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吉林大学

2016.10.14

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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
- SciFinder常见问题及解决

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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
- 总部座落于俄亥俄州的哥伦布市

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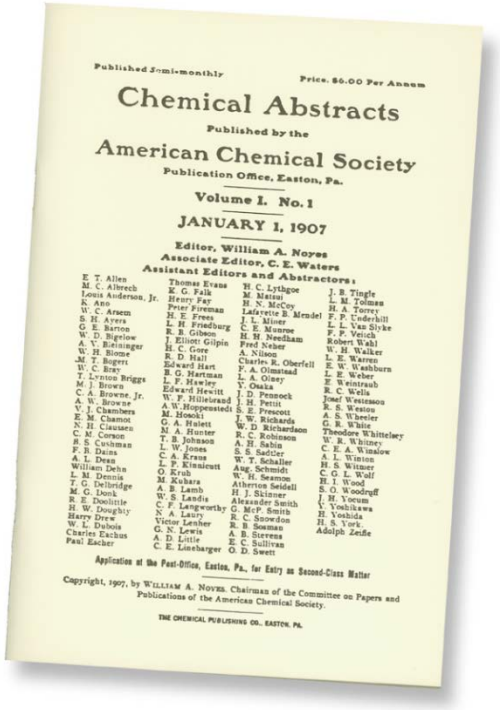
1907年，信息的汇集、管理发生了重大的变化

威廉•诺伊斯
(William A. Noyes)

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



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Chemical Abstracts

Published by the

American Chemical Society

Publication Office, Easton, Pa.

Volume I. No. 1

JANUARY 1, 1907

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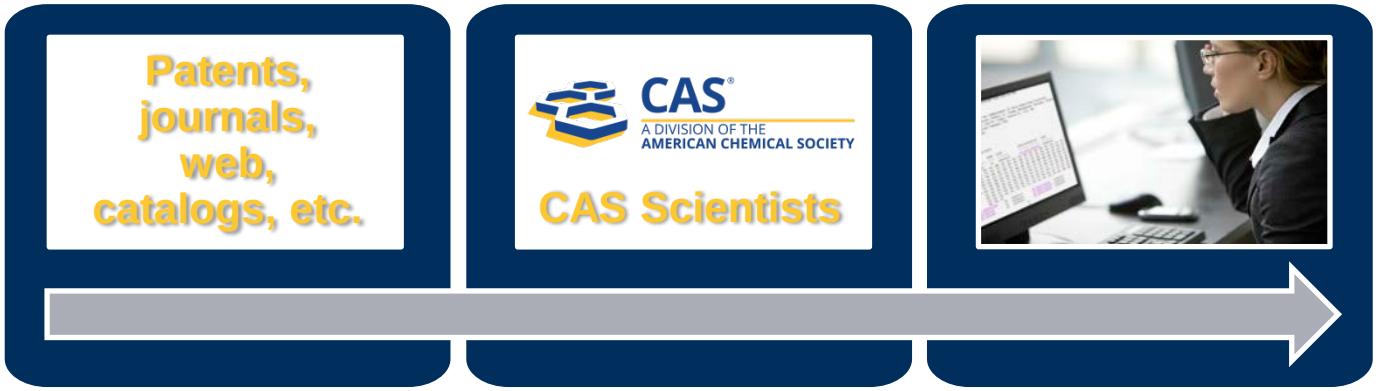

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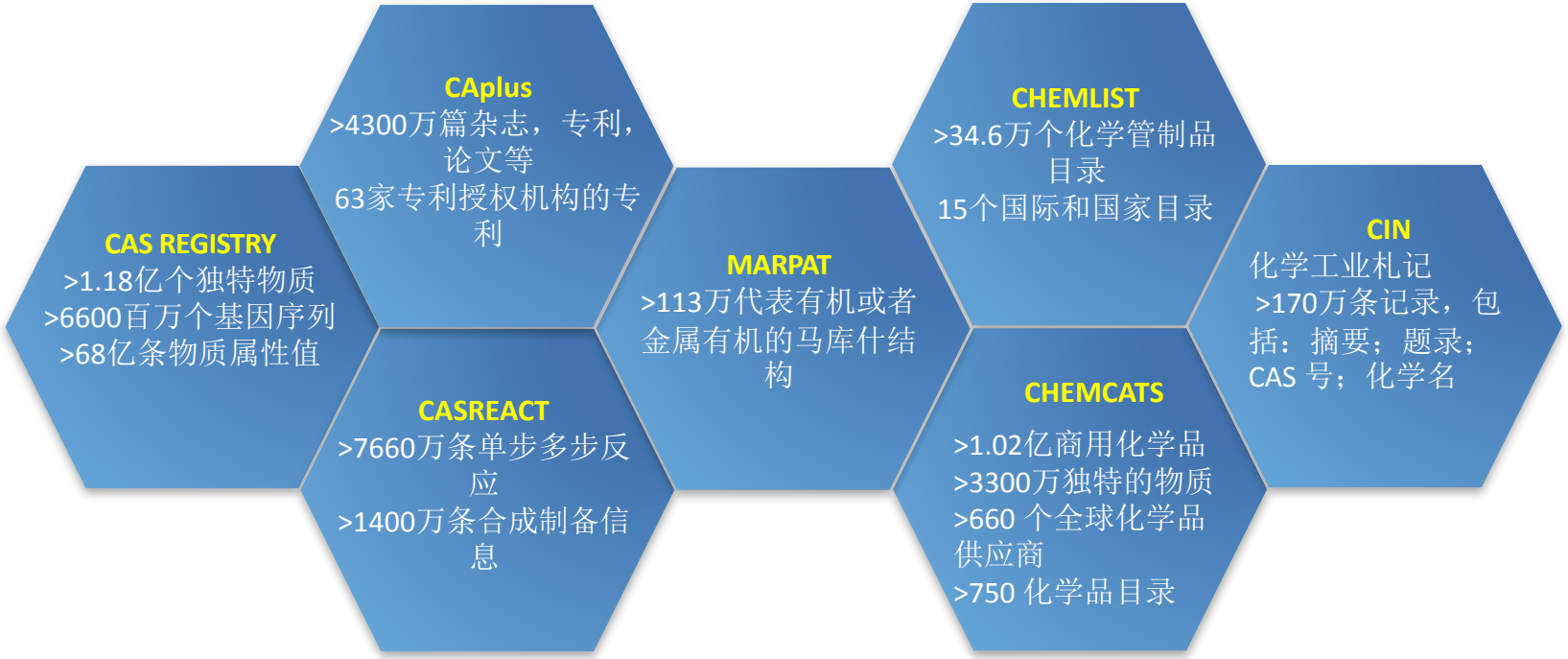

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生物化学：

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

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CAS数据库最具价值的内容——人工索引

4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia
Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751 PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014

Indexing

Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

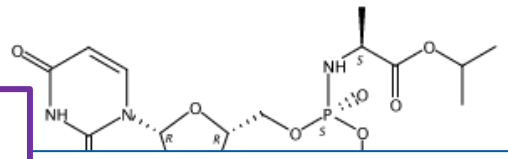
Concepts

Crystallization
Drug bioavailability
Hepatitis C
Hepatitis C virus
Homo sapiens
Human
Pharmaceutical coated tablets

Substances

1190307-88-0P Sofosbuvir
Absolute stereochemistry.

Page 2 in PATENTPAK



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

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CAS人工标引解决的问题

- 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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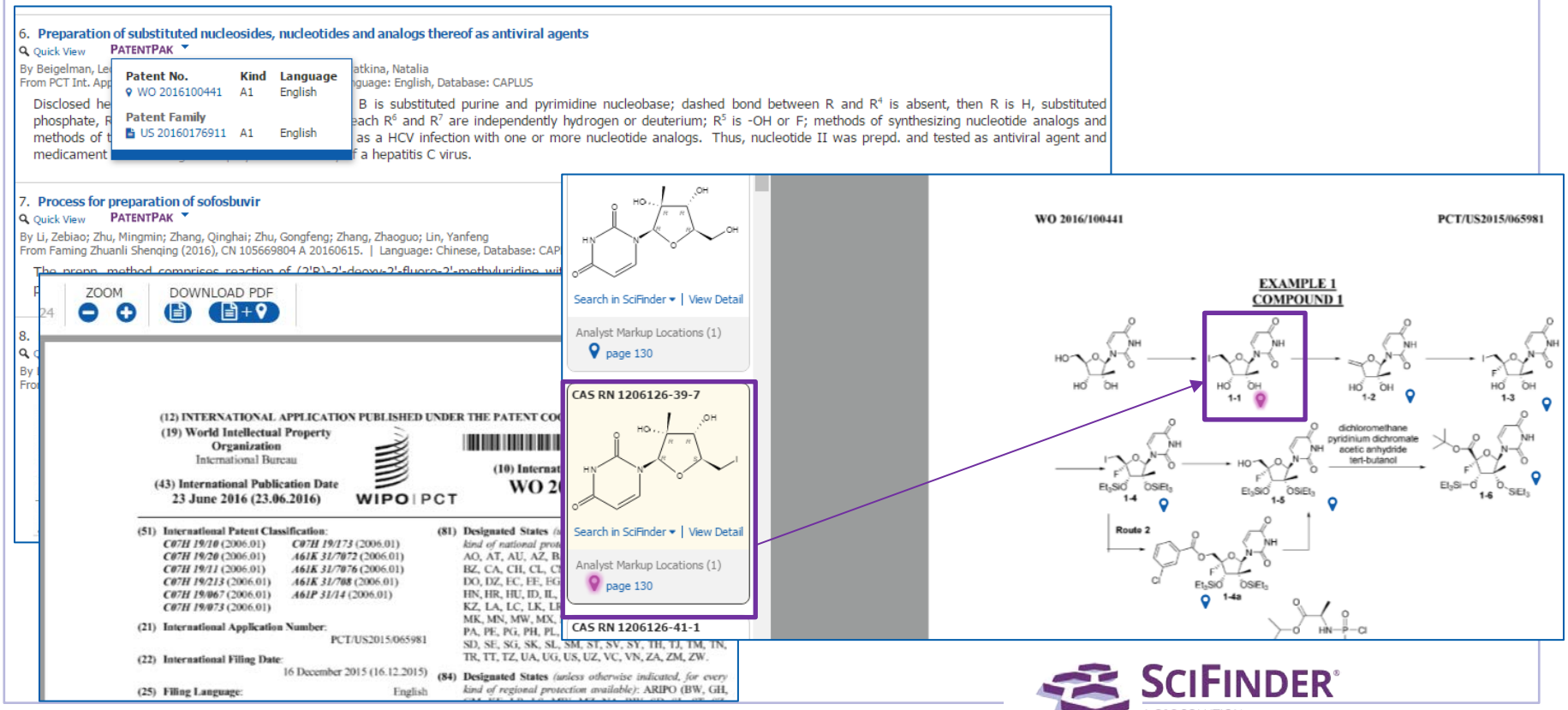

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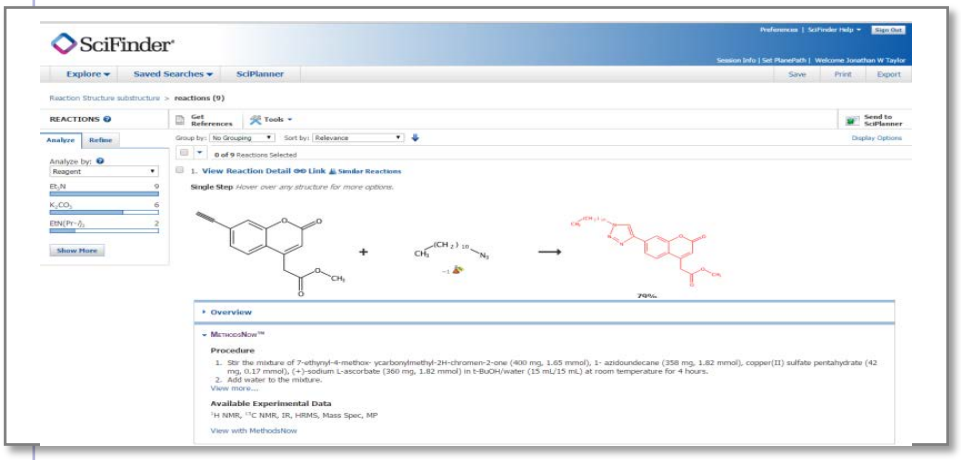
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求



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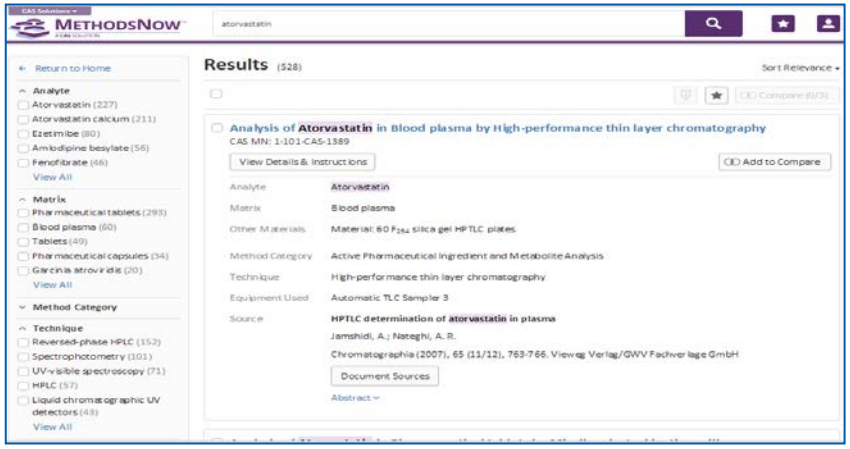

单独的分析界面

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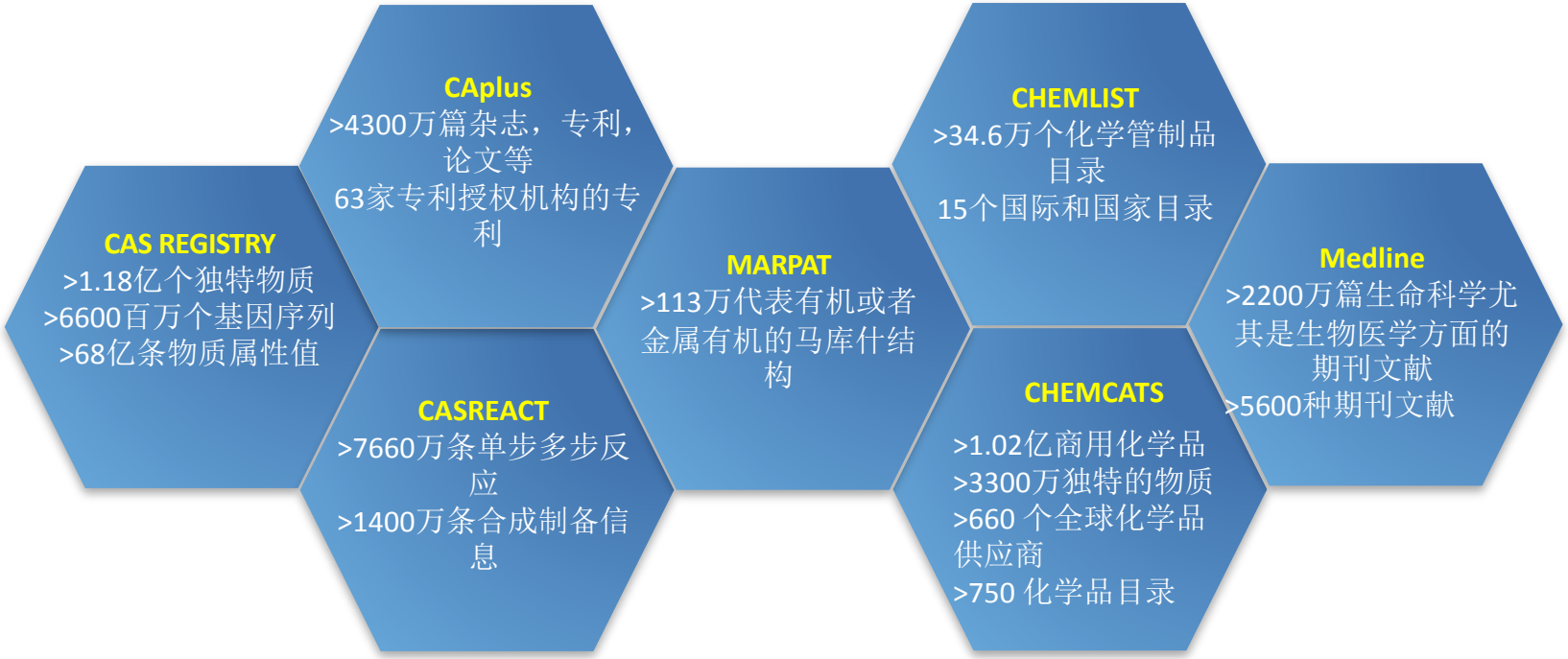

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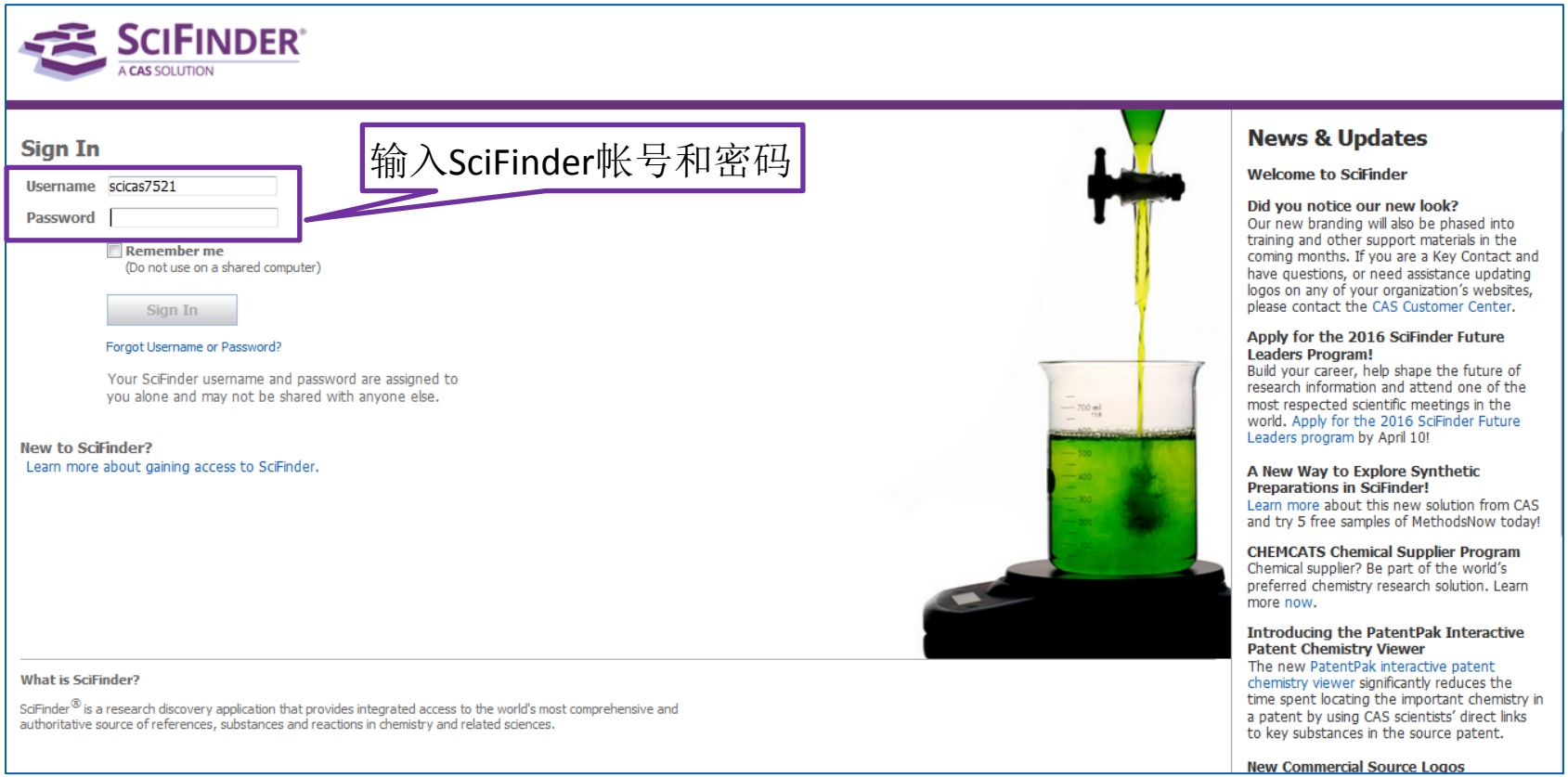

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  - 文献标识符检索
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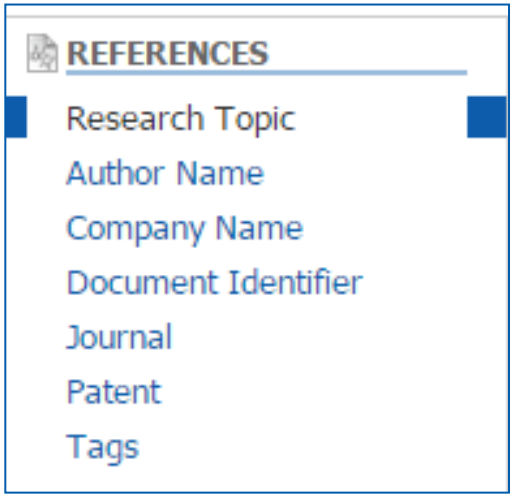

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  - 关注物质有关的文献：先获得物质，再获得文献
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文献检索——主题

主题检索：三维石墨烯的制备

检索式： prepare of 3D graphene

关键词之间用介词连接：in, with, of...

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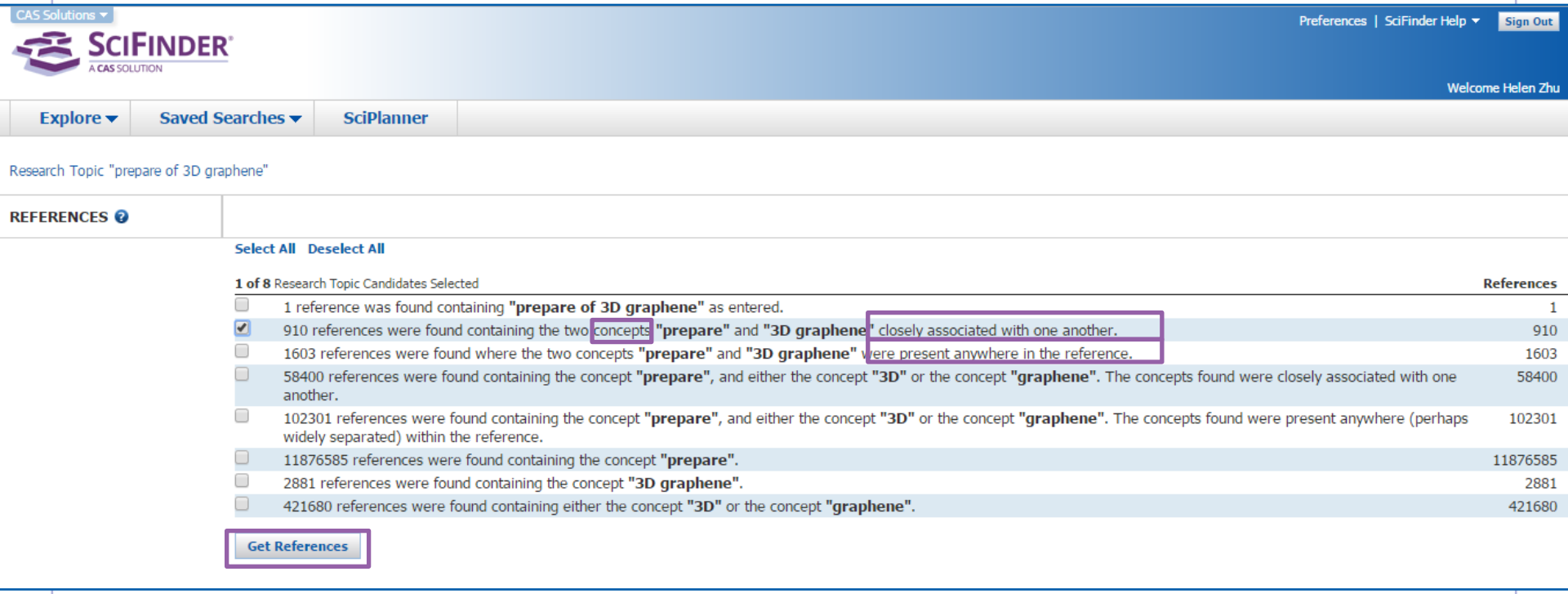
主题检索的候选项



"Concepts"表示对主题词做了同义词的扩展；

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

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

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Research Topic "prepare of 3D graphene" > **references (767)**

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Huang Wei	11
Hu Yun Hang	10
Ma Jie	10
Yu Fei	10
Dong Xiaochen	9
Chen Peng	8
Zhang Hua	8
Qu Liangti	7
Shi Gaoquan	7

Sort by: Citing References ▼ (Accession Number / Author Name / Citing References / Publication Year / Title)

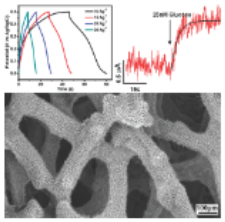
Display Options

Page: 1 of 39

1. **…lt Oxide Electrode for High-Performance Supercapacitor and Enzymeless Glucose Detection**

Quick View | Other Sources

By Dong, Xiao-Chen; Xu, Hang; Wang, Xue-Wan; Huang, Yin-Xi; Chan-Park, Mary B.; Zhang, Hua; Wang, Lian-Hui; Huang, Wei; Chen, Peng
From ACS Nano (2012), 6(4), 3206-3213. | Language: English, Database: CAPLUS



Using a simple hydrothermal procedure, cobalt oxide (Co_3O_4) nanowires were in situ **synthesized** on three-dimensional (**3D**) **graphene** foam grown by chem. vapor deposition. The structure and morphol. of the resulting **3D graphene**/Co_3O_4 composites were characterized by SEM, TEM, x-ray diffraction, and Raman spectroscopy. The **3D graphene**/Co_3O_4 composite was used as the monolithic free-standing electrode for supercapacitor application and for enzymeless electrochem. detection of glucose. The authors demonstrate that it is capable of delivering high specific capacitance of ~1100 F g^{-1} at a c.d. of 10...

2. **A Three-Dimensional Carbon Nanotube/Graphene Sandwich and Its Application as Electrode in Supercapacitors**

Quick View | Other Sources

By Fan, Zhuangjun; Yan, Jun; Zhi, Linjie; Zhang, Qiang; Wei, Tong; Feng, Jing; Zhang, Milin; Qian, Weizhong; Wei, Fei
From Advanced Materials (Weinheim, Germany) (2010), 22(33), 3723-3728. | Language: English, Database: CAPLUS

A **3D** CNT/**graphene** sandwich structures with CNT pillars grown in between the **graphene** layers had been **prepd.** by CVD. The unique structure endows the high rate transportation of electrolyte ions and electrons throughout the electrode matrix and comprehensive utilization of pseudo and double-layer capacitance, resulting in excellent electrochem. performances. The supercapacitor based on CGS exhibits 1'00 a specific capacitance of 385 F g^{-1} at 10 mV s-1 in 6 M KOH 1600 2000 soln. After 2000 cycles, a capacitance increase of ca. 20 % of the initial capacitance is obsd., indicating excellent elec...

Citing Reference: 帮助找到最重要的文献

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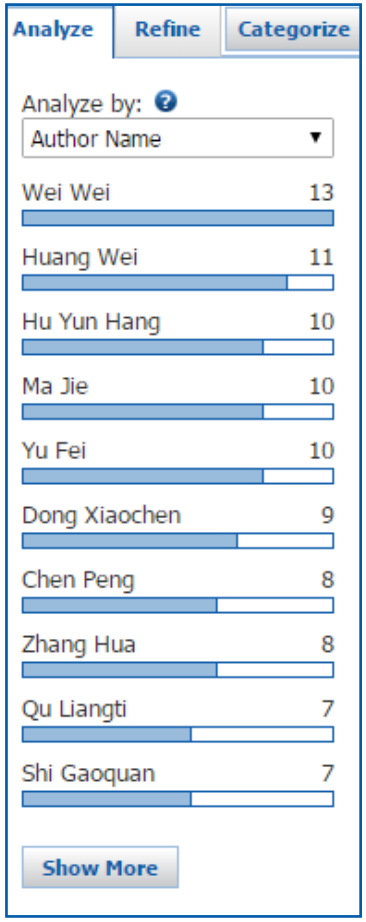
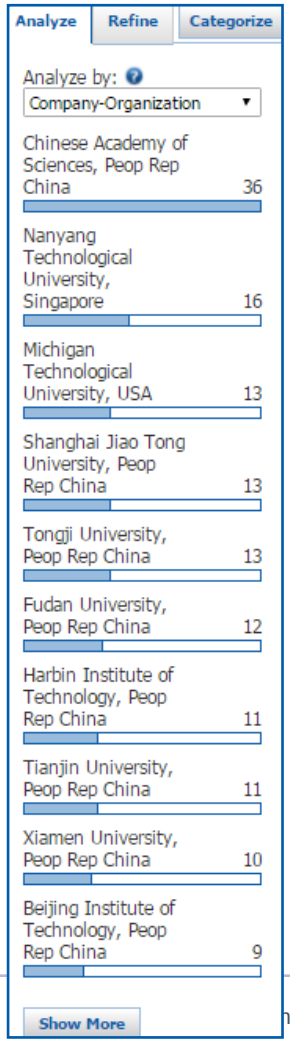
本领域研究人员



本领域研究机构、
合作伙伴、竞争对手



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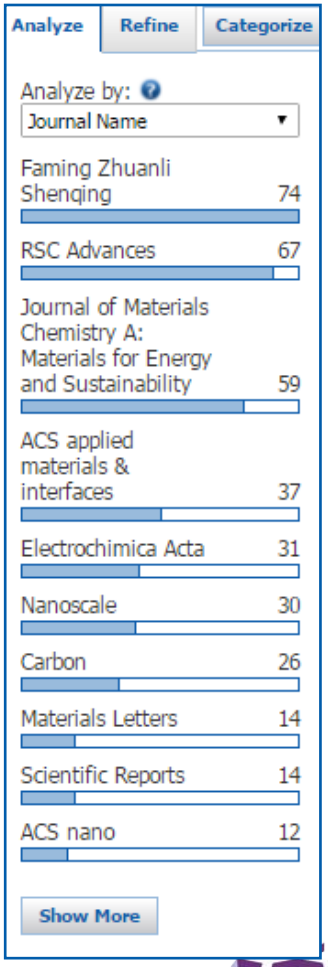

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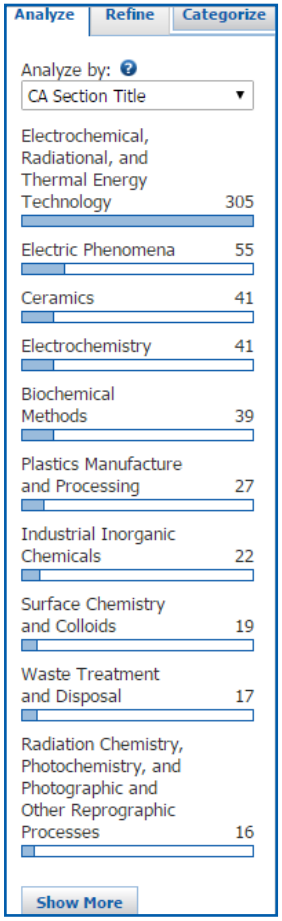

文献检索结果的Analyze

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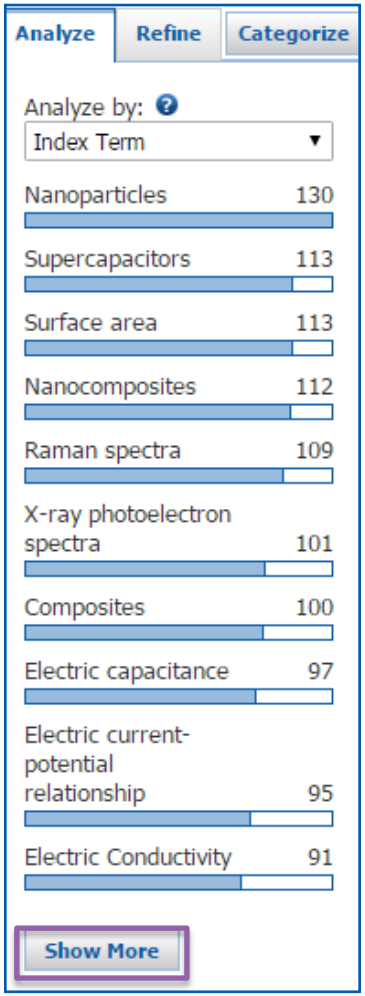

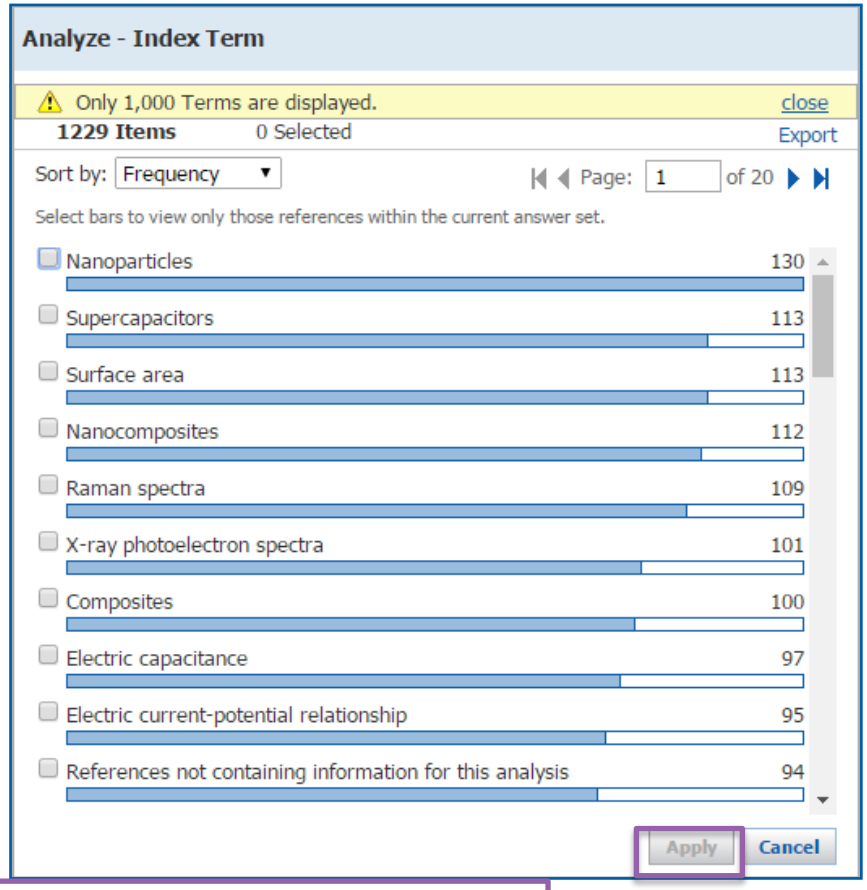

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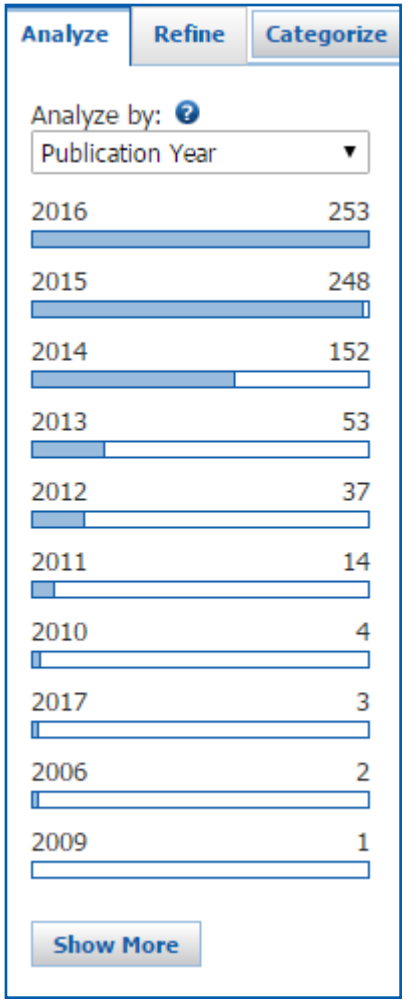

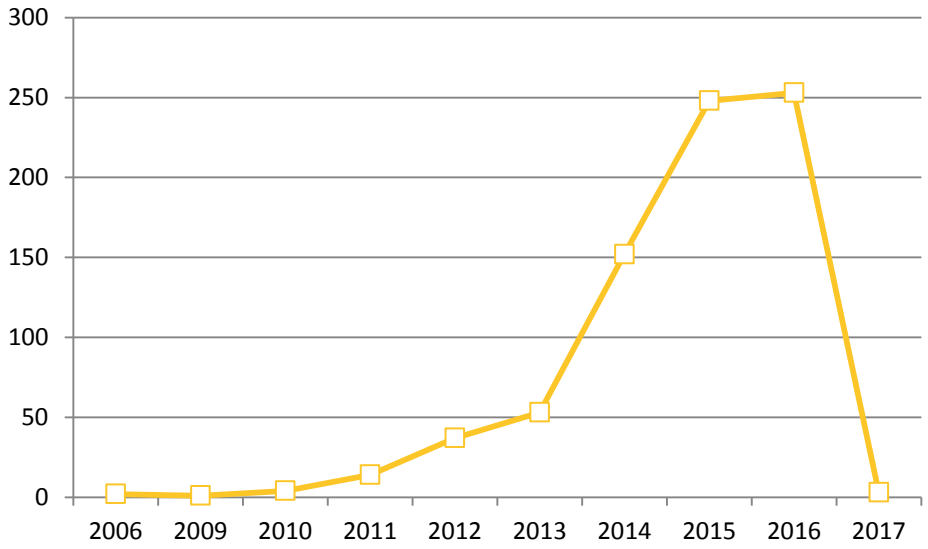

Publication Year: 分析领域发展趋势

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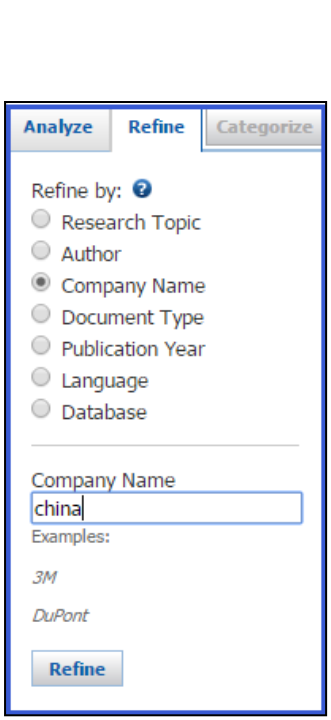

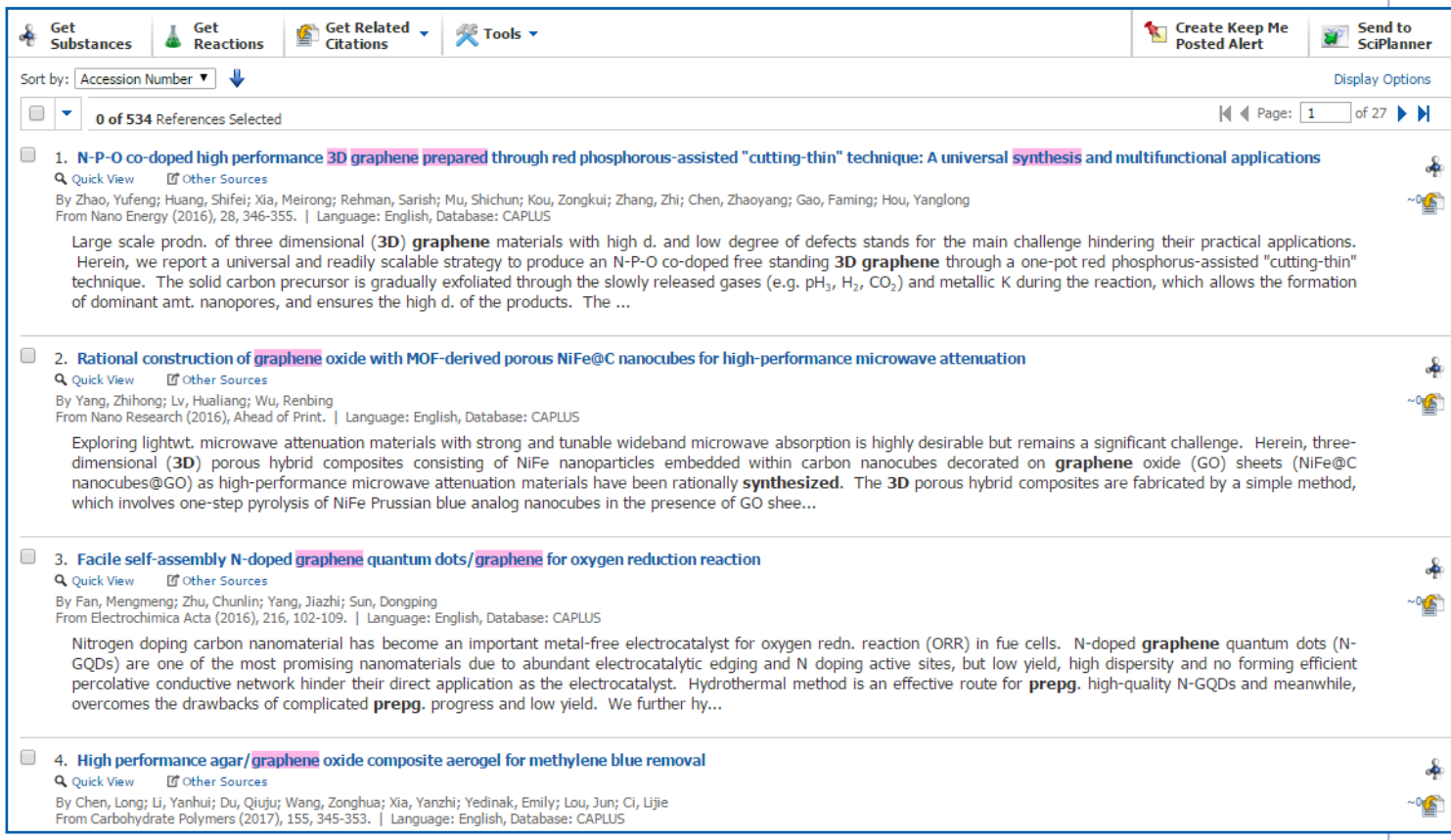

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文献检索结果的Categorize

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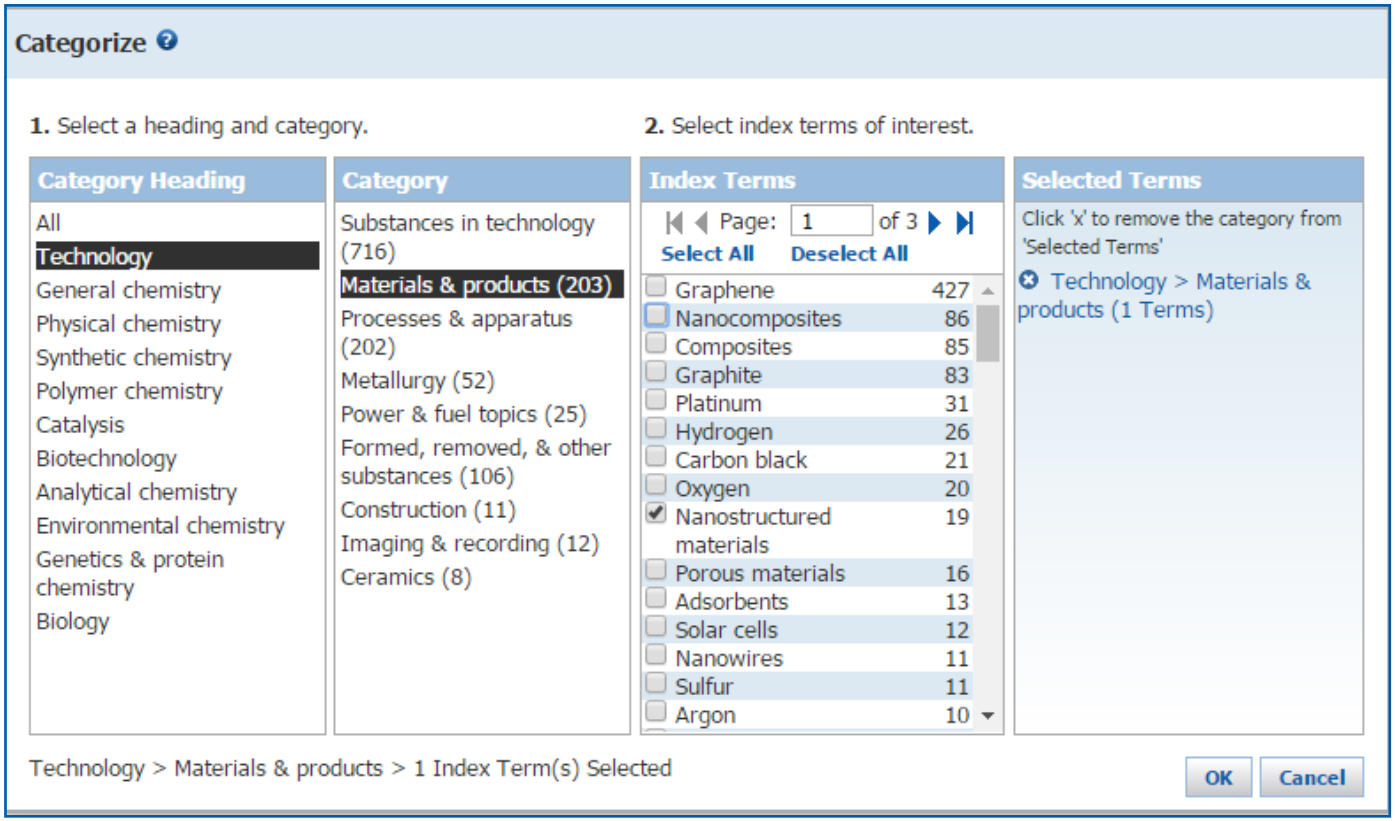

Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

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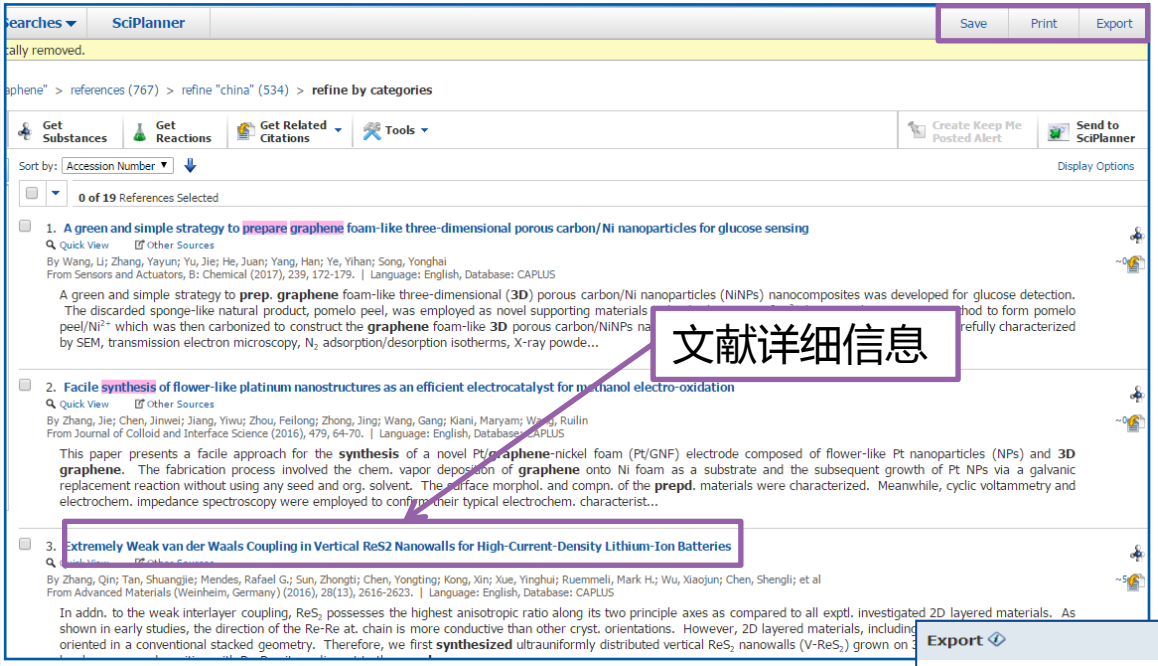

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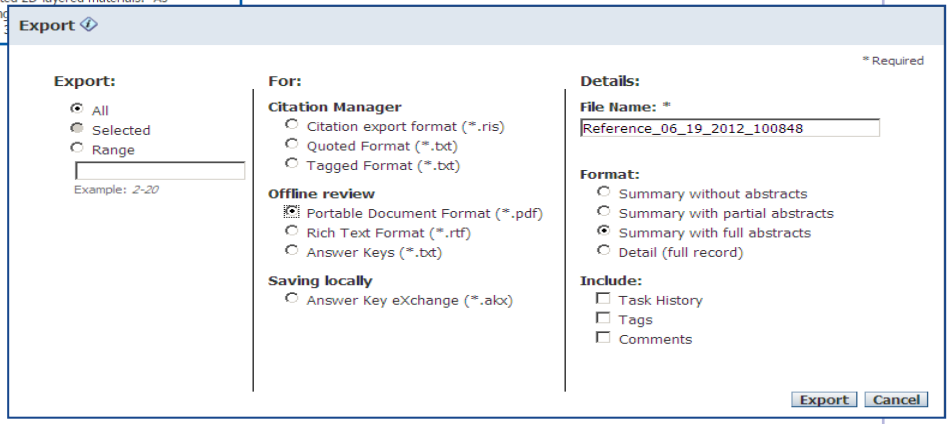
Export：导出至本地电脑。

Print：打印成PDF格式



Citation manager: 保存成RIS等格式，可导入EndNote 等文献管理工具

Offline Review：保存成PDF，RTF等格式，用于脱机浏览

SciFinder® A CAS SOLUTION

文献信息—题录、摘要、索引

3. Extremely Weak van der Waals Coupling in Vertical ReS2 Nanowalls for High-Current-Density Lithium-Ion Batteries

By: Zhang, Qin; Tan, Shuangjie; Mendes, Rafael G.; Sun, Zhongti; Chen, Yongting; Kong, Xin; Xue, Yinghui; Ruemmeli, Mark H.; Wu, Xiaojun; Chen, Shengli; Fu, Lei

In addn. to the weak interlayer coupling, ReS_2 possesses the highest anisotropic ratio along its two principle axes as compared to all exptl. investigated 2D layered materials. As shown in early studies, the direction of the Re-Re at. chain is more conductive than other cryst. orientations. However, 2D layered materials, including ReS_2, are always randomly oriented in a conventional stacked geometry. Therefore, we first synthesized ultrauniformly distributed vertical ReS_2 nanowalls (V-ReS_2) grown on 3D graphene foam (3DGF) by chem. vapor deposition with Re-Re sites adjacent to the graphene for the purpose of enhancing the cond. Meanwhile, the ReS_2 nanowalls expose more active sulfur edge sites, which improves easy lithium intercalation and deintercalation. To enhance the cond. of the whole electrode material, 3DGF was selected as template due to its high cond. and high-sp. surface area. Moreover,this favorable vertical structure shortens the pathways and facilitates fast diffusion of both Li + and electrolyte ions. As expected, the V-ReS 2 /3DGF composite demonstrated good cycling stability at high-current-densities when serving as anode material for LIBs. At the high c.d. of 1000 mA/g, the capacity of our ReS_2 /3DGF anodes still maintained over 200 mAh/g even after 500 cycles. The extremely weak vdW coupling material of ReS_2 holds great promise for practical applications in LIBs. In addn., it broadens the material choice of anode materials for other alk.-ion batteries.

Indexing

Electrochem… Energy Technology (Section52-2)

Concepts 重要概念

Battery anodes
Current density
Delithiation
Intercalation
Lithiation
Lithium-ion secondary batteries
Nanostructured materials

extremely weak van der Waals coupling in vertical ReS2 nanowalls for high-current-d. lithium-ion batteries

Substances 重要物质

12038-63-0P Rhenium sulfide

extremely weak van der Waals coupling in vertical ReS2 nanowalls for high-current-d. lithium-ion batteries

Synthetic preparation; Technical or engineered material use; Preparation; Uses

7439-93-2 Lithium, uses
1034343-98-0 Graphene

extremely weak van der Waals coupling in vertical ReS2 nanowalls for high-current-d. lithium-ion batteries

Technical or engineered material use; Uses

QUICK LINKS
0 Tags, 0 Comments

SOURCE
Advanced Materials (Weinheim, Germany)
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Issue13
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Journal; Online Computer File
2016
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ISSN:0935-9648
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COMPANY/ORGANIZATION
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CAPLUS

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LANGUAGE
English

文献详情界面包括：
1. 标题
2. 摘要
3. 文献中重要的技术术语
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
7. 参考文献
8. 链接原文

文献检索小结

- 主题检索时，使用介词 in, with, of 等作为连接词
- 根据检索要求选择合适的候选项
- 通过SciFinder 的Analyze/Refine功能来缩小检索的范围
- 尝试将不同的Analyze/Refine功能组合起来用，会有更多的收益
- 使用Categorize可以让系统来实现自动分类

SCIFINDER® A CAS SOLUTION

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
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

SciFinder检索选项——物质检索

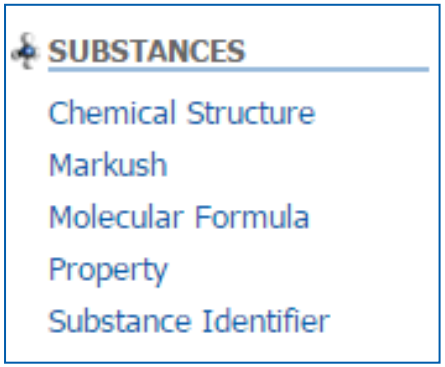
- 物质检索方法

  —结构式检索

  —分子式检索

  —理化性质检索

  —物质标识符检索：化学名称，CAS RN



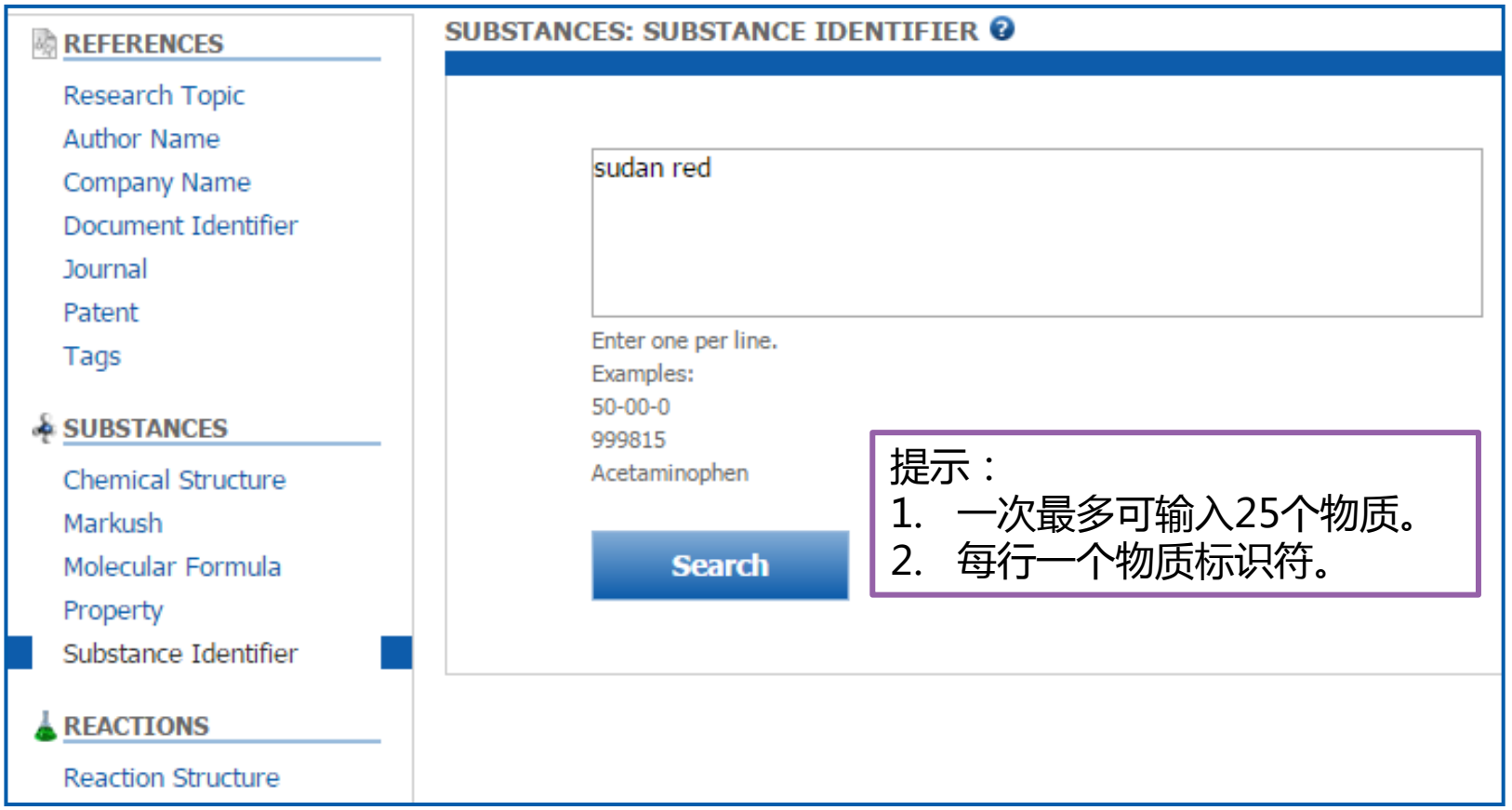
- 物质检索策略推荐

  —有机化合物，天然产物：结构检索

  —无机物，合金：分子式检索

  —高分子化合物：分子式检索和结构检索

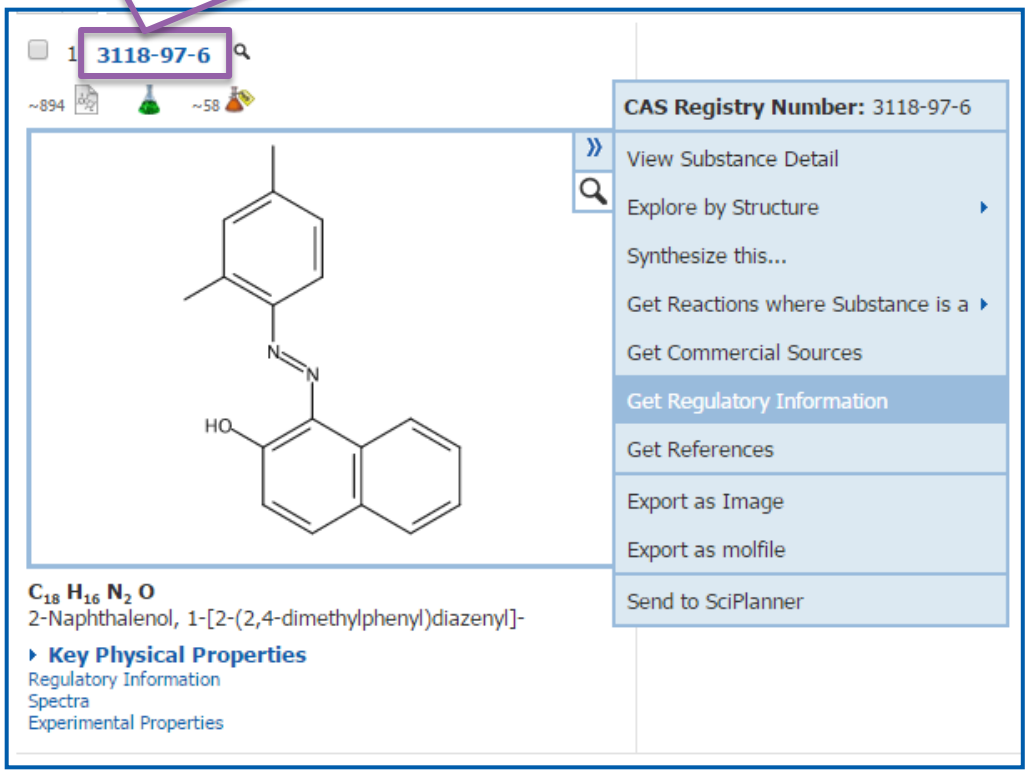
物质检索——标识符检索



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。

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

SciFinder® A CAS SOLUTION

SciFinder中的物质记录

SUBSTANCE DETAIL

Get References | Get Reactions | Get Commercial Sources

Return

由物质获得文献，反应，供应商等信息

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

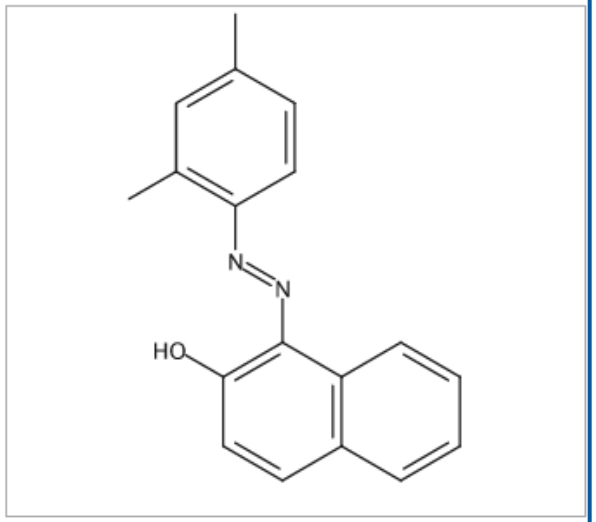
Melting Point (Experimental)
Value: 166 °C

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

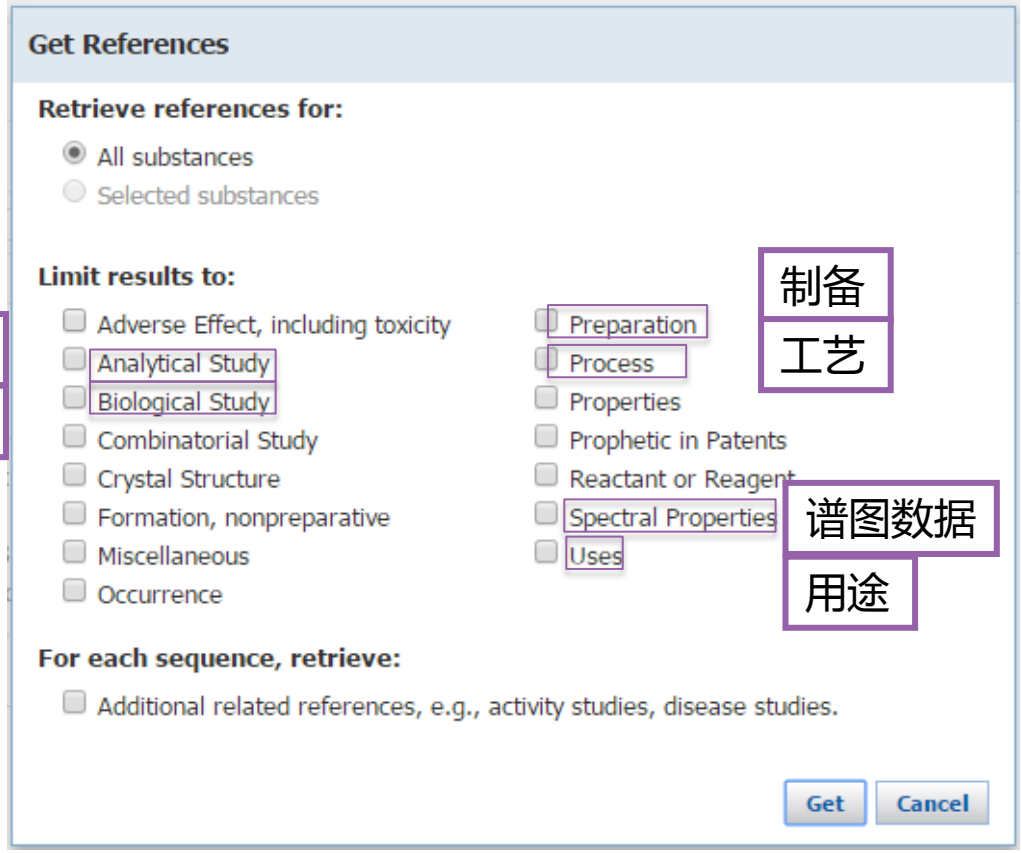
Other Names
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)
C.I. Solvent Orange 7 (7CI,8CI)
Sudan Red (6CI)
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol
AF Red No. 5
View more...



物质详情

SciFinder® A CAS SOLUTION

通过物质获得文献



分析化学

生物研究

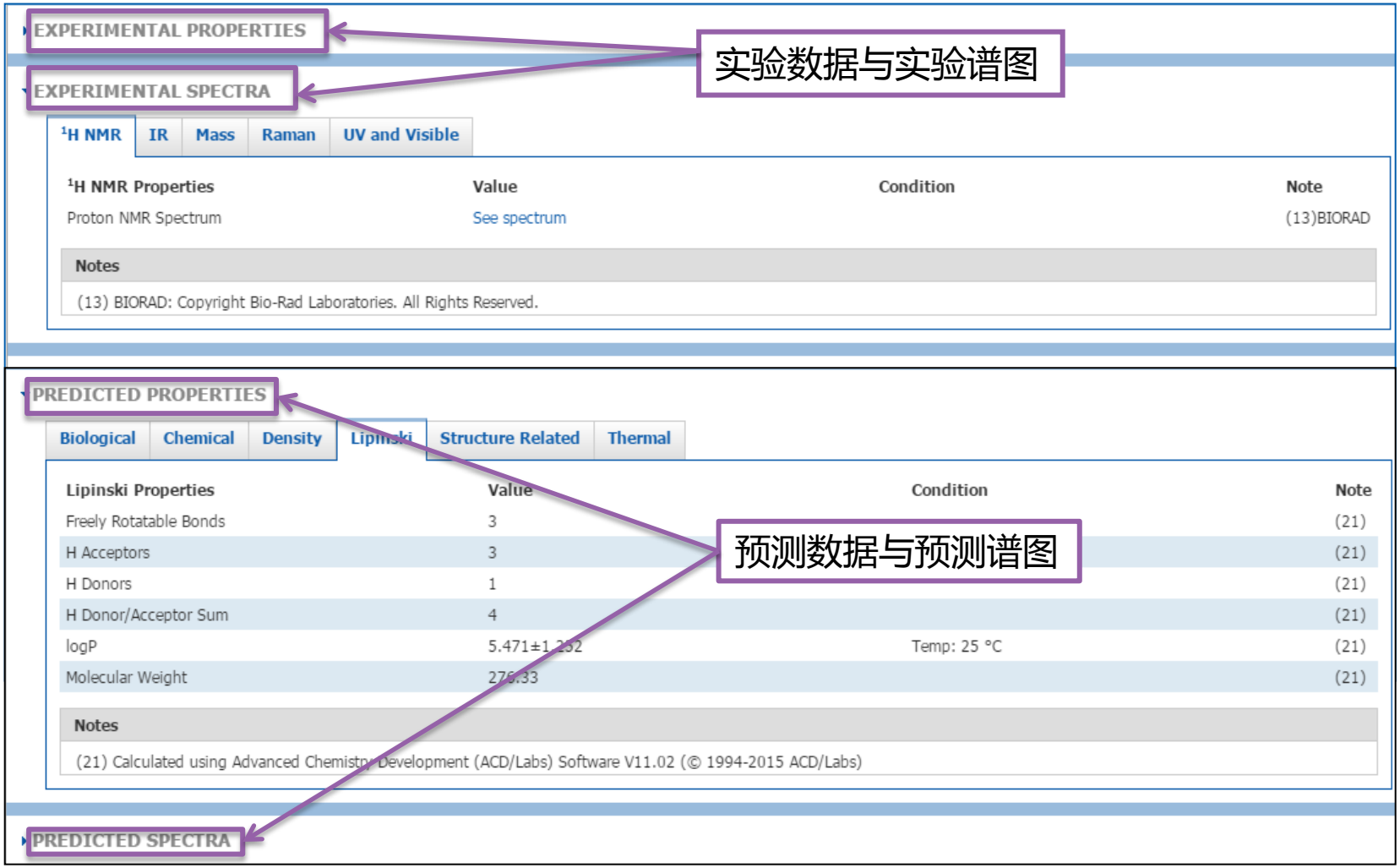
制备

工艺

谱图数据

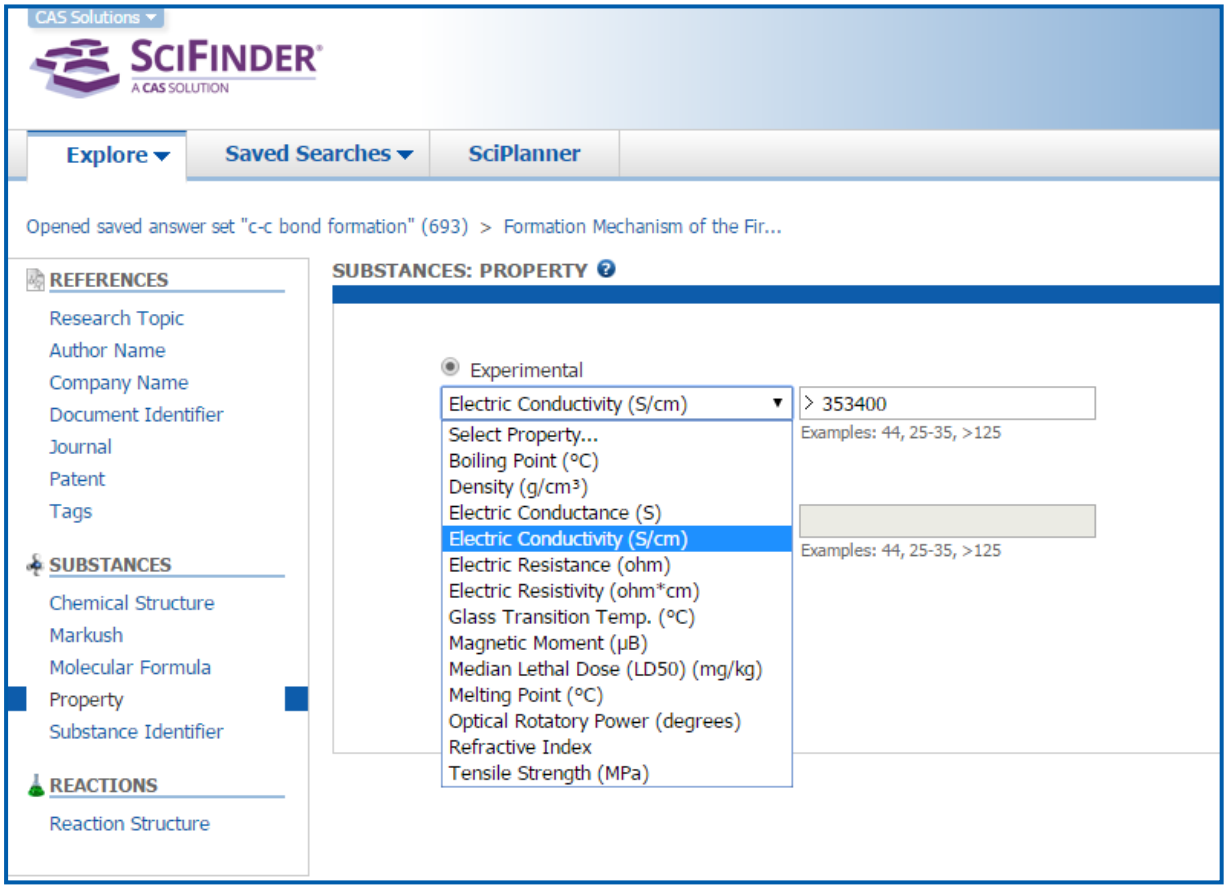
用途

SciFinder® A CAS SOLUTION



SciFinder® A CAS SOLUTION

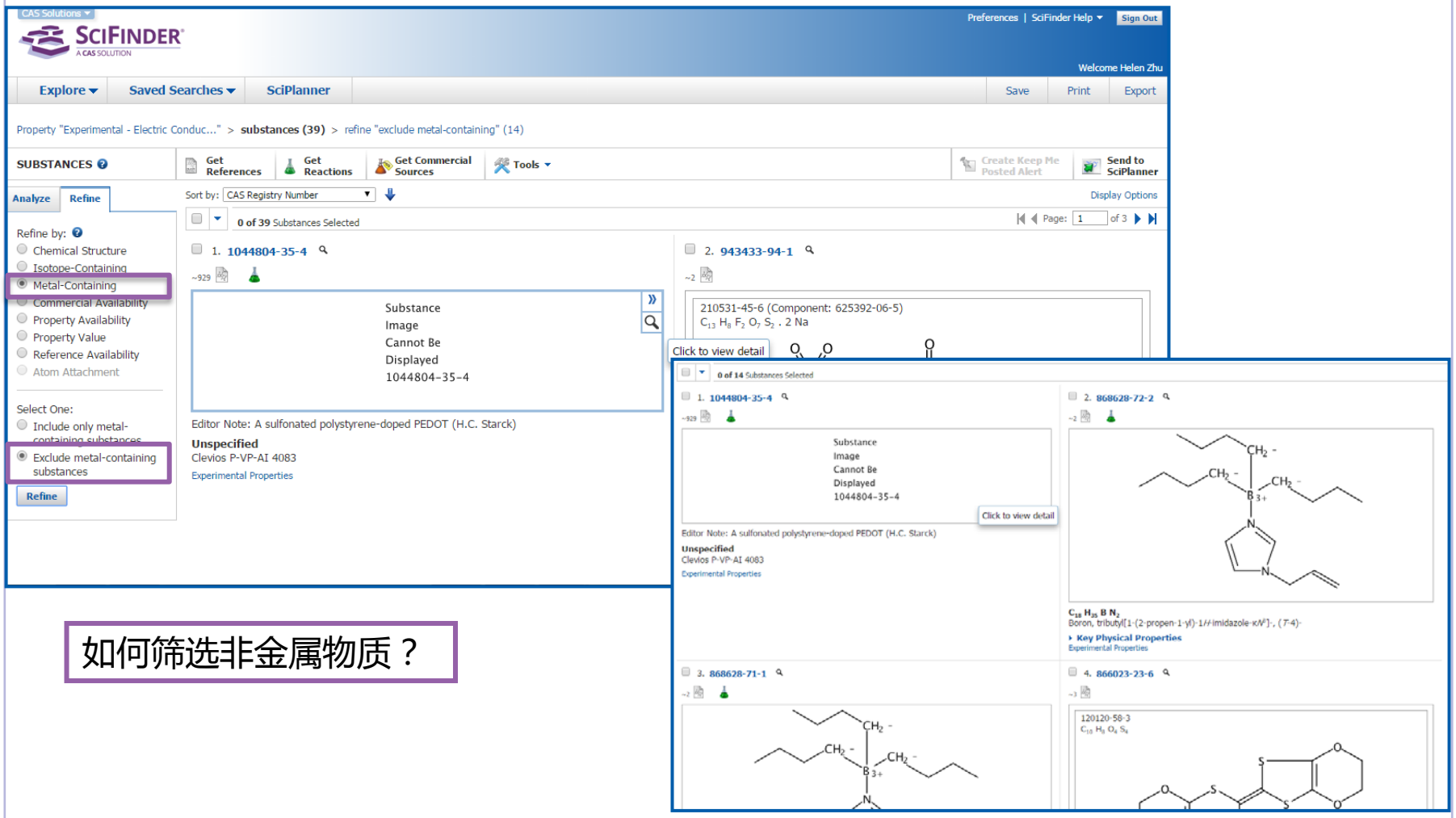
物质检索——Property explore



寻找导电率比铜的60%大的非金属材料

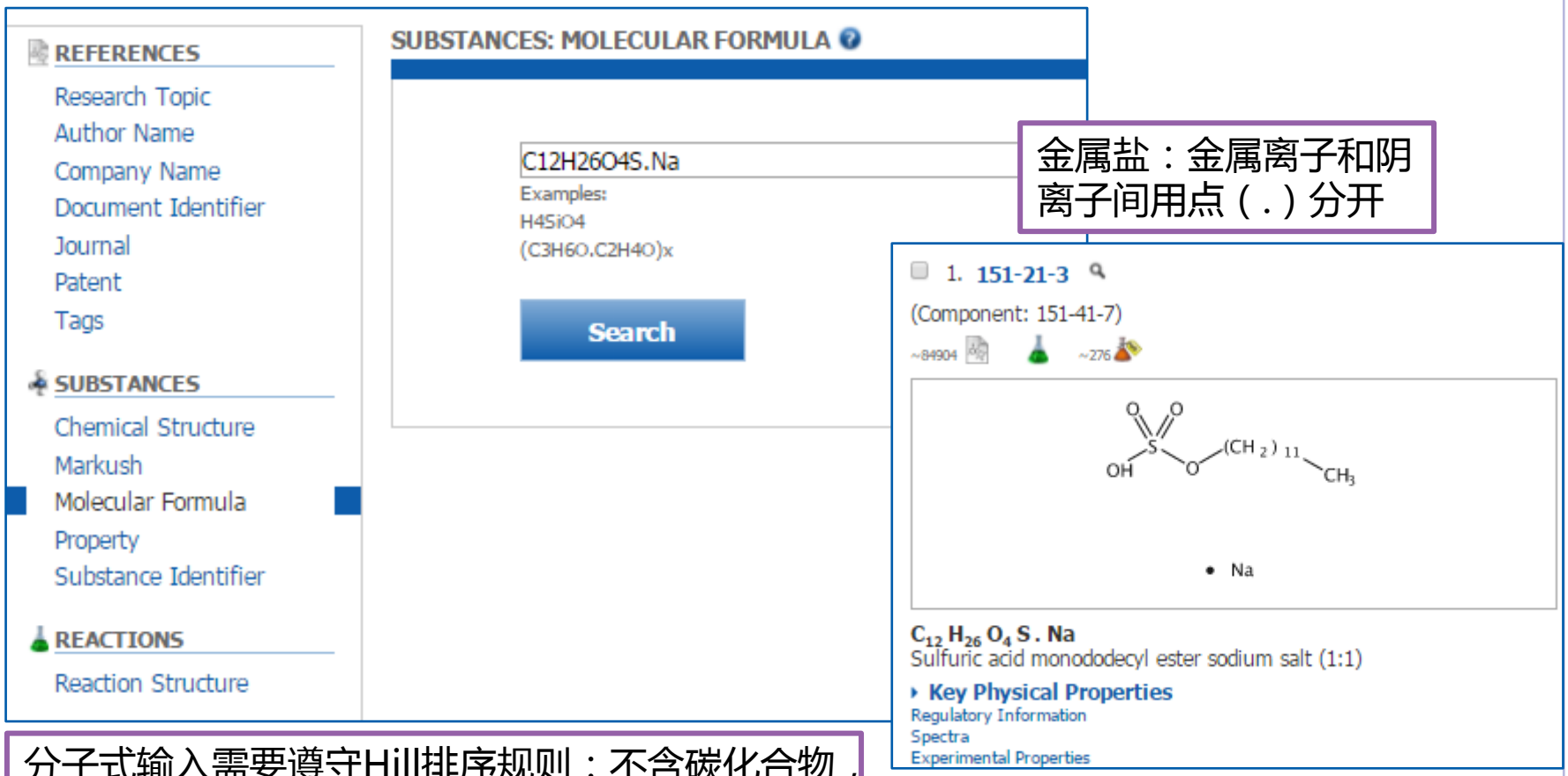
SciFinder
A CAS SOLUTION

物质结果集的筛选——Refine



如何筛选非金属物质？

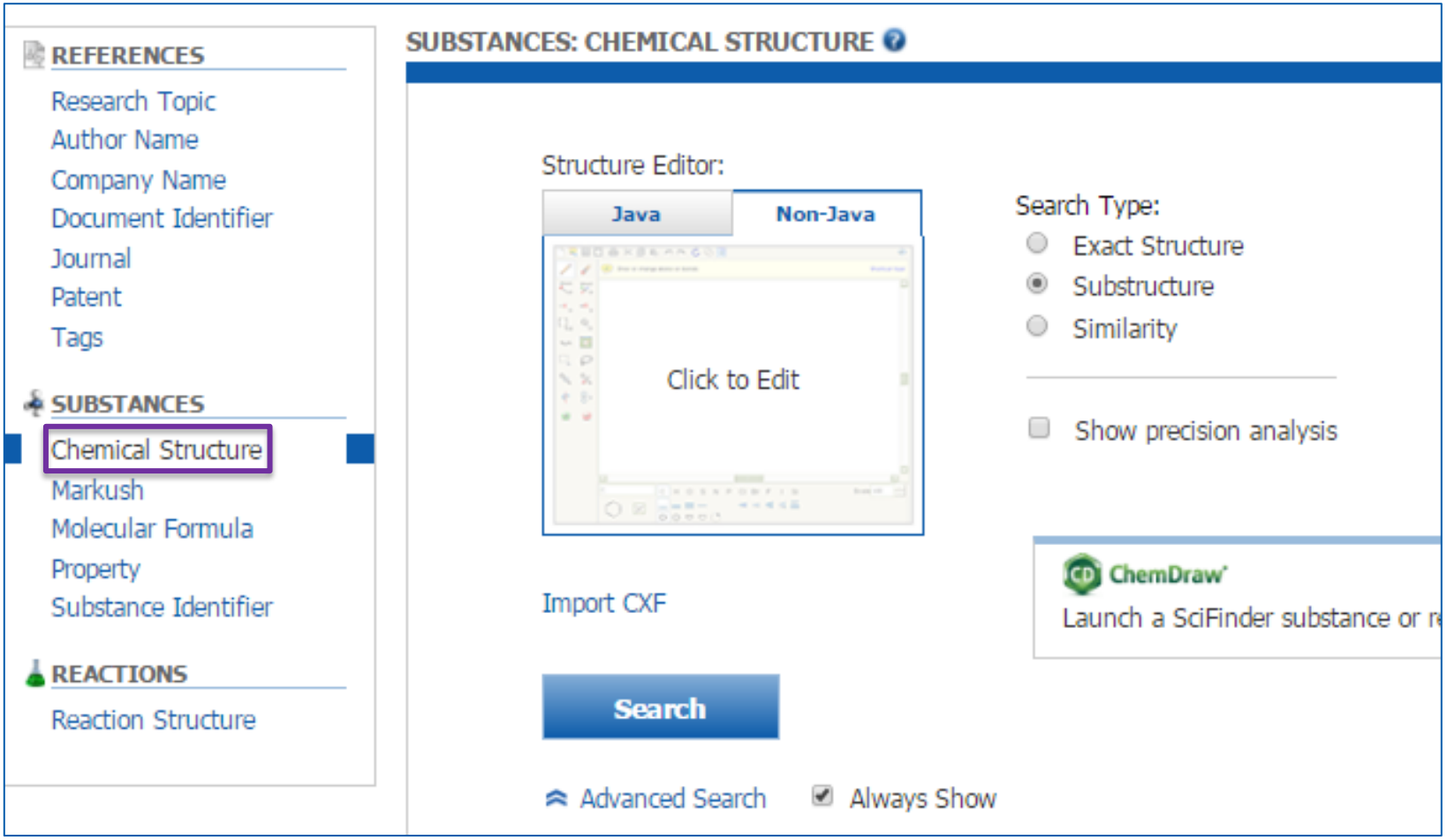
物质检索——分子式



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

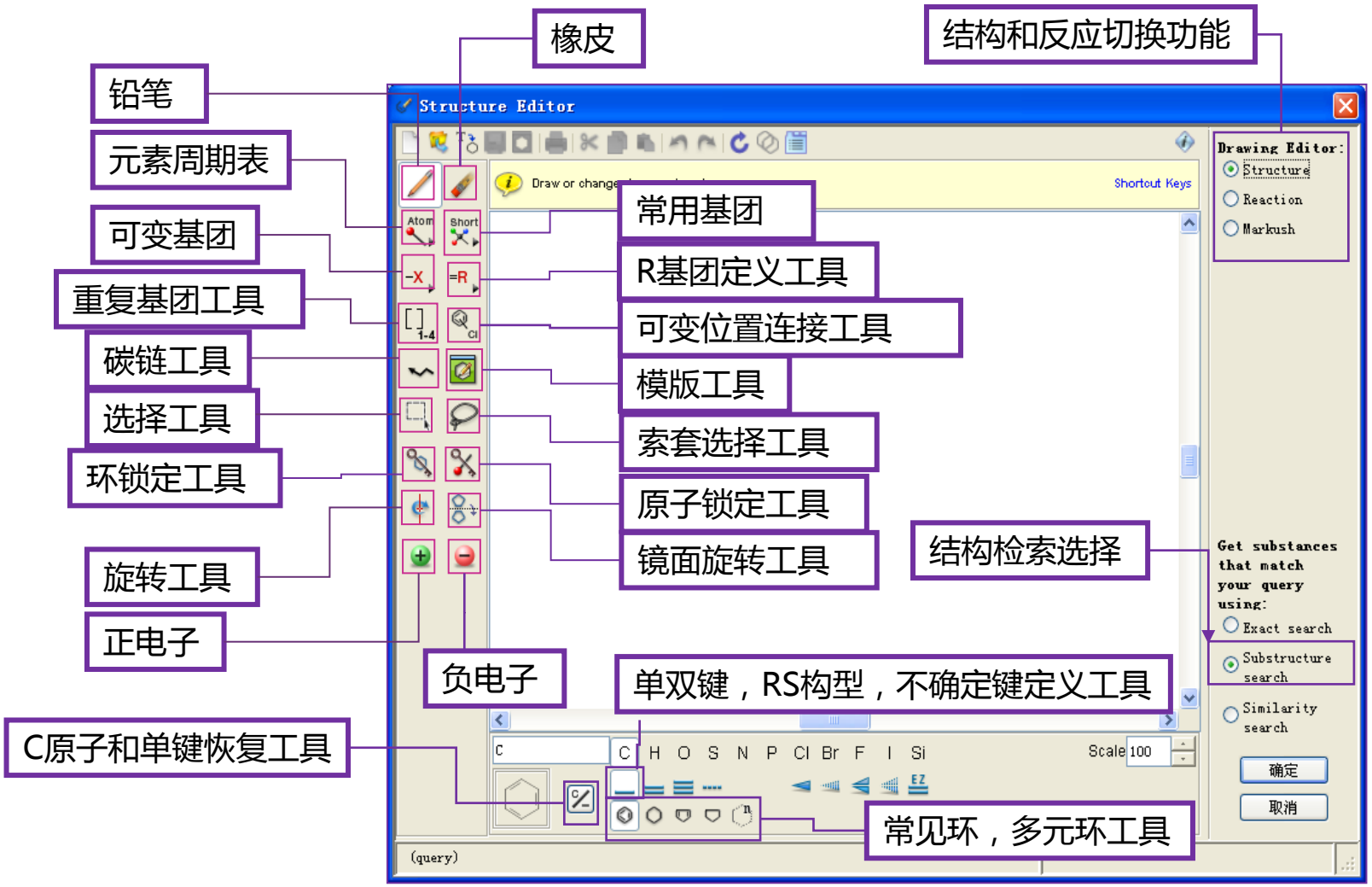
SciFinder® A CAS SOLUTION

物质检索——结构

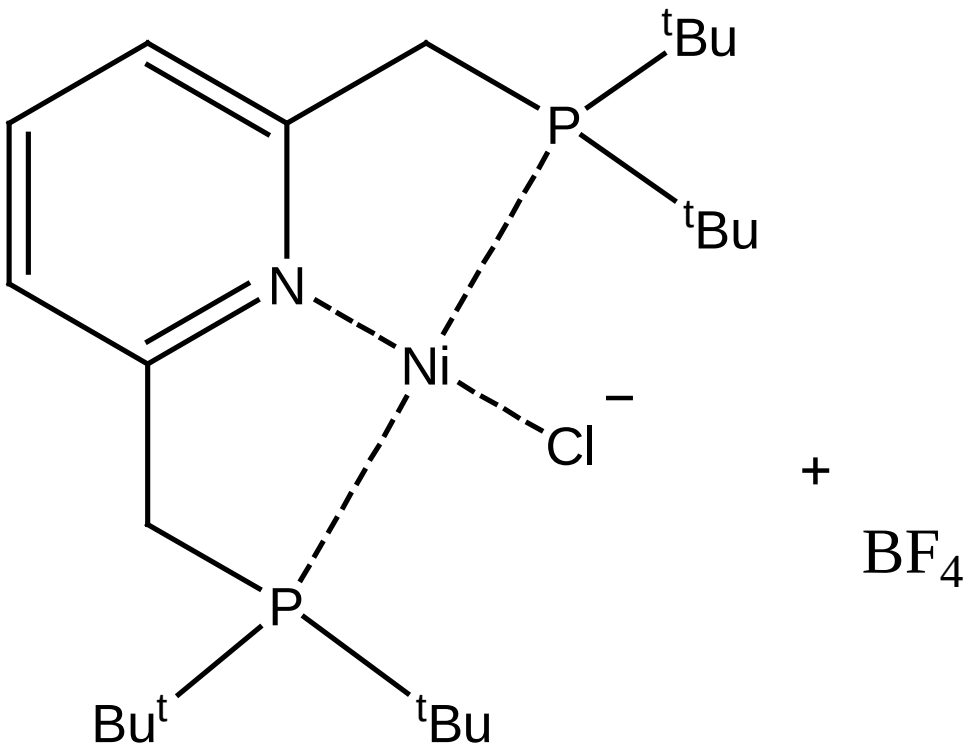


SciFinder® A CAS SOLUTION

物质检索——结构


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
C原子和单键恢复工具
负电子
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
单双键，RS构型，不确定键定义工具
常见环，多元环工具
Structure Editor
Drawing Editor:
Structure
Reaction
Markush
Shortcut Keys
Get substances that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
(query)

物质检索——精确结构检索

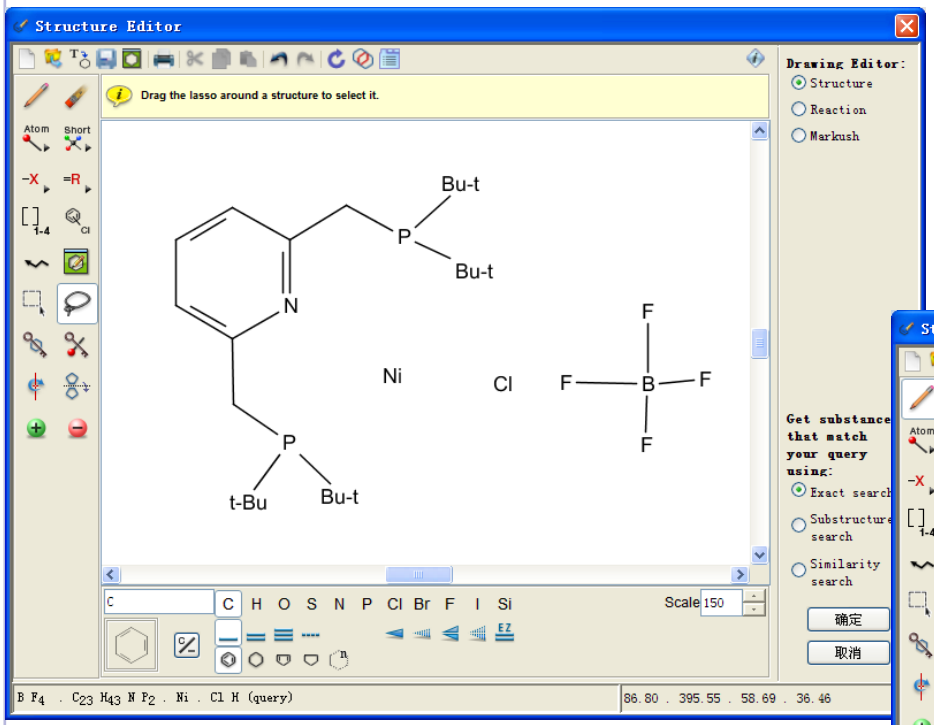


+ BF_4

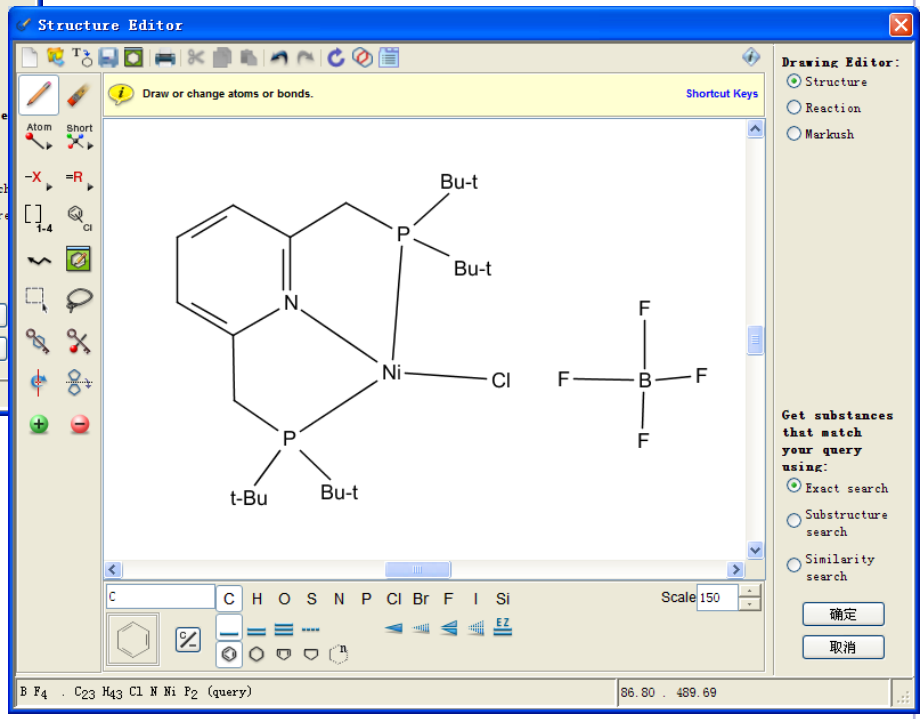
该结构中包含：

配体
金属
阳离子
阴离子

物质检索——精确结构检索



任何一种结构,使用精确结构都可以检索到

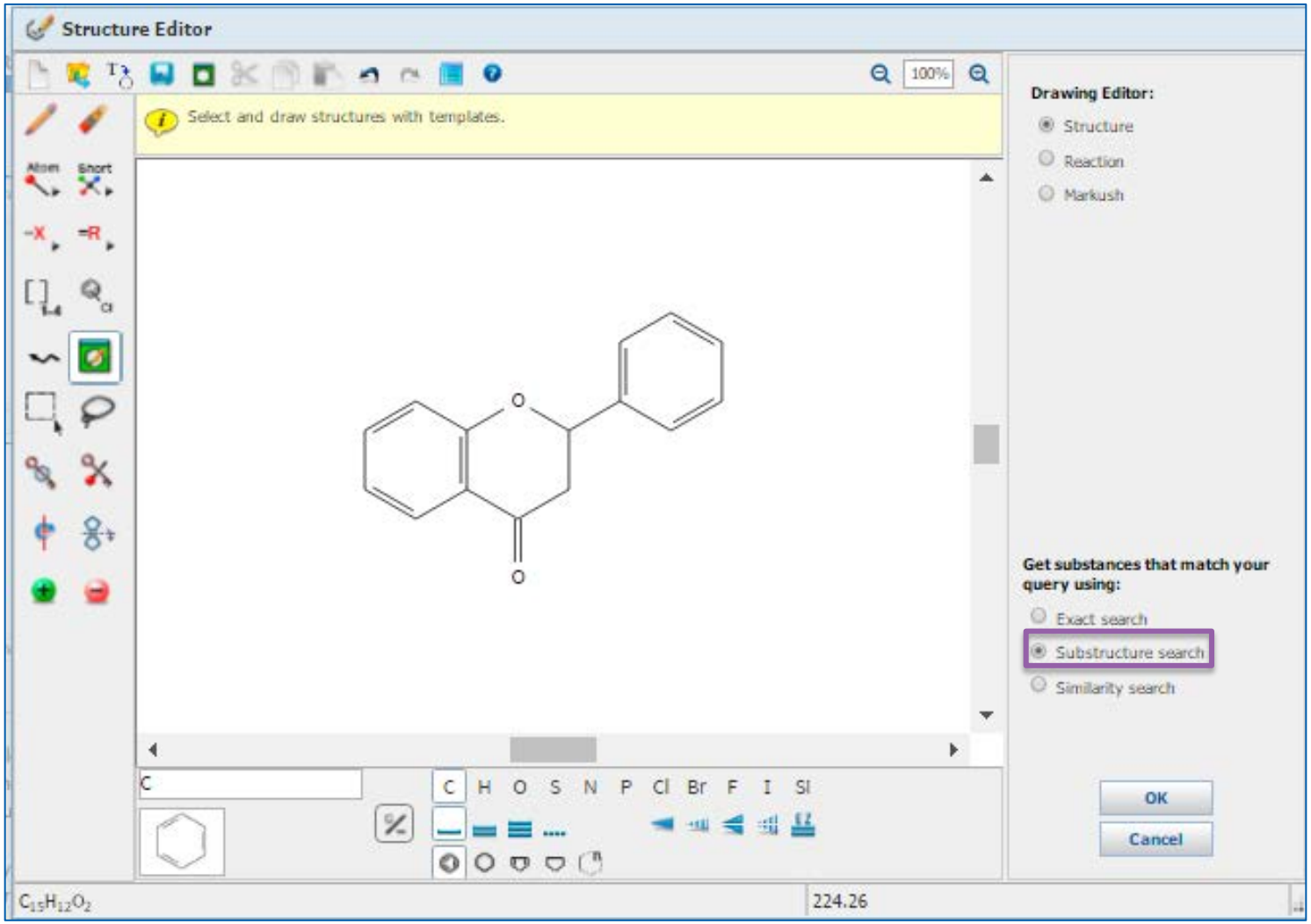


物质检索——精确结构检索

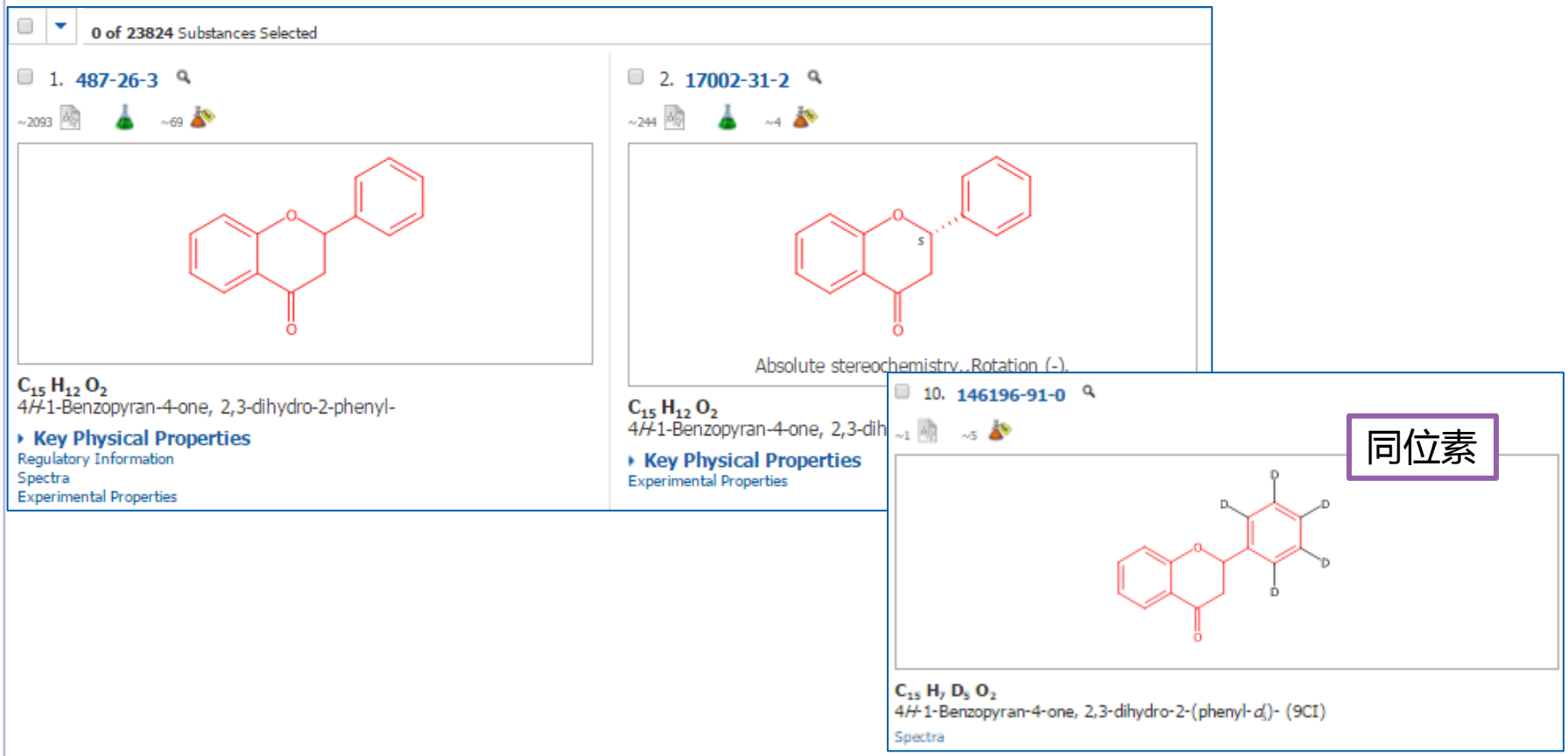
- 精确结构检索：

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


Structure Editor
100%
Select and draw structures with templates.
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search
OK
Cancel
C H O S N P Cl Br F I Si
$C_{15}H_{12}O_2$
224.26

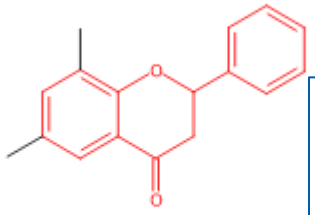
物质检索——亚结构检索


0 of 23824 Substances Selected
1. 487-26-3
~2093
~69
C15 H12 O2
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-
Key Physical Properties
Regulatory Information
Spectra
Experimental Properties
2. 17002-31-2
~244
~4
Absolute stereochemistry. Rotation (-).
C15 H12 O2
4H-1-Benzopyran-4-one, 2,3-dih
Key Physical Properties
Experimental Properties
10. 146196-91-0
~1
~5
同位素
C15 H7 D5 O2
4H-1-Benzopyran-4-one, 2,3-dihydro-2-(phenyl-d5)- (9CI)
Spectra

亚结构检索结果

281. 123251-10-5

取代物



$C_{17}H_{16}O_2$

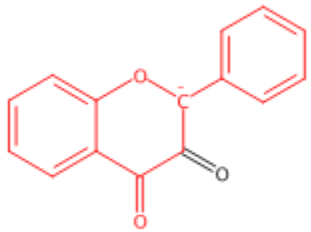
4*H*-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl

Key Physical Properties

Experimental Properties

295. 780723-19-5

离子

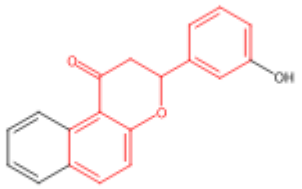


$C_{15}H_9O_3$

2*H*-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

284. 136116-23-9

稠环物质



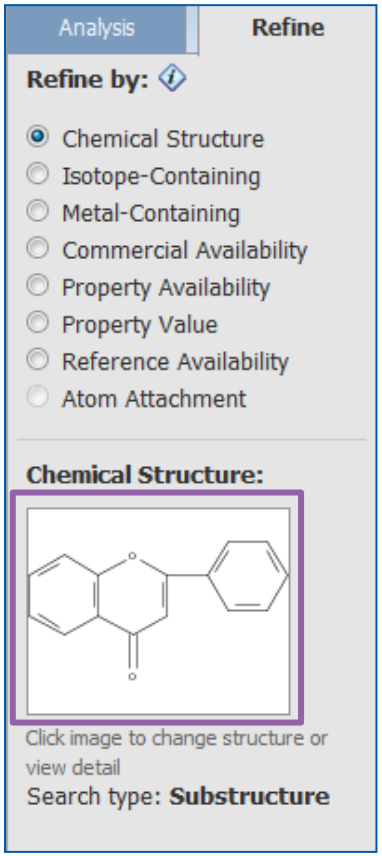
$C_{19}H_{14}O_3$

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

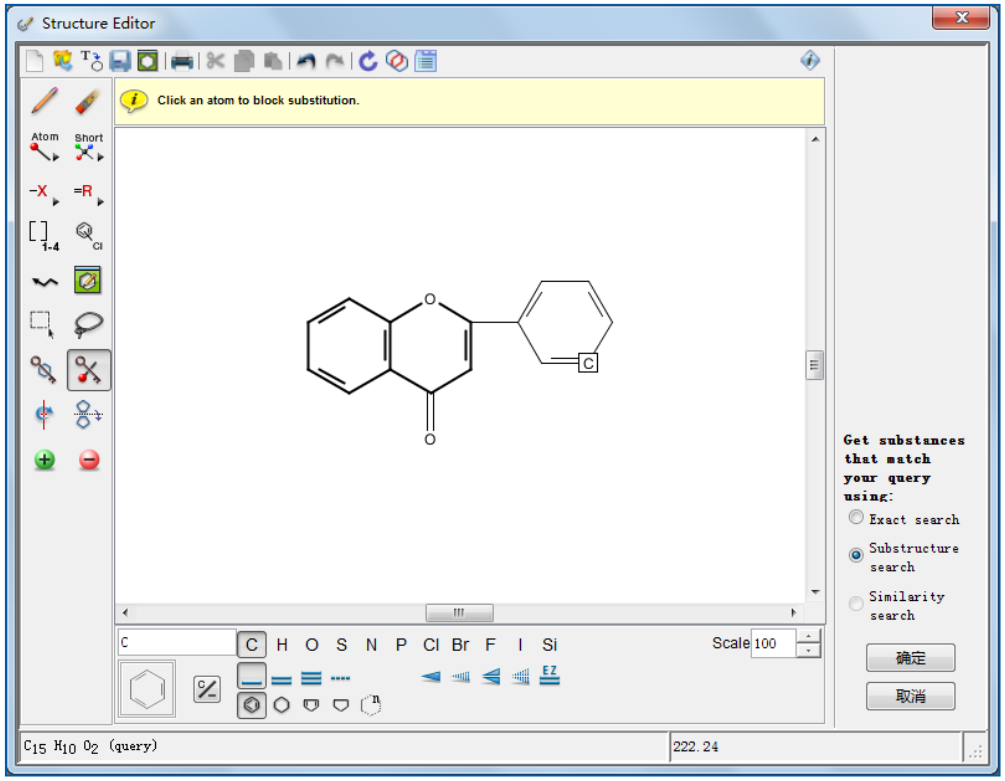
Key Physical Properties

SciFinder® A CAS SOLUTION

亚结构检索结果的限定



化学结构的再次限定



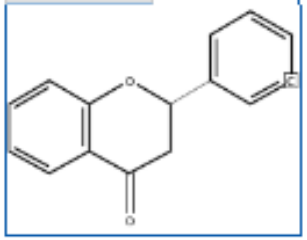
环锁定

原子锁定

亚结构检索结果的限定

Structure Editor:

Java | Non-Java



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

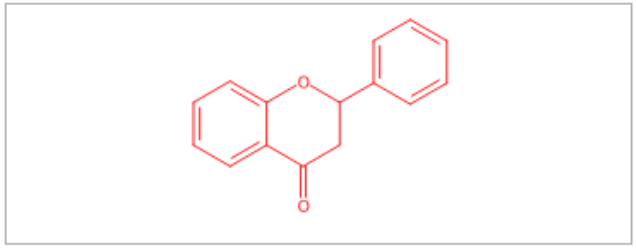
Get References | Get Reactions | Get Commercial Sources | Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. **487-26-3**

~2093 ~69

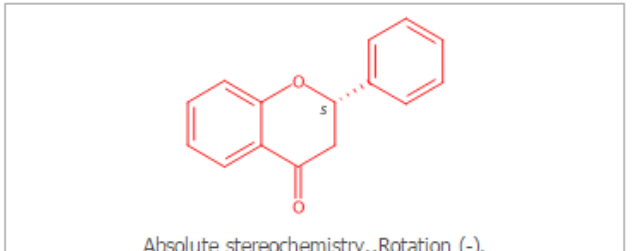


$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

▸ **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

2. **17002-31-2**

~244 ~4



Absolute stereochemistry.,Rotation (-).

$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*S*)-

▸ **Key Physical Properties**
Experimental Properties

4. **104550-32-5**

~3

5. **75524-43-5**

~2

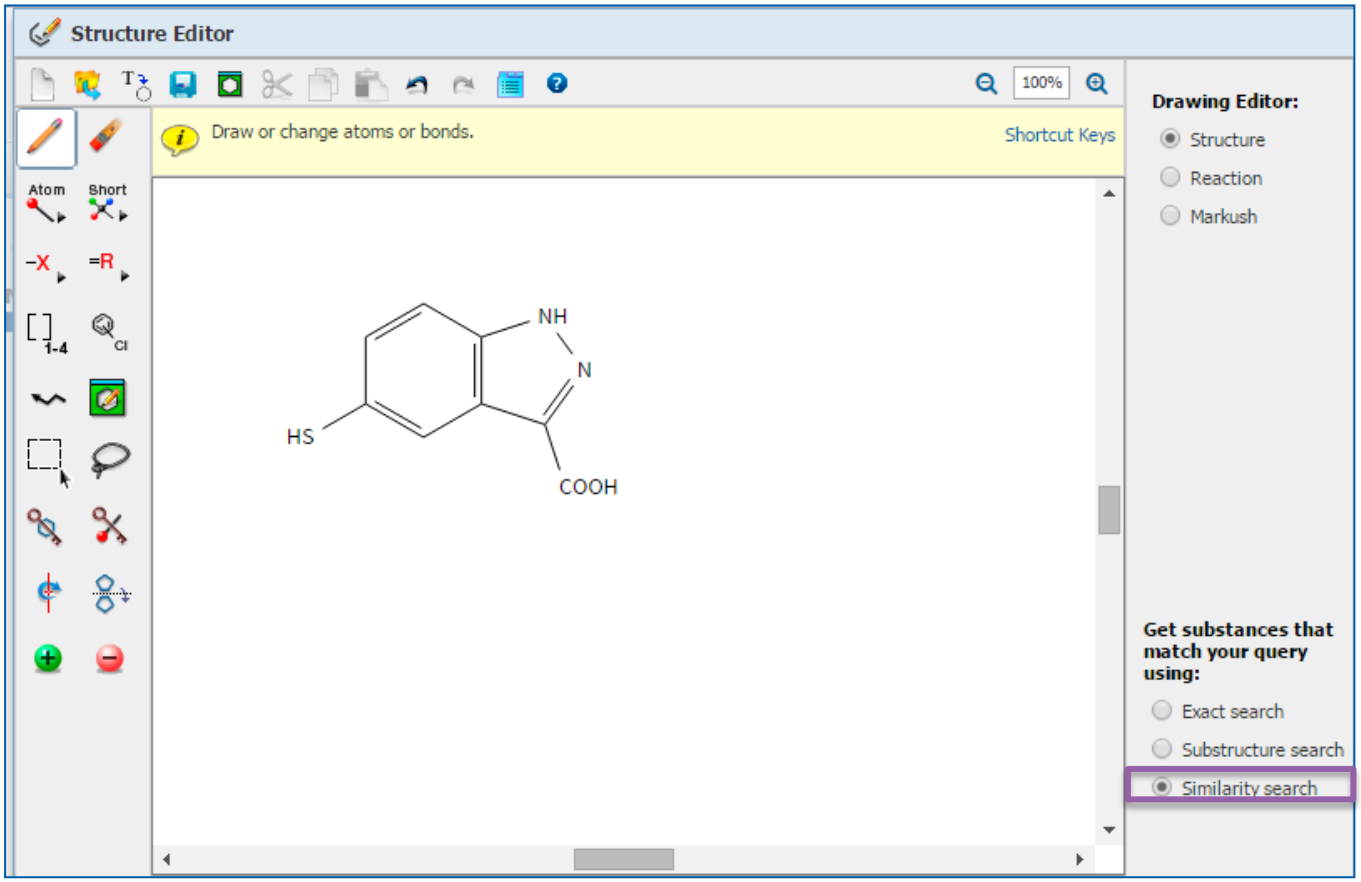
SciFinder® A CAS SOLUTION

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


Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Atom
Short
NH
N
HS
COOH
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search

相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected	Substances
≥ 99 (most similar)	0
95-98	0
90-94	0
85-89	11
80-84	34
75-79	84
70-74	267
65-69	696
0-64 (least similar)	1818

Get Substances

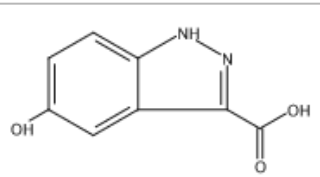
评分越高，相似度越高，结构越相似

Score: 88

1. **885518-94-5**

~1 ~35

取代基变化



$C_8H_6N_2O_3$

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

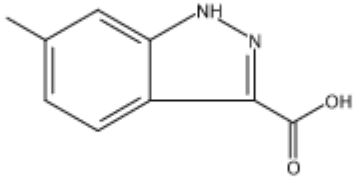
Key Physical Properties

Score: 86

5. **858227-12-0**

~7 ~41

取代基位置变化



$C_9H_8N_2O_2$

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

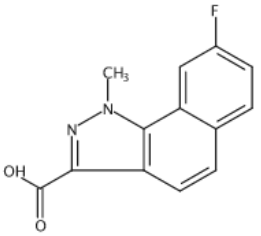
Key Physical Properties

Score: 65

541. **1100422-**

~1

母体结构变化



$C_{13}H_9FN_2O_2$

1*H*-Benz[*g*]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

Key Physical Properties

SciFinder® A CAS SOLUTION

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

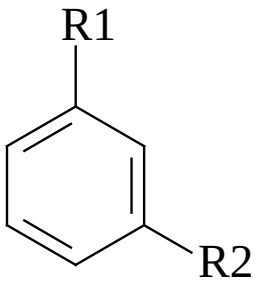
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

Markush检索

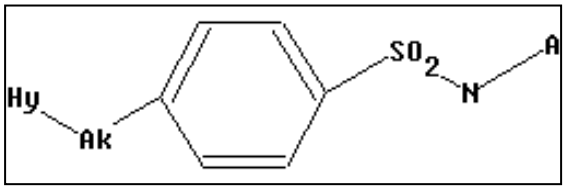
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 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，不会被分配CAS RN
  — Markush检索，能检索到通过结构检索检不到的专利

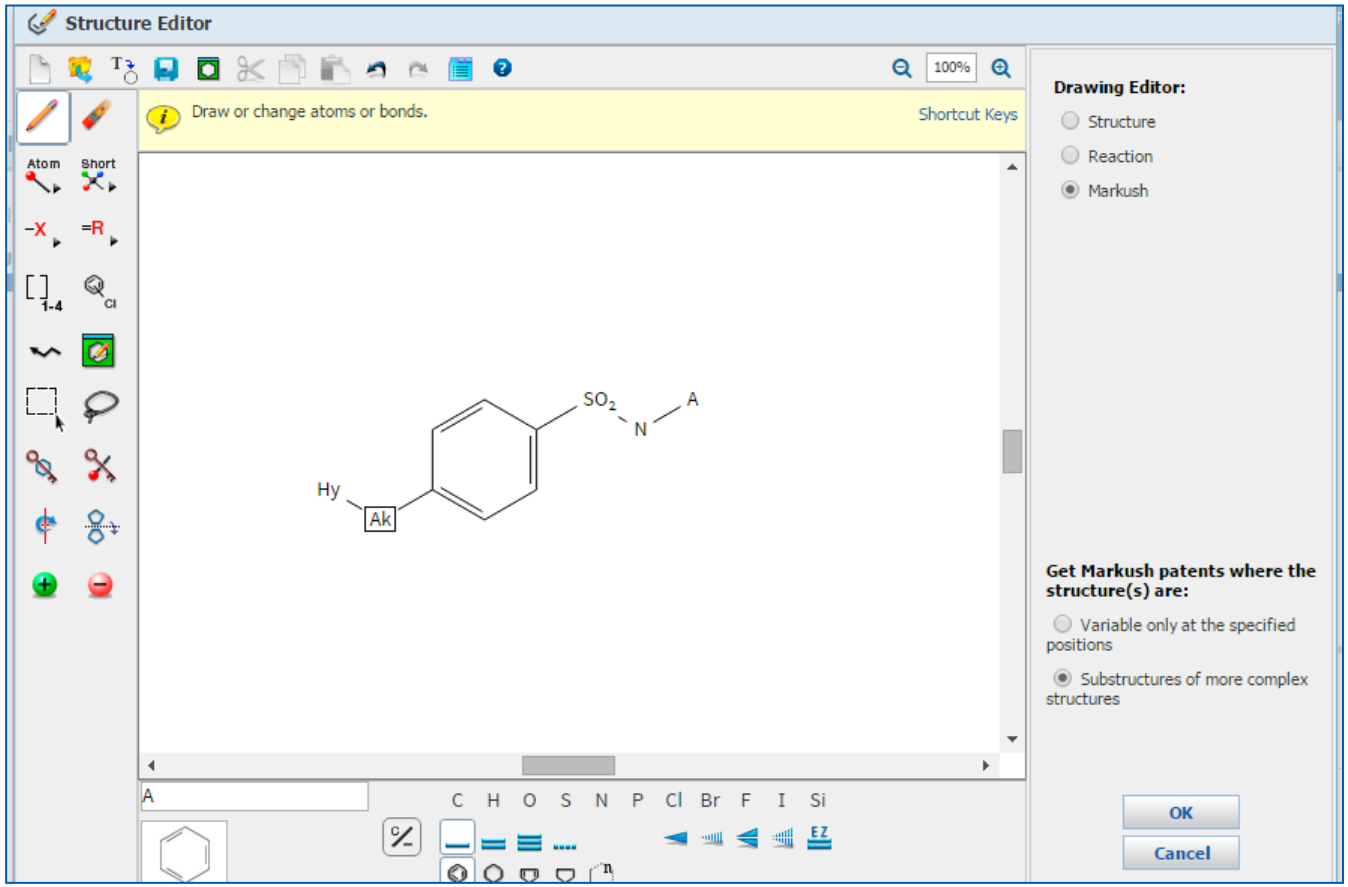


R1 = H, Br, Cl, I

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。



Markush检索

SciFinder A CAS SOLUTION

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Markush substructure > **references (1969)** > Compounds and methods for anti...

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Patent 1969

Journal 1

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0 of 1969 References Selected Page: 1 of 99

1. **Compounds and methods for anticoagulation therapy**

Quick View PATENTPAK ▾

By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen

From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

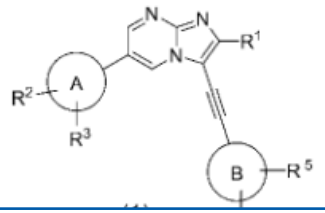
The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

2. **Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)**

Quick View PATENTPAK ▾

By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji

From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS



The title imidazo[1,2-a]pyrimidine derivs. I [R^1 = H or halogen; ring A Ph or pyridyl; R^2, R^3 (same or different) = hydrogen, halogen, C_{1-4} alkyl or C_{1-4} alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R^2 and R^3 are at the adjacent substitution position, R^2 and R^3 together with ring A form C_{5-8} carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R^4, R^5 (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^aR^b, SO_3H, $SO_2NR^aR^b$, SO_2R^b, or $NR^aSO_2R^b$; R^a, R^b (same...

全部是专利

SciFinder A CAS SOLUTION

提纲

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  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

SciFinder检索选项——反应检索

- 反应检索方法

  结构式

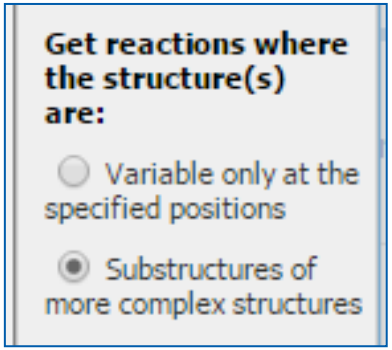
- 常用获取方法

  已知物质：由物质获取反应

  已知文献：从文献中获取反应

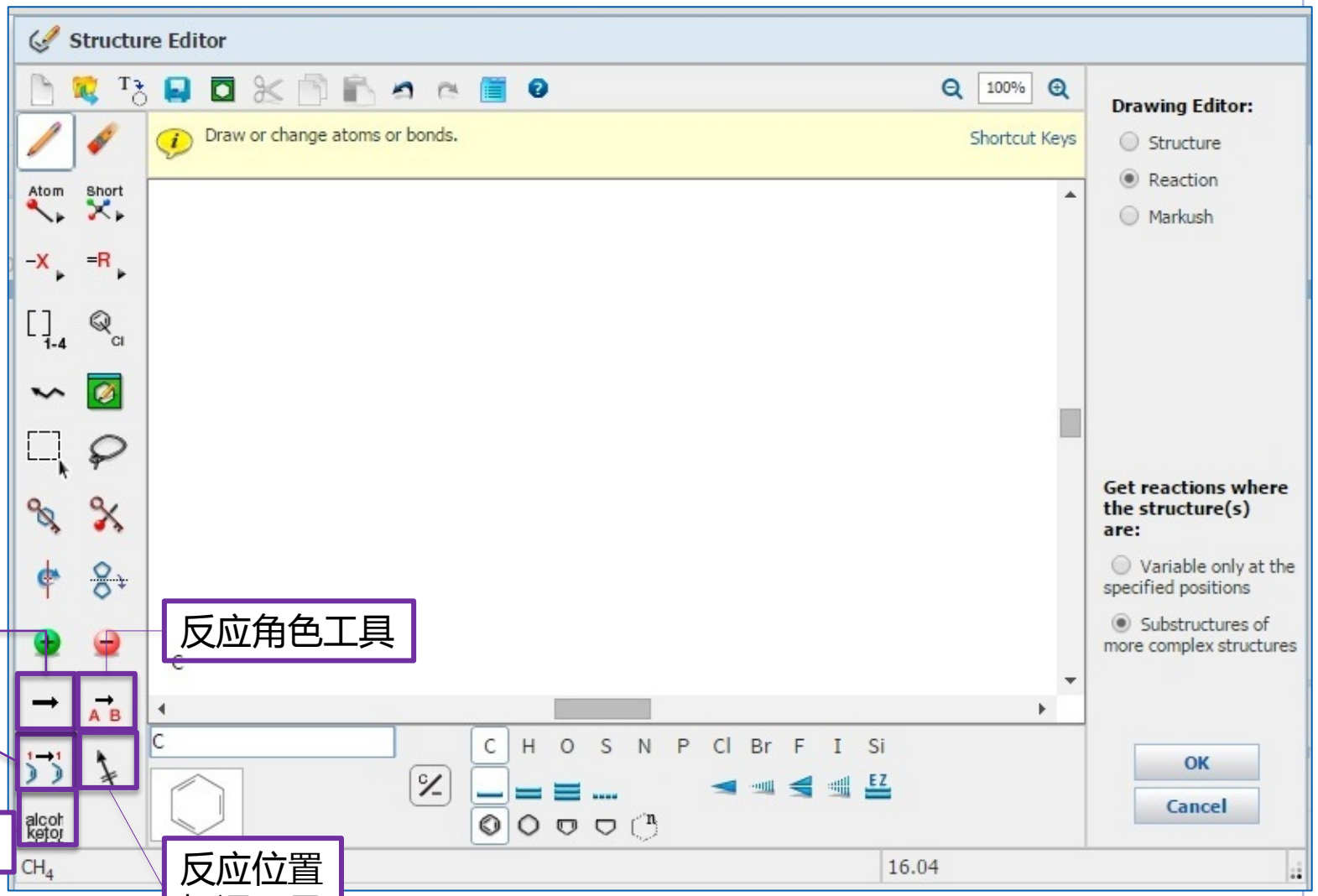
  精确结构反应检索

  亚结构反应检索



SciFinder® A CAS SOLUTION

反应绘制工具


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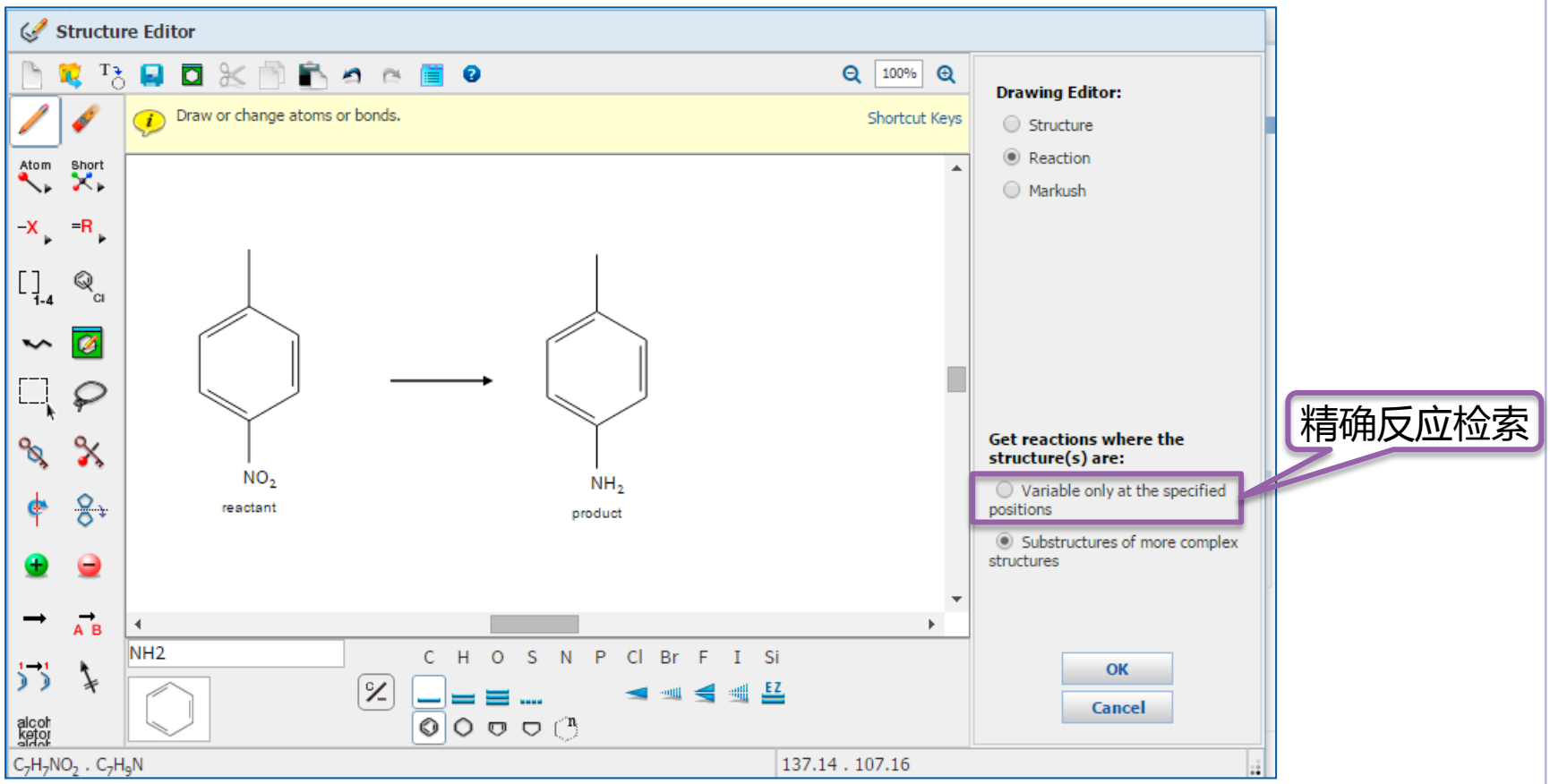
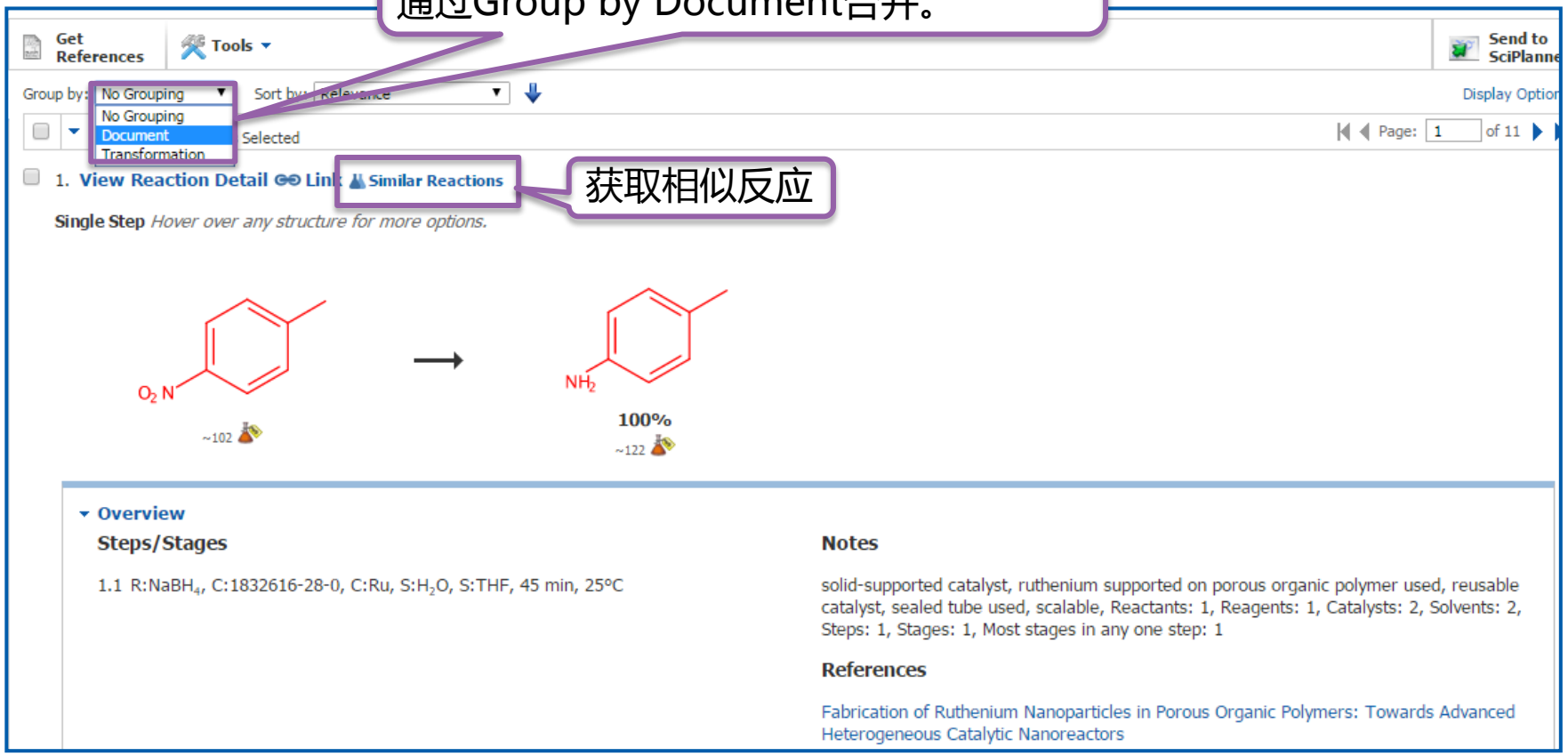
C H O S N P Cl Br F I Si
CH4
16.04
反应箭头
反应角色工具
反应原子标记工具
官能团列表
反应位置标记工具

SciFinder反应检索——精确反应检索



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。



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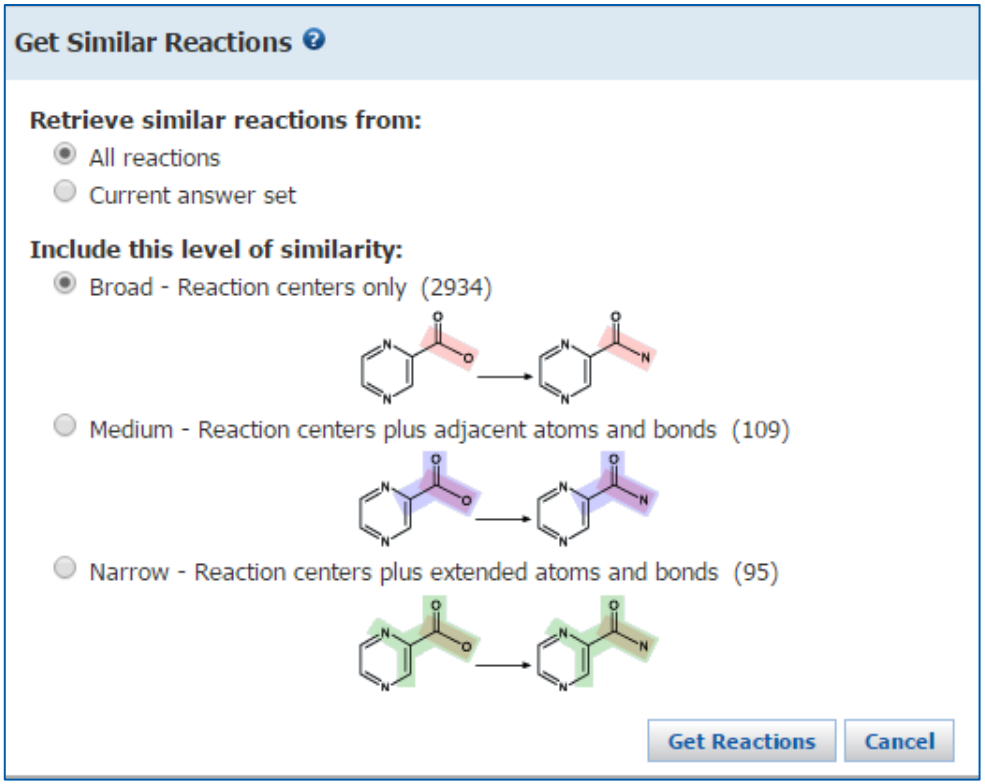
获取相似反应

选择相似反应的相似限制：

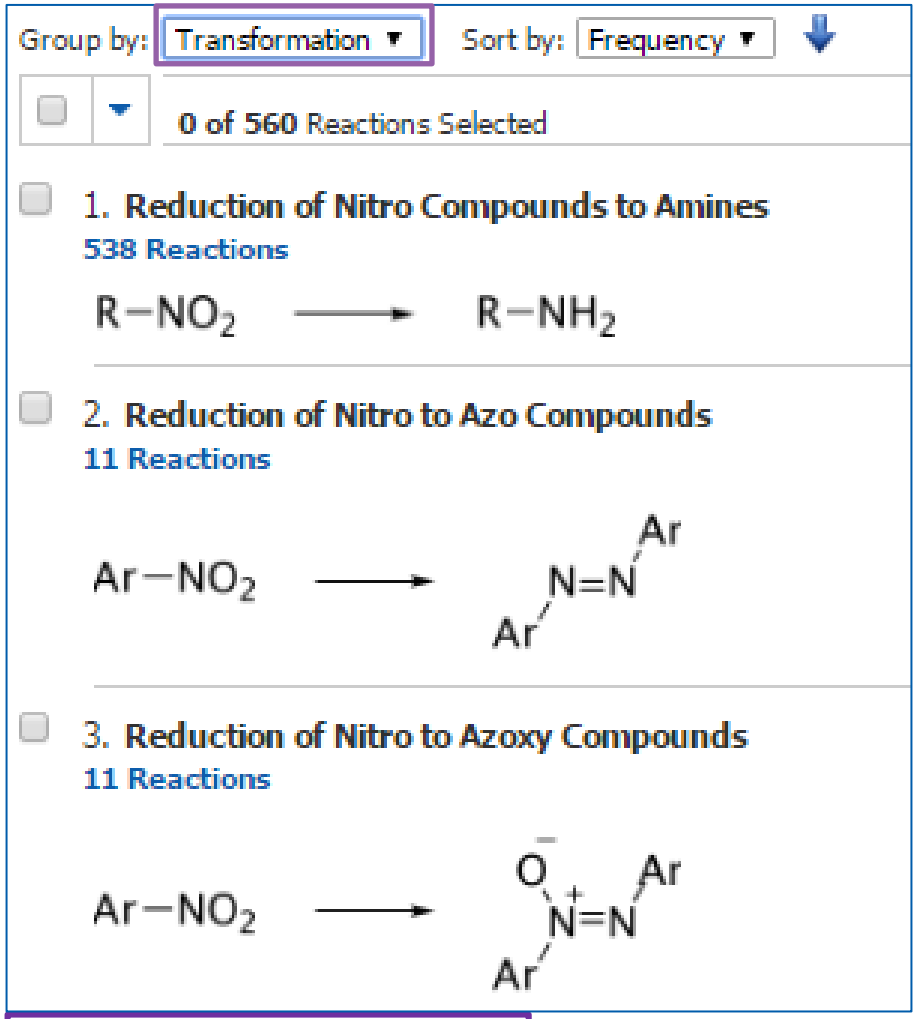
Broad：仅反应中心相似

Miedum：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键



按照反应类型排序

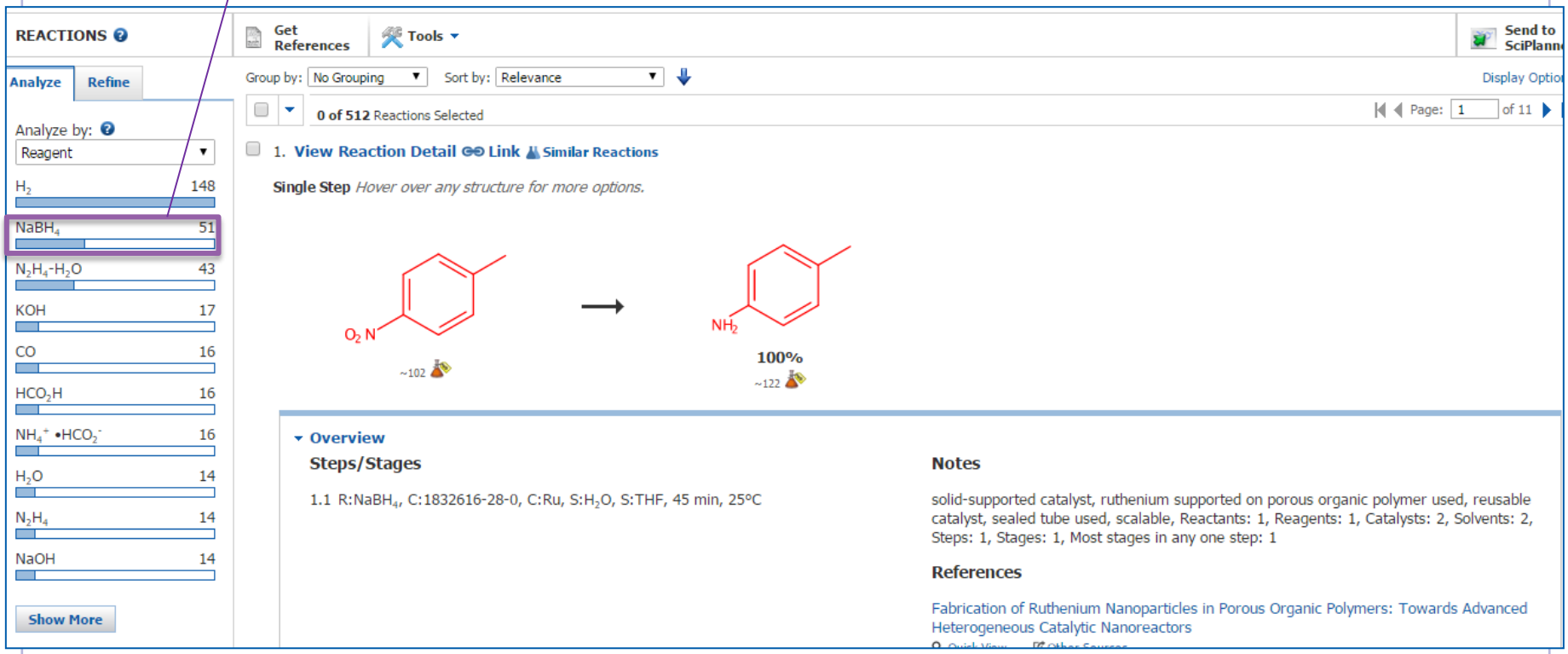


更精确的查找需要的反应

SciFinder® A CAS SOLUTION

反应检索结果的筛选

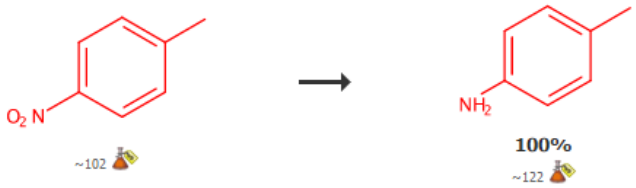
获得特定物质做还原剂的反应



SciFinder® A CAS SOLUTION

SciFinder囊括最大的反应实验过程合集

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



▾ **Overview**

Steps/Stages

1.1 R:H_2, R:Cs_2CO_3, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

Quick View Other Sources

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

▾ **Experimental Procedure**

ACS Catalysis

General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H_2 to a mixture of nitroarene (0.3 mmol), Cs_2CO_3 (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6×10^{-3} mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H_2 in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

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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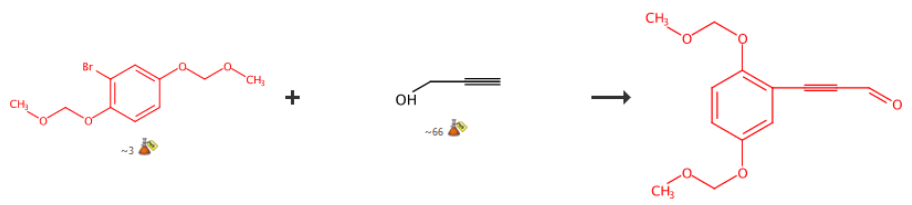
SciFinder囊括最大的反应实验过程合集

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



▾ **Overview**

Steps/Stages

1.1 C:Pd(PPh_3)$_4$, S:BuNH_2, 21 h, 100°C
2.1 R:DMSO, R:Cl(O=)CC(=O)Cl, S:CH_2Cl_2, 15 min, -78°C
2.2 S:CH_2Cl_2, -78°C; 2 h, -78°C
2.3 R:Et_3N, 30 min, -78°C; -78°C → rt
2.4 R:H_2O, R:NH_4Cl, 30 min, rt

Notes

1) key step, alternate catalyst concentration, catalyst (CuI) and tem
yield, Sonogashira coupling, 2) key intermediate, Swern oxidation, s
method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, St
Most stages in any one step: 4

References

Synthesis of Bioactive Speciosins G and P from Hexagonia speciosa
Quick View Other Sources
By Guerrero-Vasquez, Guillermo A. et al
From Journal of Natural Products, 77(9), 2029-2036; 2014

▾ **Experimental Procedure**

JOURNAL OF NATURAL PRODUCTS

Step 1

General Procedure for the Sonogashira Coupling.[8,10,11] Compounds **6a** [31] and **16** [8] were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in n-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in n-butylamine (10 mL) and $Pd(Ph_3)_4$ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured intoH_2O(80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10-50%). *3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol*[F2] (***8***). Yield 96%; colorless oil. IR (KBr) ν_{max} 3310, 2230 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, *J* = 9 and 3.0 Hz, H-5), 7.03 (1H, d, *J* = 9.0 Hz, H-6), 7.10 (1H, d, *J* = 3.0 Hz, H-3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.19 (C-2), 117.13 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1); HRESIMS *m/z* 275.0900 [M + Na]$^+$ (calcd for $C_{13}H_{16}O_5$ 275.0896).

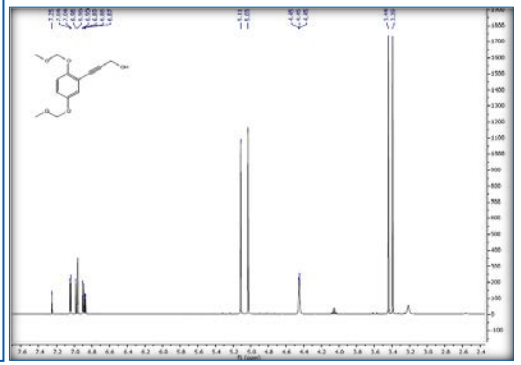
Step 2

Generation of the Key Aldehyde.[17] Oxalyl chloride (272.3 μL, 3.12 mmol) in dry CH_2Cl_2 (9 mL) was added to a stirred solution of DMSO (332 μL, 4.68 mmol) in dry CH_2Cl_2 (1.5 mL) under an argon atmosphere at -78 °C. The mixture was stirred for 15 min, and the alcohol 8 (393.5 mg, 1.56 mmol) or alcohol **17** (300 mg, 1.56 mmol) in dry CH_2Cl_2 (12 mL) was added dropwise (Note: Swern oxidation could be scaled-up to 1.56 mmol of starting material). After the starting material had been consumed (nearly 2 h), Et_3N (1.88 mL, 7.8 mmol) was added. The reaction mixture was stirred at -78 °C for a further 30 min and was allowed to warm to rt and quenched with saturated NH_4Cl and H_2O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH_2Cl_2 (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and evaporated under reduced pressure. *3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-ynal* (***9***). Yield 91%; colorless oil. IR (KBr) ν_{max} 1660, 2194 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]$^+$ (calcd for $C_{13}H_{14}O_5$ 273.0739).

Experimental Procedure:

我们可以做得更好

- 更好的阅读体验?
- 这些数字代表什么？
- 查免费的Supporting Information？可能只有图谱。



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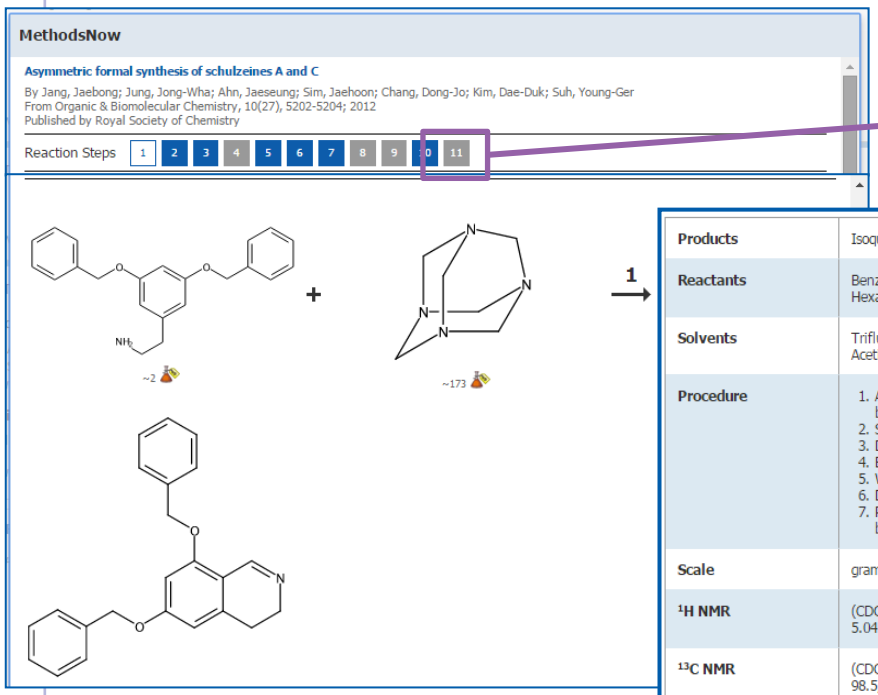
MethodsNow Synthesis



多步反应中，原文没有描述的实验过程以灰色标示

Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethylamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon 2. Stir the mixture for 3hours at 90ÊC. 3. Dilute the reaction mixture with H_2O. 4. Basify with potassium carbonate and extract with CH_2Cl_2. 5. Wash the combined organic layers with brine. 6. Dry over $MgSO_4$ and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
Scale	gram
^{1}H NMR	($CDCl_3$, 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, *J* = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
^{13}C NMR	($CDCl_3$, 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
IR	(thin film, neat) ν_{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm^{-1}
HRMS	(FAB+) calcd for $C_{23}H_{22}NO_2$ (M+H$^+$) 344.1651; found 344.1658
Mass Spec	(FAB+) *m/z* 344 (M+H$^+$)
State	yellow solid
CAS Method Number	3-614-CAS-200055

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物质信息

实验过程

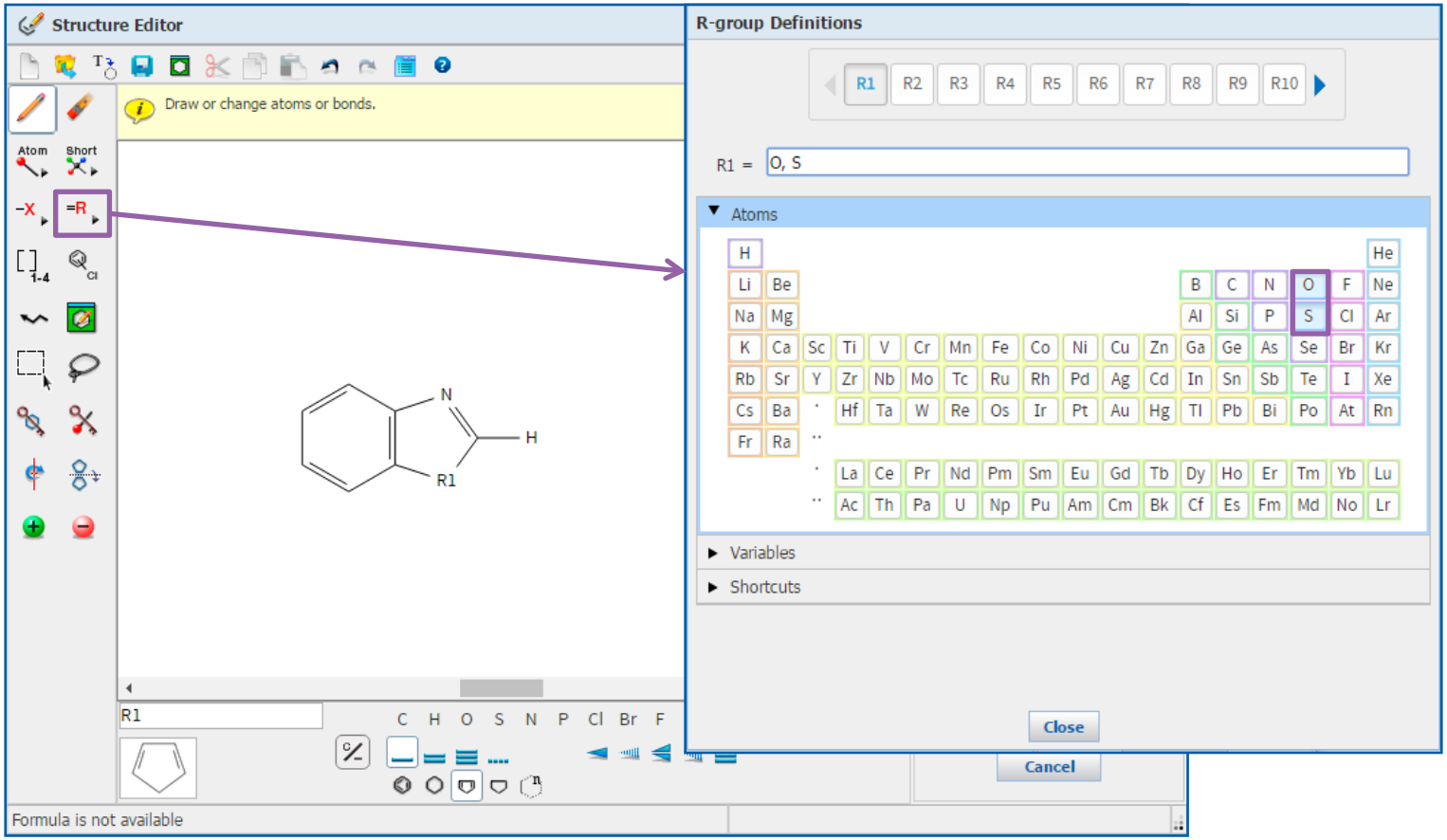
图谱信息

保存/导出方法

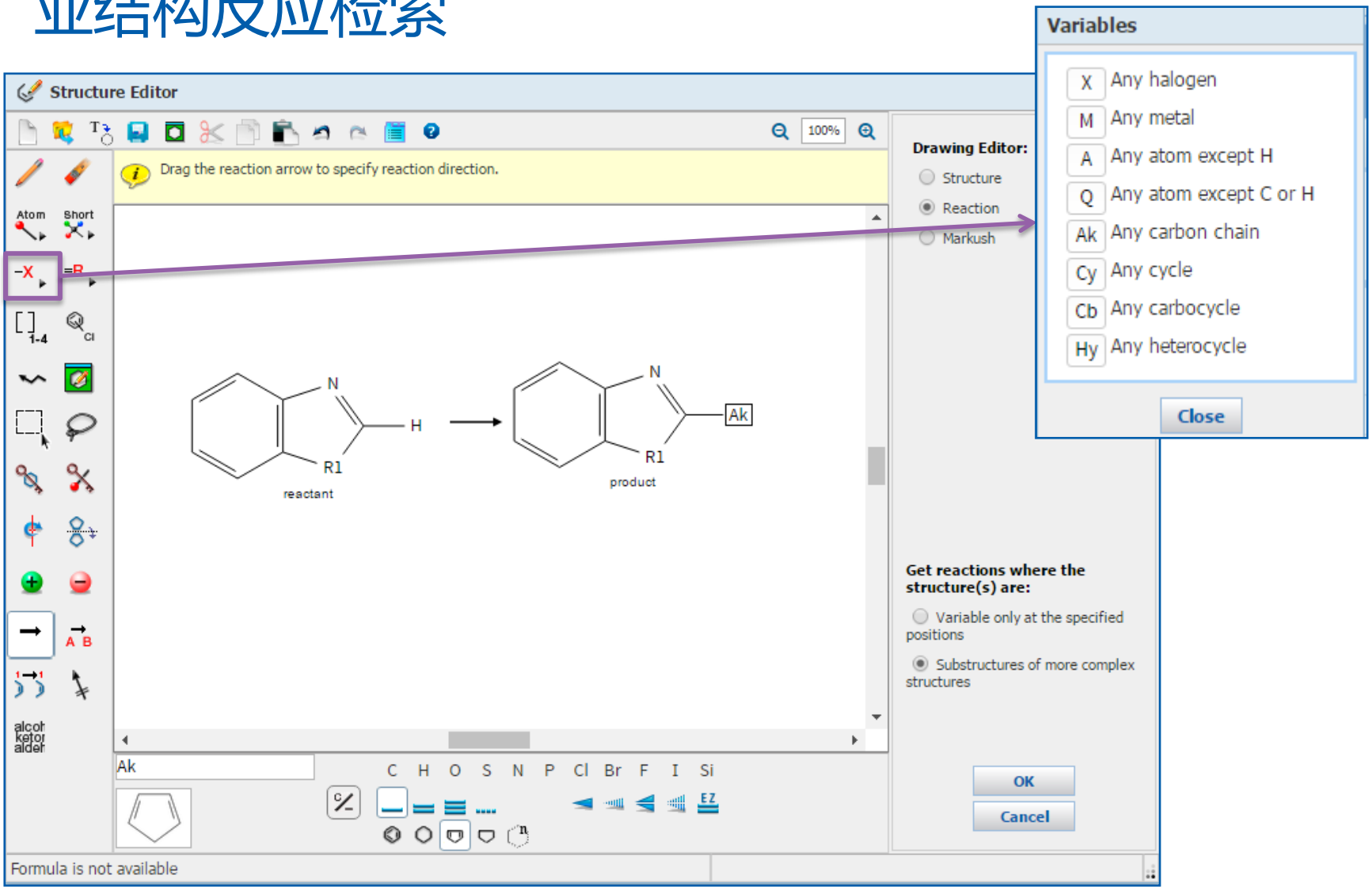
SciFinder® A CAS SOLUTION

亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化

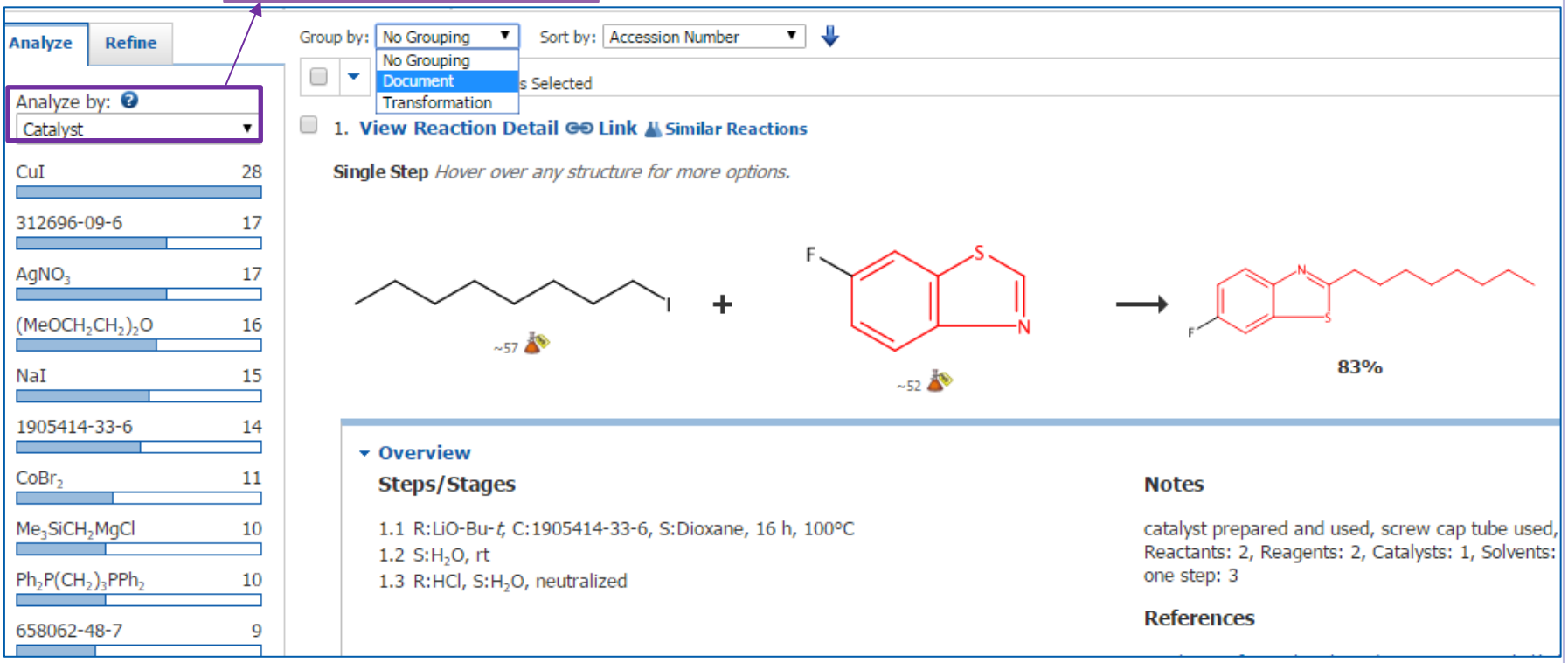


亚结构反应检索


Structure Editor
Drag the reaction arrow to specify reaction direction.
Drawing Editor:
Structure
Reaction
Markush
reactant
product
Ak
Variables
X Any halogen
M Any metal
A Any atom except H
Q Any atom except C or H
Ak Any carbon chain
Cy Any cycle
Cb Any carbocycle
Hy Any heterocycle
Close
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
Formula is not available

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应



SciFinder® A CAS SOLUTION

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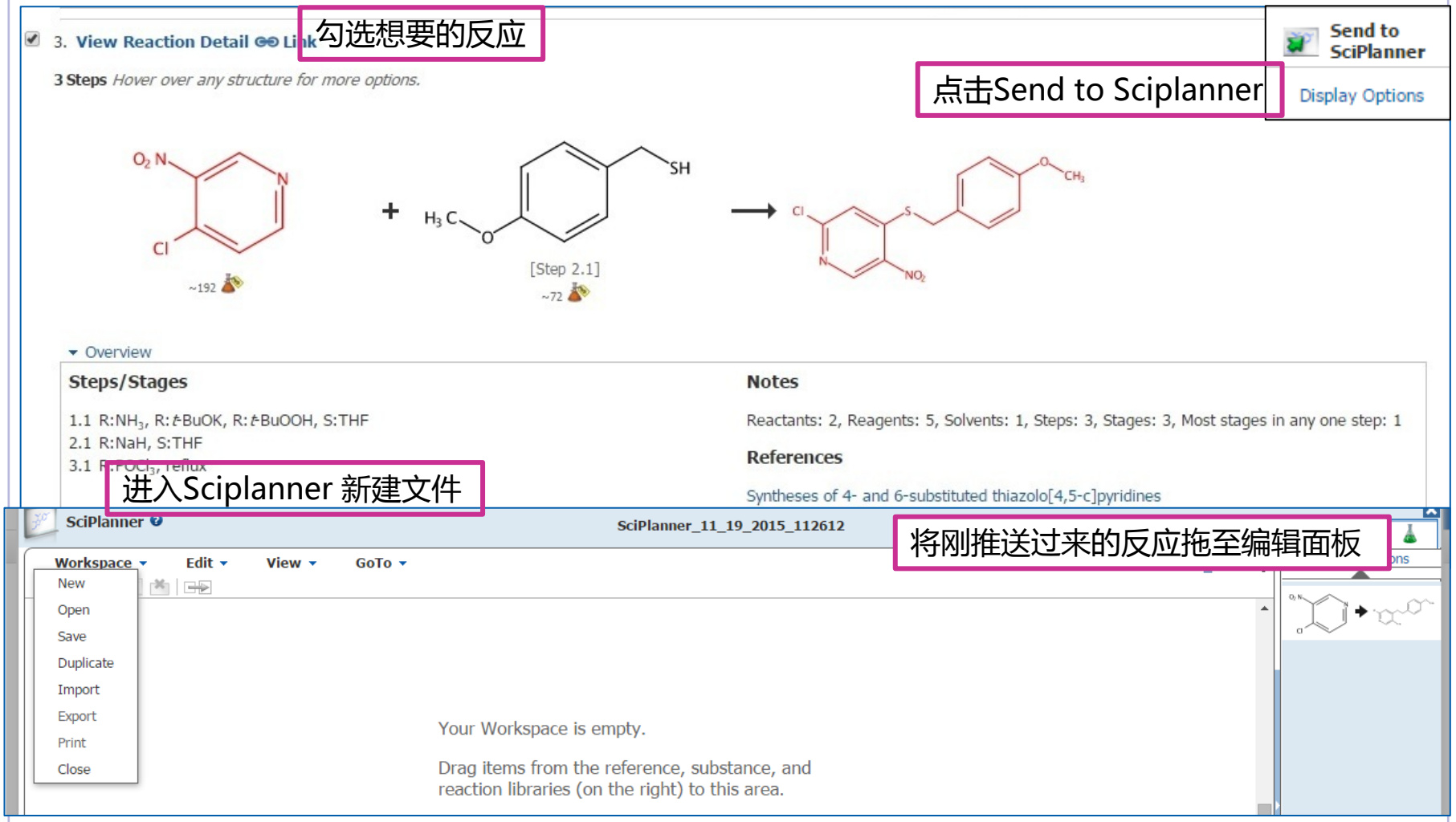
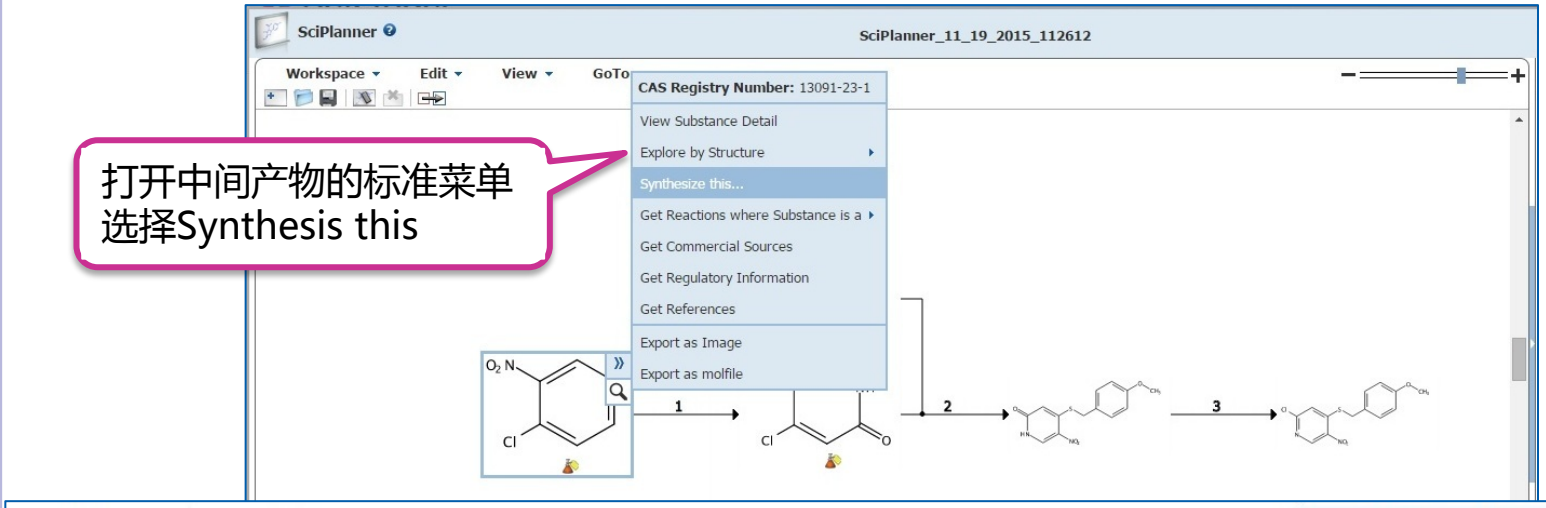
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

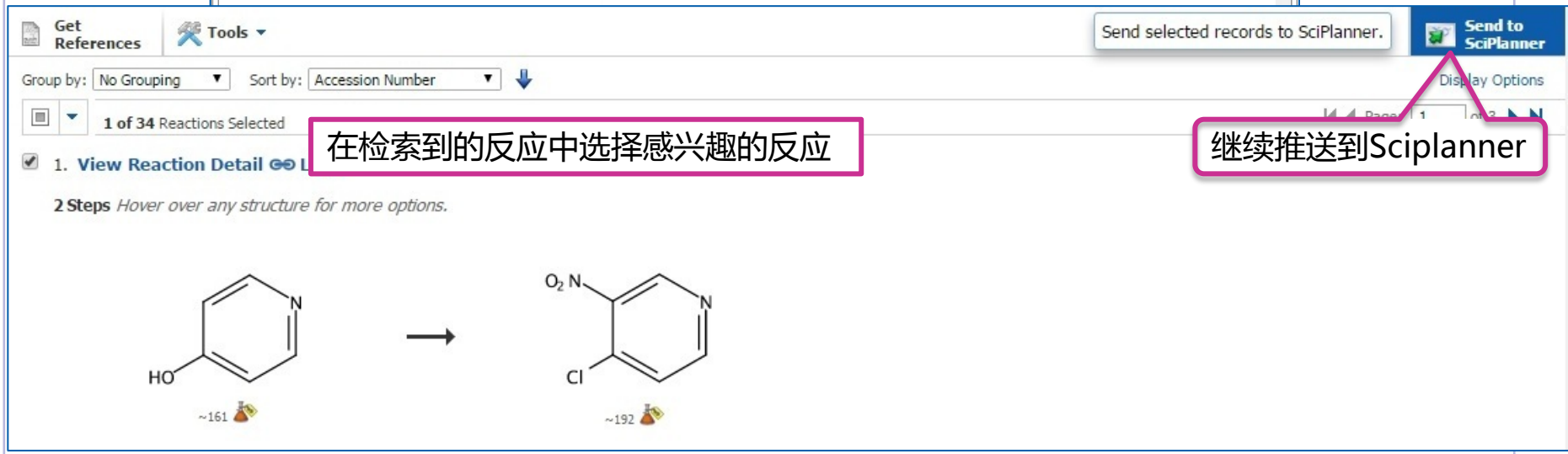
SCIFINDER® A CAS SOLUTION

SciPlanner使用简介

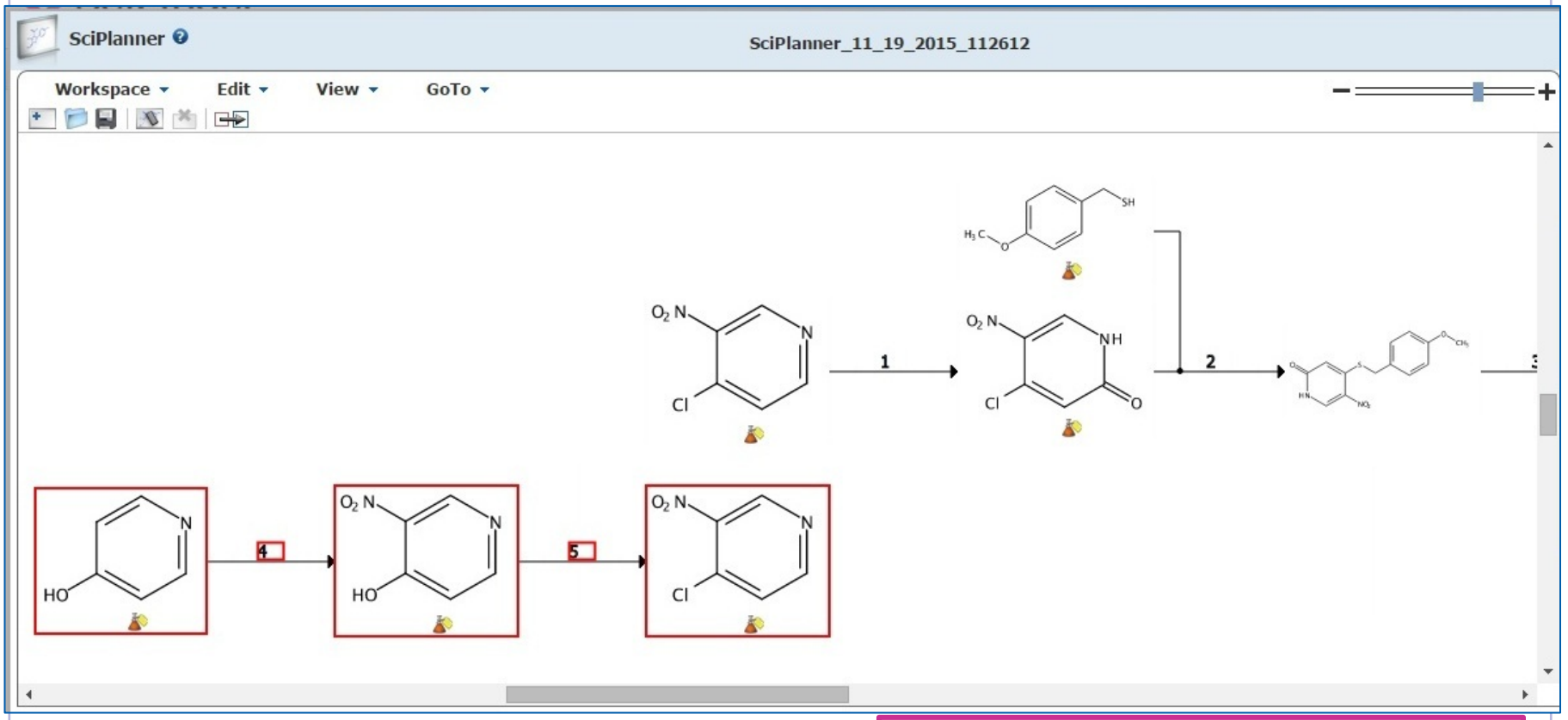


SciPlanner使用简介



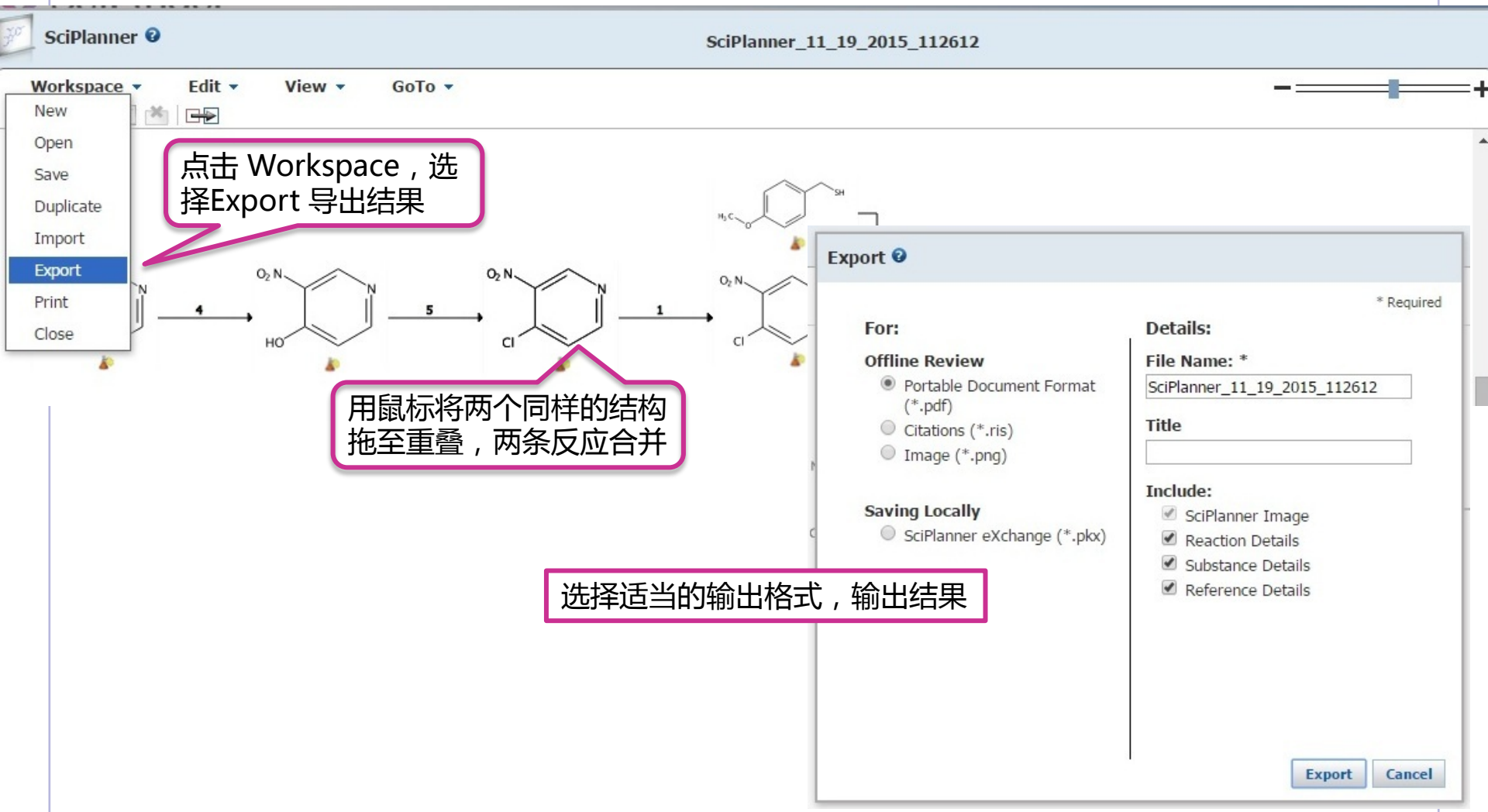


SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介



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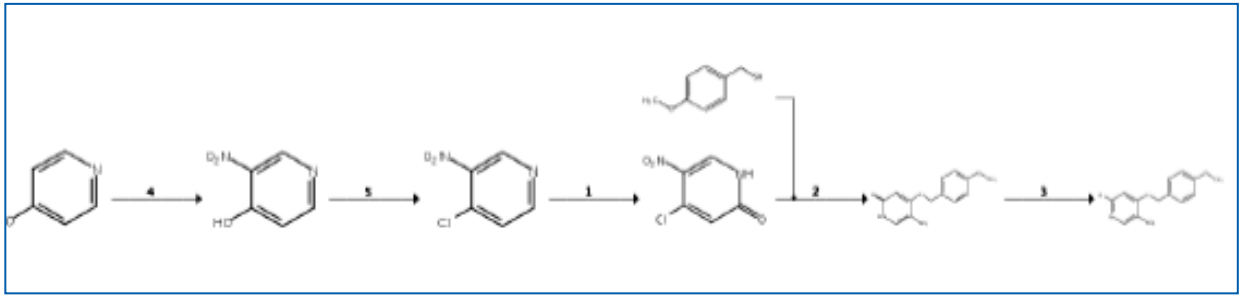
SciPlanner导出结果



Reaction	Stages		Notes	Yield
5	1.1	R:$POCl_3$, S:PhMe, 0°C → rt; 16 h, rt → 110°C	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	90%
	1.2	R:K_2CO_3, S:H_2O, cooled, pH 10	**Transformation:** 1. Formation of Alkyl Halides from Alcohols	

References

High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer 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(48), 10343-10356; 2014

Substance Information

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

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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
- SciFinder常见问题及解决

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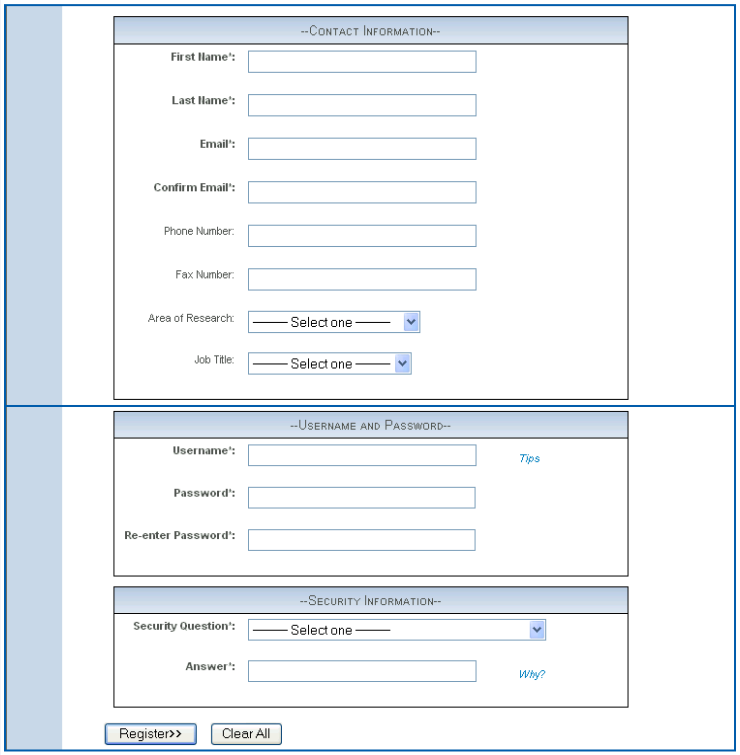
SciFinder浏览器选择建议

- 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

SCIFINDER® A CAS SOLUTION

如何获取SciFinder账号



请注意：
1.必须输入真实姓名和学校邮箱。
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 @、#、%、&、*）

例：abc@123
4.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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- 严禁将账号用于非学术研究

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