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- SciFinder简介及检索方式
  - 文献检索（PatentPak）
  - 物质检索
  - Markush检索
  - 反应检索(MethodsNow)
  - SciPlanner使用简介
- SciFinder常见问题及解决

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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division of polymer chemistry, inc American Chemical Society

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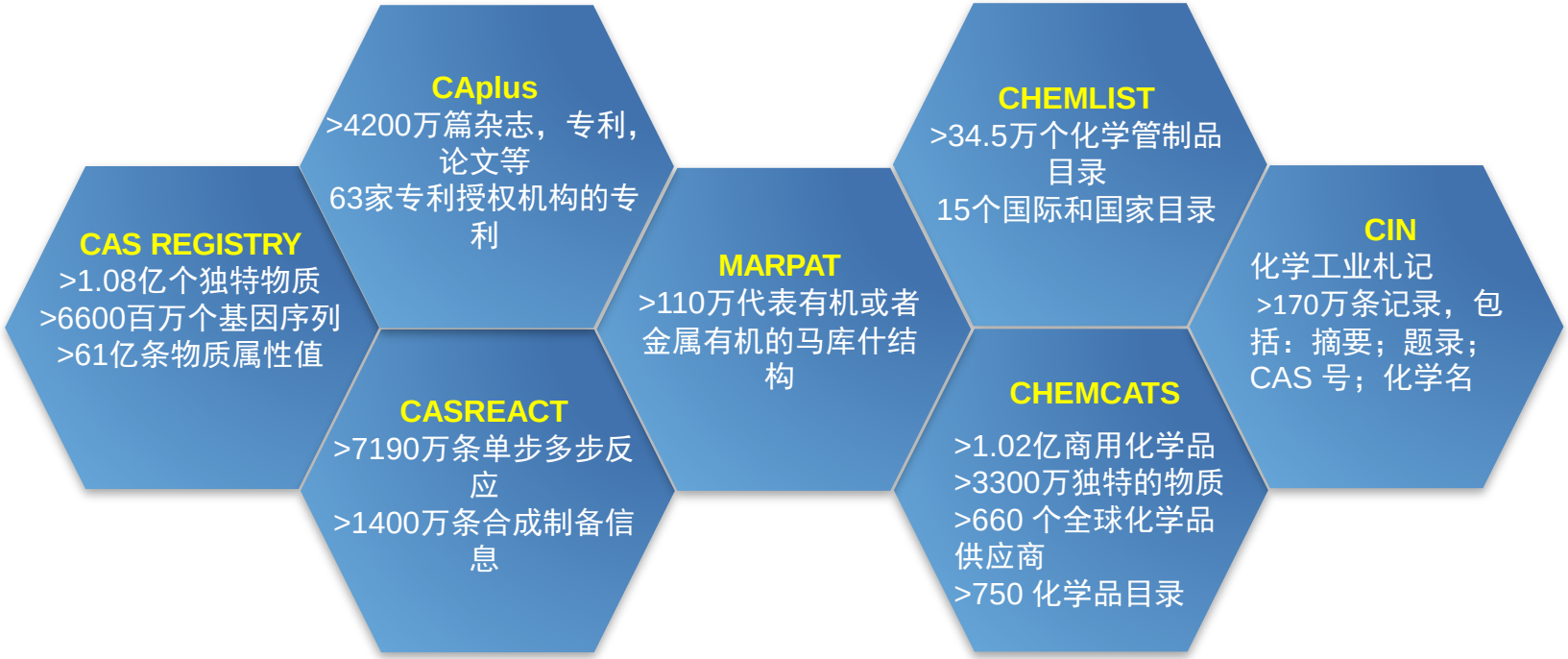

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生物化学：
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有机化学各领域：
氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：
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染料、有机颜料 ;合成橡胶 ;纺织品、纤维

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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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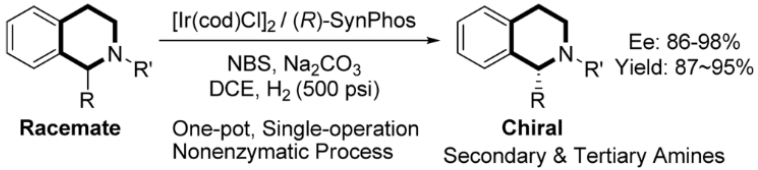
CAS数据库最具价值的内容——人工索引

1. Concise Redox Deracemization of Secondary and Tertiary Amines with a Tetrahydroisoquinoline Core via a Nonenzymatic Process

By: Ji, Yue; Shi, Lei; Chen, Mu-Wang; Feng, Guang-Shou; Zhou, Yong-Gui

A concise deracemization of racemic secondary and tertiary amines with a tetrahydroisoquinoline core has been successfully realized by orchestrating a redox process consisted of N-bromosuccinimide oxidn. and iridium-catalyzed asym. hydrogenation. This compatible redox combination enables one-pot, single-operation deracemization to generate chiral 1-substituted 1,2,3,4-tetrahydroisoquinolines with up to 98% ee in 93% yield, offering a simple and scalable synthetic technique for chiral amines directly from racemic starting materials.



Indexing

Heterocyclic Compounds (One Hetero Atom) (Section27-17)

Concepts

Enantioselective synthesis — Hydrogenation catalysts
Oxidation

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Chiral ligands

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Substances

12112-67-3 Dichlorobis(cyclooctadiene)diiridium
76189-55-4
133545-16-1
445467-61-8
503538-68-9 (S)-SynPhos
503538-69-0

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Catalyst use; Uses

QUICK LINKS
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SOURCE
Journal of the American Chemical Society
Volume137
Issue33
Pages10496-10499
Journal; Online Computer File
2015
CODEN:JACSAT
ISSN:0002-7863
DOI:10.1021/jacs.5b06659

COMPANY/ORGANIZATION
State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics
Chinese Academy of Sciences
Dalian, Peop. Rep. China
116023

ACCESSION NUMBER
2015:1340032
CAN163:331216
CAPLUS

PUBLISHER
American Chemical Society

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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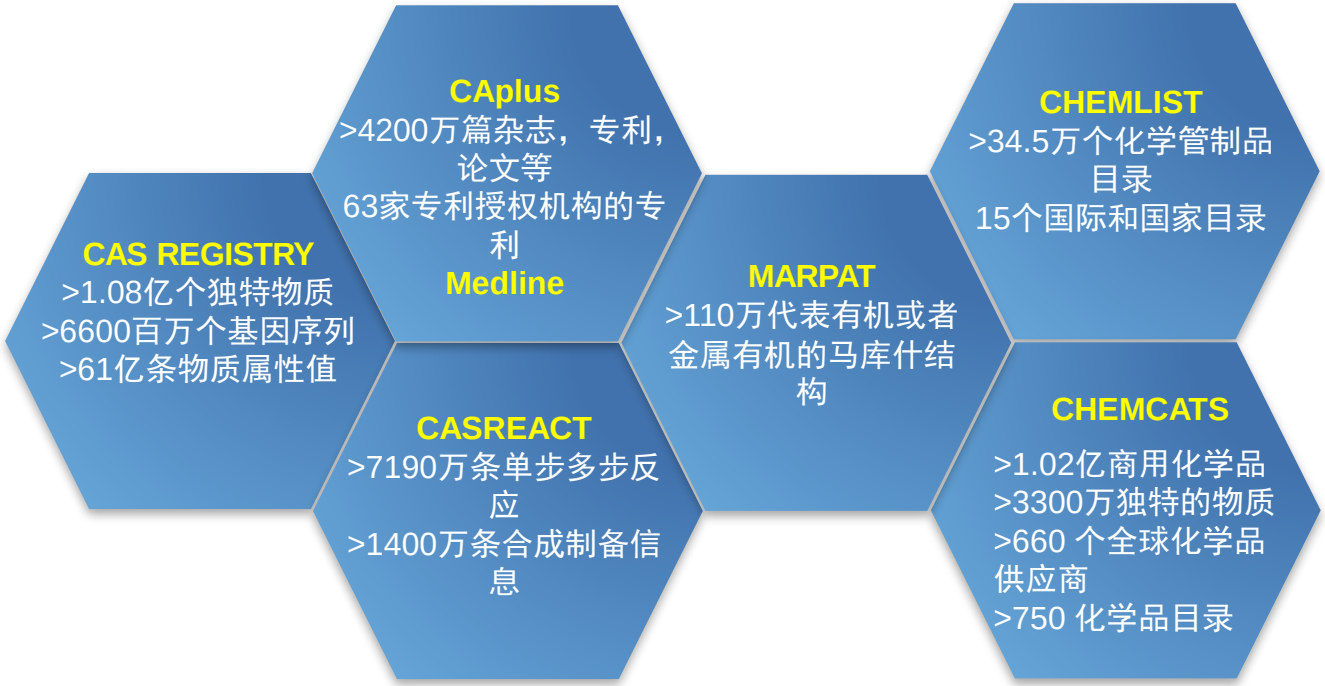

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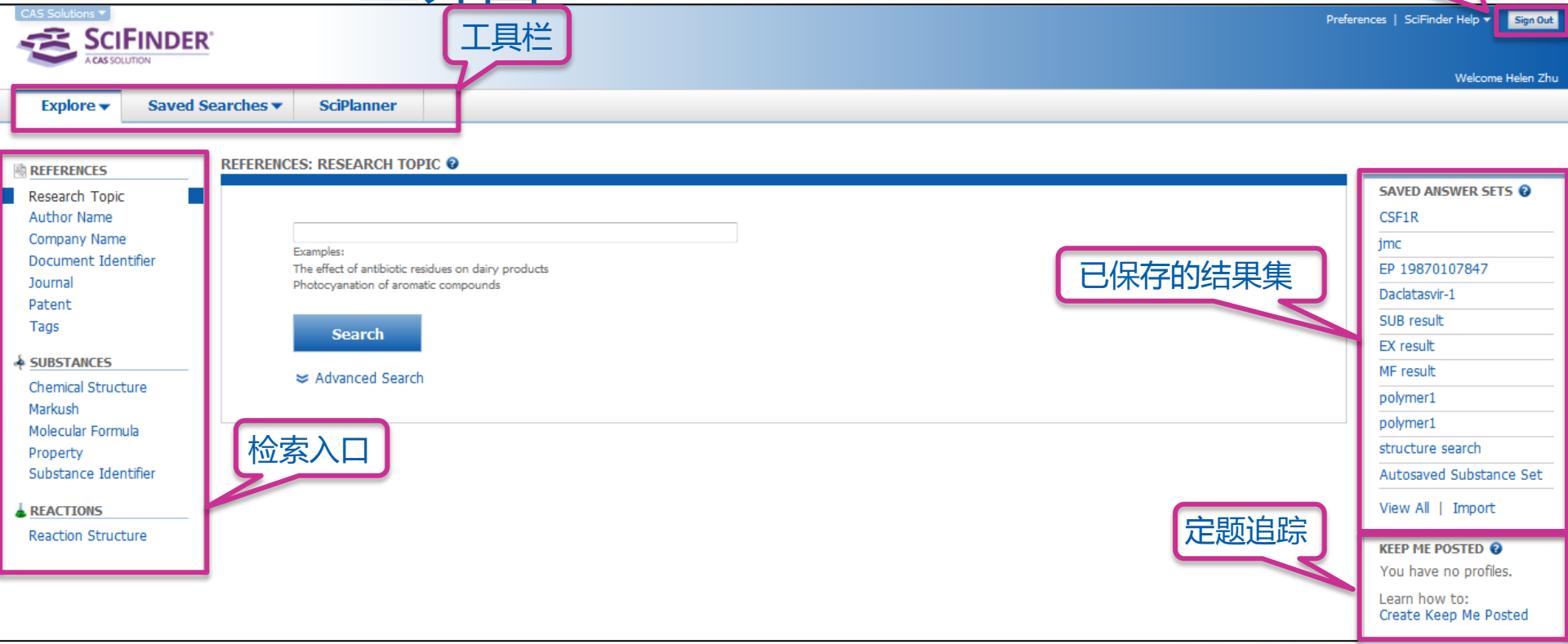

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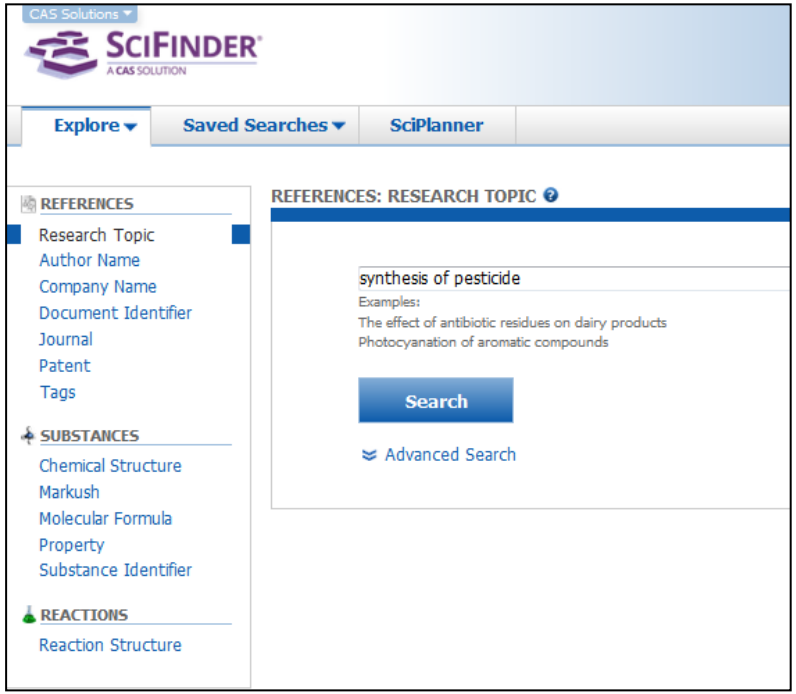
- 文献检索方法
  - 主题检索
  - 作者名检索
  - 机构名检索
  - 文献标识符检索
  - 期刊名称和专利信息（公开号，申请号等）
  - 从物质，反应获得文献

- 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
  - 关注某机构科研进展：机构名检索

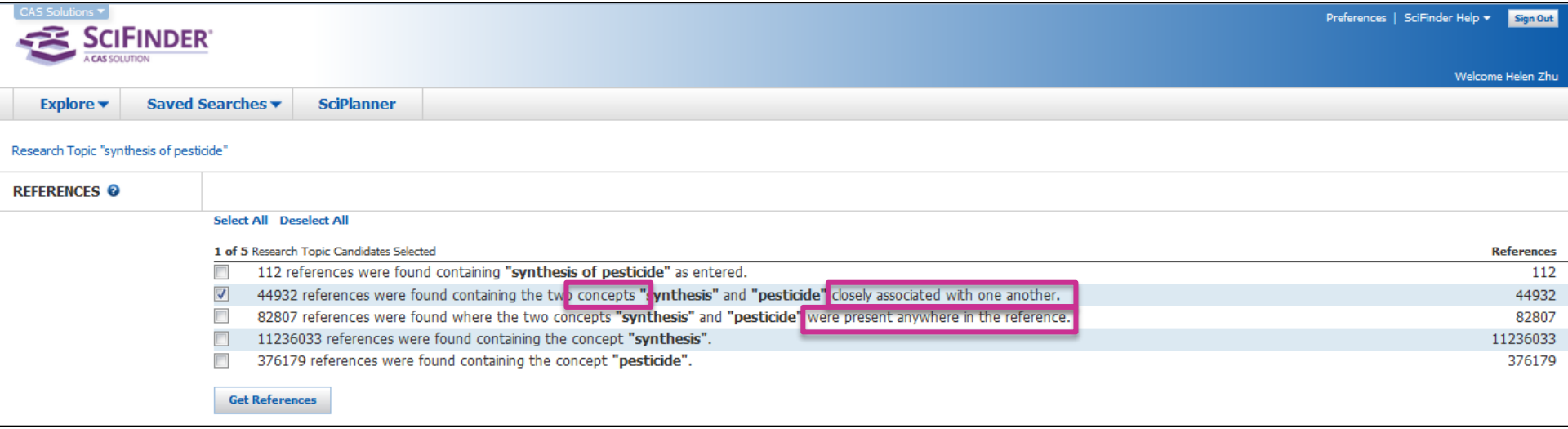
文献检索——主题: 杀虫剂的合成

- 检索式： synthesis of pesticide



关键词之间可用介词连接：in, with, of...

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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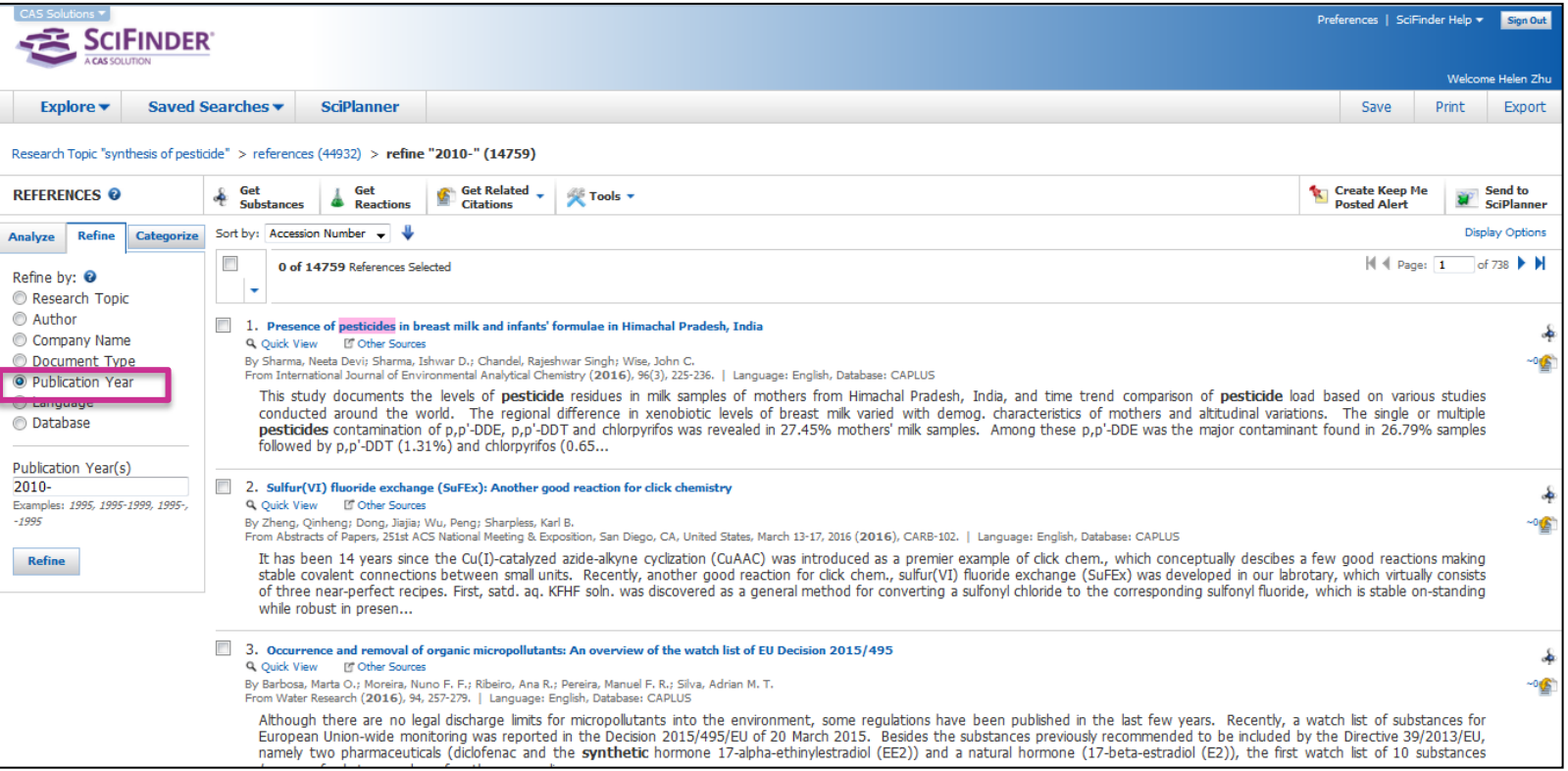
文献检索结果



Refine可以迅速获得所需文献

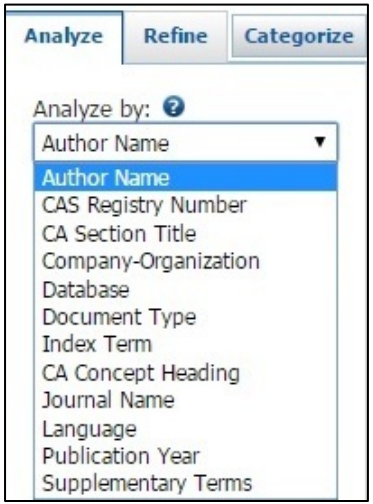
文献检索结果

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

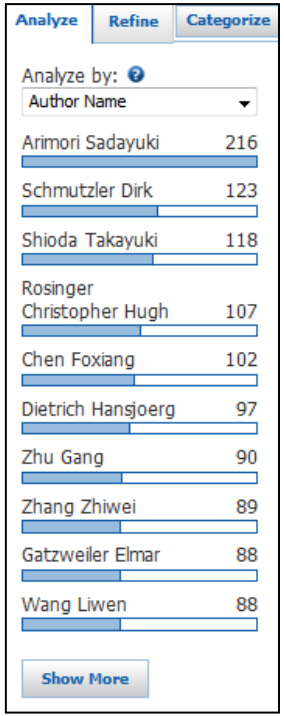
Citing Reference: 可以帮助找到最重要的文献

文献检索结果：Analyze

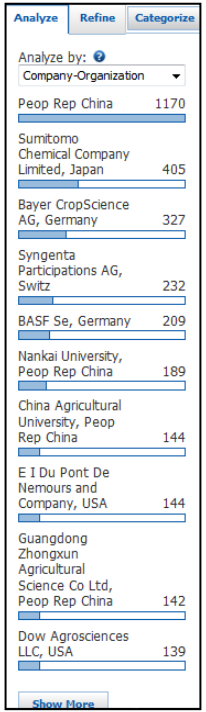
12种文献分析选项



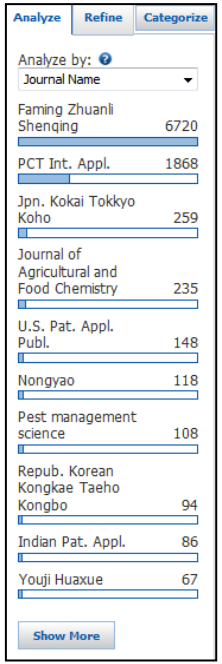
主要研究人员



主要研究机构，合作伙伴，竞争对手



主要发表期刊



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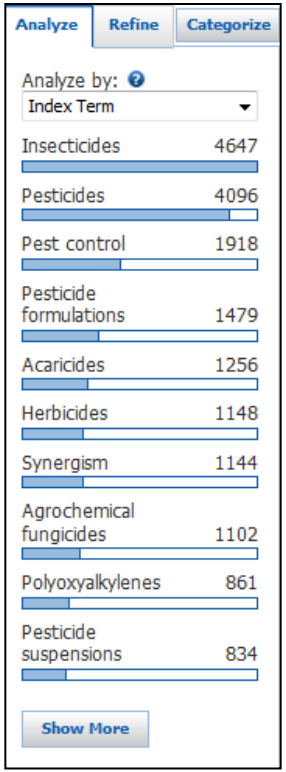
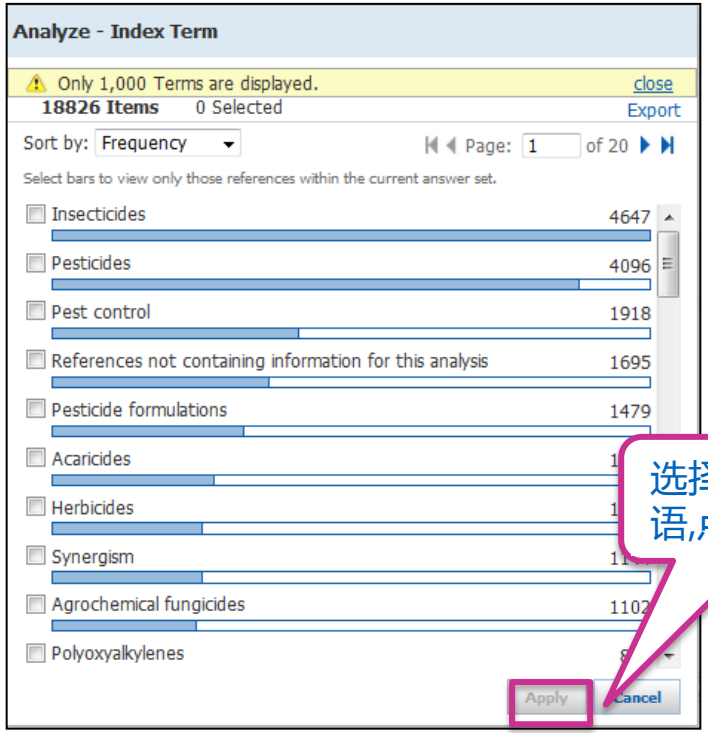
文献检索结果：Analyze



Index Term:帮助用户
全景了解本领域涉及的重要技术术语，精选文献



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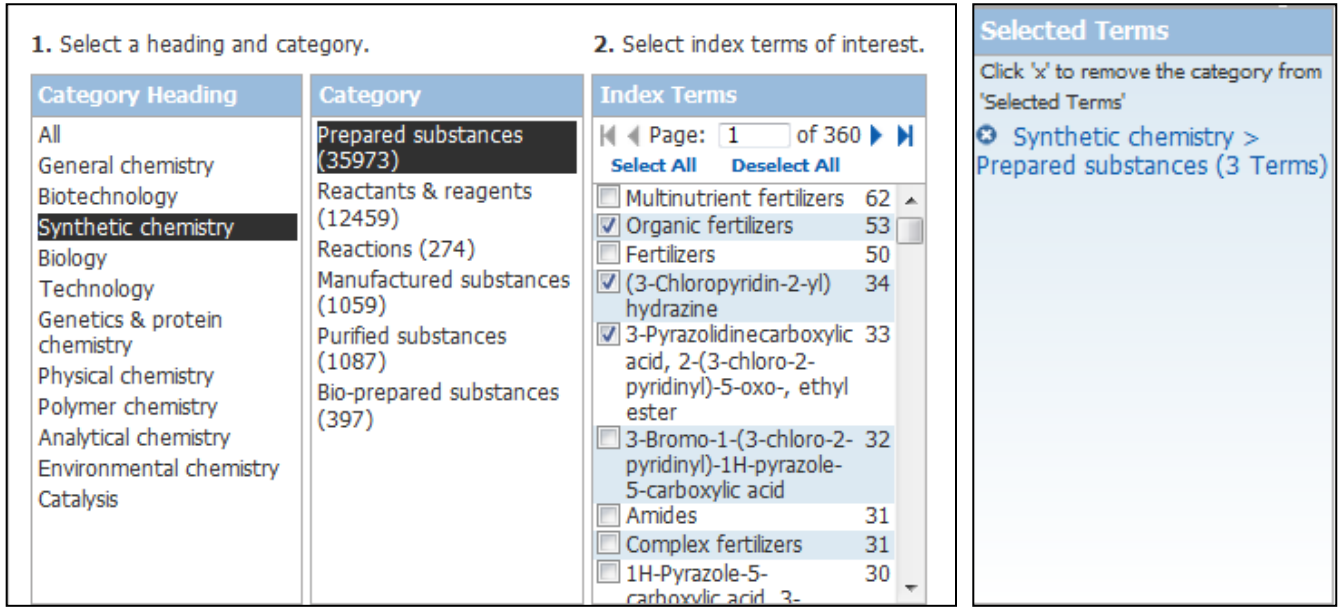
学科主分类　　学科副分类　　学科副分类涉及的重要技术术语　　选中的重要技术术语



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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。

文献信息详情

17. Plant biological source chive fertilizer maggot-eliminating pesticide

By: Li, Shi

Assignee: Qingdao Changlv Biology Research Institute, Peop. Rep. China

The title plant biol. source chive fertilizer maggot-eliminating pesticide contains effective ingredients of Nymphaea tetragona ext., chitin, plant ash, matrine, bios, and probiotics (prebiotic including Lactobacillus acidophilus, Bifidobacterium, Bacillus subtilis, and culture media raw material including soya-bean milk, wheat bran, fish bone powder, brown sugar), and is obtained through special process. The inventive plant biol. source chive fertilizer maggot-eliminating pesticide is mainly used as fertilizer in chive growth cycle to dispel chive maggot for sterilization of leek soil. There is synergistic effect of plant and biogenic cytokines, jointly being absorbed by chive, while providing nutritive substance, and avoiding chive maggot to infringe chive. The inventive plant biol. source chive fertilizer maggot-eliminating pesticide has efficient germicidal action, can purify soil, create good chive growing environment, can repair the chive injured by chem. pesticide, promote the absorption of nutritive substance, and resist chive maggot infringement, is nontoxic, easy to degrade, and pollution-free harmless, and has simple prepn., low pesticide amt., and low cost.

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PATENT INFORMATION
Apr 15, 2015
CN 104513104
A

APPLICATION
Sep 27, 2013

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 104513104 PATENTPAK	A		Apr 15, 2015	CN 2013-10448242	Sep 27,

Priority Application	
CN 2013-10448242	Sep 27, 2013

Indexing

Agrochemica

Section cross-reference(s): 19

重要技术术语

Concepts

Hormones, microbial

bios; plant biol. source chive fertilizer maggot-eliminating pesticide

Fish

bone meal of; plant biol. source chive fertilizer maggot-eliminating pesticide

Maggot

control of; plant biol. source chive fertilizer maggot-eliminating pesticide

重要物质

Substances

519-02-8 Matrine
1398-61-4 Chitin

plant biol. source chive fertilizer maggot-eliminating pesticide

Agricultural use; Biological study; Uses

57-50-1 Sucrose, biological studies

plant biol. source chive fertilizer maggot-eliminating pesticide

Biological use, unclassified; Biological study; Uses

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
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- 主题检索时，使用介词作为连接
- 尽量选择包含**Concept**和**Closed Associated with**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

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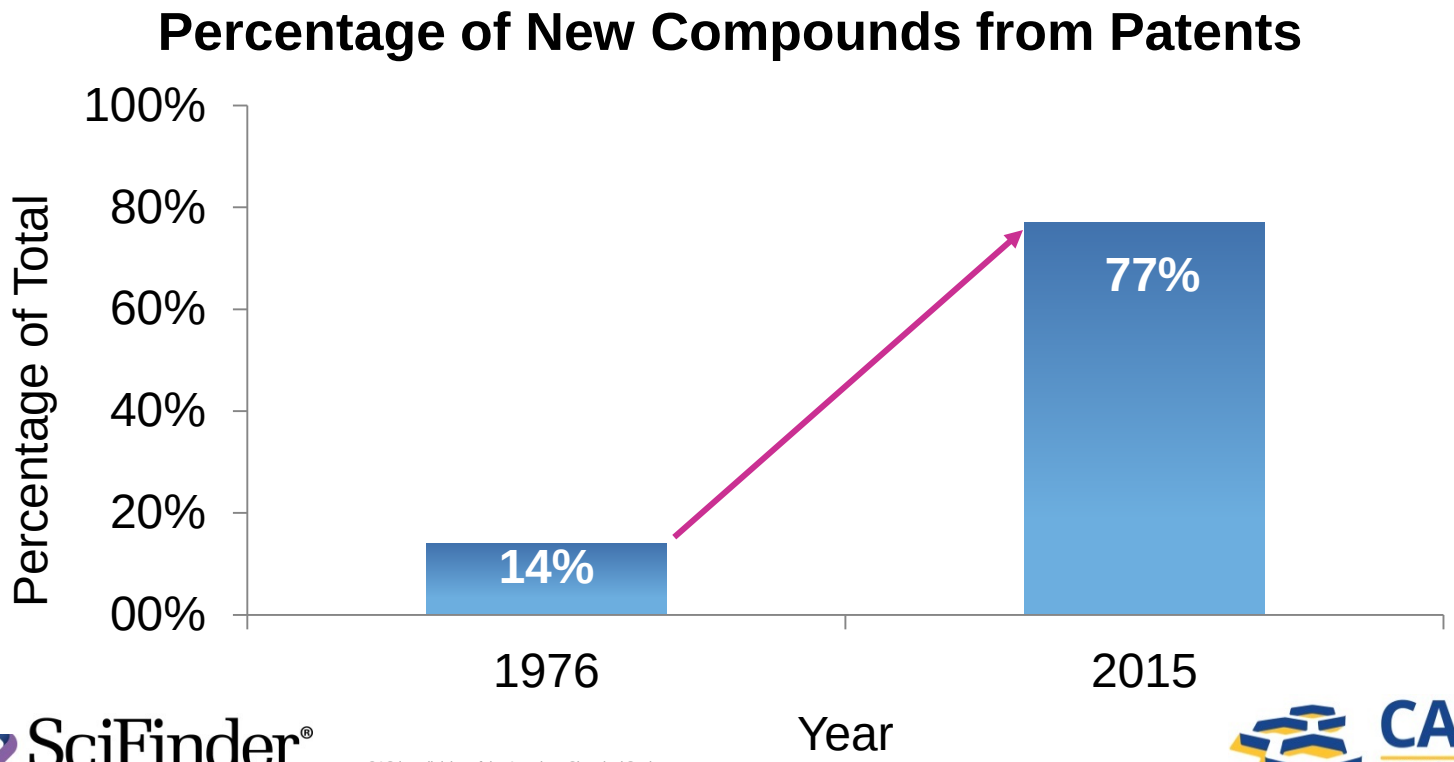

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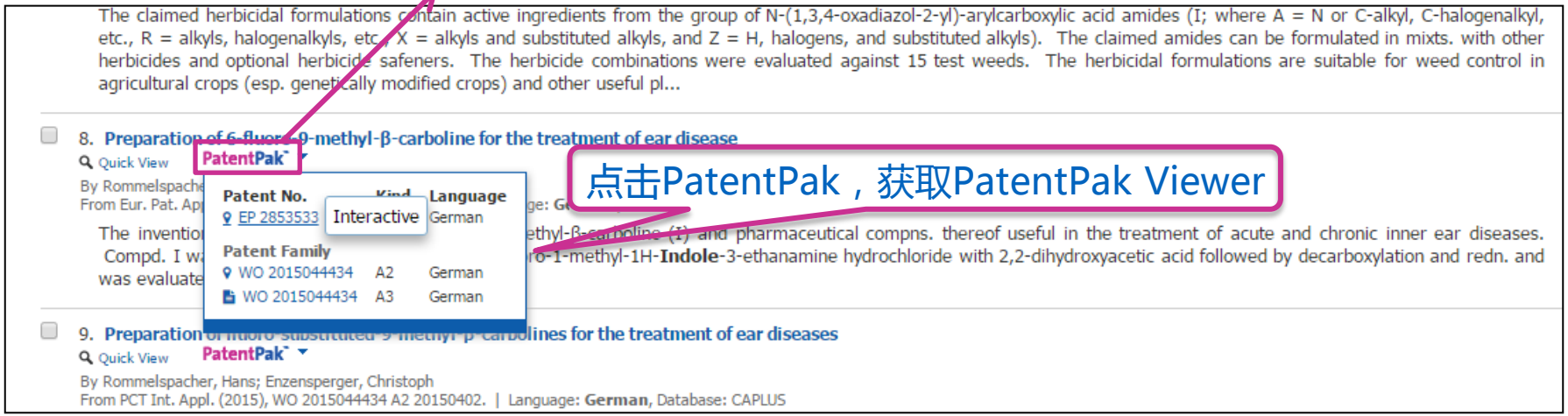

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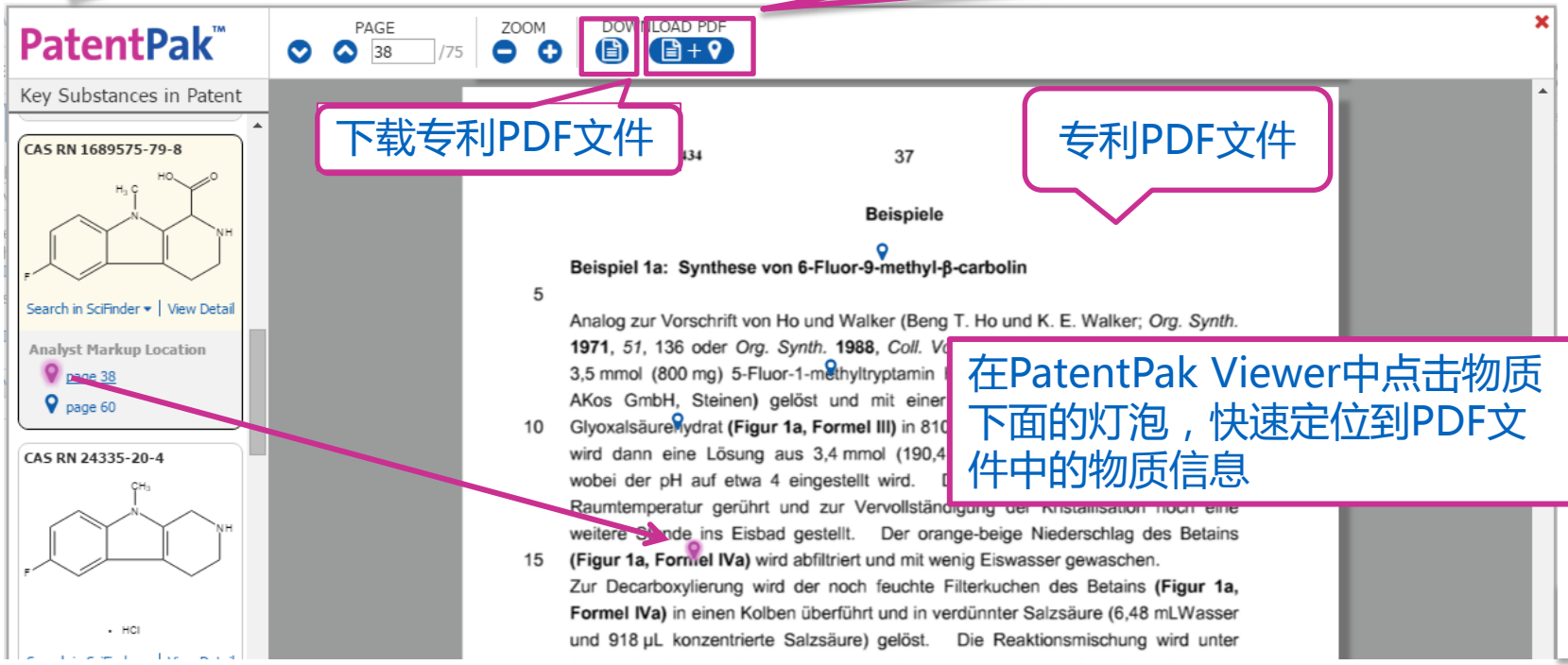

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文献检索练习

1. 检索有关合成除草剂(herbicide)的文献，该领域最大的研究机构是什么？有多少综述文献？最重要的那篇是什么？有多少篇专利？来自中国的专利有多少？主要的除草剂有哪些？
2. 检索你导师发表的文献，找出他的主要研究方向。

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  - 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
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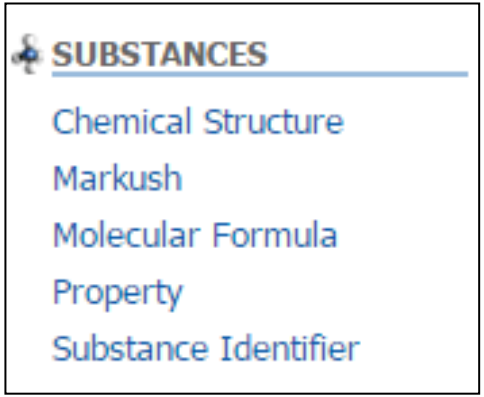
  - 高分子化合物：分子式检索和结构检索



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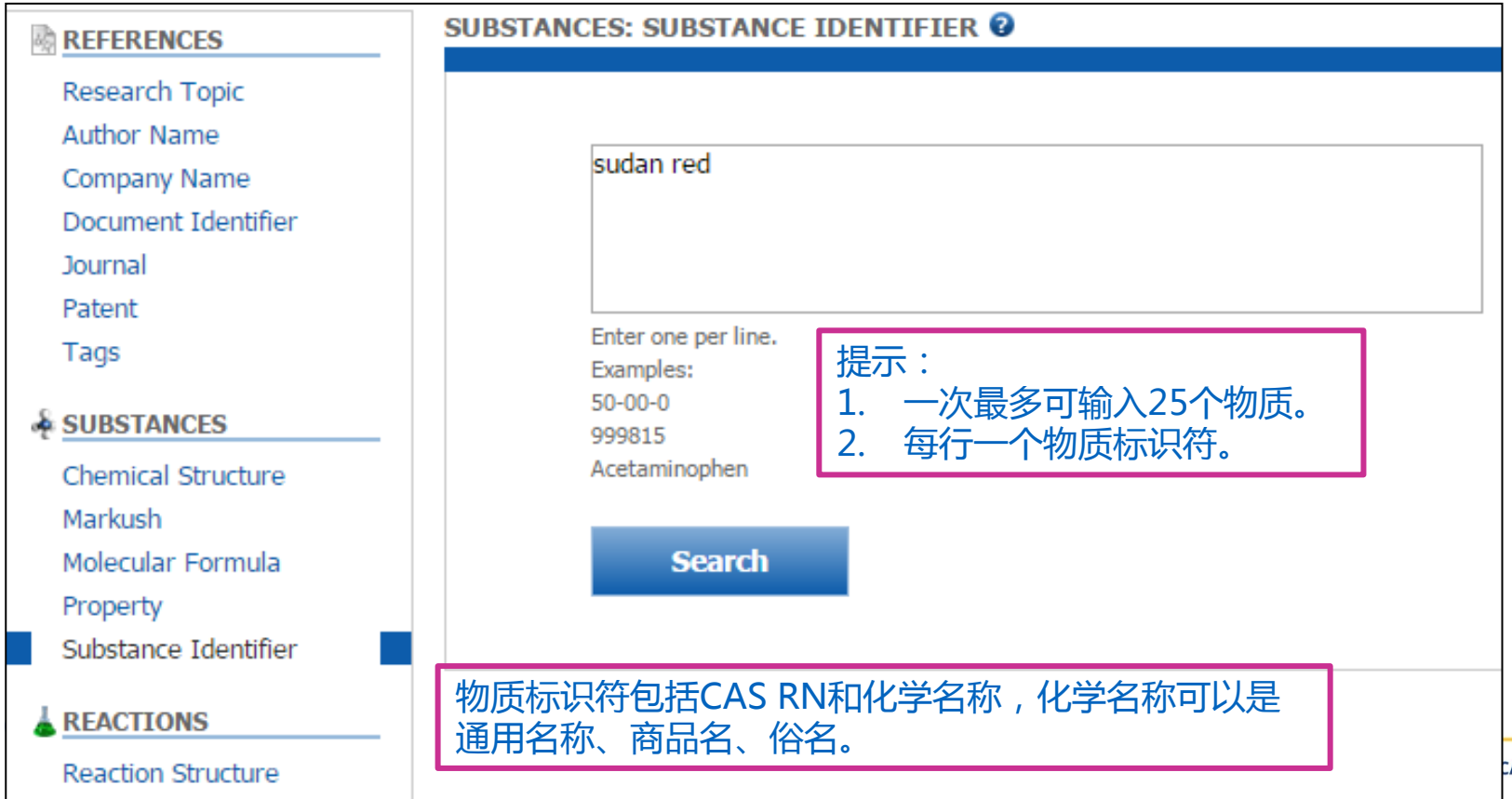
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Reaction Structure
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999815
Acetaminophen
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2. 每行一个物质标识符。
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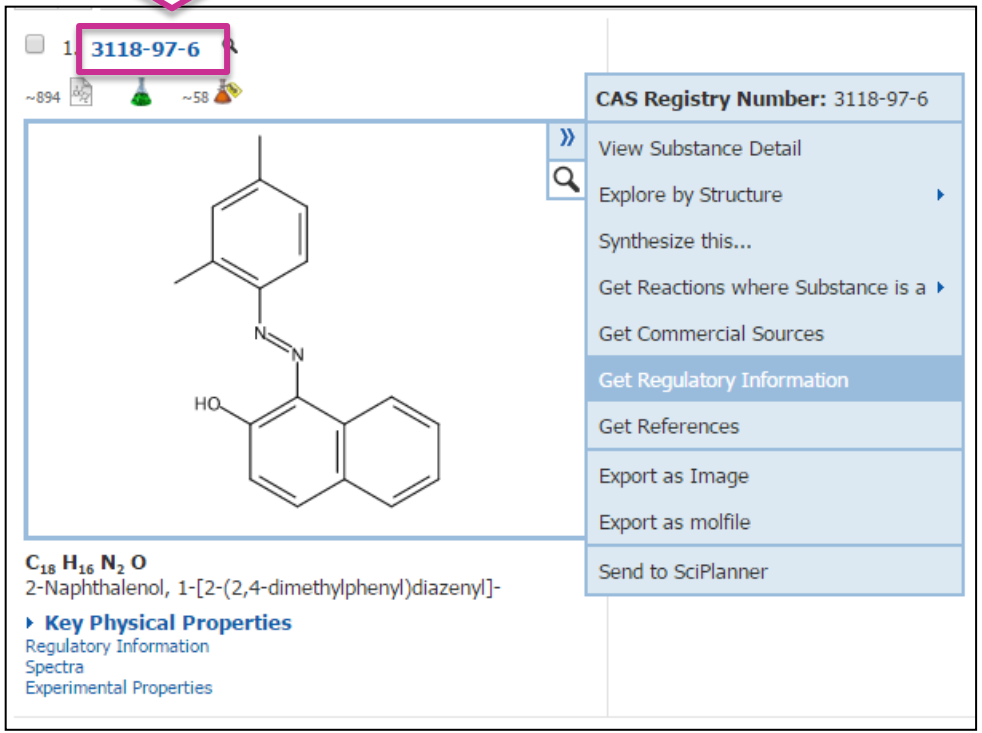
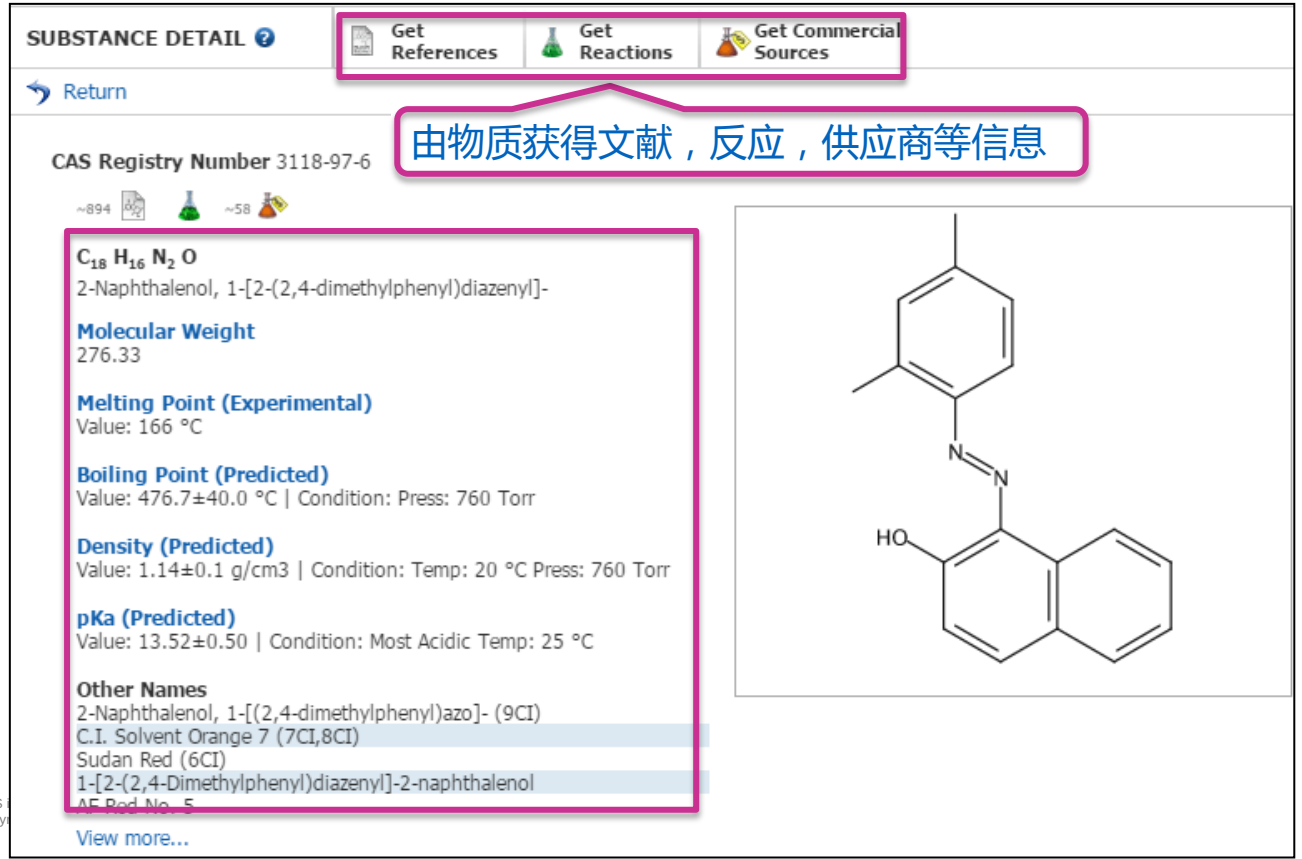
SciFinder中的物质记录

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

SciFinder中的物质记录



物质详情

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A CAS Solution

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

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

¹H 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

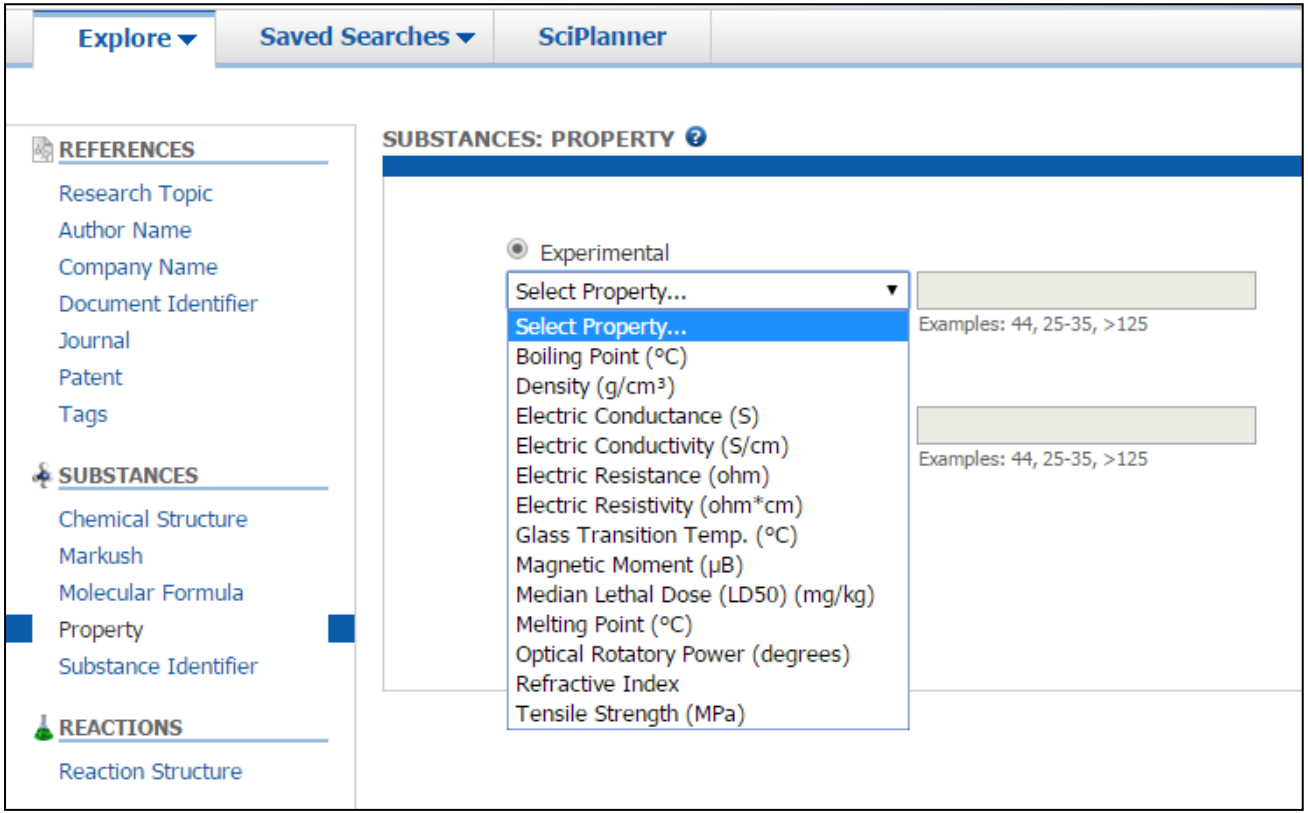
Notes

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

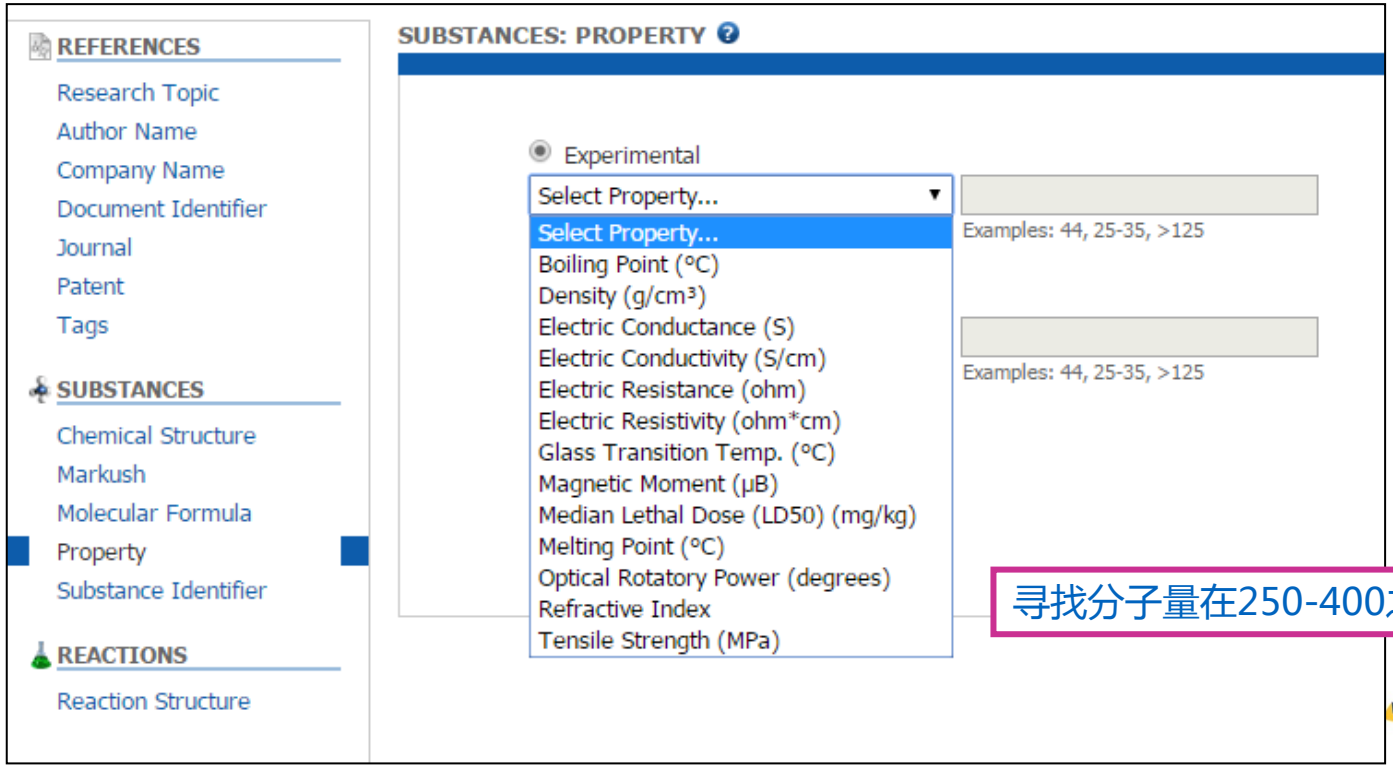
PREDICTED SPECTRA

SOCIETY

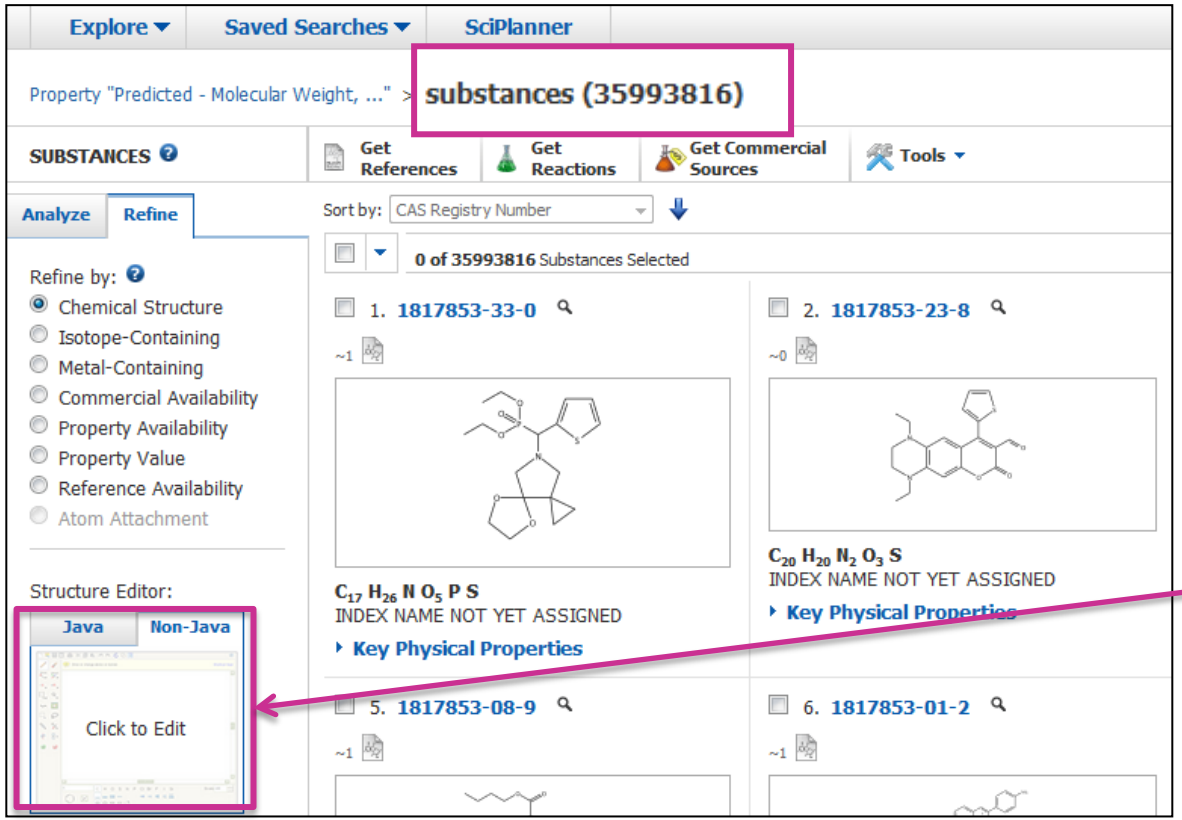
物质检索——Property explore



物质检索——Property explore



物质结果集的筛选——Refine



3500多万个结构，

如何筛选黄酮类物质？

CAS®
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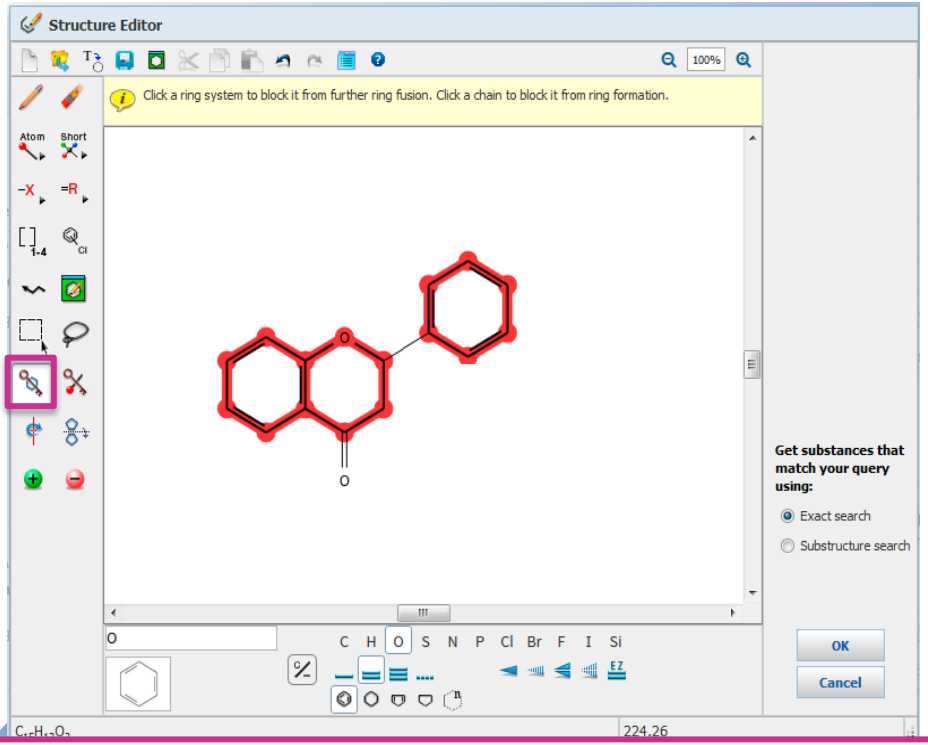
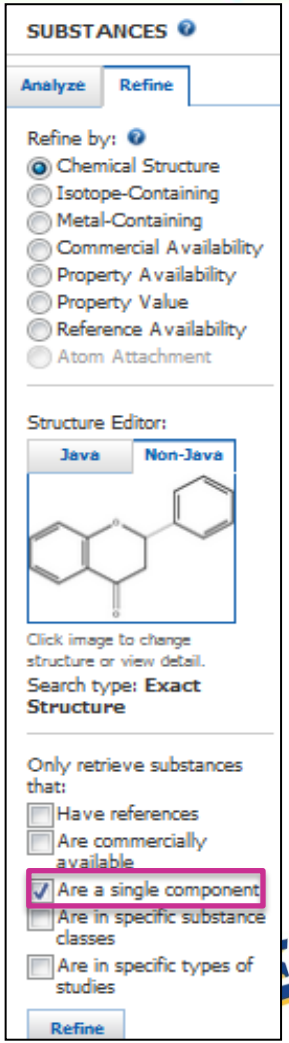
AMERICAN CHEMICAL SOCIETY

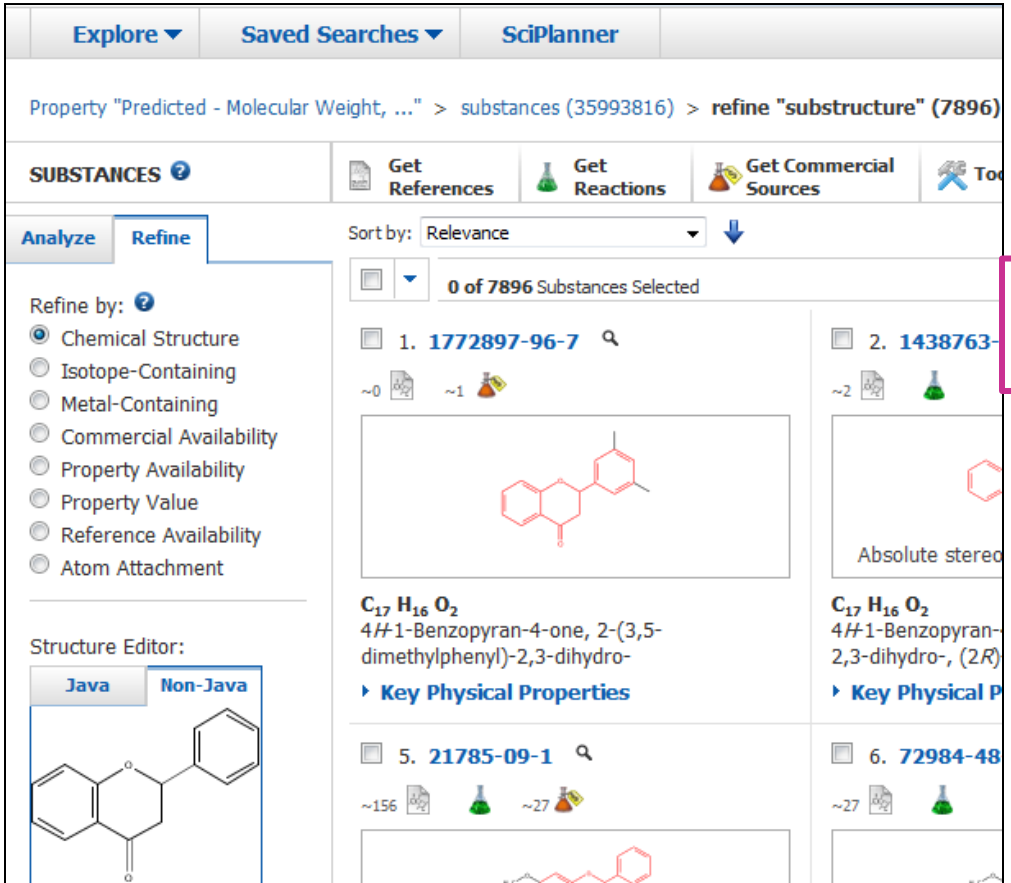
物质结果集的筛选——Refine



锁环工具：避免在被锁定的环结构上出现新的环结构



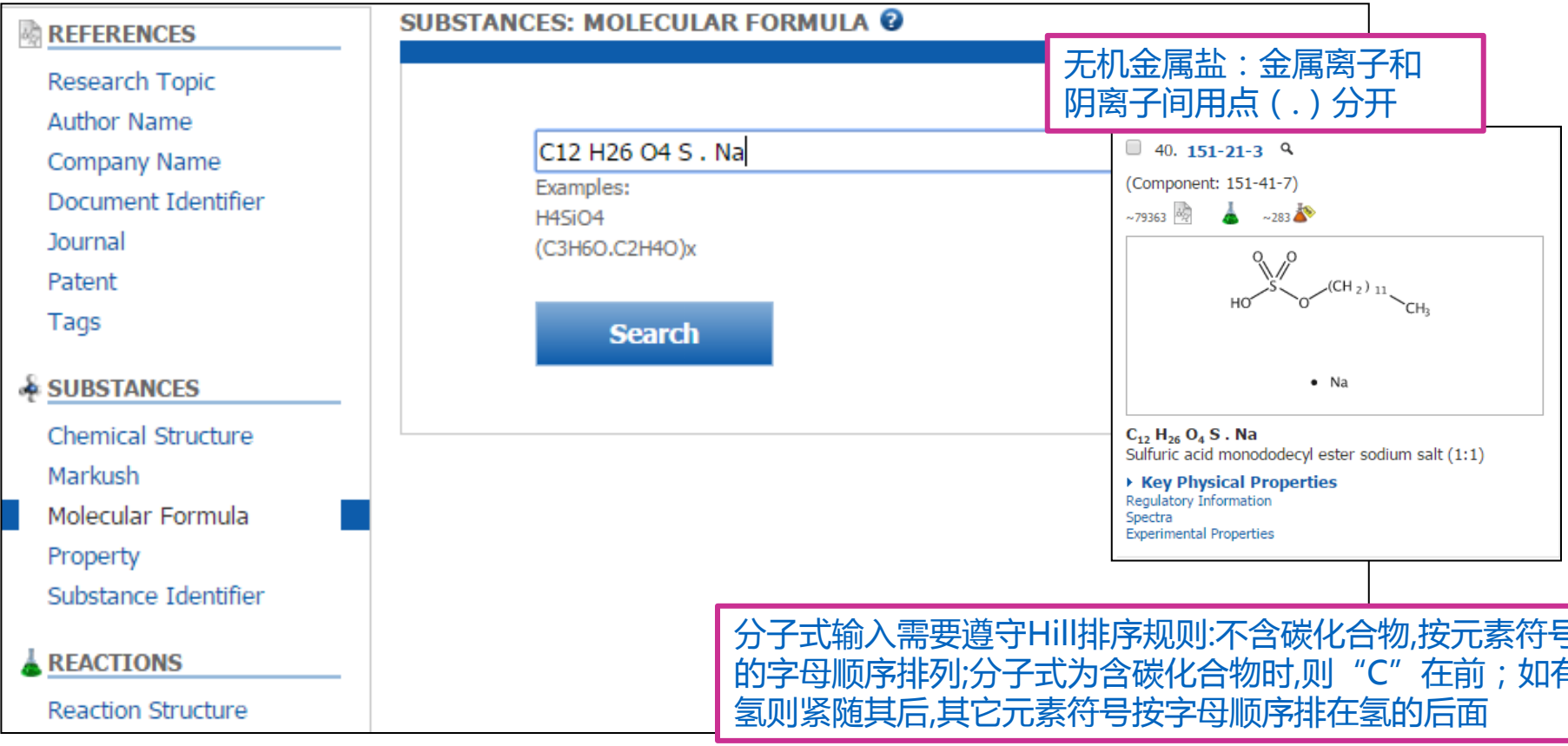
物质结果集的筛选——Refine



从3500多万个结构中

筛选出7800个黄酮类物质

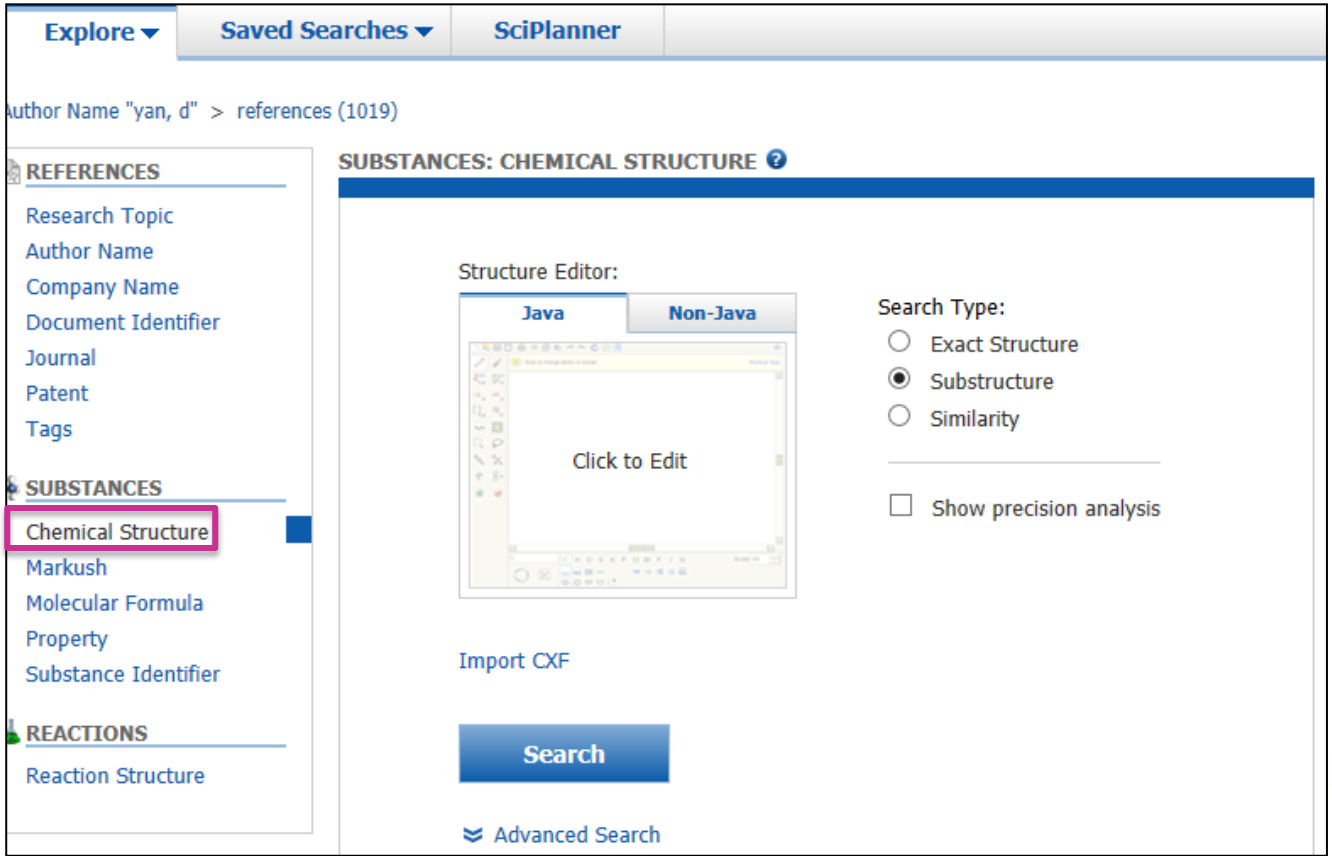
物质检索——分子式

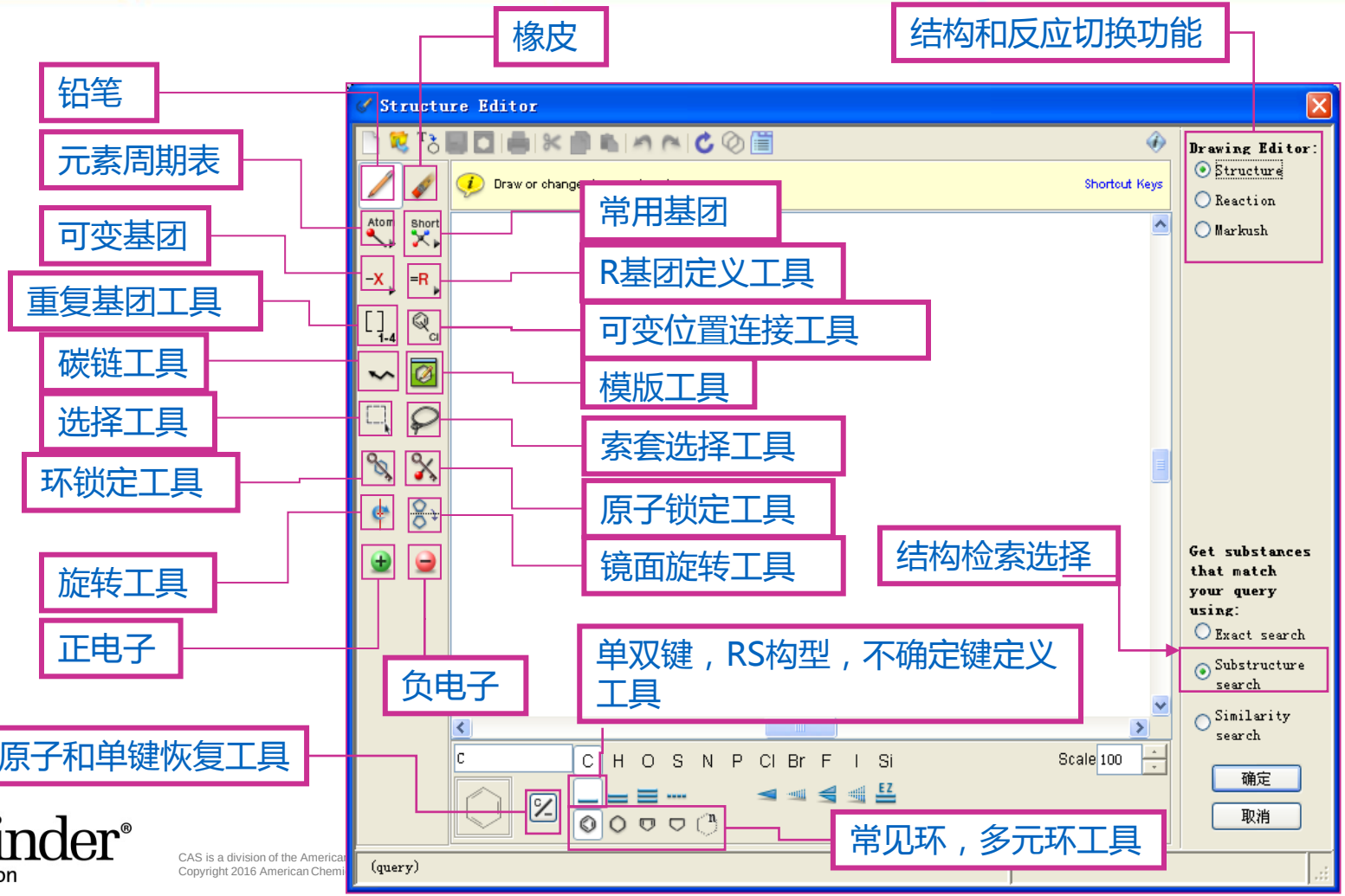


无机金属盐：金属离子和阴离子间用点（.）分开

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

物质检索——结构


Explore
Saved Searches
SciPlanner
Author Name "yan, d" > references (1019)
REFERENCES
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier
REACTIONS
Reaction Structure
SUBSTANCES: CHEMICAL STRUCTURE
Structure Editor:
Java
Non-Java
Click to Edit
Search Type:
Exact Structure
Substructure
Similarity
Show precision analysis
Import CXF
Search
Advanced Search



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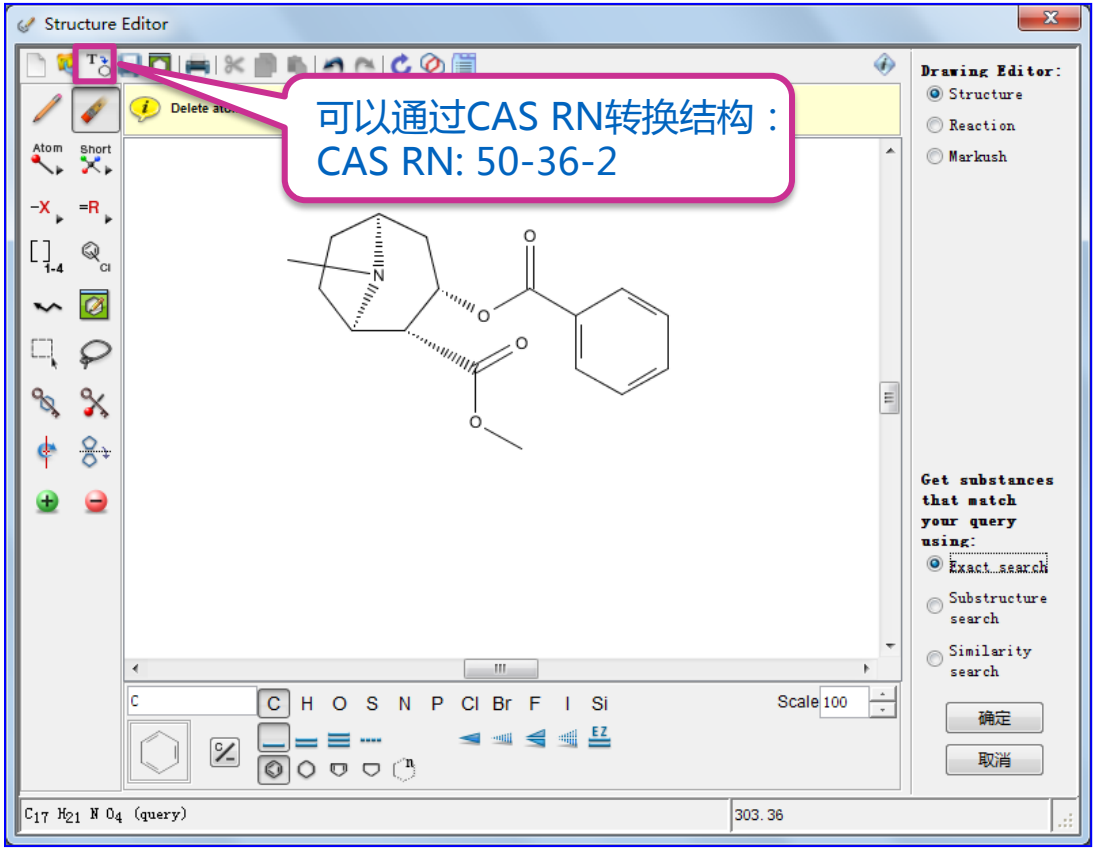
物质检索——精确结构检索



精确结构检索

浏览精确结构检索结果

可以通过分析/限定筛选结果集

Analyze | Refine

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

Select One:
- Include only metal-containing substances
- Exclude metal-containing substances

Refine

Sort by: Relevance

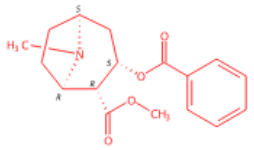
Display Optio

0 of 80 Substances Selected

Page: 1 of 2

1. 50-36-2

~20889 ~23



Absolute stereochemistry.,Rotation (-).

$C_{17}H_{21}NO_4$

8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*,2*R*,3*S*,5*S*)-

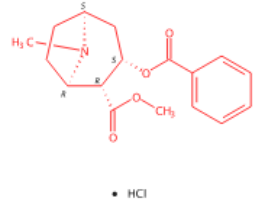
Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

可卡因

2. 53-21-4

(Component: 50-36-2)

~1700 ~27



• HCl

Absolute stereochemistry.,Rotation (-).

$C_{17}H_{21}NO_4 \cdot ClH$

8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, hydrochloride (1:1), (1*R*,2*R*,3*S*,5*S*)-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

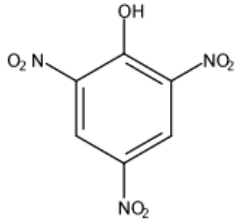
盐酸可卡因

3. 52748-70-6

~11

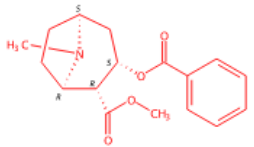
88-89-1

$C_6H_3N_3O_7$



50-36-2

$C_{17}H_{21}NO_4$



Absolute stereochemistry.,Rotation (-).

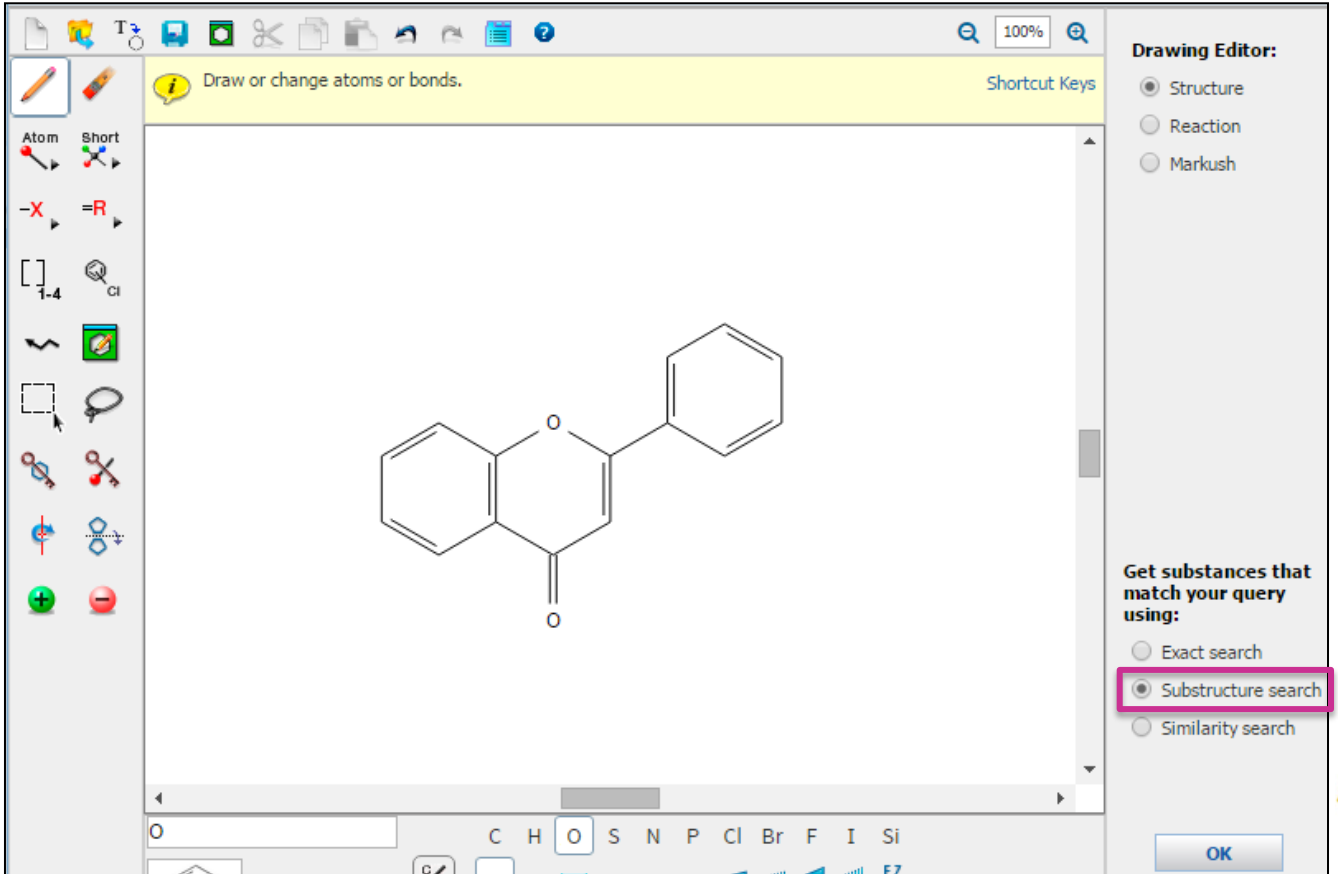
可卡因组合物

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

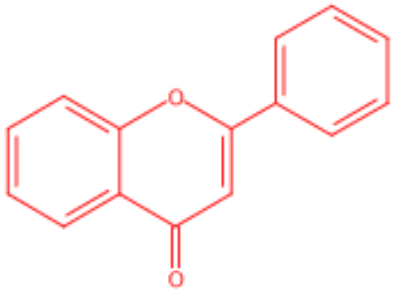

100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search
OK
C H O S N P Cl Br F I Si

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**

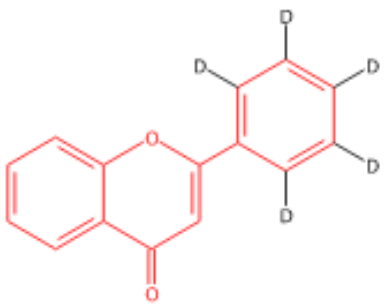
Regulatory Information

Spectra

Experimental Properties

2. 54849-75-1

~6



$C_{15}H_5D_5O_2$

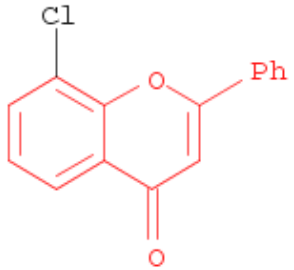
4*H*-1-Benzopyran-4-one, 2-(phenyl-d_5)-

Spectra

浏览亚结构检索结果

251. Substance Detail
1148-20-5

取代物



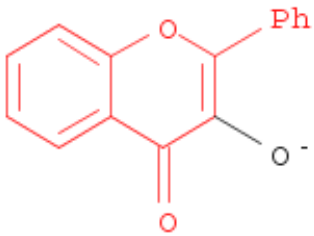
C15 H9 Cl O2
4*H*-1-Benzopyran-4-one, 8-chloro-2-phenyl-

Experimental Properties

261. Substance Detail
85481-91-0

离子

~8

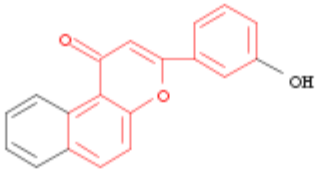


C15 H9 O3
4*H*-1-Benzopyran-4-one, 3-hydroxy-2-phenyl-, i

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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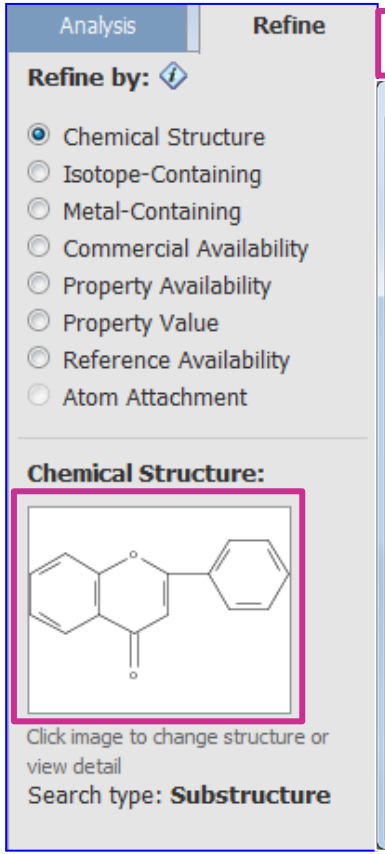
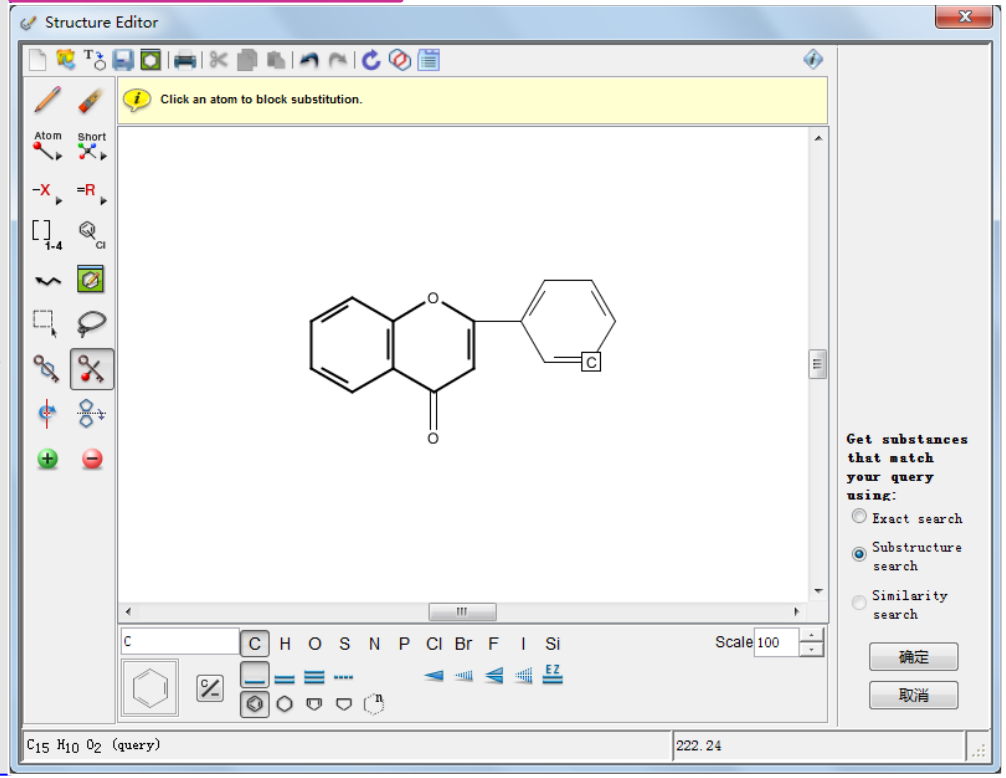
亚结构检索结果的限定工具



化学结构的再次限定

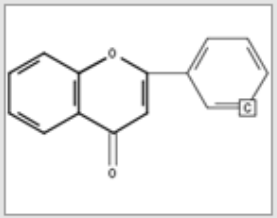


环锁定

原子锁定

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)

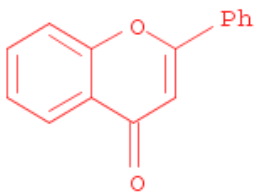
Substances | Get References | Get Reactions | Tools | Send to SciPlanner

28699 Substances | 0 Selected

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

1. Substance Detail
525-82-6

~2568



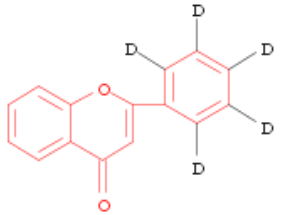
$C_{15}H_{10}O_2$

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

Spectra
Experimental Properties

2. Substance Detail
54849-75-1

~5

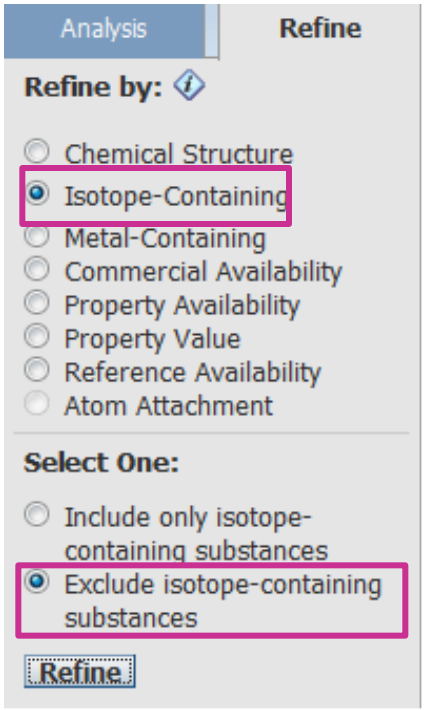


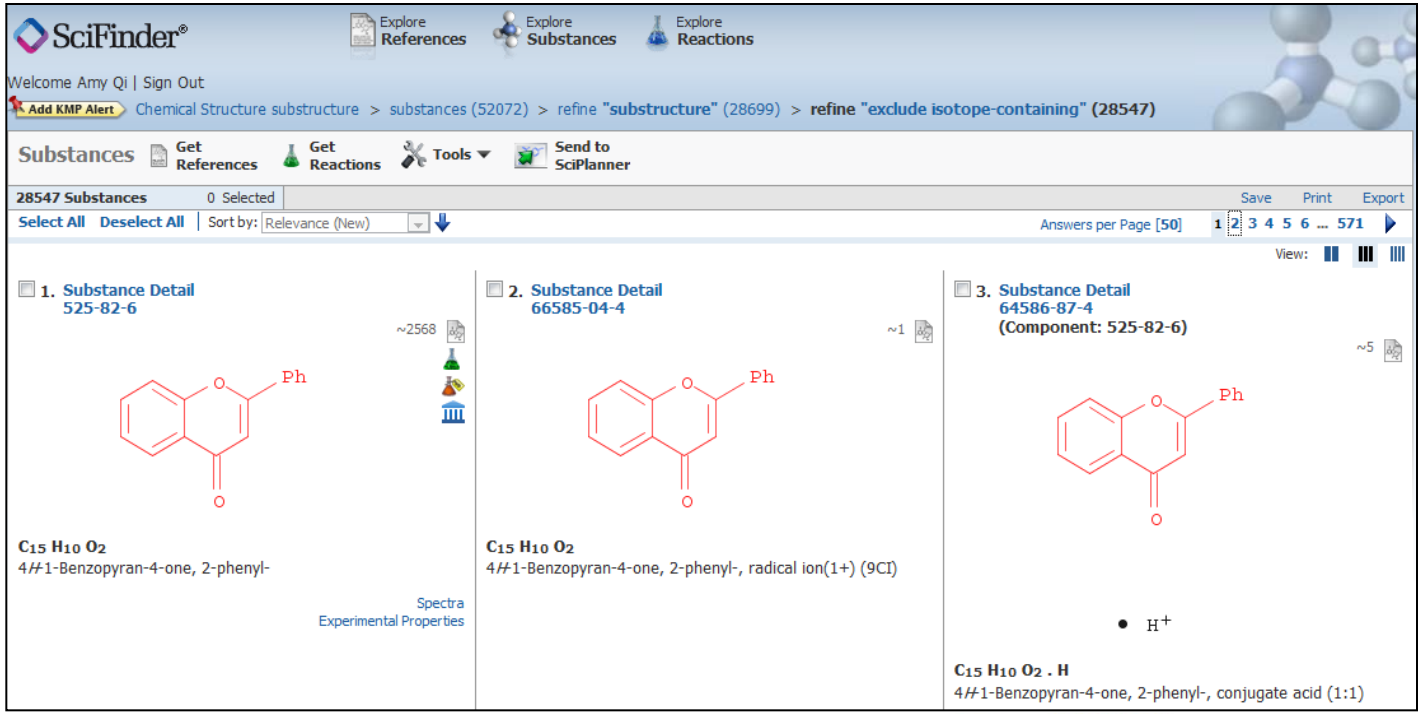
$C_{15}H_5D_5O_2$

4*H*-1-Benzopyran-4-one, 2-(phenyl-*d*5)-

Spectra

同位素去除





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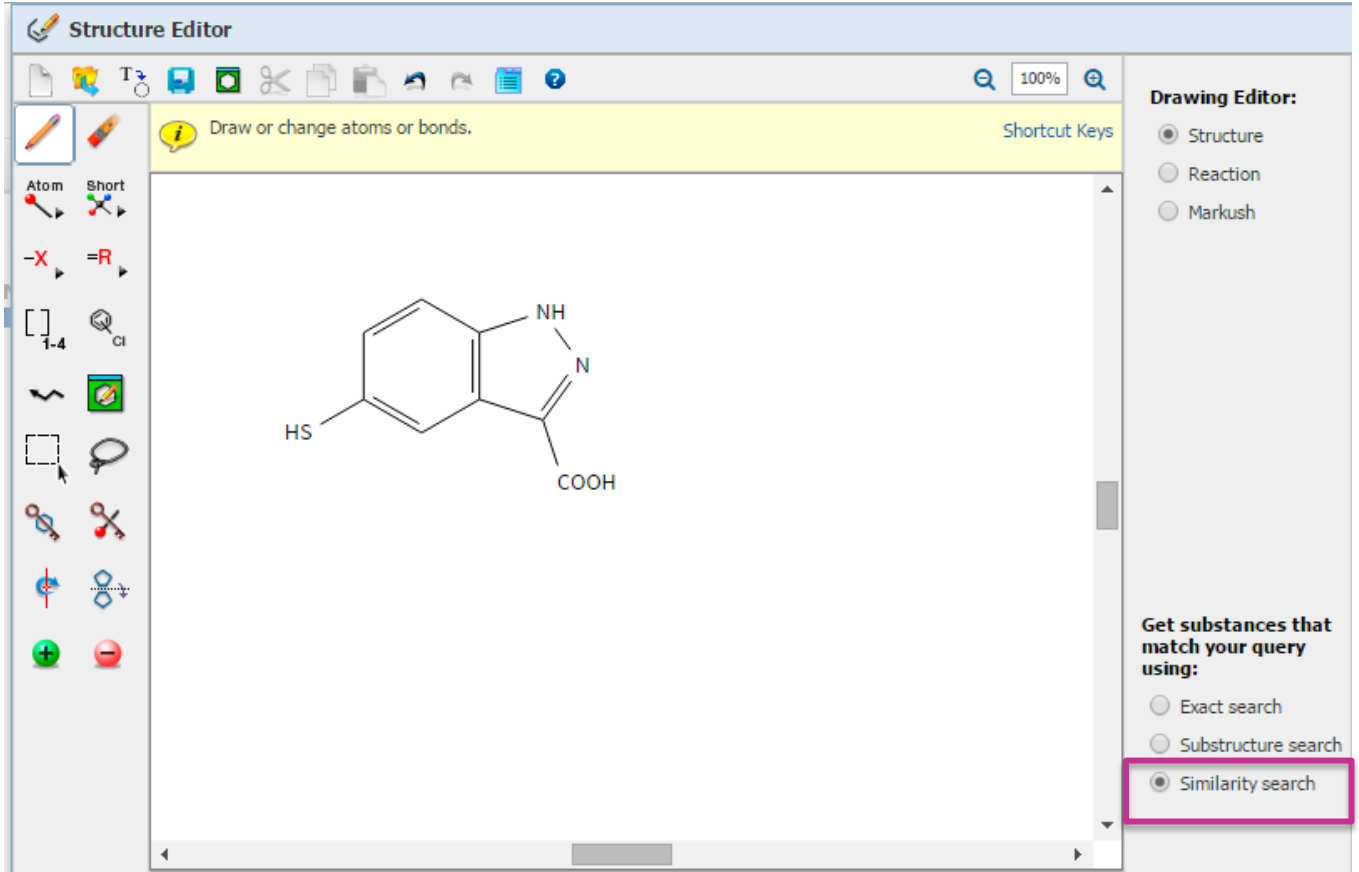
物质检索——亚结构检索

- 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
-X
=R
1-4
Cl
NH
N
HS
COOH
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search

Select All Deselect All

相似结构检索候选项

1 of 6 Similarity Candidates Selected

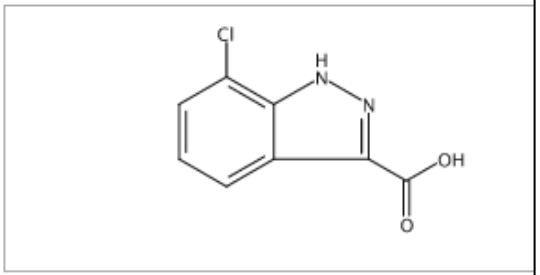
		Substances
☐	≥ 99 (most similar)	0
☐	95-98	0
☐	90-94	0
☐	85-89	11
☑	80-84	34
☐	75-79	82
☐	70-74	254
☐	65-69	633
☐	0-64 (least similar)	1636

相似度越高，结构越相似

相似结构检索结果

1. 129295-32-5

~3 ~96



$C_8 H_5 Cl N_2 O_2$

1H-Indazole [illegible]hloro-

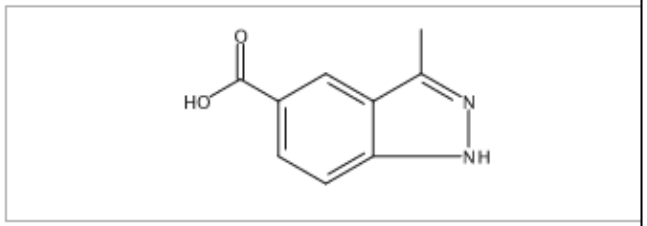
Key Phys

取代基变化

Score: 79

3. 885223-58-5

~11 ~34



$C_9 H_8 N_2 O_2$

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

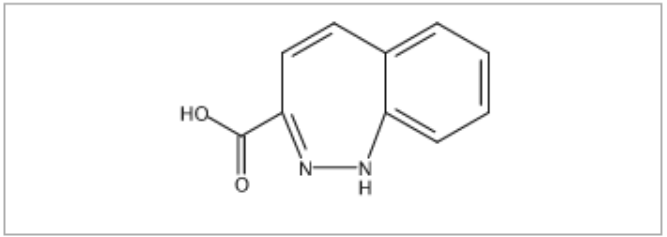
Key Pl

取代基位置变化

Score: 71

117. 72119-92-7

~1



$C_{10} H_8 N_2 O_2$

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

Key Physical Pr

Experimental Properties

母体结构变化

物质检索——相似结构检索

- 相似结构检索：

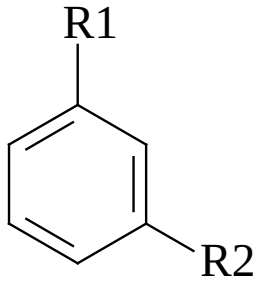
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

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

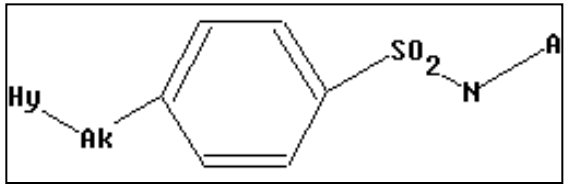
Markush检索

- 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

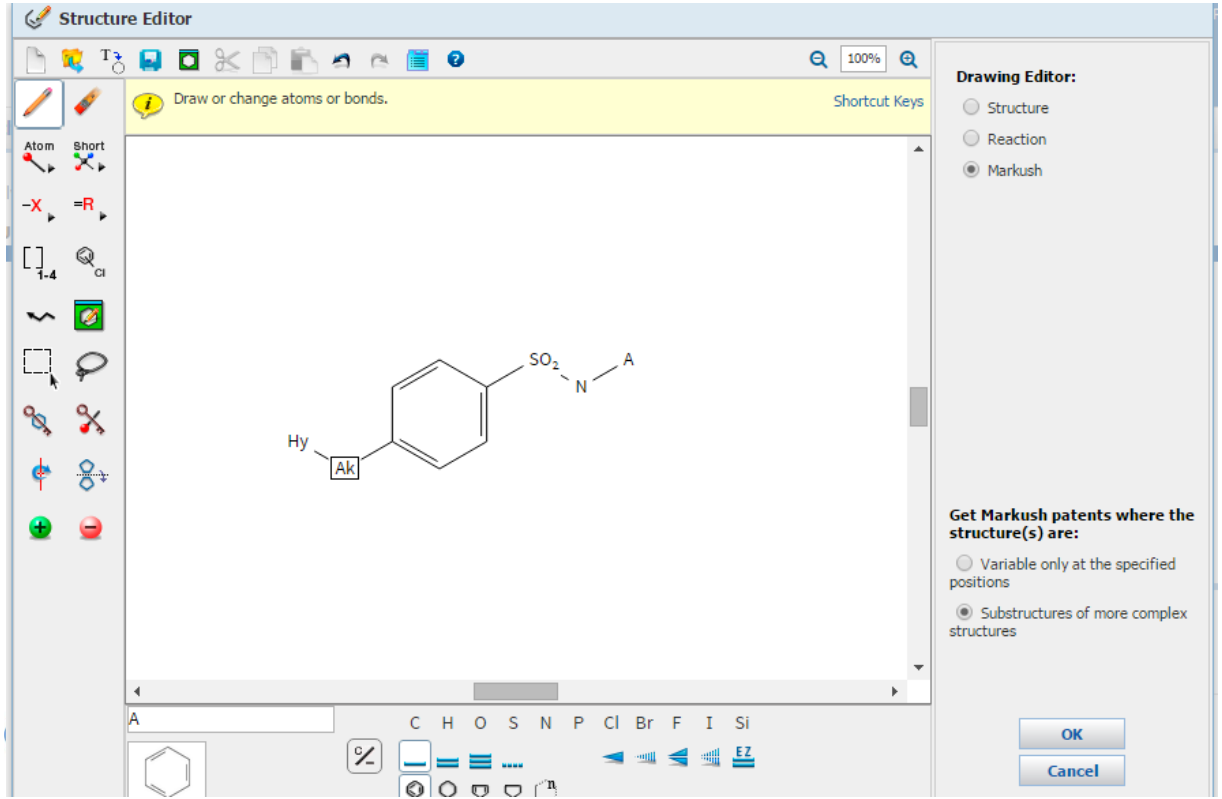


R1 = H, Br, Cl, I

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

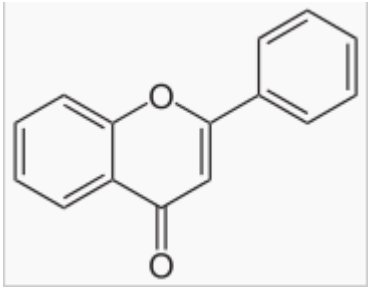


可用SciFinder中的Markush检索查看专利中化合物结构保护范围。



物质检索练习

1. 检索(NH4)Sm(SO4)2(H2O)4
2. 检索青蒿素qinghaosu，查看其HNMR谱图
3. 检索黄酮类物质

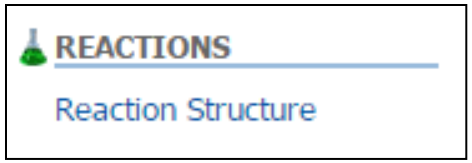


提纲

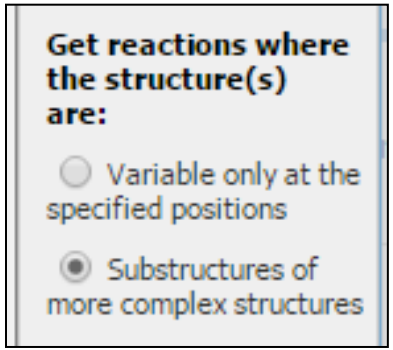
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner使用简介
- SciFinder常见问题及解决

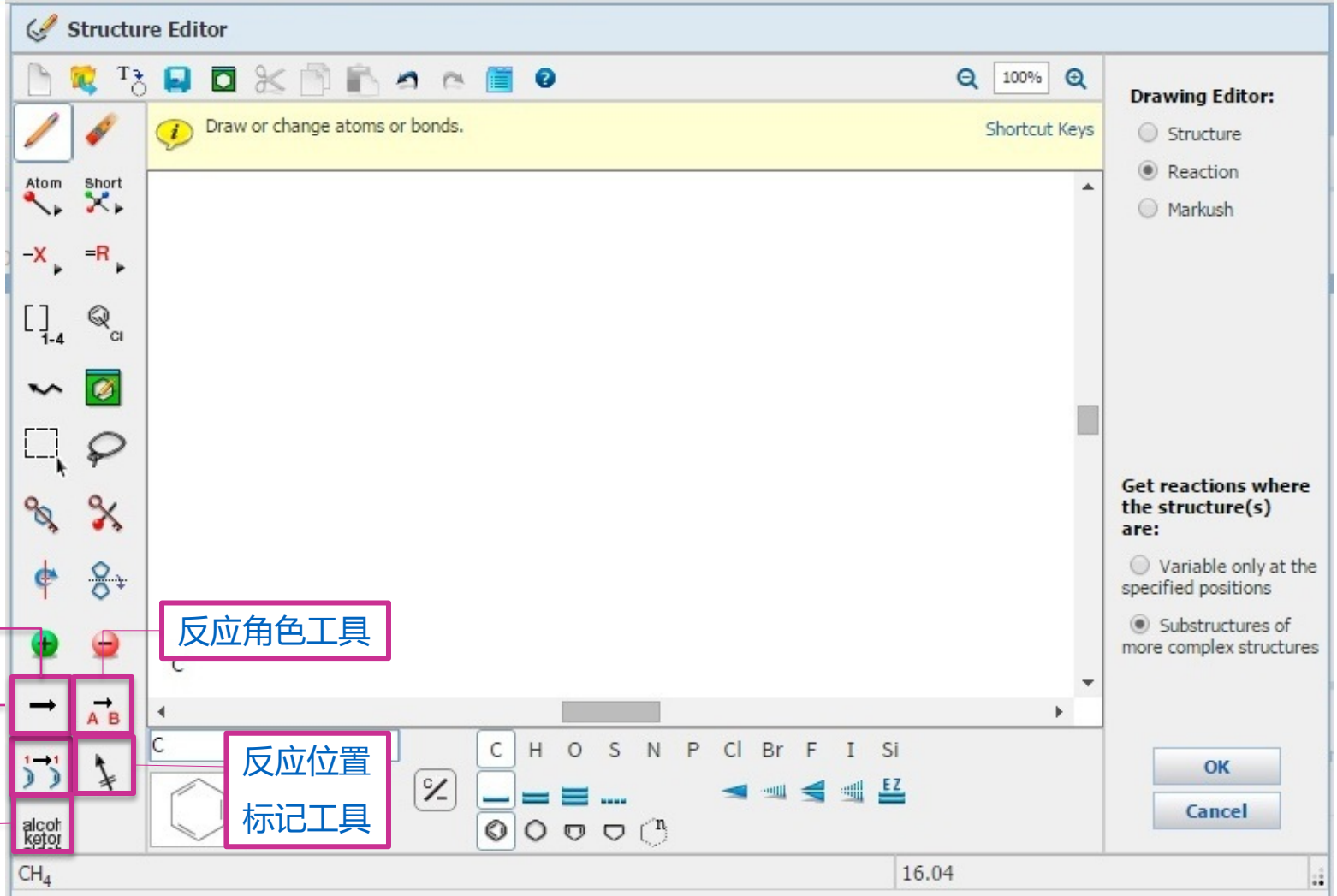
SciFinder检索选项——反应检索

- 检索选项
  - 结构式

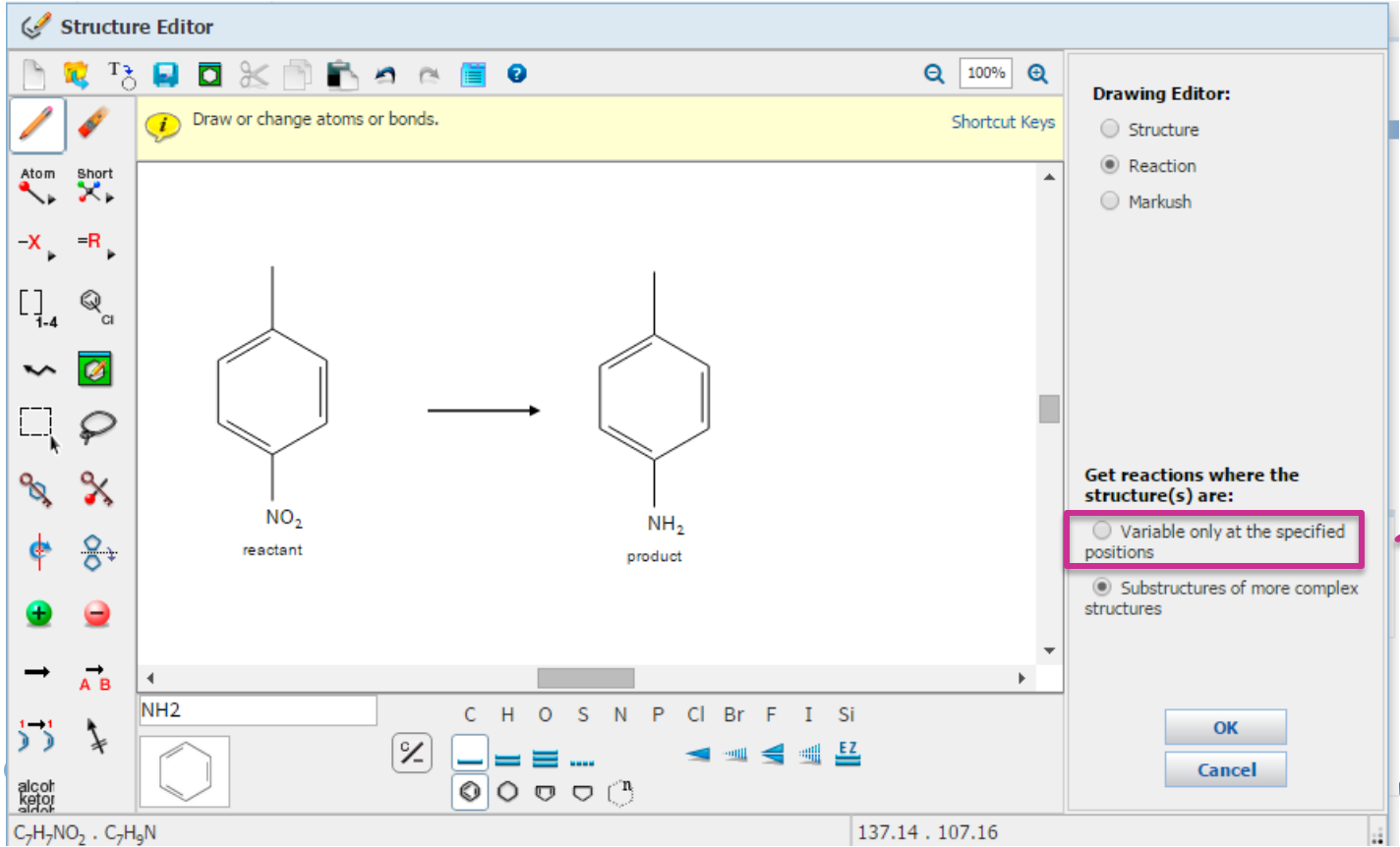


- 常用获取方法
  - 已知物质：由物质获取反应
  - 已知文献：从文献中获取反应
  - 精确结构反应检索
  - 亚结构反应检索




Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
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
反应位置标记工具
官能团列表

SciFinder反应检索——精确反应检索

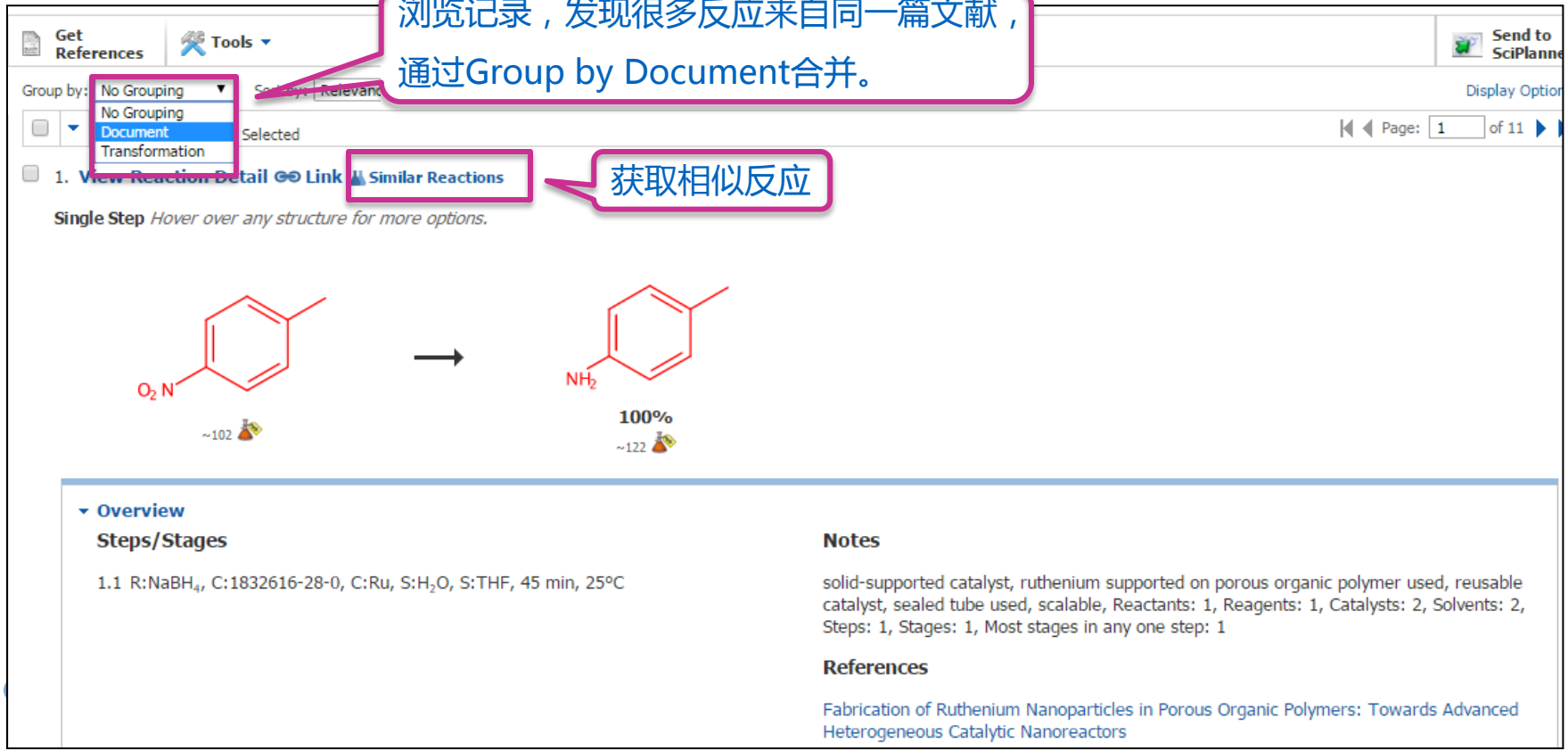


精确反应检索

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。

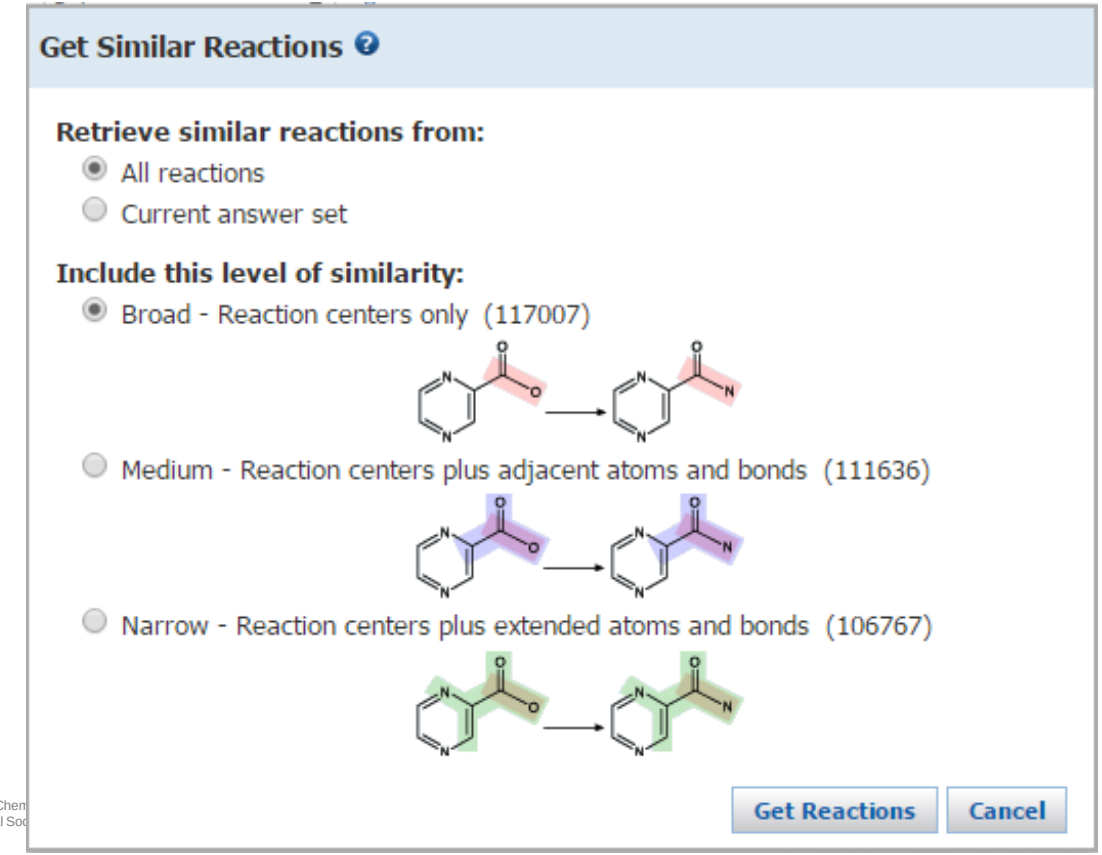
获取相似反应



获取相似反应

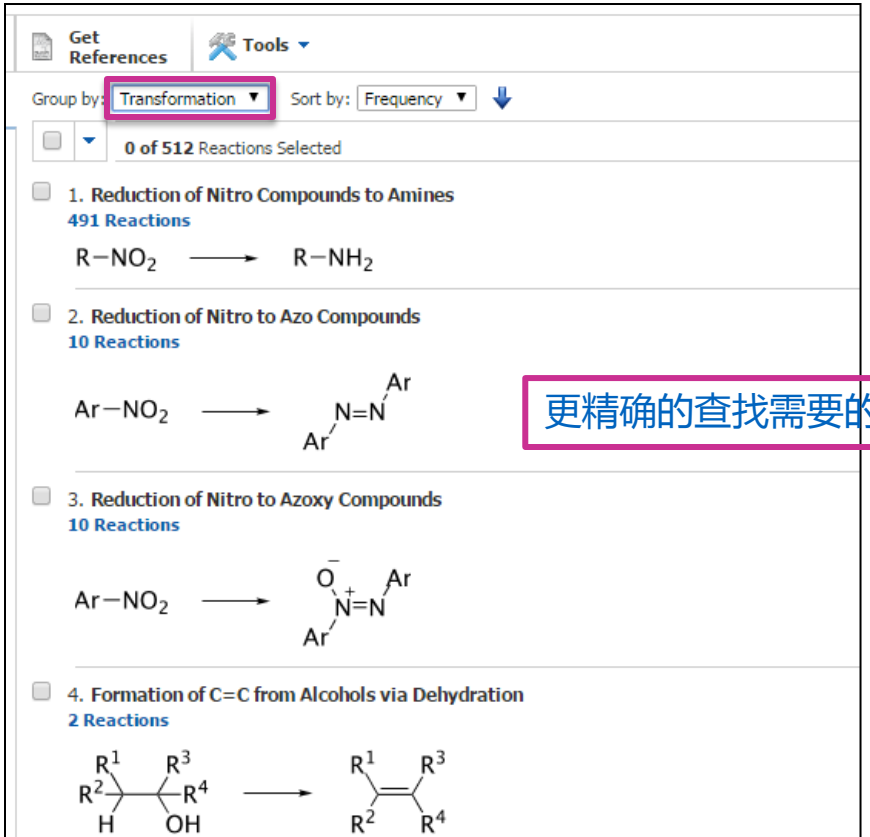
选择相似反应的相似限制：

- 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



SciFinder®
A CAS Solution

按照反应类型排序

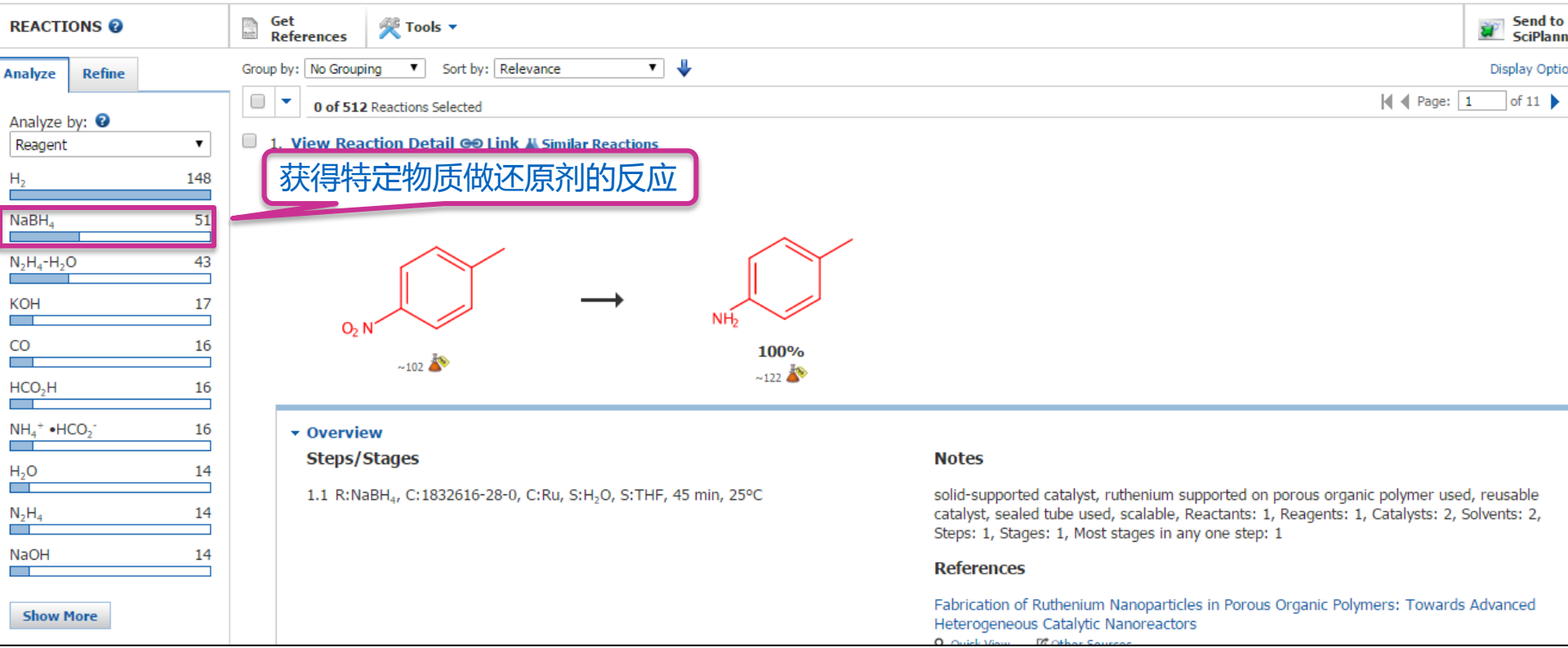


更精确的查找需要的反应

SciFinder® A CAS Solution

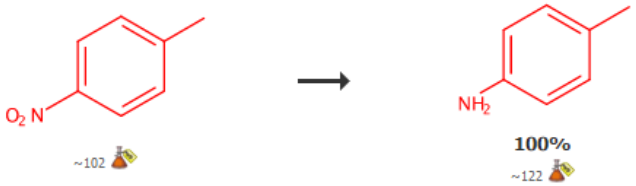
CAS® A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

反应检索结果的筛选


REACTIONS
Get References
Tools
Send to SciPlann
Analyze
Refine
Group by: No Grouping
Sort by: Relevance
Display Optio
0 of 512 Reactions Selected
Page: 1 of 11
Analyze by:
Reagent
H2 148
NaBH4 51
N2H4-H2O 43
KOH 17
CO 16
HCO2H 16
NH4+ •HCO2- 16
H2O 14
N2H4 14
NaOH 14
Show More
1. View Reaction Detail Link Similar Reactions
获得特定物质做还原剂的反应
O2N
NH2
~102
100%
~122
Overview
Steps/Stages
1.1 R:NaBH4, C:1832616-28-0, C:Ru, S:H2O, S:THF, 45 min, 25°C
Notes
solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1
References
Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

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

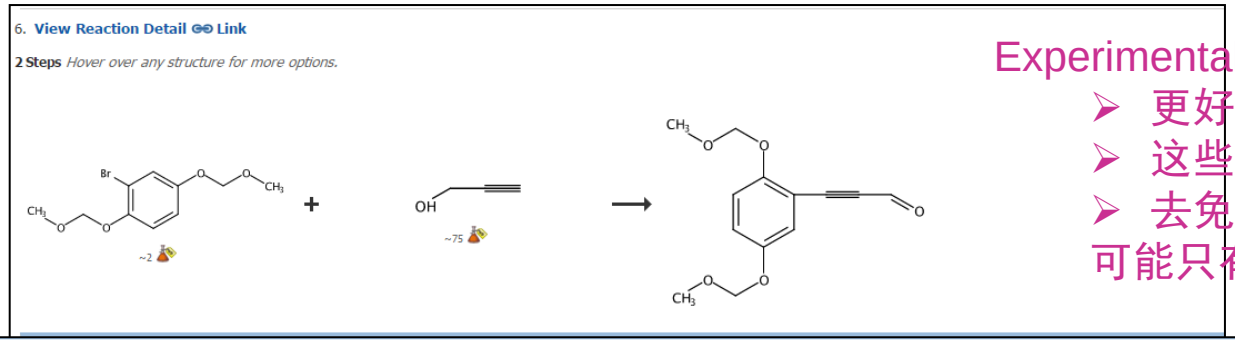
不用阅读全文，直接获得包含实验过程的反应记录

▾ **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%.

SciFinder囊括最大的反应实验过程合集



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?
- 去免费的Supporting Information查?

可能只有图谱。

Experimental Procedure

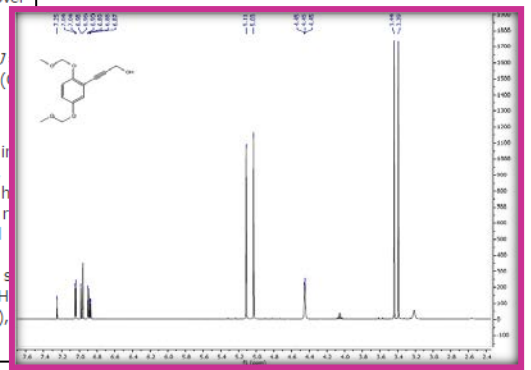
JOURNAL OF NATURAL PRODUCTS

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 into H_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*[12] (**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 (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) i 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 h 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 r 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).

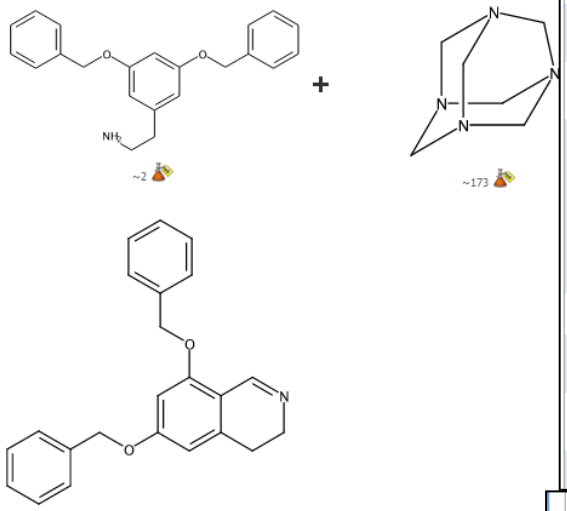


MethodsNow

Asymmetric formal synthesis of schulzeines A and C

By Jang, Jaebong; Jung, Jong-Wha; Ahn, Jaeseung; Sim, Jaehoon; Chang, Dong-Jo; Kim, Dae-Duk; Suh, Young-Ger
From Organic & Biomolecular Chemistry, 10(27), 5202-5204; 2012
Published by Royal Society of Chemistry

Reaction Steps 1 2 3 4 5 6 7 8 9 10 11



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

Print/Export Close

多步反应中，原文没有
描述的实验过程以灰色展示

物质信息

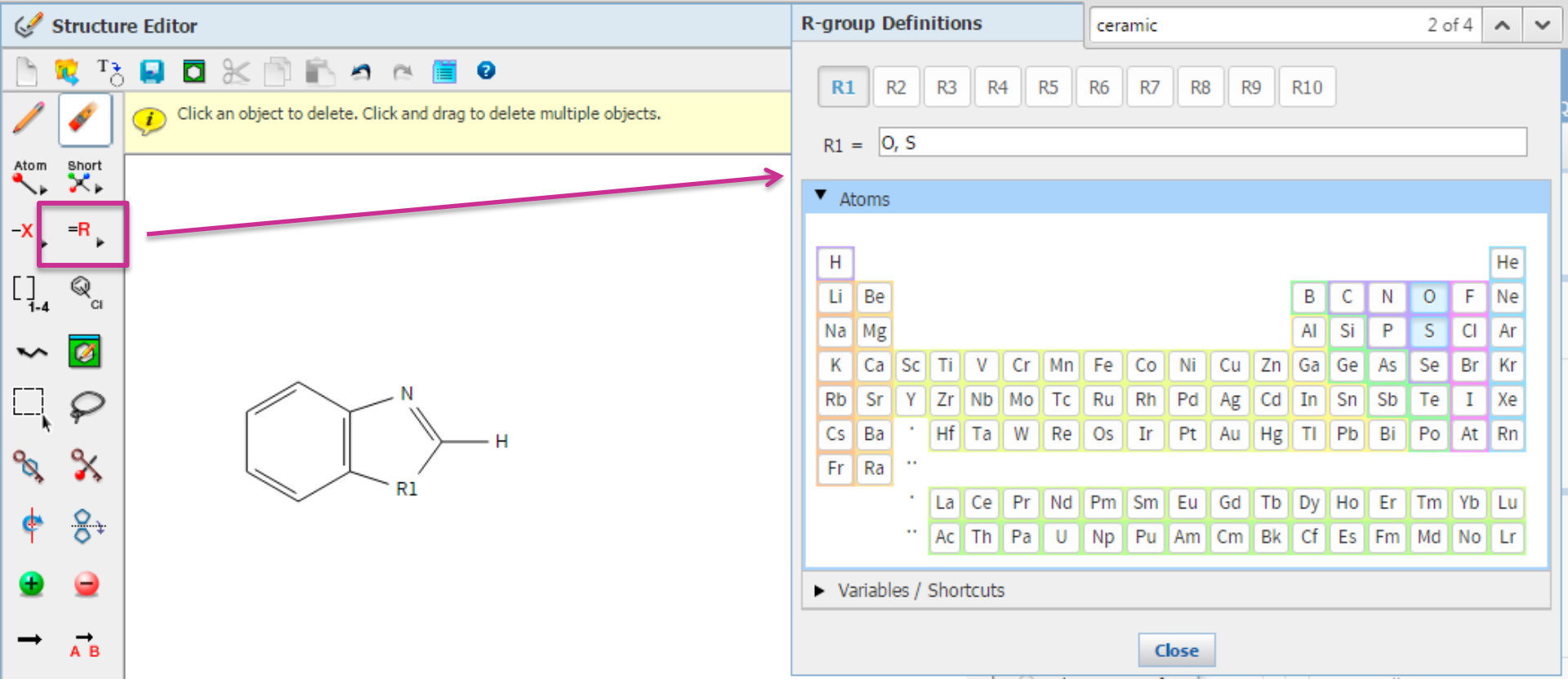
实验过程

图谱信息

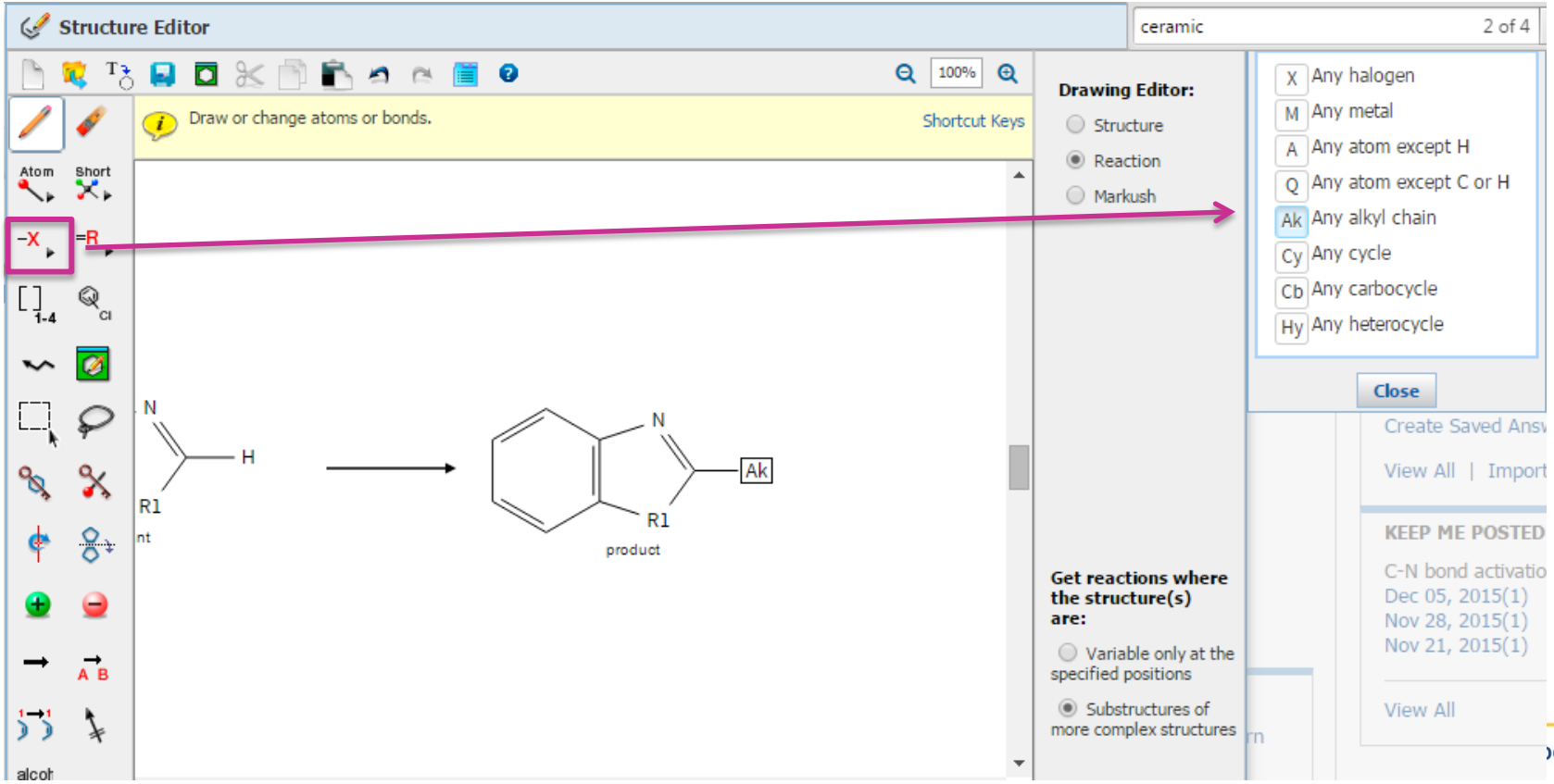
保存/导出方法

SciFinder® A CAS Solution

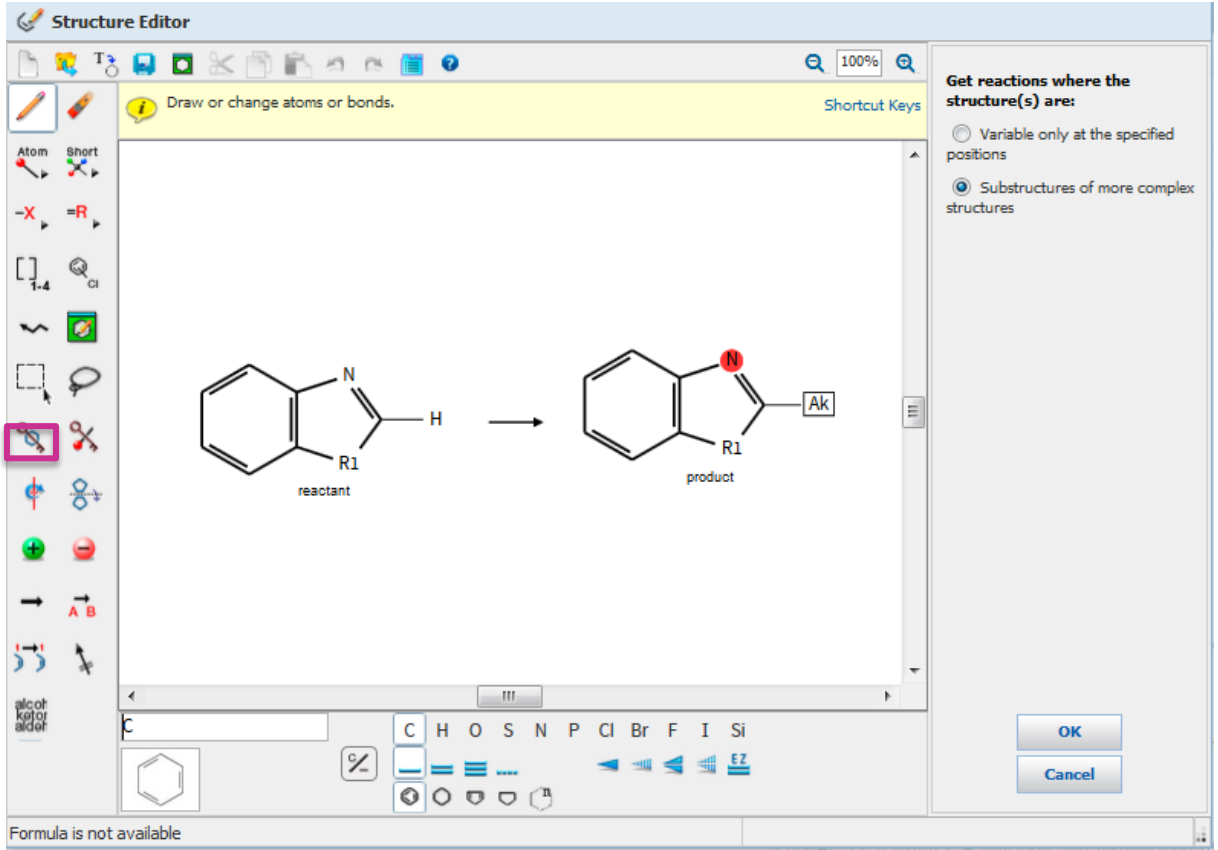
亚结构反应检索——通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索——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——通过C-H活化对苯并噻唑或者恶唑进行烷基化



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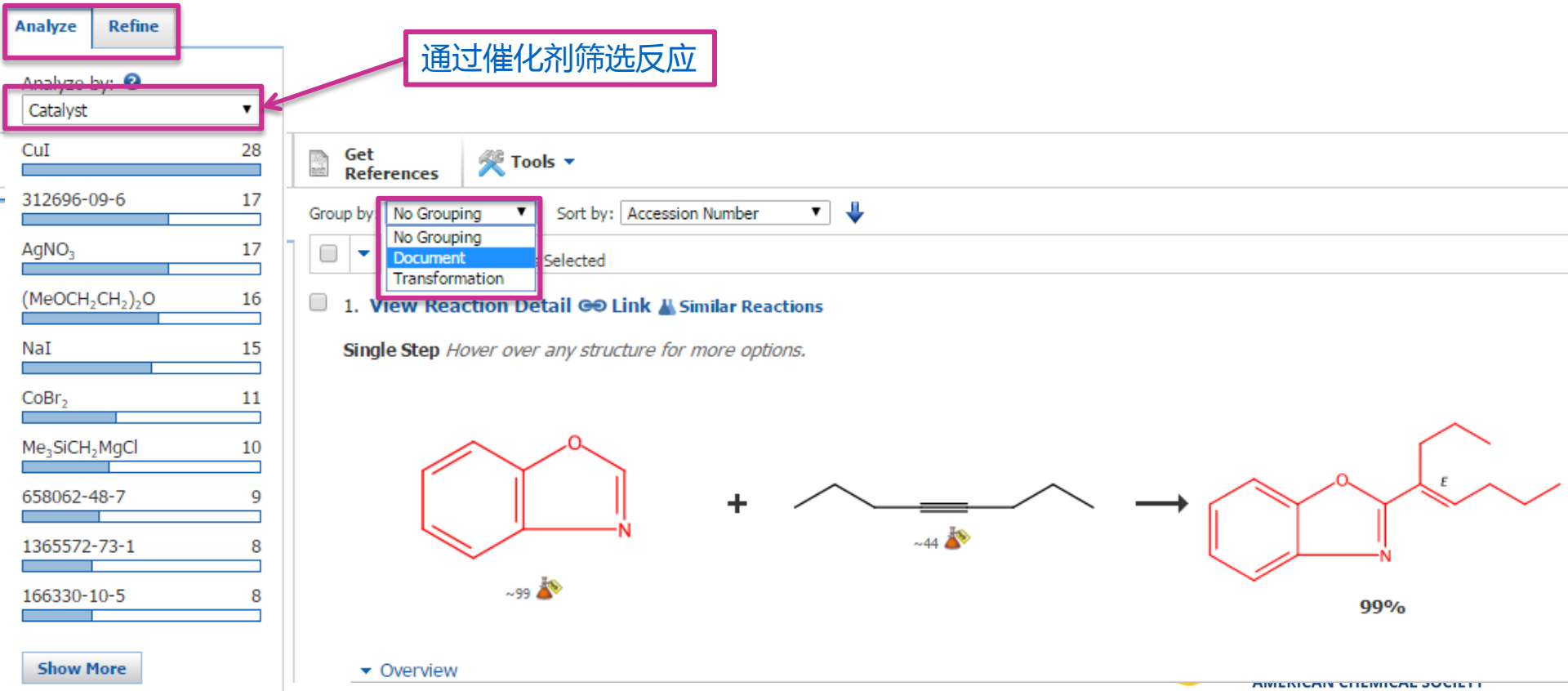
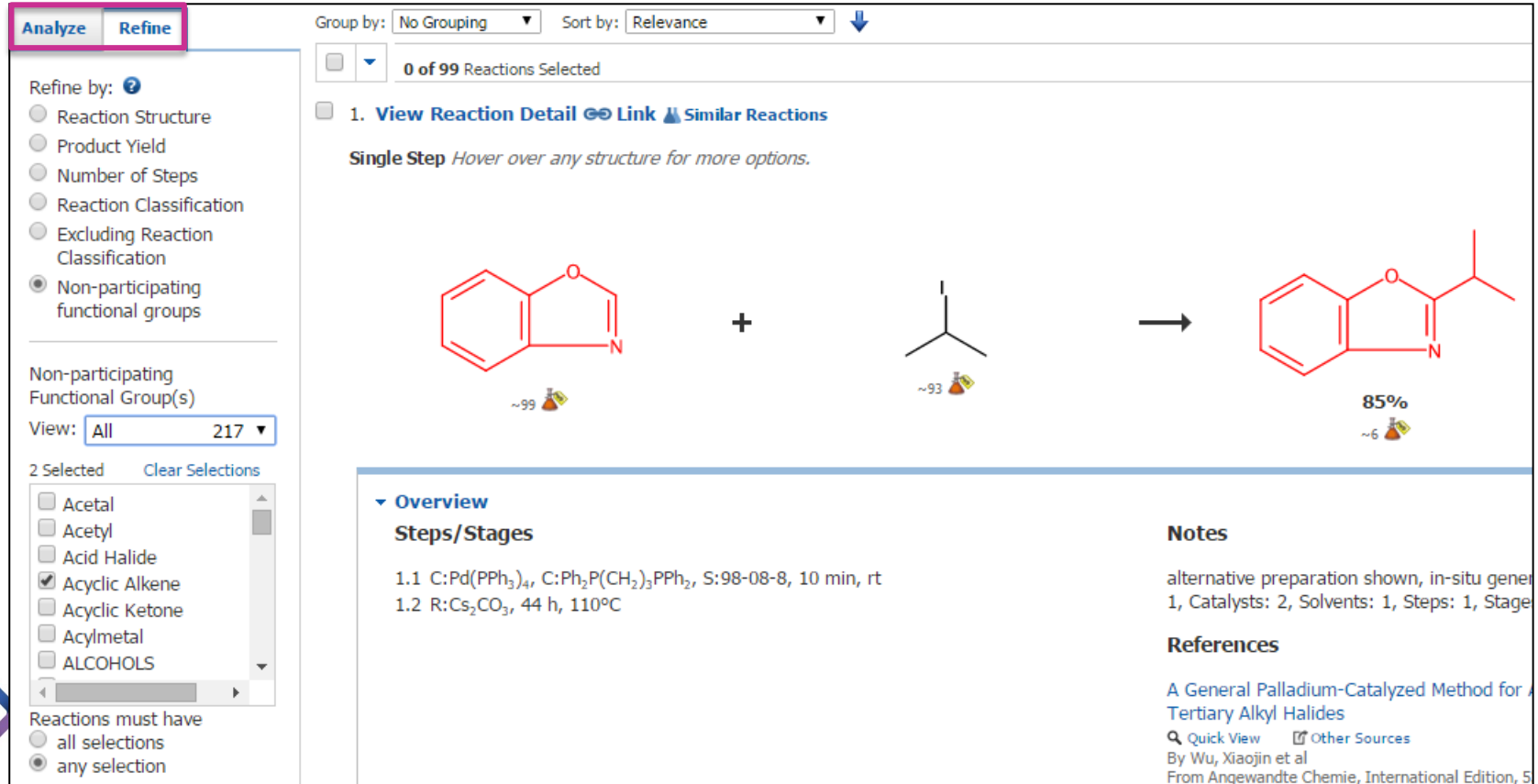
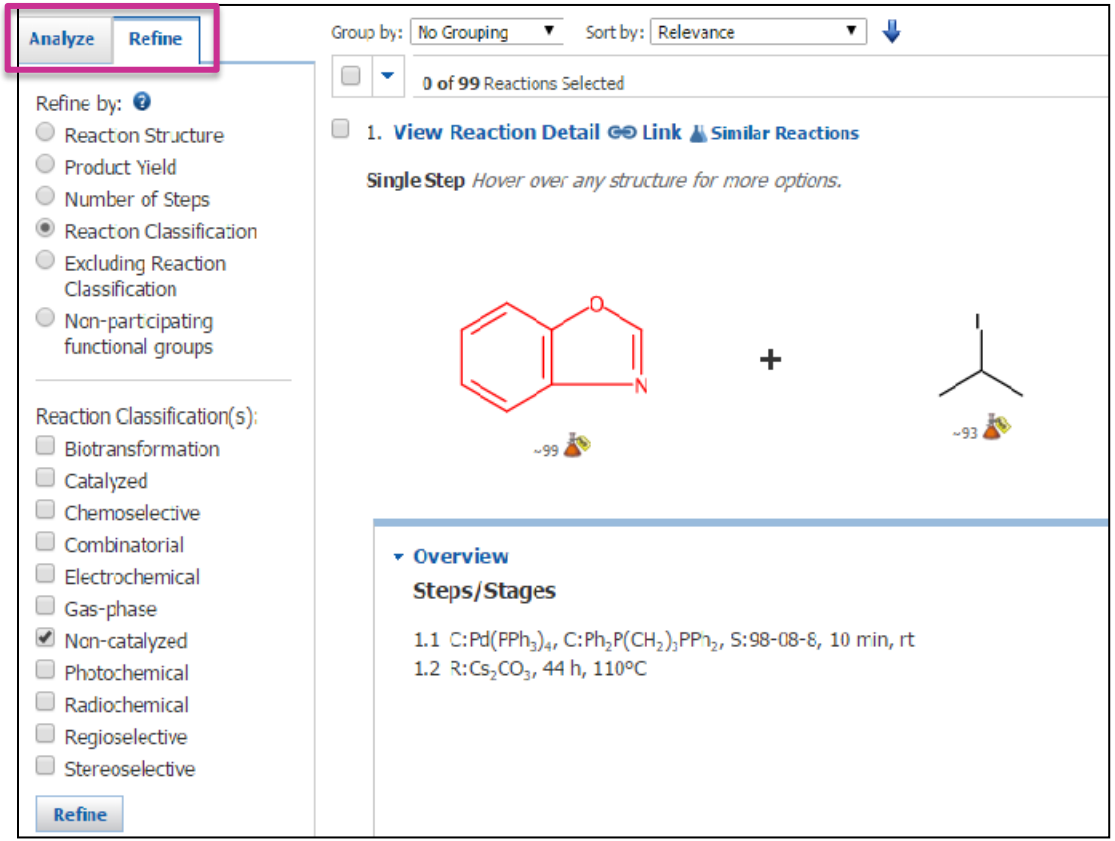


通过后处理工具筛选反应



通过后处理工具筛选反应



反应检索练习

1. 检索苯甲醛氧化成苯甲酸的反应，有哪些常用的氧化剂？用高锰酸钾做氧化剂的反应条件？

2. 底物上有伯羟基和仲羟基，寻找伯羟基氧化成醛而仲羟基不变的反应条件？

提纲

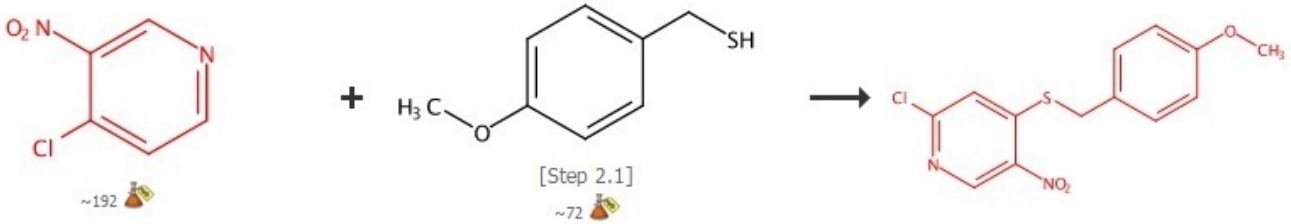
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner使用简介
- SciFinder常见问题及解决

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

SciPlanner

SciPlanner_11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

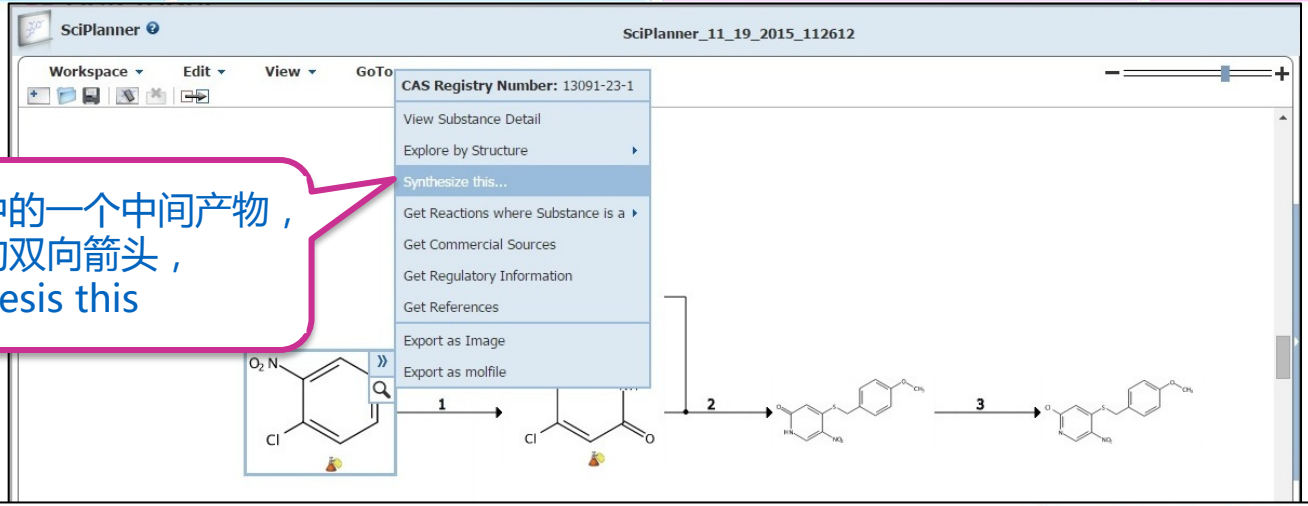
workspace 下新建一个文件

Clear Reactions

进入Sciplanner，将刚推送过来的反应拖动到屏幕中间

Your Workspace is empty.

Drag items from the reference, substance, and reaction libraries (on the right) to this area.



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

Get References | Tools | Send selected records to SciPlanner. | Send to SciPlanner

Group by: No Grouping | Sort by: Accession Number | Display Options

1 of 34 Reactions Selected | Page: 1 of 3

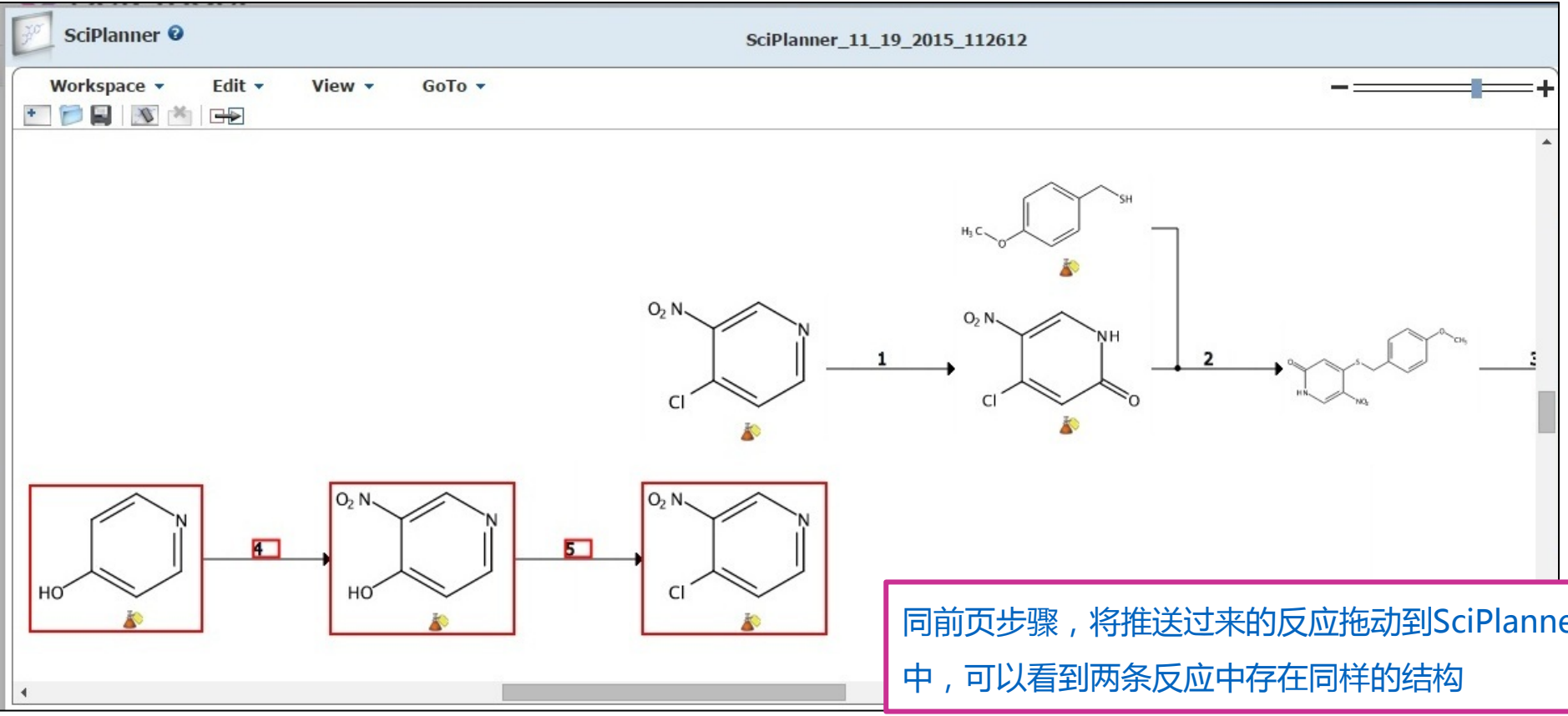
1. View Reaction Detail Link

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

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

关于SciPlanner使用简介



SciPlanner

SciPlanner_11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

点击 Workspace，选择其中的 Export 输出结果

用鼠标将两个同样的结构拖动至重叠状态，两条反应合并

Export

* Required

For:

Offline Review
- Portable Document Format (*.pdf)
- Citations (*.ris)
- Image (*.png)

Saving Locally
- SciPlanner eXchange (*.pkx)

Details:

File Name: *
SciPlanner_11_19_2015_112612

Title

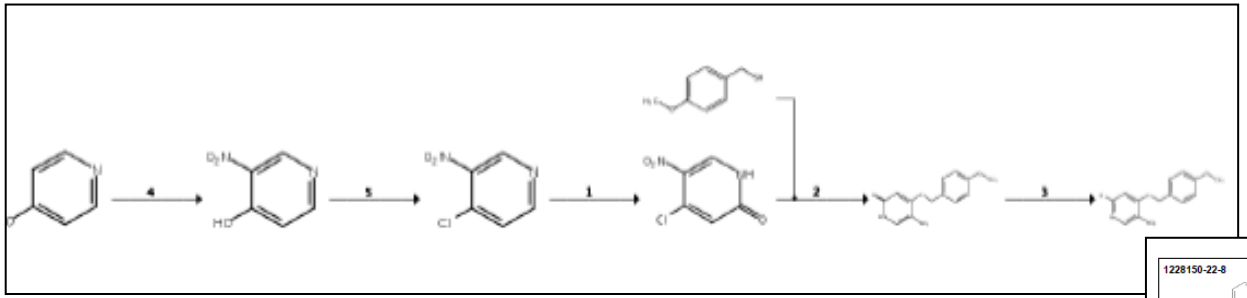
Include:
- SciPlanner Image
- Reaction Details
- Substance Details
- Reference Details

Export Cancel

选择适当的输出格式，输出结果

SciFinder®
A CAS Solution

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 $C_{13}H_{14}N_2O_4S$ 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		

SciFinder® A CAS Solution

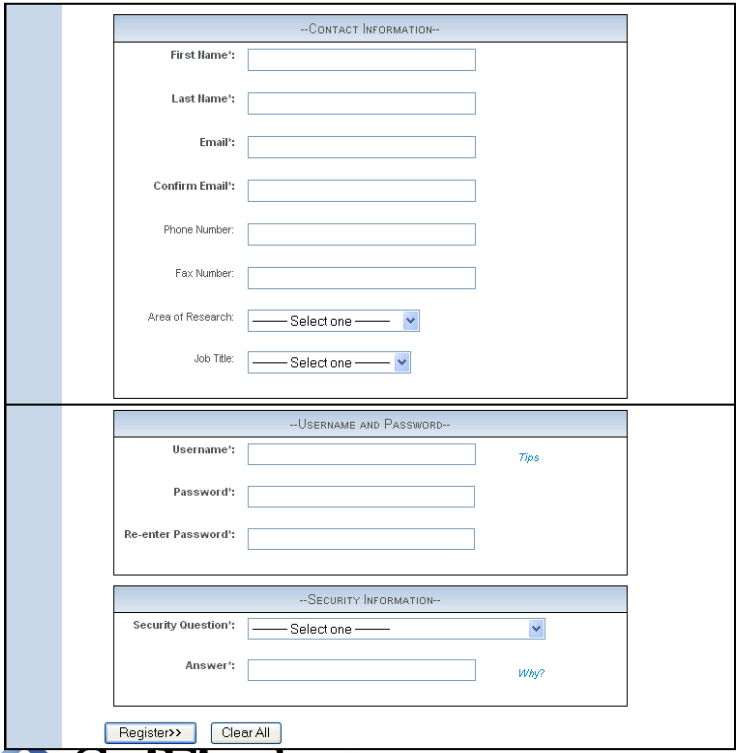
提纲

- 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使用简介
- SciFinder常见问题及解决

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 @、#、%、&、*）

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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- 严禁账号分享
- 严禁将账号用于非学术研究

美国化学文摘社北京代表处

010-62508026

china@acsi.info

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谢 谢！

朱传娴
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