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SciFinder Web使用介绍

俞靓

SciFinder培训专员

2014.12

提纲

- 介绍
  - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索
- **SciFinder Web的注册**

美国化学文摘社—Chemical Abstracts Service

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

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- 物质报道文献，回溯到1802年
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Chemical Substances

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- >1万种科技期刊的覆盖
- 63家专利发行机构的专利
- 1997年以来的3.65亿条引文记录
- 回溯到1800年
- 每天更新

References from MEDLINE®
- > 1900万条生命科学相关文献
- > 5600 期刊
- 回溯到1946年
- 每天更新

References

Markush Structures
- >102万专利中的Markush结构
- 回溯到1961年
- 每天更新

Markush Structures

SciFinder

Reactions

CASREACT®
- CAS提供的反应信息包含:
  - 反应中的结构信息
  - 反应中所有物质的CAS No
  - 详细的反应条件
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- >1340万物质合成制备信息
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- 反应条件起始于 2003
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- 全球范围内的法规信息
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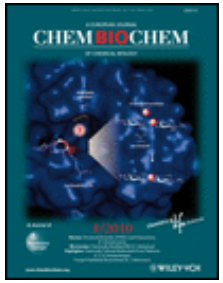

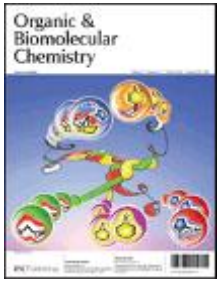

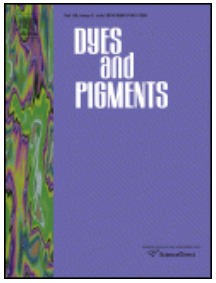

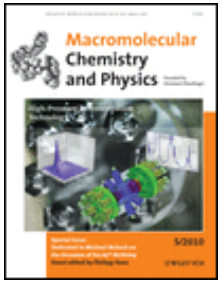

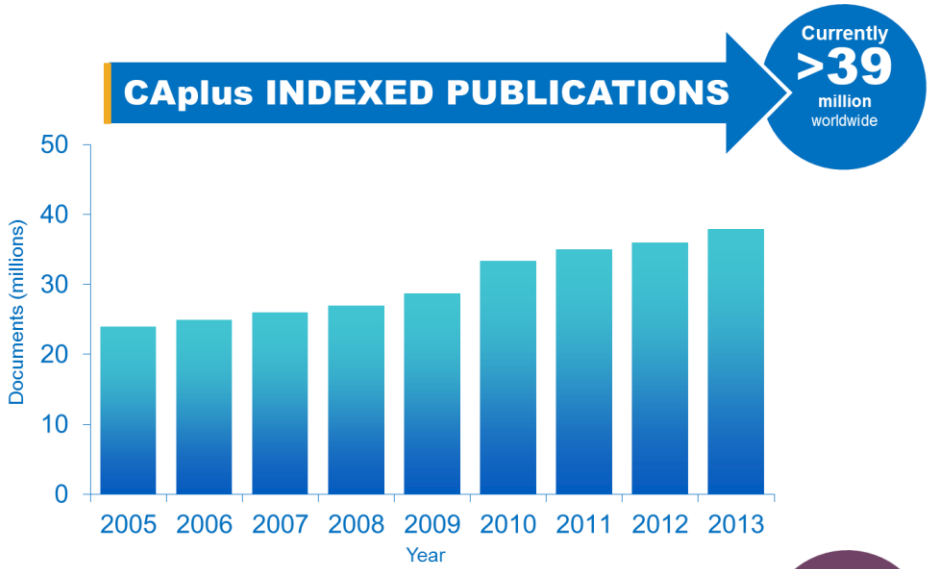

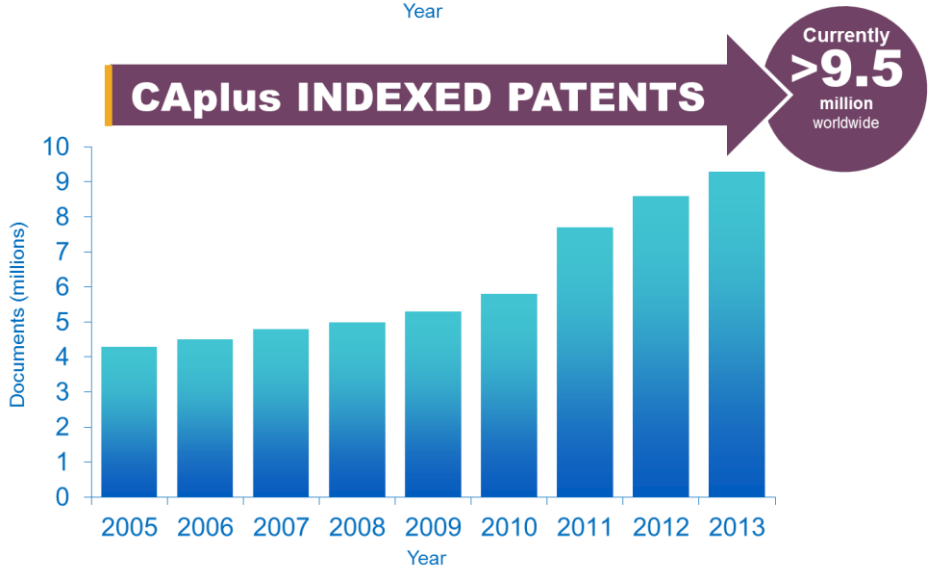

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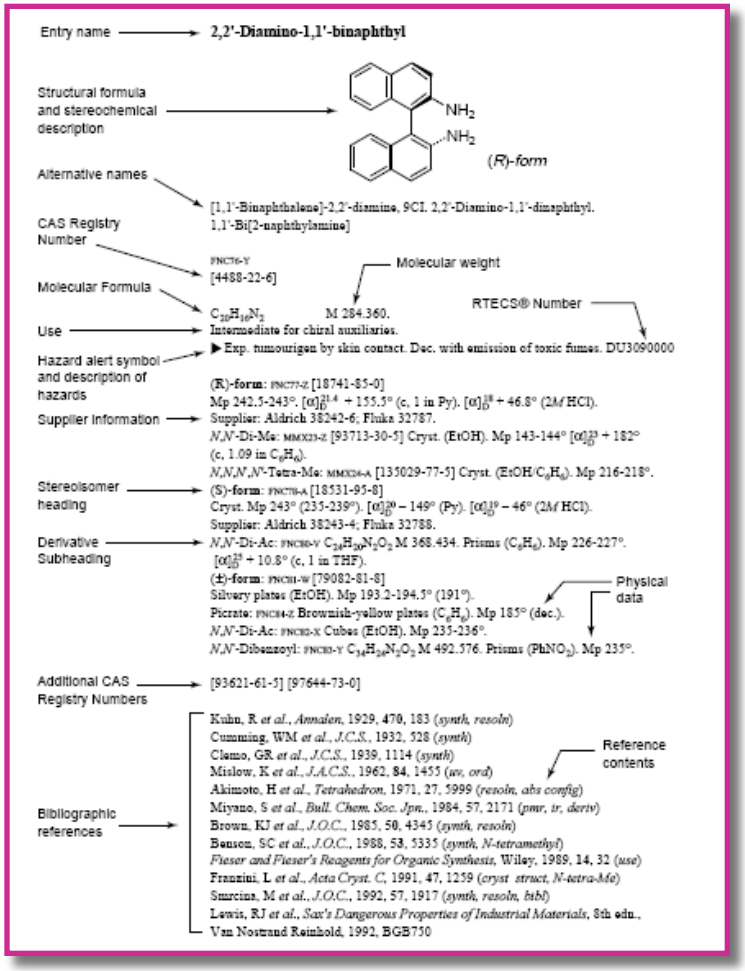

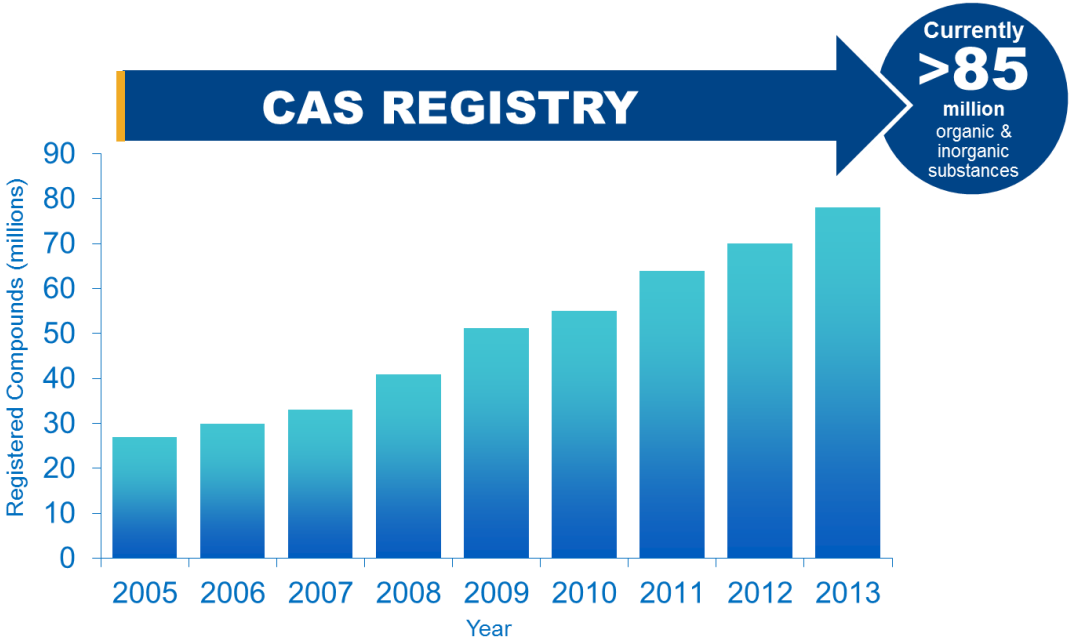

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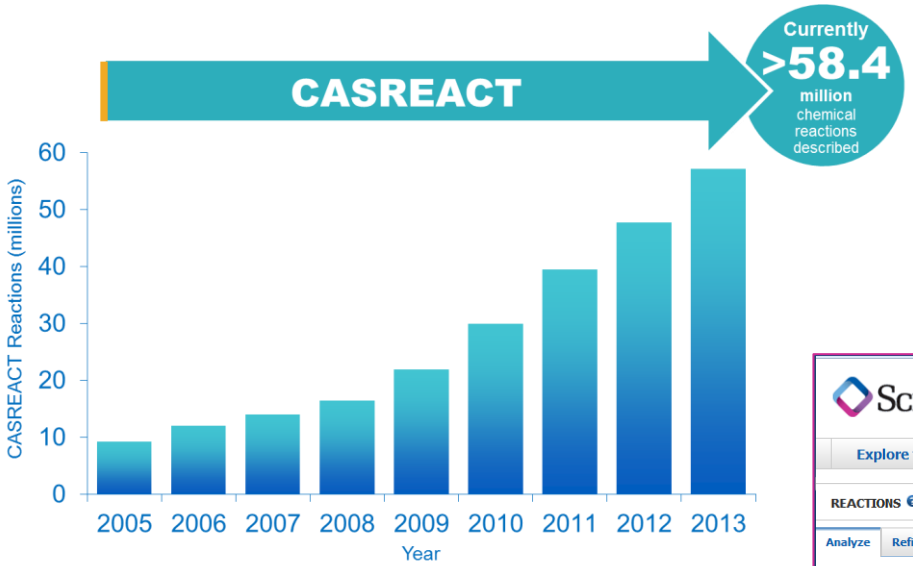

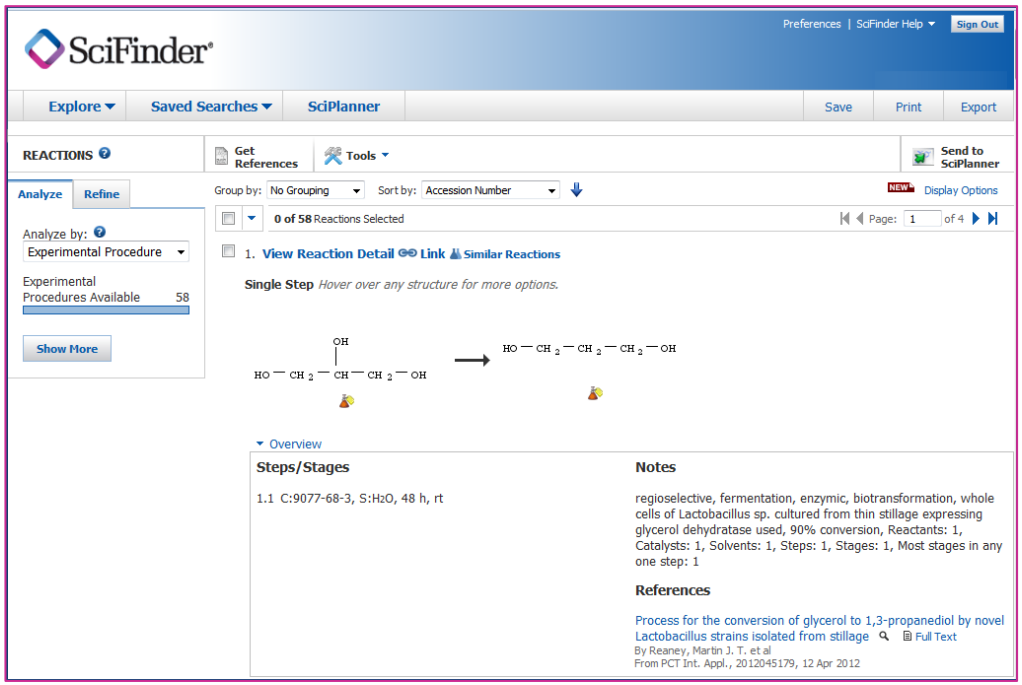

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提纲

- 介绍
  - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
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1. Selective oxidation of light alkanes: interaction between the catalyst and the gas phase on different classes of catalytic materials

By: Cavani, F.; Trifiro, F.

A review, with 202 refs., on the selective oxidn. of light ($C_{\leq 6}$) alkanes to bulk and industrial chems., with emphasis on catalyst-gas phase interactions. Attention was given mainly to: (1) the role of the redox properties of transition metal oxide-based systems, and (2) the contribution of radical-type, homogeneous and heterogeneously-initiated homogeneous reactions over nonreducible metal oxide and noble metal catalysts. Other topics included: (1) key factors in selective oxidn. of light alkanes, (2) bulk and surface properties of catalysts, (3) oxidative dehydrogenation, (4) control of oxygen supply to the catalyst, (5) non-redox-type metal oxides (e.g., alk. earth oxides, rare earth oxides, boron oxides, tin oxides, and silica). Some research examples are: (1) oxidn. of propane to acrylic acid and isobutane to methacrylic acid over Keggin-type heteropolymolybdates, (2) oxidative dehydrogenation of alkanes to alkenes over vanadium oxide-based catalysts, and (3) oxidn. of butane and pentane over vanadyl pyrophosphate.

Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-0)

Section cross-reference(s): 35, 45

Concepts

Redox reaction catalysts

catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Alkaline earth oxides | Rare earth oxides

catalysts contg.; catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Catalyst use; Properties; Uses

Substances

12026-66-3
58834-75-6

catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Catalyst use; Uses

1303-86-2 Boron oxide, uses
1332-29-2 Tin oxide
7631-86-9 Silica, uses

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Catalysis Today
Volume51
Issue3-4
Pages561-580
Journal; General Review
1999
CODEN:CATTEA
ISSN:0920-5861
DOI:10.1016/S0920-5861(99)00041-3

COMPANY/ORGANIZATION

Dipartimento di Chimica Industriale e dei Materiali
Bologna, Italy 40136

ACCESSION NUMBER

1999:340014
CAN131:159478
CAPLUS

PUBLISHER

Elsevier Science B.V.

Citations

Bielanski, A; Oxygen in Catalysis 1991
Haber, J; ACS Symp Series 1996, 638, 20
Oyama, S; ACS Symp Series 1996, 638, 2
Lee, J; Catal Rev-Sci Eng 1988, 30, 249
Kung, H; Adv Catal 1994, 40, 1
Vedrine, J; Catal Today 1997, 33, 3
Vedrine, J; Catal Today 1996, 32, 115
Busca, G; Catal Today 1996, 32, 133
Cavani, F; Catalysis 1994, 11, 246
Albonetti, S; Catal Rev-Sci Eng 1996, 38, 413
Sokolovskii, V; Catal Rev-Sci Eng 1990, 32, 1
Delmon, B; Catalysts in Petroleum Refining and Petrochemical Industries 1995 1996
Burch, R; J Mol Catal A 1995, 100, 13
Schmidt, L; Chem Eng Sci 1994, 49, 3981
Kung, H; ACS Symp Series 1993, 523, 387
Trifiro, F; Selective Partial Oxidation of Hydrocarbons and Related Oxidations 1994
Trifiro, F; Oxidative dehydrogenation and alternative dehydrogenation processes 1993
Cavani, F; Catal Today 1995, 24, 307

一篇完整的文献界面包括：

1. 题录信息
2. 摘要信息
3. 文献中重要的概念
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质，反应，引文等
7. 文献中的引文信息

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  - 从物质，反应获得文献

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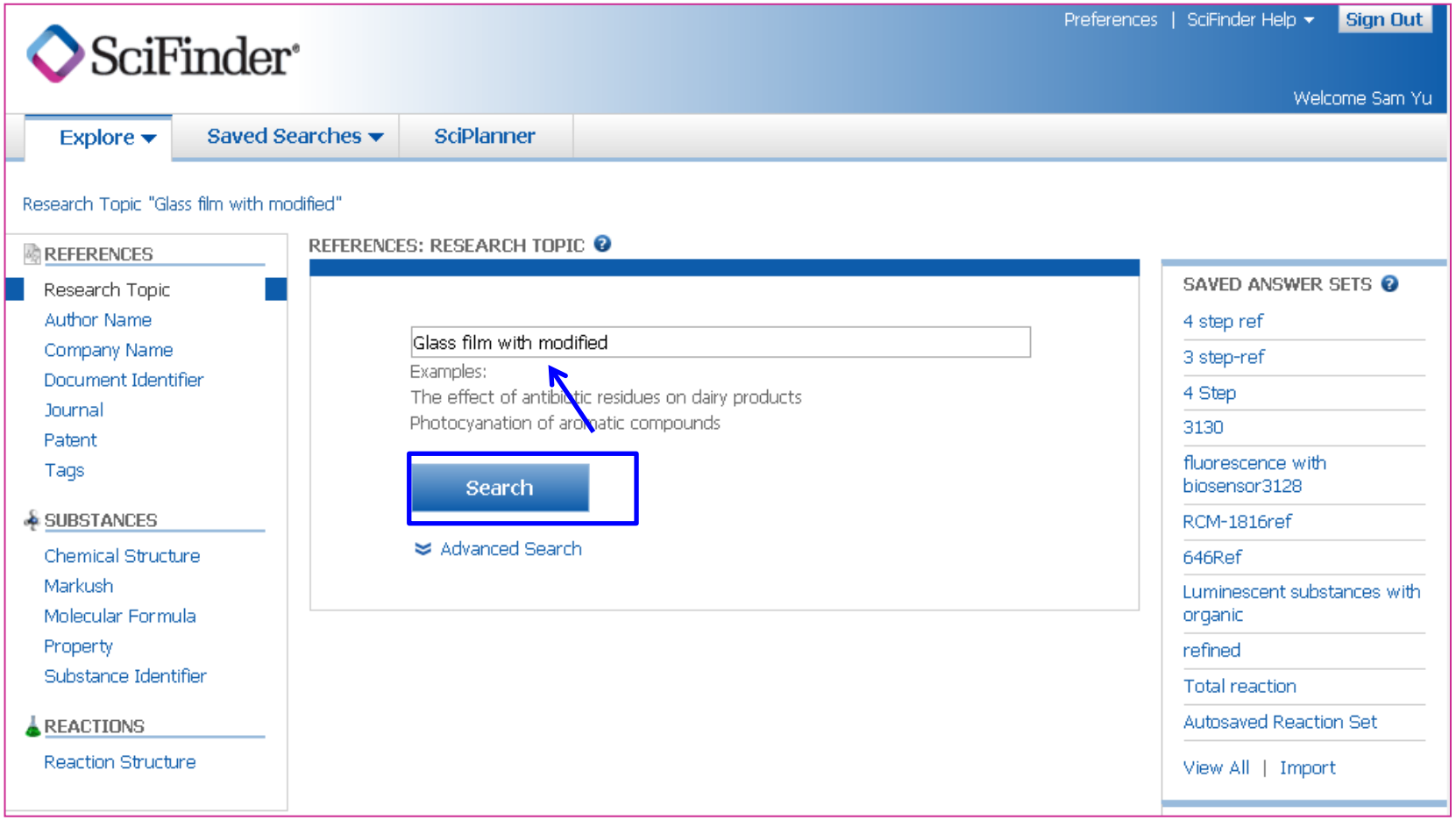
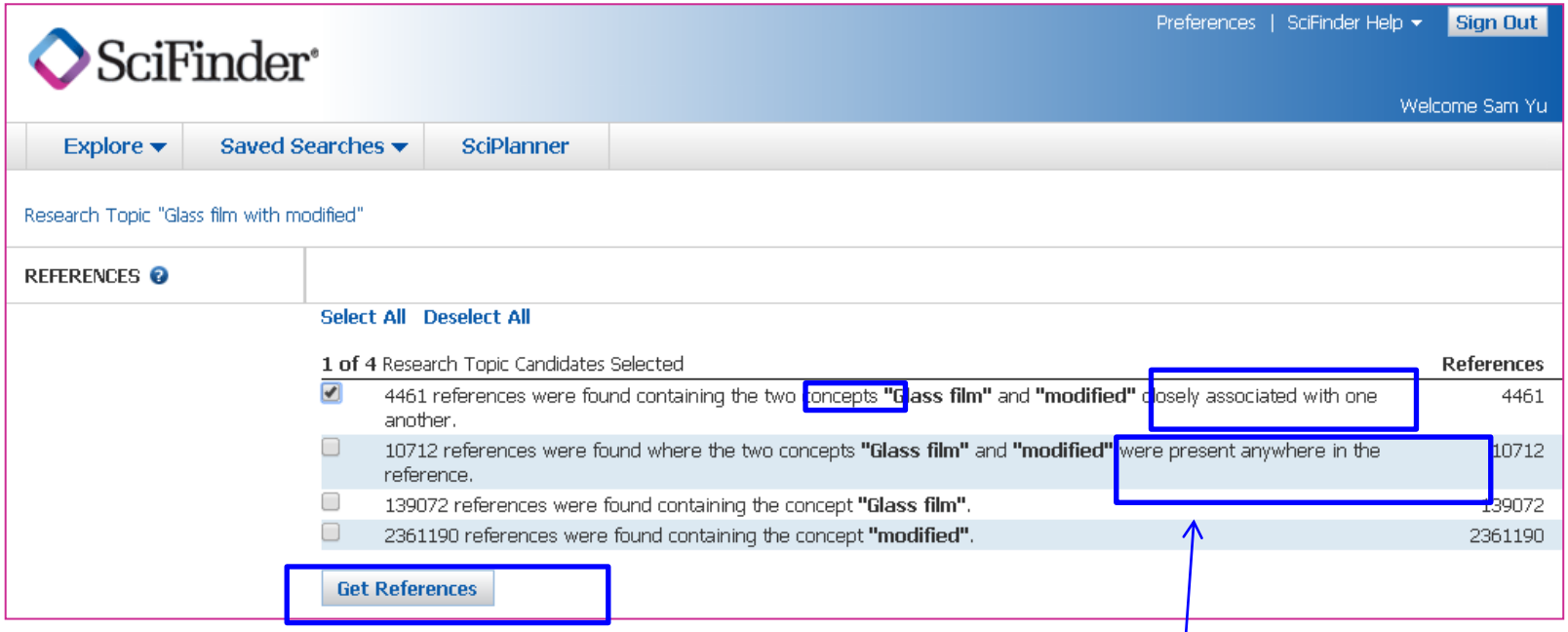
  - 关注物质有关的文献———-先获得物质，再获得文献
  - 关注某科研人员的文献——-作者名检索

SciFinder Web中的主题检索

主题： glass film with modified（玻璃贴膜的改进）



主题检索的候选项



“Concept”表示做了同意词的扩展

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Huang Ke Jing	24

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1. Non-enzymatic glucose biosensor based on copper oxide-reduced graphene oxide nanocomposites synthesized from water-isopropanol solution
Quick View | Full Text
By Wang, Xiaolin; Liu, Enli; Zhang, Xiaoli
From Electrochimica Acta (2014), 130, 253-260. | Language: English, Database: CAPLUS
A novel, stable and sensitive non-enzymic glucose biosensor based on nanocomposites of copper oxide (CuO) and the reduced graphene oxide (rGO) was developed. A facile, green and effective chem. method was employed to synthesize the CuO-rGO nanocomposites in a mixt. soln. of water-isopropanol. During the synthesis process, isopropanol acted as both solvent and reductant. oxide (GO) sheets through electrostatic force and rGO without any addn. of strong redn. agents...

2. Direct electrochemistry and electrocatalysis of poly(ethylene glycol diglycidyl ether) and gold na hydrogen peroxide and nitric oxide
Quick View | Full Text
By Li, Fangping; Nie, Mingzhe; He, Xiulan; Fei, Junjie; Di
From Microchimica Acta (2014), Ahead of Print. | Lan

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Huang Ke Jing	24
John S Abraham	24
Li Jing	24

1. ystalline diamond thin-films as stable, biologically active substrates
Quick View | Full Text
By Yang, Wensha; Auciello, Orlando; Butler, James E.; Cai, Wei; Carlisle, John A.; Gerbi, Jennifer E.; Gruen, Dieter M.; Knickerbocker, Tanya; Lasseter, Tami L.; Russell, John N.; et al
From Nature Materials (2002), 1(4), 253-257. | Language: English, Database: CAPLUS
~528

Diamond, because of its elec. and chem. properties, may be a suitable material for integrated sensing and signal processing. But methods to control chem. or biol. **modifications** on diamond surfaces have not been established. Here, we show that nanocryst. diamond thin-**films** covalently **modified** with DNA oligonucleotides provide an extremely stable, highly selective platform in subsequent surface hybridization processes. We used a photochem. **modification** scheme to chem. **modify** clean, H-terminated nanocryst. diamond surfaces grown on silicon substrates, producing a homogeneous layer of amine gro...

2. **An ESCA study of the termination of the passivation of elemental metals**
Quick View | Full Text
By Barr, Tery L.
From Journal of Physical Chemistry (1978), 82(16), 1801-10. | Language: English, Database: CAPLUS
~321

A detailed ESCA study was made of the passivation of 16 metals which were allowed to oxidize (passivate) to completion in room-temp. air. Particular attention was paid to the characteristics of the final (satn.) layer that terminates the rapid oxidn. and provides the initial barrier to corrosion and other forms of metallic degrdn. The passivation of some of these metals (A) terminates with a micro thin (few Å) layer of the metal in its highest oxidn. state, whereas the bulk of the passivation **film** is largely composed of an oxide of a lower oxidn. state. On the other

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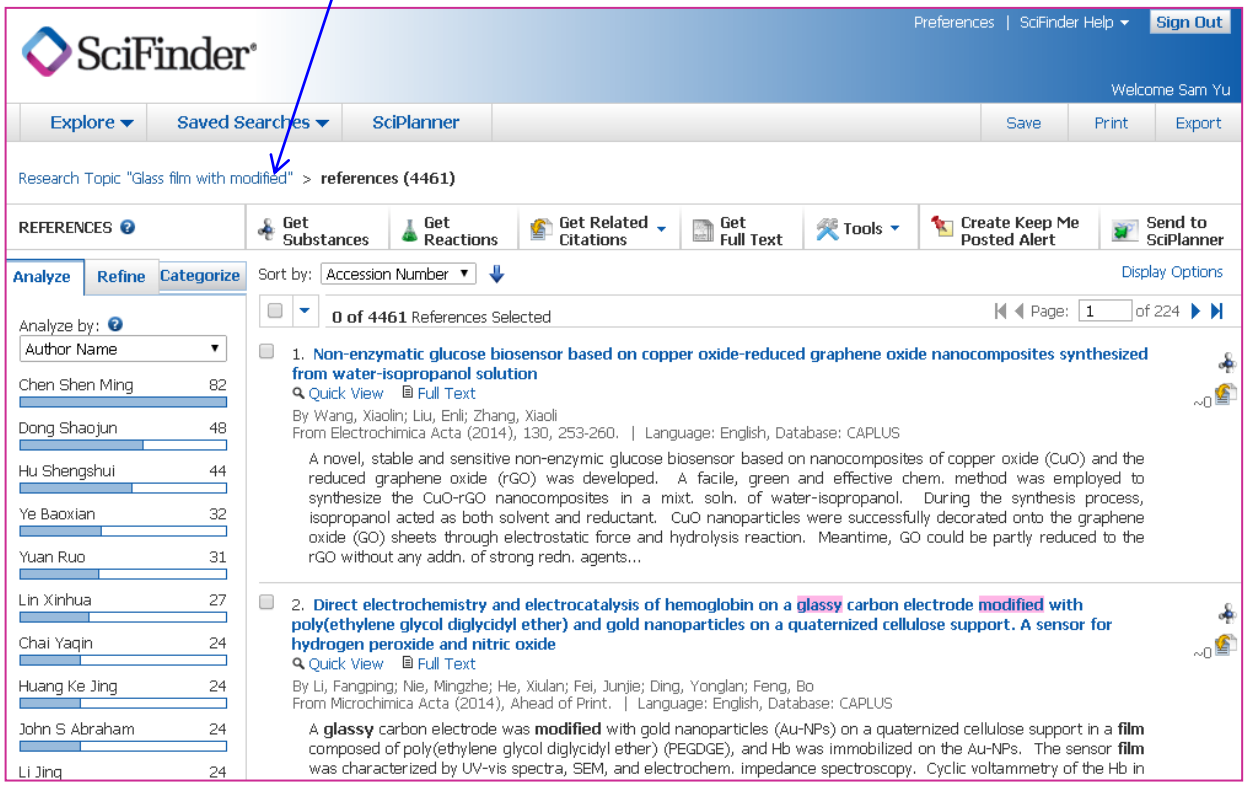

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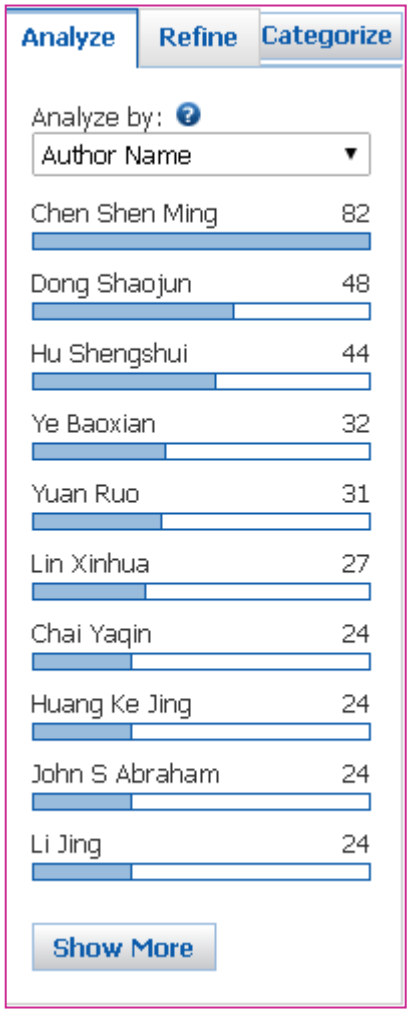
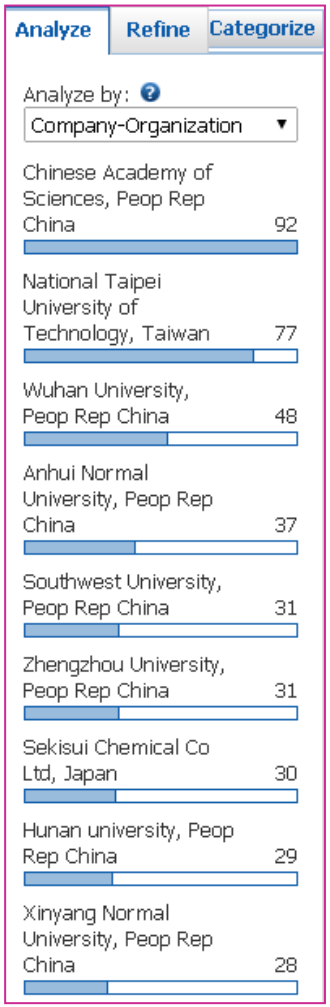
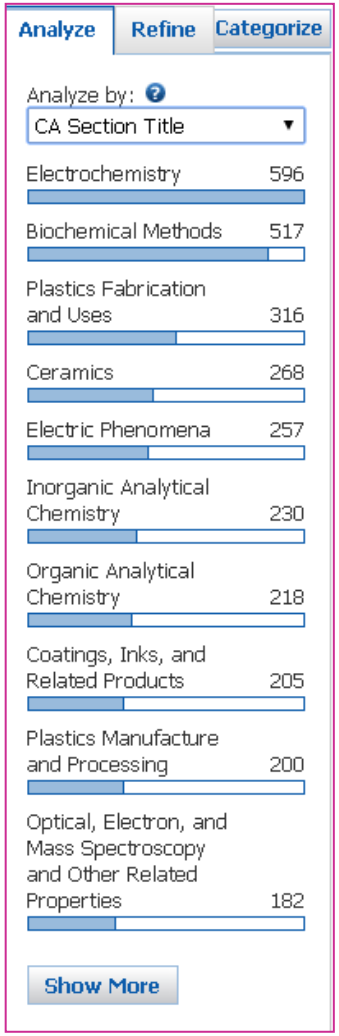


主要研究机构，合作伙伴，竞争对手



主要的学科领域



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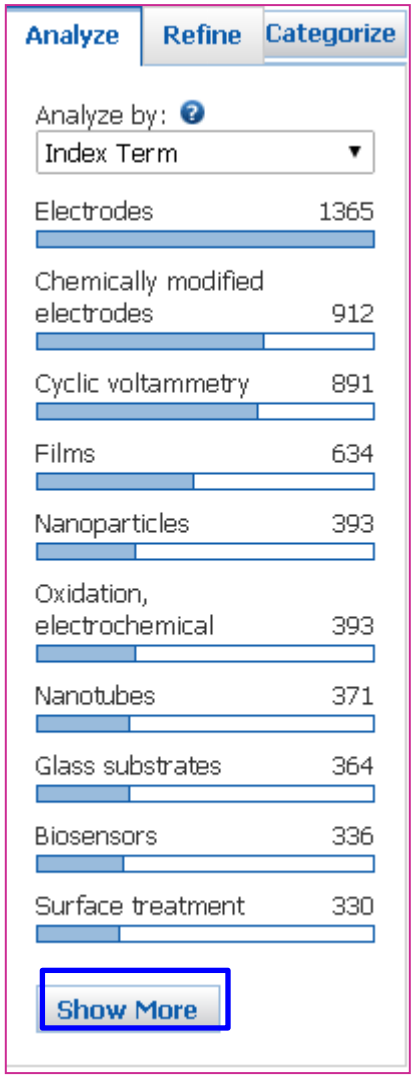

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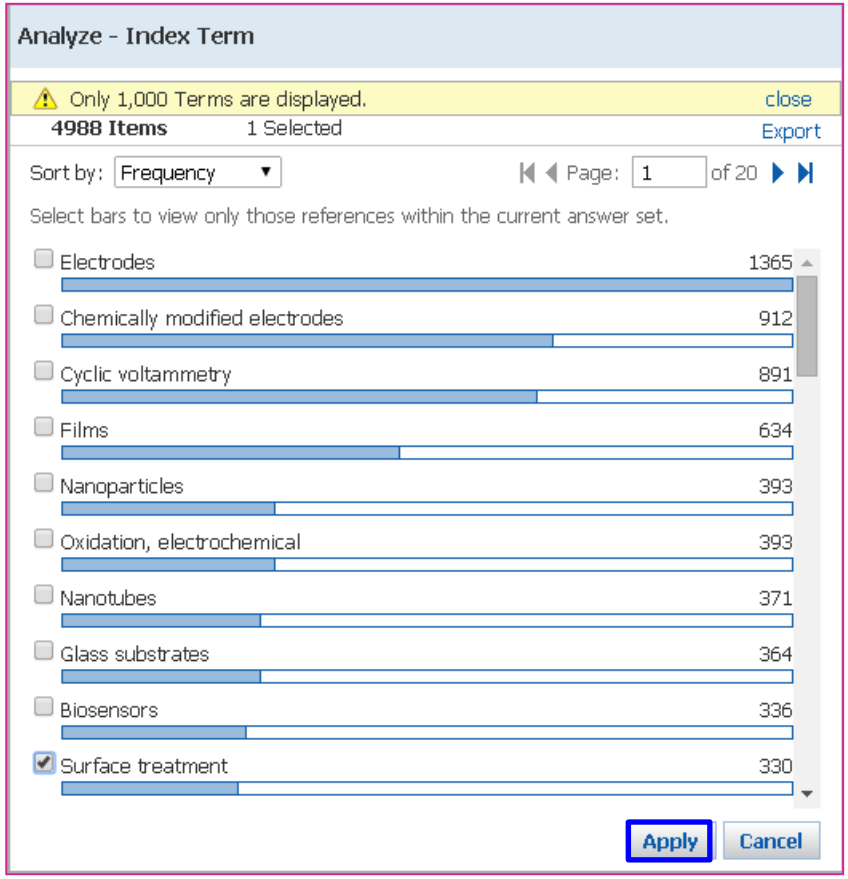

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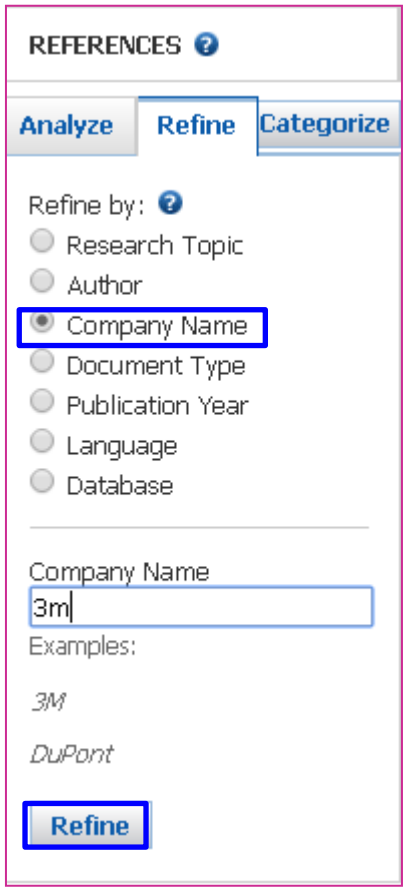

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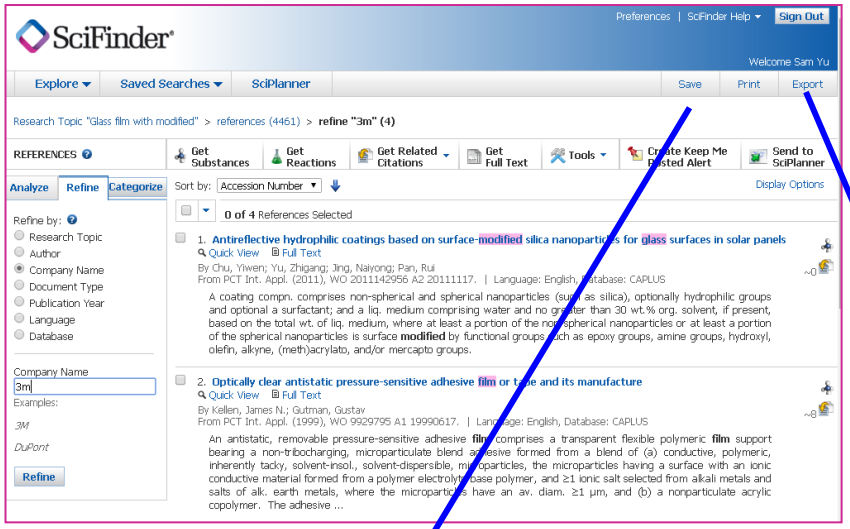

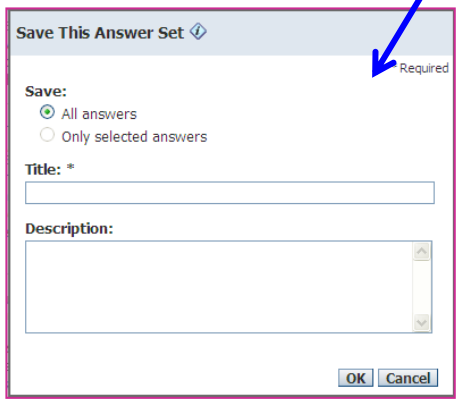

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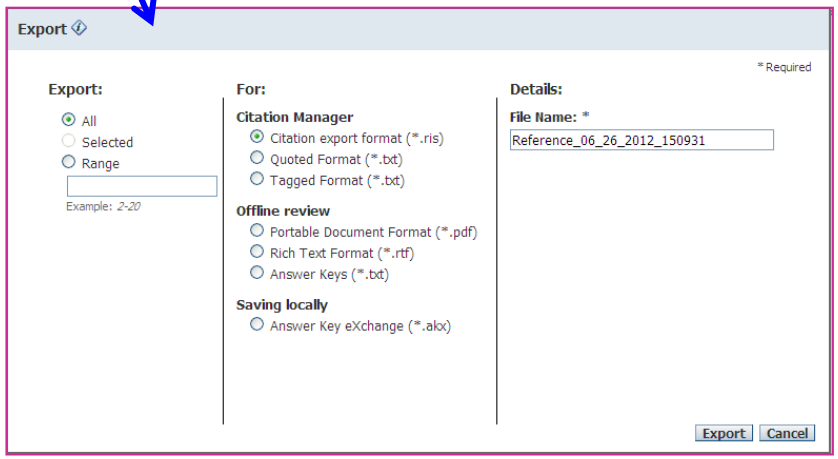

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By Li, Fangping; Nie, Mingzhe; He, Xiulan; Fei, Junjie; Ding, Yonglan; Feng, Bo
From Microchimica Acta (2014), Ahead of Print. | Language: English, Database: CAPLUS
A **glassy** carbon electrode was **modified** with gold nanoparticles (Au-NPs) on a quaternized cellulose support in a **film** composed of poly(ethylene glycol diglycidyl ether) (PEGDGE), and Hb was immobilized on the Au-NPs. The sensor **film**

Categorize系统分类功能，基于Index Term，对文献依学科方向进行分类

SciFinder中的Categorize

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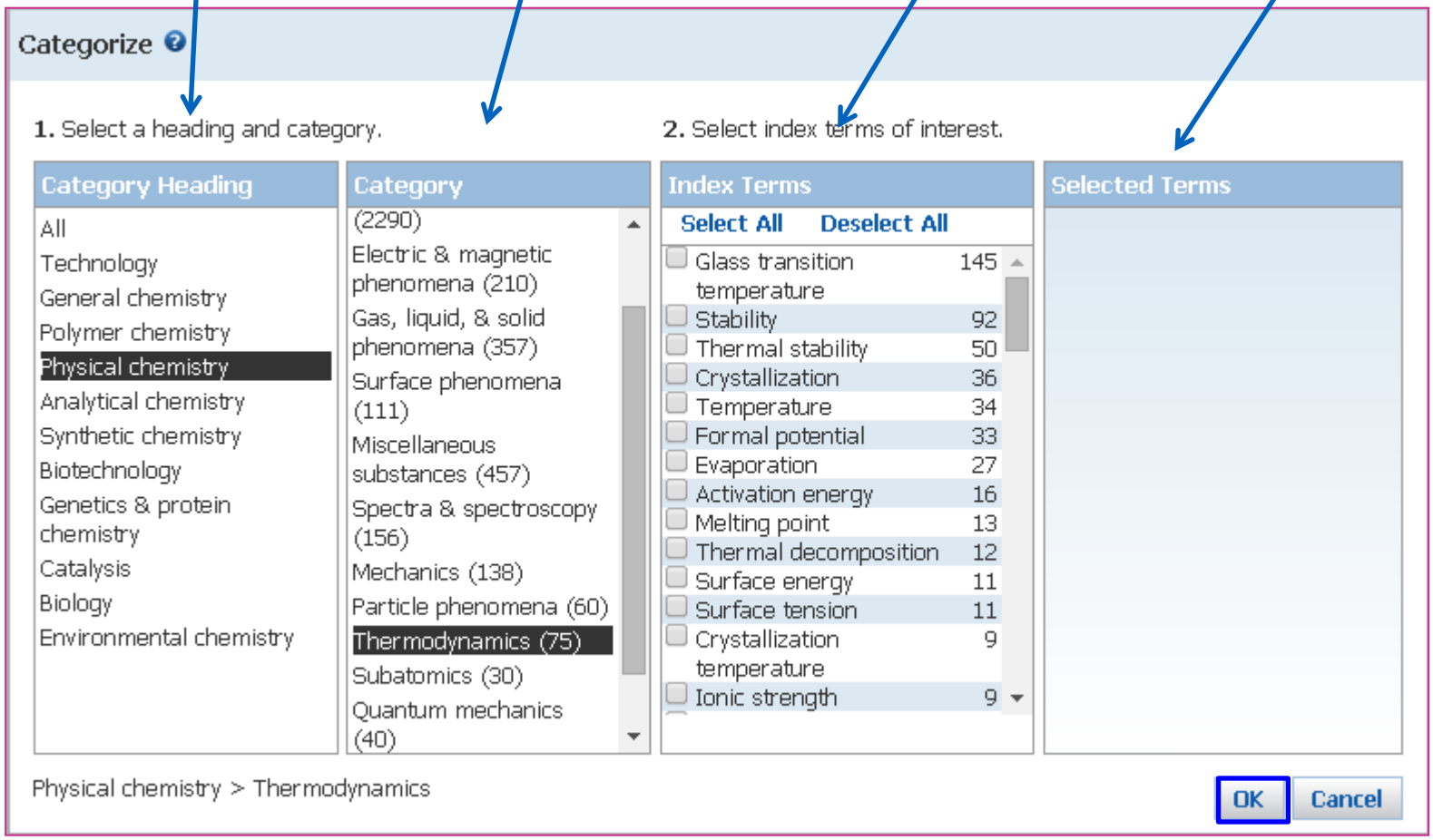


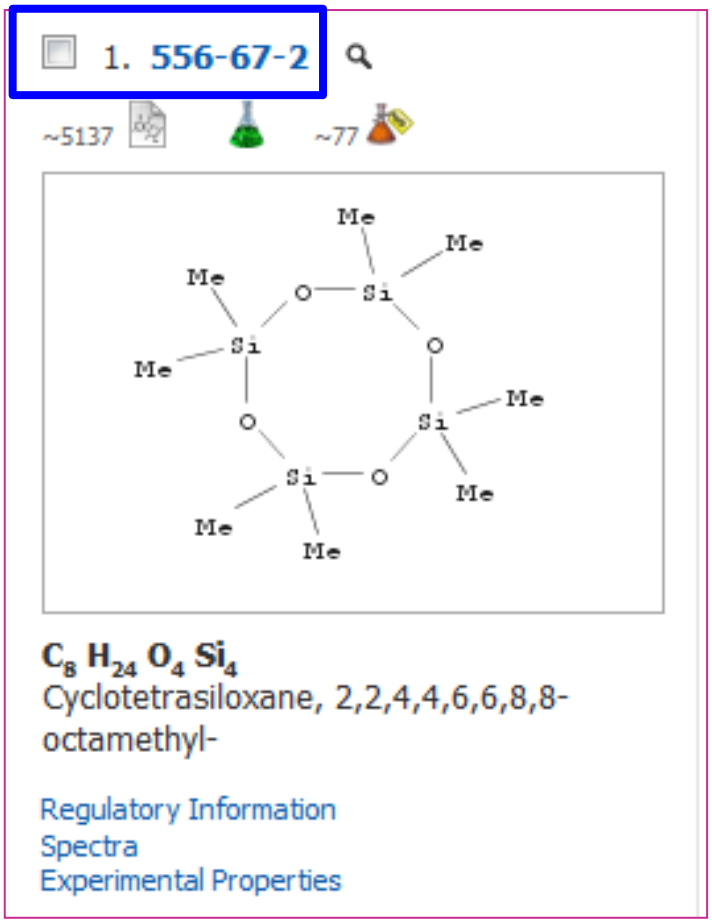
主题检索小结

- 关键词之间用介词链接，With，Of，In，On
- 建议2-3个关键词，最多不超过5个
- 候选项选择包含Concept和Closed associated with的选项
- 可以使用KMP时时跟踪文献
- 可以使用Citing Reference排序获得被引次数最多的文献
- 尽可能多的使用Analyze，Refine，功能对文献进行处理
- 使用Categorize对文献进行系统分类
- 可以使用历史导航条返回任意检索界面

提纲

- 介绍
  - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索
- **SciFinder Web的注册**

SciFinder中的物质结果界面



一个完整的物质结果界面包含：

- 物质详情连接
- 文献连接
- 反应连接
- 商品信息连接
- 管制品信息连接
- 谱图连接
- 实验性质连接

SciFinder中的物质详情界面

CAS Registry Number 556-67-2

~5,137 ~77

$C_8H_{24}O_4Si_4$

Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-

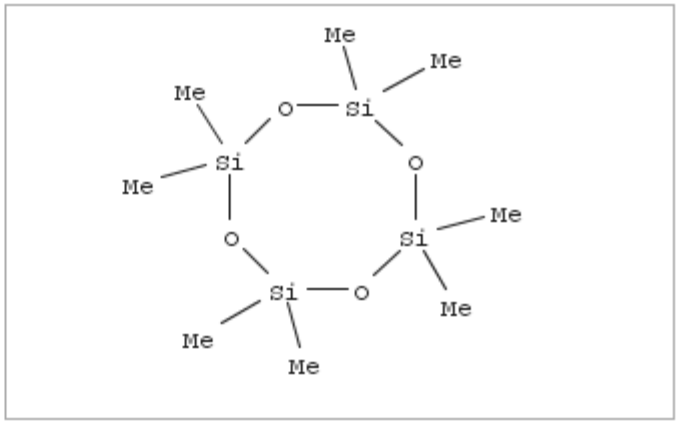
Molecular Weight
296.62

Melting Point (Experimental)
Value: 17.5 °C

Boiling Point (Experimental)
Value: 175 °C

Density (Experimental)
Value: 0.9558 g/cm3

Other Names
Cyclotetrasiloxane, octamethyl- (8CI,9CI)
Abil K 4
Cyclic dimethylsiloxane tetramer
D 4
DC 244
View more...



SciFinder中的实验性质和实验谱图

EXPERIMENTAL PROPERTIES

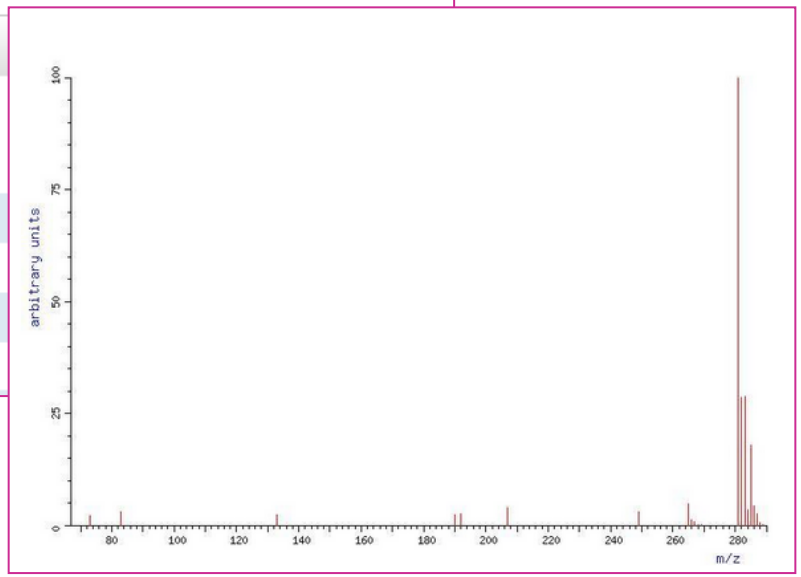
Biological | Chemical | Density | Flow and Diffusion | Interface | Lipinski | Optical and Scattering | Thermal

Density Properties	Value	Condition	Note
Density	1.06 g/cm3		(28)CAS
Density	0.96 g/cm3		(22)NIOSH
Density	0.9561 g/cm3	Temp: 20 °C	(4)CAS
Density	0.9561 g/cm3	Temp: 420 °C	(15)CAS
Density	0.956 g/cm3		(8)GELEST

EXPERIMENTAL SPECTRA

^{1}H NMR | ^{13}C NMR | Hetero NMR | IR | Mass | Raman | UV and Visible

Mass Properties	Value	Condition
Mass Spectrum	See spectrum	
Mass Spectrum	See spectrum	
Mass Spectrum	See spectrum	
Mass Spectrum	See spectrum	
Mass Spectrum	See spectrum	

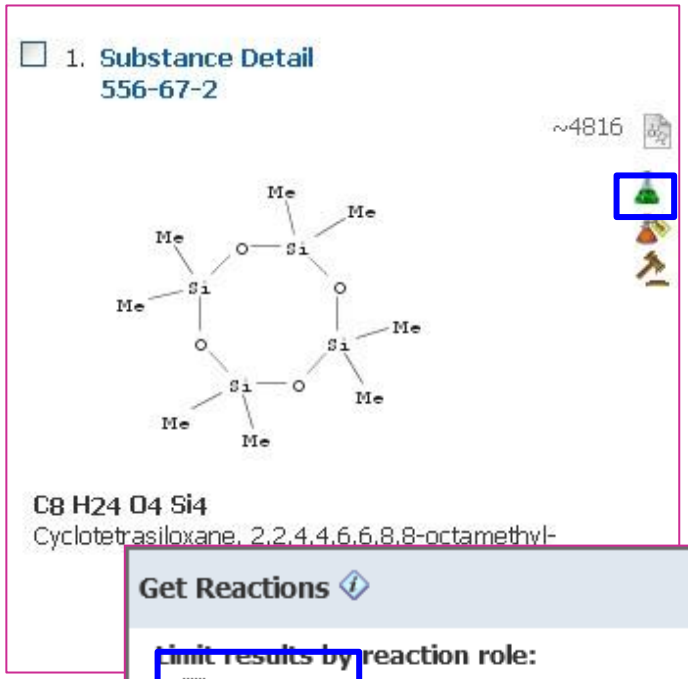


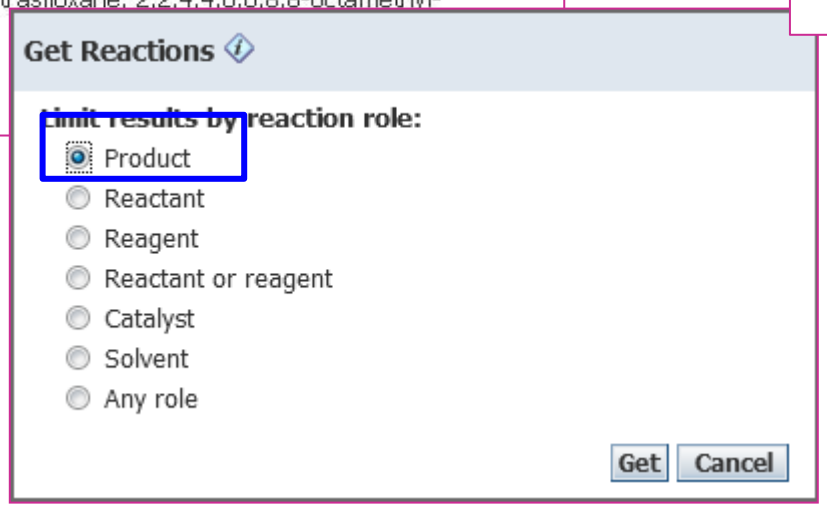
SciFinder中依据物质角色所作的文献分类

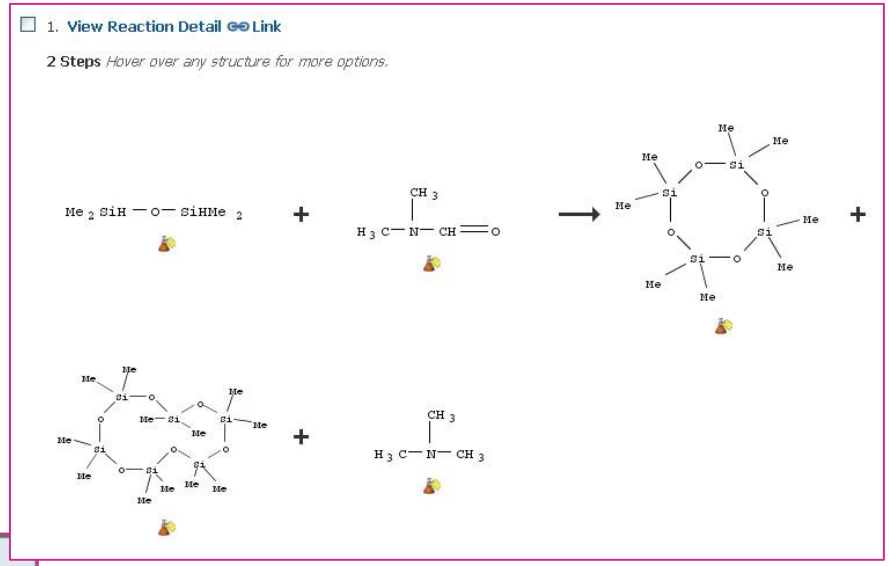
CAS REFERENCE ROLES

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

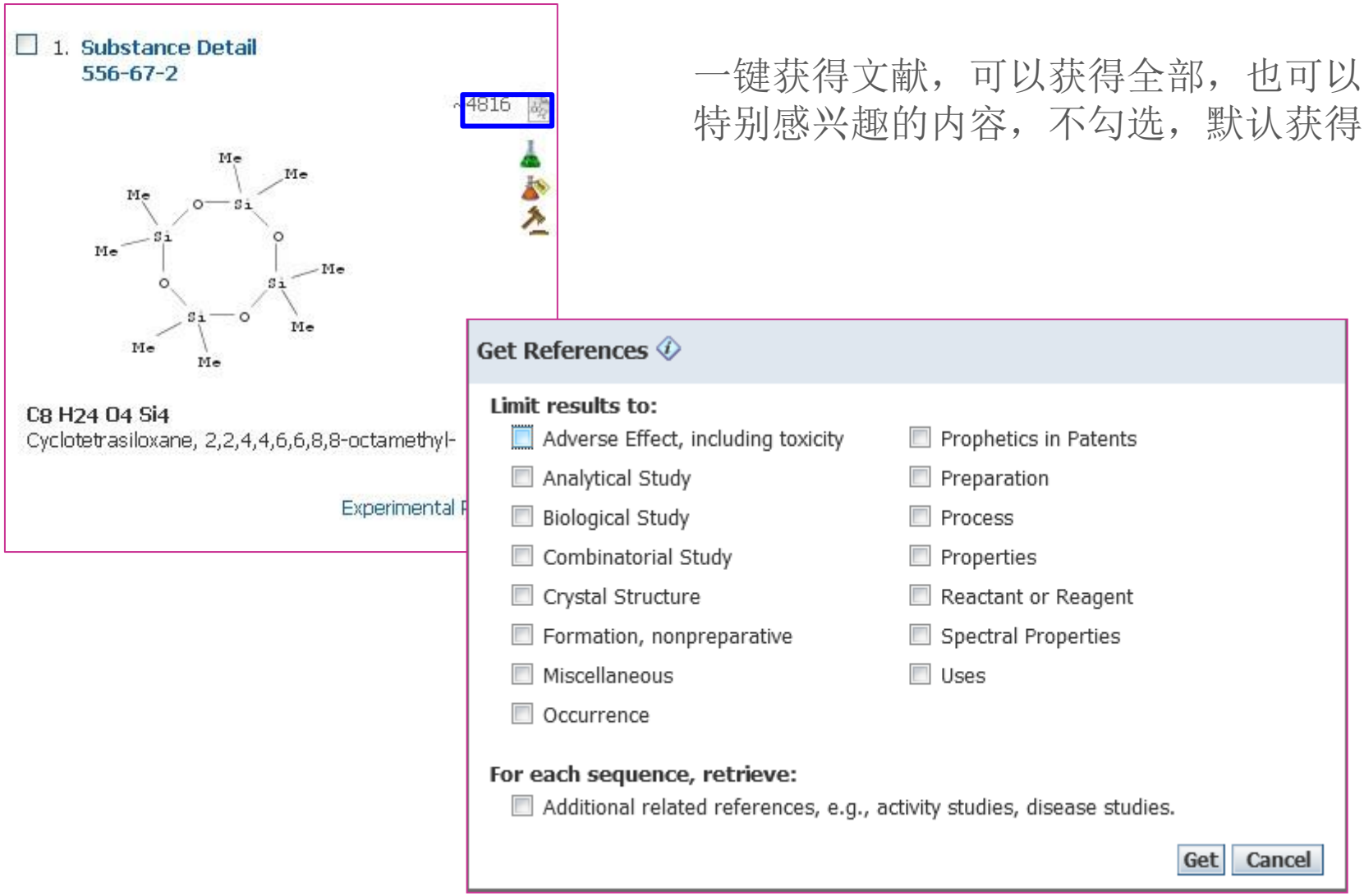
物质有关的反应







物质有关的文献信息

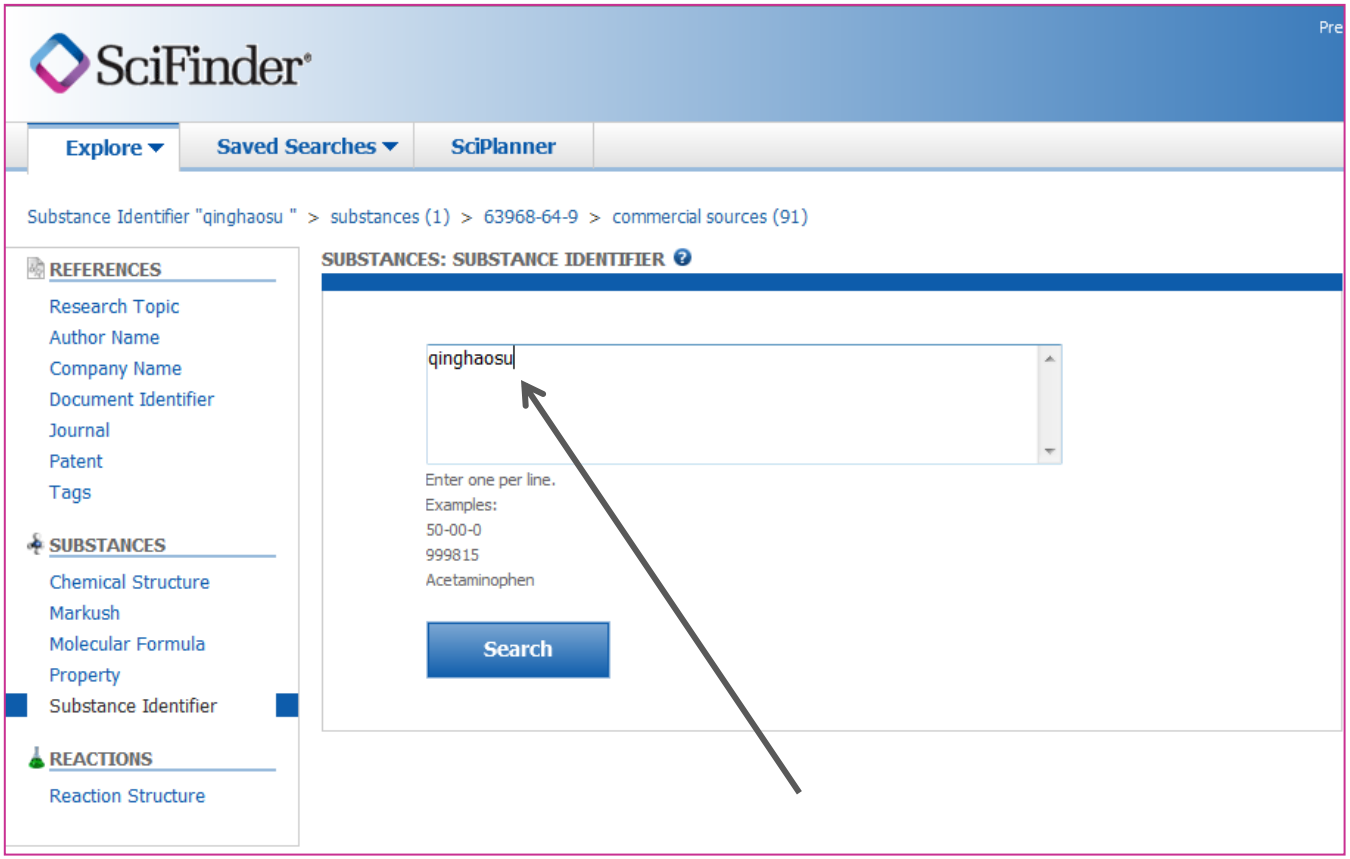


一键获得文献，可以获得全部，也可以勾选特别感兴趣的内容，不勾选，默认获得全部

SciFinder中的物质检索方法

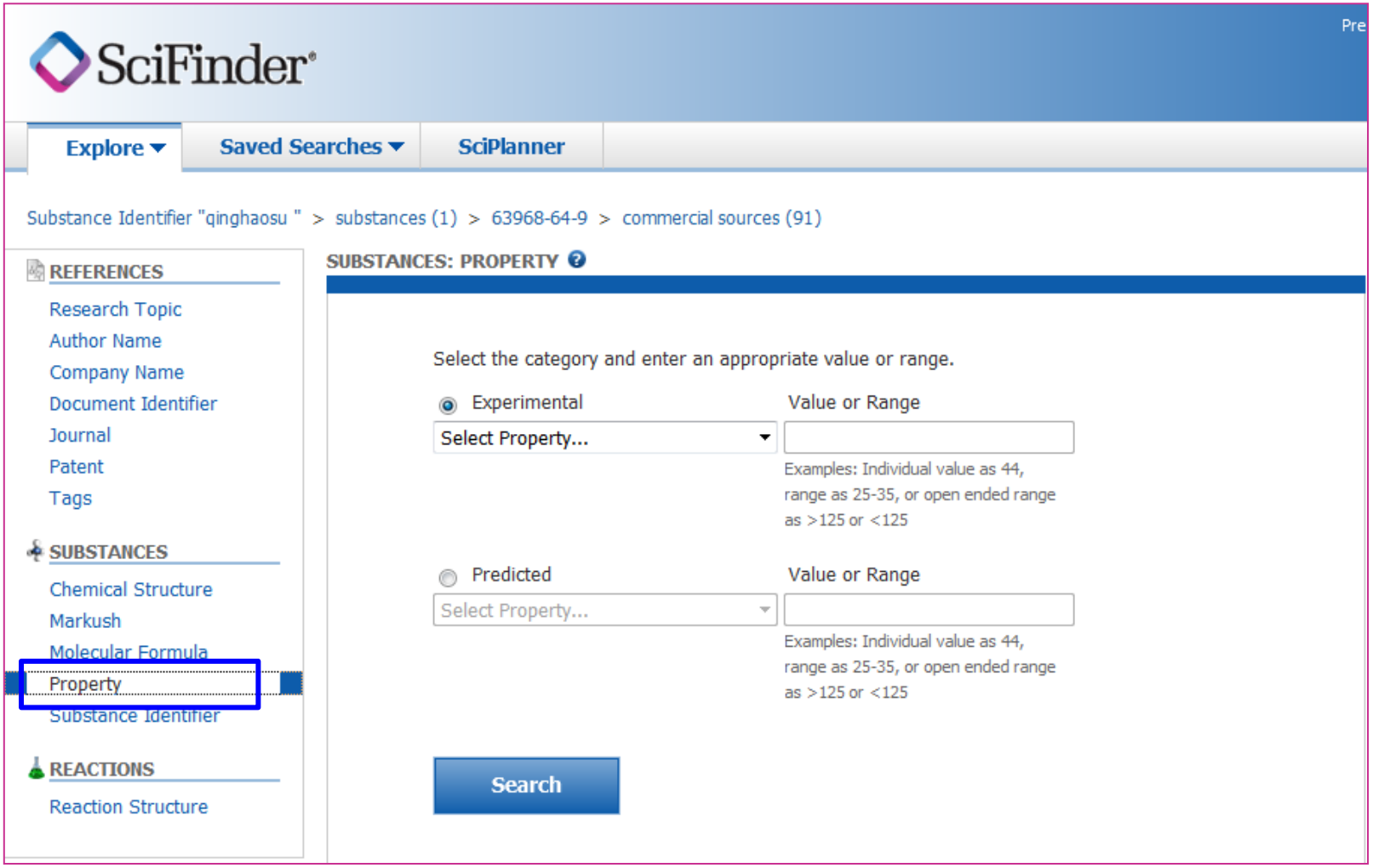
- 功能方面
  - 物质名称，CAS No
  - 分子式
  - 结构式
  - 理化性质
- 推荐的物质检索功能
  - 有机物，天然产物及衍生物 ---结构比较方便
  - 无机物 ---分子式比较方便
  - 高分子化合物 ---首先分子式，其次结构

物质名称检索

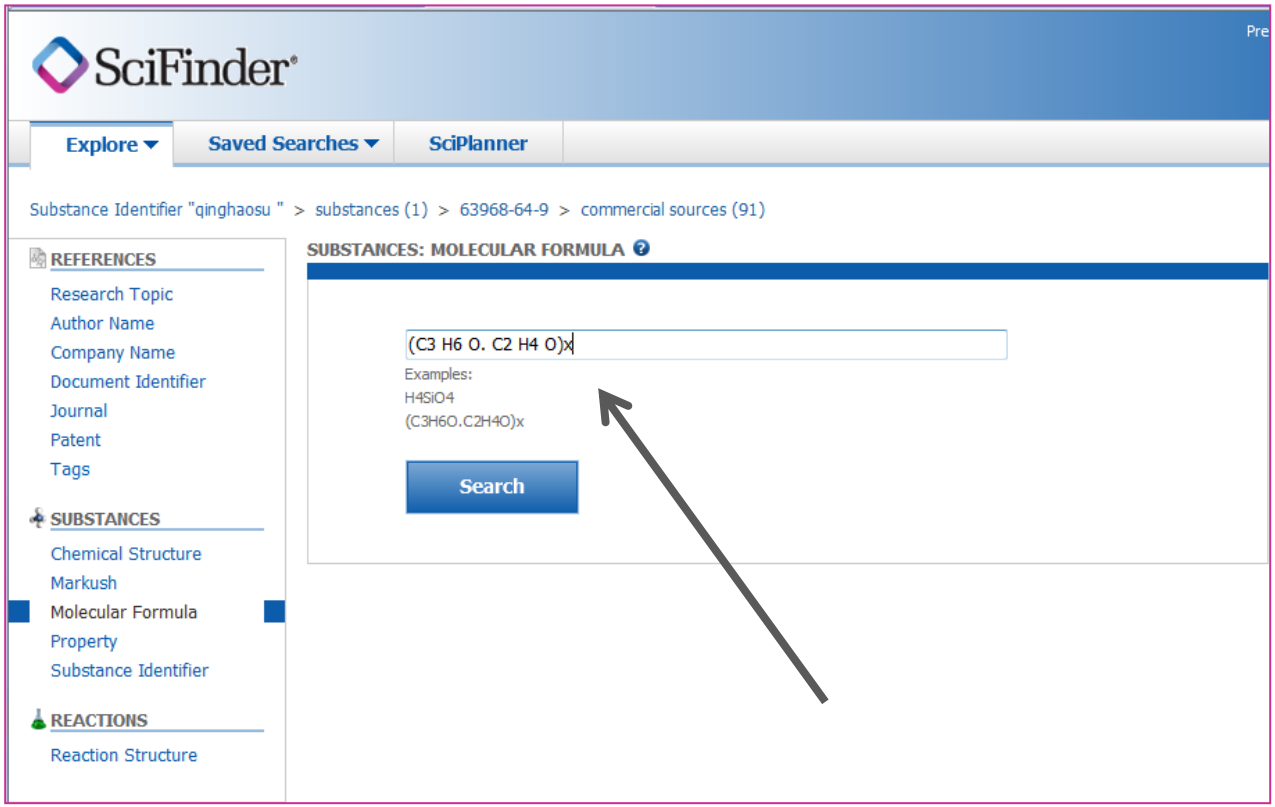


直接输入物质的名称，CAS No，俗名，都能检索，一次最多检索25个物质，用换行换开

理化性质检索

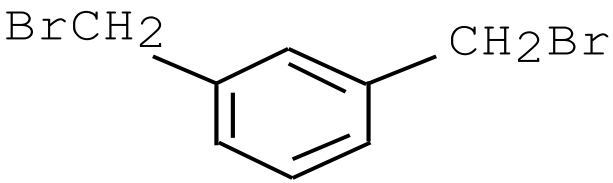


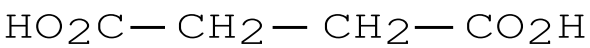
分子式检索



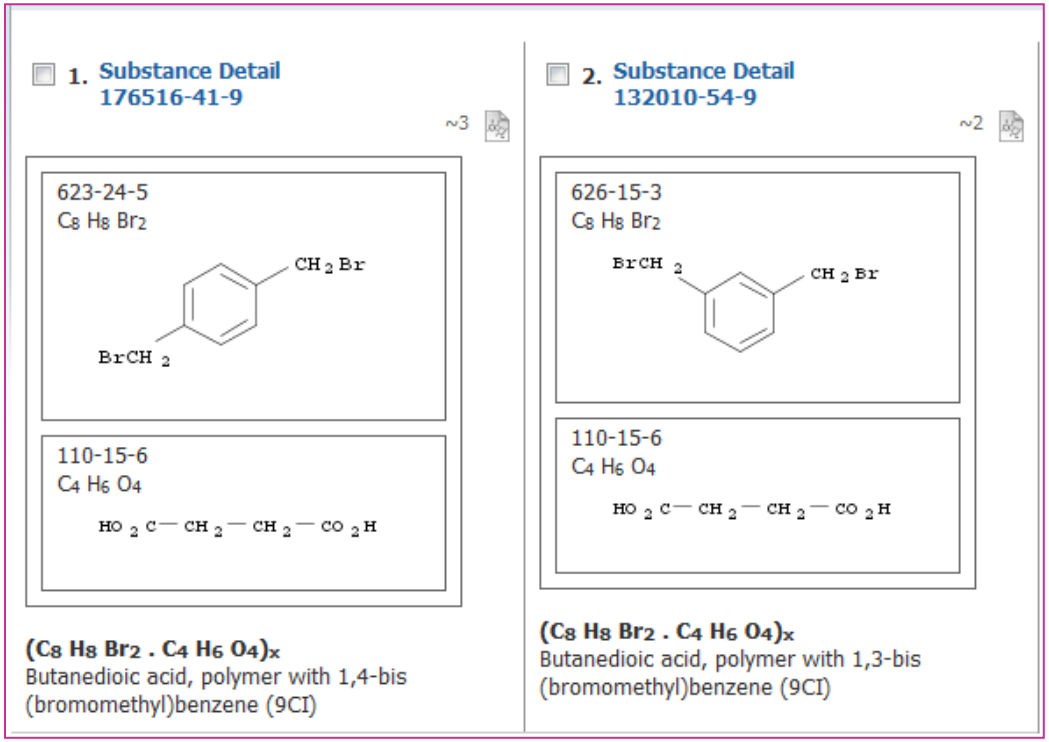
分子式的检索，需要按照HILL排序进行

只知道起始原料的聚合物

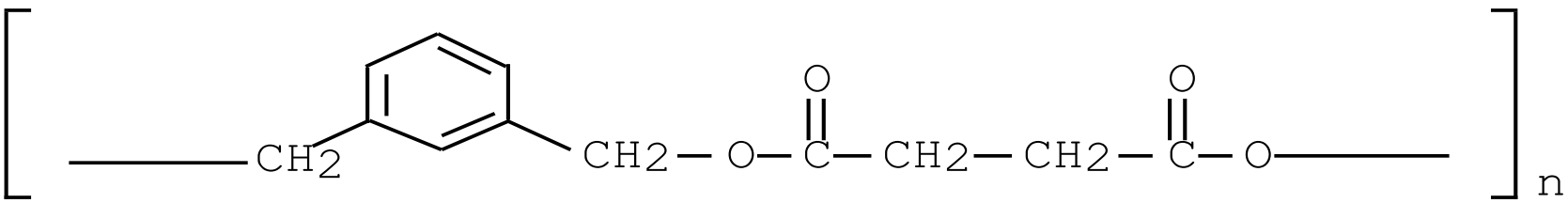




(C8 H8 Br2 . C4 H6 O4)x



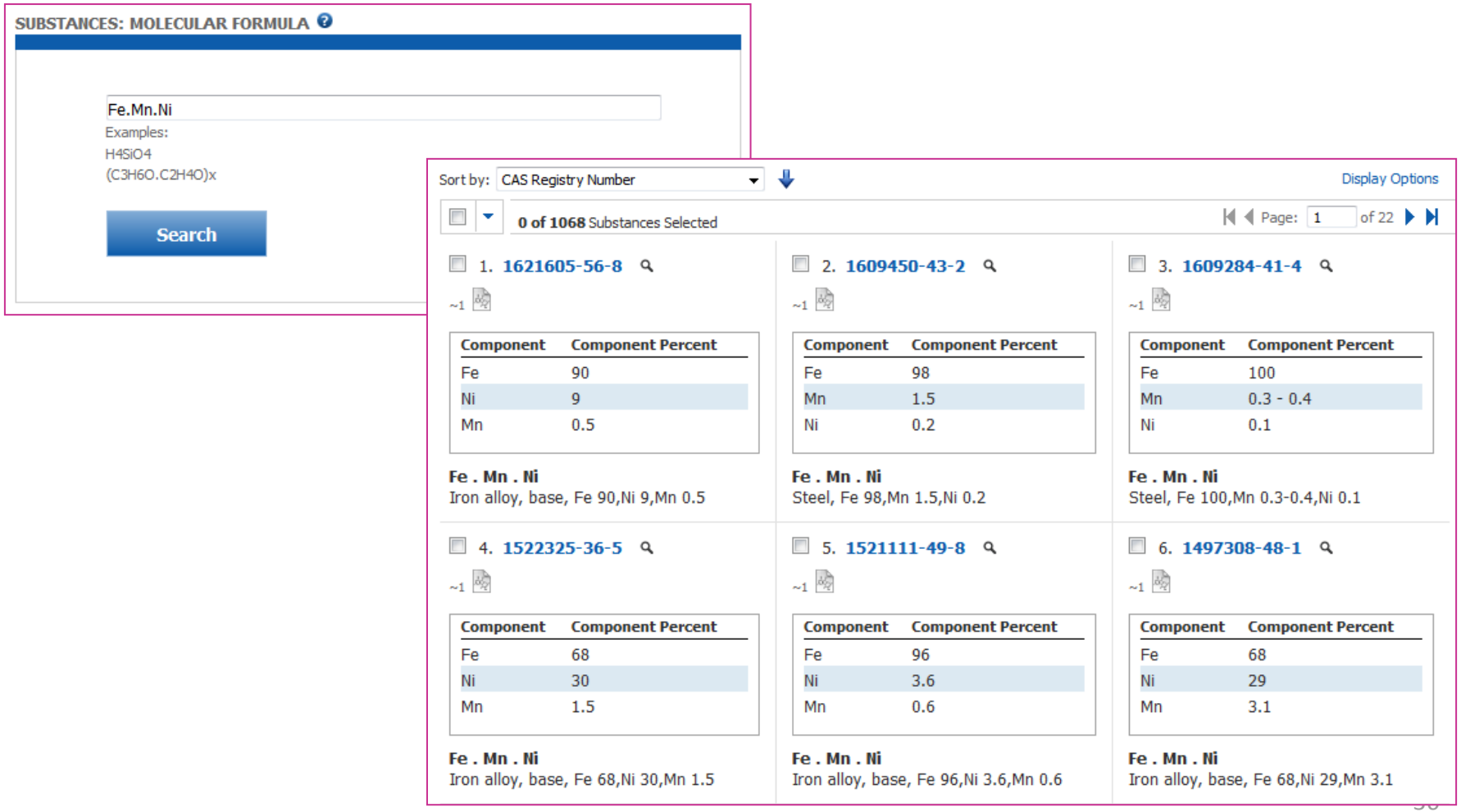
知道最终SRU的检索



(C12 H12 O4)n

合金的检索

- 检索铁镍锰合金
- Fe.Mn.Ni



Tabular Inorganic Substance的检索

- 检索Al0.33 Fe0.07 Mg0.67 (CO3)0.02 (CN)0.43 (OH)2
- 使用以下的分子式检索：C N . C O3 . Al . Fe . H O . Mg

SUBSTANCES: MOLECULAR FORMULA

C N . C O3 . Al . Fe . H O . Mg

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

Sort by: CAS Registry Number

Display Options

0 of 12 Substances Selected

1. **156348-99-1**

Component	Component Ratio
HO	2
Mg	0.83
Fe	0.02
Al	0.17
CO3	0.05
CN	0.12

C N . C O_3 . Al . Fe . H O . Mg
Aluminum iron magnesium carbonate cyanide hydroxide ($Al_{0.17}Fe_{0.02}Mg_{0.83}(CO_3)_{0.05}(CN)_{0.12}(OH)_2$)

2. **154948-24-0**

Component	Component Ratio
HO	2
Mg	0.57
Fe	0.09
Al	0.43
CO3	0.03
CN	0.55

C N . C O_3 . Al . Fe . H O . Mg
Aluminum iron magnesium carbonate cyanide hydroxide ($Al_{0.43}Fe_{0.09}Mg_{0.57}(CO_3)_{0.03}(CN)_{0.55}(OH)_2$)

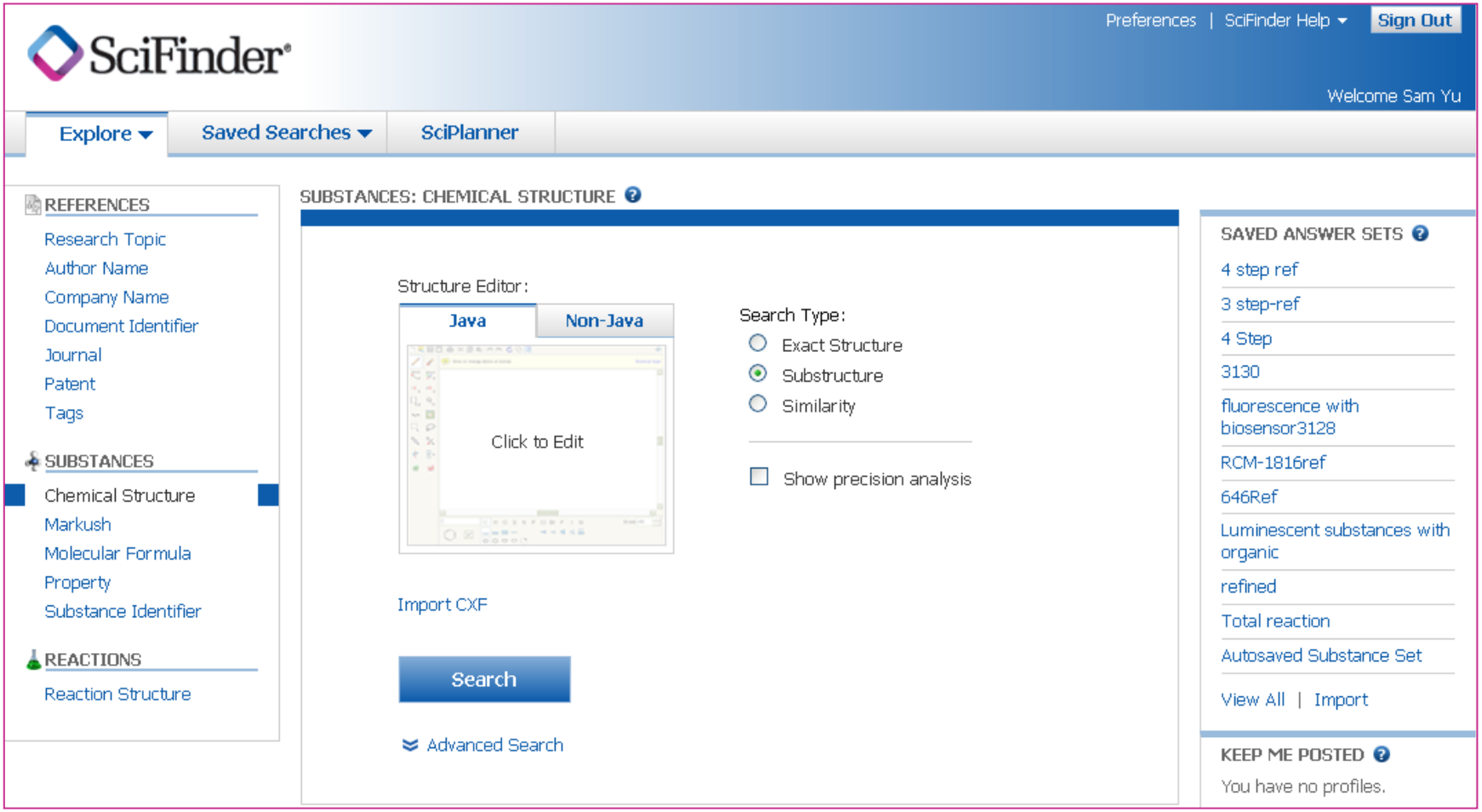
3. **154948-23-9**

Component	Component Ratio
HO	2
Mg	0.67
Fe	0.07
Al	0.33
CO3	0.02
CN	0.43

C N . C O_3 . Al . Fe . H O . Mg
Aluminum iron magnesium carbonate cyanide hydroxide ($Al_{0.33}Fe_{0.07}Mg_{0.67}(CO_3)_{0.02}(CN)_{0.43}(OH)_2$)

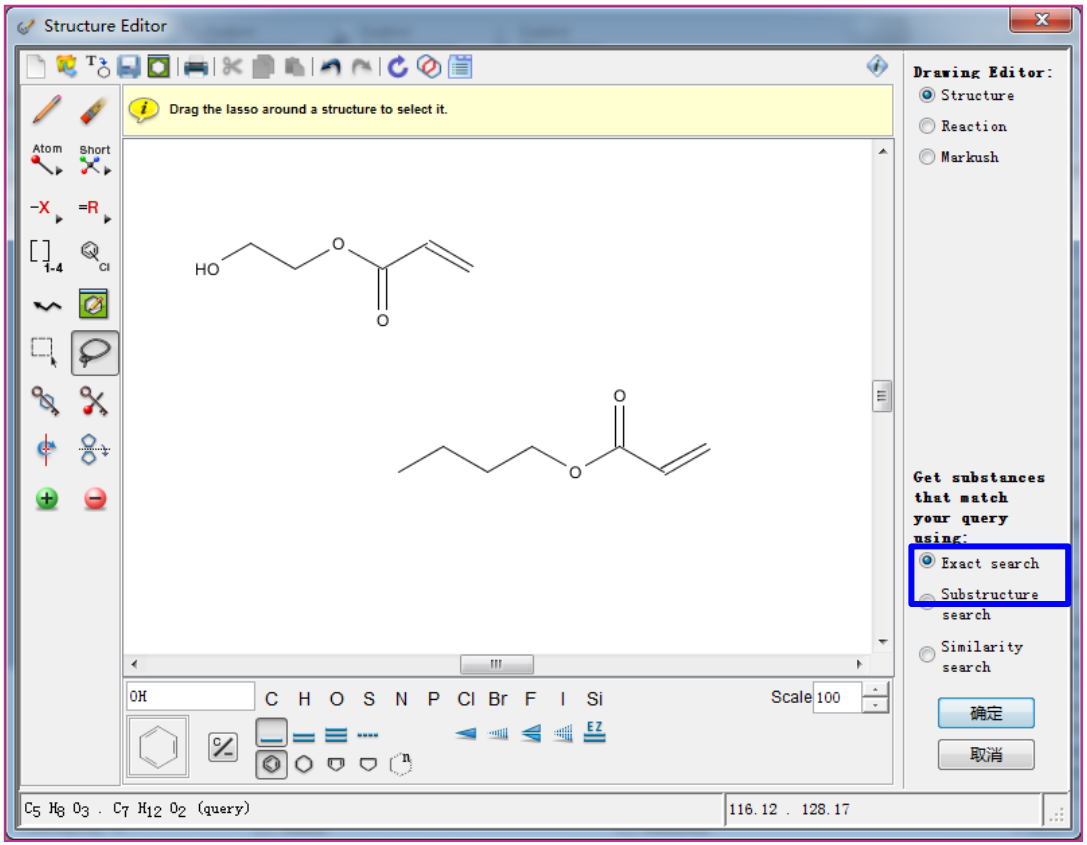
结构式检索—精确检索

SciFinder®
The choice for chemistry research.™



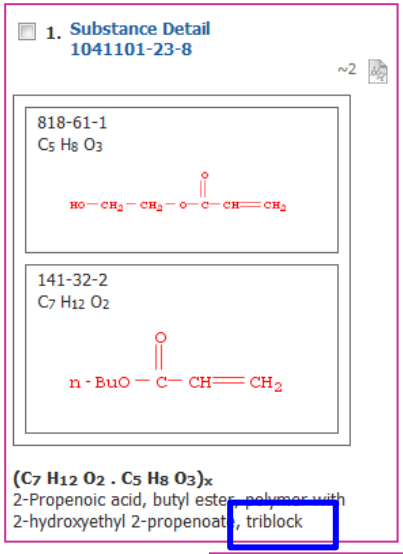
知道起始原料的聚合物检索

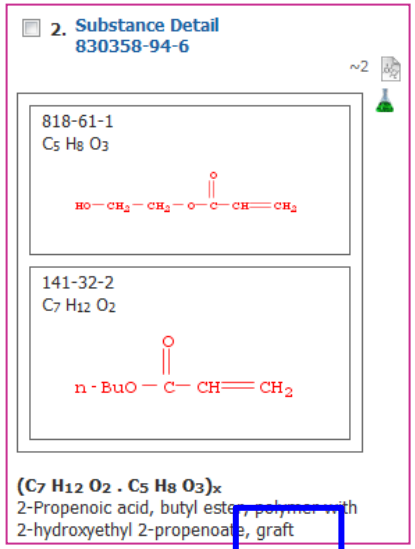
- 检索由丙烯酸丁酯（Butyl acrylate）和丙烯酸羟乙酯（2-hydroxyethyl acrylate）聚合产生的聚合物
- 只绘制单体，精确结构

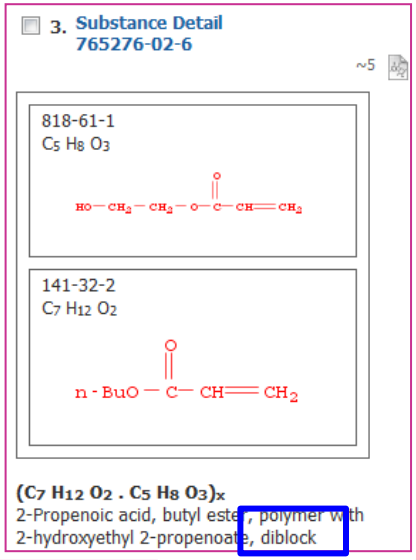


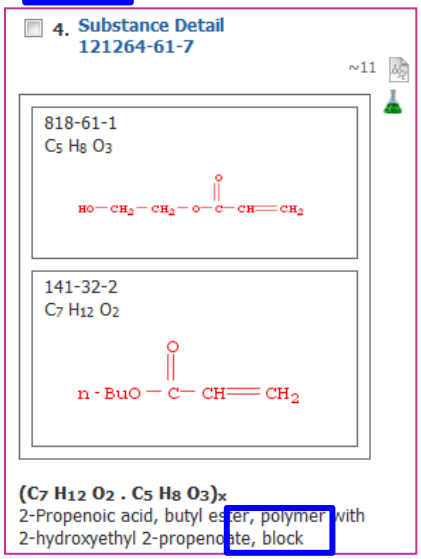
使用精确结构检索

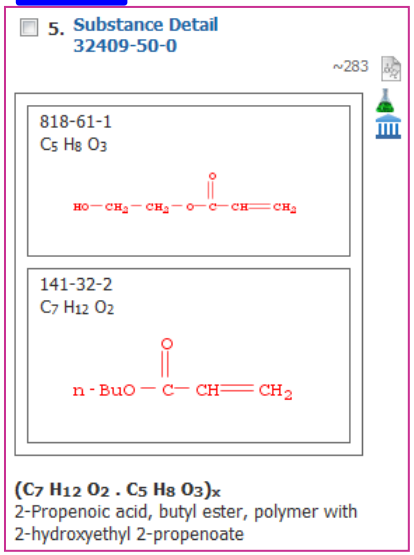
检索结果—看名字得到区别





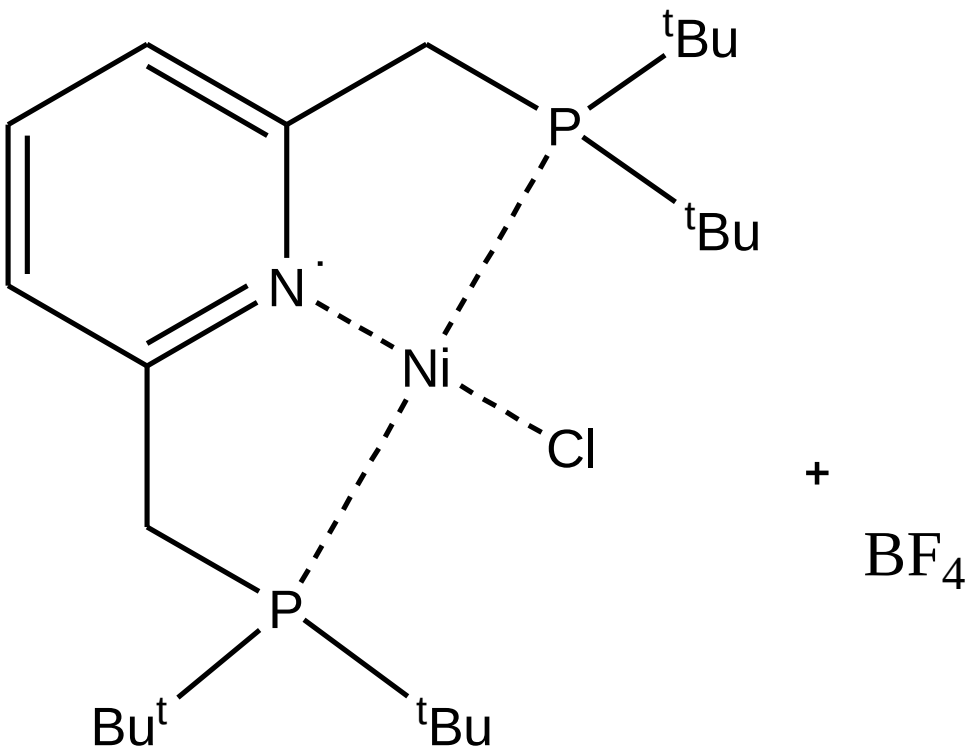






Triblock，Graft，Diblock，Block，无序

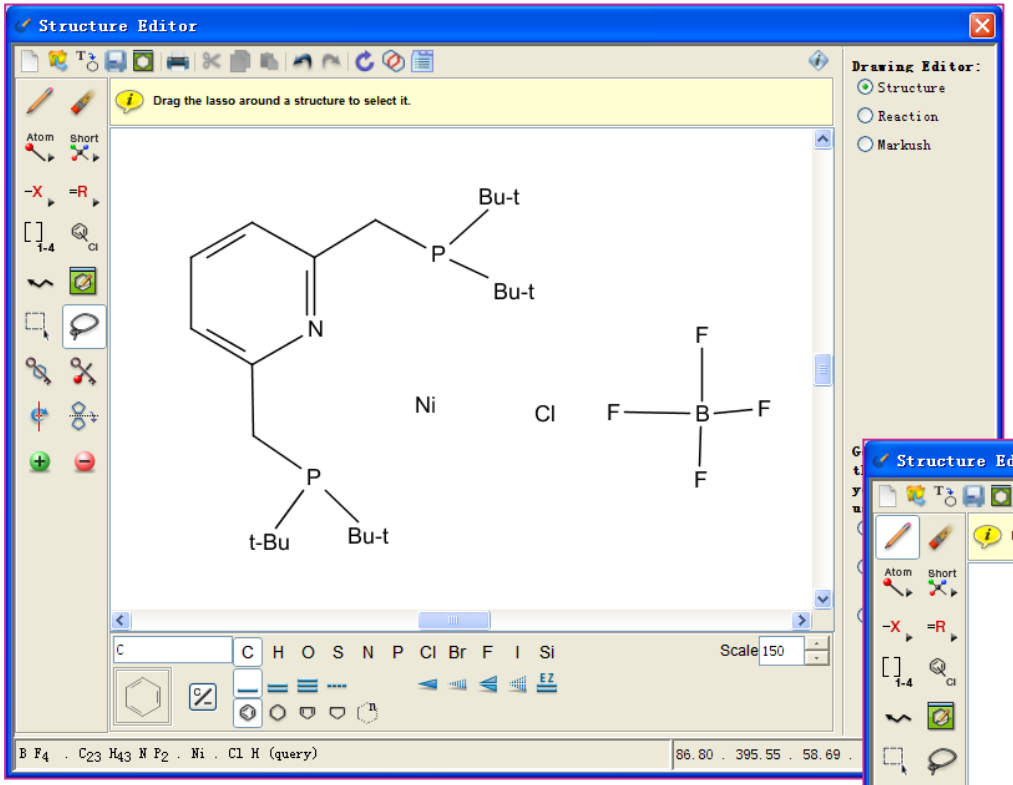
精确结构检索—检索金属配合物



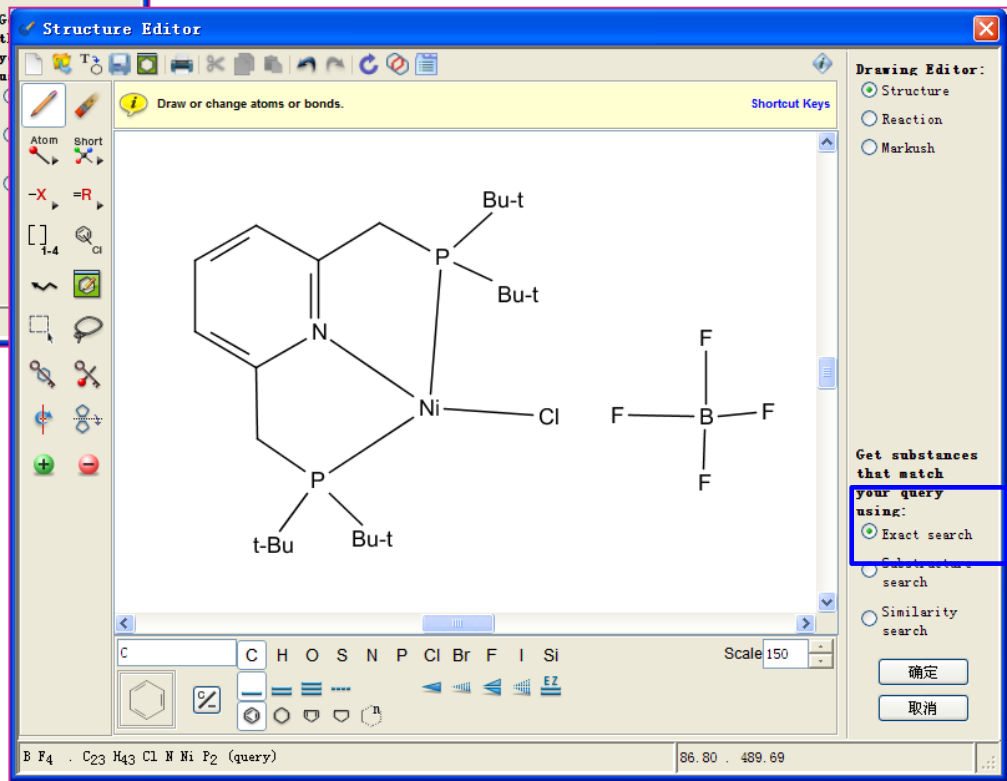
该结构中包含：

配体
金属
阳离子
阴离子

检索界面



任何一种结构，使用精确结构都可以检索到

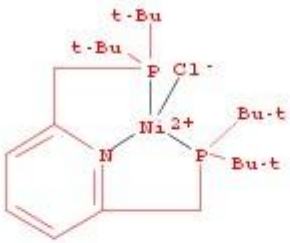


SciFinder中的结果

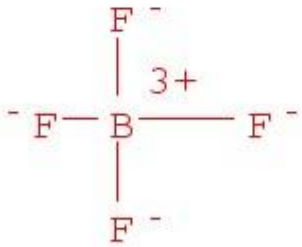
1. **Substance Detail**
   1136166-99-8

~1

1136166-98-7
C23 H43 Cl N Ni P2

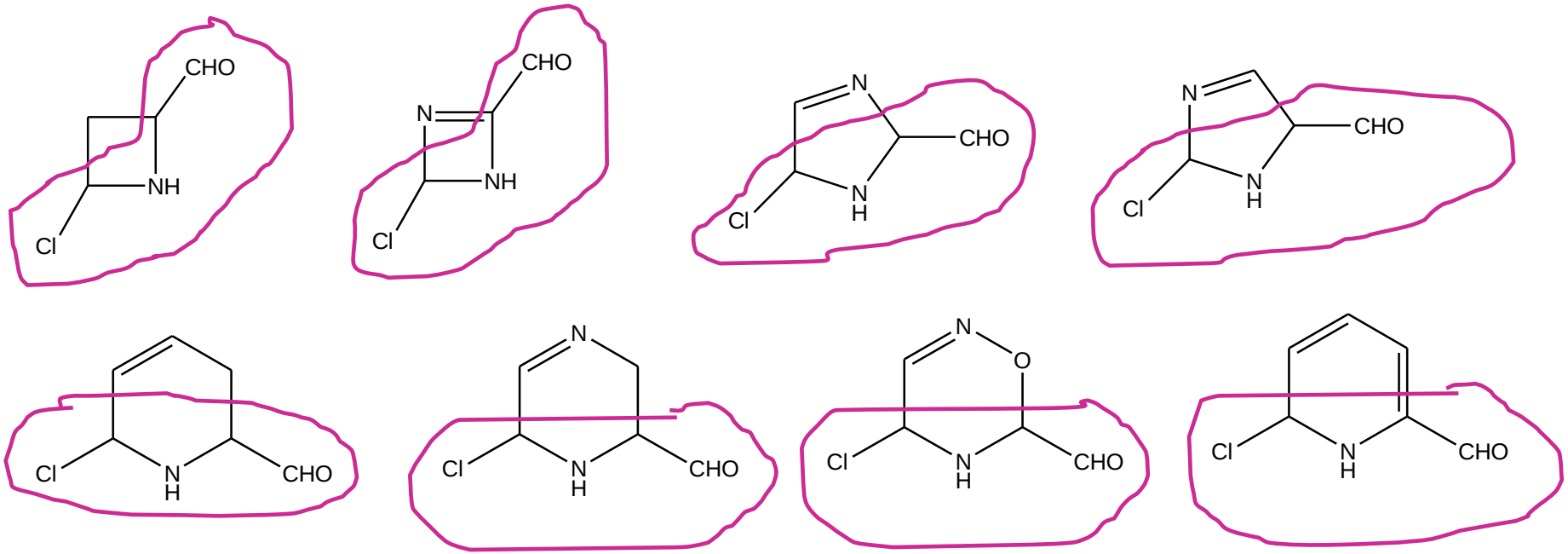


14874-70-5
B F4



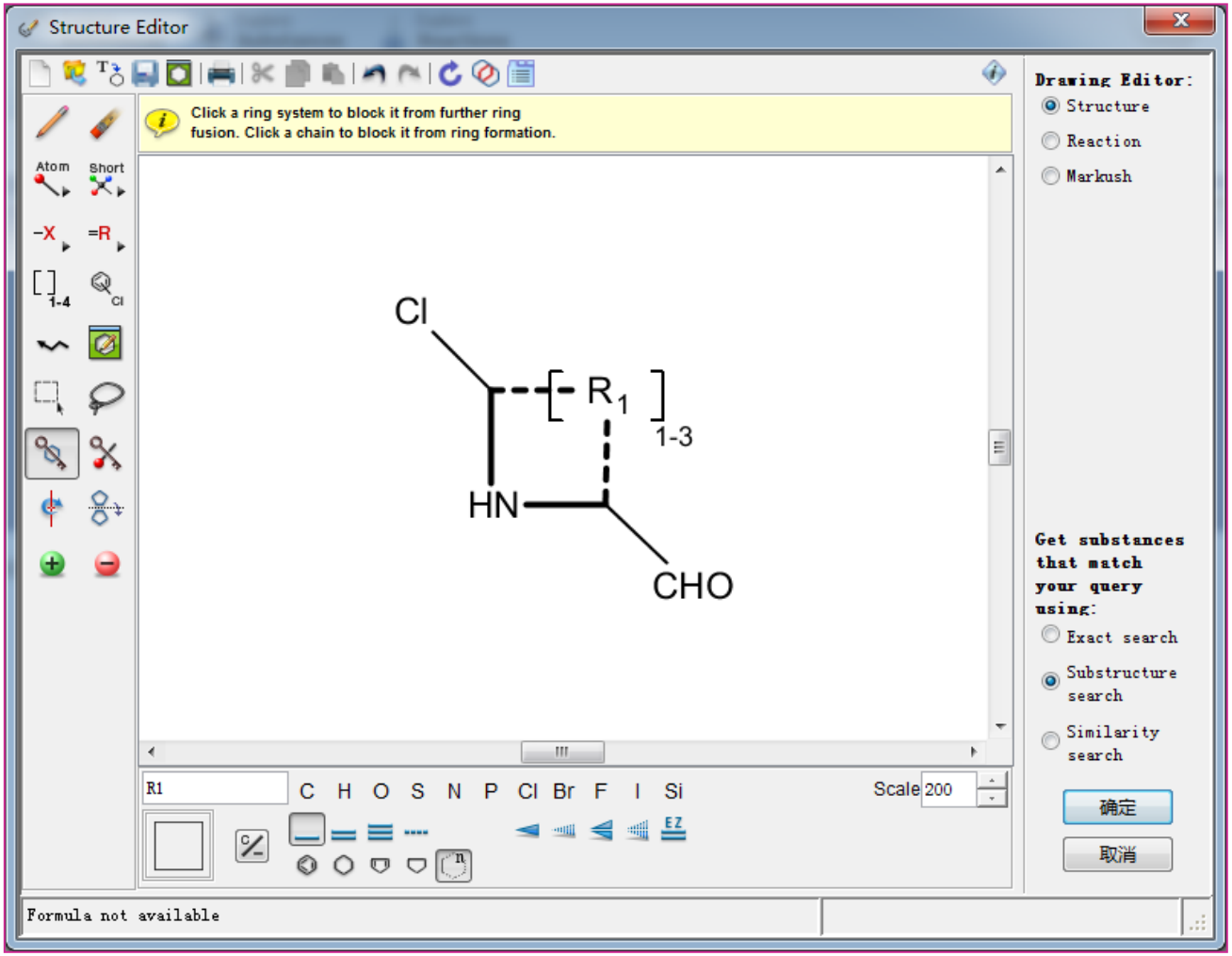
C23 H43 Cl N Ni P2 . B F4
Nickel(1+), [2,6-bis[[bis(1,1-dimethylethyl) phosphino-κ*P*]methyl]pyridine-κ*N*]chloro-, (*SP*-4-3)-, tetrafluoroborate(1-) (1:1)

我想获得以下的一系列物质



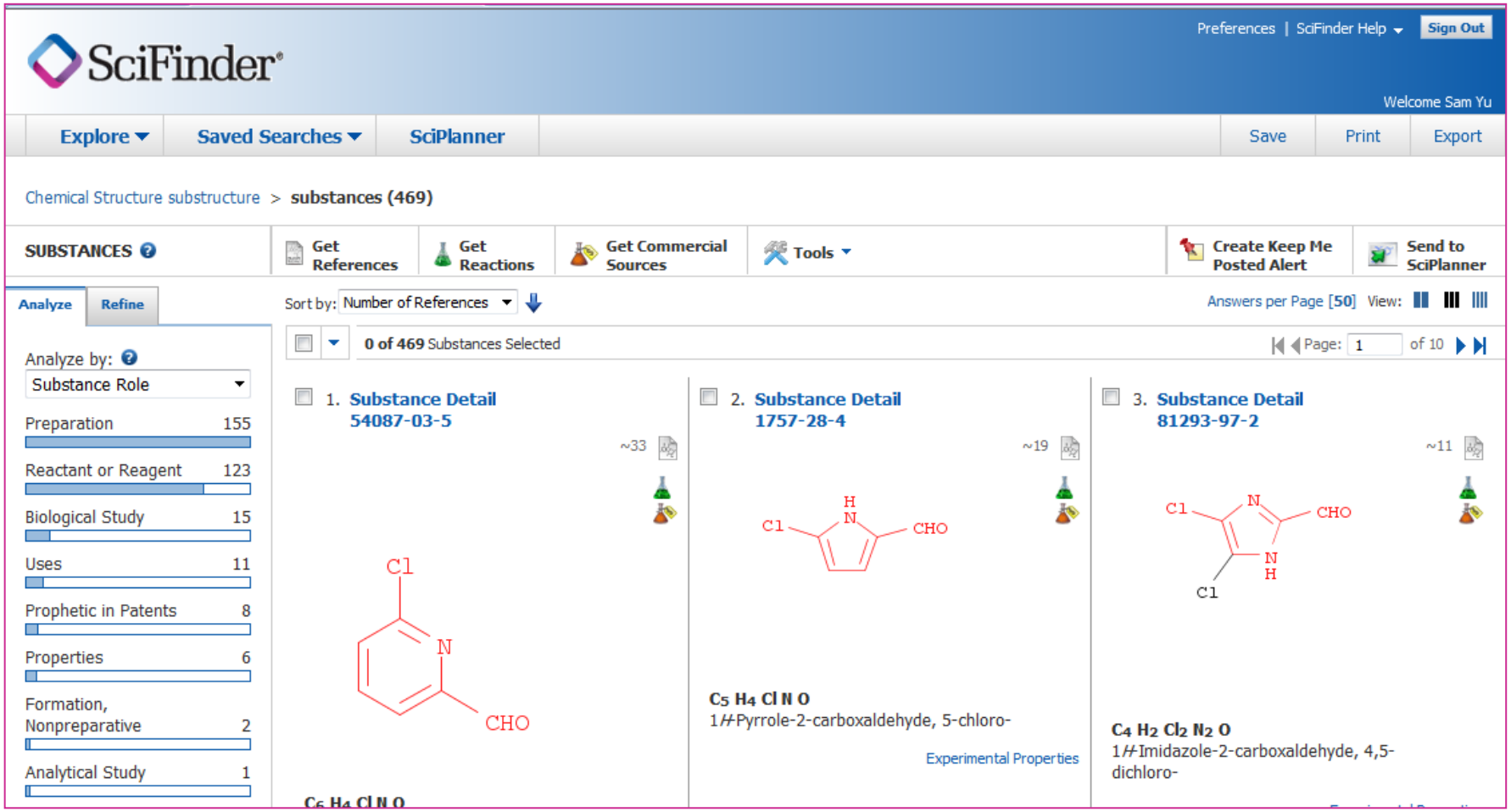
。 。 。 。 。 。

结构定义



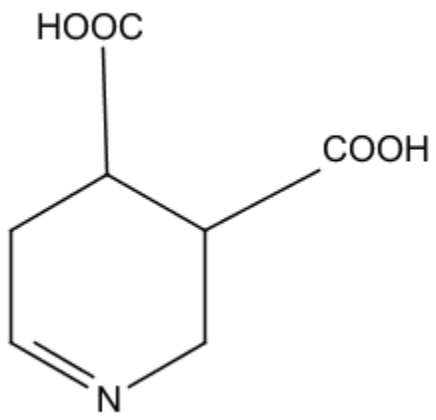
用亚结构检索获得所有的物质

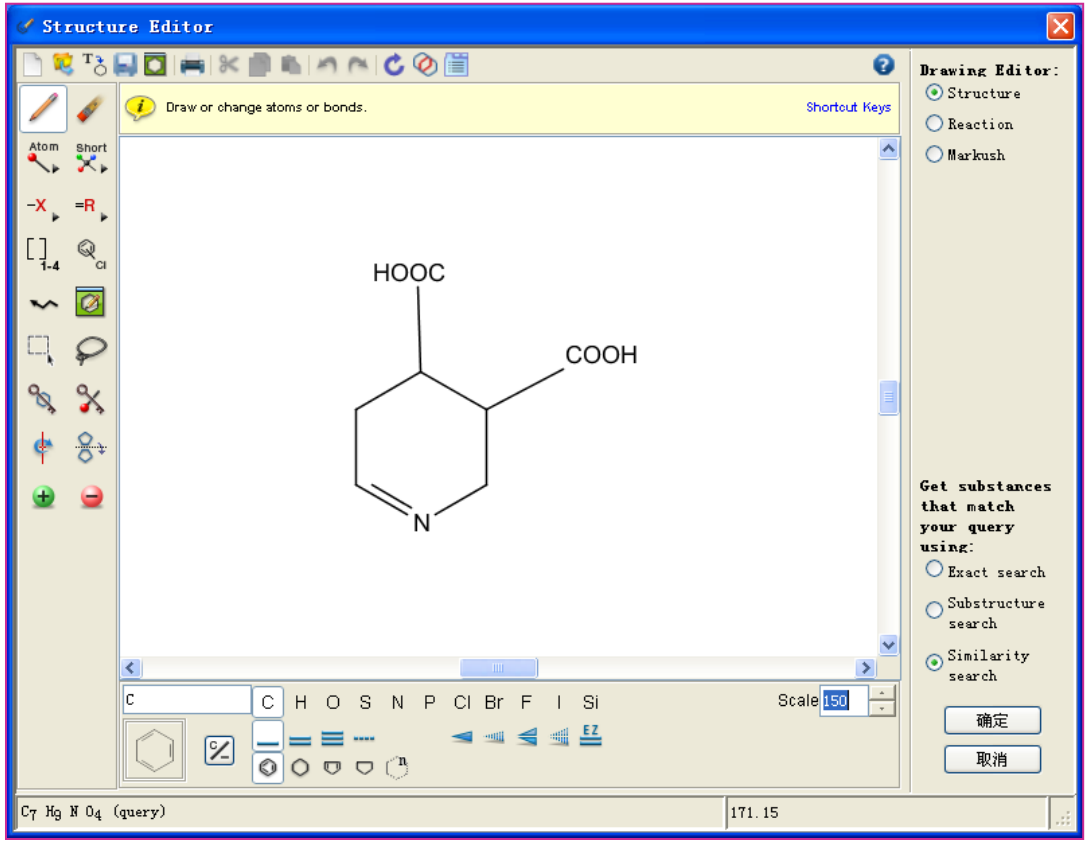
亚结构检索结果



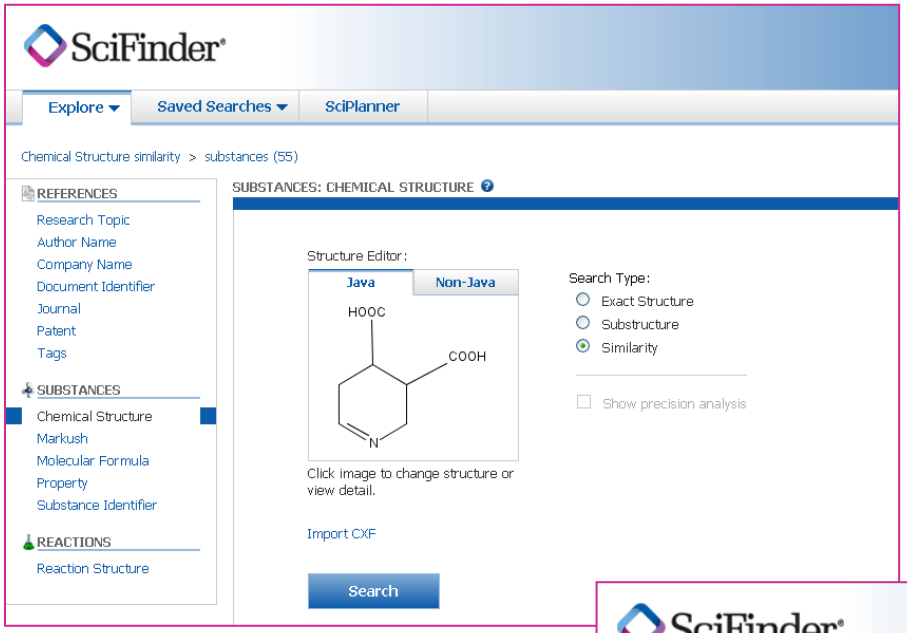
相似结构检索

这是一个不存在的化合物，有没有办法通过寻找类似物的方法，找到这个化合物的合成方法

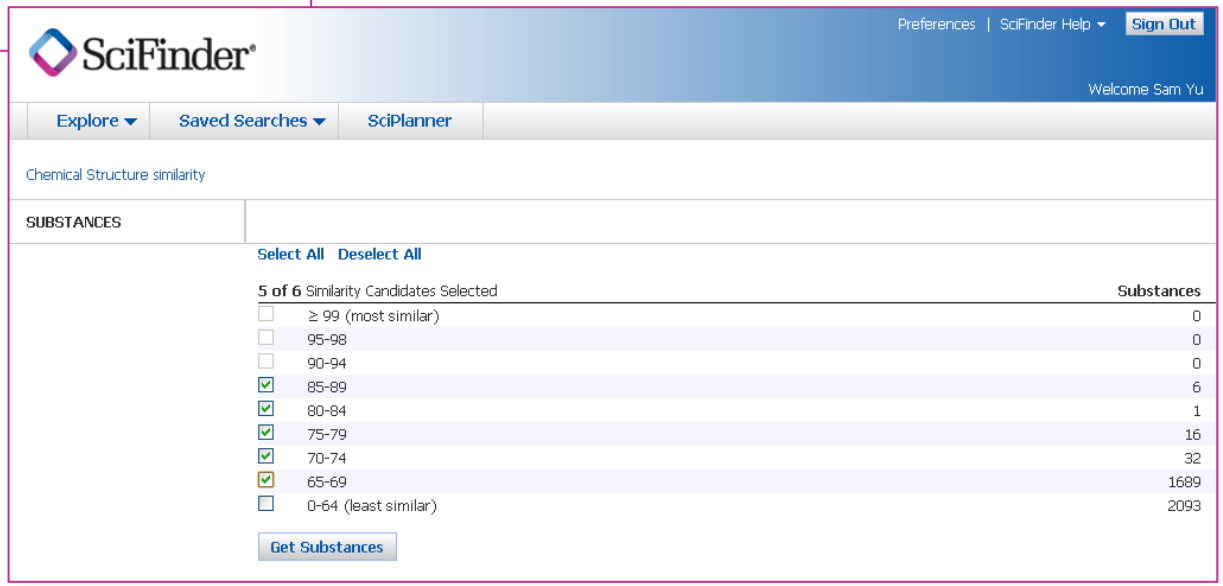




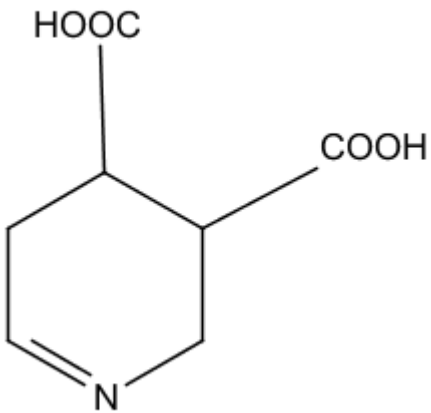
相似结构检索

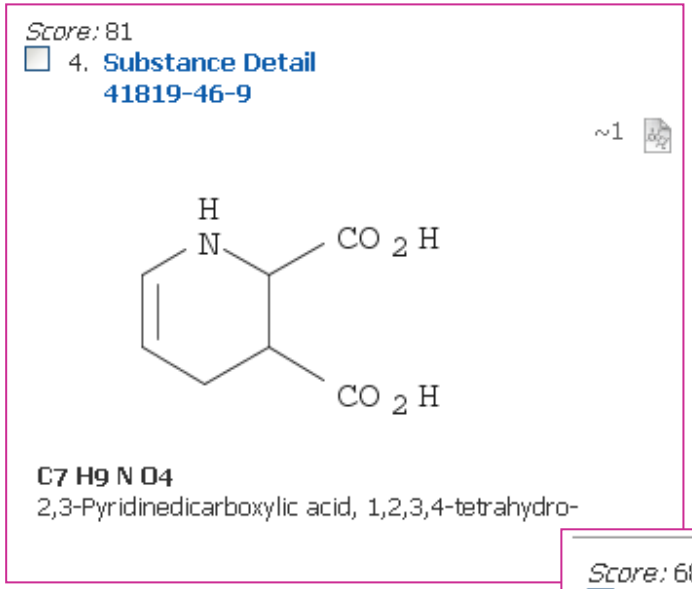


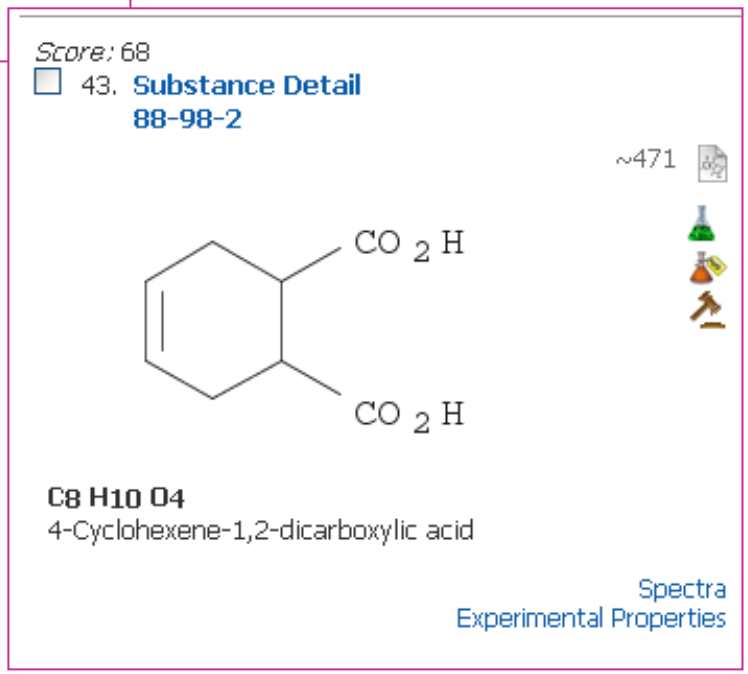
SciFinder会依据相似度给出相似度表格，选择高分值的看



和原本结构相似的结构







结构存在相似，但又不一样，可依据这些化合物的制备方法，制备目标化合物

精确结构，亚结构，相似结构检索区别

- 精确结构
  - 检索到结构的盐，混合物，配合物，聚合物等
  - 母体结构不能改变，不能修饰

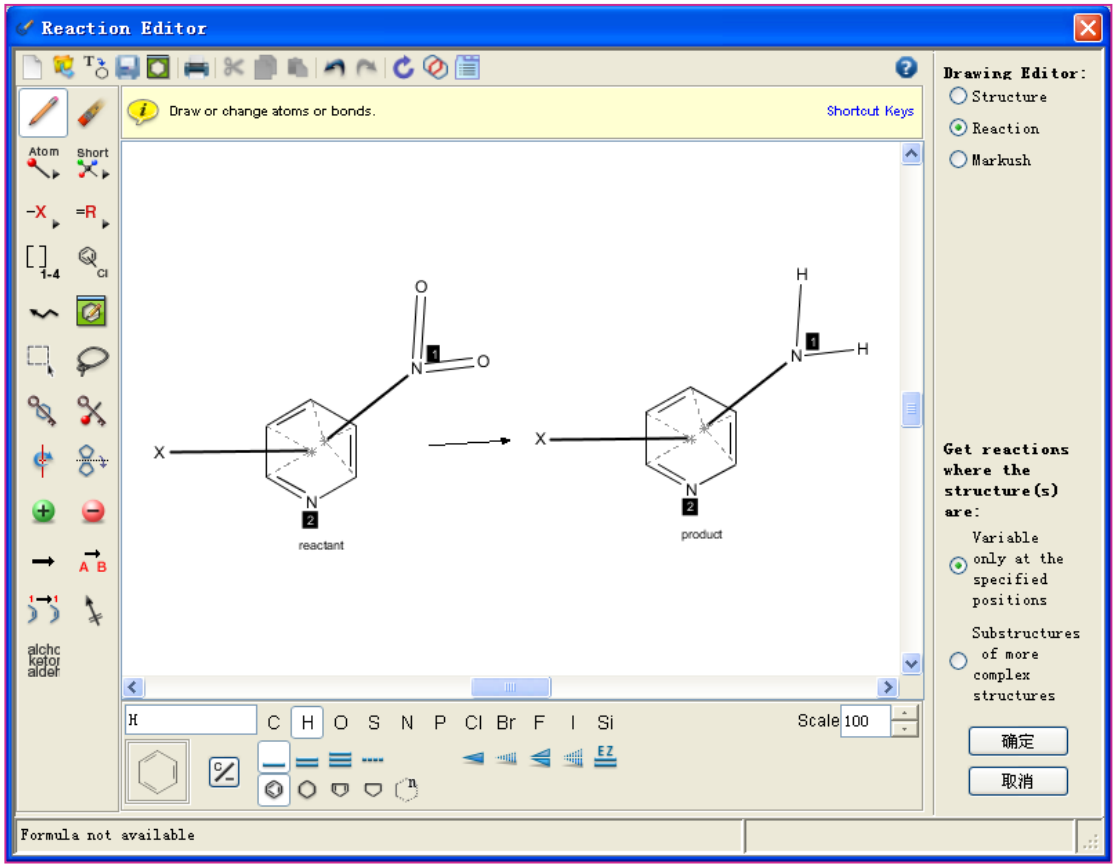
- 亚结构
  - 检索到结构的本身，衍生物结构
  - 母体结构不能改变，但可以修饰

- 相似结构
  - 检索到和结构本身相似度在60分以上的物质
  - 母体结构可以改变，可以修饰，用相似度控制结果范围

提纲

- 介绍
  - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索
- **SciFinder Web的注册**

SciFinder反应检索

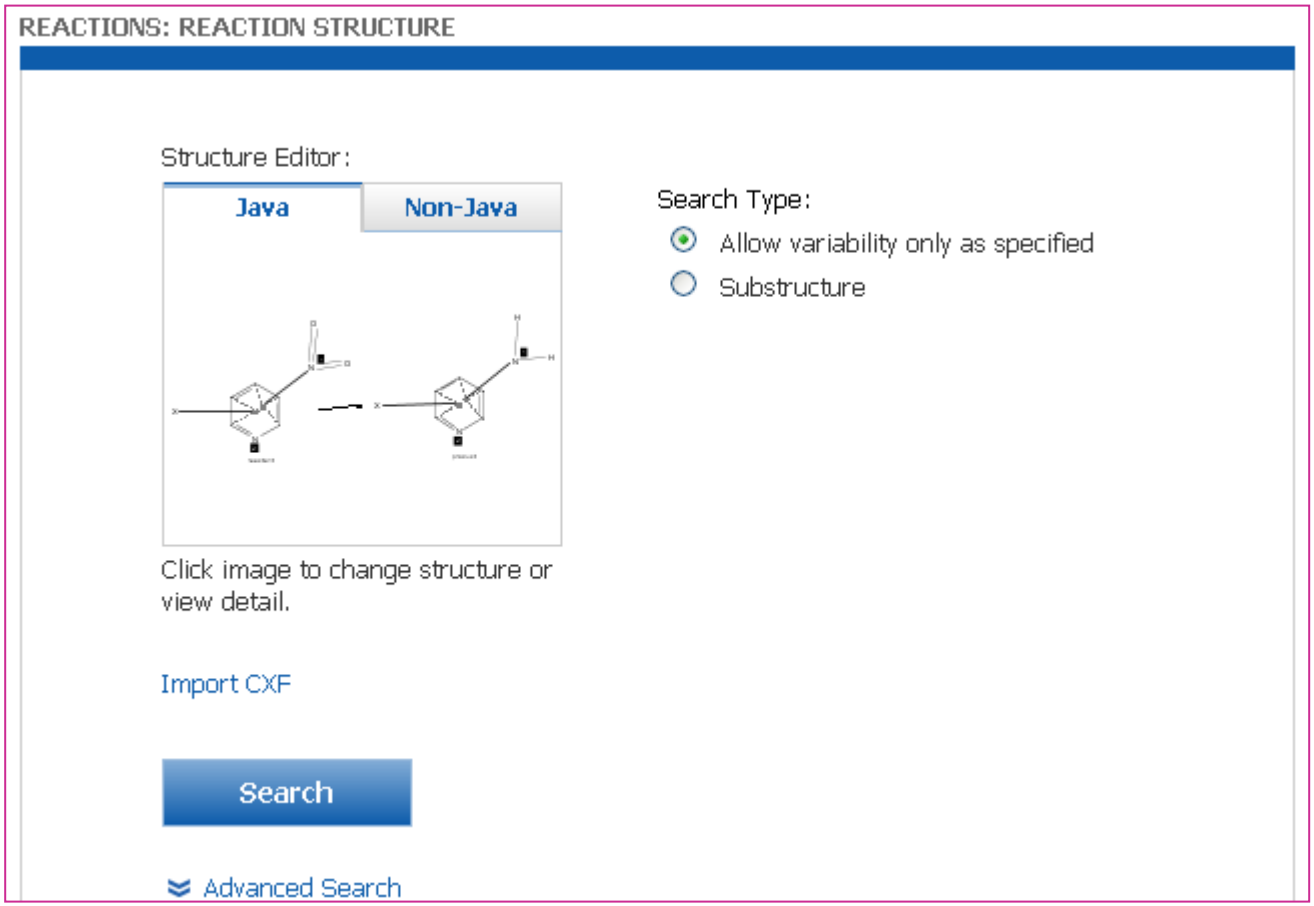


检索要求：

1：吡啶环2，3，4位上存在一个硝基还原成氨基

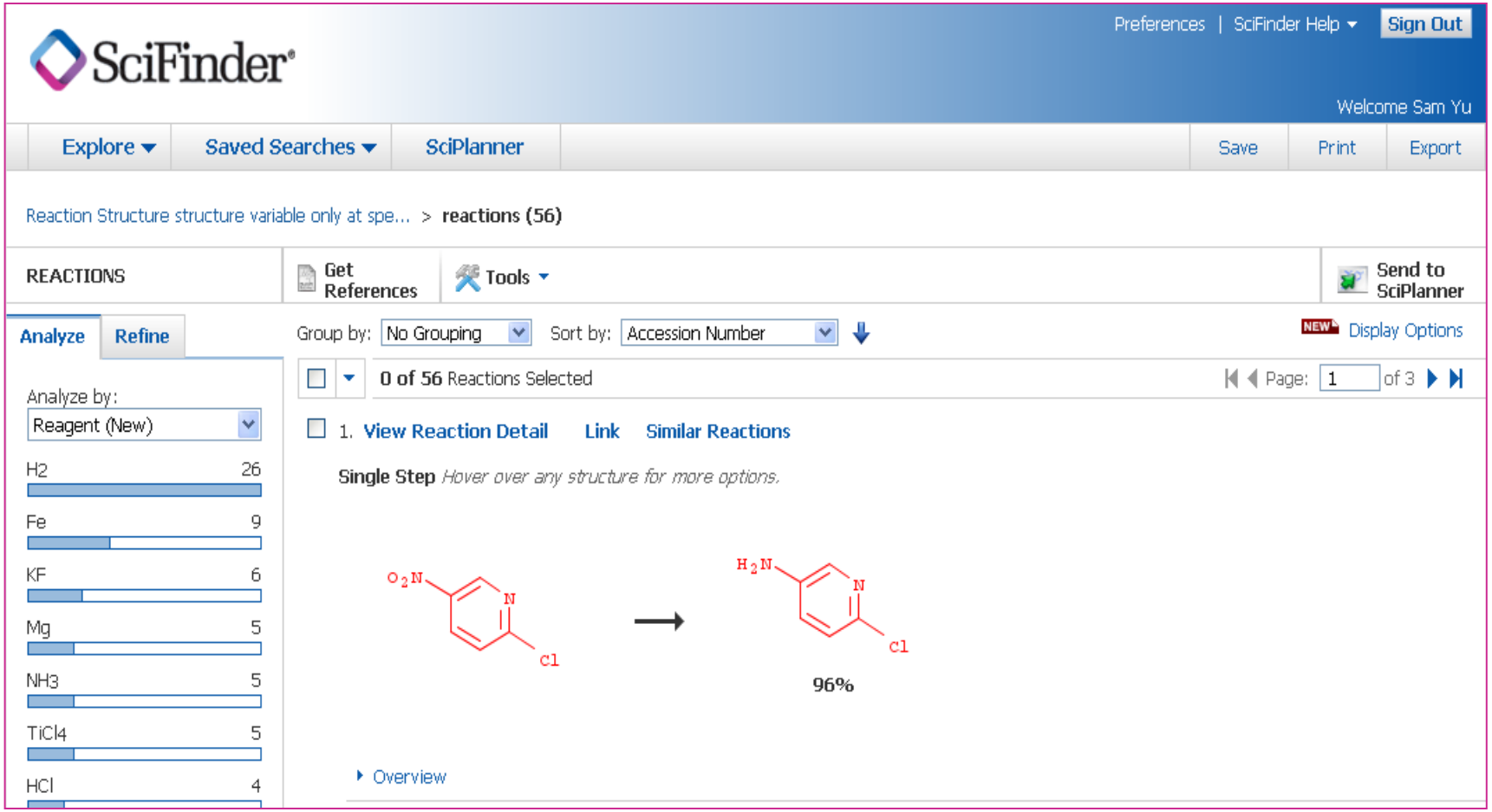
2：吡啶环5，6位上存在一个卤素

SciFinder Web中的检索

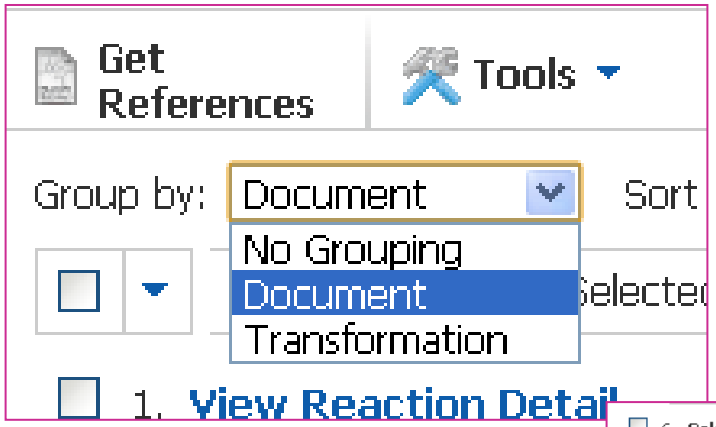


如果之前选择检索模式，可以在此处进行修改

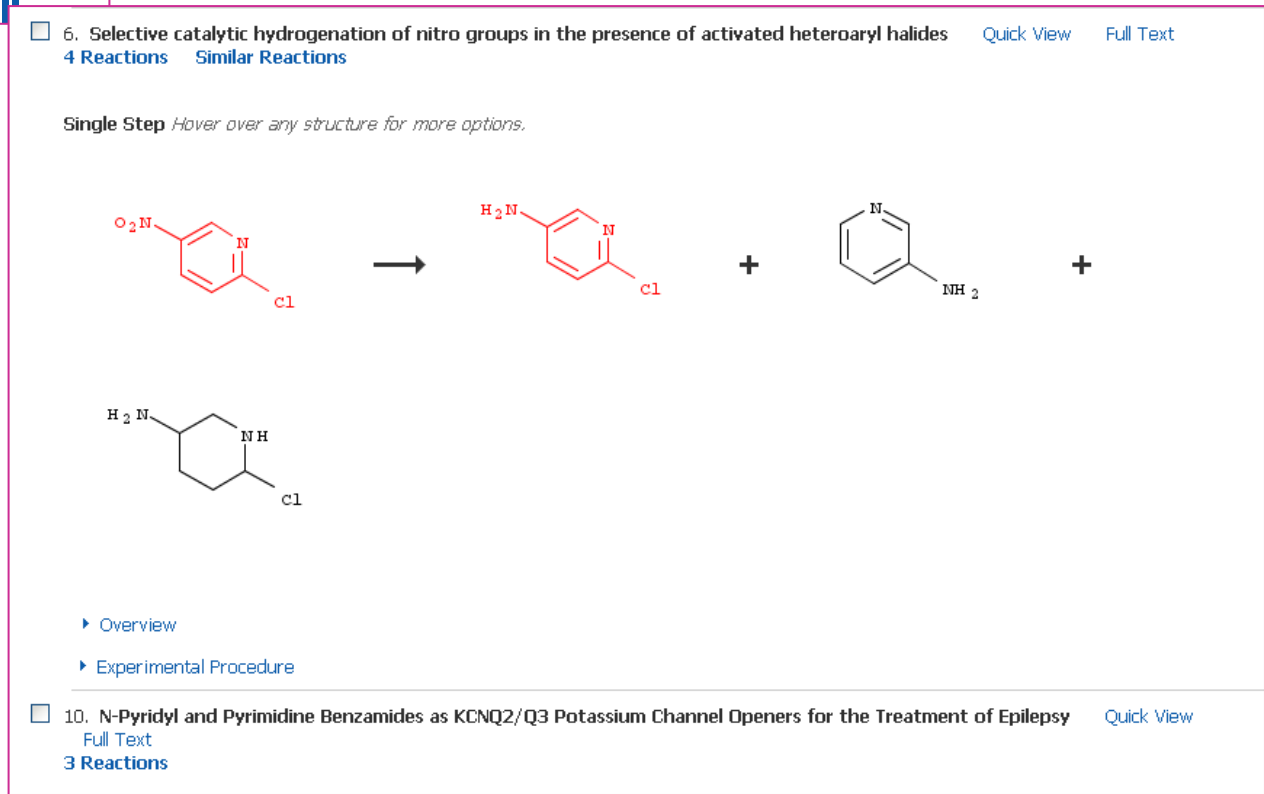
SciFinder中的检索结果



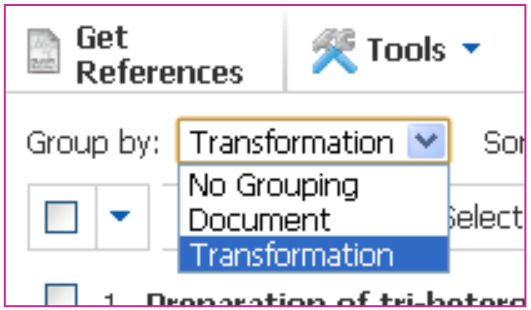
Group By Document

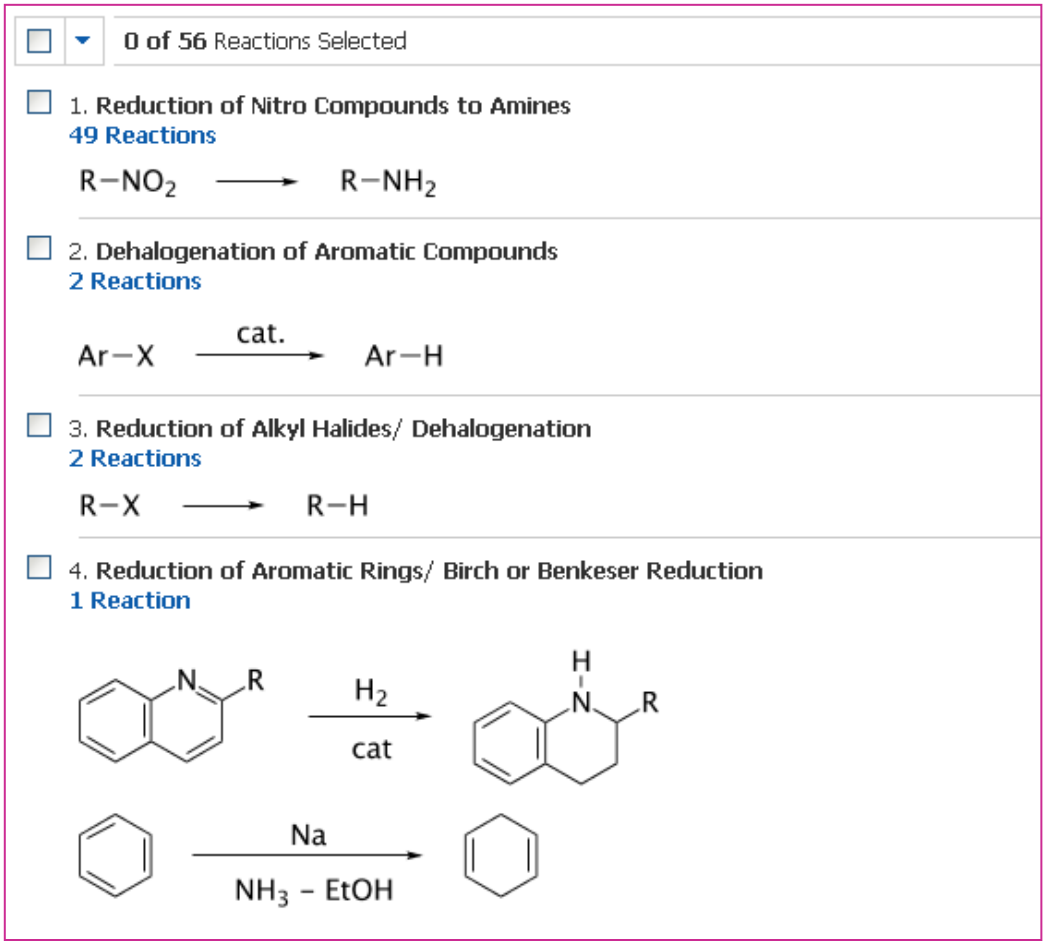


Group By Document将来自同篇文献的反应合并



Group By Transformation





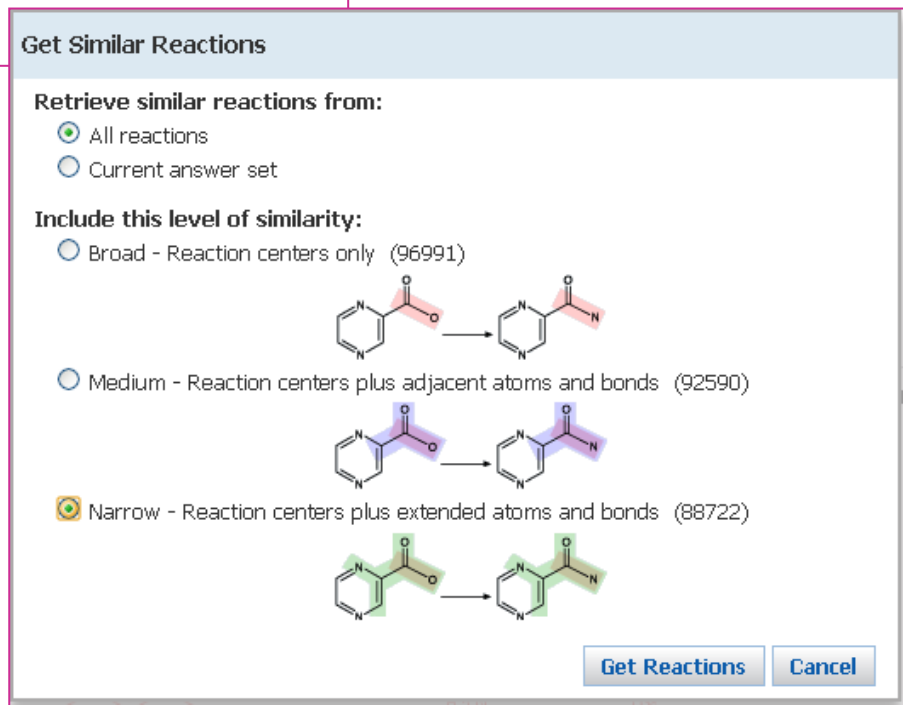
将所有同类型变化的反应合并

Similary Reaction

1. **Preparation of tri-heterocyclic derivatives as Flt3 kinase inhibitors** Quick View Full Text
1 Reaction Similar Reactions

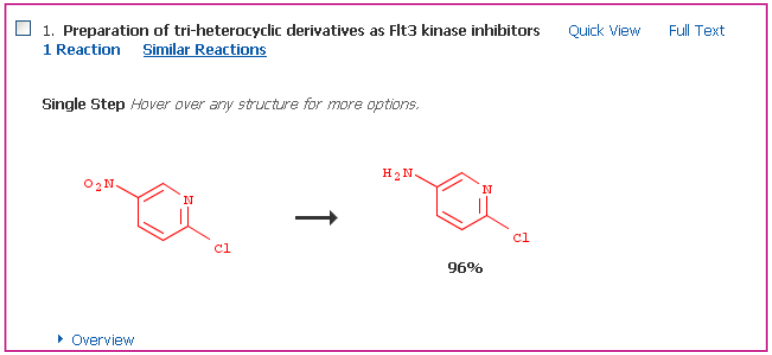
Single Step *Hover over any structure for more options.*

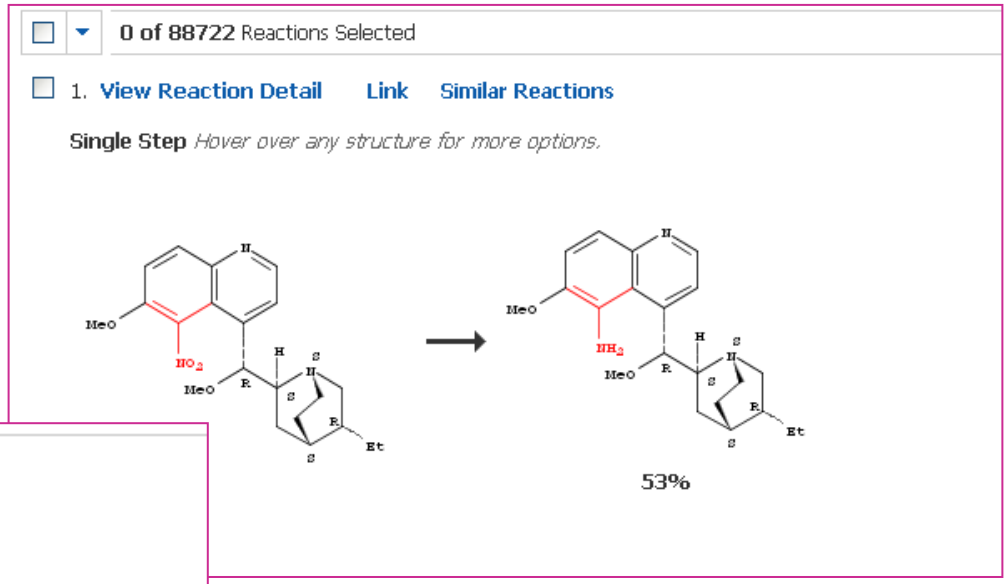
Overview

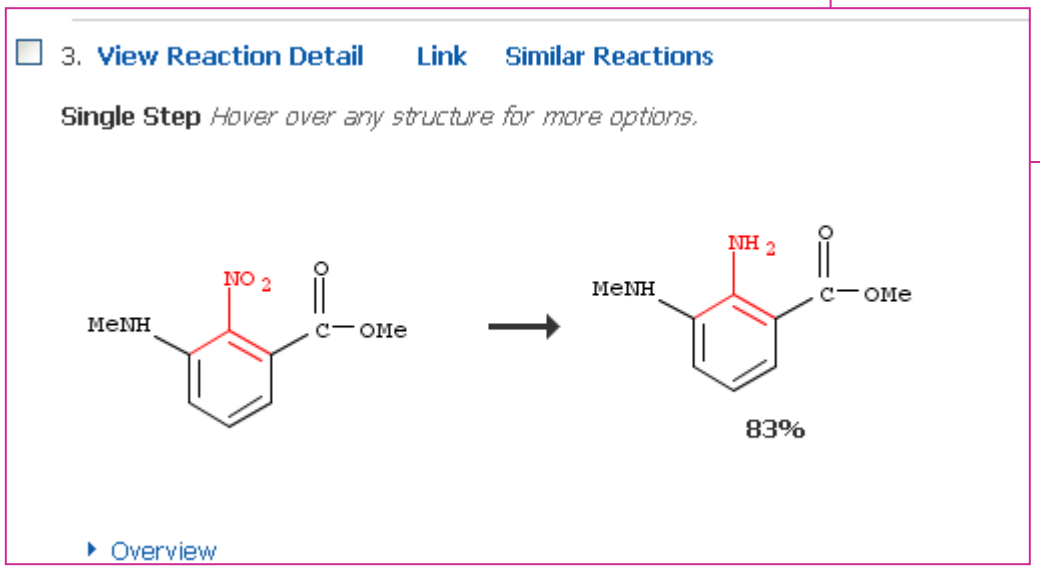


对单步反应提供相似反应检索，
Broad：仅反应中心相同
Medium：反应中心和附属原子相同
Narrow：反应中心及扩展原子和键相同

相似反应结果

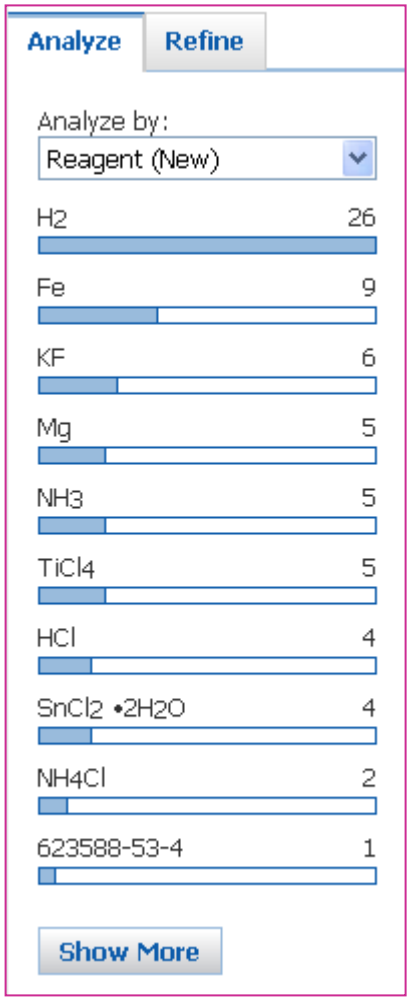


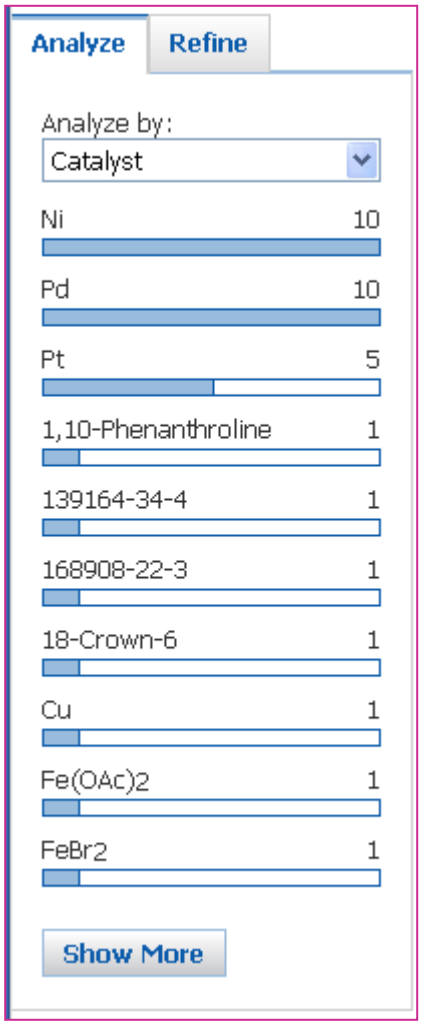


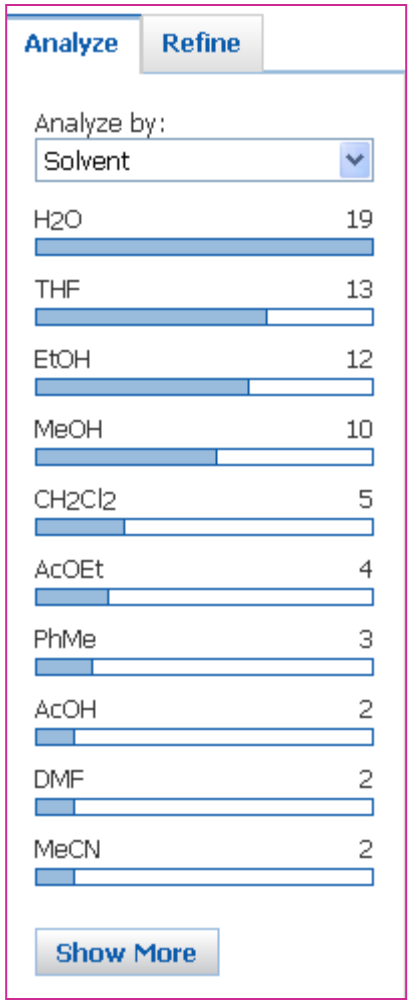


这些都和原有的反应，在反应中心，及扩展的原子和键上是一致的

SciFinder Web中的反应后处理







提纲

- 介绍
  - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索
- **SciFinder Web的注册**

SciFinder Web的注册和登陆

SciFinder Web的系统要求

Windows用户支持IE 9.x或者FireFox 2.x

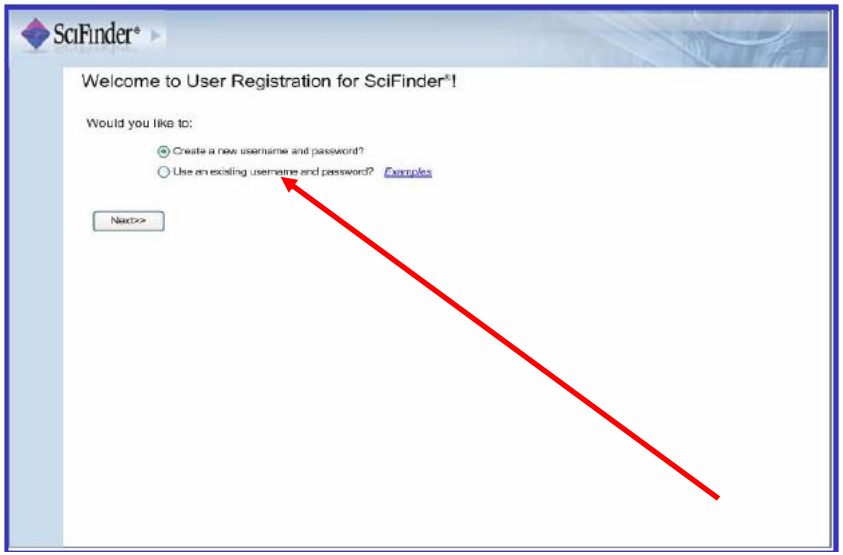
Mac 用户支持 Firefox 和 Safari

Java 安装（初次使用结构时自动安装，建议安装Java 7）

在图书馆相关页面上找到SciFinder Web注册用的网址

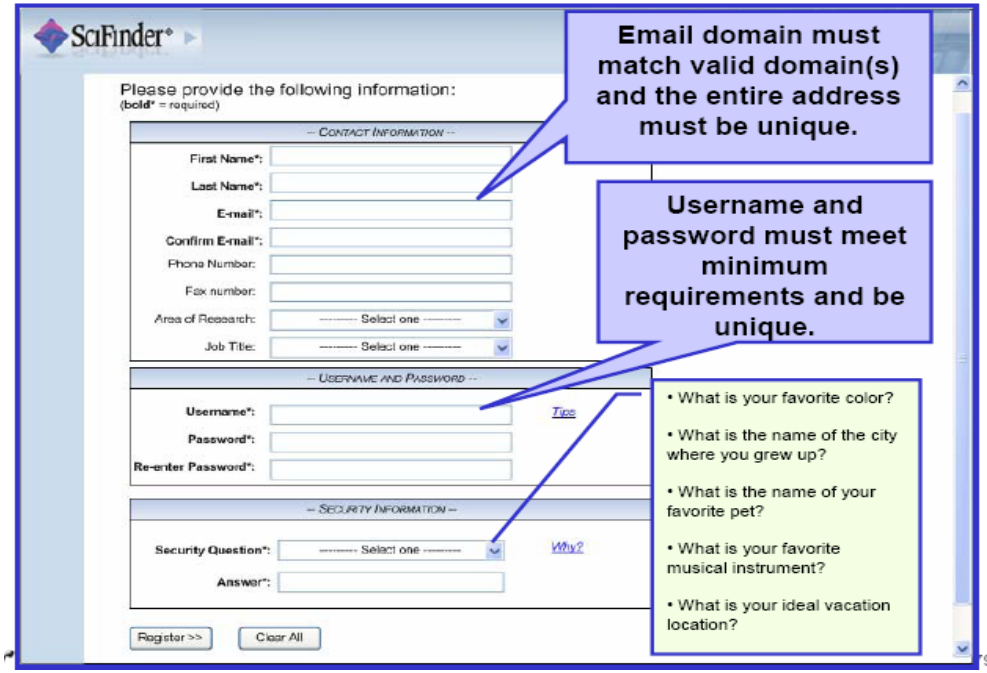
千万别用360浏览器，用其他浏览器的时候，也请关闭360安全卫士

点击URL创建SciFinder Web账号



开始创建SciFinder Web帐号

创建ID所用的IP不能是代理服务器的IP



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：

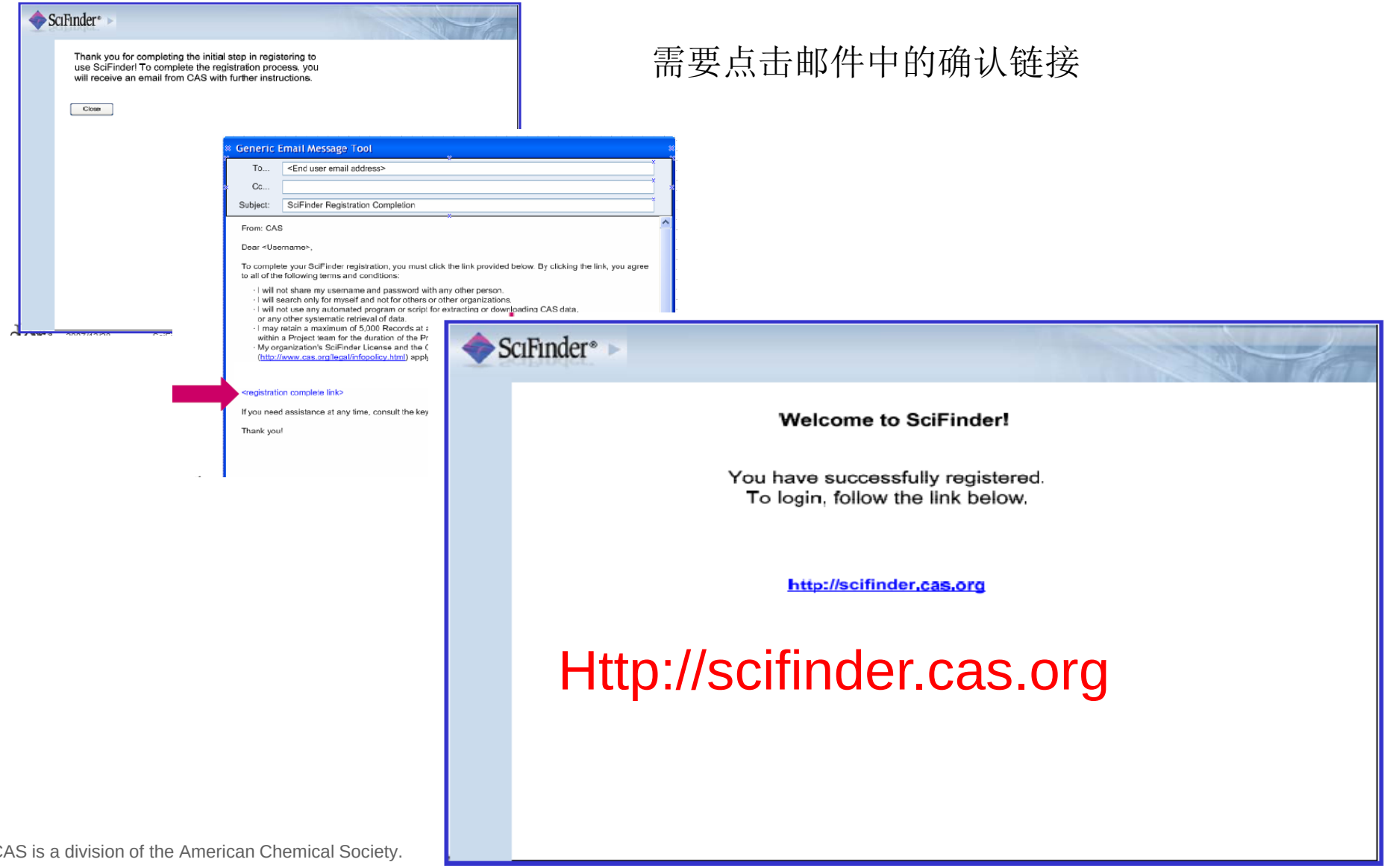
必须包含 7-15 个字符，并且至少包含三个以下字符：

字母　　混合的大小写字母

数字　　非字母数字的字符（例如 @、#、%、&、*）

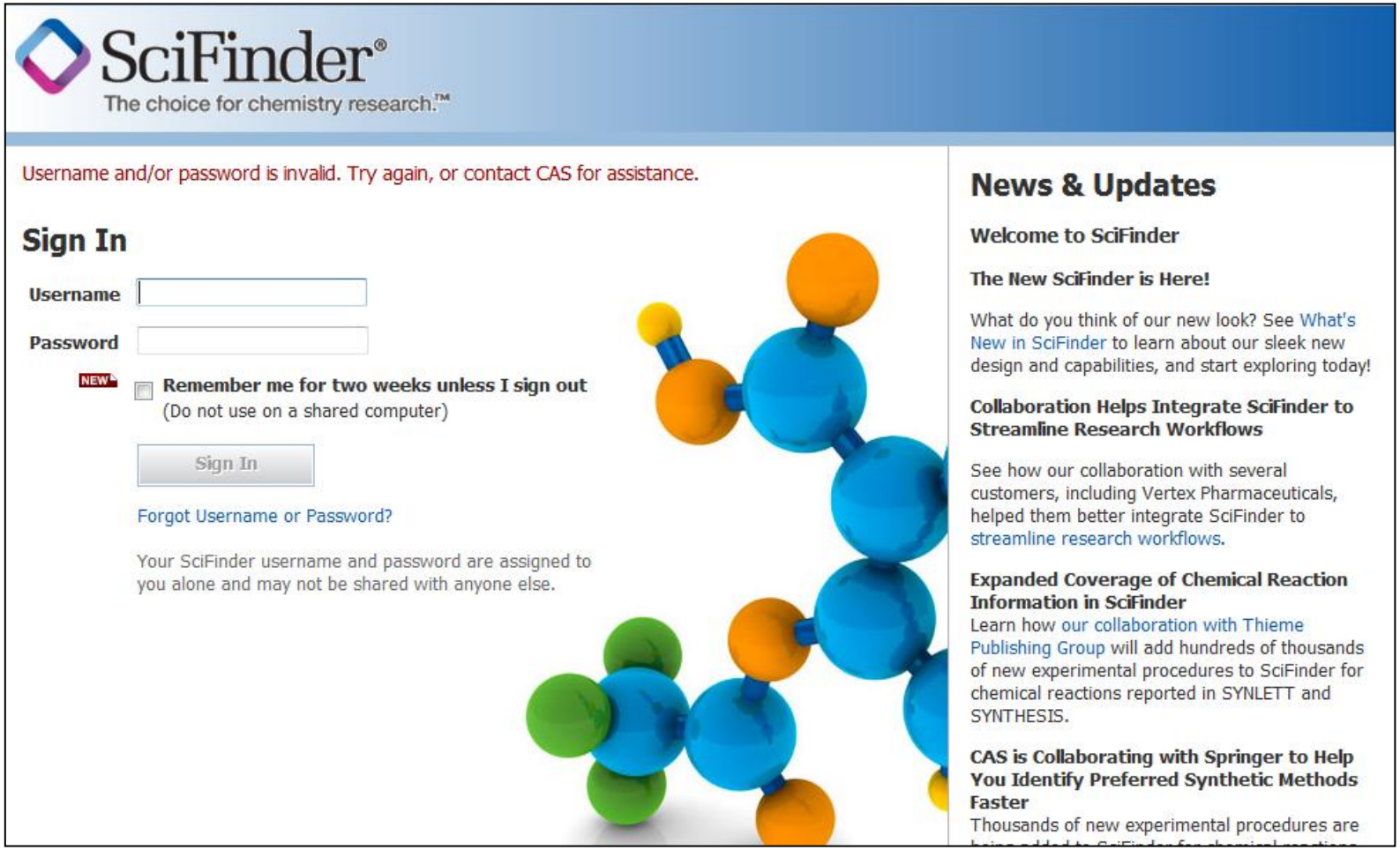
密码设置小技巧：
1：不要和账号中有重复的字符
2：密码格式最好是abc@123

对新ID的Email确认



需要点击邮件中的确认链接

SciFinder Web 常见问题



账号或密码错误，请在username处填写，截图，并与图书馆联系

SciFinder Web 常见问题

任何需要反馈给图书馆的问题，都请点击测试IP地址的链接

http://www.cas.org/cgi-bin/casip

Your IP address comes across to CAS as: **210.32.9.45**

将页面截图下来，一并发给图书馆

SciFinder使用注意事项

1. 单次下载只能下载50条记录，严禁过量下载SciFinder中的记录，如遇大量记录，请使用Analyze/Refine工具缩小检索范围，或使用Save功能，保存在网上
2. 请合理使用SciFinder，检索完，点击Sign Out退出
3. SciFinder使用南方答疑群：207211509(群满）， 258225168（新群）
4. 不能使用360浏览器登录SciFinder，即使在使用其他浏览器的时候，也请关闭360有关的任何软件

Thank You

俞靓

SciFinder 培训专员

Mail：Sam@igroup.com.cn

Tel:021-64453167-8004