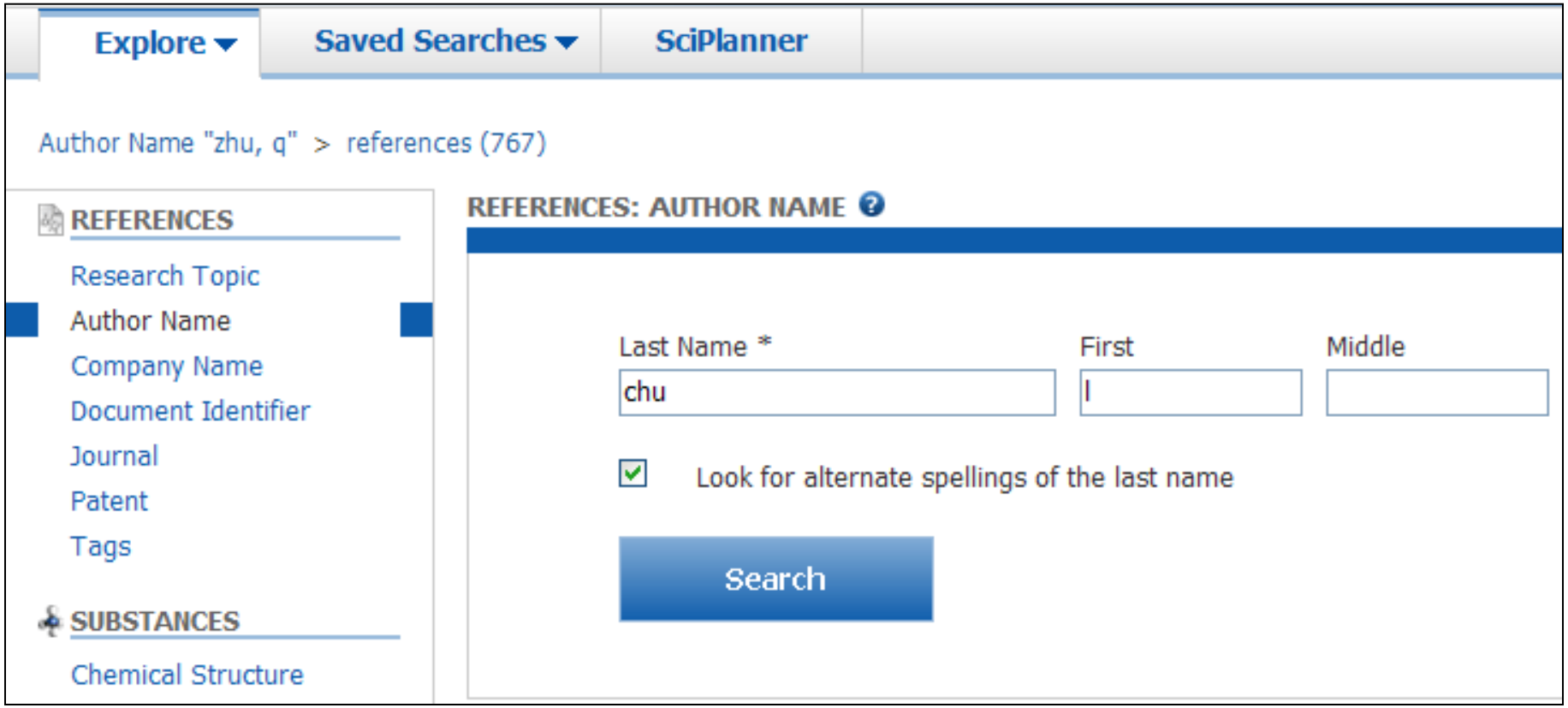
Export：将检索结果保存到桌面



1.保存成RIS格式，用于EndNote的文献管理工具。

2.保存成PDF、RTF格式，用于脱机浏览。选择summary可保存500条记录，选择detail可保存100条记录。


SciFinder®
Explore References
Explore Substances
Explore Reactions
保存结果
Saved Answer Sets
KMP Alert Results
Help
History
Welcome hu jing | Sign Out
Add KMP Alert
Research Topic "pva in wastewater of treat" > references (710) > remove 9 references (701)
References
Get Substances
Get Reactions
Get Related
Tools
Analysis
Refine
Analyze by:
Author Name
701 References
3 Selected
Save
Print
Export
9 duplicates were removed.To remove duplicates automatically, visit Preferences.
Select All
Deselect All
Sort by:
Accession Number
Answers per Page [20]
1 2 3 4 5 6 ... 36
1. Project of leather wastewater treatment by UASB and two-stage SBR
By Jiang, Qingyuan
From Guangdong Huagong (2011), 38(6), 160-161, 144. Language: Chinese, Database: CAPLUS
UASB and two stage SBR was adopted to treat leather wastewater. With influent COD
treatment, the wastewater reached the I class std. of "Integrated Wastewater Disch
were 99 %, 98.6 % and 97.4 %.
Save This Answer Set
* Required
Save:
All answers
Only selected answers
Title: *
PVA wastewater treat
Description:
OK
Cancel


Explore
Saved Searches
SciPlanner
Author Name "zhu, q" > references (767)
REFERENCES
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
SUBSTANCES
Chemical Structure
REFERENCES: AUTHOR NAME
Last Name *
First
Middle
chu
l
Look for alternate spellings of the last name
Search

2 of 365 Author Name Candidates Selected	References
CHU	6
CHU L	155
CHU L A	1
CHU L C	42
CHU L C Y	1
CHU L D	2
CHU L E	1
CHU L F	4
CHU L H	17
CHU L H L	1
CHU L H X	1
CHU L J	1
CHU L K	26
CHU L L	35

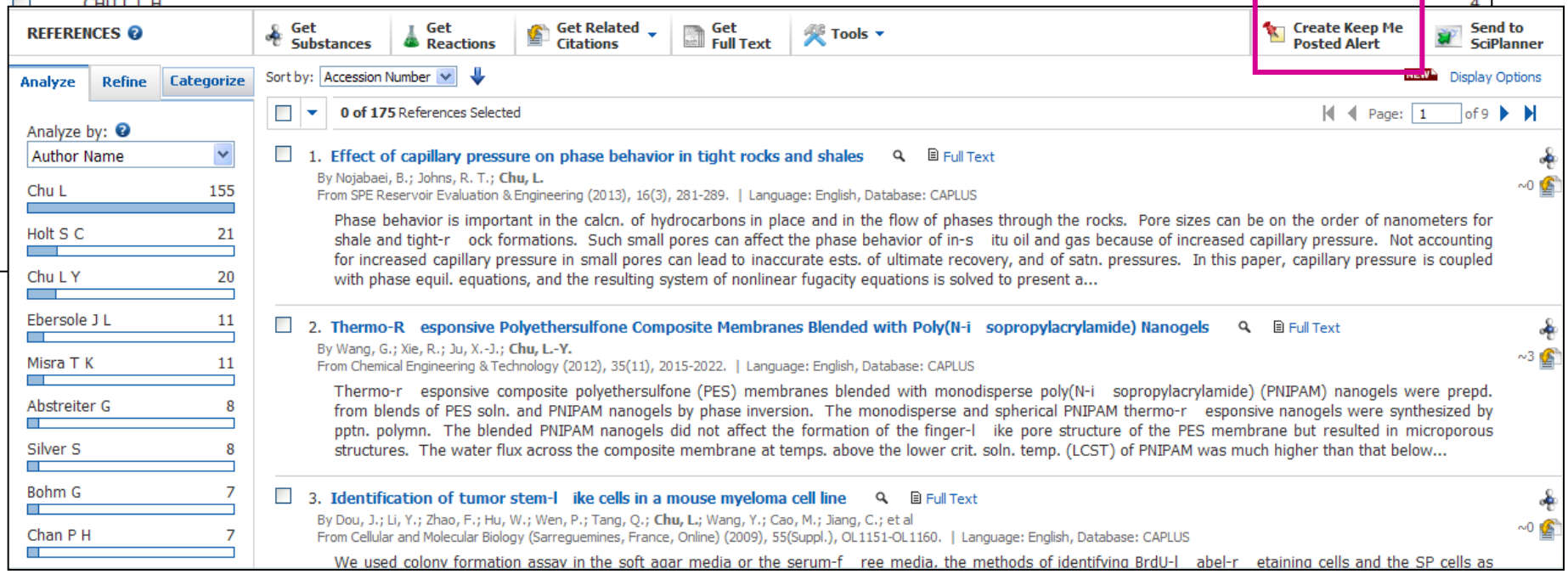
CHU L,

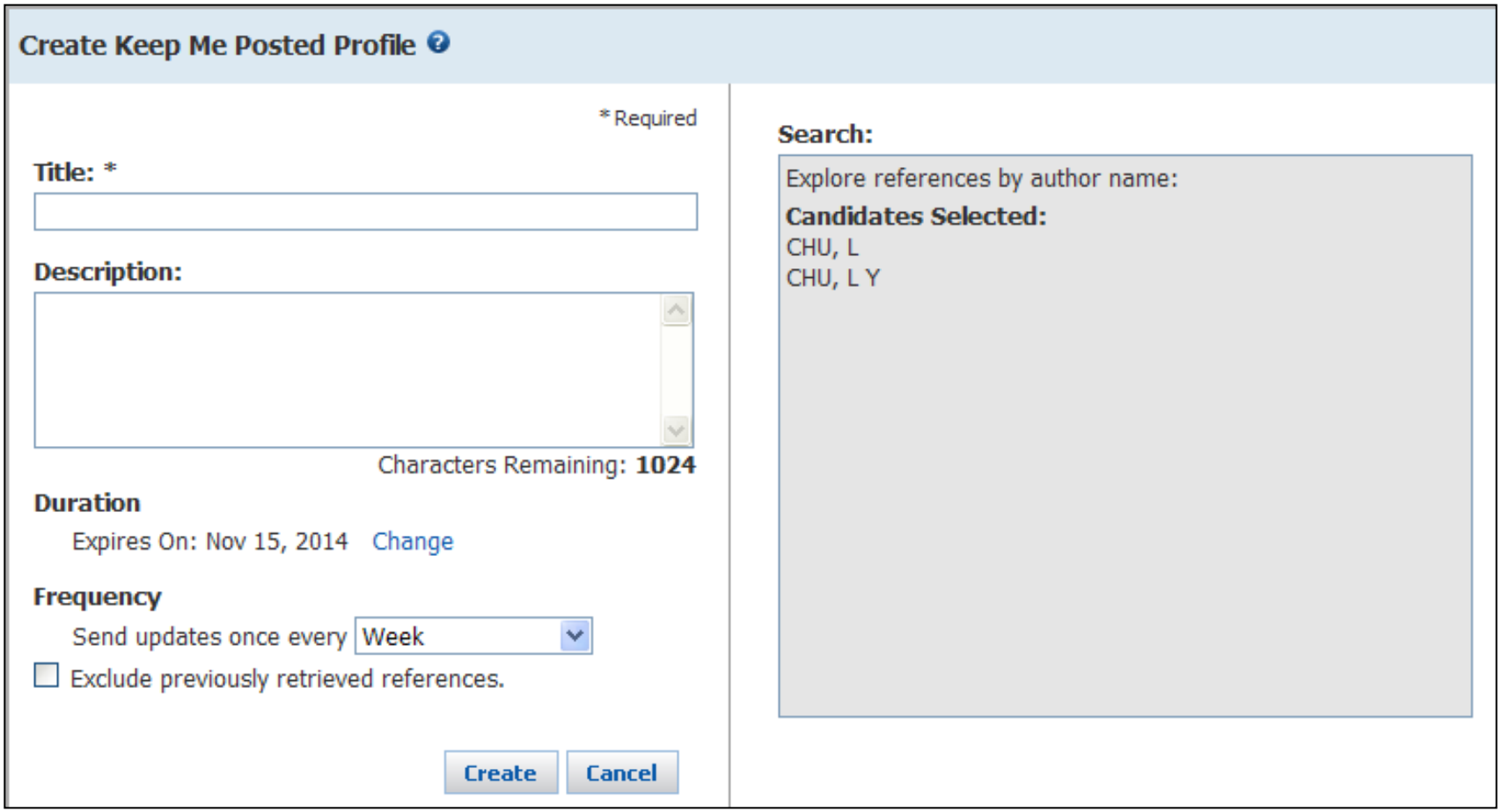
CHU L Y,

CHU LIANG YIN,

CHU LIANGYIN

KMP-跟踪文献





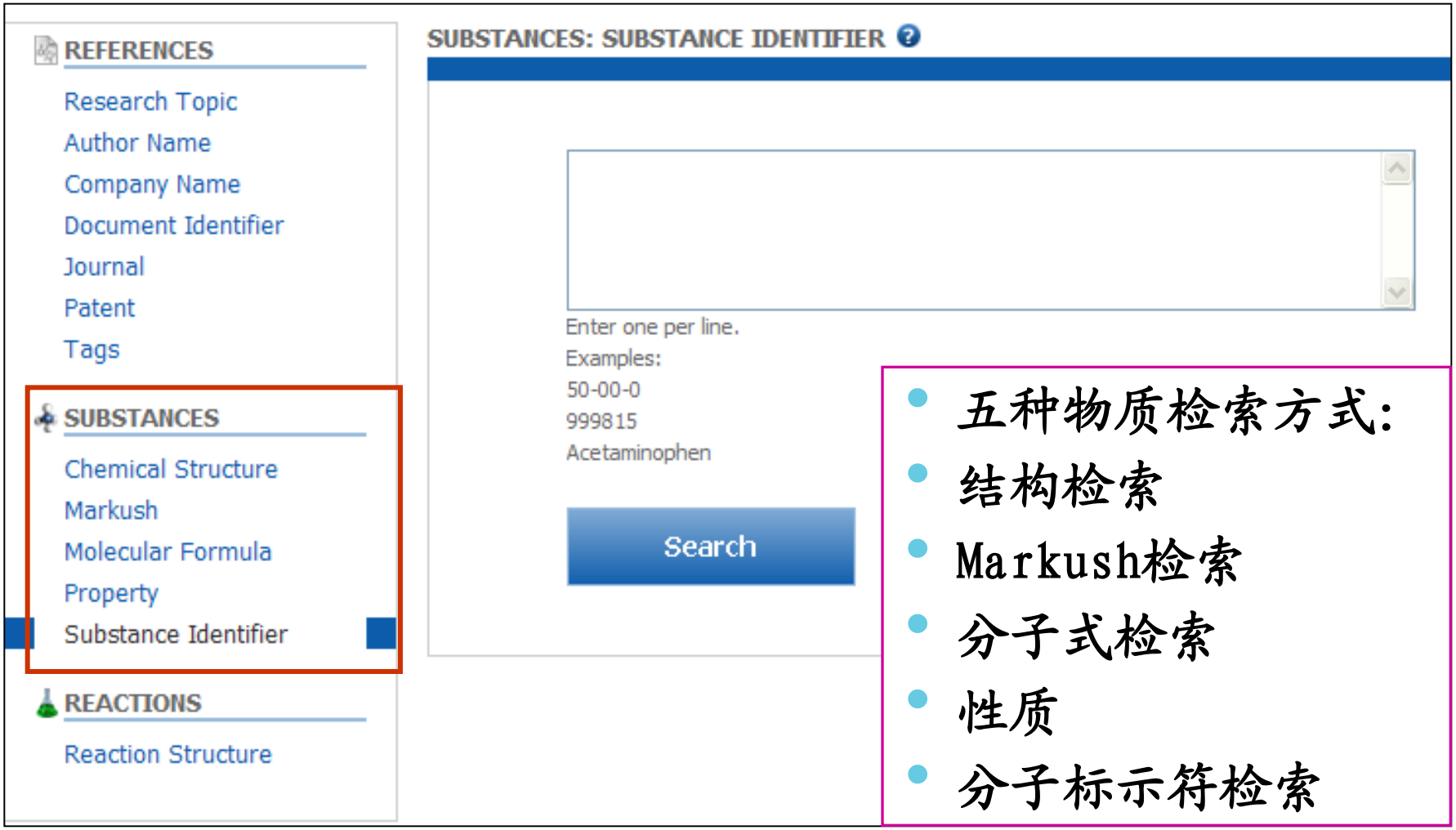
KMP：对关注的领域随时保持关注

文献检索小结

- 检索主题时用介词连接检索词。
- 检索结果项，应尽量选择含“concepts”和“associated with”项。
- 可通过Refine和Analyze项缩小检索结果范围。
- 使用Categorize可将检索结果按不同主题分类。
- 作者名检索时姓写全，名写首字母，得到文献后依Organization分析

检索方式

文献　　物质　　反应

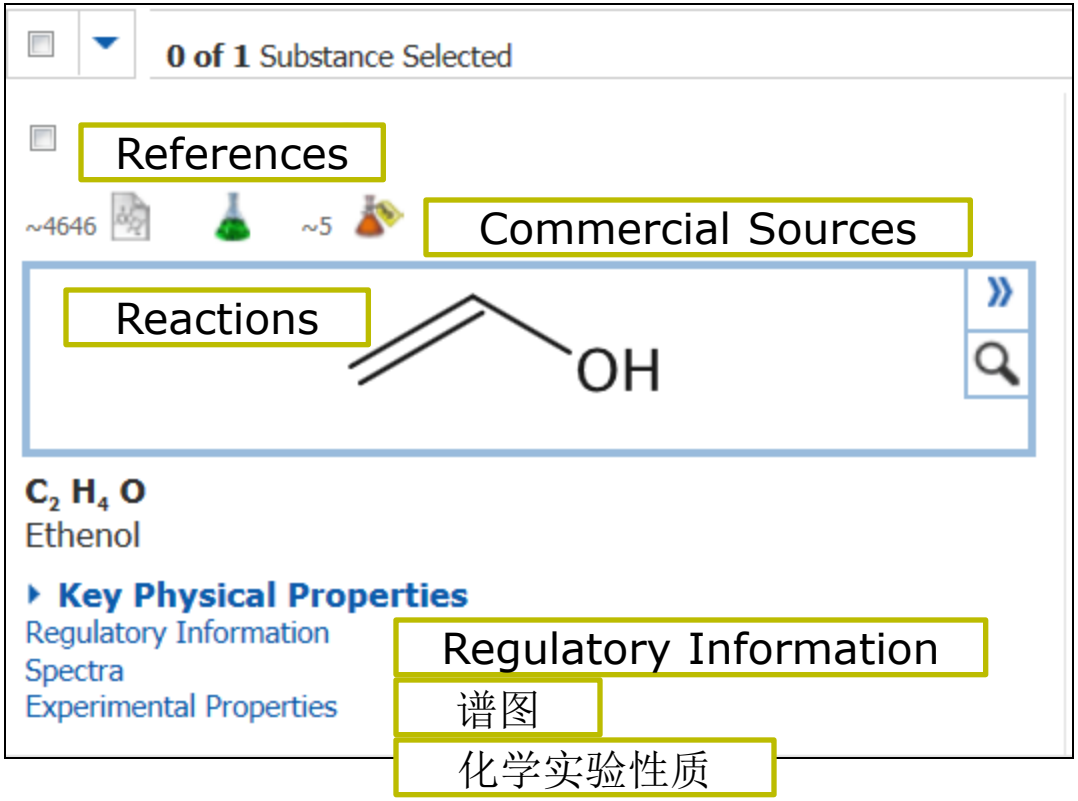

REFERENCES
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier
REACTIONS
Reaction Structure
SUBSTANCES: SUBSTANCE IDENTIFIER
Enter one per line.
Examples:
50-00-0
999815
Acetaminophen
Search
五种物质检索方式:
结构检索
Markush检索
分子式检索
性质
分子标示符检索

1. 标示符检索

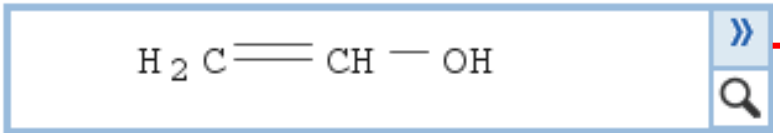
可以通过输入物质的名称、CA号、俗名、商品名进行检索

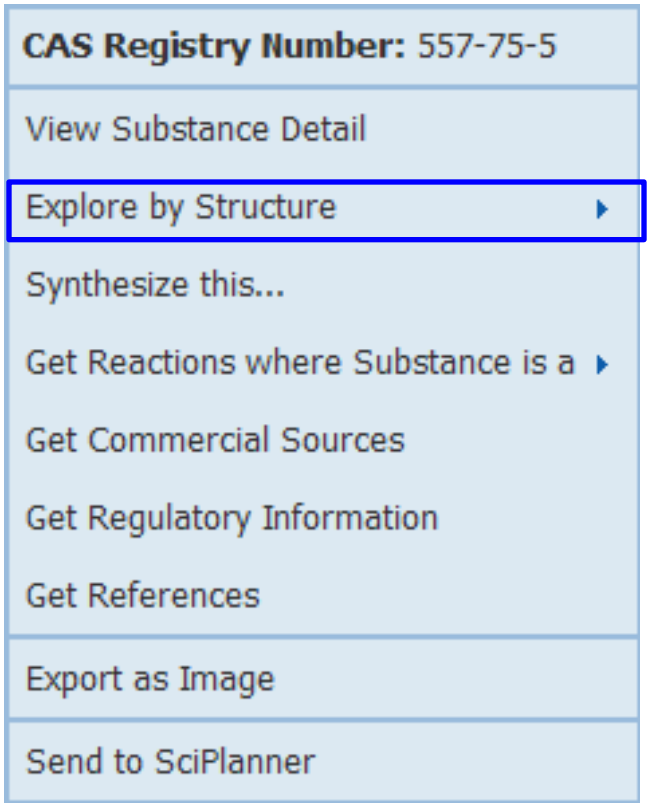
规则：1. 每次最多可输入25个物质名称，每行1个。

Scifinder中的物质信息



详细列出“乙烯醇”的文献数量、化学反应、销售厂商、法规信息





转入结构检索或反应检索

在SciFinder中，鼠标滑过物质，可以打开物质的标准菜单，从而获得与物质相关的所有内容

CAS Registry Number 557-75-5

~4,646 ~5

C_2H_4O

Ethenol

Molecular Weight
44.05

Melting Point (Experimental)
Value: 9 °C

Boiling Point (Experimental)
Value: 101 °C

Density (Predicted)
Value: 0.813±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 10.50±0.50 | Condition: Most Acidic Temp: 25 °C

Other Names
Vinyl alcohol (8CI)
Acetaldehyde enol
Hydroxyethene
Hydroxyethylene

CAS号
分子式
结构式
分子质量
熔点
沸点
化学名
别名

物质来源，相关文献篇数和类型

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Combinatorial Study		✓		
Formation, Nonpreparative	✓	✓		✓
Miscellaneous	✓			
Occurrence	✓	✓	✓	
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents			✓	
Reactant or Reagent	✓	✓	✓	✓
Uses	✓	✓	✓	✓

按照CAS Role分类的专利、非专利文献列表。对某类文献感兴趣，仅需点击交叉处的　即可方便快捷地获取。

预测数据与实验数据

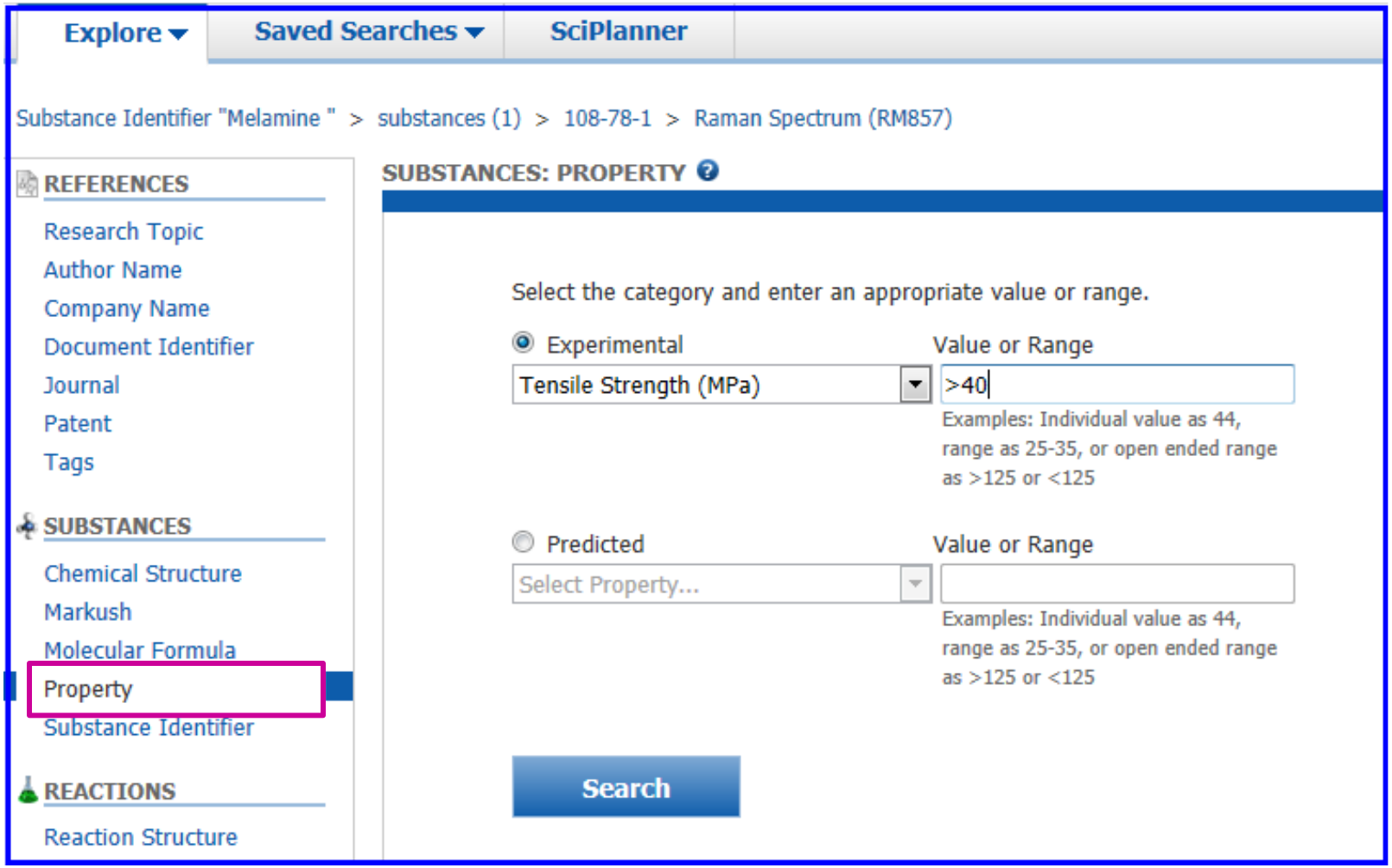
Top

Biological Properties	Value	Condition	Note
Bioconcentration Factor	1.79	pH 1 Temp: 25 °C	(15)
Bioconcentration Factor	1.79	pH 2 Temp: 25 °C	(15)
Bioconcentration Factor	1.79	pH 3 Temp: 25 °C	(15)
Bioconcentration Factor	1.79	pH 4 Temp: 25 °C	(15)
Bioconcentration Factor	1.79	pH 5 Temp: 25 °C	(15)
Bioconcentration Factor	1.79	pH 6 Temp: 25 °C	(15)
Bioconcentration Factor	1.79	pH 7 Temp: 25 °C	(15)
Bioconcentration Factor	1.78	pH 8 Temp: 25 °C	(15)
Bioconcentration Factor	1.73	pH 9 Temp: 25 °C	(15)
Bioconcentration Factor	1.36	pH 10 Temp: 25 °C	(15)

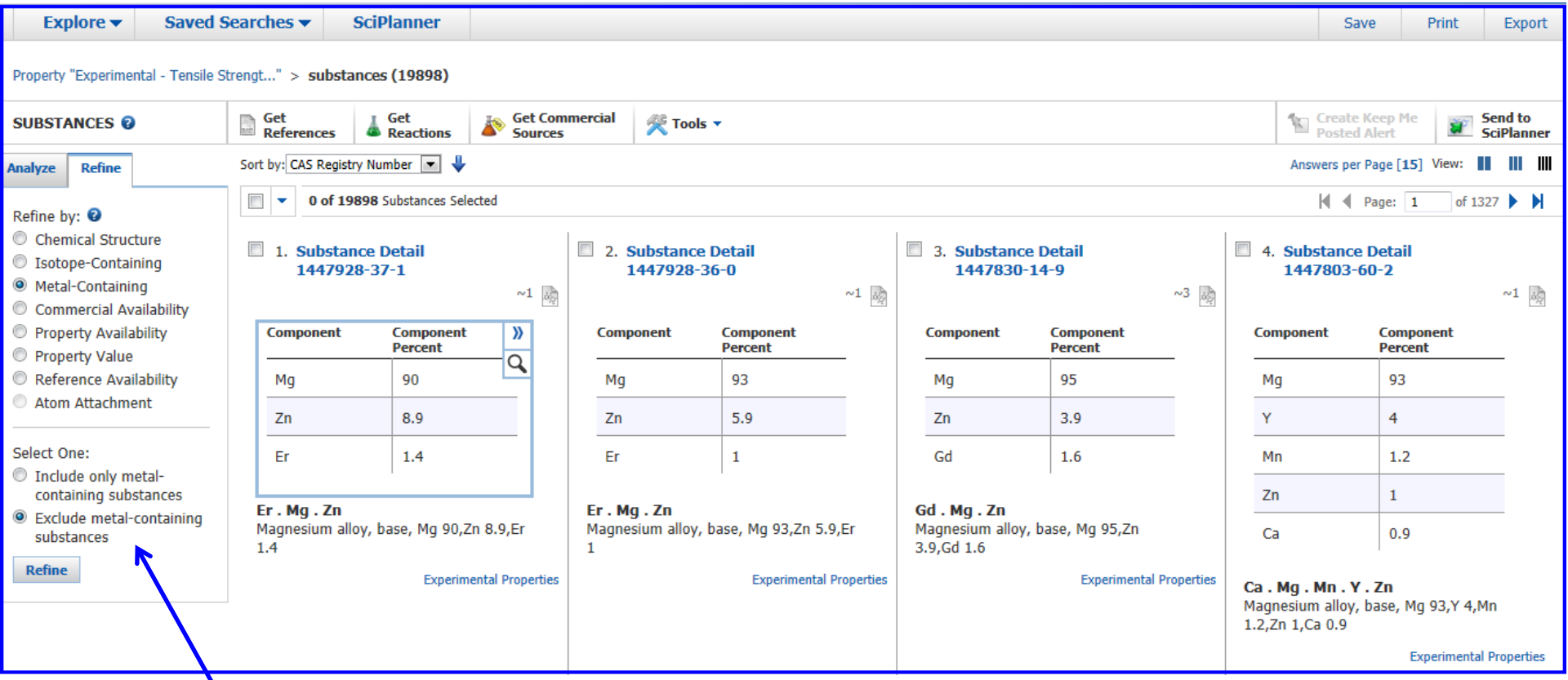
Top

Chemical Properties	Value	Condition	Note
Koc	52.8	pH 1 Temp: 25 °C	(15)
Koc	52.8	pH 2 Temp: 25 °C	(15)
Koc	52.8	pH 3 Temp: 25 °C	(15)
Koc	52.8	pH 4 Temp: 25 °C	(15)
Koc	52.8	pH 5 Temp: 25 °C	(15)
Koc	52.8	pH 6 Temp: 25 °C	(15)
Koc	52.8	pH 7 Temp: 25 °C	(15)
Koc	52.6	pH 8 Temp: 25 °C	(15)
Koc	51.2	pH 9 Temp: 25 °C	(15)
Koc	40.1	pH 10 Temp: 25 °C	(15)
logD	0.63	pH 1 Temp: 25 °C	(15)

2. 性质检索



寻找比PVC的拉伸强度大的有机材料



通过Refine快速排除具有某类性质的物质

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

Property "Experimental - Tensile Strengt..." > substances (19898) > **refine "exclude metal-containing" (2284)**

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

Analyze | Refine

Sort by: CAS Registry Number | Answers per Page [15] | View:

0 of 2284 Substances Selected | Page: 1 of 153

Analyze by: Substance Role

Properties	2211
Preparation	1952
Uses	881
Process	745
Reactant or Reagent	364
Biological Study	240
Analytical Study	196
Miscellaneous	187
Occurrence	143
Formation, Nonpreparative	141

Show More

1. **Substance Detail**
1356571-12-4

~2

Substance Image Cannot Be Displayed

1356571-12-

Unspecified
Iron alloy, base, (X50MnAl25-5)

Experimental Properties

2. **Substance Detail**
1346871-45-1

~2

Substance Image Cannot Be Displayed

1346871-45-

Editor Note: A two-part epoxy resin adhesive (Henkel Adhesives)

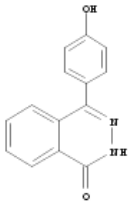
Unspecified
Hysol EA 9380.05

Experimental Properties

3. **Substance Detail**
1339943-97-3

~1

152594-70-2
$C_{14}H_{10}N_2O_2$



92-88-6
$C_{12}H_{10}O_2$

90-98-2

4. **Substance Detail**
1332830-93-9

~1

Substance Image Cannot Be Displayed

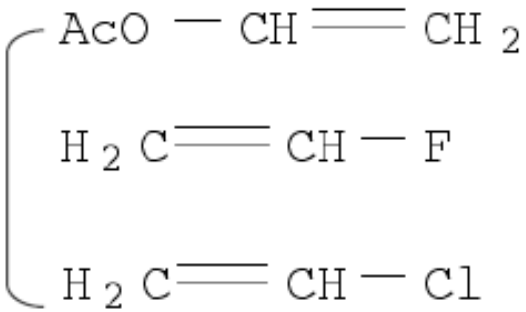
1332830-93-

Unspecified
Iron alloy, base, (04Kh19N5G11M2AFB)

Experimental Properties

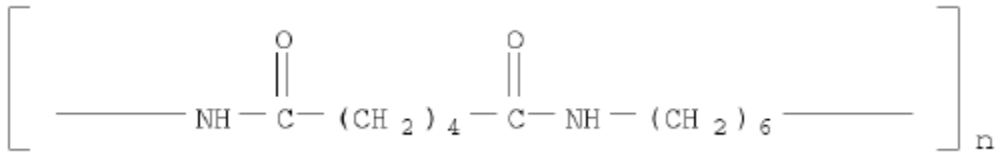
3. 分子式检索

（1）只知道起始原料-聚合物括号表示，组分间用点分开，括号外用x表示。



例:(C4H6O2.C2H3Cl.C2H3F)x

（2）知道结构重复单元-外括号用n表示



(C12H22N2O2)n

（3）无机盐：按照混合物的方法检，使用Dot-disconnect将不同组分连接

例：H2SO4.Na

分子式输入规则-Hill排序：

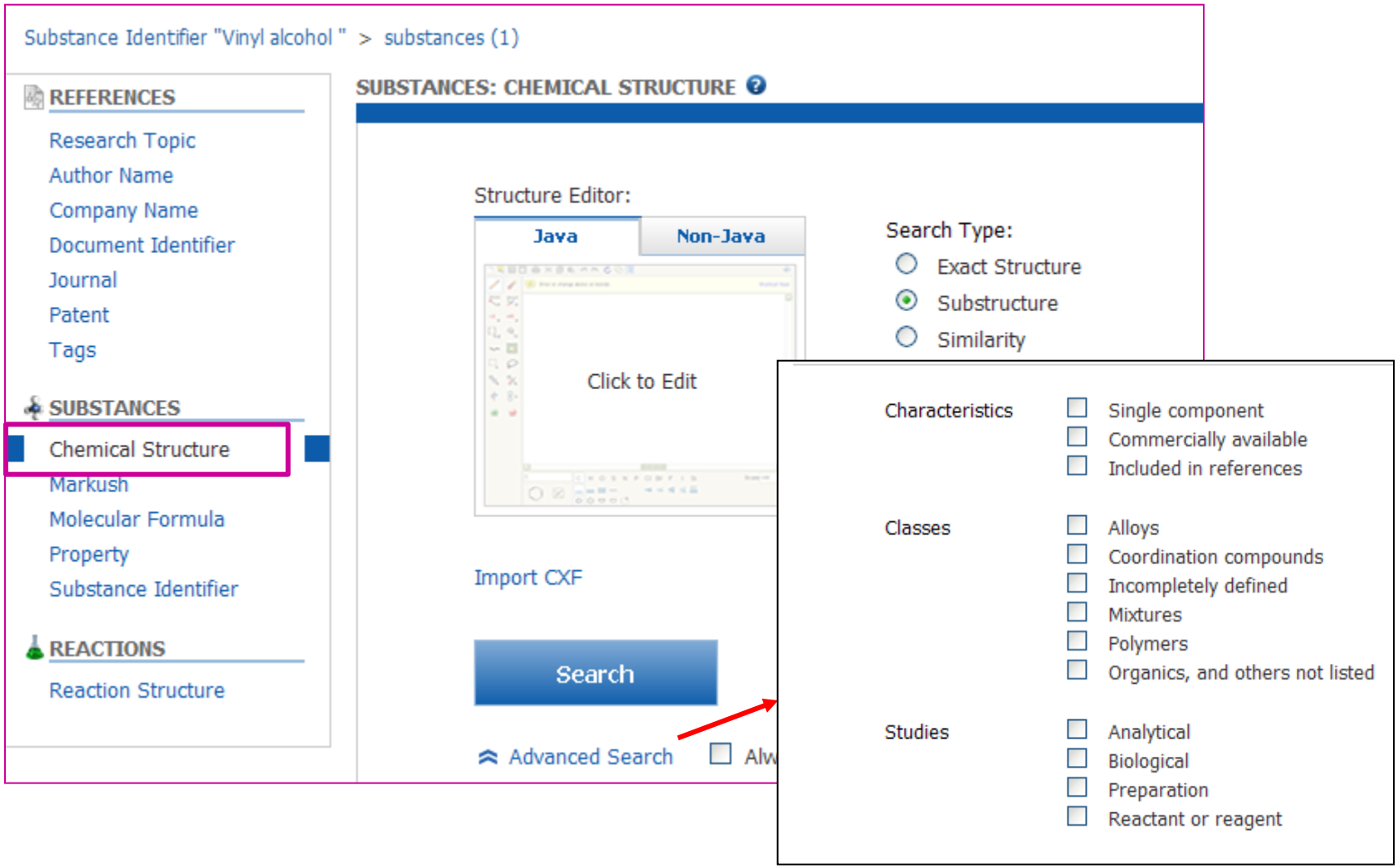
1）不含碳的化合物，分子式按元素符号的字母顺序排列。

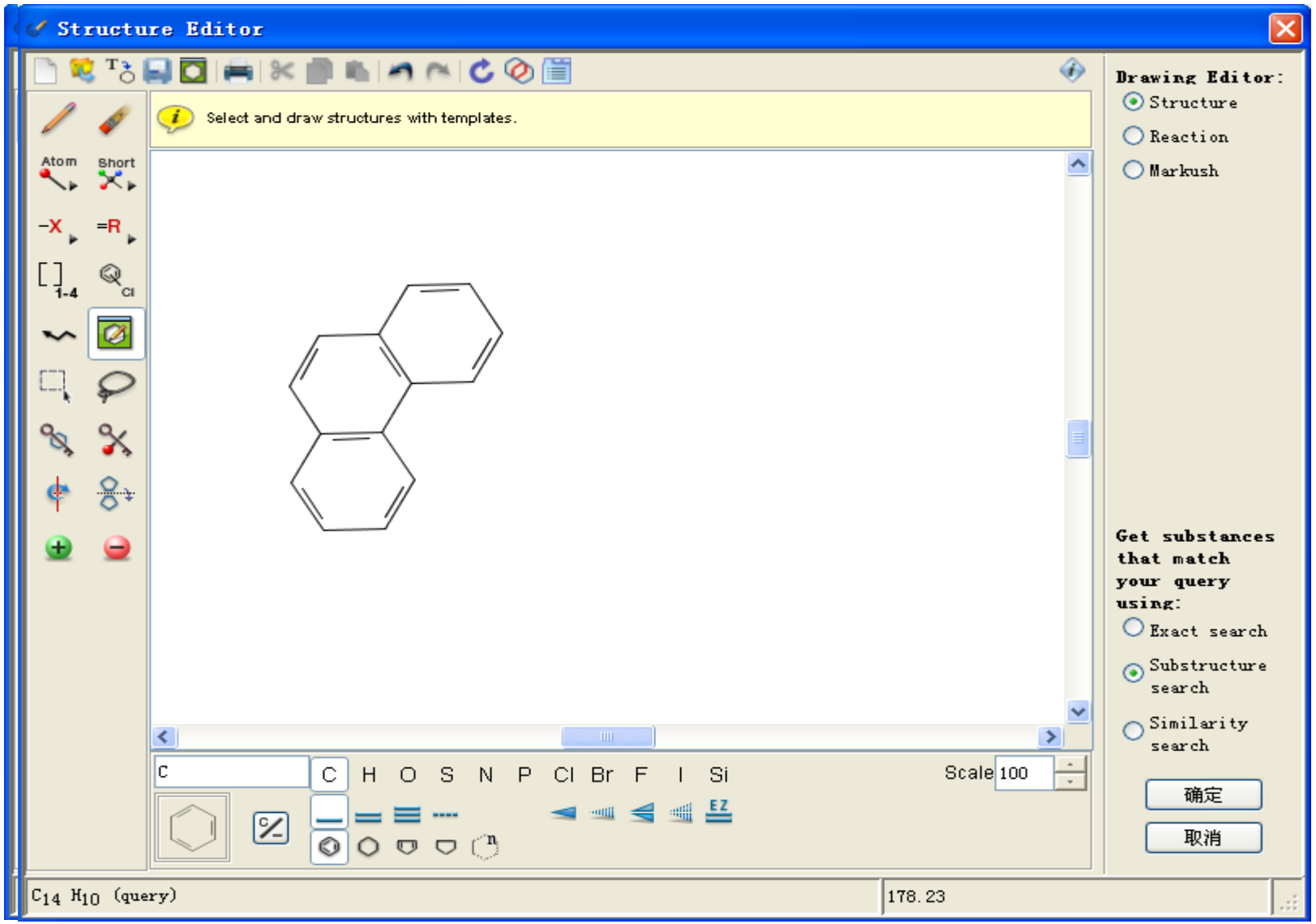
2）含碳的化合物，则“C”在前。

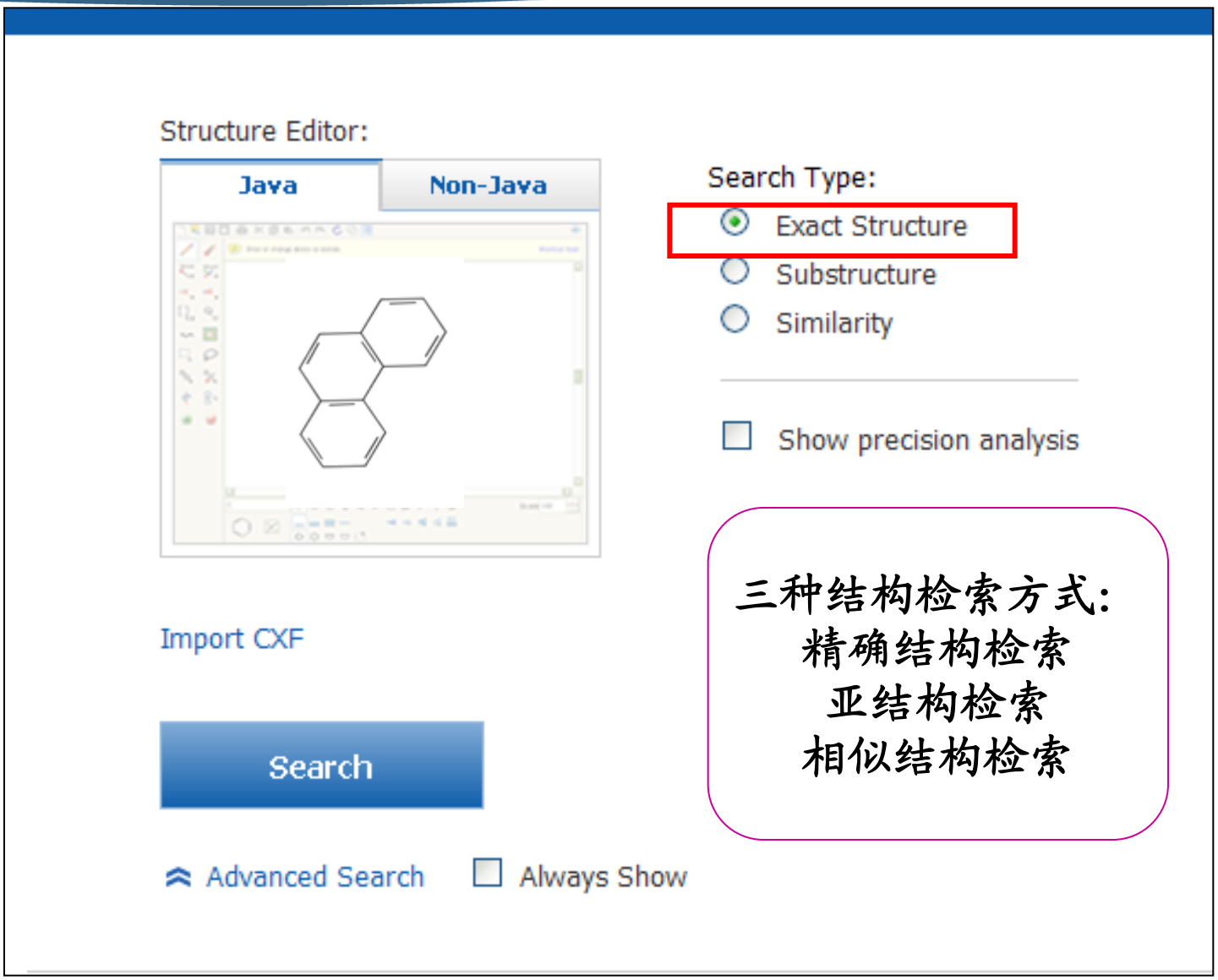
3）如有“H”则紧随其后，其他元素符号按照字母顺序排列在氢后。

4. 结构式检索

只了解一个化学结构式，怎样获得具体的物质信息？




Structure Editor
Select and draw structures with templates.
Atom
Short
-X
=R
1-4
Cl
C H O S N P Cl Br F I Si
Scale 100
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
C14 H10 (query)
178.23


Structure Editor:
Java
Non-Java
Search Type:
Exact Structure
Substructure
Similarity
Show precision analysis
Import CXF
Search
Advanced Search
Always Show
三种结构检索方式:
精确结构检索
亚结构检索
相似结构检索

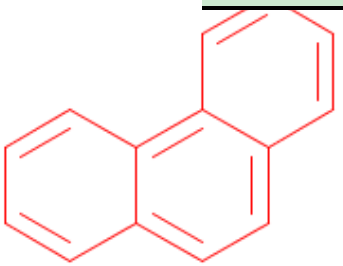
精确结构检索

551 Substances 0 Selected

Select All Deselect All | Sort by: CAS Registry Number

CAS Registry Number
Number of References
Molecular Weight
Molecular Formula

1. Substance Detail
1336891-83-8
(Component: 85-01-8)



● 3 K

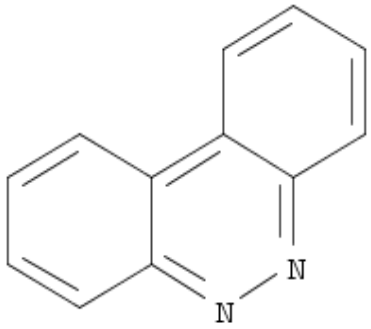
C14 H10 . 3 K

Phenanthrene, potassium salt (1:3)

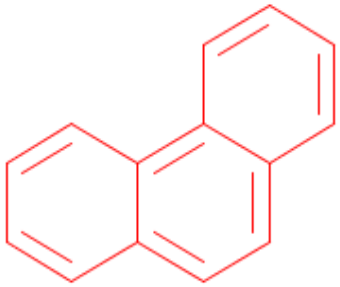
~1 References
Reactions
Commercial Sources

$_3{}^{+}N-(CH_2)_9-Me$

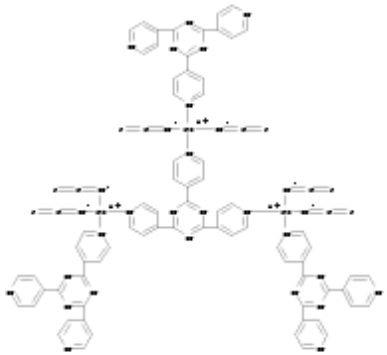
230-17-1
$C_{12}H_8N_2$



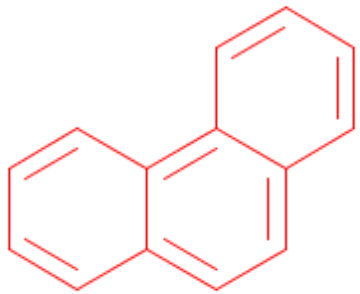
85-01-8
$C_{14}H_{10}$



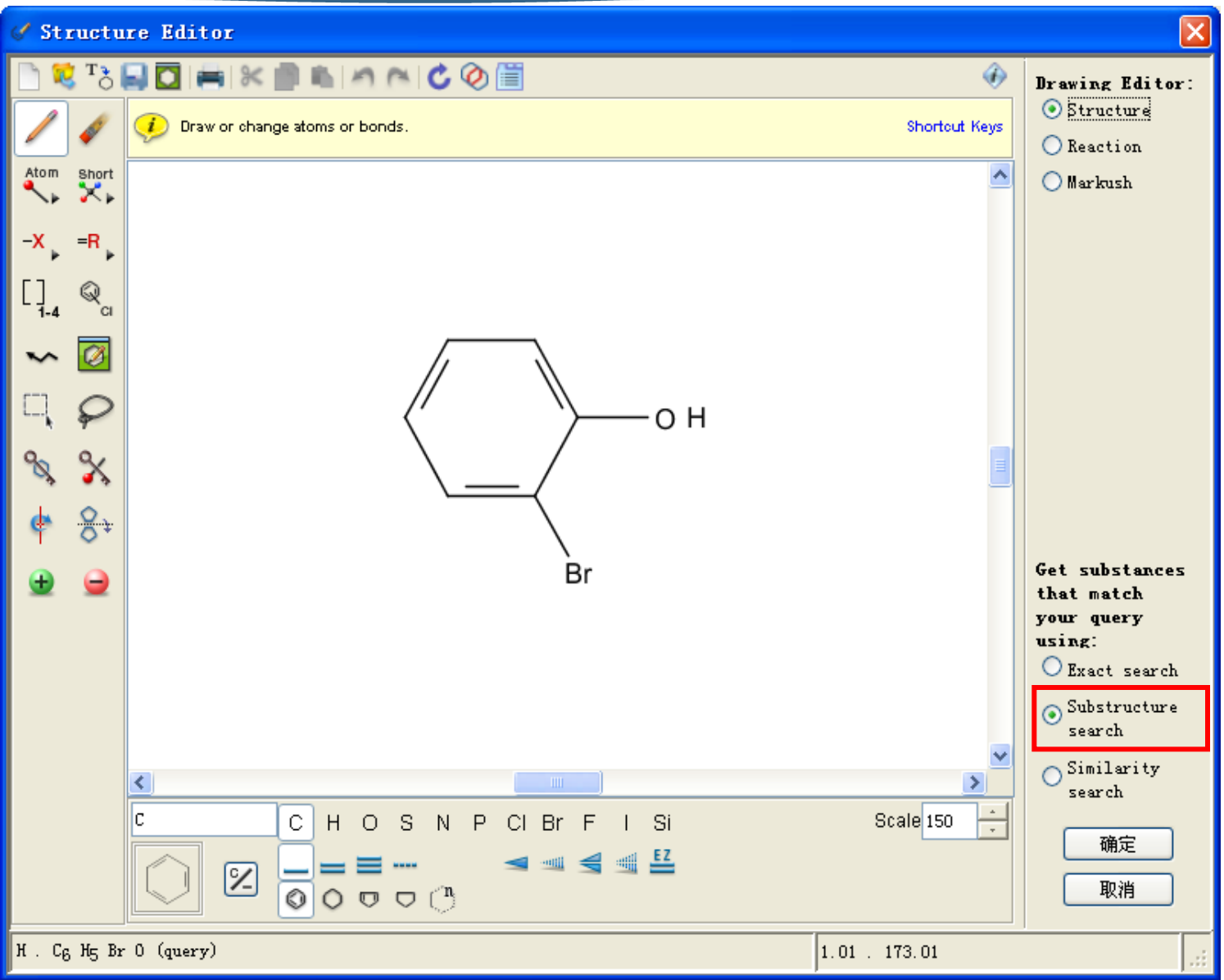
1252019-62-7
$C_{78}H_{48}Co_3N_{30}S_6$



85-01-8
$C_{14}H_{10}$

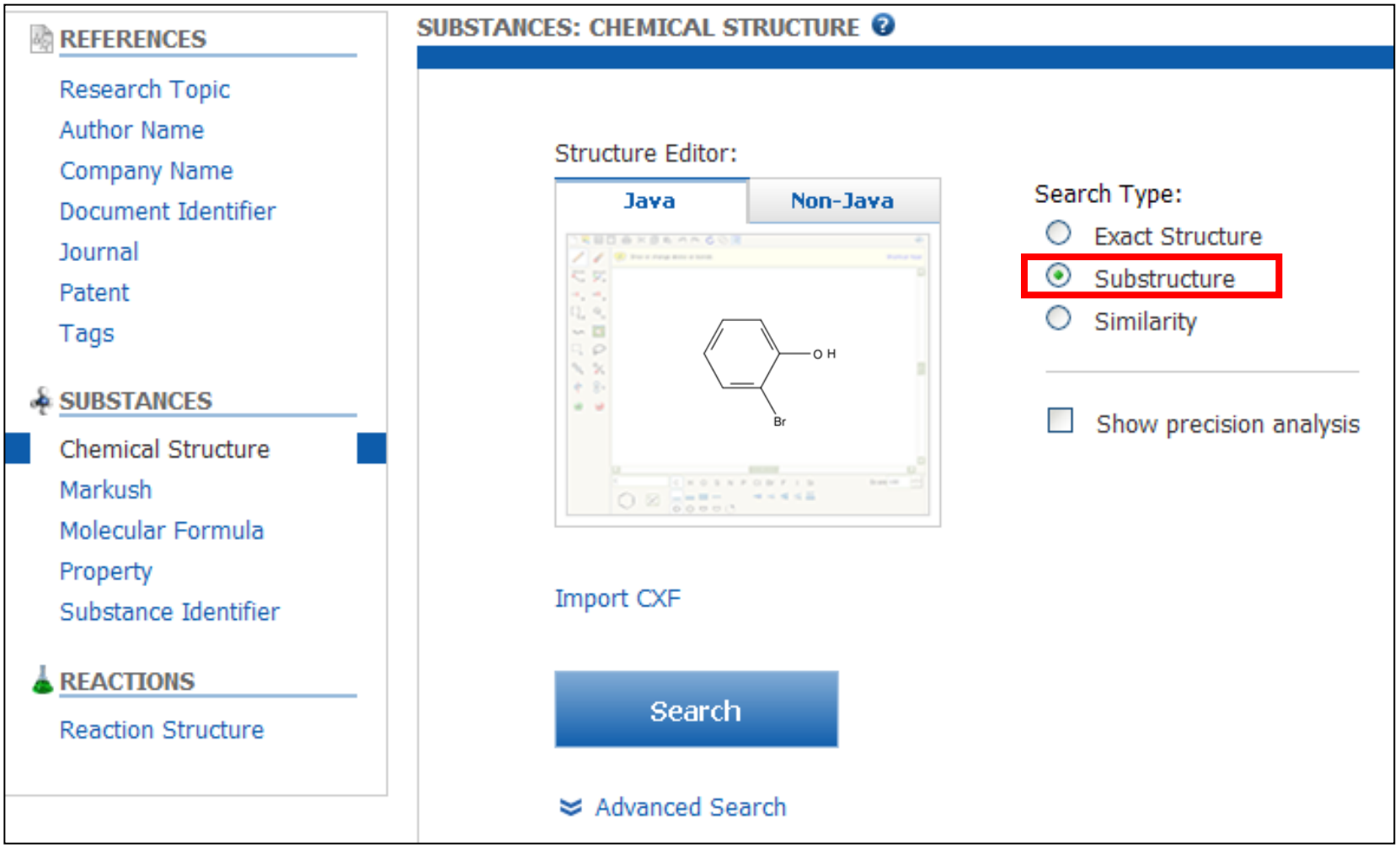


亚结构检索

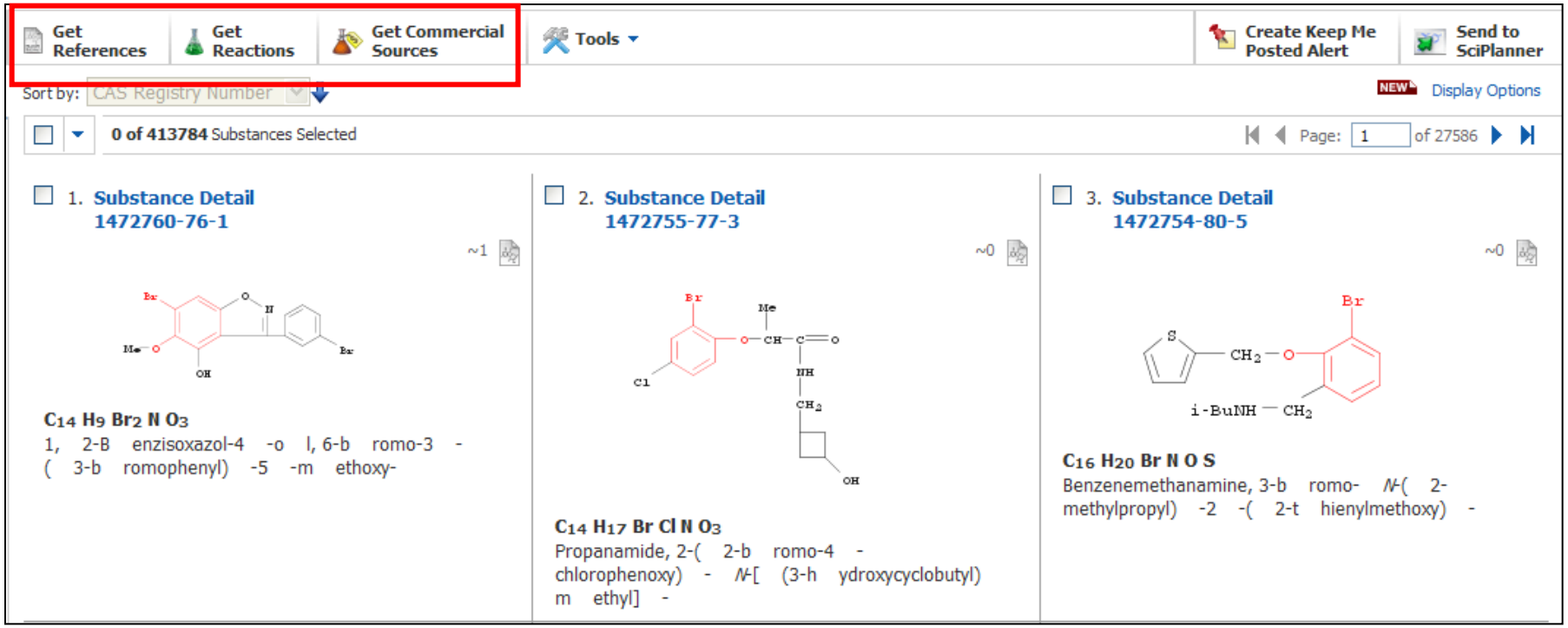


亚结构检索

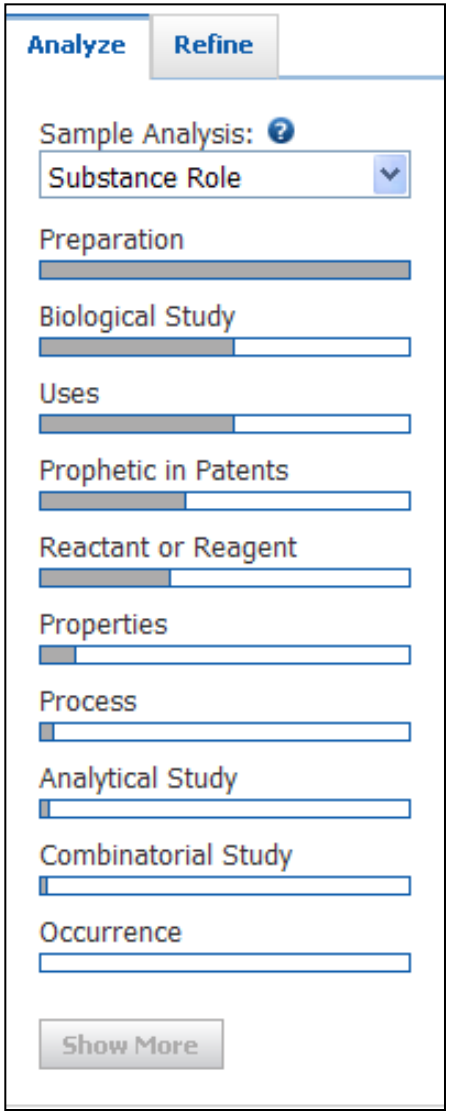
查找特定母核结构的一类物质

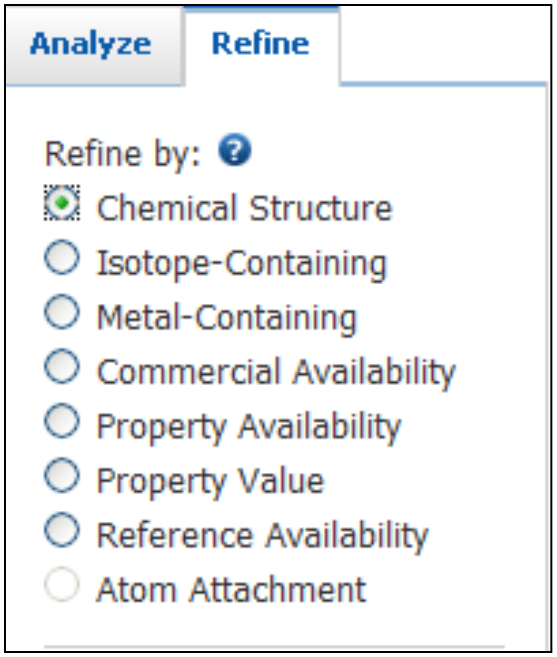

REFERENCES
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier
REACTIONS
Reaction Structure
SUBSTANCES: CHEMICAL STRUCTURE
Structure Editor:
Java
Non-Java
O H
Br
Search Type:
Exact Structure
Substructure
Similarity
Show precision analysis
Import CXF
Search
Advanced Search

获得与物质有关的文献、反应、商品信息。



物质检索分析限定工具





七种限定功能：

1 结构修饰

2 同位素包含

3 金属包含

4 商业来源

5 理化性质

6 文献来源

7 原子附属性

Analysis | **Refine**

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Contai
- Commercial
- Property Ava
- Property Val
- Reference A
- Atom Attach

可精选物质的熔点、沸点、PH值等信息

Select a property on the left, and specify values or limits on the right. Repeat for multiple properties.

Properties - 1 selected

Experimental

- Boiling Point
- Melting Point

Predicted

- H Acceptors
- H Donors
- Molecular Weight
- logP
- Freely Rotatable Bonds
- Bioconcentration Factor
- Boiling Point
- Density
- Enthalpy of Vaporization
- Flash Point
- H Acceptor/Donor Sum
- Koc
- logD
- Mass Intrinsic Solubility

Values - Predicted pKa

Specify range:

0.0 to 14.0

Min: Max:

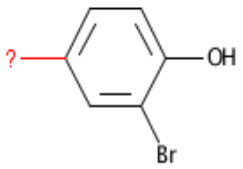
Limit by:

- Most acidic
- Most basic

Analysis | Refine

Refine by:

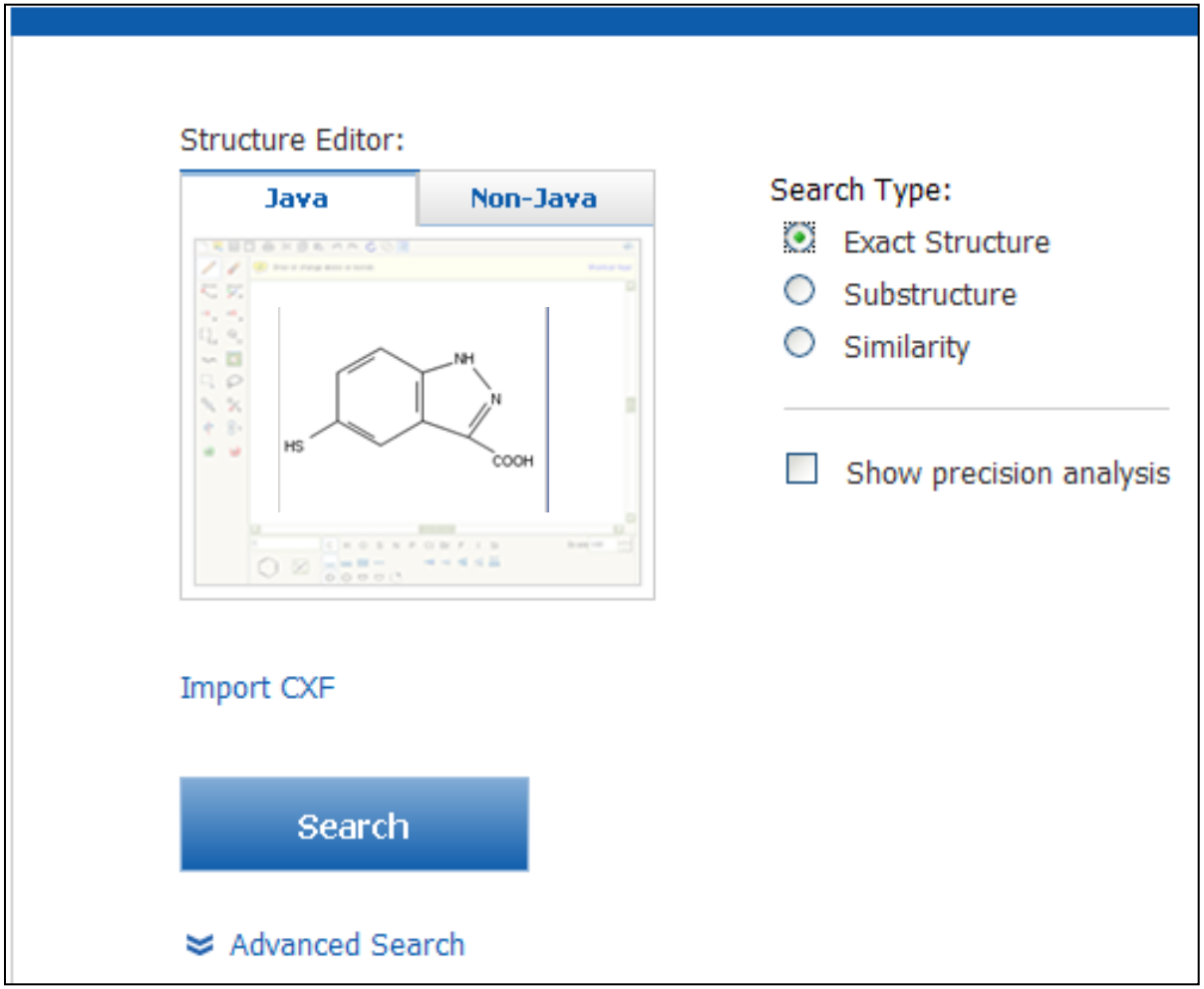
- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment



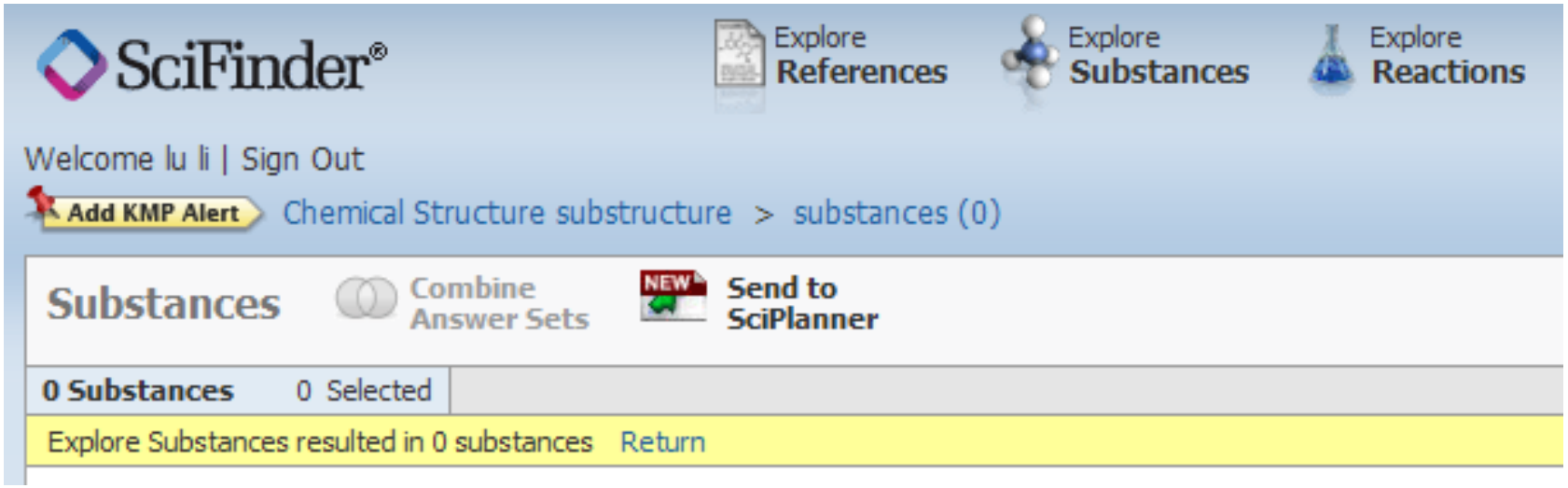
精炼指定处（问号处）所带的元素

? =

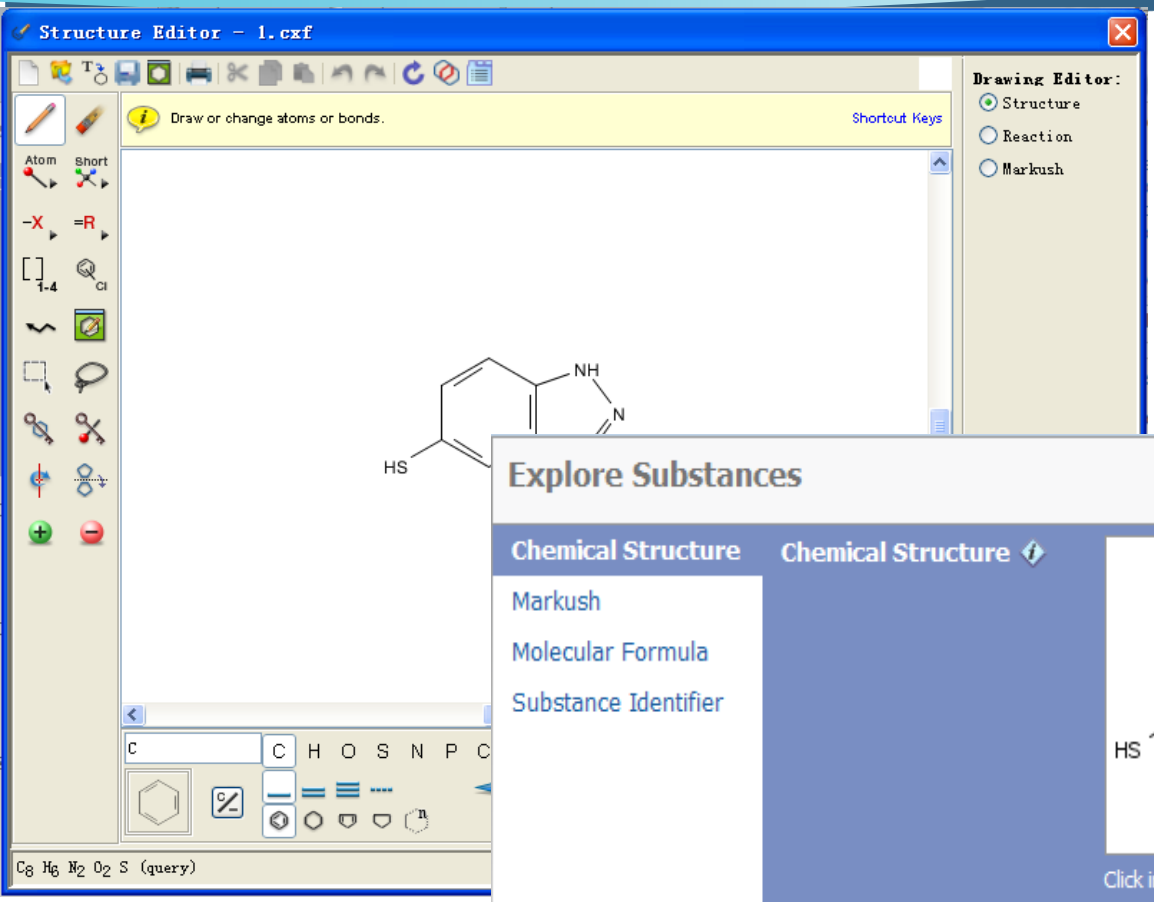
相似结构检索

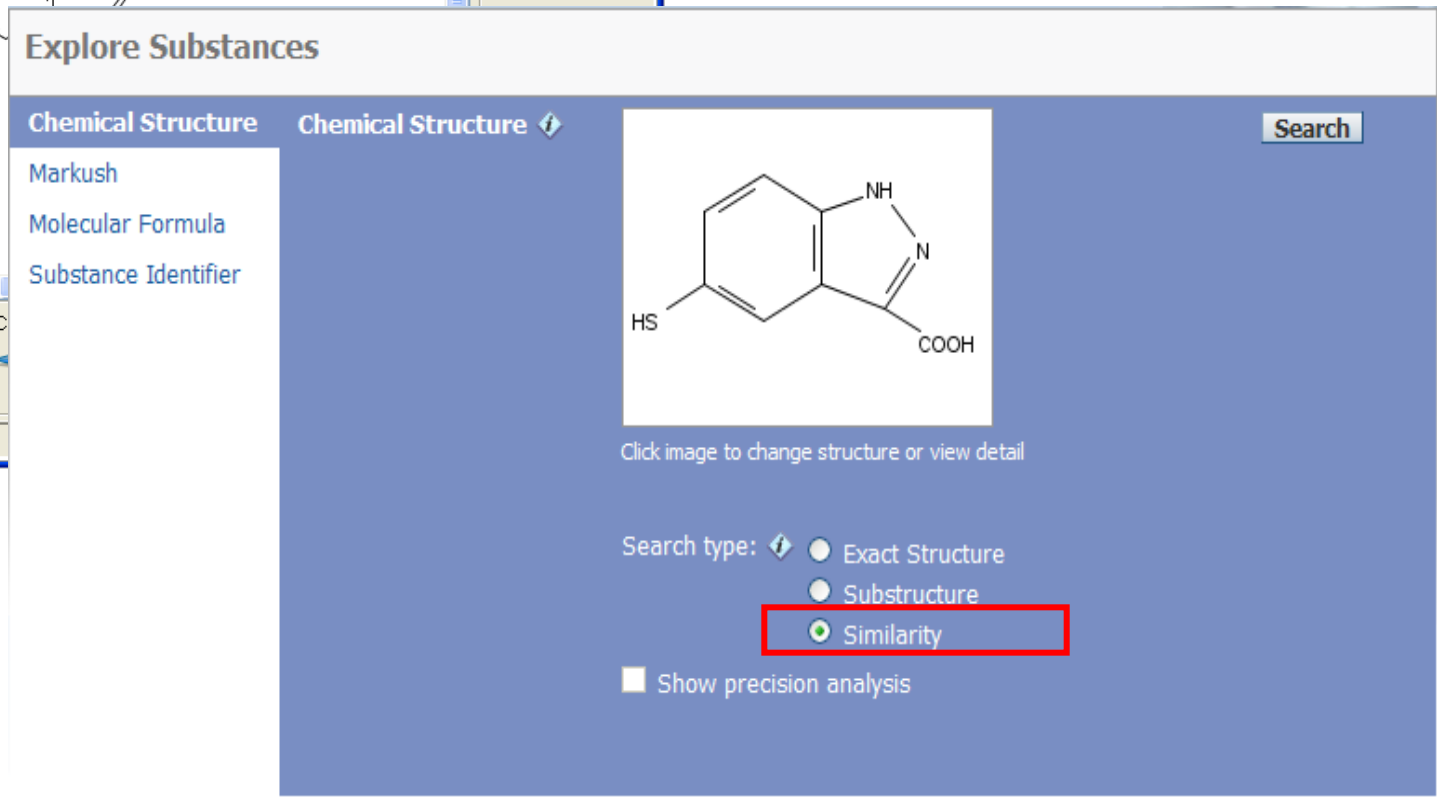


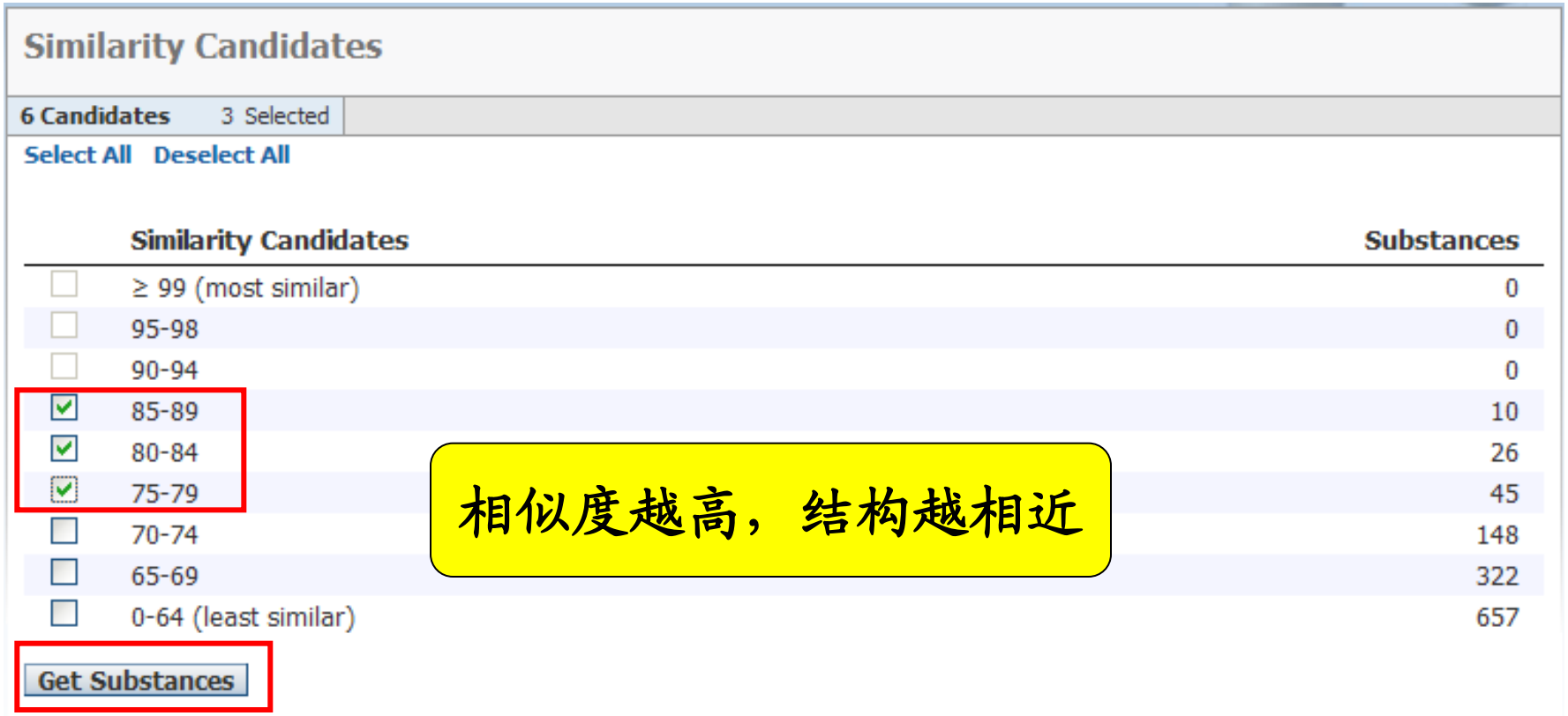
想要合成一种设计的新物质



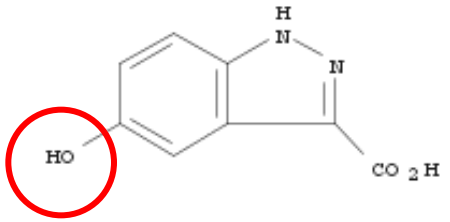
检索结果为0，新物质，未合成过可通过相似物质的反应，得到新物质的合成可能性。


Structure Editor - 1.cxf
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
NH
N
HS
C H O S N P C
C8 H8 N2 O2 S (query)


Explore Substances
Chemical Structure
Markush
Molecular Formula
Substance Identifier
Chemical Structure
Search
NH
N
HS
COOH
Click image to change structure or view detail
Search type:
Exact Structure
Substructure
Similarity
Show precision analysis


Similarity Candidates
6 Candidates
3 Selected
Select All
Deselect All
Similarity Candidates
Substances
≥ 99 (most similar) 0
95-98 0
90-94 0
85-89 10
80-84 26
75-79 45
70-74 148
65-69 322
0-64 (least similar) 657
Get Substances
相似度越高，结构越相近

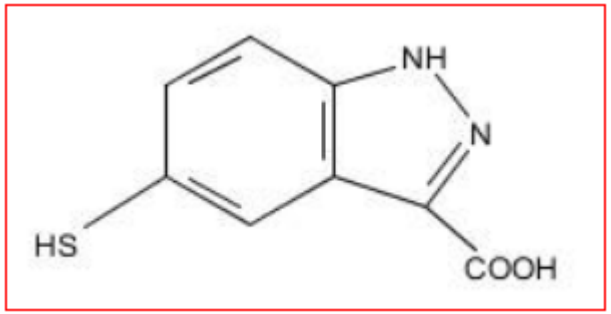
1. **Substance Detail** *Score:* 88
885518-94-5



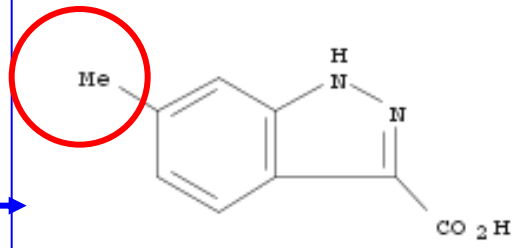
C8 H6 N2 O3

1H-Indazole-3-carboxylic acid, 5-hydroxy

取代基不同



4. **Substance Detail** *Score:* 86
858227-12-0



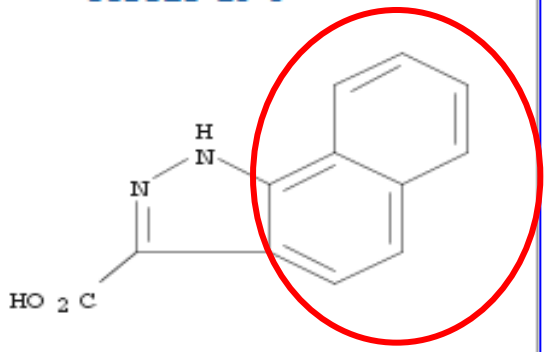
C9 H8 N2 O2

1H-Indazole-3-carboxylic acid, 6-methyl-

取代基和位置不同

母核结构不同

64. **Substance Detail** *Score:* 76
665020-19-9



C12 H8 N2 O2

1H-Benz[g]indazole-3-carboxylic acid

5. Makrush检索

- 具体物质[Specific Substance]：

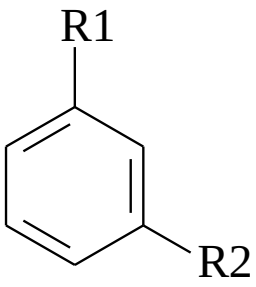
  以具体化学结构所陈述的特定物质，会被标示CAS No.

- 预测性物质[Prophetic Substance]：

  使用Markush结构所陈述的预测物质，一个Markush可以陈述上百或上千的化学物质

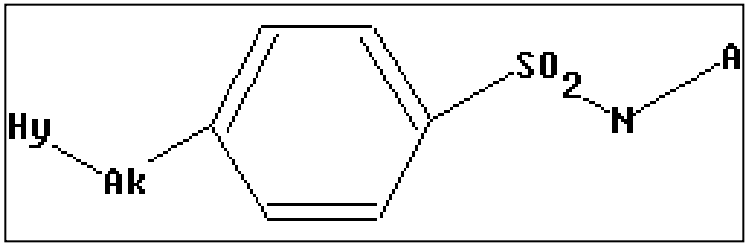
  Patent 中所陈述的预测物质，不会被标示CAS No.

  Markush检索，能检索到通过结构检索检不到的专利

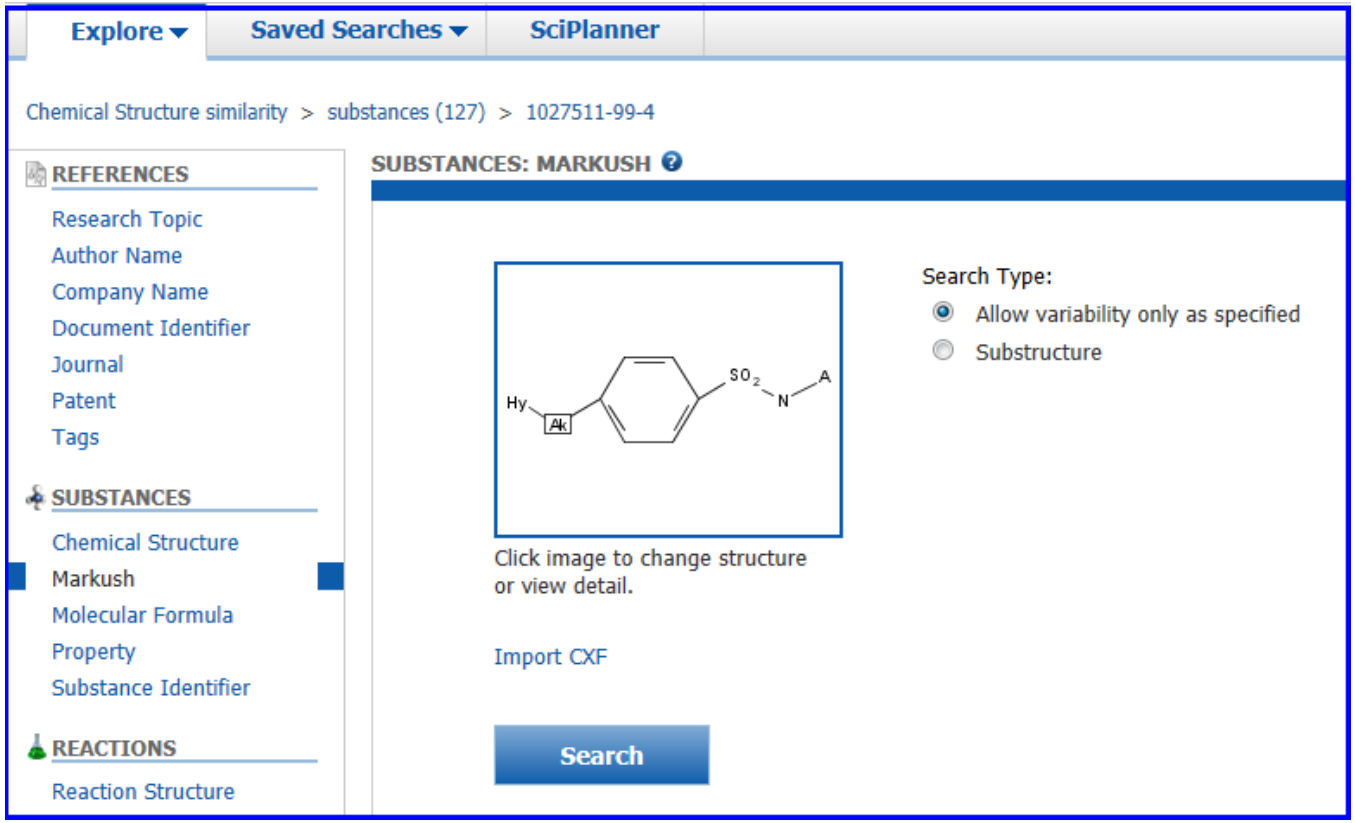


R1 = H, Br, Cl, I

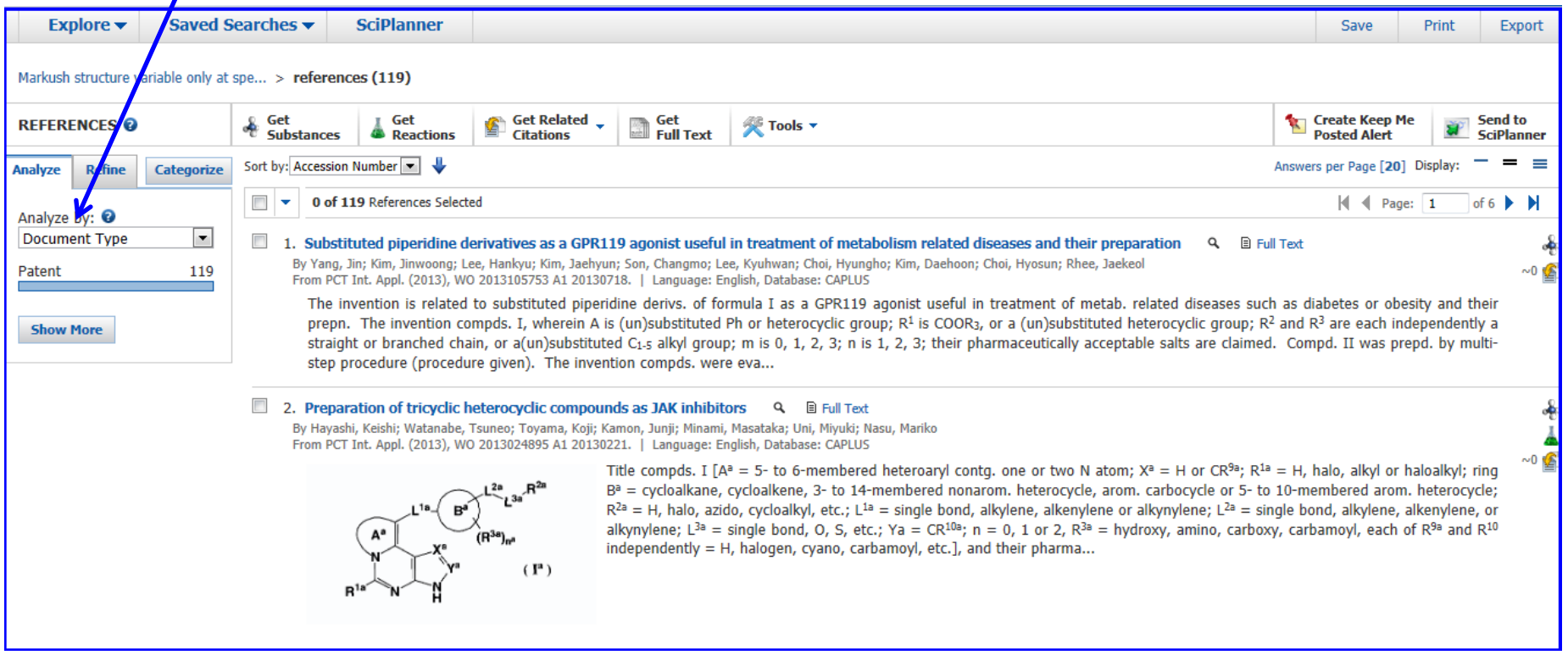
R2 = Br, Cl, I, —CH_2–halogen, —CH(–CH_3)–halogen,



SciFinder中的Markush检索能帮助做初步的专利评估。



全部是专利文献


Explore
Saved Searches
SciPlanner
Save
Print
Export
Markush structure variable only at spe... > references (119)
REFERENCES
Get Substances
Get Reactions
Get Related Citations
Get Full Text
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Categorize
Sort by: Accession Number
Answers per Page [20] Display:
Analyze by:
Document Type
Patent 119
Show More
0 of 119 References Selected
Page: 1 of 6
1. Substituted piperidine derivatives as a GPR119 agonist useful in treatment of metabolism related diseases and their preparation
Full Text
By Yang, Jin; Kim, Jinwoong; Lee, Hankyu; Kim, Jaehyun; Son, Changmo; Lee, Kyuhwan; Choi, Hyungho; Kim, Daehoon; Choi, Hyosun; Rhee, Jaekeol
From PCT Int. Appl. (2013), WO 2013105753 A1 20130718. | Language: English, Database: CAPLUS
The invention is related to substituted piperidine derivs. of formula I as a GPR119 agonist useful in treatment of metab. related diseases such as diabetes or obesity and their prepn. The invention compds. I, wherein A is (un)substituted Ph or heterocyclic group; R1 is COOR3, or a (un)substituted heterocyclic group; R2 and R3 are each independently a straight or branched chain, or a(un)substituted C1-5 alkyl group; m is 0, 1, 2, 3; n is 1, 2, 3; their pharmaceutically acceptable salts are claimed. Compd. II was prepd. by multi-step procedure (procedure given). The invention compds. were eva...
2. Preparation of tricyclic heterocyclic compounds as JAK inhibitors
Full Text
By Hayashi, Keishi; Watanabe, Tsuneo; Toyama, Koji; Kamon, Junji; Minami, Masataka; Uni, Miyuki; Nasu, Mariko
From PCT Int. Appl. (2013), WO 2013024895 A1 20130221. | Language: English, Database: CAPLUS
Title compds. I [Aa = 5- to 6-membered heteroaryl contg. one or two N atom; Xa = H or CR9a; R1a = H, halo, alkyl or haloalkyl; ring Ba = cycloalkane, cycloalkene, 3- to 14-membered nonarom. heterocycle, arom. carbocycle or 5- to 10-membered arom. heterocycle; R2a = H, halo, azido, cycloalkyl, etc.; L1a = single bond, alkylene, alkenylene or alkynylene; L2a = single bond, alkylene, alkenylene, or alkynylene; L3a = single bond, O, S, etc.; Ya = CR10a; n = 0, 1 or 2, R3a = hydroxy, amino, carboxy, carbamoyl, each of R9a and R10 independently = H, halogen, cyano, carbamoyl, etc.], and their pharma...

结构检索小结

精确结构检索：

获得物质的盐、聚合物、配合物等，母体结构不能改变，不能修饰

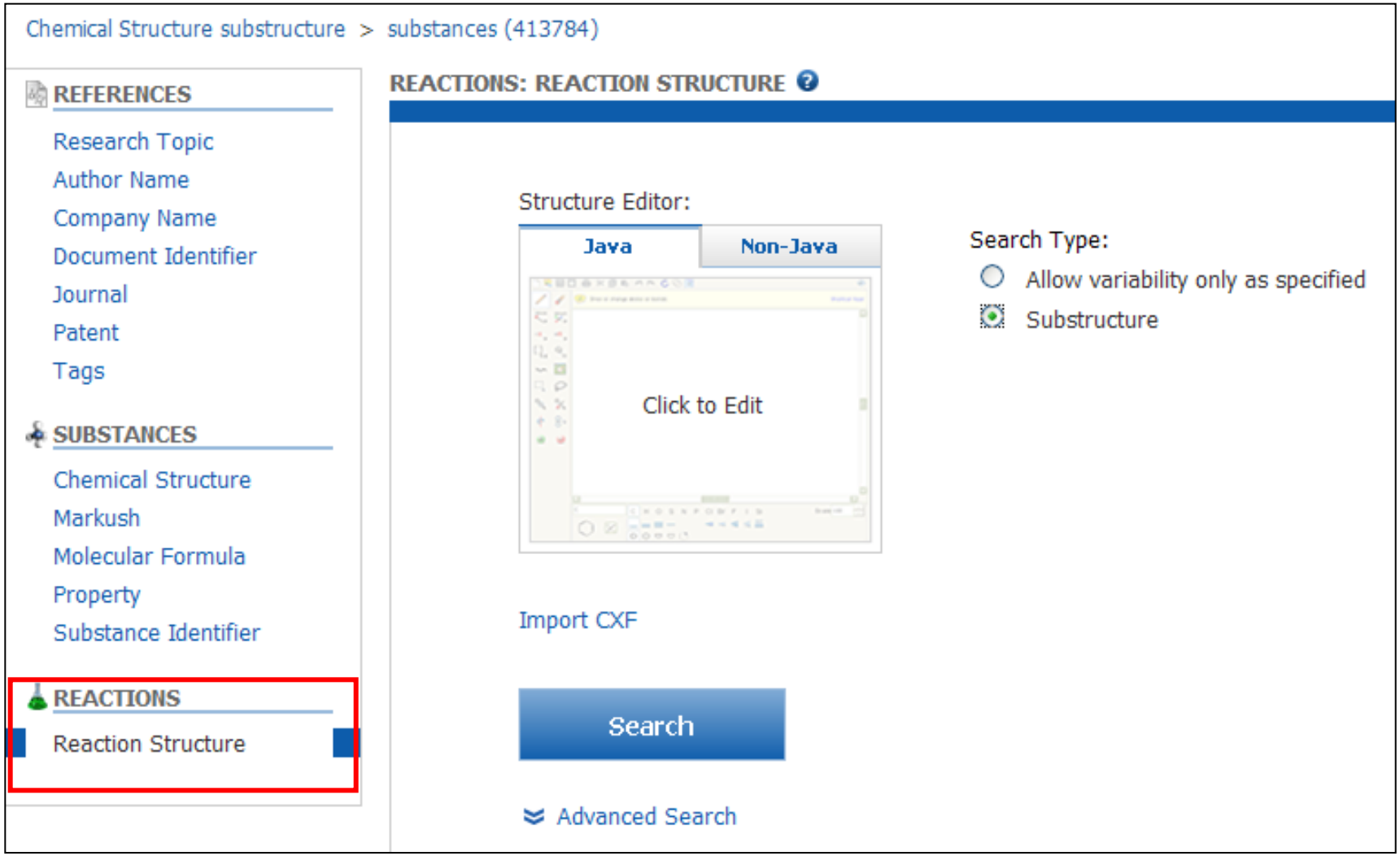
亚结构检索：

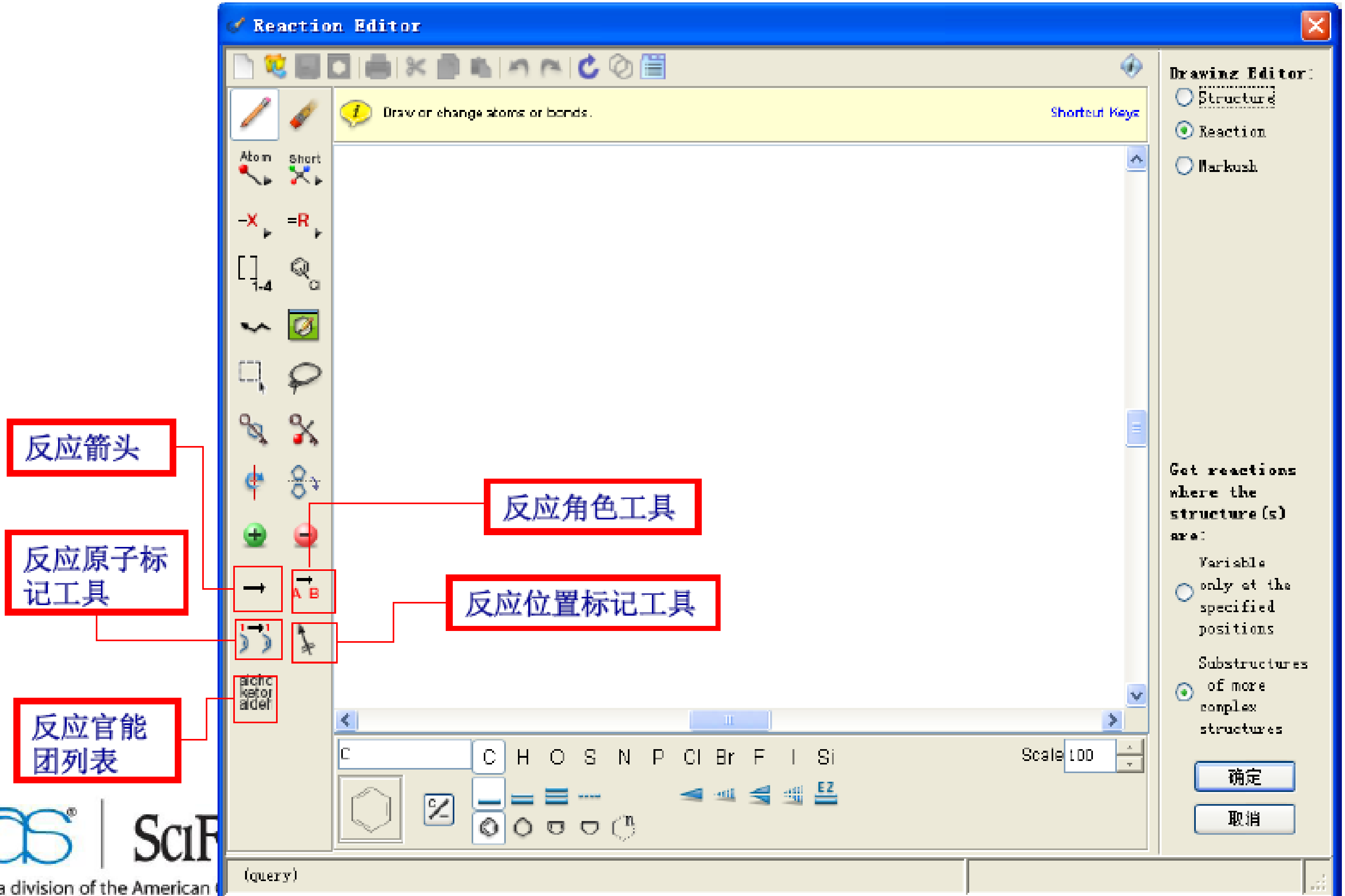
所画的结构必须存在，母体结构不能修改，但可以修饰。

相似结构检索：

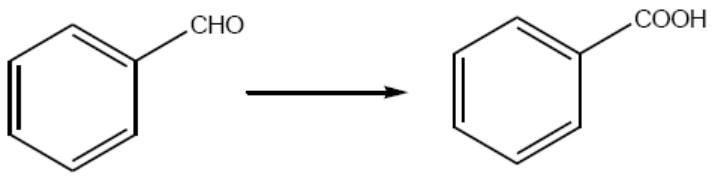
母体结构可以修改，可以修饰，相似度来控制获得的结果。

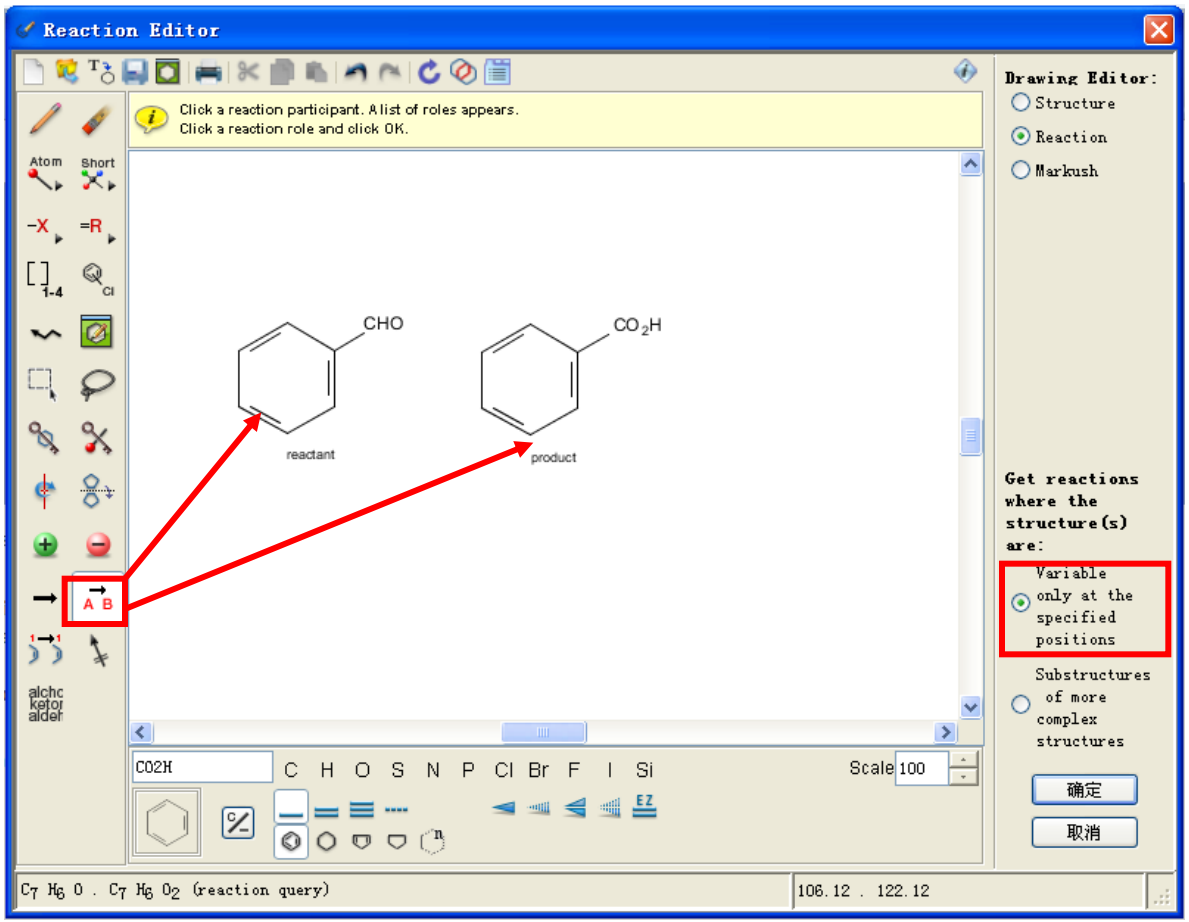
检索方式-反应检索


Chemical Structure substructure > substances (413784)
REFERENCES
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier
REACTIONS
Reaction Structure
REACTIONS: REACTION STRUCTURE
Structure Editor:
Java
Non-Java
Click to Edit
Search Type:
Allow variability only as specified
Substructure
Import CXF
Search
Advanced Search

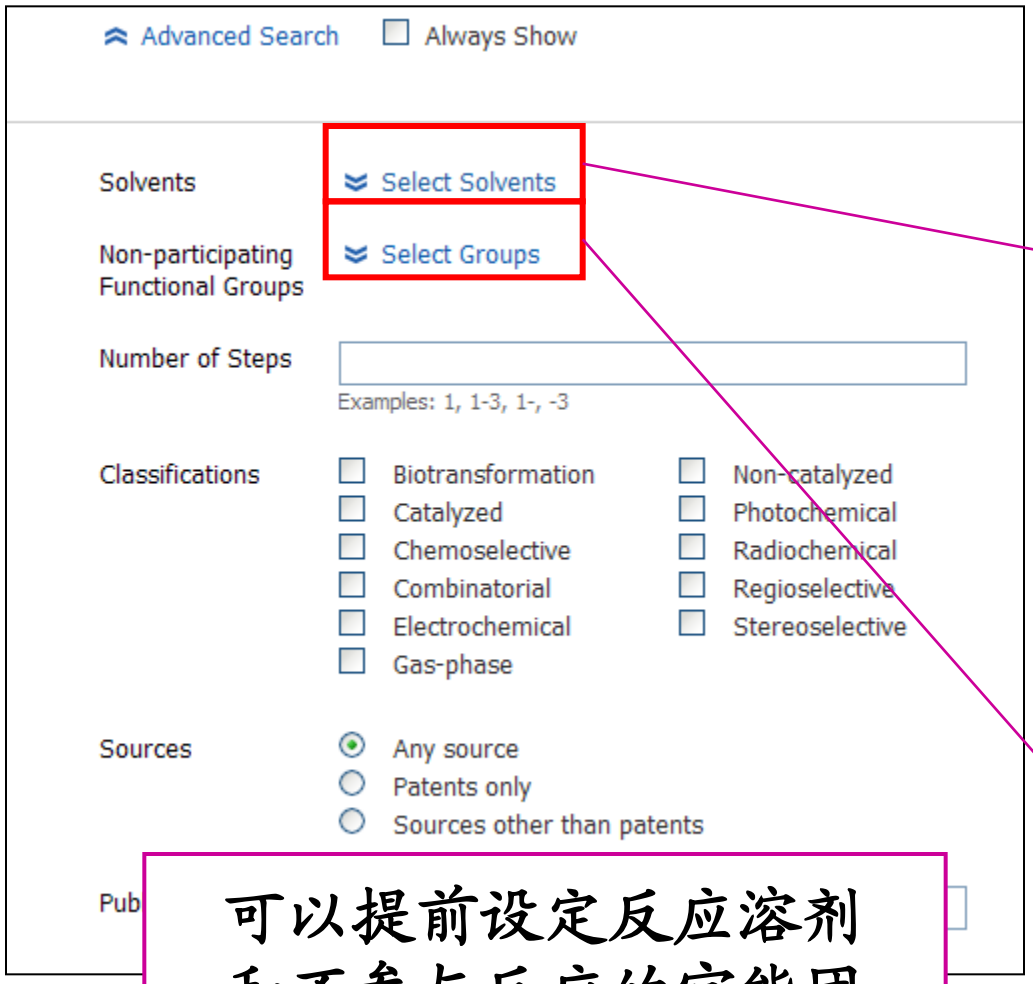


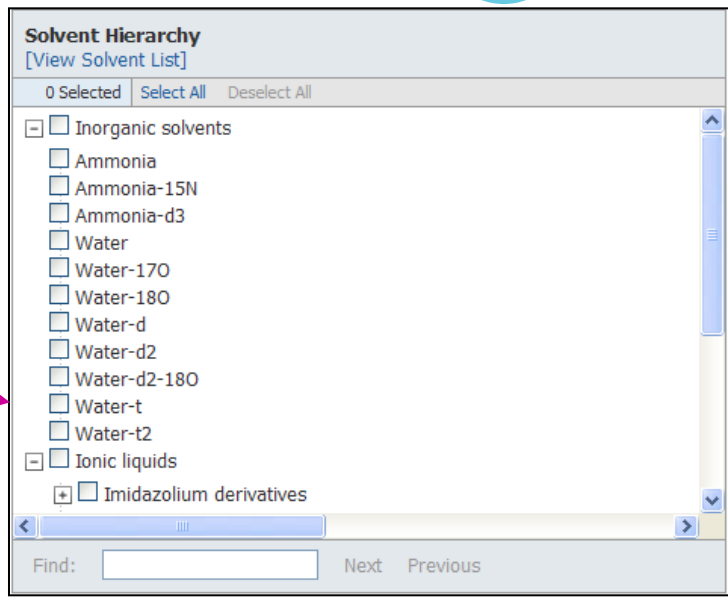
SciF
S is a division of the American

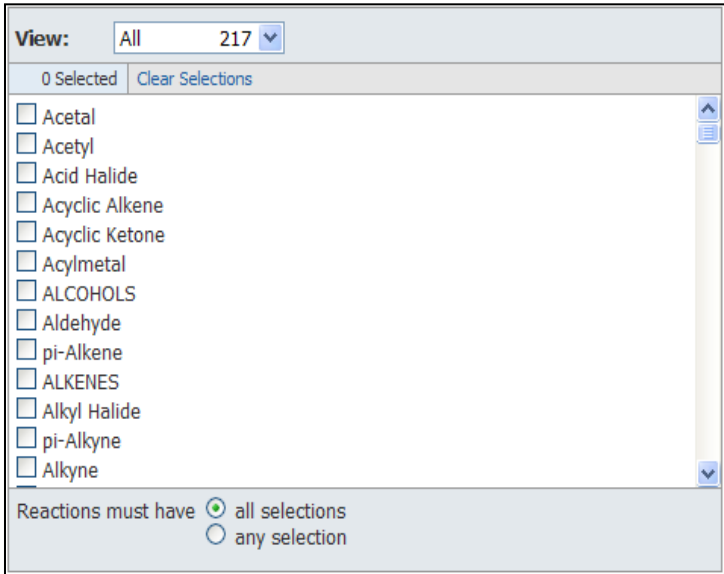




精确物质检索获得特定的物质反应







可以提前设定反应溶剂
和不参与反应的官能团

Reactions | Get References | Tools | NEW Send to SciPlanner

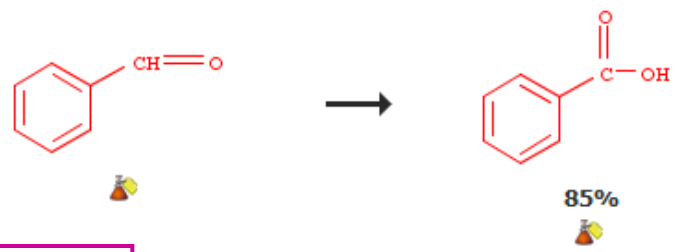
320 Reactions | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Relevance | Answers per Page [15] | 1 2 3 4 5 6 ... 22

Display:

1. View Reaction Detail | Link | Similar Reactions

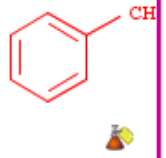
Single Step *Hover over any structure for more options.*



Overview

2. View Reaction D

Single Step *Hover o*



Overview

Overview

Steps/Stages

1.1 R:H_2O_2, C:69289-47-0, S:H_2O, rt; rt → 80°C; 2.5 h, 80°C; 24 h, cooled

Notes

optimization study, optimized on catalyst, reagent, reaction time, temperature, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Synthesis of Keggin compound [(CH2)5NH2]4SiMo12O40 and synthesis of benzoic acid by catalytic oxidation with it

By Ding, Yuansheng et al

From Jingxi Shiyou Huagong, 27(3), 19-22; 2010

Full Text

Analysis | Refine

Analyze by:

Catalyst

Click bar to view only those reactions within the current answer set

Na_2WO_4	14
Au	12
$Bu_4N^+ \cdot Br^-$	5
12304-65-3	4
141556-45-8	4
18-Crown-6	4

查看实验过程

Reactions | Get References | Tools | NEW Send to SciPlanner

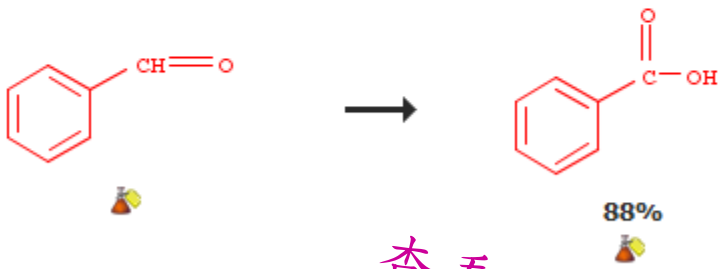
20 Reactions 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Relevance | Answers per Page [15] 1 2

Display:

1. View Reaction Detail | Link | Similar Reactions

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



查看实验过程

▸ Overview

▸ Experimental Procedure

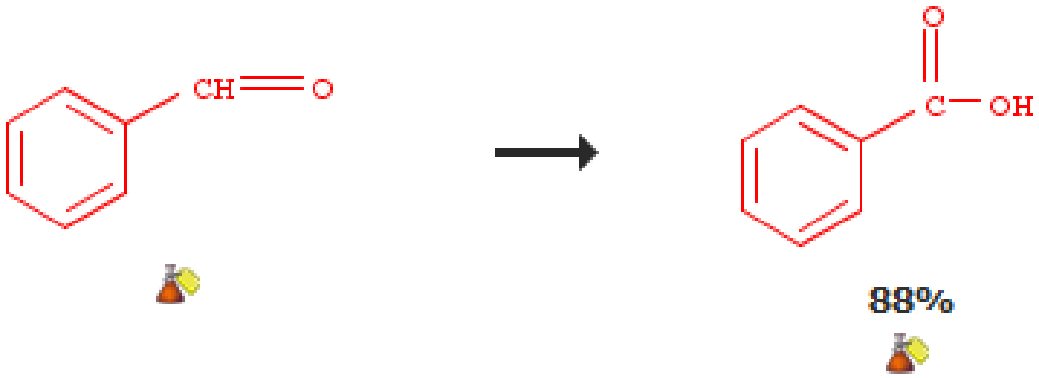
▾ Experimental Procedure

Organic LETTERS

General/Typical Procedure: (a) Synthesis of carboxylic acids:- DBU(20 mol %) was added to a suspension of the 1,3-dimesityl imidazolinium chloride (15 mol %) and aldehyde(1 mmol) in dry THF. A slow stream of CO_2 was passed through this solution for 15 minutes. The reaction mixture was quenched with hydrochloric acid (1N, 5ml) and extracted with dichloromethane (3x4 ml). The organic layer was washed with brine, dried with Na_2SO_4, filtered and concentrated. The concentrated residue was subjected to column chromatography on a silica gel (100-200 mesh) column using 90:10 hexane-ethyl acetate solvent mixture as eluent to afford corresponding carboxylic acid. Compound 3c, yield 88% ^1H NMR (500 MHz, $CDCl_3$) δ 8.13-8.11 (m, 2H) 7.61-7.59 (m, 1H) 7.49-7.46 (m, 1H) ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.0, 133.7, 130.3, 129.4, 128.4

获得反应中心相似的反应

1. **View Reaction Detail** **Link** **Similar Reactions**
Single Step *Hover over any structure for more options.*



- Overview
- Experimental Procedure

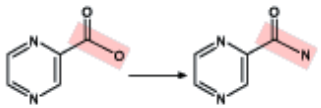
Get Similar Reactions

Retrieve similar reactions from:

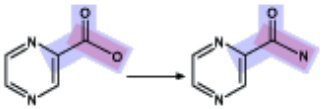
- (•) All reactions
- ( ) Current answer set

Include this level of similarity:

- ( ) Broad - Reaction centers only (9316)



- ( ) Medium - Reaction centers plus adjacent atoms and bonds (4176)



- (•) Narrow - Reaction centers plus extended atoms and bonds (3458)

Broad: 反应中心相似

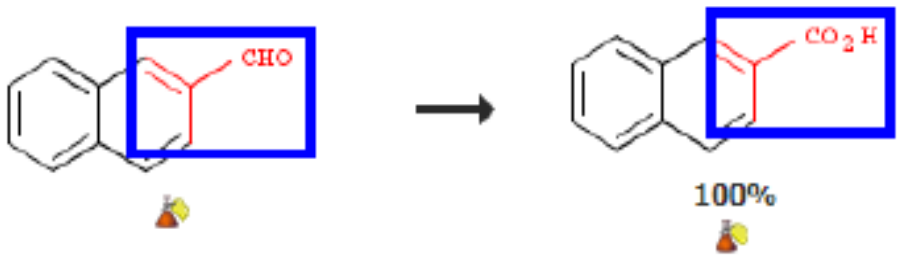
Medium: 反应中心及附属原子和健

Narrow: 反应中心及扩展的原子和健

Display:

1. View Reaction Detail Link Similar Reactions

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



▸ Overview

补充问题

并发用户已满，请稍后再试

用户名或密码错误，请在username处填写，截图，并与图书馆联系

THANK YOU

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Email：hu.jing@scu.edu.cn