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美国化学文摘社北京代表处

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# 提 纲

- 美国化学文摘社简介
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# 美国化学文摘社—Chemical Abstracts Service

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

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# CAS-构建最高质量的化学数据库

arXiv.org

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

Cornell University Library

U.S. Patent Office

Patents, journals, web, catalogs, etc.

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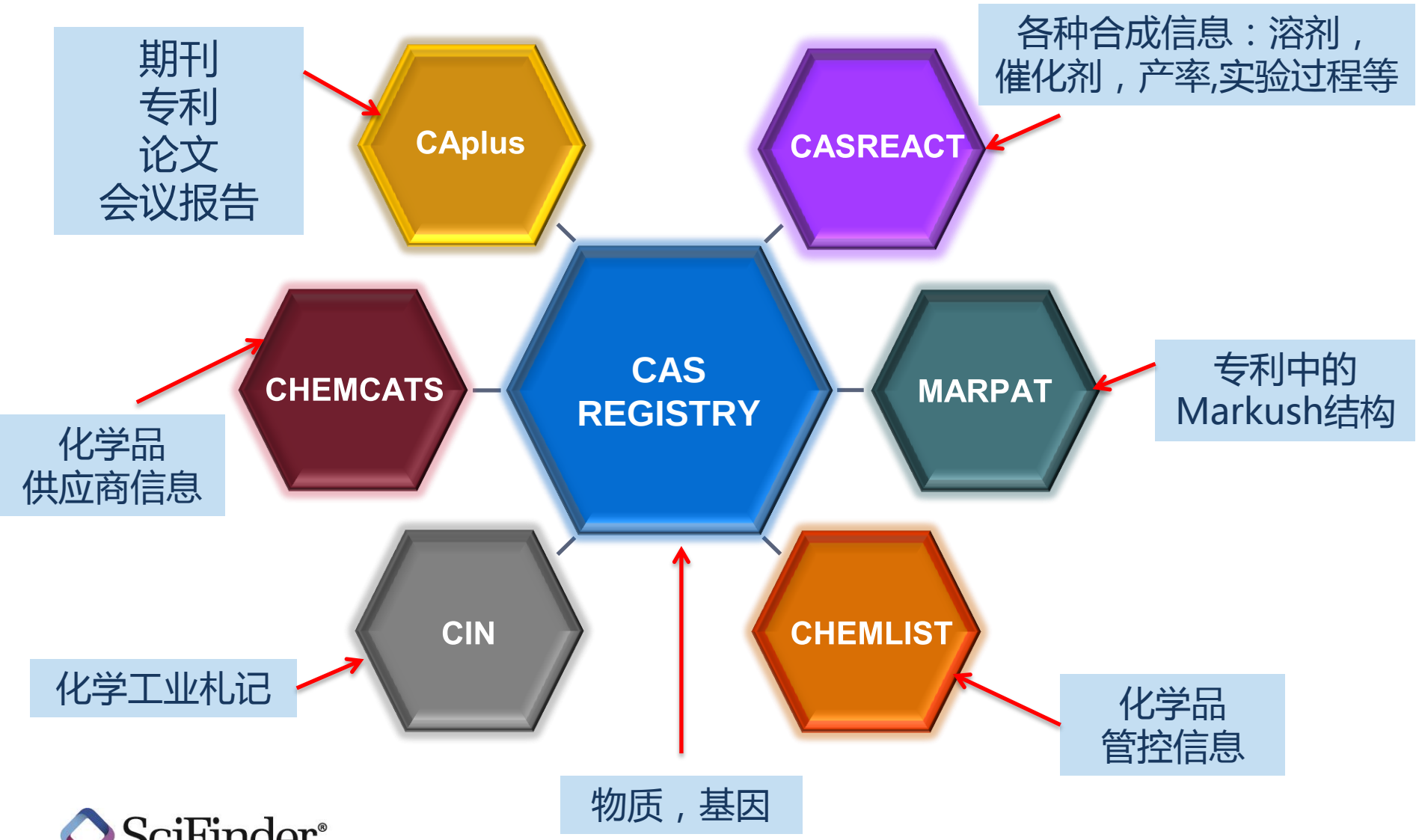


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# CAS数据库——源于化学，超越化学

**生物化学**：
农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

**有机化学各领域：**
氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

**大分子化学各领域：**
纤维素、木质素、造纸;涂料、墨水
染料、有机颜料 ;合成橡胶 ;纺织品、纤维

**应用化学各领域 ：**
大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

**物理、无机、分析化学各领域：**
表面化学,催化剂,相平衡,核现象,电化学

a

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# CAS数据库最具价值的内容—人工索引

## 12. Cobalt-Catalyzed Reductive Allylation of Alkyl Halides with Allylic Acetates or Carbonates

By: Qian, Xin; Auffrant, Audrey; Felouat, Abdellah; Gosmini, Corinne

A new route for the direct allylation of various alkyl halides catalyzed by simple cobalt(II) bromide has been developed. This method is efficient for the coupling of a large variety of alkyl halides (primary, secondary and tertiary) with substituted allylic acetates and carbonates and provides good to excellent yields with good functional group tolerance.

### Indexing

General Organic Chemistry (Section21-2)

**Concepts**

Allylic compounds

acetates, carbonates; prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates

Reactant; Synthetic preparation; Preparation; Reactant or reagent

Alcohols

allyl; prepn. of olefins via cobalt catalyzed r
acetates or allylic carbonates

Reactant; Reactant or reagent

Bromoalkanes

Alkenes

prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates

Synthetic preparation; Preparation

Allylation

Allylation catalysts

reductive; prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates

**Substances**

7789-43-7 Cobalt(II) bromide

prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates

Catalyst use; Uses

4407-36-7 trans-Cinnamyl alcohol
5332-06-9 4-Bromobutyronitrile
6940-78-9 1-Bromo-4-chlorobutane
7697-09-8 1-Bromobicyclo[2.2.2]octane
14660-52-7 Ethyl 5-bromopentanoate
25260-60-0
33884-43-4 2(2-Bromoethyl)-1,3-dioxane
57006-69-6
74036-95-6
166953-64-6 Benzyl 4-bromopiperidine-1-carboxylate

prepn. of olefins via cobalt catalyzed reductive allylation of alkyl halides with allylic acetates or allylic carbonates

Tips:

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

# CAS人工索引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好的解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term，CAS RN，CAS Role），提高效率，启发思路。

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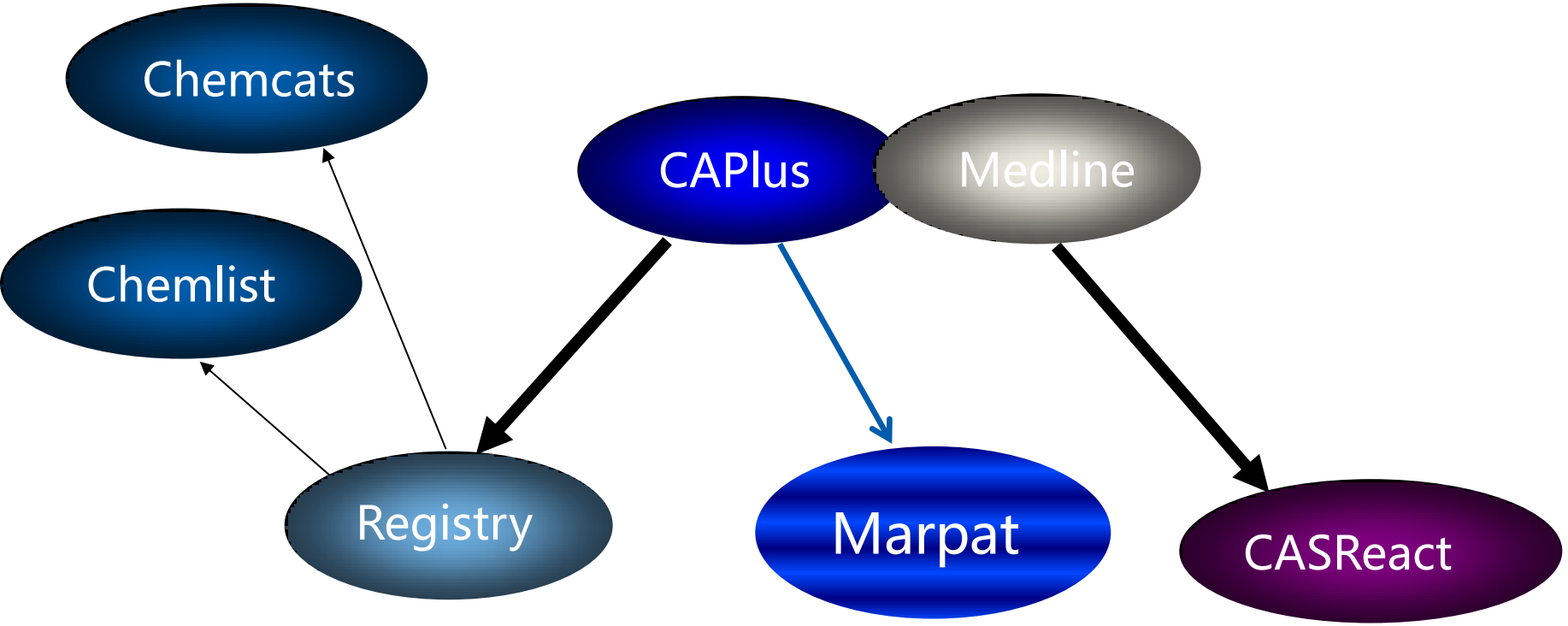


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Password

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(Do not use on a shared computer)

Sign In

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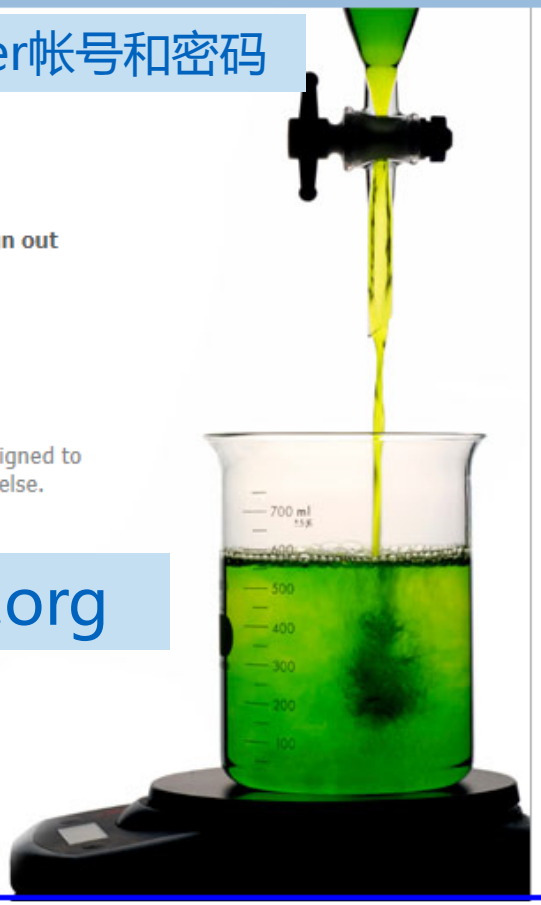
https://scifinder.cas.org



## News & Updates

**Welcome to SciFinder**

**A New Non-Java Structure Editor is Now Available in SciFinder**

SciFinder now features a non-Java version of the CAS Structure Editor, a new option for your substance and reaction searching! Start searching with the new editor today. Plus, we've added a new option to Analyze reaction answer sets by reagent, along with other enhancements. See all that's new in the latest release.

**Learn about this year's Nobel Prize-winning chemistry research with SciFinder**

By now you've heard that Martin Karplus, Michael Levitt and Arieh Warshel were awarded the 2013 Nobel Prize in Chemistry. But did you know that much of their Nobel Prize-winning research can be found in SciFinder? Check out a few examples of their most highly cited articles.

**Watch Part 3 of Our New Science in the News Podcast on Molecular Gastronomy**

In part 3 of our Science in the News podcast on molecular gastronomy, find out why SciFinder is essential to food chemistry research. Watch it now and don't forget to catch all three parts of

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  - 文献标示符检索
  - 期刊名称和专利信息（公开号，申请号等）
  - 从物质，反应获得文献


- 检索策略推荐
  - 关注某特定领域的文献：主题检索
  - 关注物质有关的文献：先获得物质，再获得文献
  - 关注某科研人员的文献：作者名检索
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# 文献检索—主题: Suzuki催化反应

## 检索式： Suzuki reaction with catalyst


关键词之间可用介词连接：
in, with, of…

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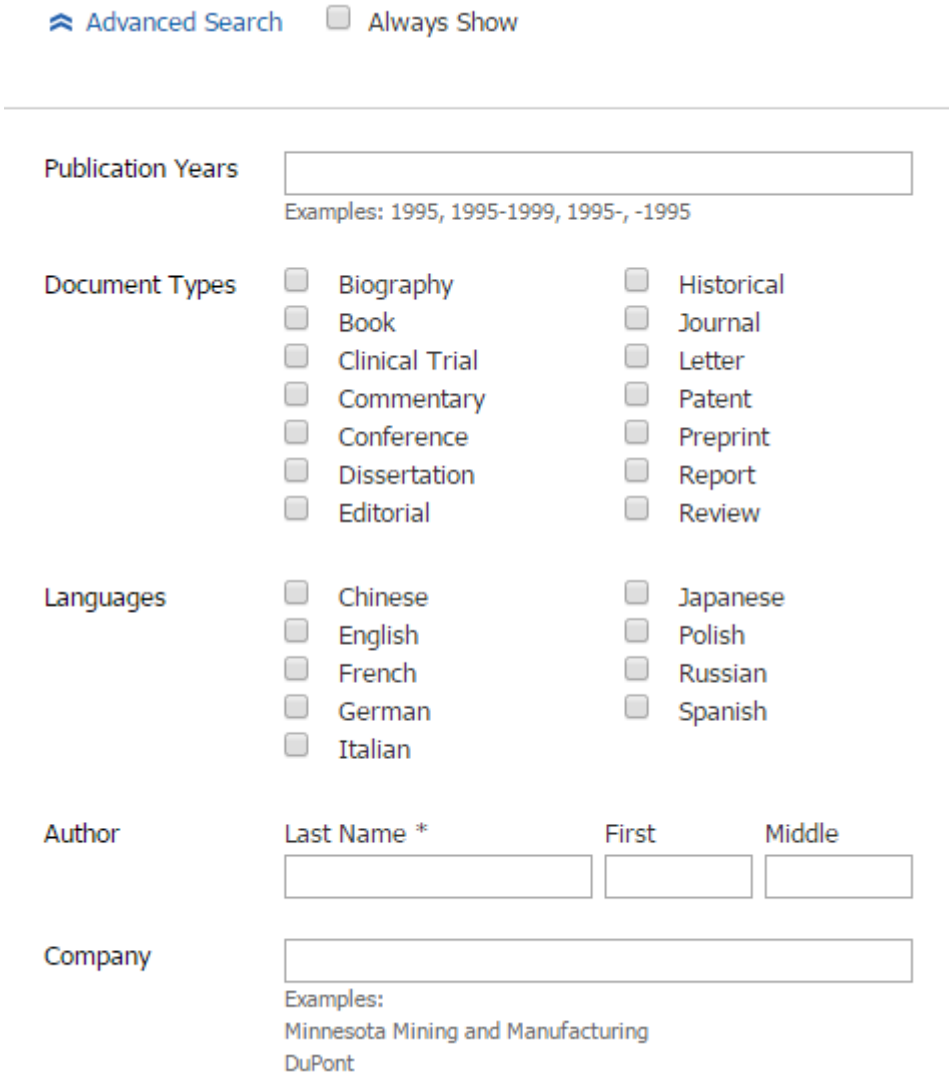
# 文献检索—主题: Suzuki催化反应

## 检索式： Suzuki reaction with catalyst

提前限制出版年限、文献类型、语言等

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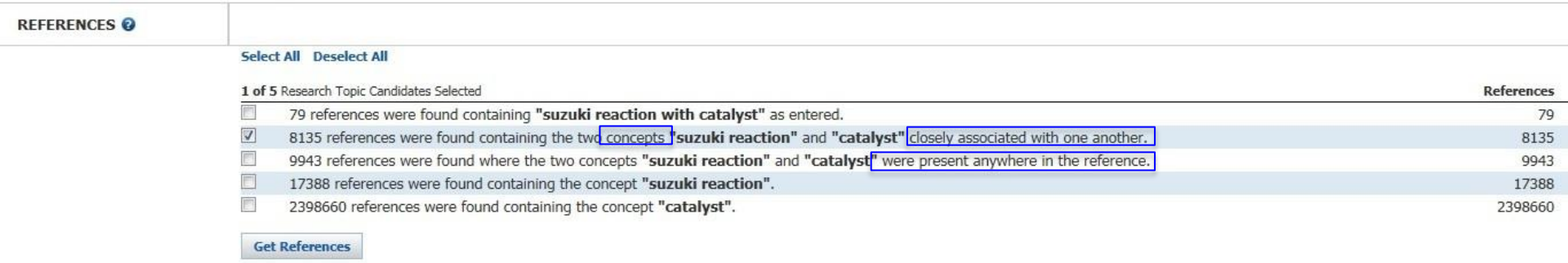
# 主题检索的候选项




“Concepts”表示对主题词做了同义词的扩展；

“Closely associated with one another”表示同时出现在一个句子中或同时作为索引词；

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

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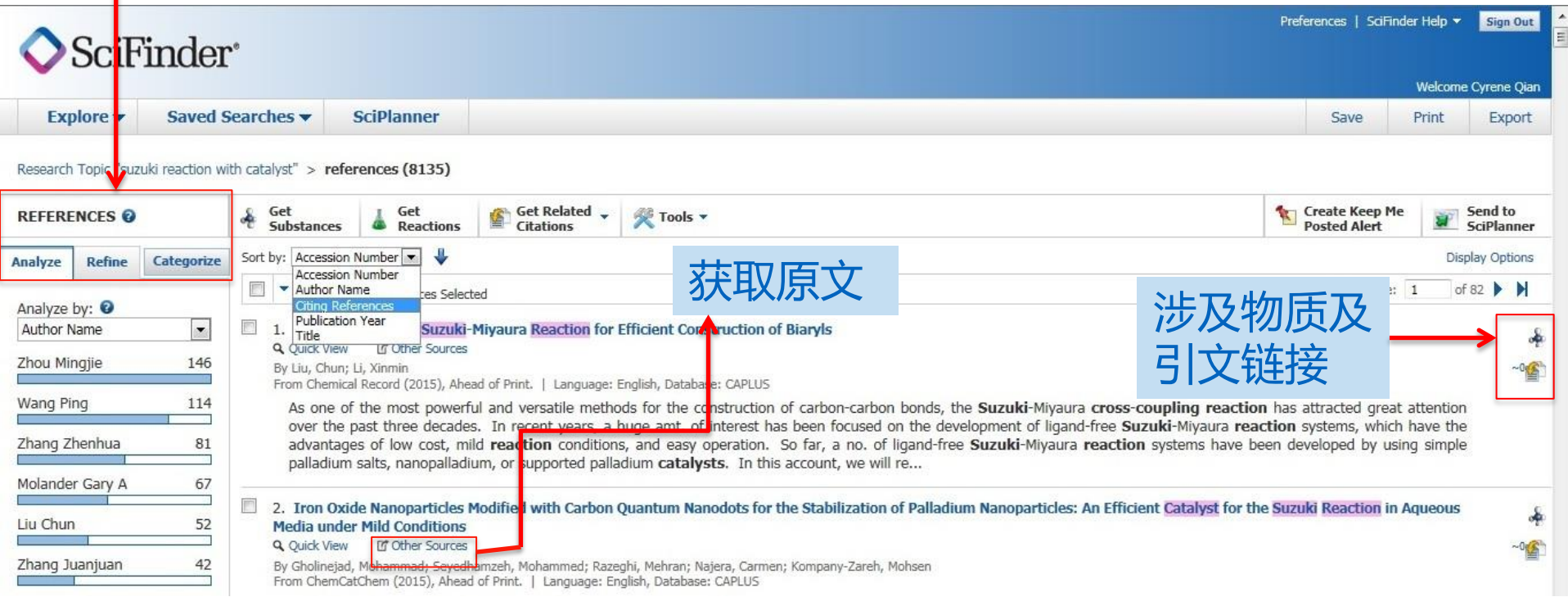
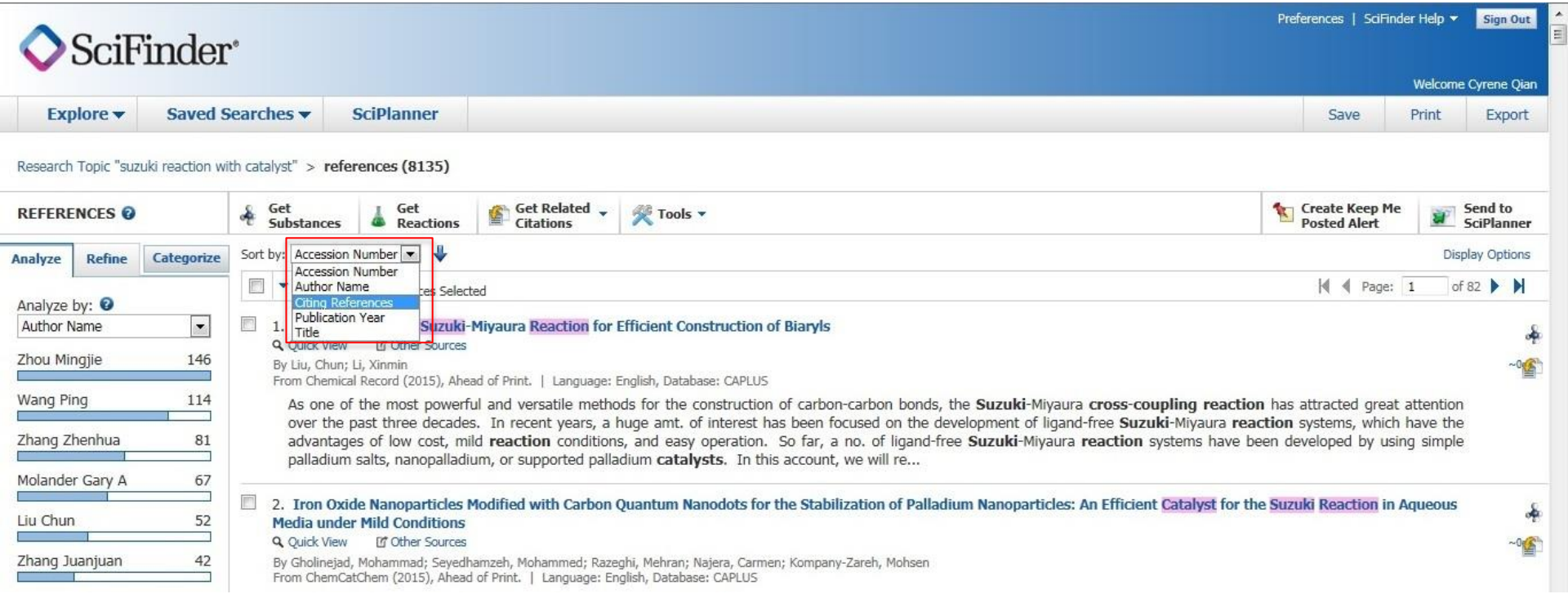
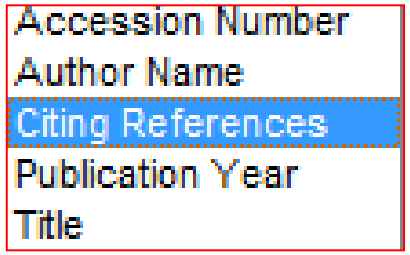
# 文献检索结果

文献处理工具



# 文献结果的排序功能




5种排序方式，可以按照进入数据库的时间、作者名、引文排序、公开年限、标题对文献检索结果进行重新排序

Citing Reference: 可能帮助找到最重要的文献

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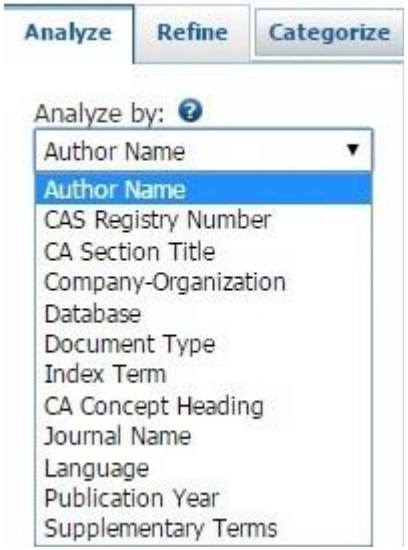
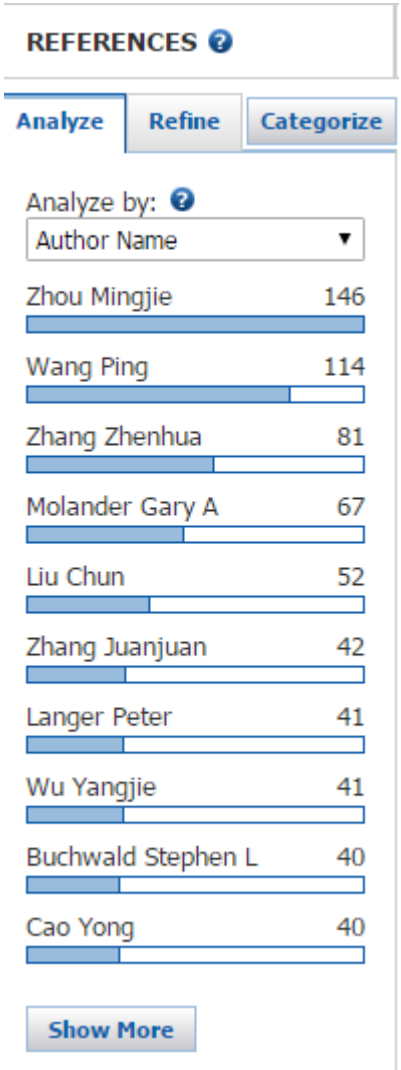
# 文献检索结果：Analyze

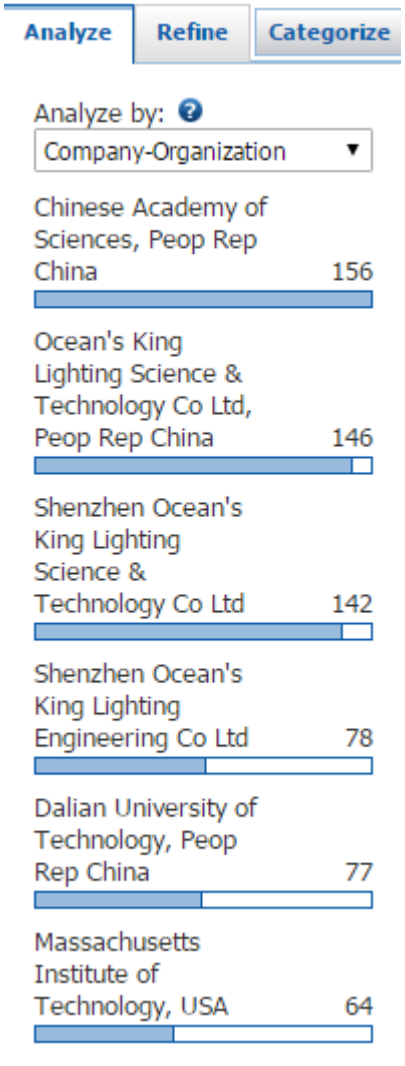
12种文献分析工具



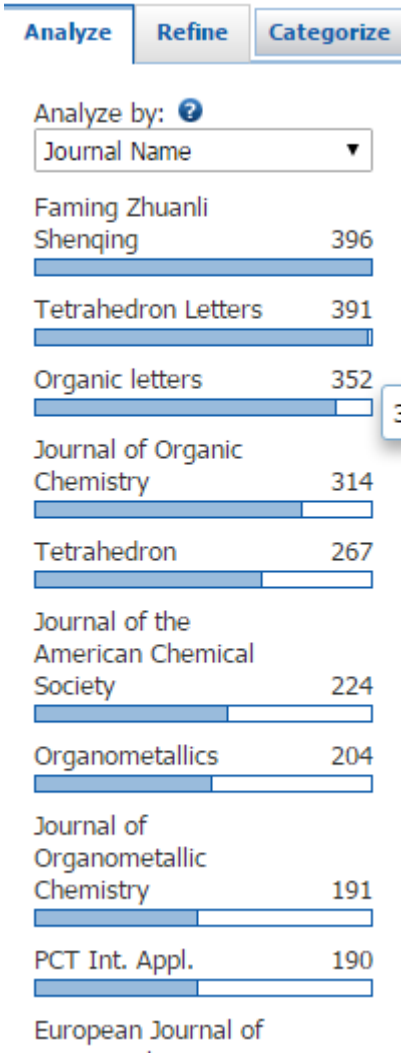

领域内主要研究人员，专家




主要研究机构，合作伙伴，竞争对手




主要的期刊

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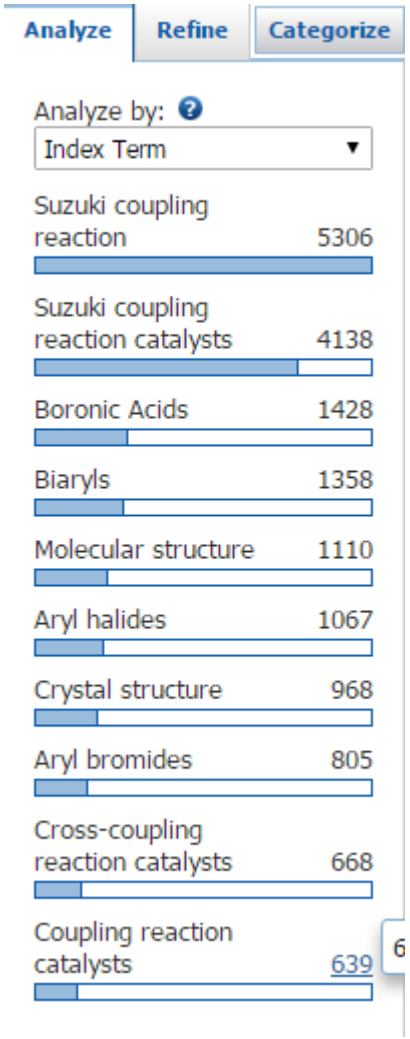
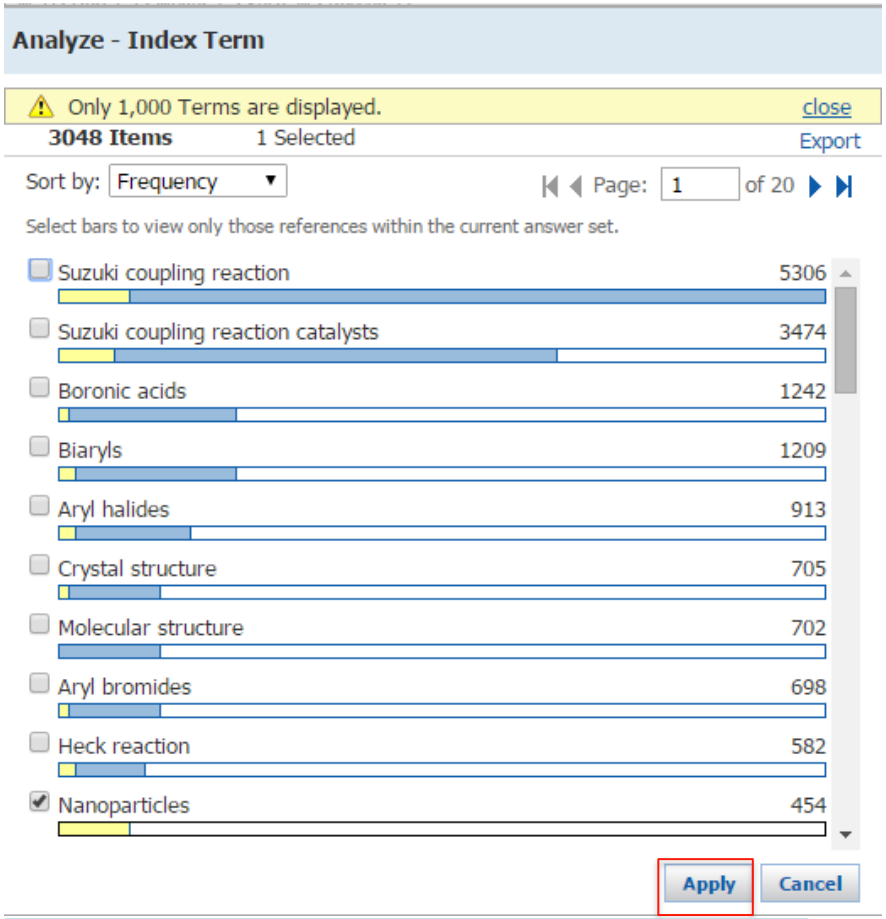
# 文献检索结果的Analyze




Index Term：

帮助用户全景了解文献内容，精选文献




选择感兴趣的内容，点击Apply

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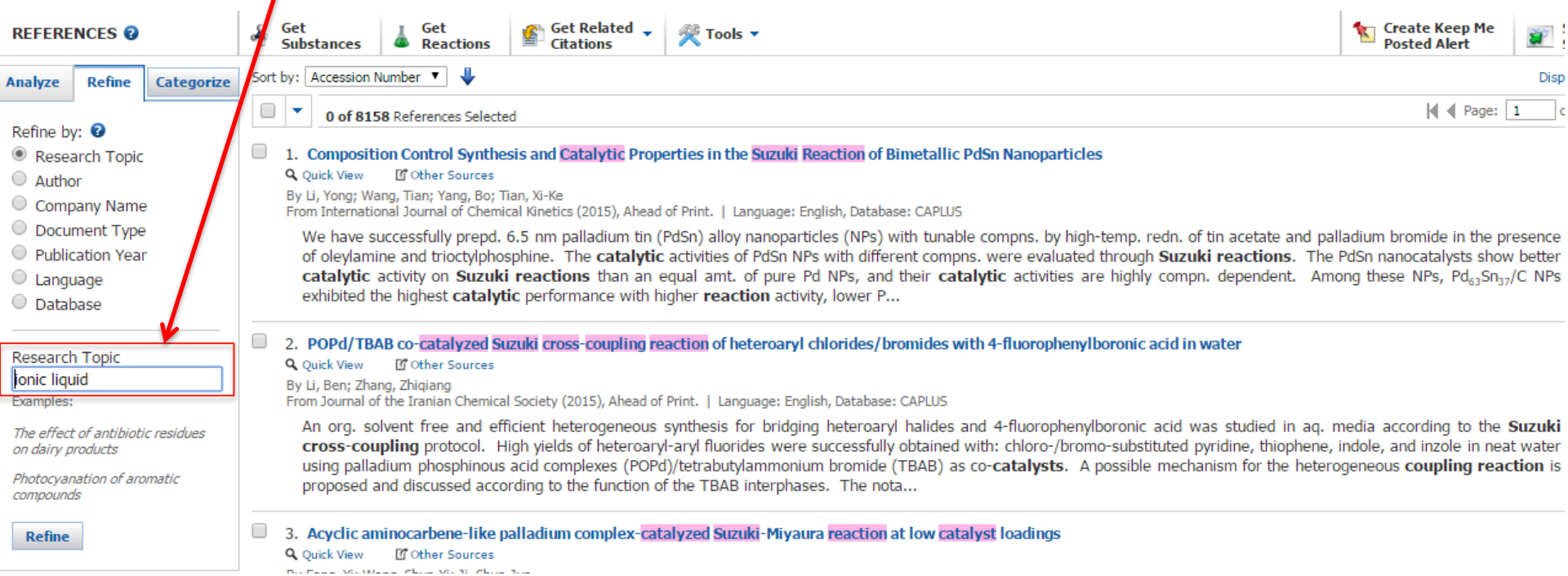
# 文献检索结果的Refine

六种限定工具，包括主题词、作者姓名、机构名称、出版年代、语言、所属数据库

在结果中筛选主题带有“ionic liquid”的文献

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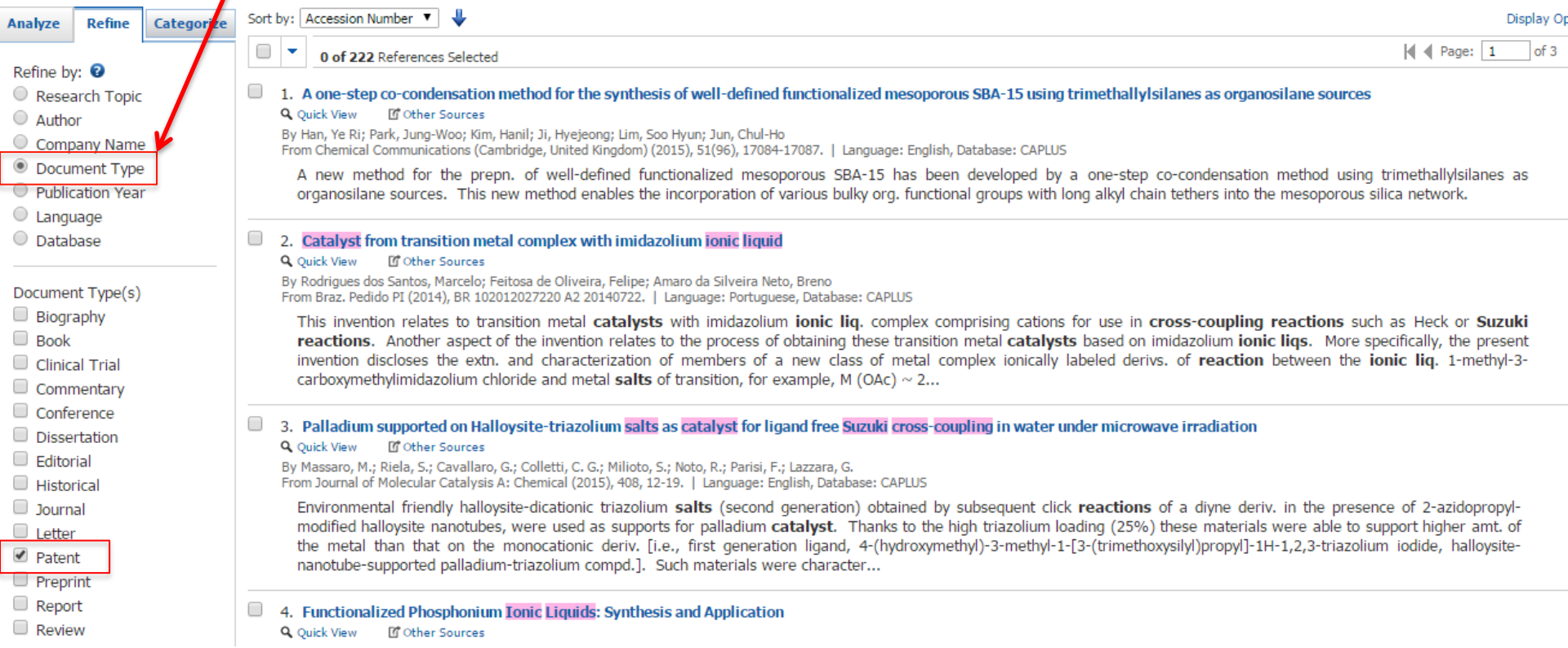
# 文献检索结果的Refine

在结果中筛选专利文献

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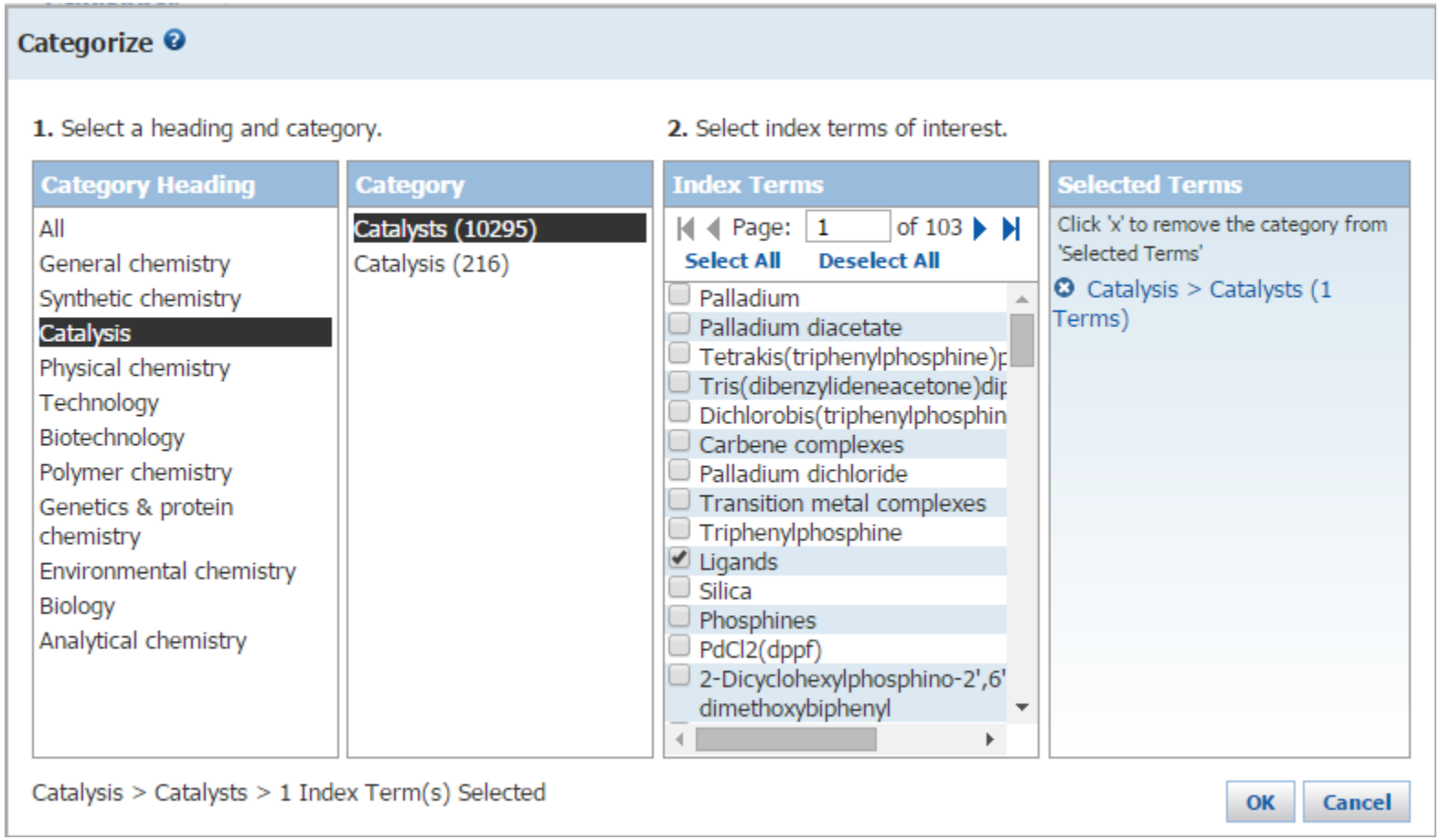
# 文献检索结果的Categorize

学科主分类　　学科副分类　　学科副分类涉及的重要技术术语　　选中的重要技术术语




Categorize系统分类功能，基于学科对文献进行自动分类，帮助用户精准定位所关注的学科和技术术语。

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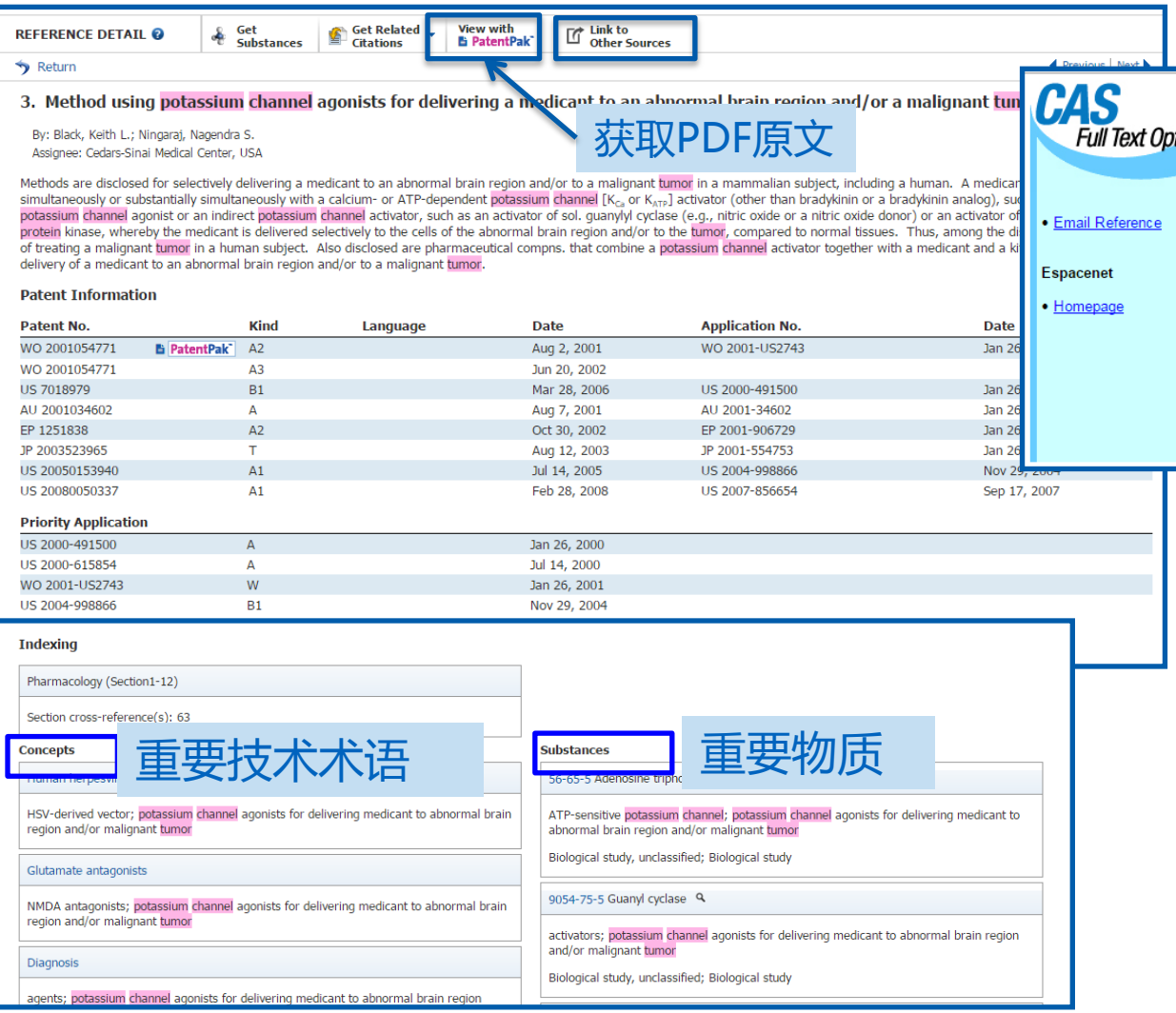
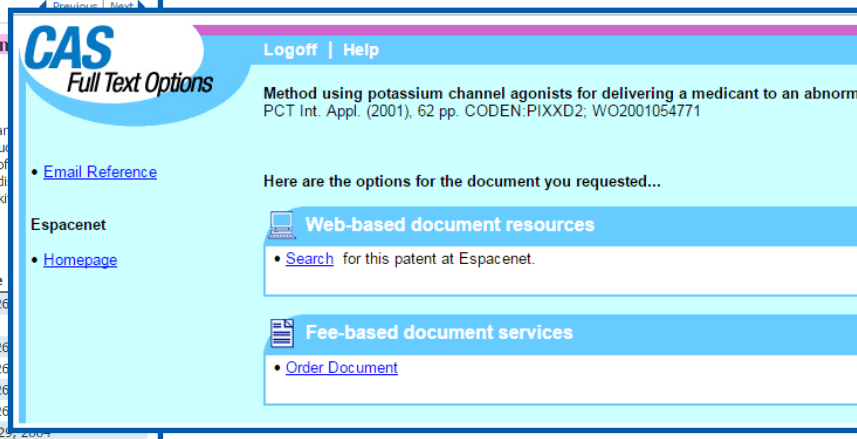
# 文献信息详情




一篇完整的文献界面包括：

1. 题录信息
2. 摘要信息
3. 文献中重要的技术术语
4. 文献中重要的物质
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7. 参考文献

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# PatentPak——专利流程解决方案


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# PatentPak——专利流程解决方案

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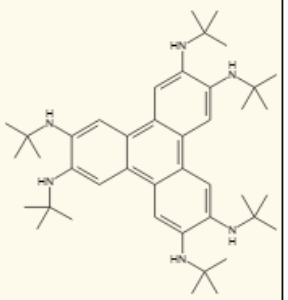
Key Substances in Patent

CAS RN 1448428-20-3



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Analyst Markup Location

page 20

CAS RN 1448428-12-3

1*H*-Triphenyleno[2,3-*d*:6,7-*d*':10,11-*d*'']triimidazolium, 1,3,6,8,11,13-hexakis(1,1-dimethylethyl)-8,13-dihydro-, tetrafluoroborate(1-) (1:3)

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Analyst Markup Location

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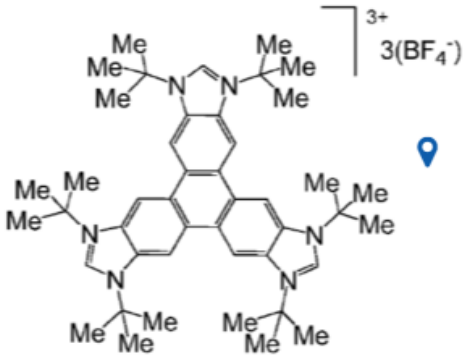
PAGE 20 /44 ZOOM DOWNLOAD PDF

15 **Ejemplo 1.** Obtención de **I** ($R_1$ = *terc*-butilo)



En un matraz de fondo redondo se disuelve la hexaamina **IV** (R = *terc*-butilo) (590 mg, 0,902 mmol) en 40 mL de $HC(OEt)_3$. Seguidamente se añade ácido tetrafluorobórico (solución etérea al 54 %; 0,36 mL, 2,977 mmol) y se deja 20 agitando a 110ºC durante 16 horas. A continuación, se añaden 100 mL de dietil éter. La sal formada se separa mediante filtración. Tras precipitar con acetonitrilo/dietil éter, el compuesto **I** se obtiene puro como un sólido beige. Rendimiento: 820 mg, 95 %.

$^1$H NMR (300 MHz, DMSO-$d_6$, 303 K): δ 9.19 (s, 6H, CH$_{arom}$), 9.16 (s, 3H

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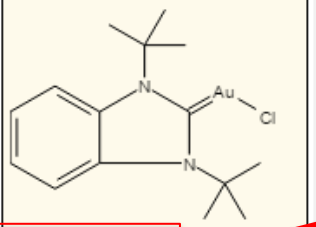
# PatentPak---专利流程解决方案

PatentPak™ PAGE 29 /44 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 1504582-75-5



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Analyst Markup Location

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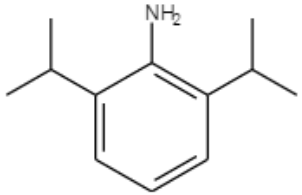
CAS RN 24544-04-5



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Analyst Markup Location

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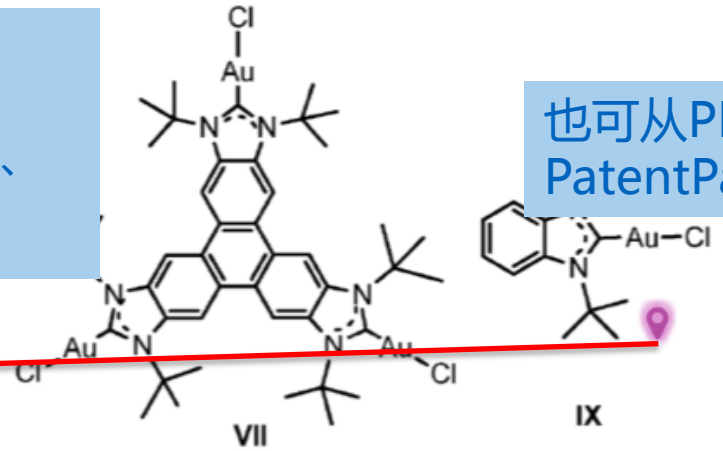
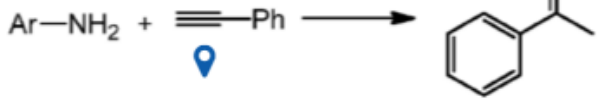


VII



IX



| Entrada | Ar | Catalizador | Rendimiento (%) |
|---|---|---|---|
| 1 | 2,6-*i*Pr$_2$C$_6$H$_3$ | VII | 95 |
| 2 | 2,6-*i*Pr$_2$C$_6$H$_3$ | IX | 82 |

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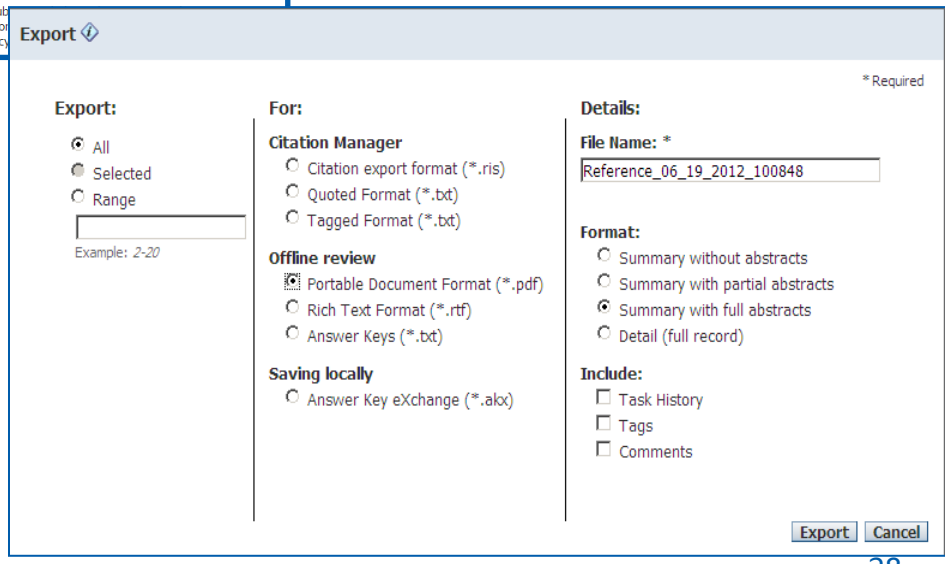
Export：导出至本地电脑，保存为PDF格式

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# 文献检索小结

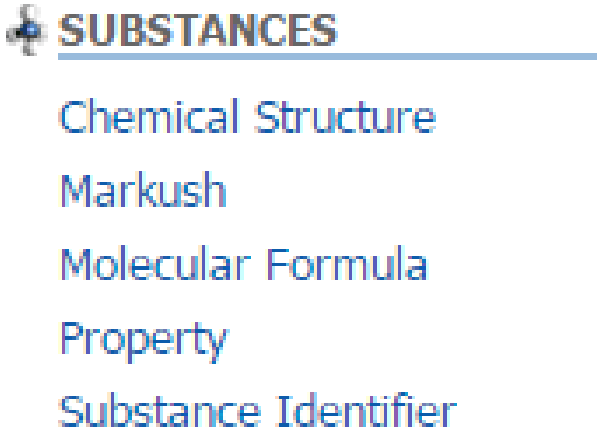
- 主题检索时，使用介词作为连接 (of, with, in…)
- 可用Analyze对本领域文献进行全景分析，获取到研究进展，同行等信息
- 可用Refine快速获取到所需信息
- 可用Categorize实现精准定位学科信息
- 通过PatentPak快速定位专利文件中的物质，实现专利原文与PatentPak的互动，极大节省时间，提高效率

# 提 纲

- 美国化学文摘社及SciFinder简介
- SciFinder的检索和后处理
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner使用简介
- SciFinder常见问题及解决

# SciFinder检索选项——物质检索

- 物质检索方法
  - 结构式检索
  - Markush结构检索
  - 分子式检索
  - 理化性质检索
  - 物质标识符检索：化学名称，CAS RN




- 物质检索策略推荐
  - 有机物化合物、天然产物：结构检索
  - 无机化合物、合金：分子式检索
  - 高分子化合物：分子式检索和结构检索

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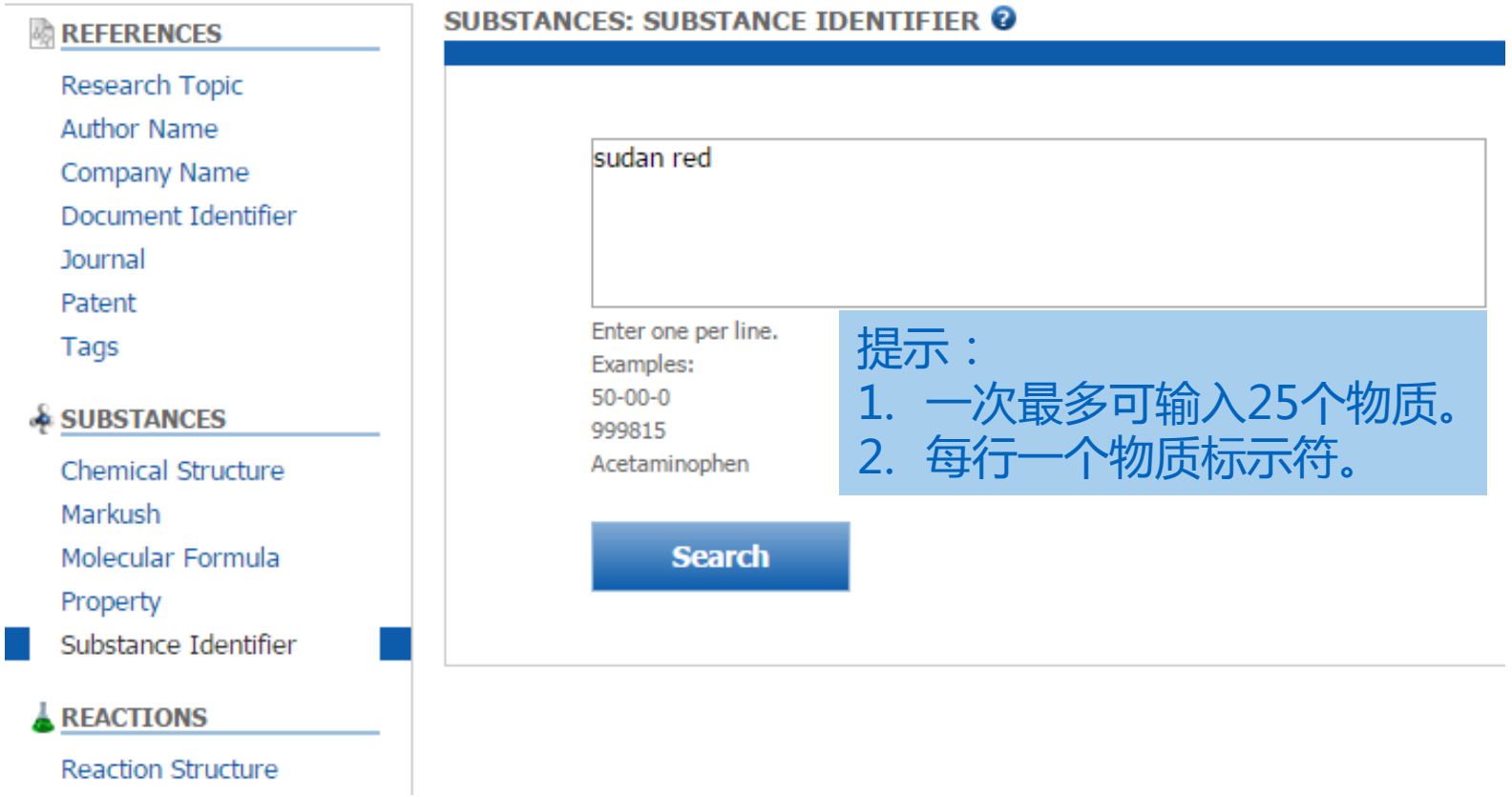
# 物质检索--标识符检索




物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

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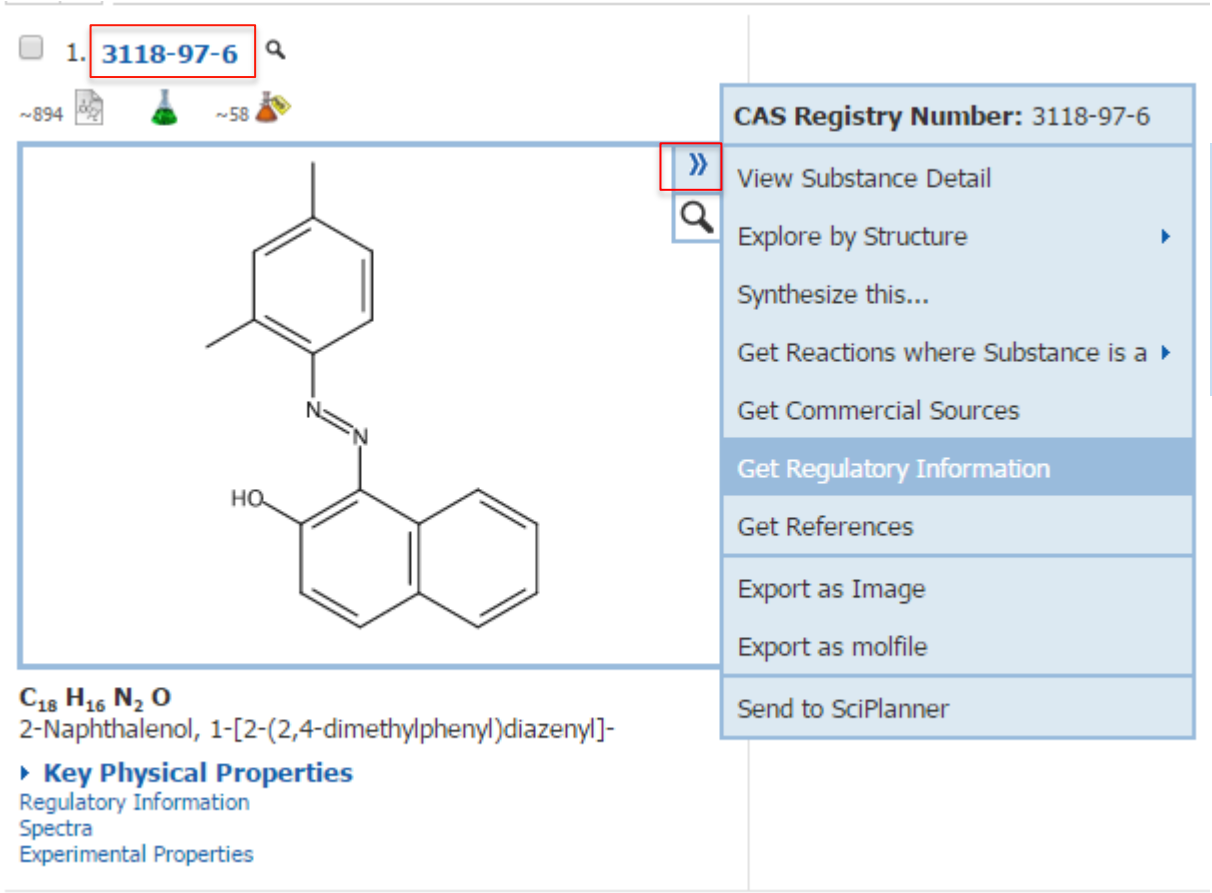
# SciFinder中的物质记录

## 点击CAS RN 获得物质详细信息




在SciFinder中，鼠标滑过物质，即可打开物质标准菜单，获得与物质相关的所有内容

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由物质获得文献，反应，供应商等信息

SUBSTANCE DETAIL

Get References | Get Reactions | Get Commercial Sources

Return

**CAS Registry Number** 3118-97-6

~894 ~58

$C_{18}H_{16}N_2O$

2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

**Molecular Weight**
276.33

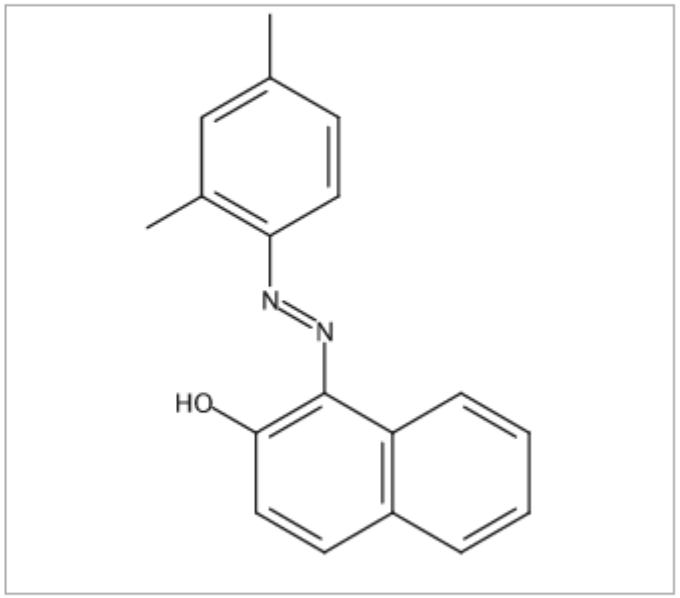
**Melting Point (Experimental)**
Value: 166 °C

**Boiling Point (Predicted)**
Value: 476.7±40.0 °C | Condition: Press: 760 Torr

**Density (Predicted)**
Value: 1.14±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

**pKa (Predicted)**
Value: 13.52±0.50 | Condition: Most Acidic Temp: 25 °C

**Other Names**
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)
C.I. Solvent Orange 7 (7CI,8CI)
Sudan Red (6CI)
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol
AF Red No. 5
View more...




物质详情

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EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

[1]H NMR | IR | Mass | Raman | UV and Visible

| [1]H NMR Properties | Value | Condition | Note |
|---|---|---|---|
| Proton NMR Spectrum | See spectrum | | (13)BIORAD |

**Notes**

(13) BIORAD: Copyright Bio-Rad Laboratories. All Rights Reserved.

PREDICTED PROPERTIES

Biological | Chemical | Density | Lipinski | Structure Related | Thermal

| Lipinski Properties | Value | Condition | Note |
|---|---|---|---|
| Freely Rotatable Bonds | 3 | | (21) |
| H Acceptors | 3 | | (21) |
| H Donors | 1 | | (21) |
| H Donor/Acceptor Sum | 4 | | (21) |
| logP | 5.471±1.252 | Temp: 25 °C | (21) |
| Molecular Weight | 276.33 | | (21) |

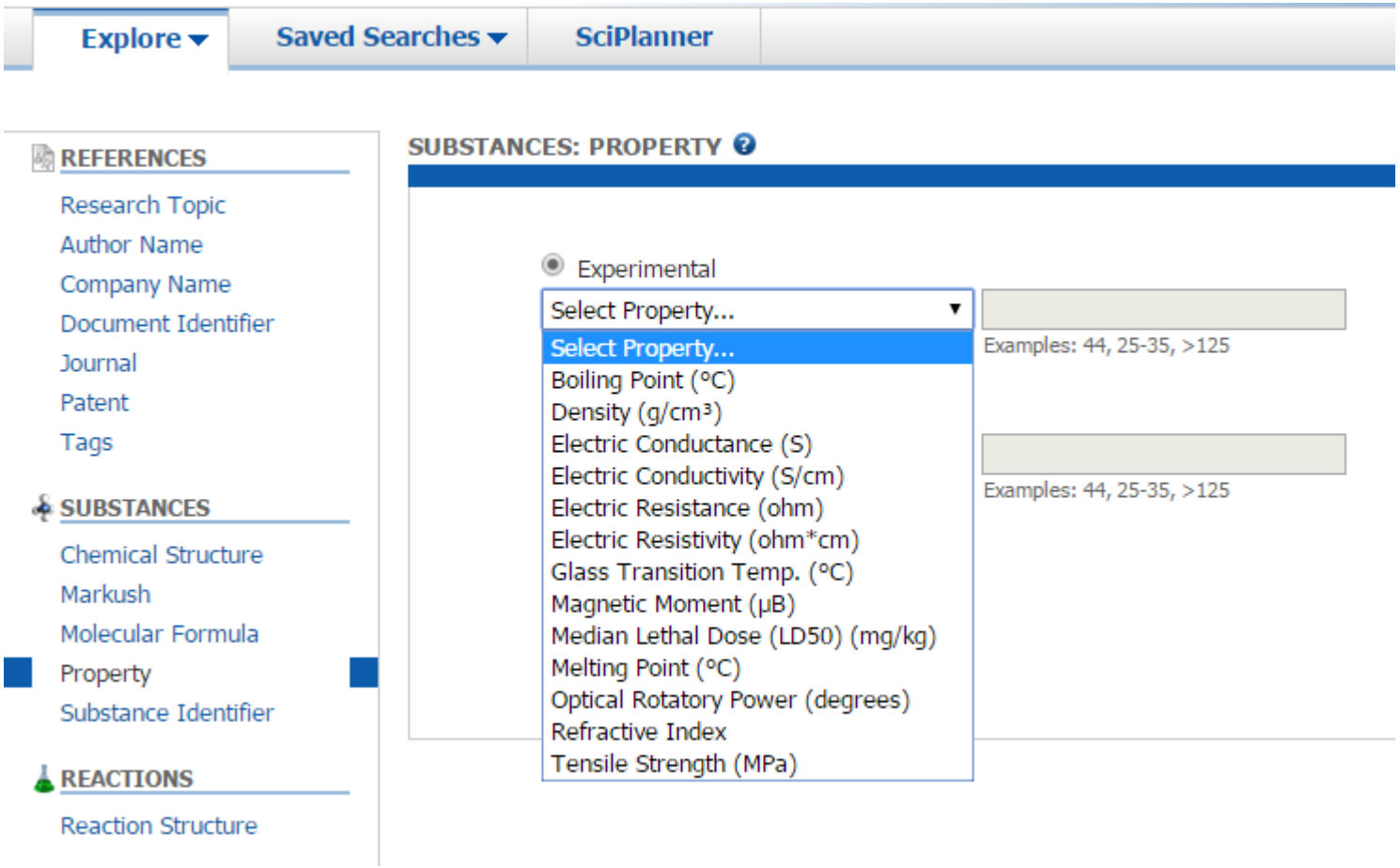
预测数据与预测谱图

**Notes**

(21) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2015 ACD/Labs)

PREDICTED SPECTRA

# 物质检索--Property explore

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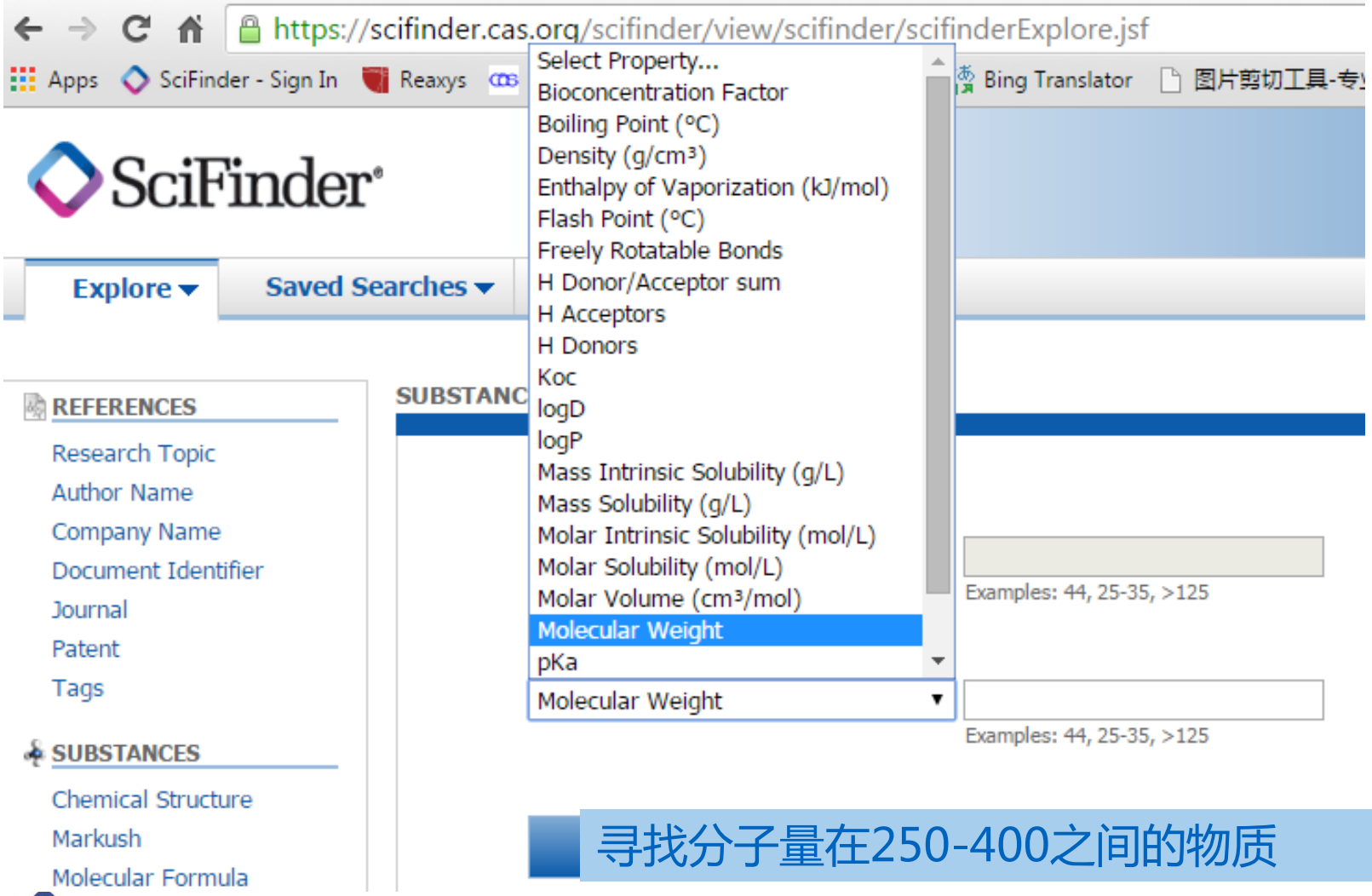
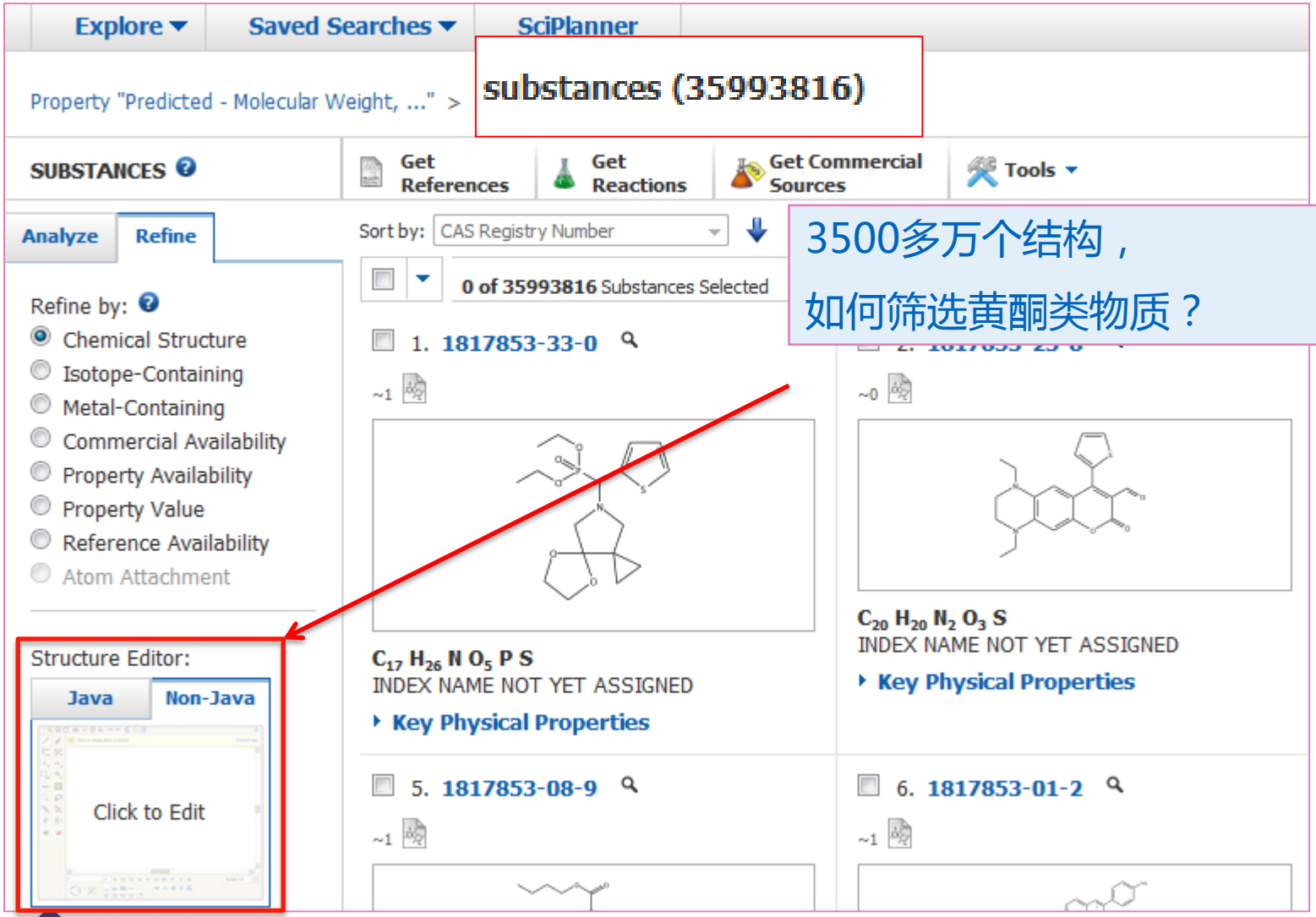
# 物质检索--Property explore




寻找分子量在250-400之间的物质

# 物质结果集的筛选--Refine




3500多万个结构，

如何筛选黄酮类物质？

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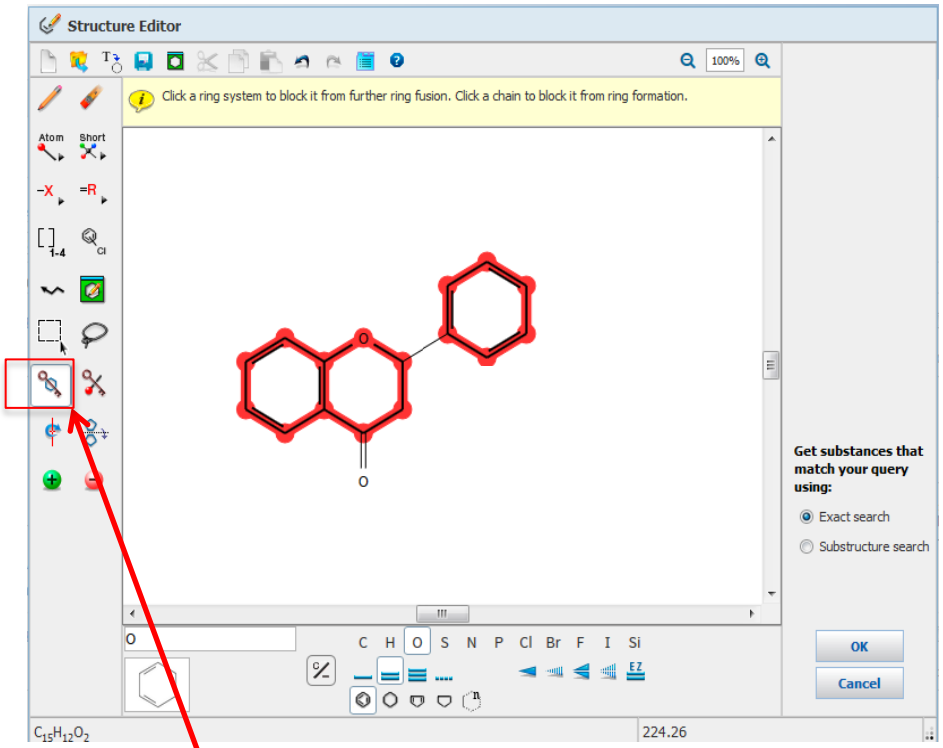
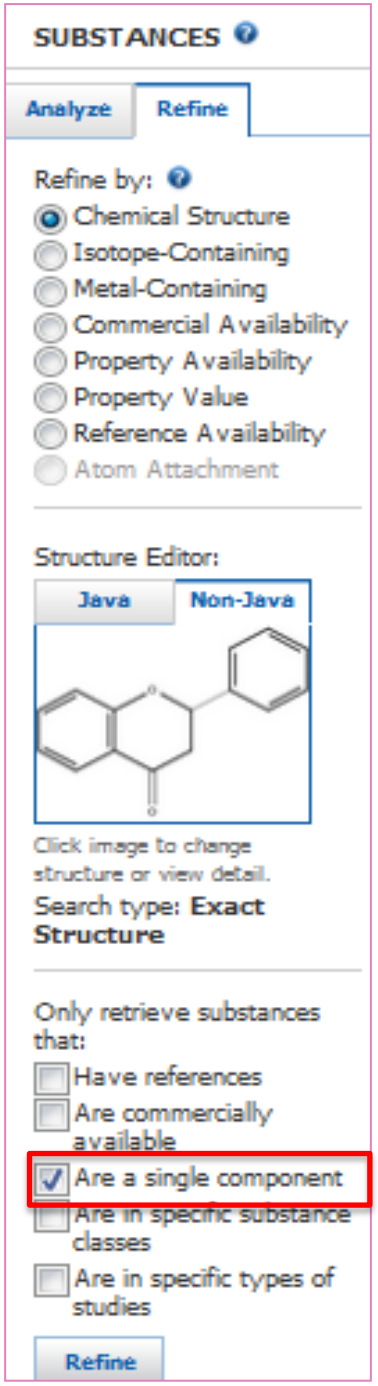
# 物质结果集的筛选--Refine




锁环工具：避免在现有环结构基础上出现新的稠环结构

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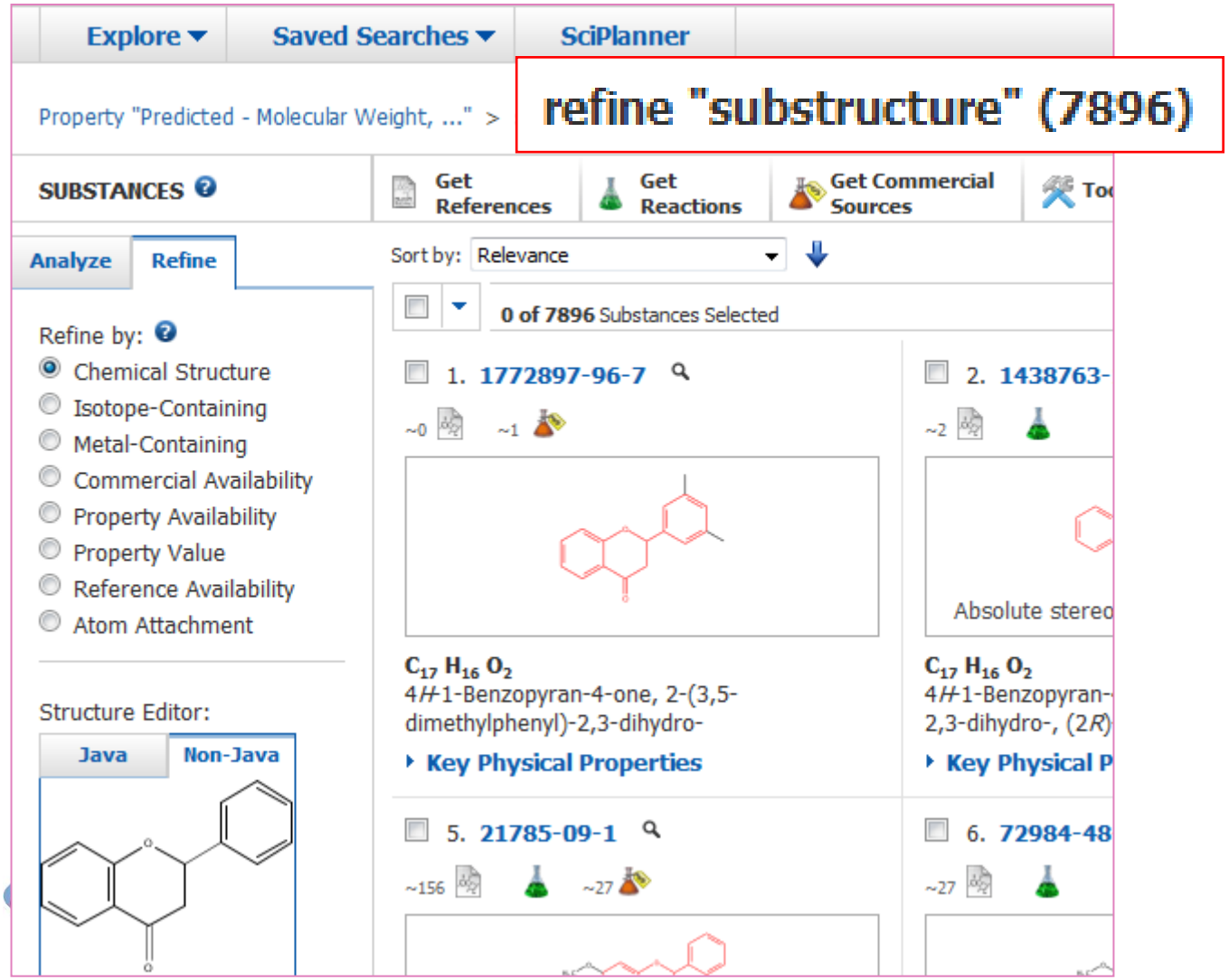
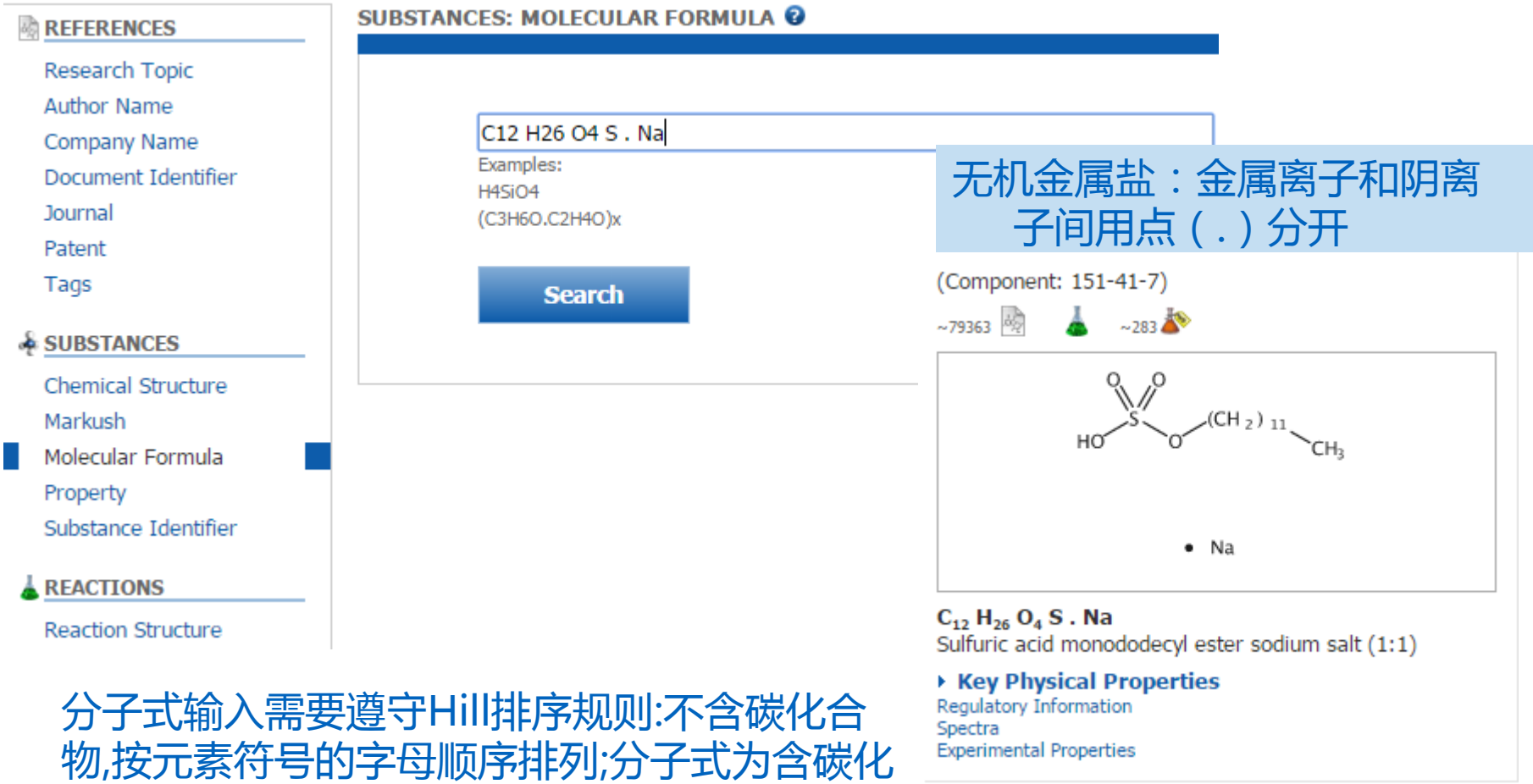
# 物质结果集的筛选--Refine

从3500多万个结构筛选出7800个黄酮类物质



# 物质检索—分子式




分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前；如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面

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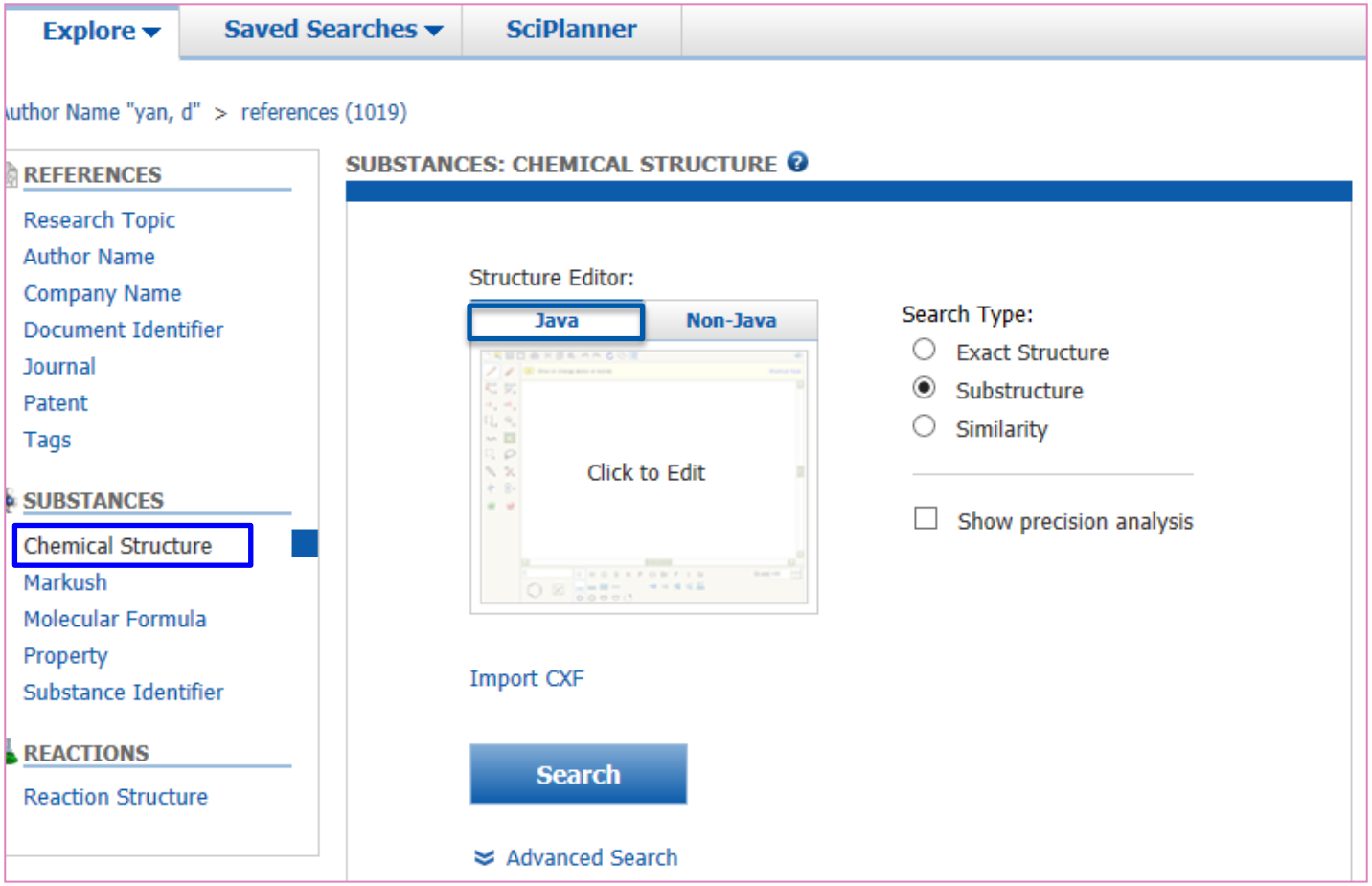
# 物质检索--结构

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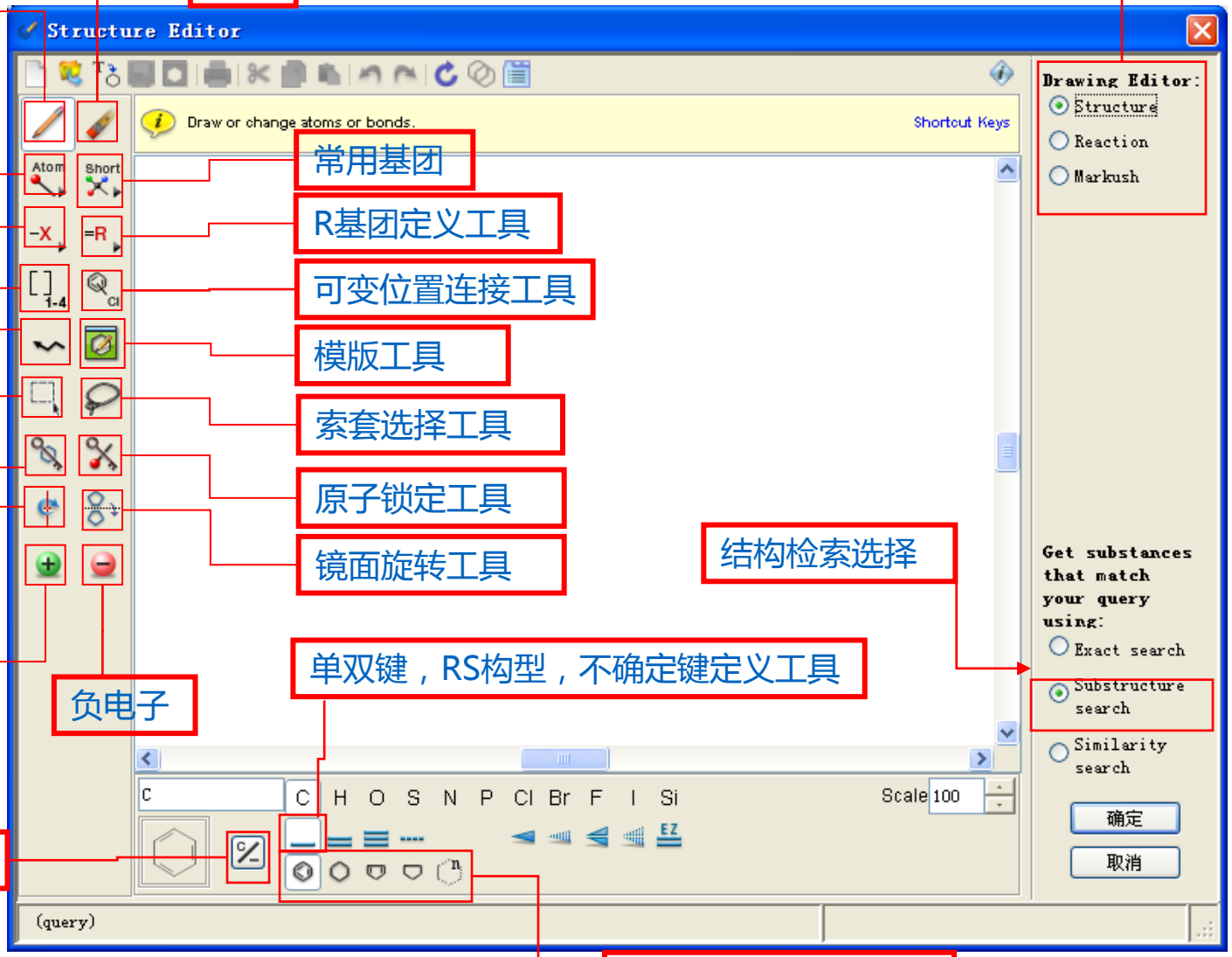
# SciFinder结构编辑器




铅笔

橡皮

结构和反应切换功能

元素周期表

可变基团

重复基团工具

碳链工具

选择工具

环锁定工具

旋转工具

正电子

常用基团

R基团定义工具

可变位置连接工具

模版工具

索套选择工具

原子锁定工具

镜面旋转工具

结构检索选择

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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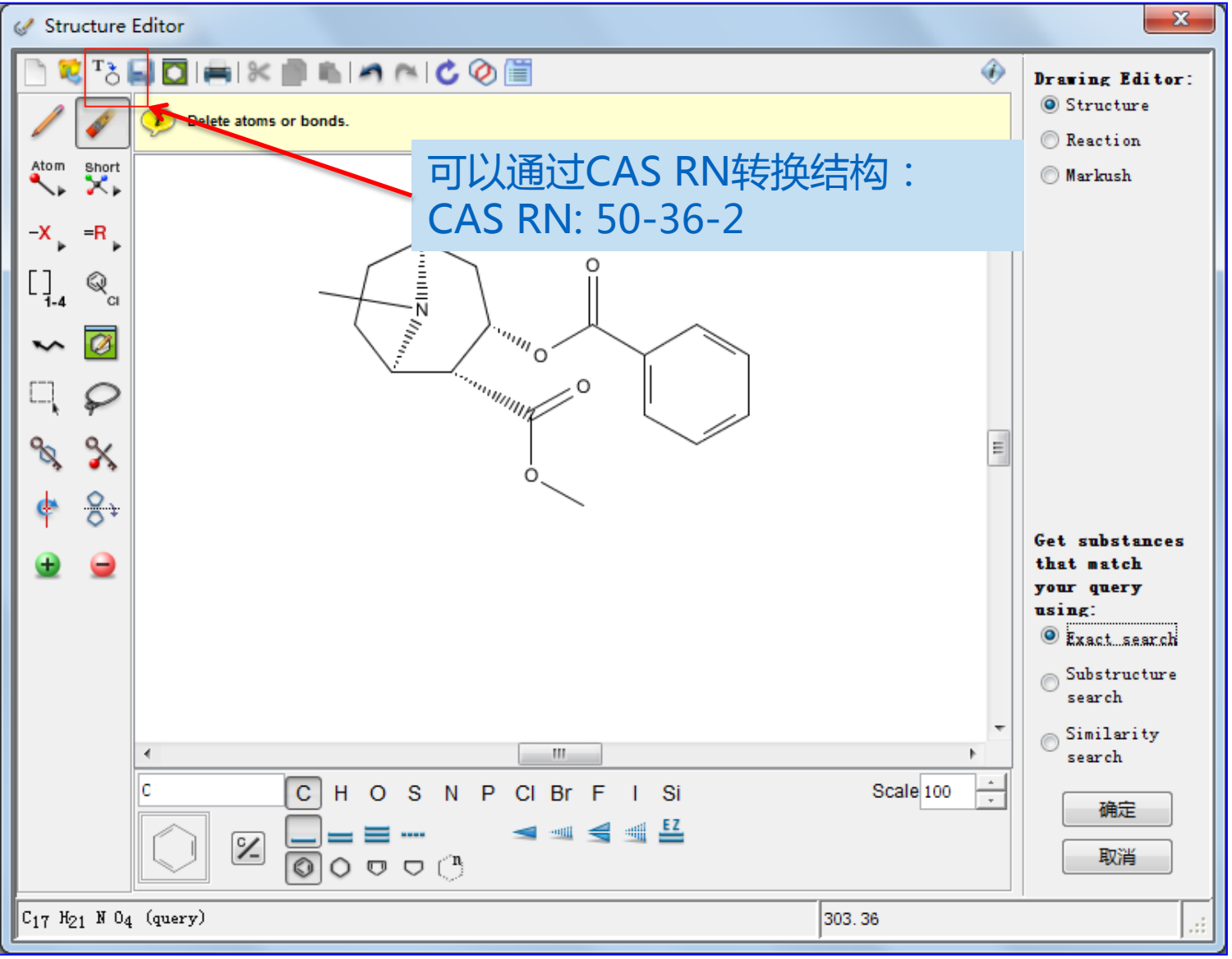
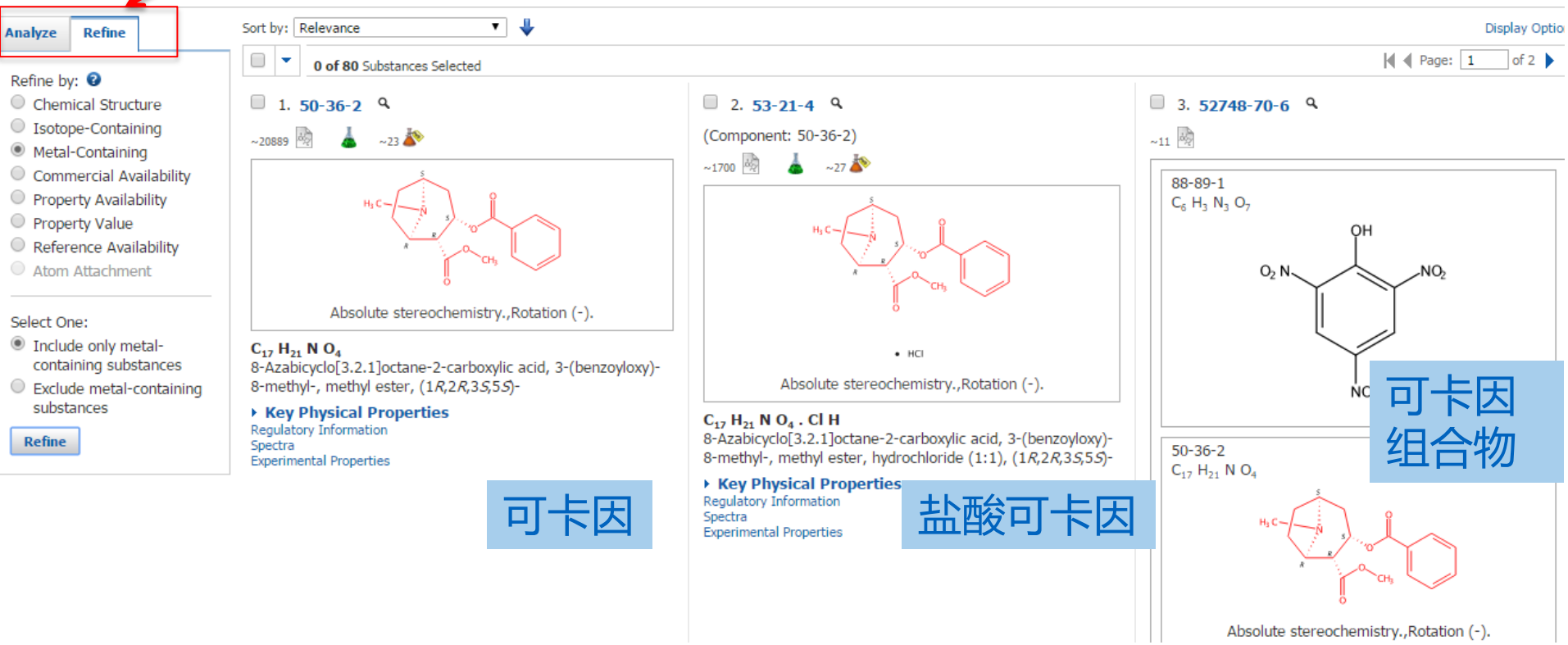
# 物质检索——精确结构检索




精确结构检索

# 浏览精确结构检索结果

可以通过分析限定再处理检索结果

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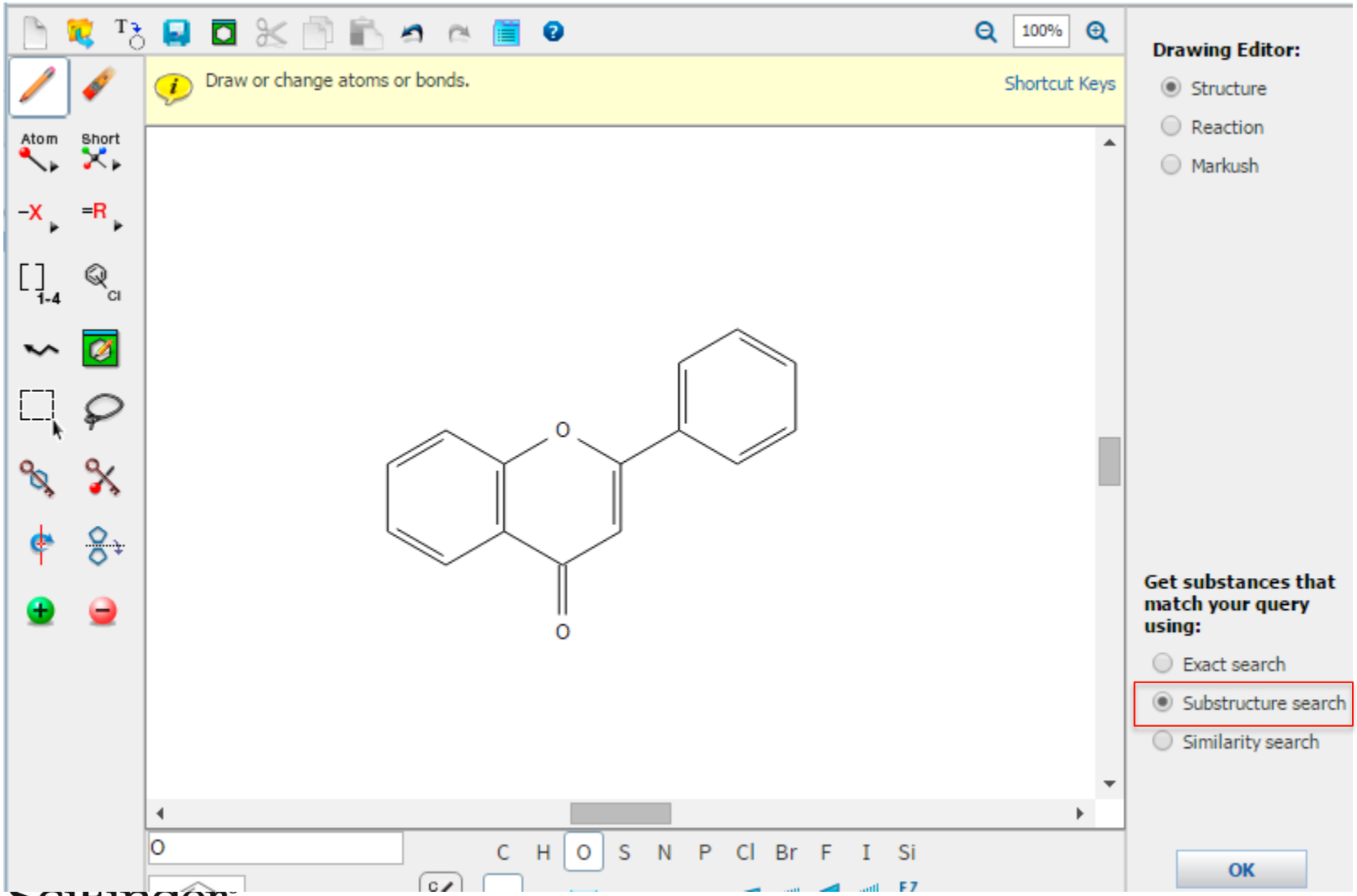
# 物质检索——精确结构检索

- 精确结构检索：

  获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

# 物质检索——亚结构检索

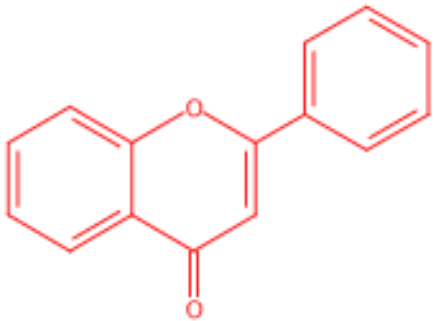

100%
Draw or change atoms or bonds.
Shortcut Keys
Atom
Short
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search
OK
C H O S N P Cl Br F I Si

# 物质检索——亚结构检索

**0 of 63231** Substances Selected

1. **525-82-6**

~3509 ~78



$C_{15}H_{10}O_2$

4*H*-1-Benzopyran-4-one, 2-phenyl-

**Key Physical Properties**

Regulatory Information

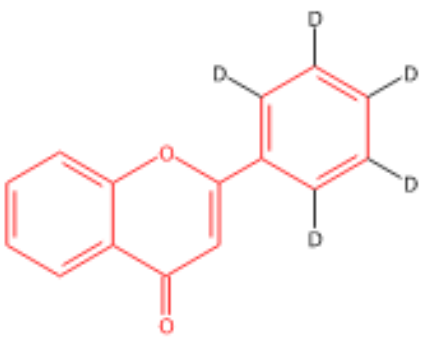
Spectra

Experimental Properties

2. **54849-75-1**

~6

同位素



$C_{15}H_5D_5O_2$

4*H*-1-Benzopyran-4-one, 2-(phenyl-$d_5$)-

Spectra

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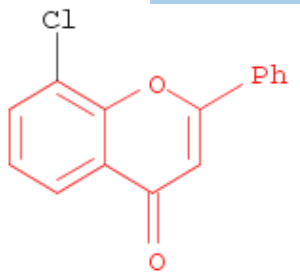
# 浏览亚结构检索结果

251. Substance Detail
1148-20-5

取代物

~16

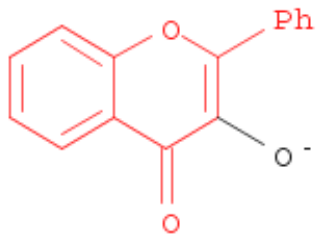



**C15 H9 Cl O2**
4*H*-1-Benzopyran-4-one, 8-chloro-2-phenyl-

261. Substance Detail
85481-91-0

离子

~8

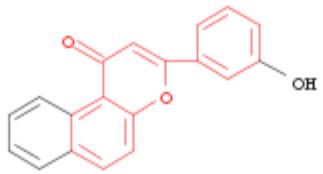



**C15 H9 O3**
4*H*-1-Benzopyran-4-one, 3-hydroxy-2-phenyl-, ion(

273. Substance Detail
136116-17-1

稠环物质

~2




**C19 H12 O3**
1*H*-Naphtho[2,1-*b*]pyran-1-one, 3-(3-hydroxyphenyl)-

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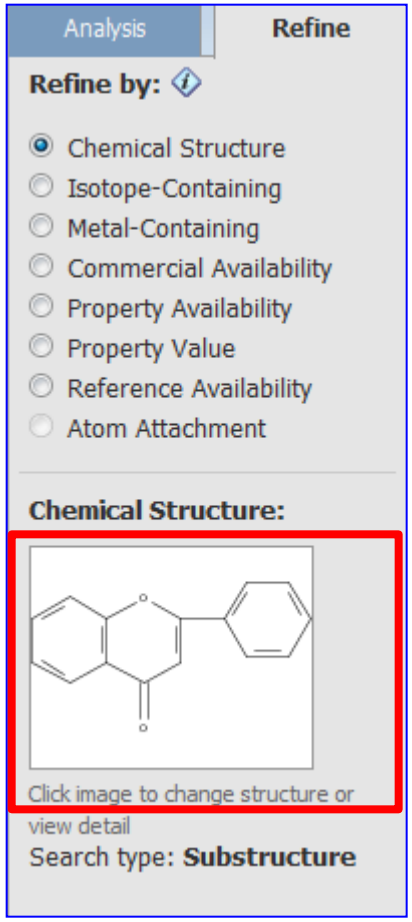
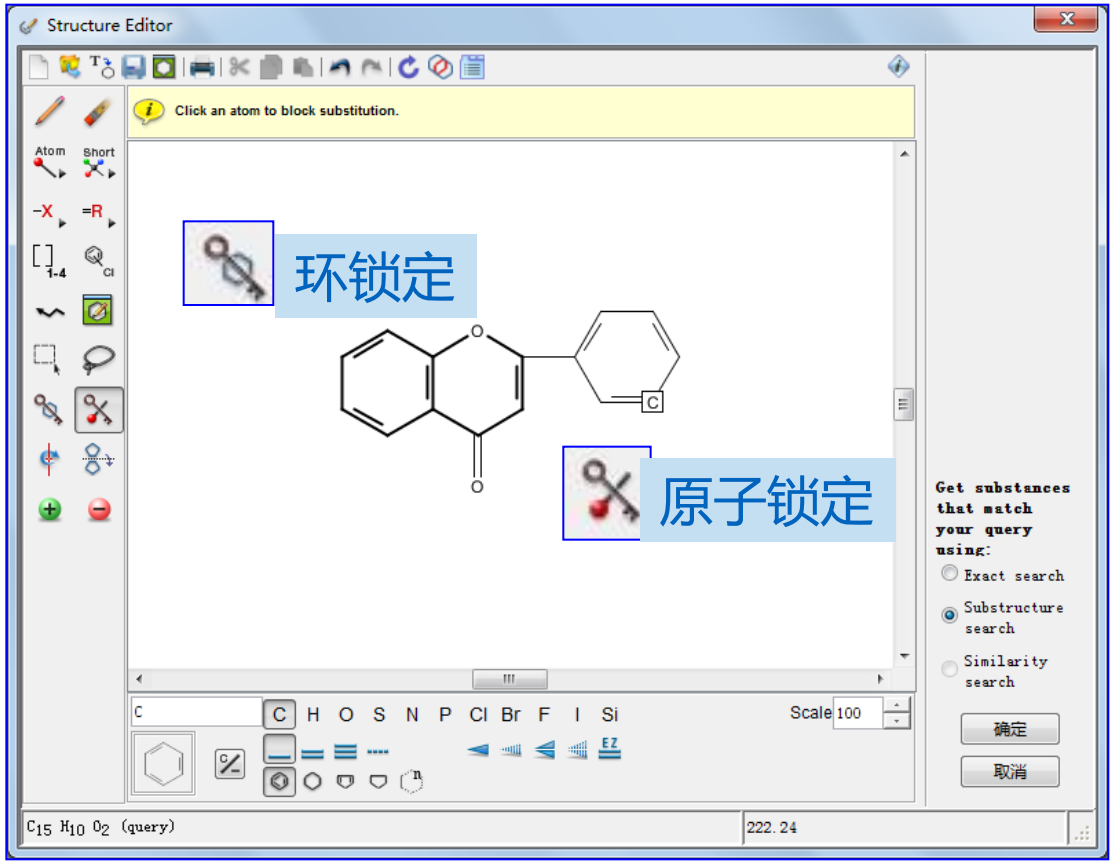
# 亚结构检索结果的限定工具




## 化学结构的再次限定

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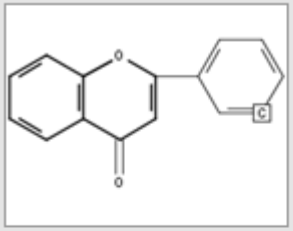
# 化学结构的再次限定

**Chemical Structure:**



Click image to change structure or view detail

Search type: **Substructure**

**Only retrieve substances that:**

- [x] Have references
- [ ] Are commercially available
- [x] Are a single component
- [ ] Are in specific substance classes
- [ ] Are in specific types of studies

Refine

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome Amy Qi | Sign Out

Add KMP Alert | Chemical Structure substructure > substances (52072) > refine "substructure" (28699)

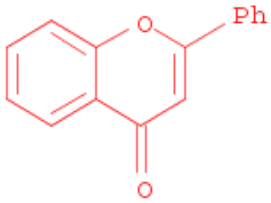
Substances | Get References | Get Reactions | Tools | Send to SciPlanner

28699 Substances | 0 Selected

Select All | Deselect All | Sort by: Relevance (New)

1. **Substance Detail**
   **525-82-6**

~2568

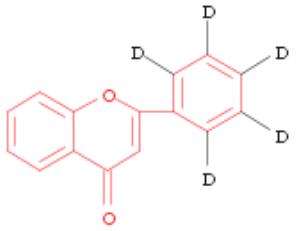



**$C_{15}H_{10}O_2$**
4*H*-1-Benzopyran-4-one, 2-phenyl-

Spectra
Experimental Properties

2. **Substance Detail**
   **54849-75-1**

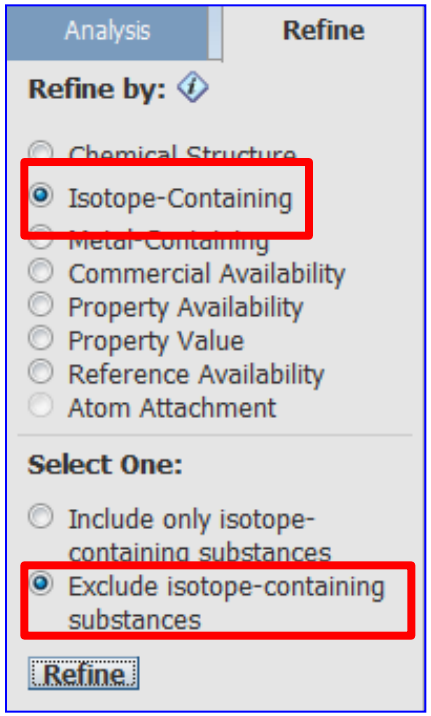
~5



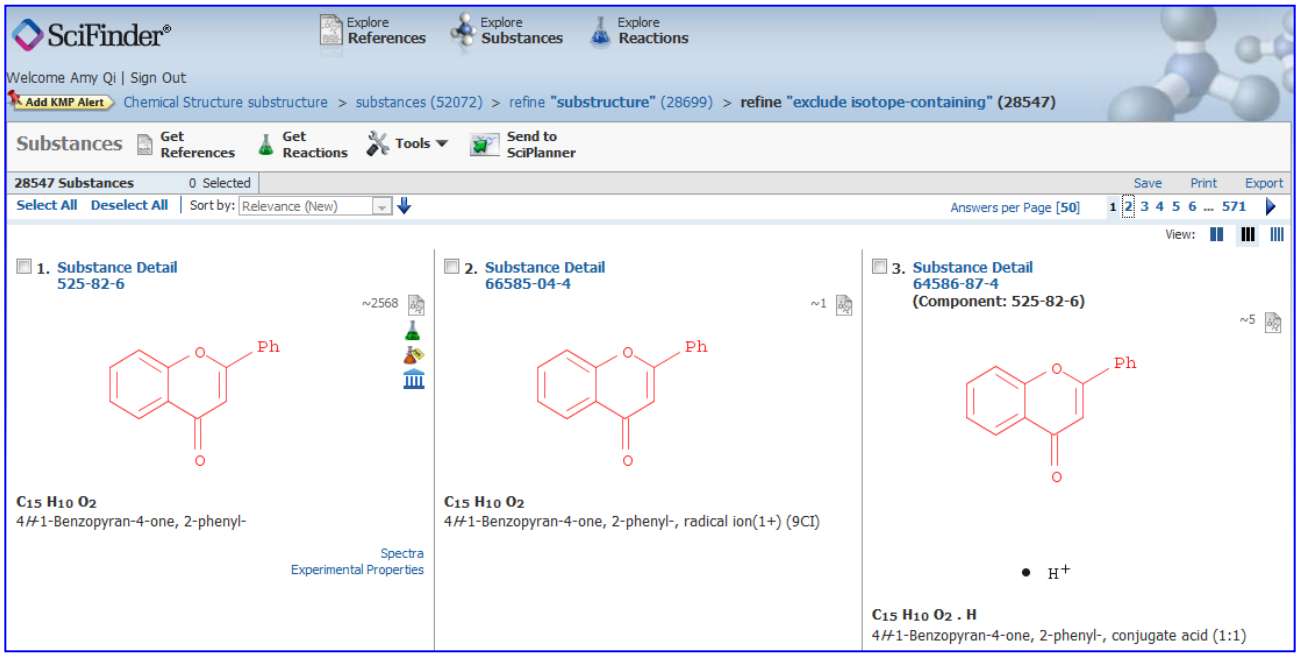

**$C_{15}H_5D_5O_2$**
4*H*-1-Benzopyran-4-one, 2-(phenyl-*d*5)-

Spectra

# 同位素去除


Analysis
Refine
Refine by:
Chemical Structure
Isotope-Containing
Metal-Containing
Commercial Availability
Property Availability
Property Value
Reference Availability
Atom Attachment
Select One:
Include only isotope-containing substances
Exclude isotope-containing substances
Refine

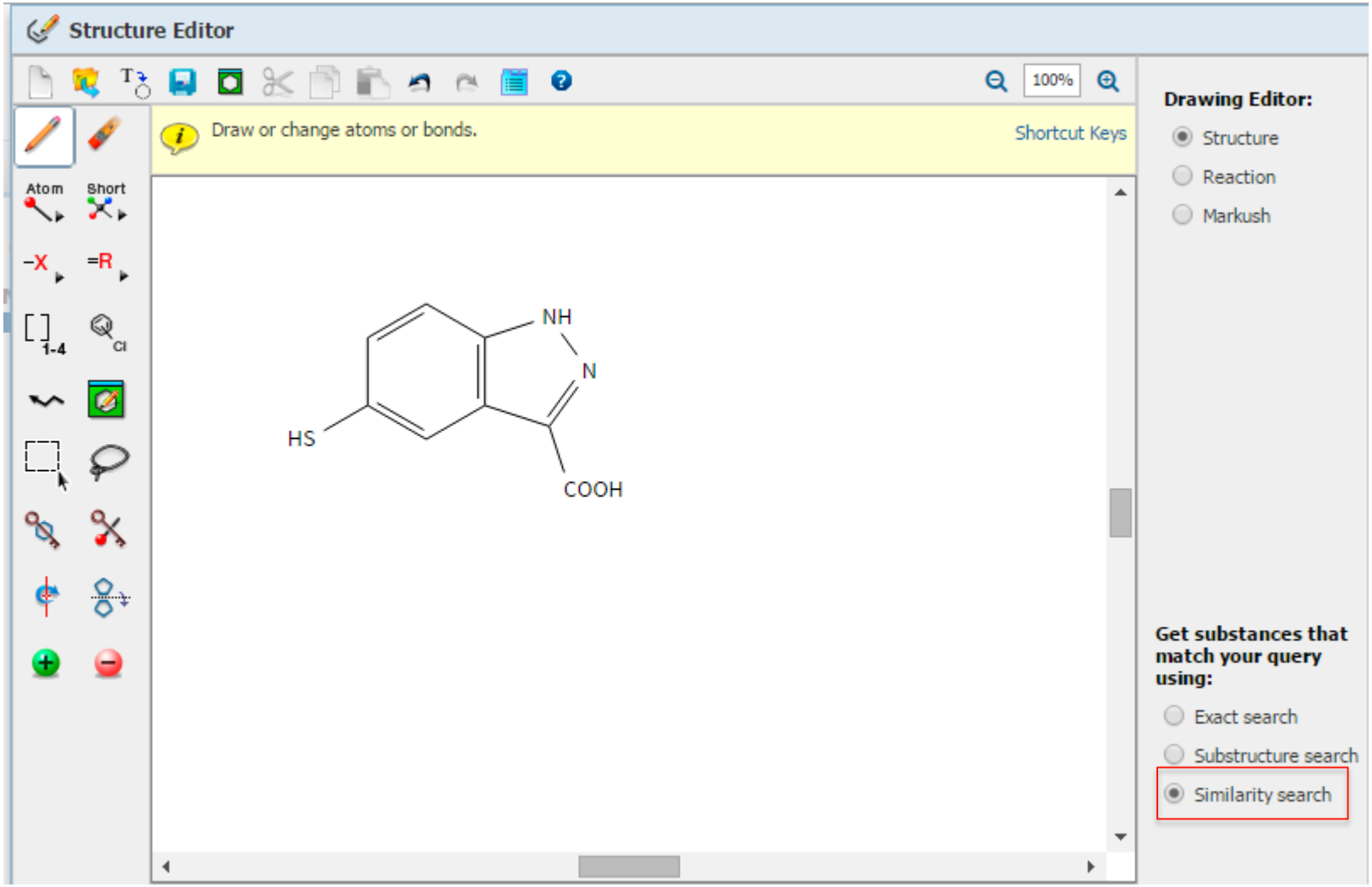
去除同位素


SciFinder
Explore References
Explore Substances
Explore Reactions
Welcome Amy Qi | Sign Out
Add KMP Alert
Chemical Structure substructure > substances (52072) > refine "substructure" (28699) > refine "exclude isotope-containing" (28547)
Substances
Get References
Get Reactions
Tools
Send to SciPlanner
28547 Substances
0 Selected
Save
Print
Export
Select All
Deselect All
Sort by: Relevance (New)
Answers per Page [50]
1 2 3 4 5 6 ... 571
View:
1. Substance Detail
525-82-6
~2568
Ph
O
O
C15 H10 O2
4H-1-Benzopyran-4-one, 2-phenyl-
Spectra
Experimental Properties
2. Substance Detail
66585-04-4
~1
Ph
O
O
C15 H10 O2
4H-1-Benzopyran-4-one, 2-phenyl-, radical ion(1+) (9CI)
3. Substance Detail
64586-87-4
(Component: 525-82-6)
~5
Ph
O
O
H+
C15 H10 O2 . H
4H-1-Benzopyran-4-one, 2-phenyl-, conjugate acid (1:1)

# 物质检索——亚结构检索

- 亚结构检索：
  包括精确结构检索结果，及被检索结构的修饰结构

# 物质检索——相似结构检索

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# 相似结构检索候选项

Select All  Deselect All

| 1 of 6 Similarity Candidates Selected | Substances |
|---|---|
| ≥ 99 (most similar) | 0 |
| 95-98 | 0 |
| 90-94 | 0 |
| 85-89 | 11 |
| 80-84 | 34 |
| 75-79 | 82 |
| 70-74 | 254 |
| 65-69 | 633 |
| 0-64 (least similar) | 1636 |

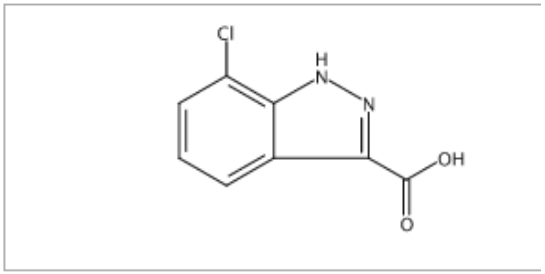
Get Substances

相似度越高，结构越相似

# 相似结构检索结果

1. 129295-32-5

~3  ~96




$C_8H_5ClN_2O_2$

1*H*-Indazole-3-carboxylic acid, 7-chloro-

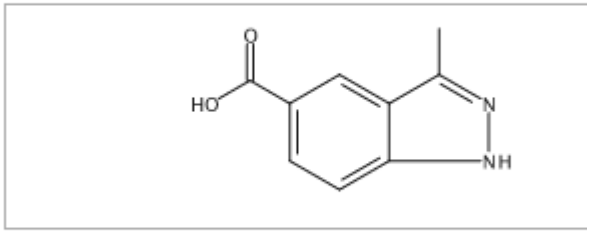
Key Physical P

取代基变化

*Score:* 79

3. 885223-58-5

~11  ~34




$C_9H_8N_2O_2$

1*H*-Indazole-5-carboxylic acid, 3-methyl-

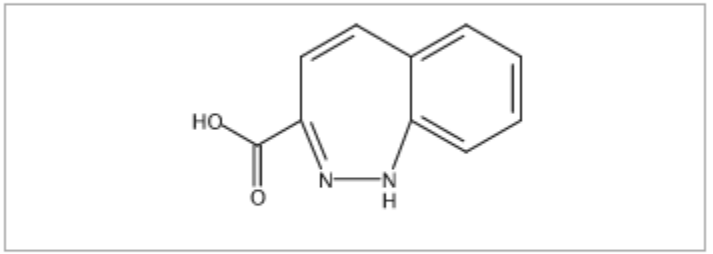
Key Physic

取代基位置变化

*Score:* 71

117. 72119-92-7

~1




$C_{10}H_8N_2O_2$

1*H*-1,2-Benzodiazepine-3-carboxylic acid

Key Physical Properties

Experimental Properties

母体结构变化

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# 物质检索——相似结构检索

- 相似结构检索：

  获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

# 提 纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner使用简介
- SciFinder常见问题及解决

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- 具体物质[Specific Substance]：

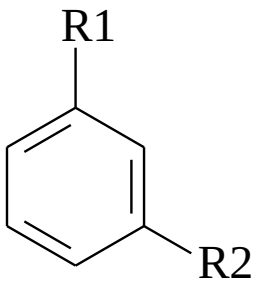
  以具体化学结构陈述的特定物质，会被标示CAS RN

- 预测性物质[Prophetic Substance]：

  使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质

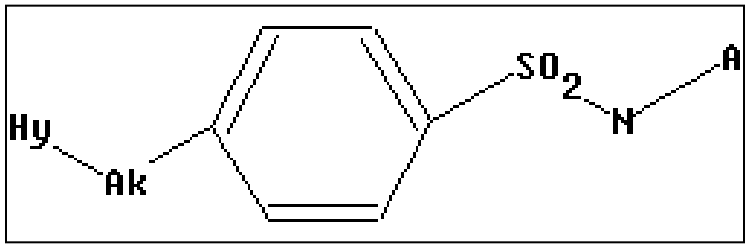
  专利中所陈述的预测物质，不会被标示CAS RN

  Markush检索，能检索到通过结构检索检不到的专利

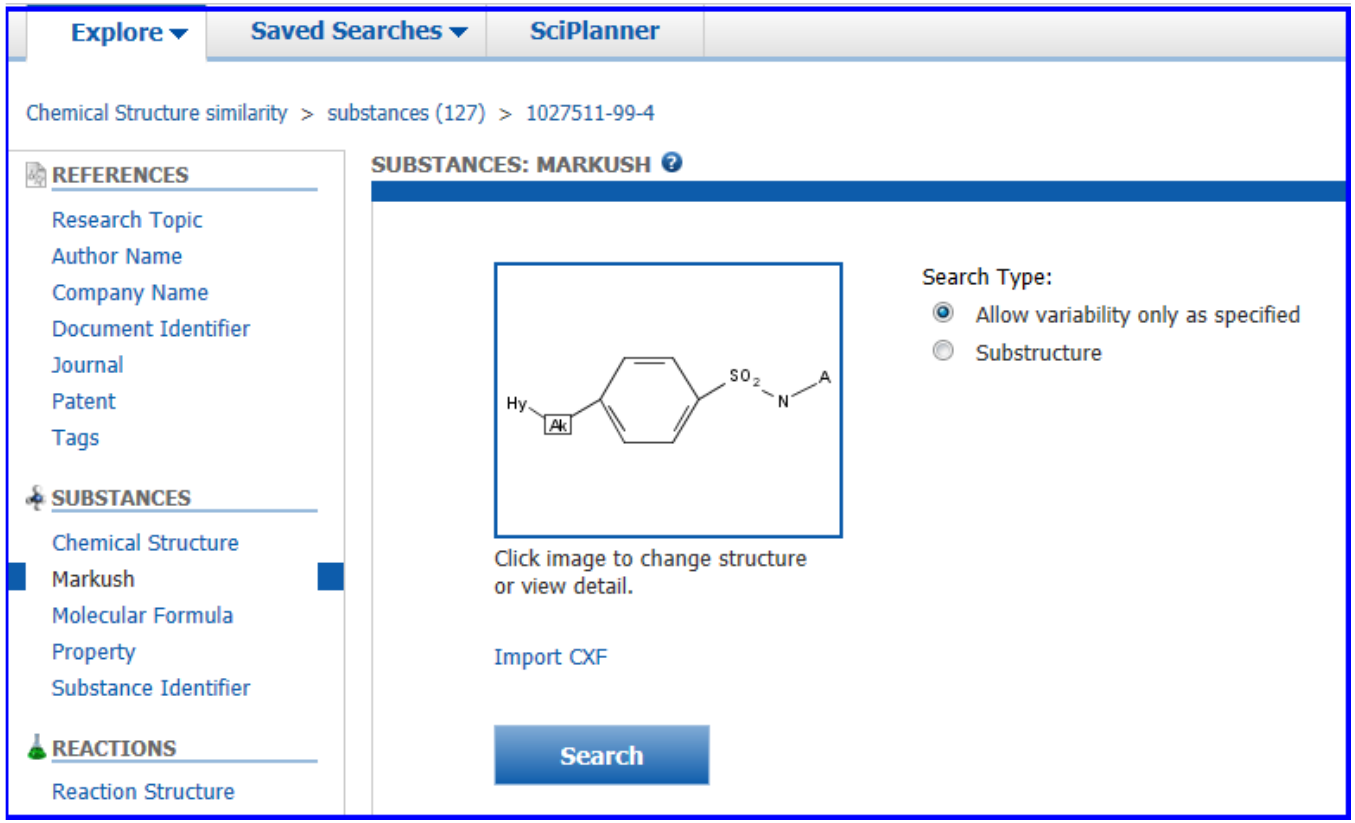



R1 = H, Br, Cl, I

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




可用SciFinder中的Markush检索查看专利中化合物结构保护范围。

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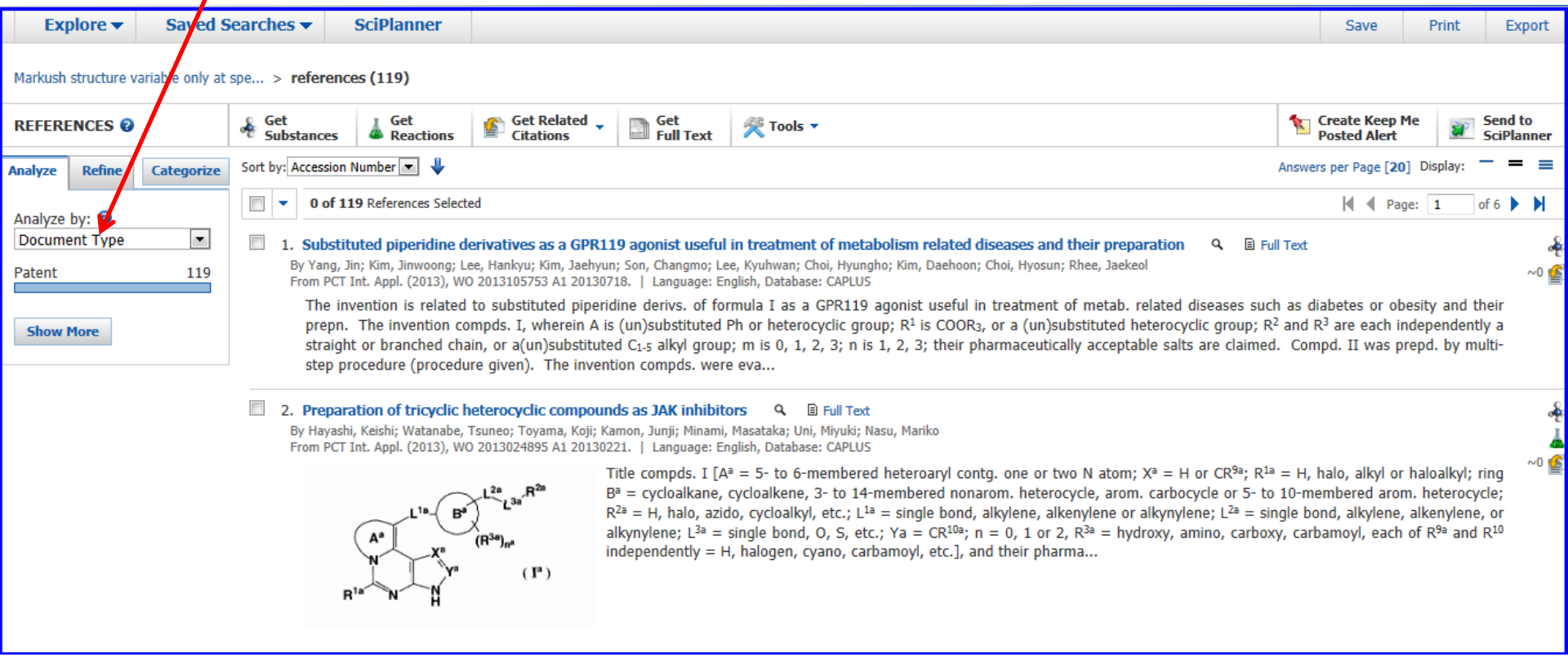
# 全部是专利文献

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- SciFinder常见问题及解决

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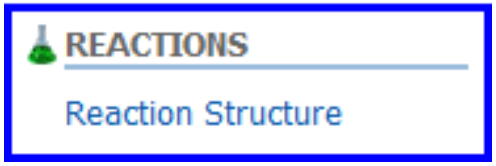
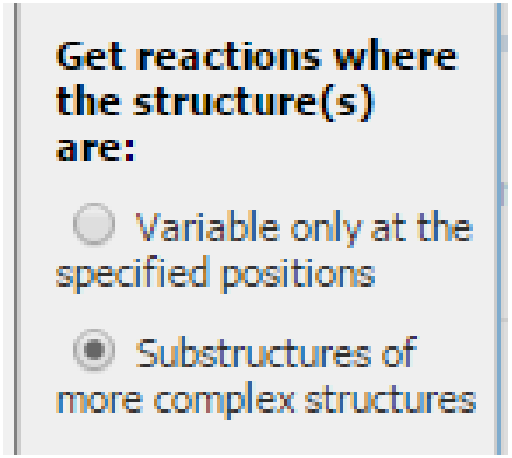
# SciFinder检索选项——反应检索

- 功能方面
  - 结构式




- 常用检索方法
  - 已知物质：由物质获取反应
  - 已知文献：从文献中获取反应
  - 精确结构反应检索
  - 亚结构反应检索

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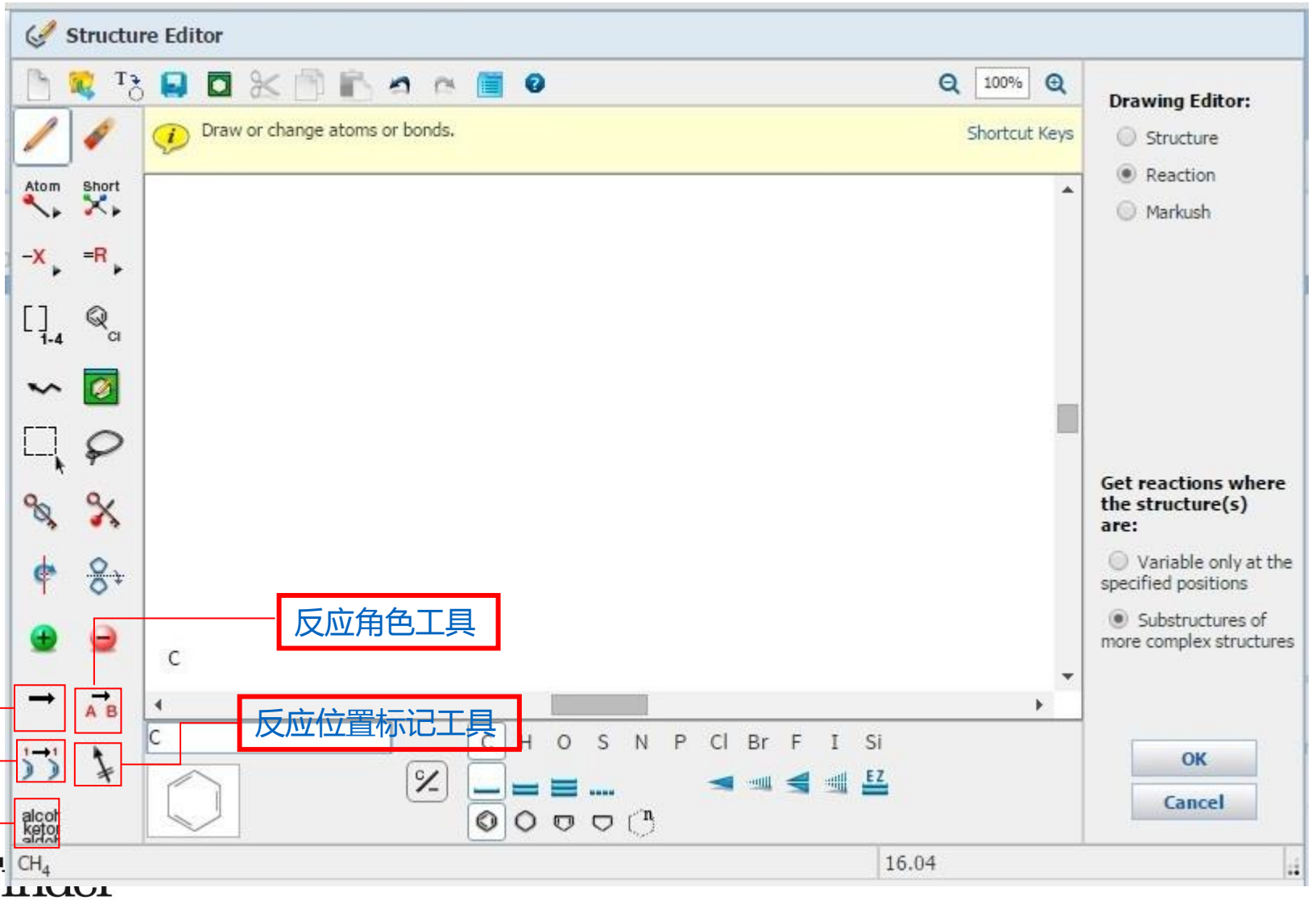
# Scifinder 中反应定义工具

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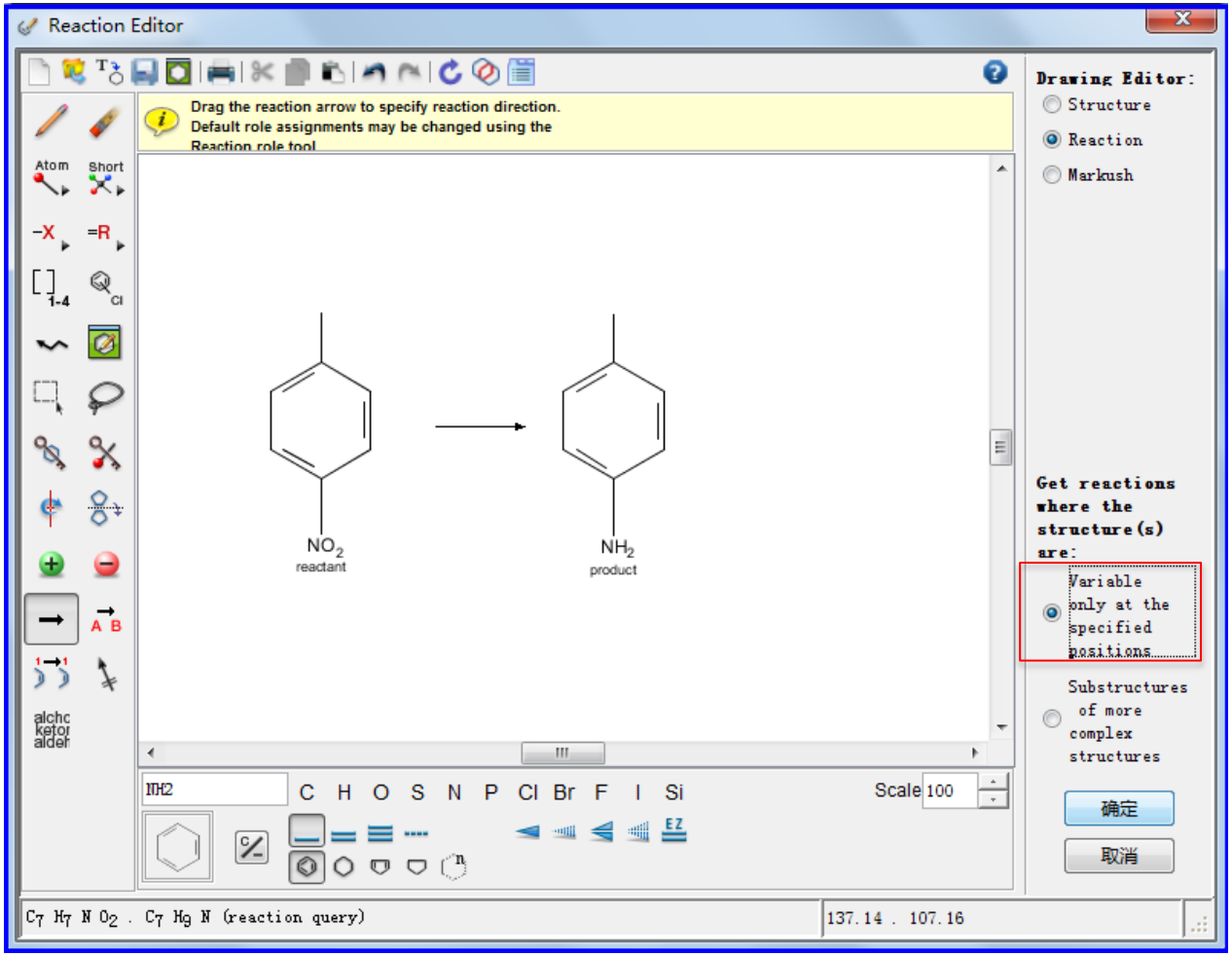
# SciFinder反应检索——精确反应检索




精确反应检索

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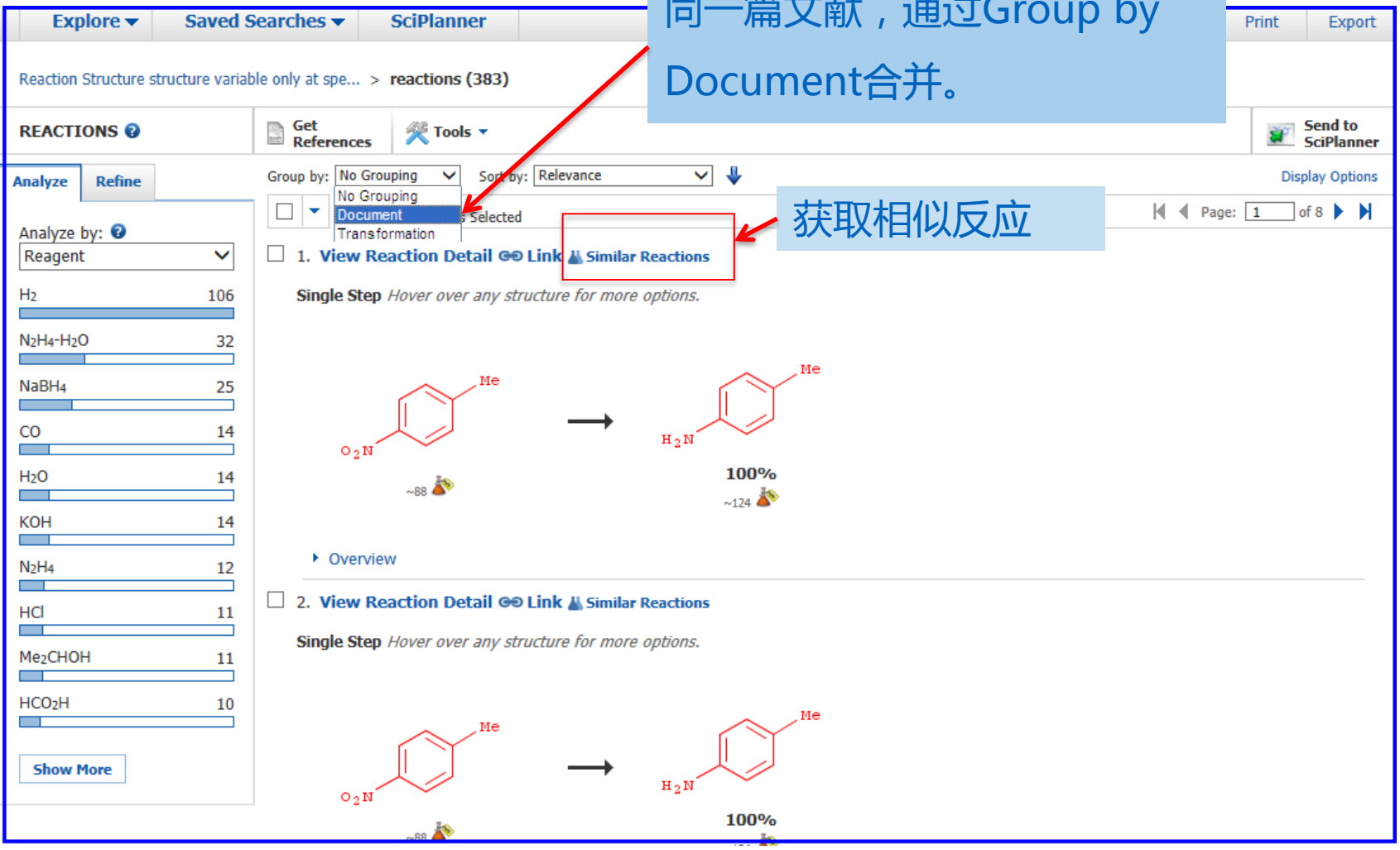
# 反应检索结果

浏览记录，发现很多反应来自同一篇文献，通过Group by Document合并。

获取相似反应

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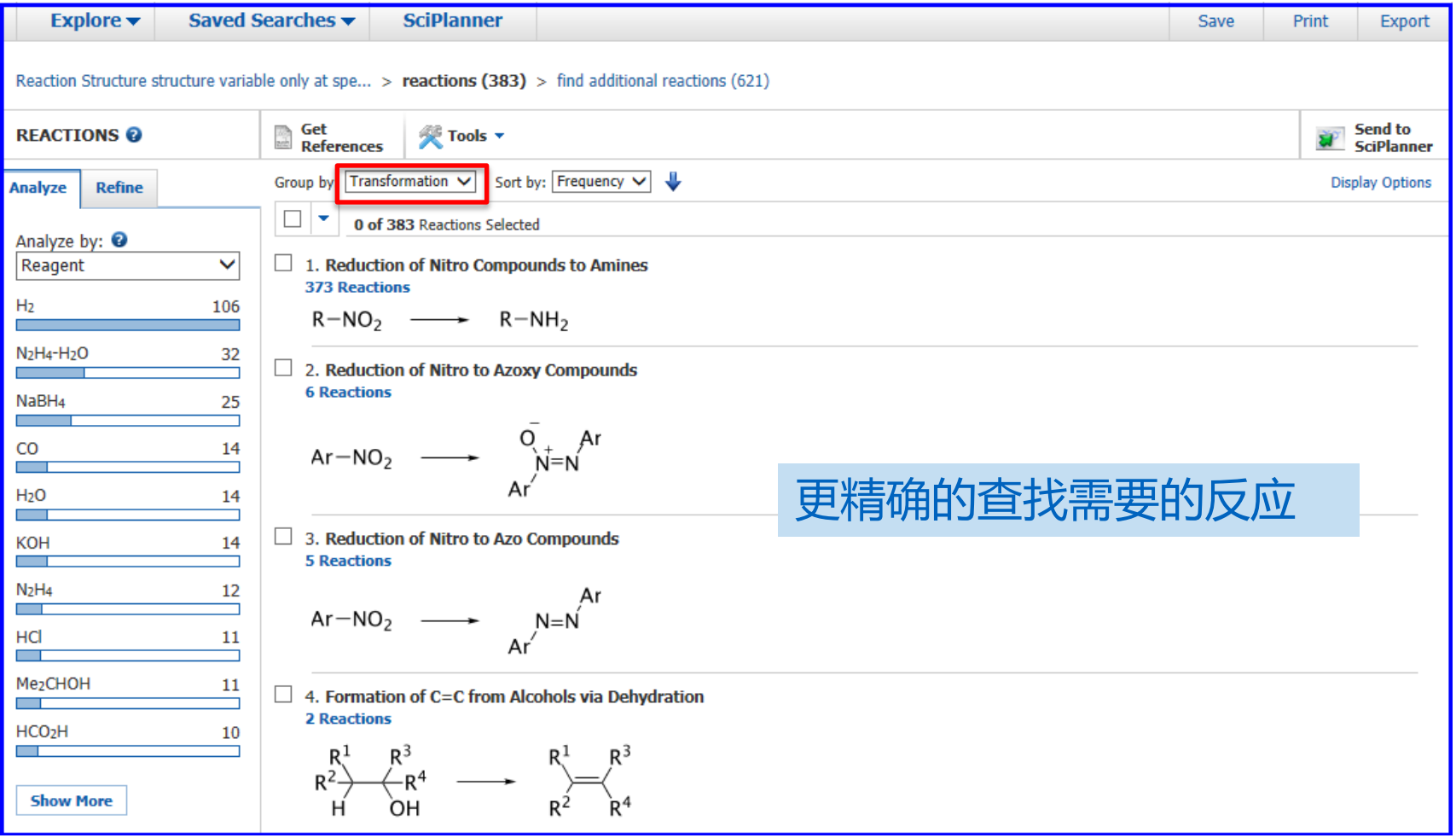
# 按照反应类型排序

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# 反应过程

37. **Polymeric PEG35k-Pd Nanoparticles: Efficient and Recyclable Catalyst for Reduction of Nitro Compounds** Quick View Full Text

1 Reaction Similar Reactions

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


Overview

Experimental Procedure

Taylor & Francis Online

General/Typical Procedure: **Typical Experiment Procedure for the Reduction of Aromatic Reduction Compounds** Reduction of nitroarenes was performed in a 10 ml, round-bottom flask in the presence of nitroarenes (entries 1-14) (1.0 mmol), polymeric PEG35k-Pd NPs (1 mol % polymeric PEG35k-Pd NPs), and hydrazine hydrate (5 equivalents) in an open atmosphere at 90 °C. After the reaction was completed, polymeric PEG35k-Pd NPs were removed by centrifugation. The solution was filtered through a pad of Celite, and then saturated aqueous $NaHCO_3$ (10 ml) was added to the filtrate and extracted with ethyl acetate. The combined organic layers were dried over anhydrous $Na_2SO_4$, concentrated under reduced pressure, and purified by the column chromatography to give the aniline derivatives. Products were characterized by $^1H$ NMR and $^{13}C$ NMR and mass spectra. The removed polymeric PEG35k-Pd NPs were washed with water and diethyl ether, dried under vacuum, and then reused. Entry 2: Yield: 99%.

不用阅读全文，直接获得包含实验过程的反应记录

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# 反应检索结果的筛选


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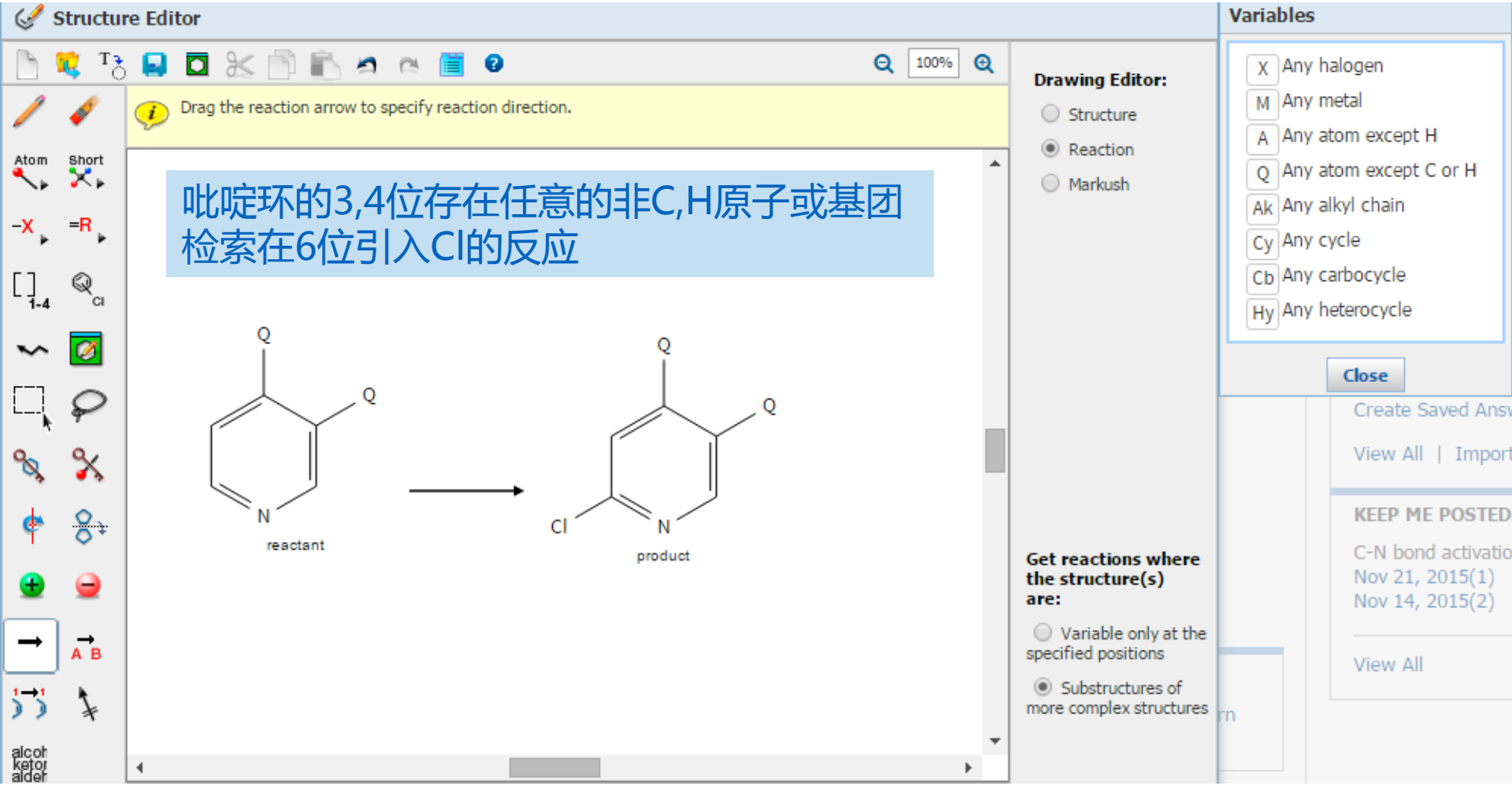
# SciFinder反应检索——亚结构反应检索

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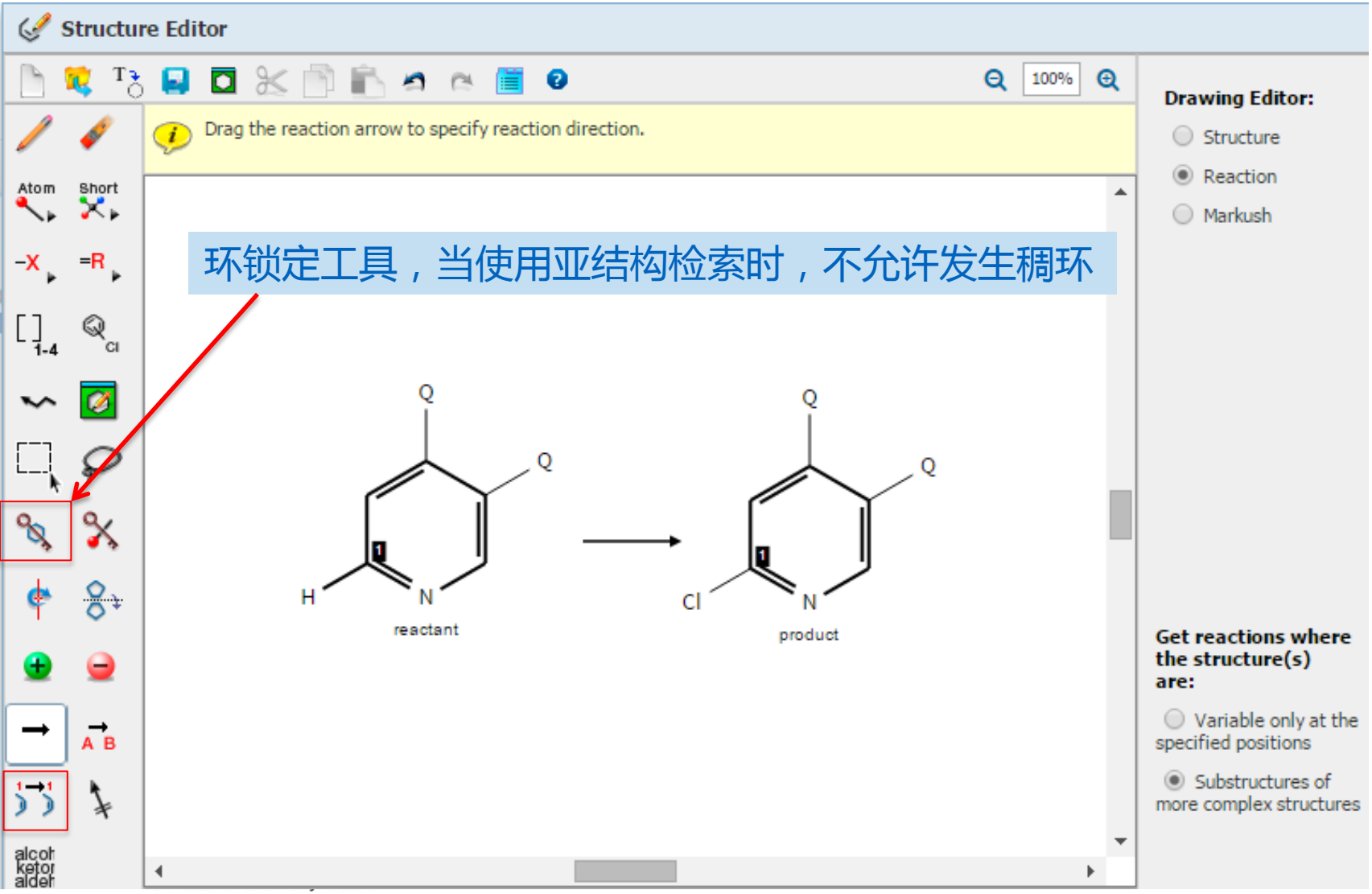
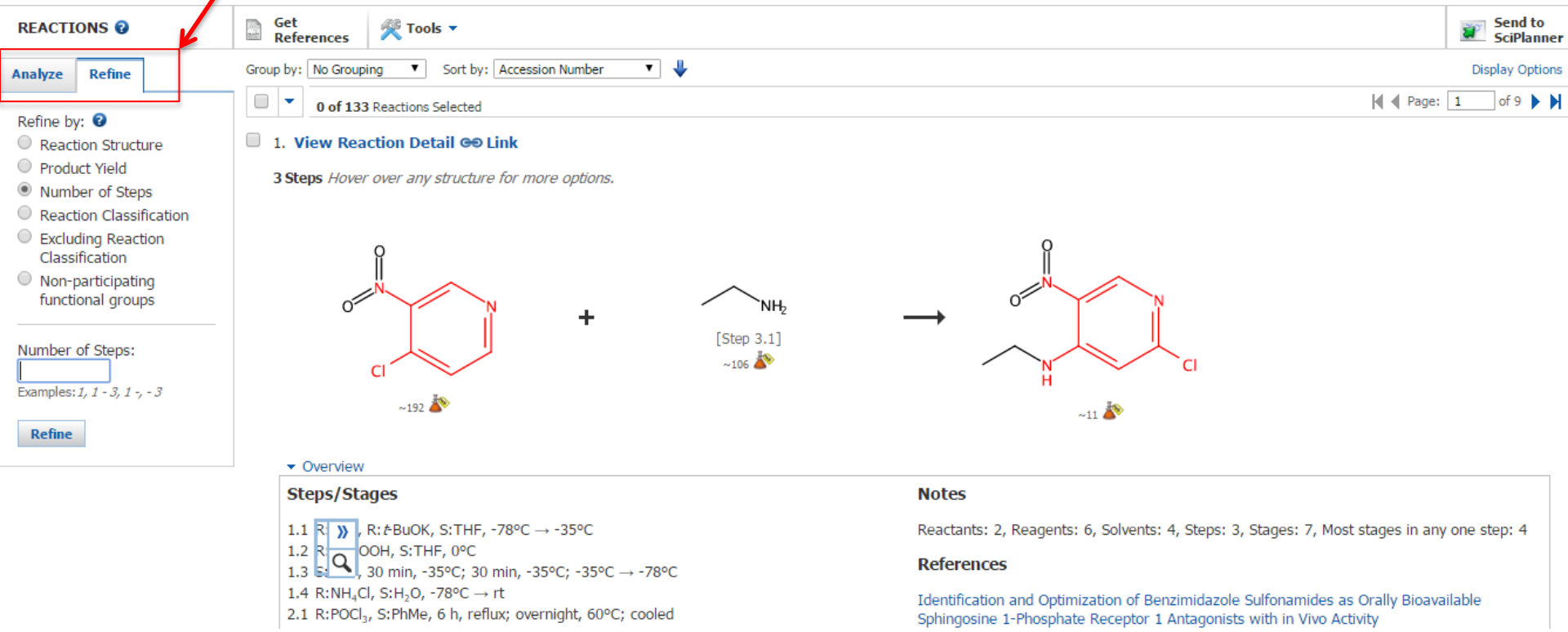
# SciFinder反应检索——亚结构反应检索



# 亚结构反应检索结果

通过Analyze或者Refine处理检索结果

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# 关于SciPlanner使用简介

3. View Reaction Detail Link

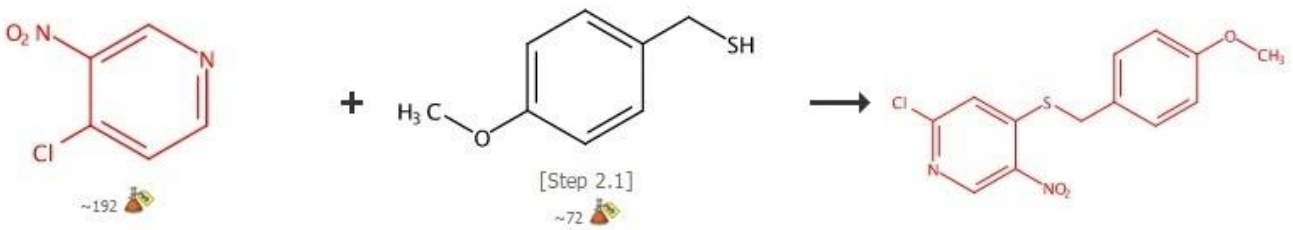
勾选想要的反应

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

点击Send to Sciplanner

Send to SciPlanner

Display Options




Overview

**Steps/Stages**

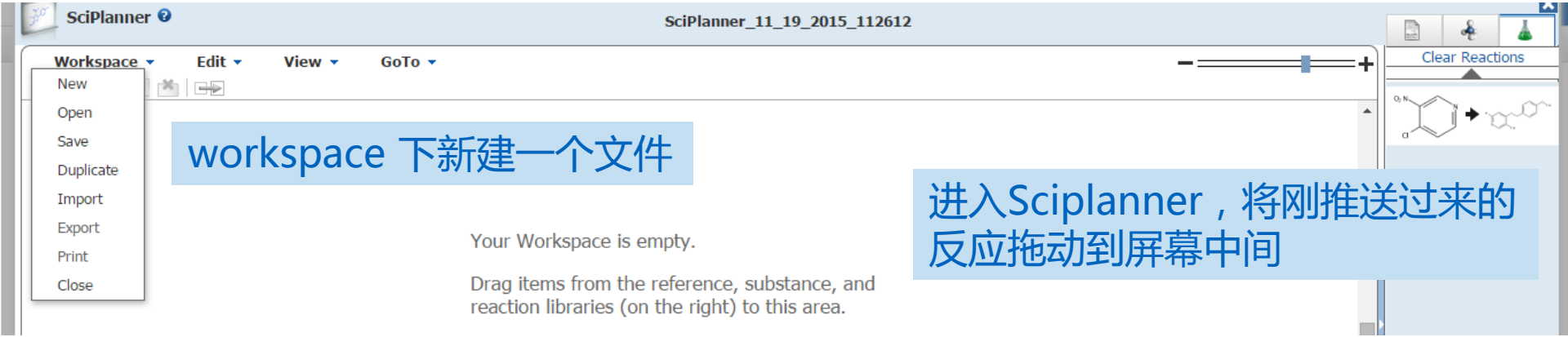
1.1 R:$NH_3$, R:*t*-BuOK, R:*t*-BuOOH, S:THF
2.1 R:NaH, S:THF
3.1 R:$POCl_3$, reflux

**Notes**

Reactants: 2, Reagents: 5, Solvents: 1, Steps: 3, Stages: 3, Most stages in any one step: 1

**References**

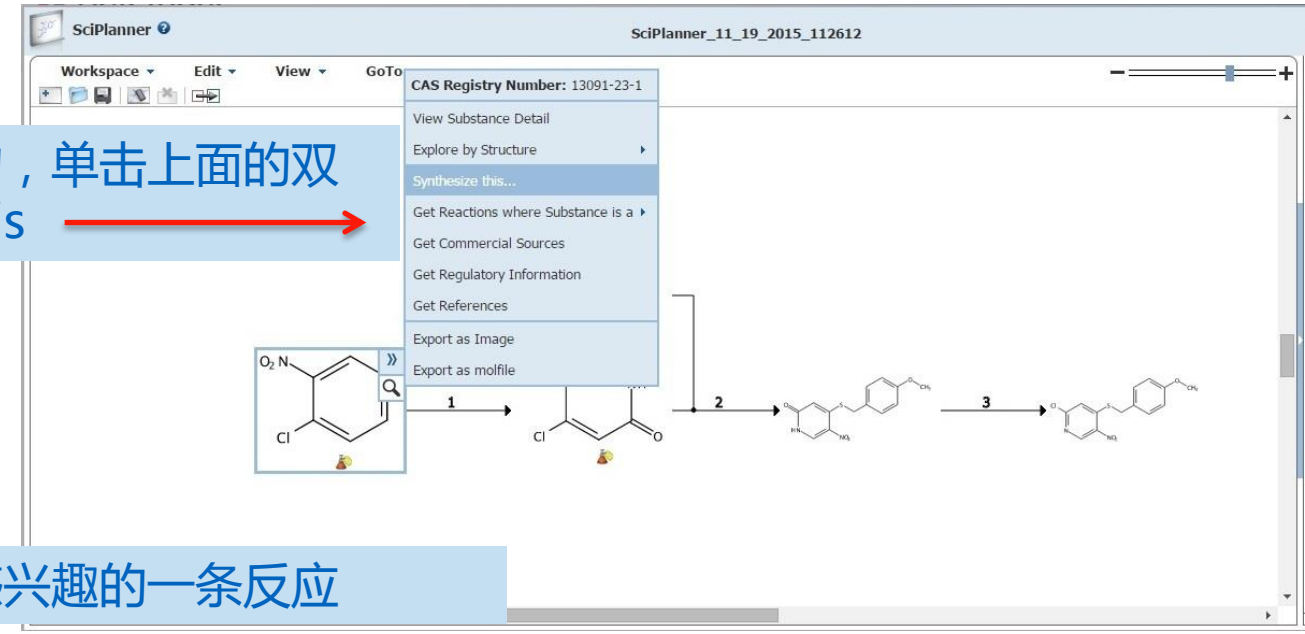
Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines
Quick View Other Sources
By Huang, Yuhua et al
From Tetrahedron Letters, 51(21), 2800-2802; 2010



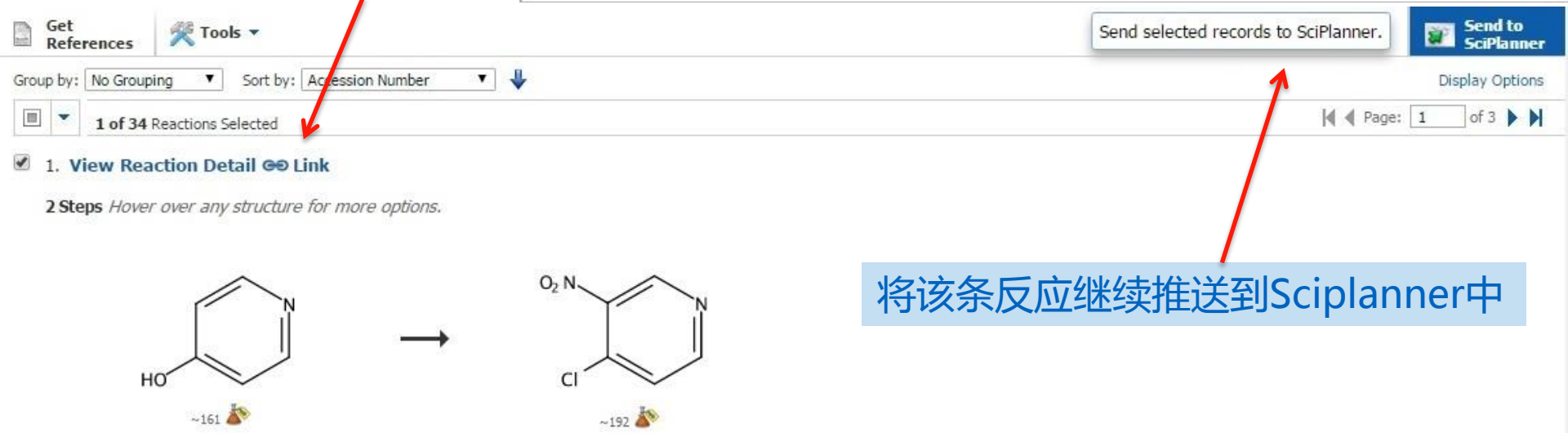

workspace 下新建一个文件

进入Sciplanner，将刚推送过来的反应拖动到屏幕中间

点击反应中的一个中间产物，单击上面的双向箭头，选择Synthesis this




在检索到的反应中，选择感兴趣的一条反应




将该条反应继续推送到Sciplanner中

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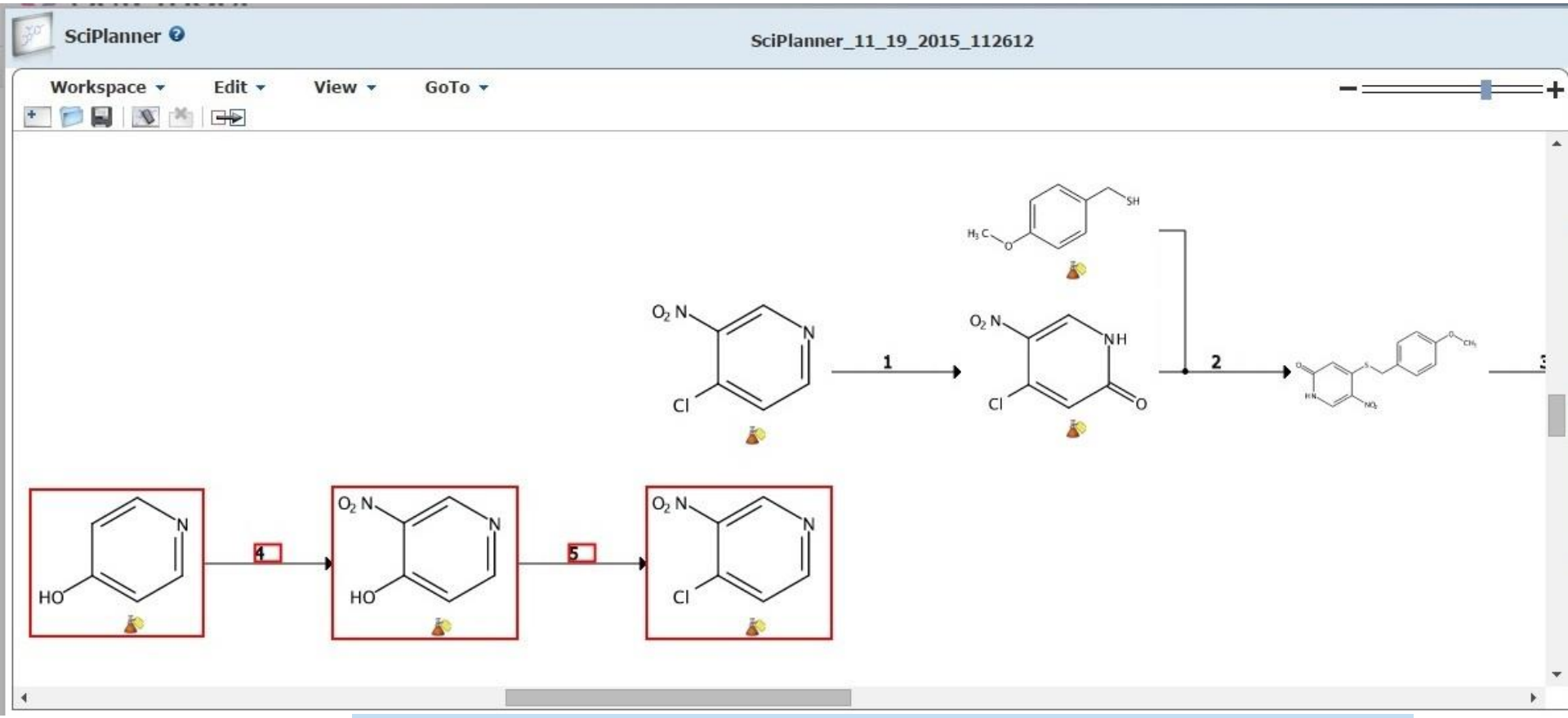


同前页步骤，将推送过来的反应拖动到SciPlanner中，可以看到两条反应中存在同样的结构

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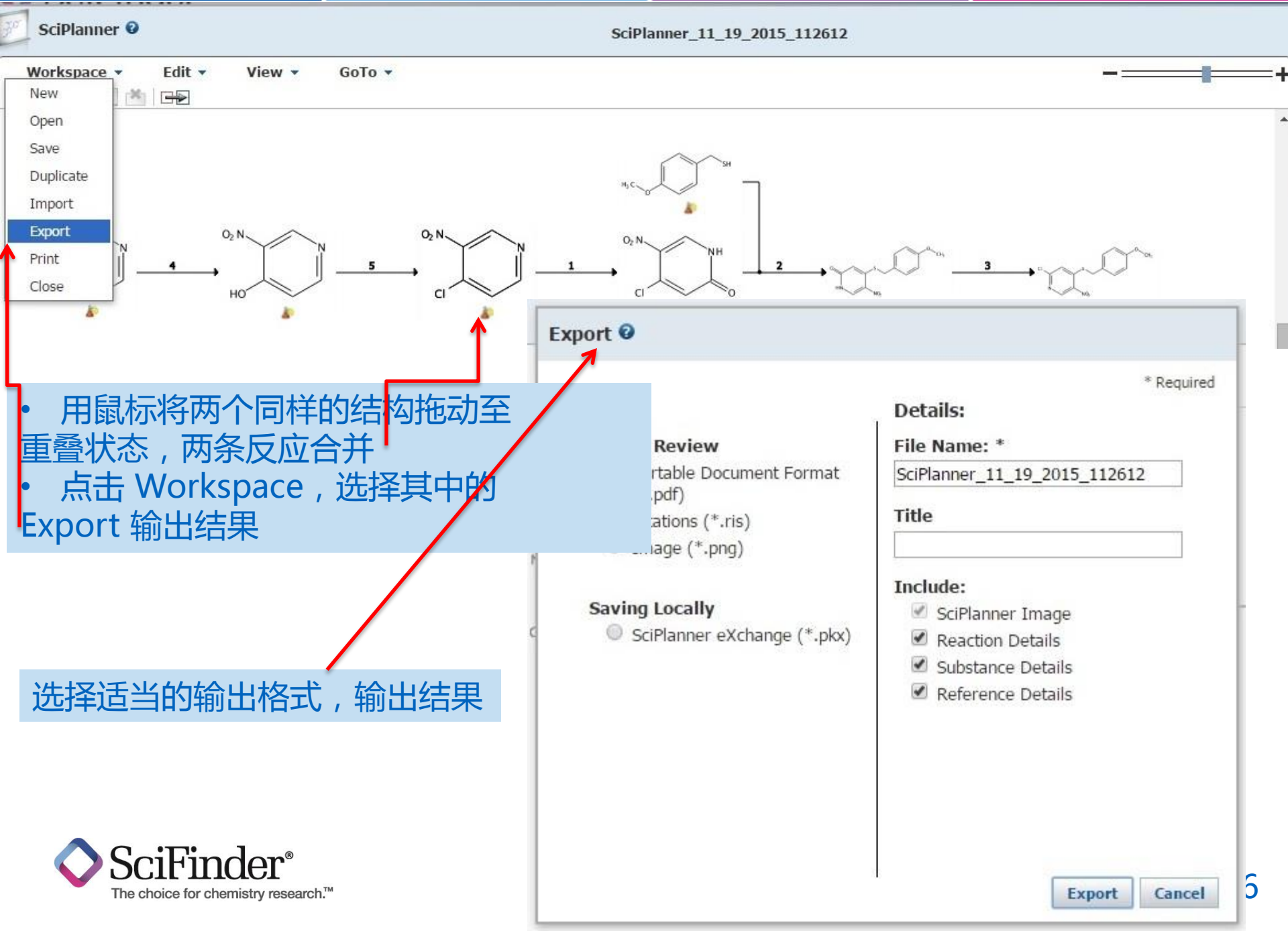


- 用鼠标将两个同样的结构拖动至重叠状态，两条反应合并
- 点击 Workspace，选择其中的 Export 输出结果

选择适当的输出格式，输出结果

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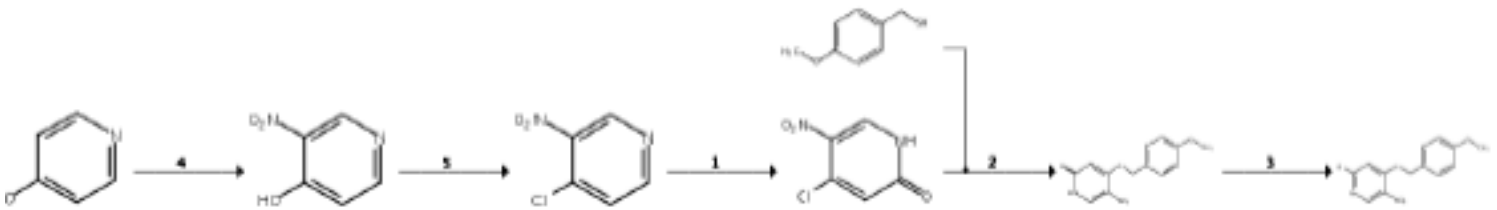
# SciPlanner导出结果



| Reaction | Stages | Notes |
|---|---|---|
| 5 | 1.1 R:$POCl_3$, S:PhMe, 0°C → rt; 16 h, rt → 110°C<br>1.2 R:$K_2CO_3$, S:$H_2O$, cooled, pH 10 | Reactants: 1, Reagents: 2<br>Solvents: 2, Steps: 1, Stag<br>**Transformation:**<br>1. Formation of Alkyl Hal from Alcohols |

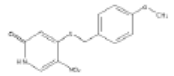
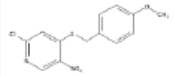
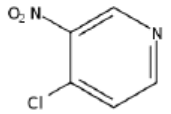
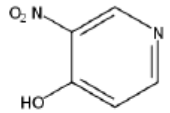
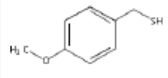
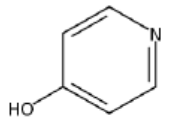
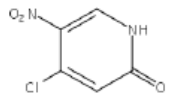
**References**

High color rendering index and color stable hybrid white efficient OLEDs with a double en structure using a single phosphorescence dopant of heteroleptic platinum complexes

By Poloek, Anurach et al

From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(4 2014

**Substance Information**

| | | |
|---|---|---|
| **1228150-22-8**<br>  <br>$C_{13}H_{12}N_2O_4S$<br>2(1*H*)-Pyridinone, 4-[[(4-methoxyphenyl)methyl]thio]-5-nitro-<br>**Related Info:**<br>~ 2 References<br>Reactions | **1228150-23-9**<br>  <br>$C_{13}H_{11}ClN_2O_3S$<br>Pyridine, 2-chloro-4-[[(4-methoxyphenyl)methyl]thio]-5-nitro-<br>**Related Info:**<br>~ 2 References<br>Reactions | **13091-23-1**<br>  <br>$C_5H_3ClN_2O_2$<br>Pyridine, 4-chloro-3-nitro-<br>**Related Info:**<br>~ 391 References<br>Reactions<br>~ 190 Commercial Sources<br>Regulatory Information |
| **5435-54-1**<br>  <br>$C_5H_4N_2O_3$<br>4-Pyridinol, 3-nitro-<br>**Related Info:**<br>~ 113 References<br>Reactions<br>~ 197 Commercial Sources<br>Regulatory Information | **6258-60-2**<br>  <br>$C_8H_{10}OS$<br>Benzenemethanethiol, 4-methoxy-<br>**Related Info:**<br>~ 749 References<br>Reactions<br>~ 71 Commercial Sources<br>Regulatory Information | **626-64-2**<br>  <br>$C_5H_5NO$<br>4-Pyridinol<br>**Related Info:**<br>~ 1351 References<br>Reactions<br>~ 160 Commercial Sources<br>Regulatory Information |
| **850663-54-6**<br>  <br>$C_5H_3ClN_2O_3$<br>2(1*H*)-Pyridinone, 4-chloro-5-nitro-<br>**Related Info:**<br>~ 22 References<br>Reactions<br>~ 136 Commercial Sources | | |

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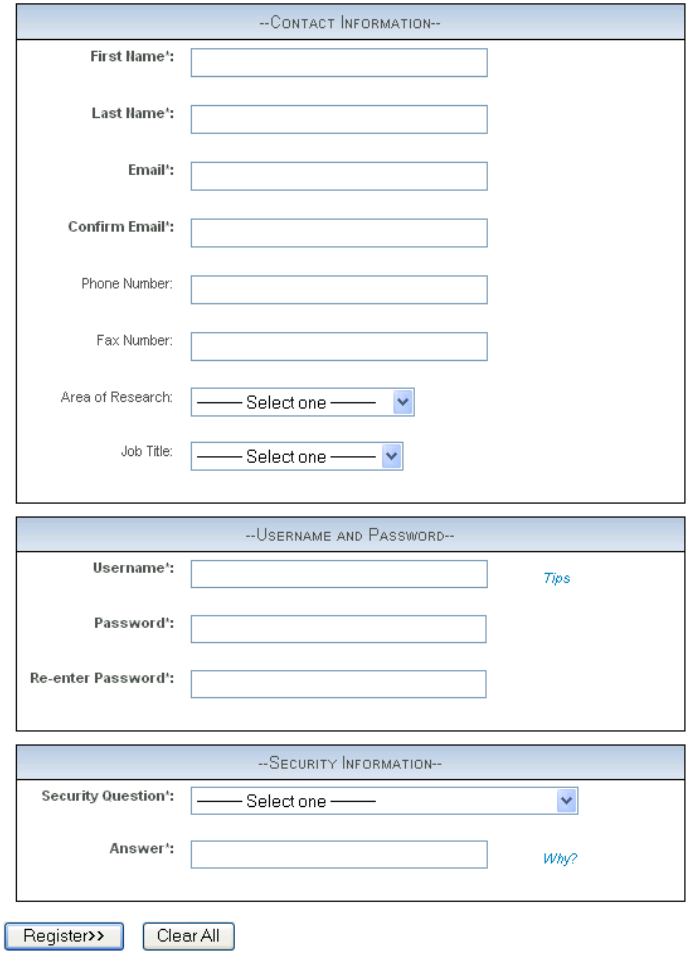
# SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

# 如何获取SciFinder账号




请注意：

1.必须输入真实姓名和域名邮箱。

2.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）

3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：

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

3.从下拉列表中选择一个密码提示问题并给出答案。单击 Register（注册）。

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# 如何获取SciFinder账号

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?respKey=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.

打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

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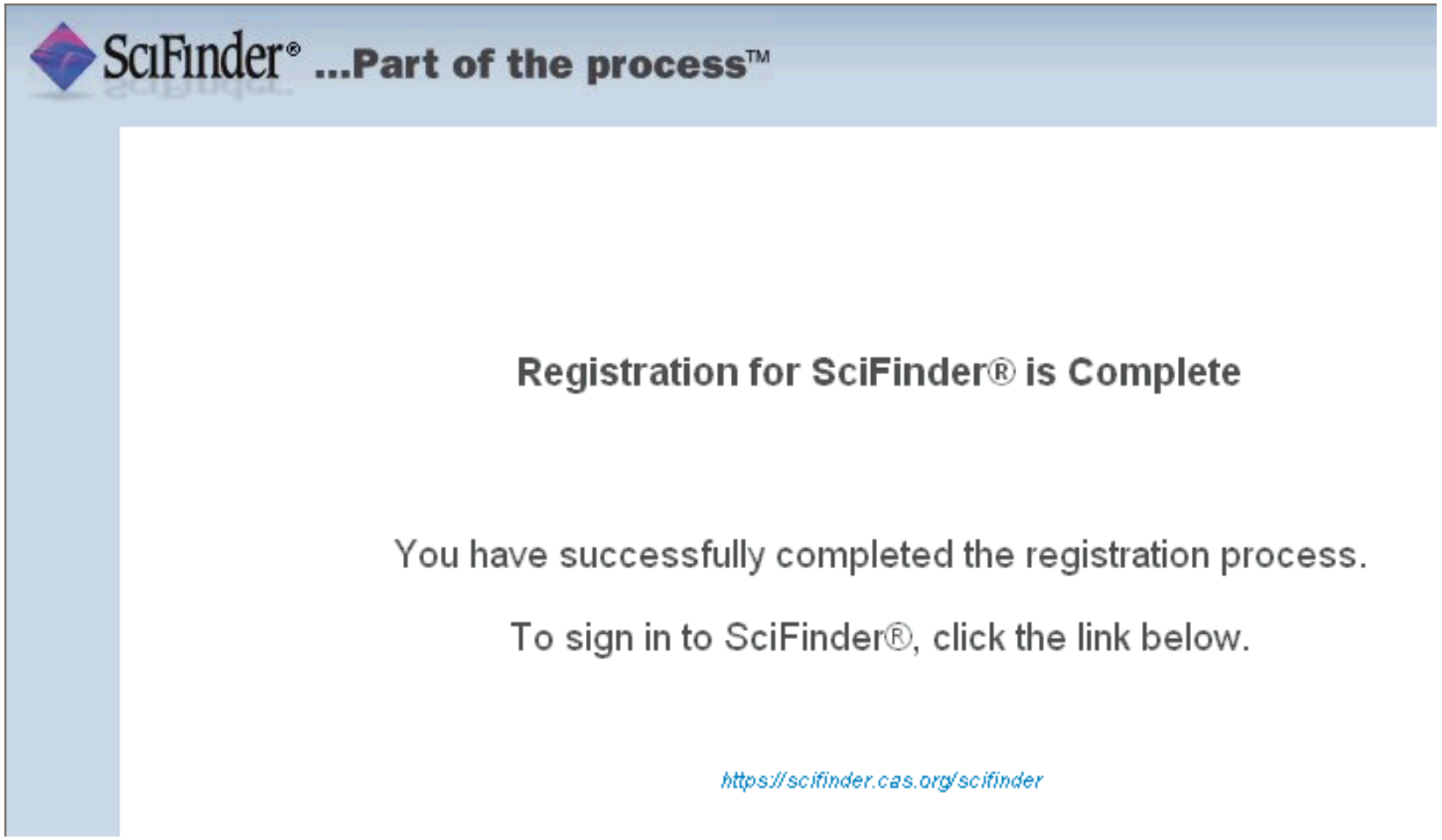


至此，账号注册成功，登录scifinder.cas.org开始使用SciFinder

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# SciFinder使用注意事项

- 一人注册一个帐号
- 严禁过量下载
- 严禁帐号分享
- 严禁将帐号用于非学术研究

# SciFinder常见问题


并发用户数已满，请稍后再试

# SciFinder常见问题

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Username and/or password is invalid. Try again, or contact CAS for assistance.

**Sign In**

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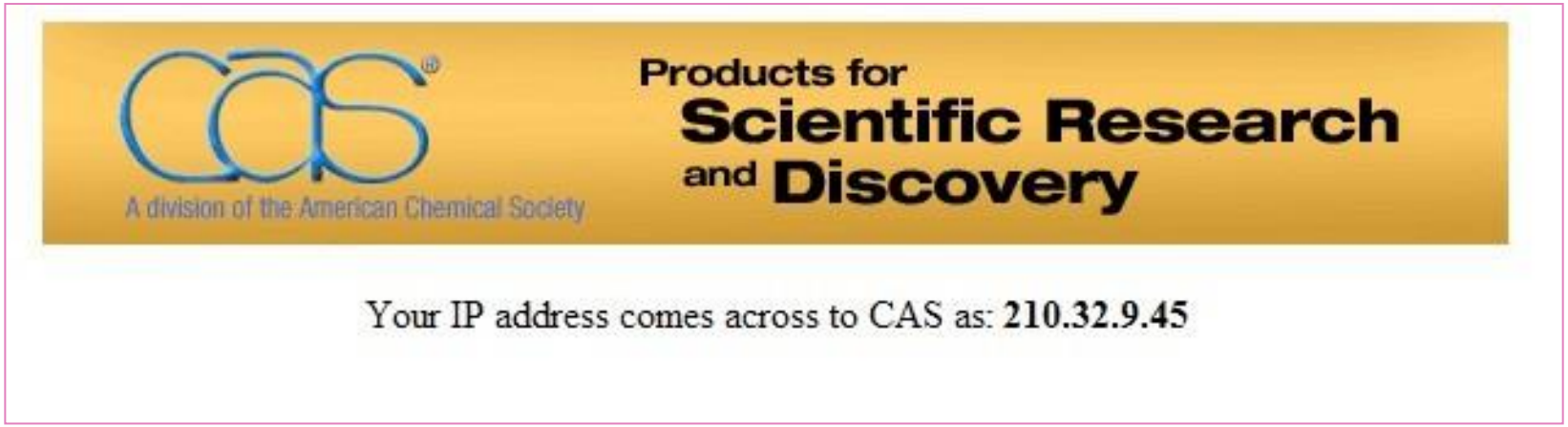
# SciFinder常见问题

任何需要反馈给图书馆的问题，都需点击测试IP地址的链接，并将页面做成截图，一并发给图书馆

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



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