朱传娴
客户顾问
hzhu@acs-i.org

如何使用SciFinder获取医药信息

湖北医药学院

2019.6.4

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

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

SciFinder® A CAS SOLUTION

CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水
染料、有机颜料 ;合成橡胶 ;纺织品、纤维

应用化学各领域 ：

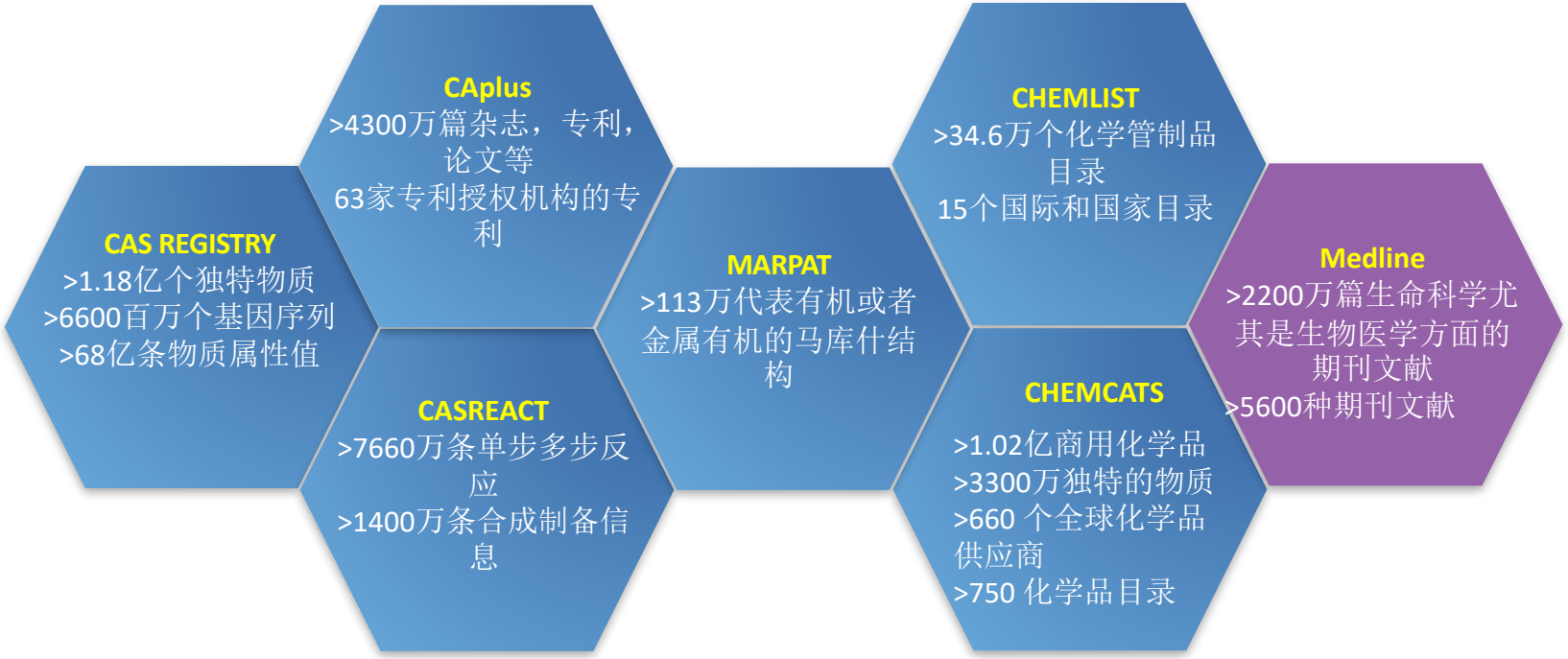
大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学

SciFinder® A CAS SOLUTION

SciFinder覆盖的数据库



SciFinder® A CAS SOLUTION

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

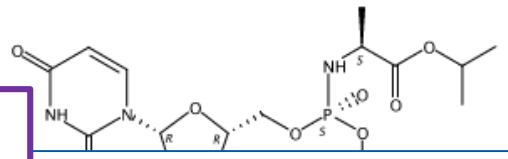
Concepts

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

SCIFINDER® A CAS SOLUTION

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。

SCIFINDER® A CAS SOLUTION

提纲

- 美国化学文摘社简介
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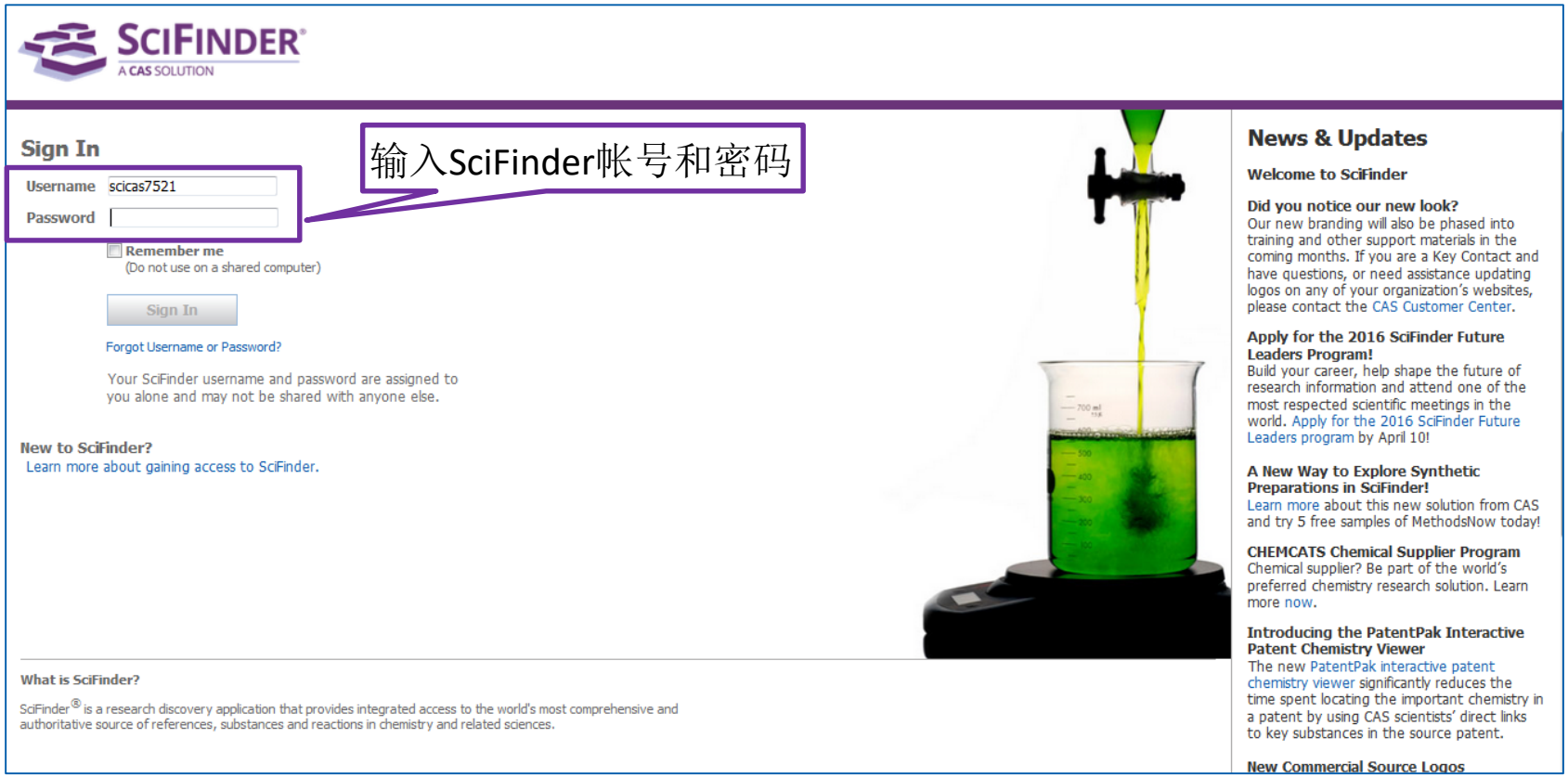
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

SciFinder登录网址: https://scifinder.cas.org/



SCIFINDER®
A CAS SOLUTION

SciFinder主界面

SciFinder检索——文献检索

- 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

SCIFINDER® A CAS SOLUTION

文献检索——主题

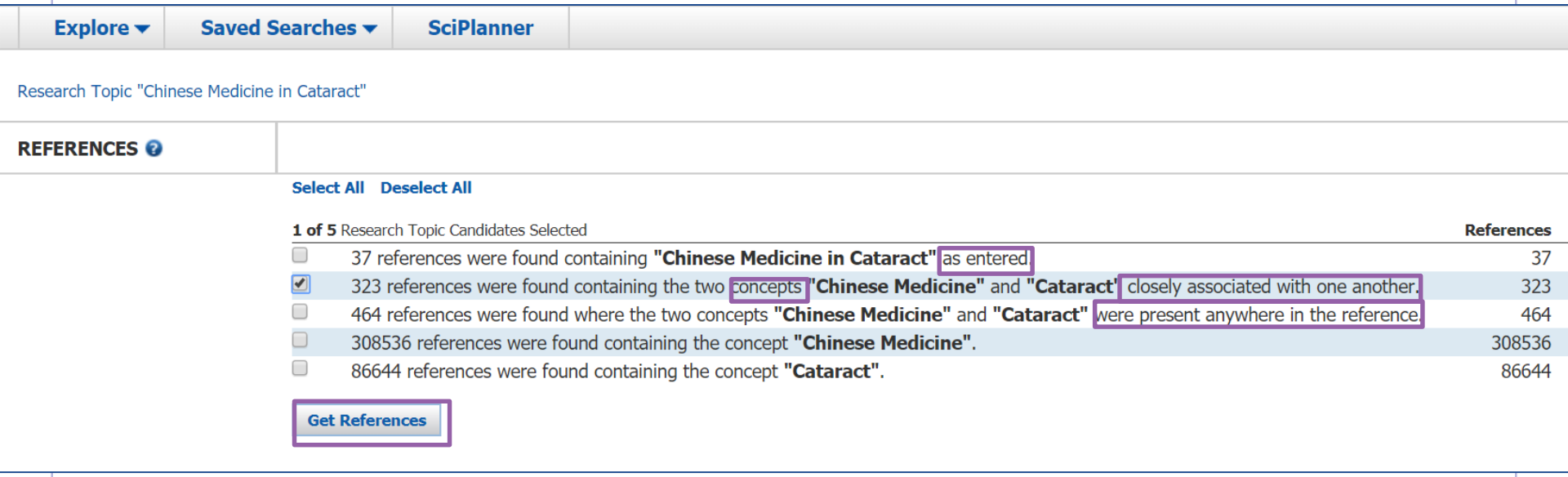
主题检索：中药在白内障治疗中的应用

检索式： Chinese Medicine in Cataract

关键词之间用介词连接：in, with, of...

SCIFINDER
A CAS SOLUTION

主题检索的候选项



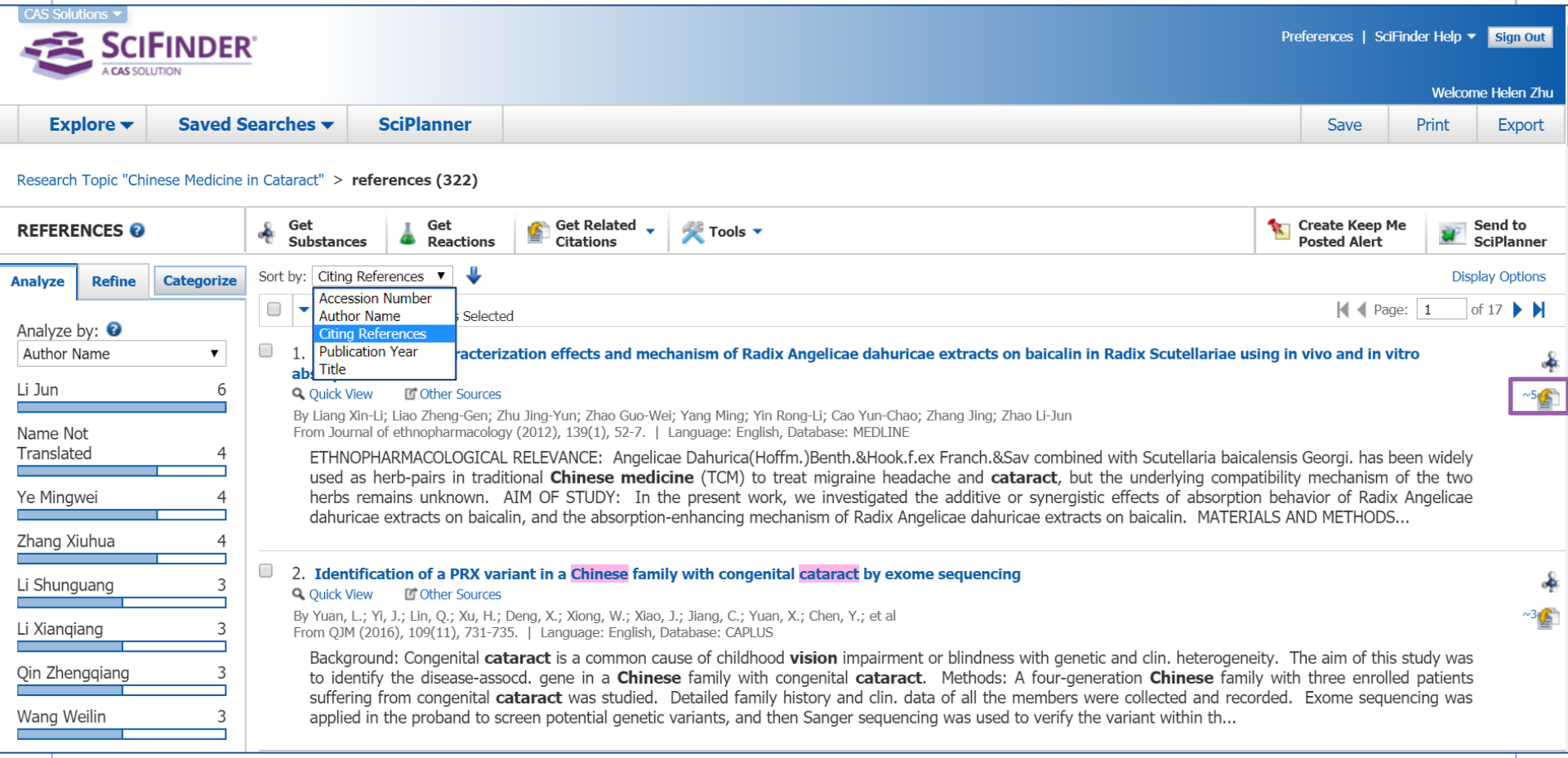
"Concepts"表示对主题词做了同义词的扩展；

"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；

SciFinder® A CAS SOLUTION

按被引次数排序— Citing References



Citing Reference: 帮助找到最重要的文献

SciFinder A CAS SOLUTION

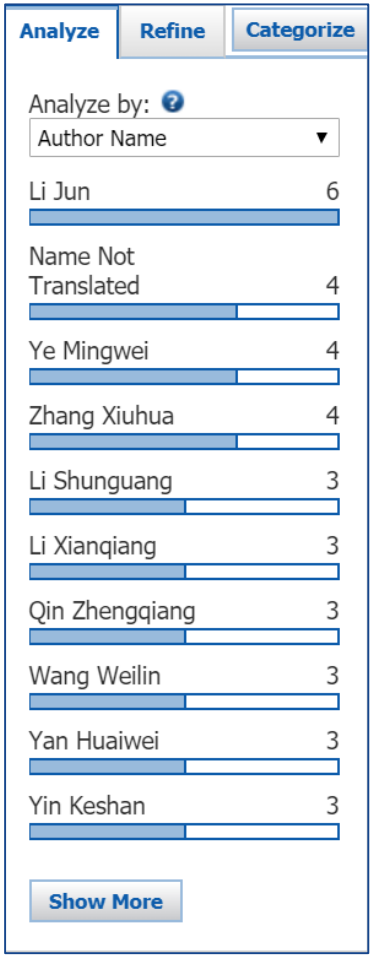
文献检索结果

SciFinder提供强大的文献处理工具，帮助处理文献

SciFinder A CAS SOLUTION

文献检索结果的Analyze

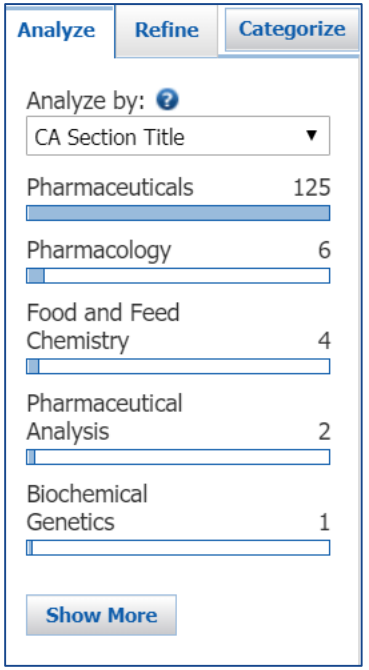
本领域研究人员



本领域研究机构、合作伙伴、竞争对手

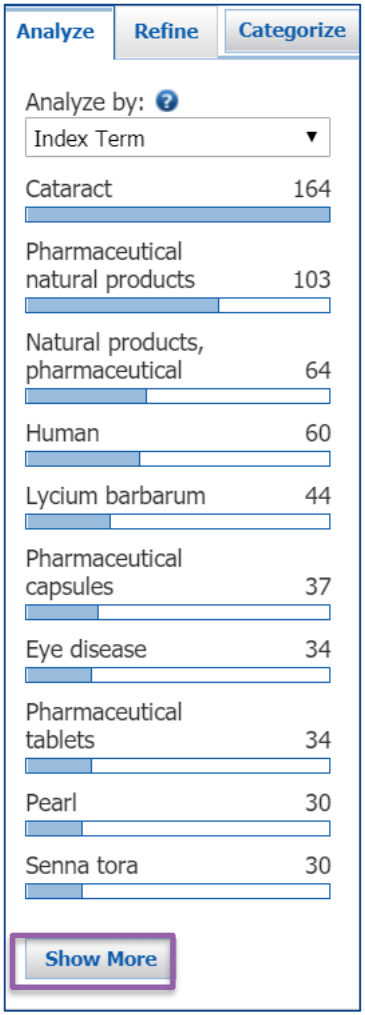
期刊

涉及学科领域



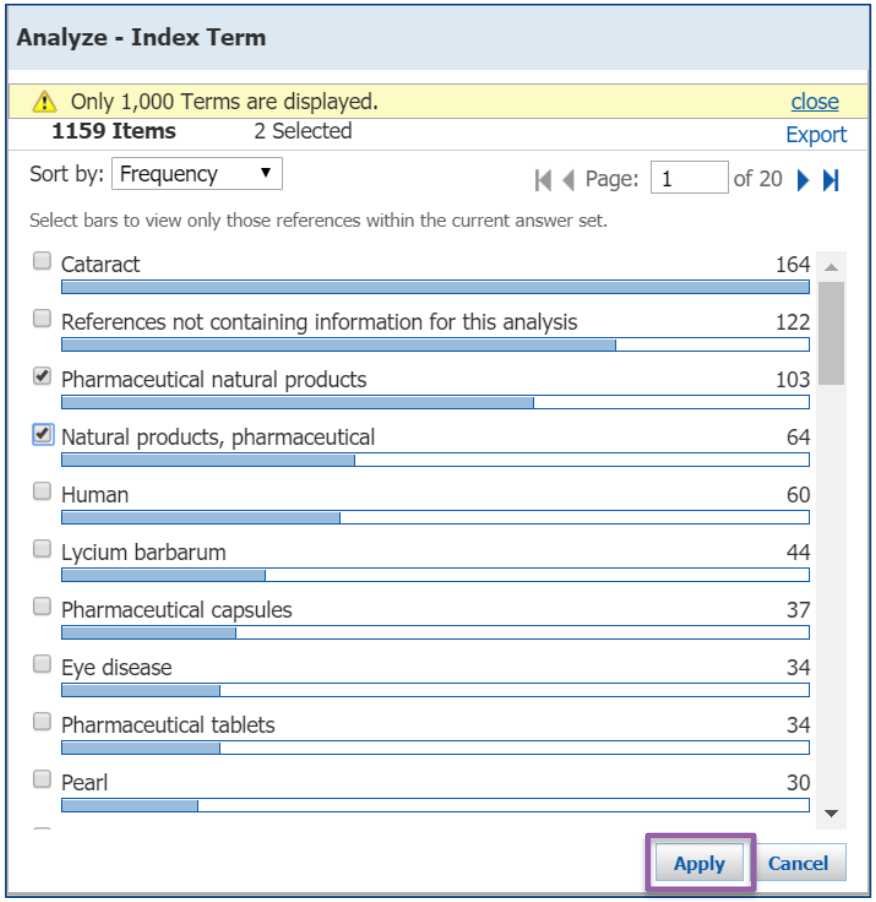
SciFinder® A CAS SOLUTION

文献检索结果的Analyze



Index Term：

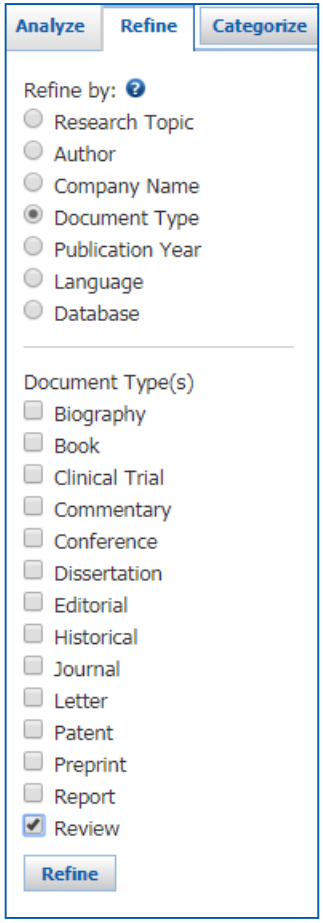
帮助用户了解涉及到的重要技术术语，并修正检索词

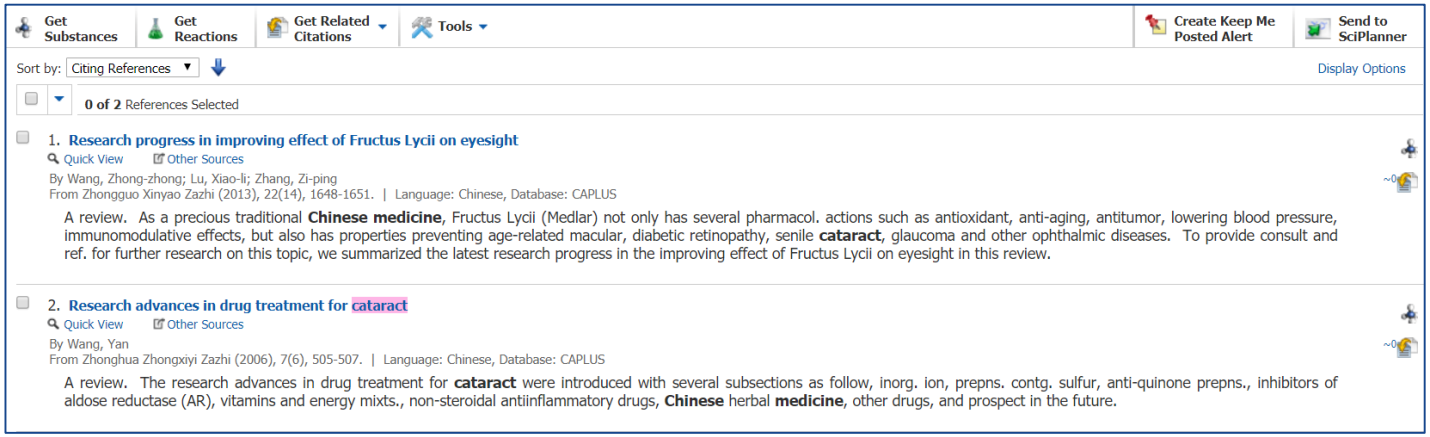


选择感兴趣的内容，点击Apply

SciFinder® A CAS SOLUTION

文献检索结果的Refine



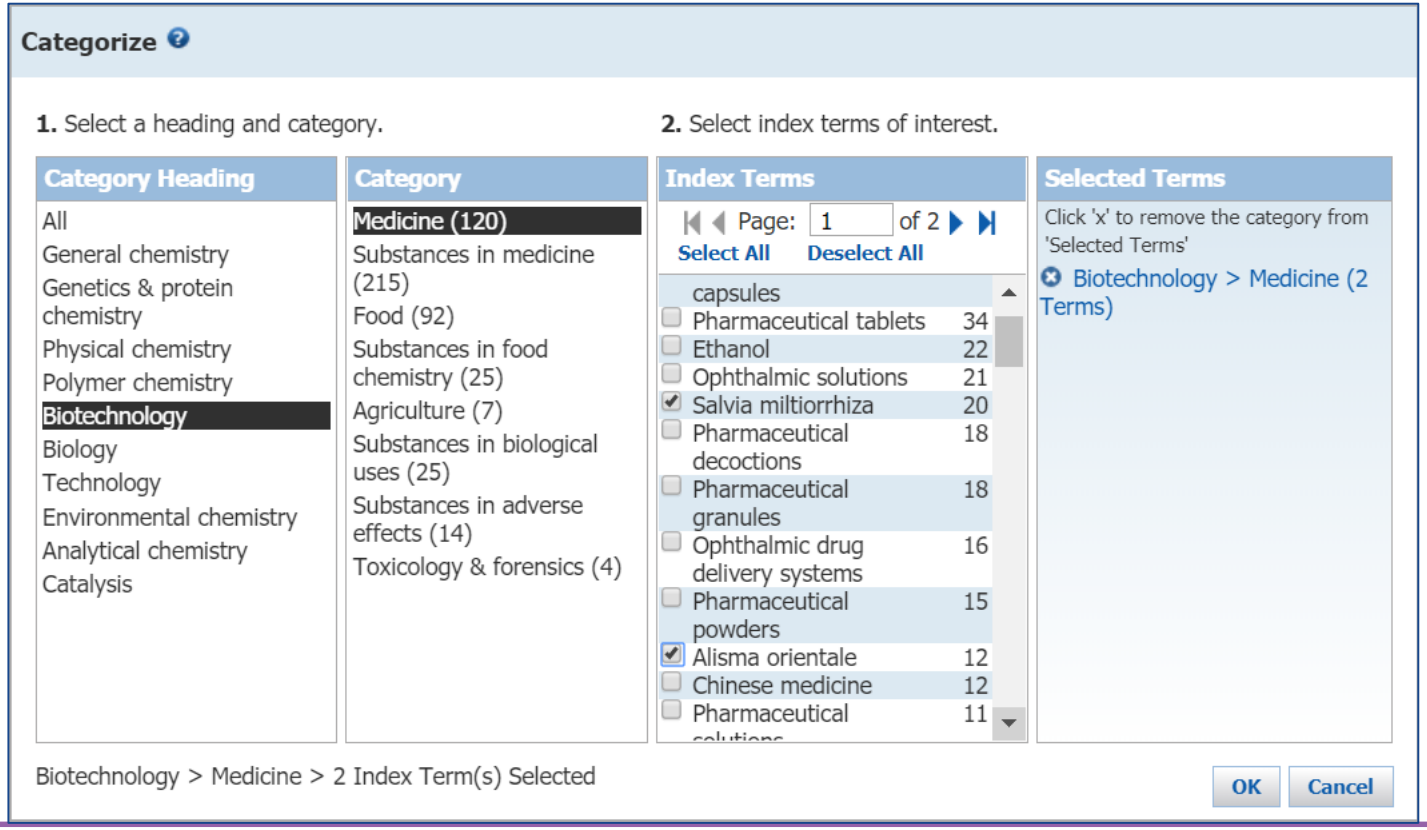


Refine：帮助用户迅速获得需要的文献

SciFinder® A CAS SOLUTION

文献检索结果的Categorize

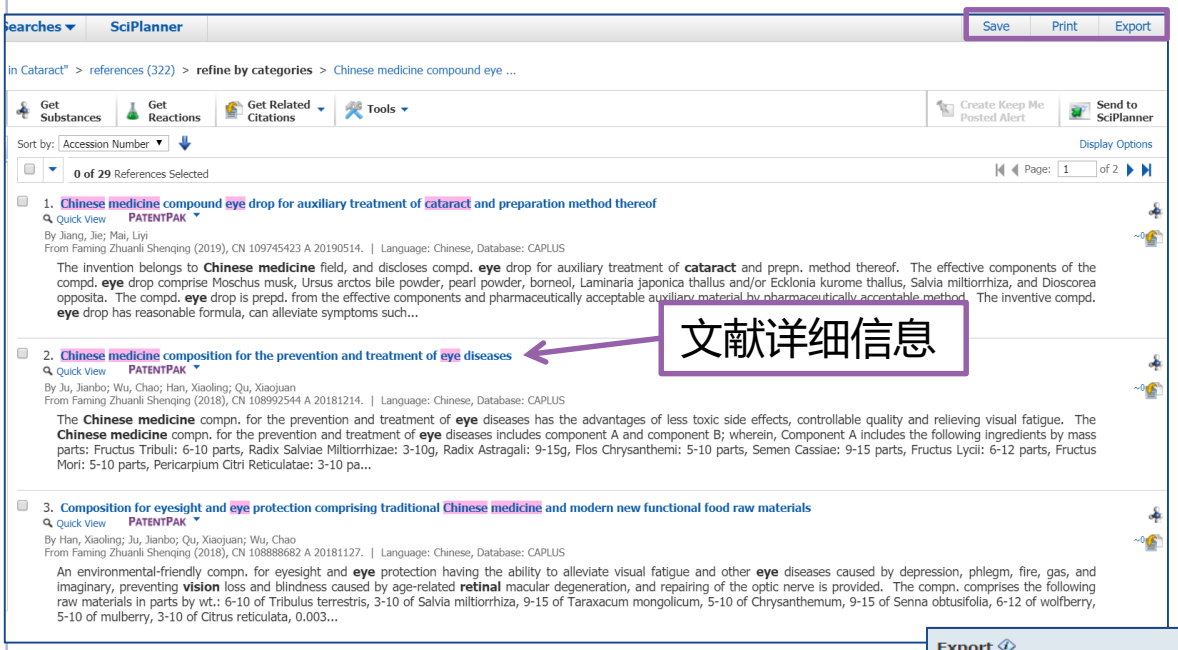
学科领域主分类　　学科领域副分类　　Index Term　　选中的Index Term



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。

SciFinder® A CAS SOLUTION

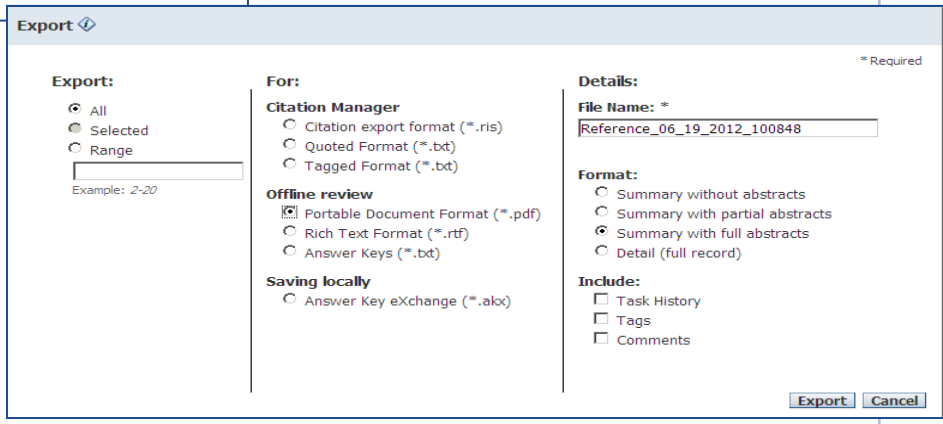
结果集的保存— Save, Print, Export



Save：保存在服务器上，方便以后登陆查看，每次可存1万条记录。

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

2. Chinese medicine composition for the prevention and treatment of eye diseases

By: Ju, Jianbo; Wu, Chao; Han, Xiaoling; Qu, Xiaojuan
Assignee: Xi'an Libang Pharmaceutical Co., Ltd., Peop. Rep. China

The Chinese medicine compn. for the prevention and treatment of eye diseases has the advantages of less toxic side effects, controllable quality and relieving visual fatigue. The Chinese medicine compn. for the prevention and treatment of eye diseases includes component A and component B; wherein, Component A includes the following ingredients by mass parts: Fructus Tribuli: 6-10 parts, Radix Salviae Miltiorrhizae: 3-10g, Radix Astragali: 9-15g, Flos Chrysanthemi: 5-10 parts, Semen Cassiae: 9-15 parts, Fructus Lycii: 6-12 parts, Fructus Mori: 5-10 parts, Pericarpium Citri Reticulatae: 3-10 parts, Xanthophyll: 0.003-0.012 part, Acer truncatum Bunge seed oil: 1-3 parts, zeaxanthin: 0.001-0.0044 part, milk: 20-50 parts, egg liq.: 5-20 parts, and plant juice: 2-5 parts.

Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
CN 108992544	PDF | PDF+ | Viewer	A		Dec 14, 2018	CN 2018-11062718	Sep 12, 2018

Priority Application

CN 2018-11062718	Sep 12, 2018

Indexing

Pharmaceu

Concepts 重要概念

Pharmaceutical natural products

Chaihu; Chinese medicine compn. for the prevention and treatment of eye diseases

Acer truncatum
Asthenopia
Adenophora
Buddleja

Substances 重要物质

557-04-0 Magnesium stearate	Page 7 in PATENTPAK
9004-32-4 Sodium carboxymethylcellulose	Page 7 in PATENTPAK
9004-53-9 Dextrin	Page 8 in PATENTPAK
9004-61-9 Hyaluronic acid	Page 7 in PATENTPAK
9063-38-1 Sodium Carboxymethyl starch	Page 7 in PATENTPAK

Chinese medicine compn. for the prevention and treatment of eye diseases

Modifier or additive use; Therapeutic use; Biological study; Uses

472-70-8 Cryptoxanthin	Page 2 in PATENTPAK
507-70-0	Page 2 in PATENTPAK
1309-38-2 Magnetitum, biological studies	Page 2 in PATENTPAK
7235-40-7 β-Carotene	Page 2 in PATENTPAK
11103-57-4 Vitamin A	Page 2 in PATENTPAK

QUICK LINKS
0 Tags, 0 Comments

PATENT INFORMATION
Dec 14, 2018
CN 108992544
A

APPLICATION
Sep 12, 2018
CN 2018-11062718

PRIORITY
Sep 12, 2018
CN 2018-11062718

SOURCE
Faming Zhuanli Shenqing
16pp.
Patent
2018
CODEN:CNXXEV

ACCESSION NUMBER
2018:2488106
CAN170:140195
CAPLUS

LANGUAGE
Chinese

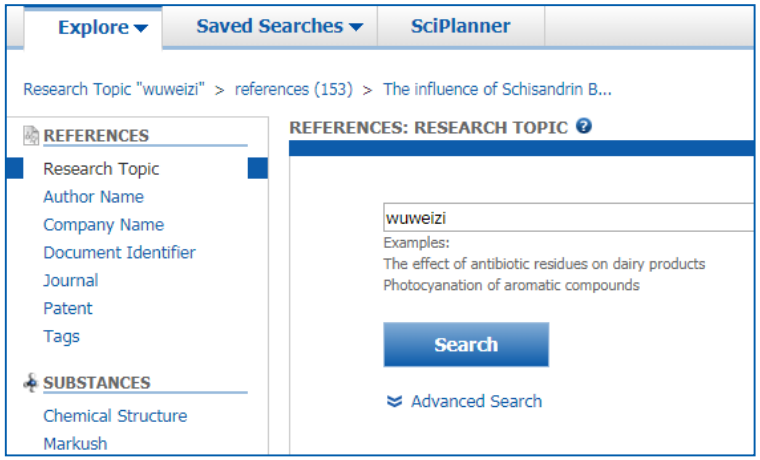
文献详情界面包括：
1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质，反应
7. 参考文献
8. 链接原文

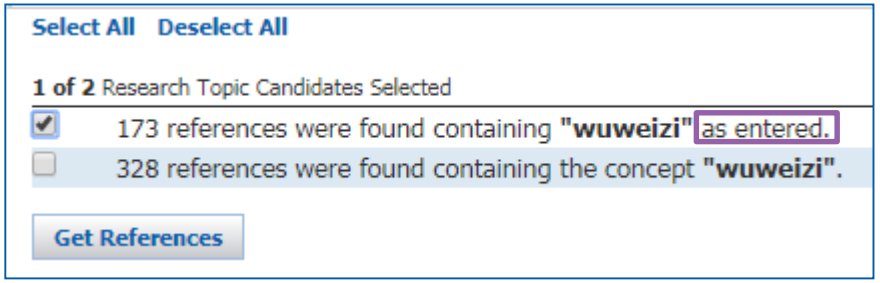
文献检索——中草药

主题检索：五味子

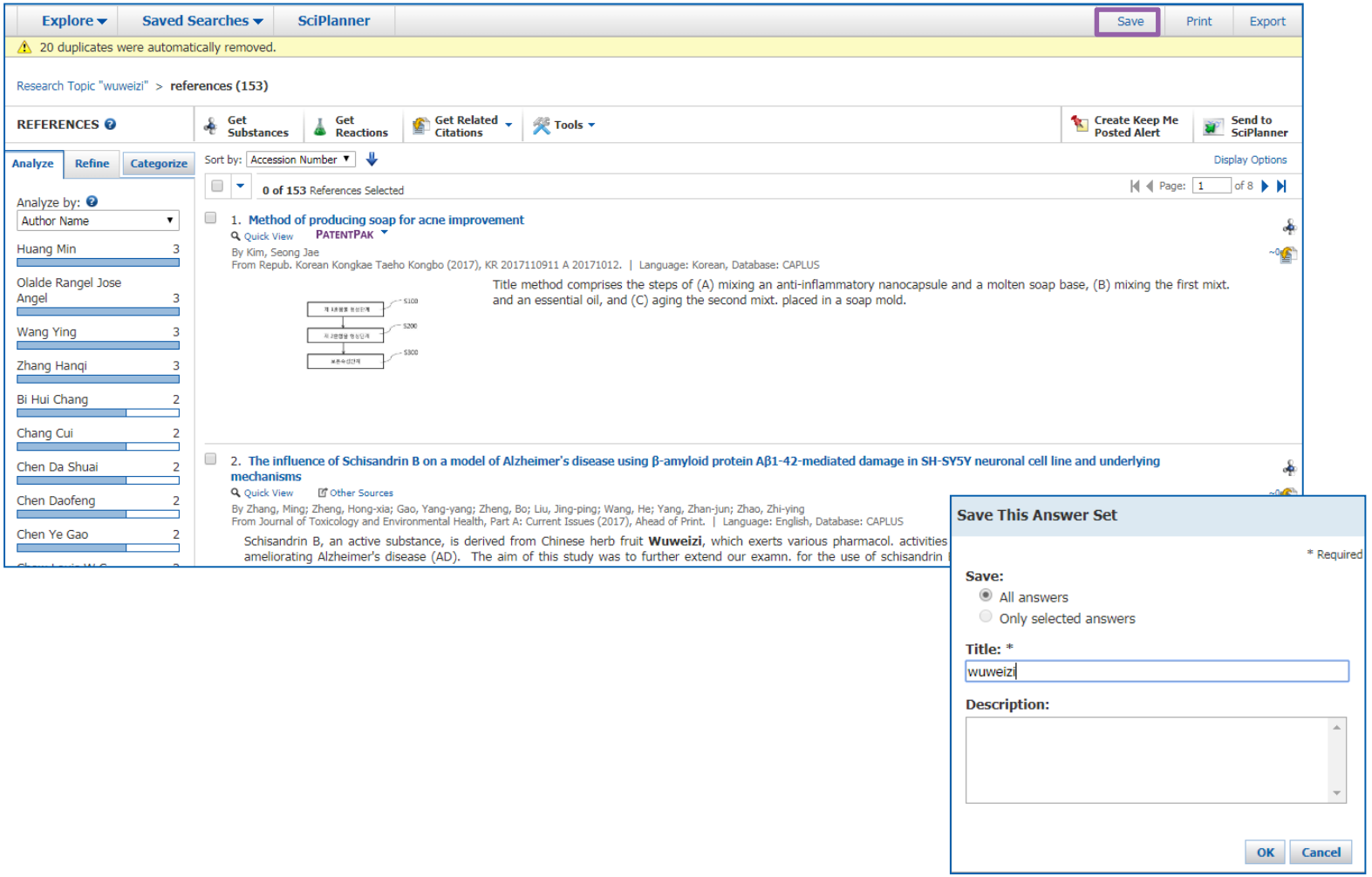
检索式： Wuweizi，Schisandra chinensis

第一步：中文名检索



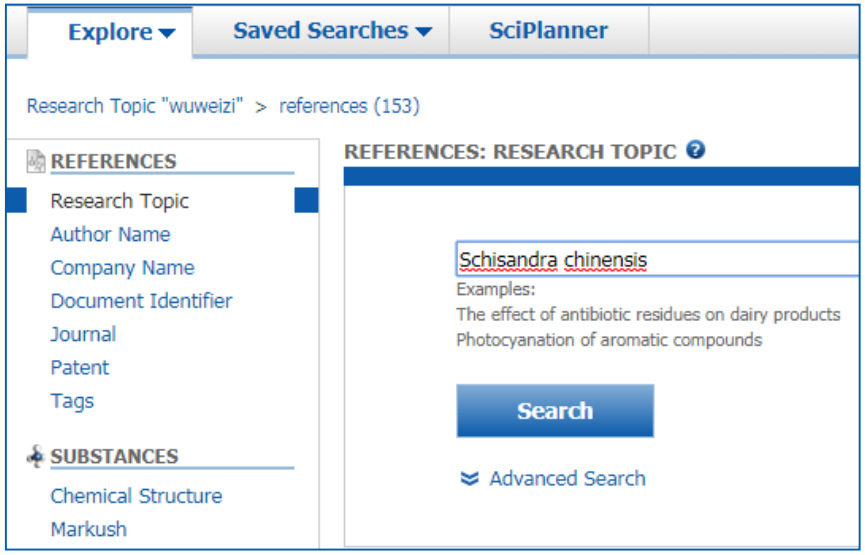


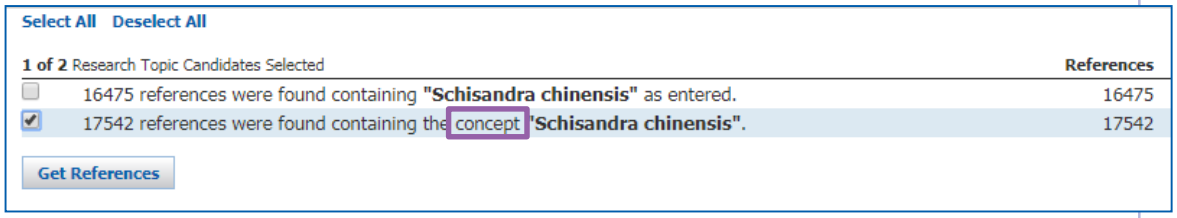
文献检索——中草药


Explore
Saved Searches
SciPlanner
Save
Print
Export
20 duplicates were automatically removed.
Research Topic "wuweizi" > references (153)
REFERENCES
Get Substances
Get Reactions
Get Related Citations
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Categorize
Sort by: Accession Number
Display Options
0 of 153 References Selected
Page: 1 of 8
Analyze by:
Author Name
Huang Min 3
Olalde Rangel Jose Angel 3
Wang Ying 3
Zhang Hanqi 3
Bi Hui Chang 2
Chang Cui 2
Chen Da Shuai 2
Chen Daofeng 2
Chen Ye Gao 2
1. Method of producing soap for acne improvement
Quick View
PATENTPAK
By Kim, Seong Jae
From Repub. Korean Kongkae Taeho Kongbo (2017), KR 2017110911 A 20171012. | Language: Korean, Database: CAPLUS
Title method comprises the steps of (A) mixing an anti-inflammatory nanocapsule and a molten soap base, (B) mixing the first mixt. and an essential oil, and (C) aging the second mixt. placed in a soap mold.
2. The influence of Schisandrin B on a model of Alzheimer's disease using β-amyloid protein Aβ1-42-mediated damage in SH-SY5Y neuronal cell line and underlying mechanisms
Quick View
Other Sources
By Zhang, Ming; Zheng, Hong-xia; Gao, Yang-yang; Zheng, Bo; Liu, Jing-ping; Wang, He; Yang, Zhan-jun; Zhao, Zhi-ying
From Journal of Toxicology and Environmental Health, Part A: Current Issues (2017), Ahead of Print. | Language: English, Database: CAPLUS
Schisandrin B, an active substance, is derived from Chinese herb fruit Wuweizi, which exerts various pharmacol. activities
ameliorating Alzheimer's disease (AD). The aim of this study was to further extend our examn. for the use of schisandrin
Save This Answer Set
* Required
Save:
All answers
Only selected answers
Title: *
wuweizi
Description:
OK
Cancel

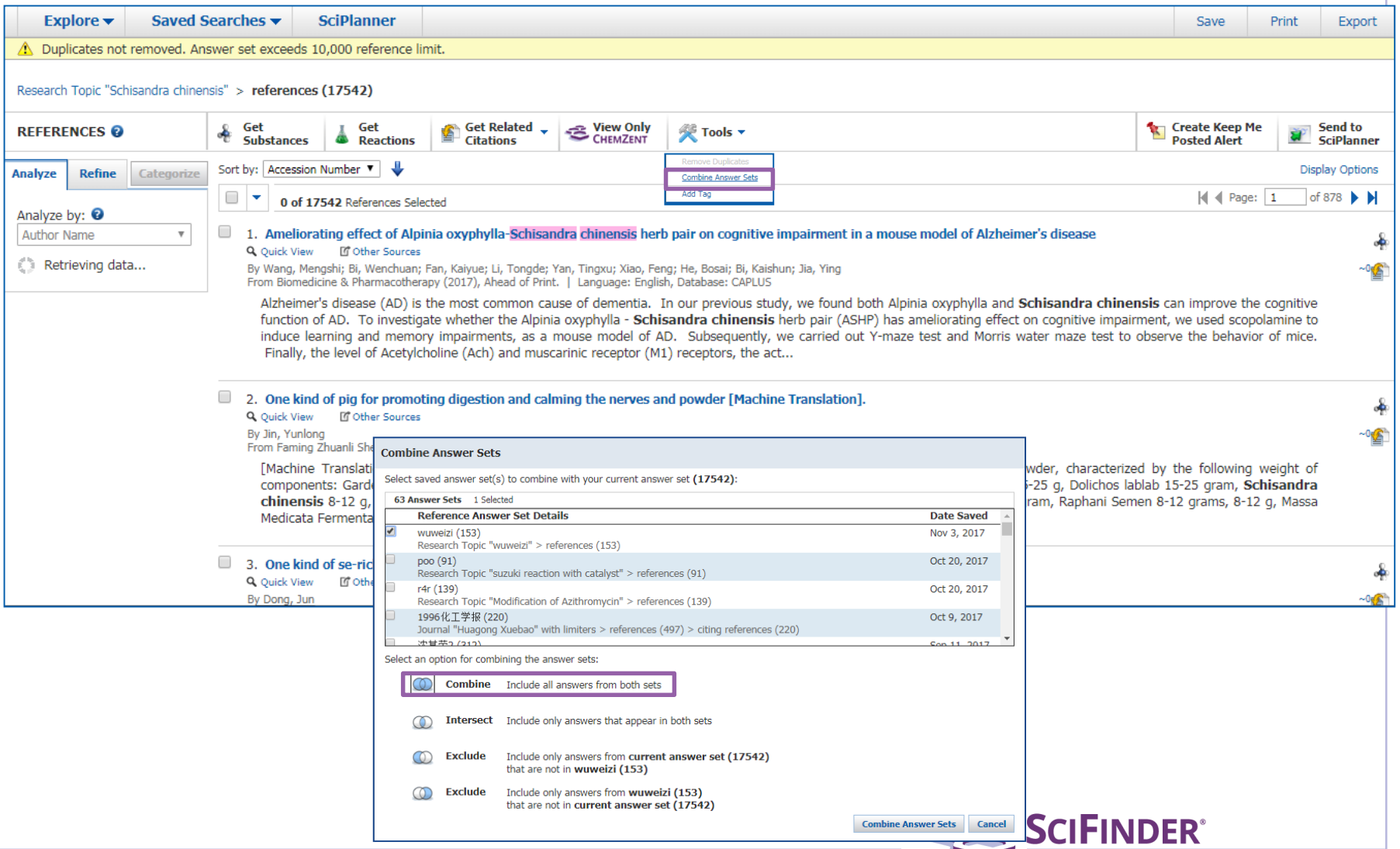
文献检索——中草药

第二步：拉丁名检索

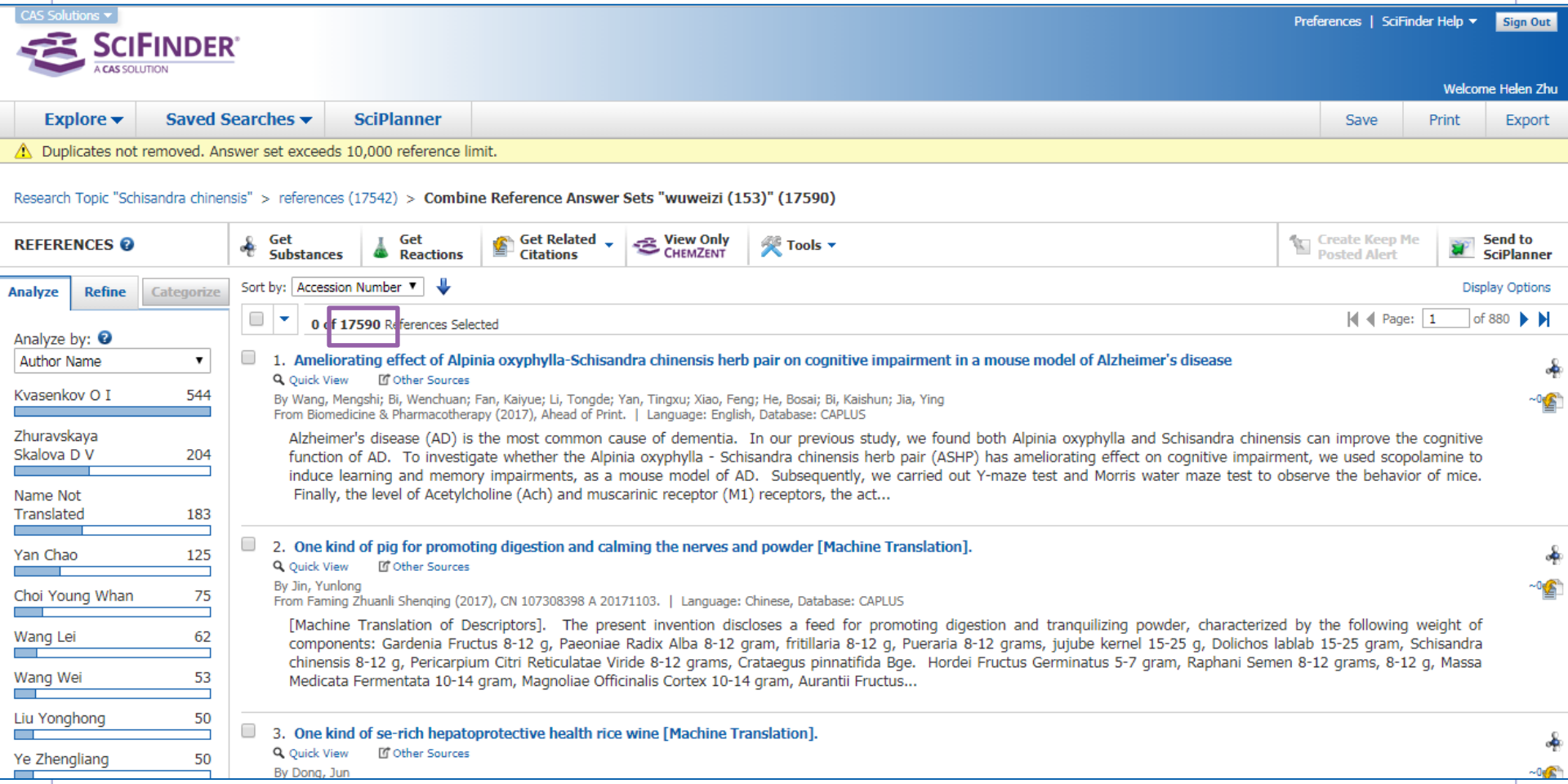




文献检索——中草药


Explore
Saved Searches
SciPlanner
Save
Print
Export
Duplicates not removed. Answer set exceeds 10,000 reference limit.
Research Topic "Schisandra chinensis" > references (17542)
REFERENCES
Get Substances
Get Reactions
Get Related Citations
View Only CHEMZENT
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Categorize
Sort by: Accession Number
Remove Duplicates
Combine Answer Sets
Add Tag
Display Options
0 of 17542 References Selected
Page: 1 of 878
Analyze by:
Author Name
Retrieving data...
1. Ameliorating effect of Alpinia oxyphylla-Schisandra chinensis herb pair on cognitive impairment in a mouse model of Alzheimer's disease
Quick View
Other Sources
By Wang, Mengshi; Bi, Wenchuan; Fan, Kaiyue; Li, Tongde; Yan, Tingxu; Xiao, Feng; He, Bosai; Bi, Kaishun; Jia, Ying
From Biomedicine & Pharmacotherapy (2017), Ahead of Print. | Language: English, Database: CAPLUS
Alzheimer's disease (AD) is the most common cause of dementia. In our previous study, we found both Alpinia oxyphylla and Schisandra chinensis can improve the cognitive function of AD. To investigate whether the Alpinia oxyphylla - Schisandra chinensis herb pair (ASHP) has ameliorating effect on cognitive impairment, we used scopolamine to induce learning and memory impairments, as a mouse model of AD. Subsequently, we carried out Y-maze test and Morris water maze test to observe the behavior of mice. Finally, the level of Acetylcholine (Ach) and muscarinic receptor (M1) receptors, the act...
2. One kind of pig for promoting digestion and calming the nerves and powder [Machine Translation].
Quick View
Other Sources
By Jin, Yunlong
Combine Answer Sets
Select saved answer set(s) to combine with your current answer set (17542):
63 Answer Sets 1 Selected
Reference Answer Set Details
Date Saved
wuweizi (153)
Research Topic "wuweizi" > references (153)
Nov 3, 2017
poo (91)
Research Topic "suzuki reaction with catalyst" > references (91)
Oct 20, 2017
r4r (139)
Research Topic "Modification of Azithromycin" > references (139)
Oct 20, 2017
1996化工学报 (220)
Journal "Huagong Xuebao" with limiters > references (497) > citing references (220)
Oct 9, 2017
Select an option for combining the answer sets:
Combine
Include all answers from both sets
Intersect
Include only answers that appear in both sets
Exclude
Include only answers from current answer set (17542) that are not in wuweizi (153)
Exclude
Include only answers from wuweizi (153) that are not in current answer set (17542)
Combine Answer Sets
Cancel

文献检索——中草药



全面的结果集

SciFinder
A CAS SOLUTION

文献检索小结

- 主题检索时，使用介词 in, with, of 等作为连接词
- 跟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
- 中草药的检索需要分别检中文名和拉丁名

SCIFINDER® A CAS SOLUTION

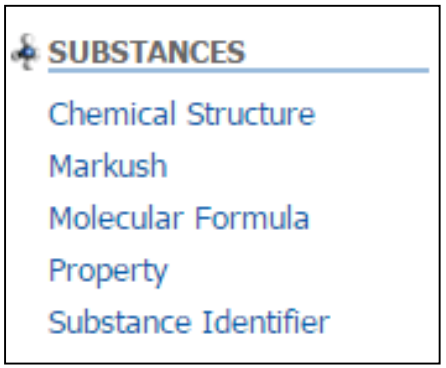
提纲

- 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

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物质检索——标识符检索

提示：
1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

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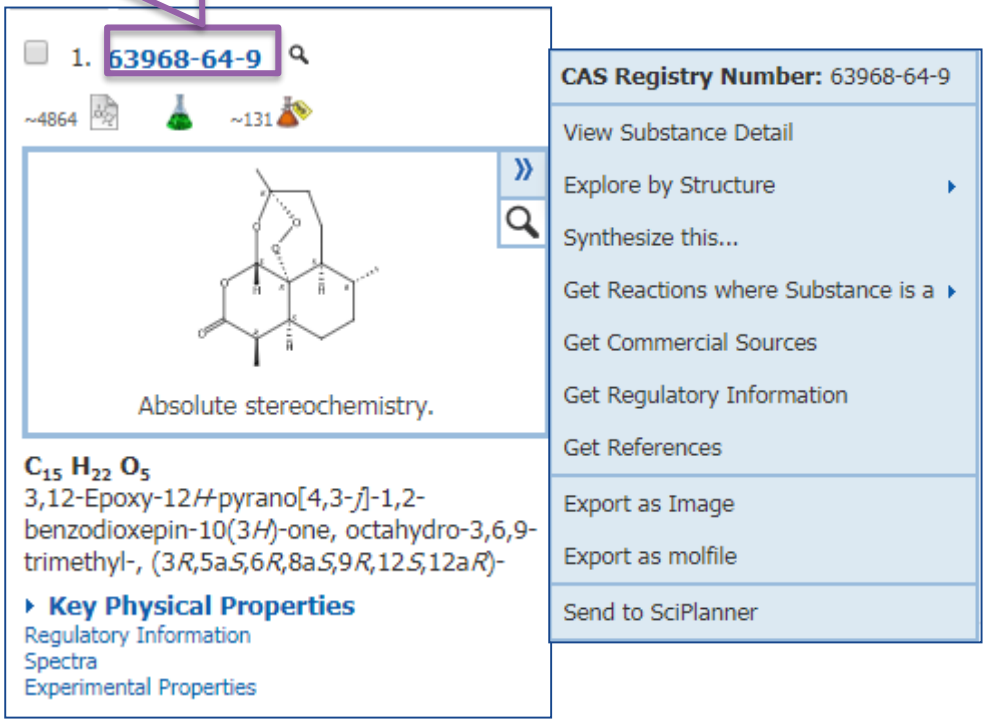
SciFinder中的物质记录

点击CAS RN 获得物质详细信息



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

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 63968-64

~4,864 ~131

$C_{15}H_{22}O_5$

3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-

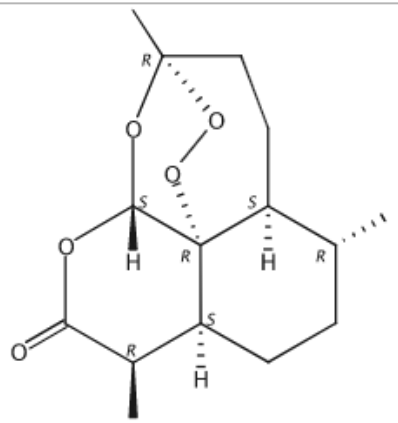
Molecular Weight
282.33

Melting Point (Experimental)
Value: 156-157 °C

Boiling Point (Predicted)
Value: 389.9±42.0 °C | Condition: Press: 760 Torr

Density (Experimental)
Value: 1.300 g/cm3

Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3α,5aβ,6β,8aβ,9α,12β,12a*R**)]-
(3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Arteannuin
(+)-Artemisinin
(+)-Qinghaosu
View more...



Absolute stereochemistry.

物质详情

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

¹H NMR | ¹³C NMR | Hetero NMR | IR | Mass | Raman | UV and Visible | Additional Spectra

¹³C NMR Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(3)ACD
Carbon-13 NMR Spectrum	See spectrum		(4)ACD
Carbon-13 NMR Spectrum	See full text	1 of 8	(5)CAS

Notes

(3) ACD: Spectral data were obtained from Advanced Chemistry Development, Inc.

(4) Han, Jaehong; Journal of Natural Products 2001, V64(9), P1201-1205 CAPLUS

(5) Yadav, J. S.; Tetrahedron 2010, V66(11), P2005-2009 CAPLUS

预测数据与预测谱图

PREDICTED PROPERTIES

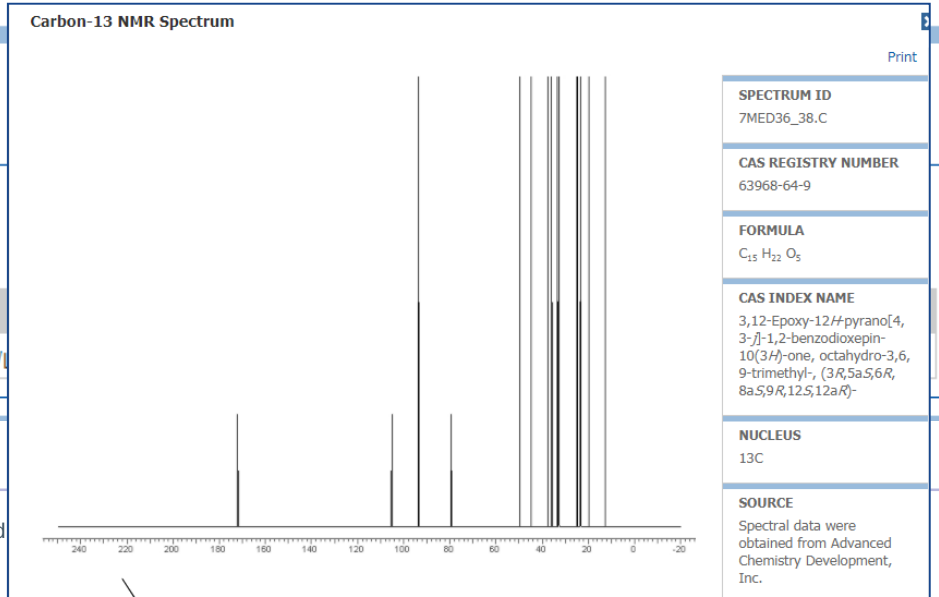
PREDICTED SPECTRA

¹H NMR | ¹³C NMR

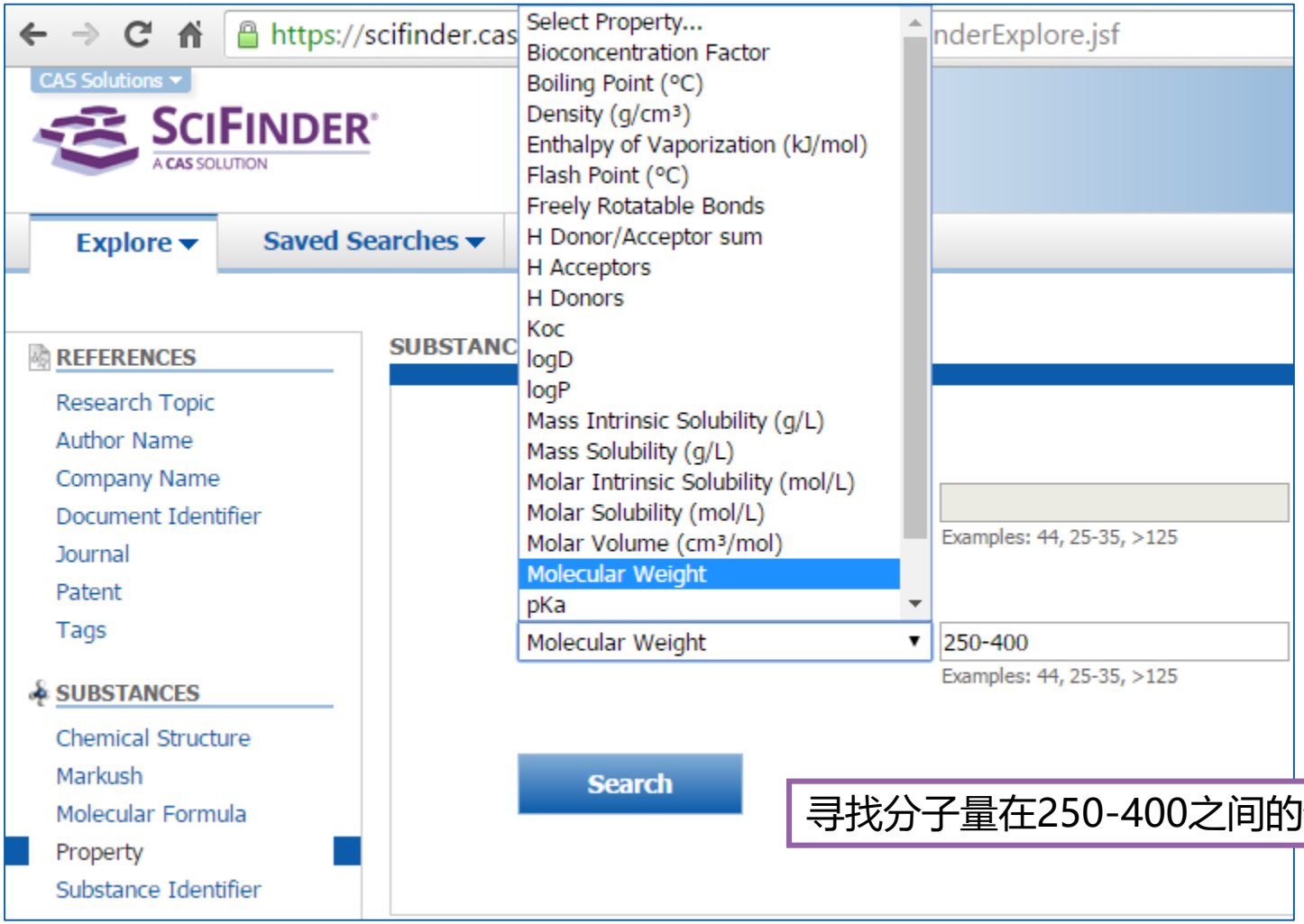
¹H NMR Properties	Value
Proton NMR Spectrum	See spectrum

Notes

(28) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/L



物质检索——Property explore



寻找分子量在250-400之间的物质

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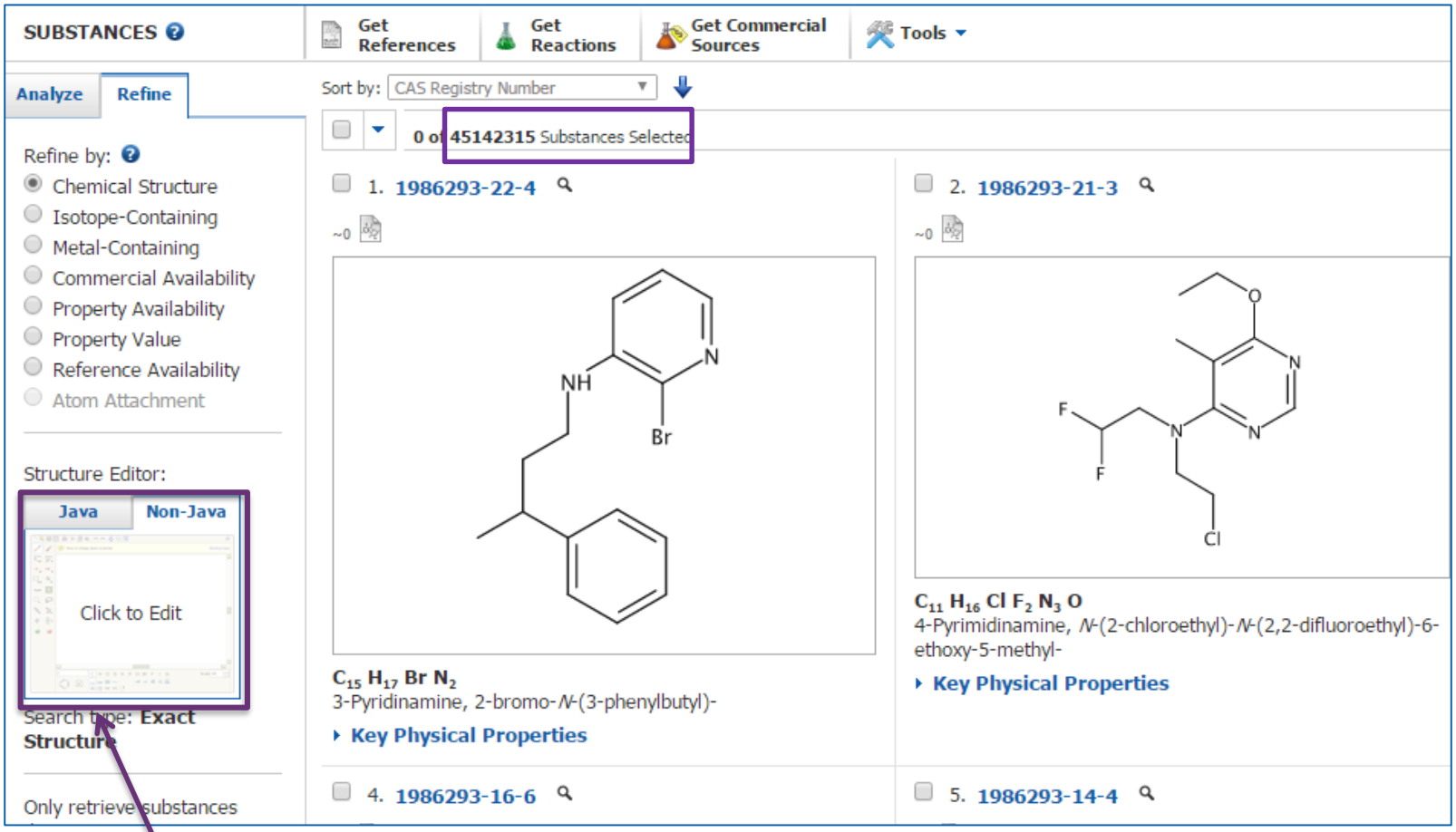
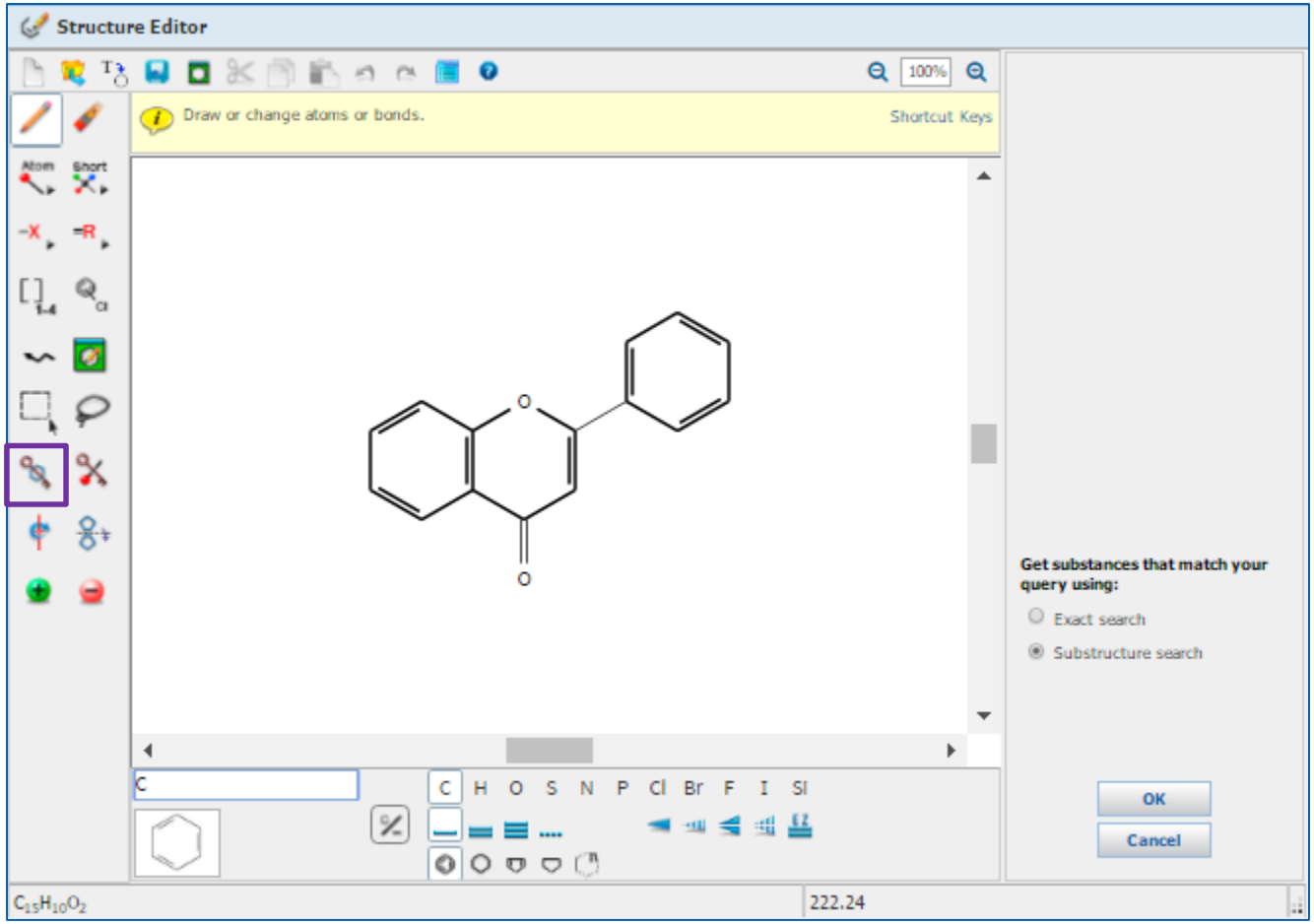
物质结果集的筛选——Refine

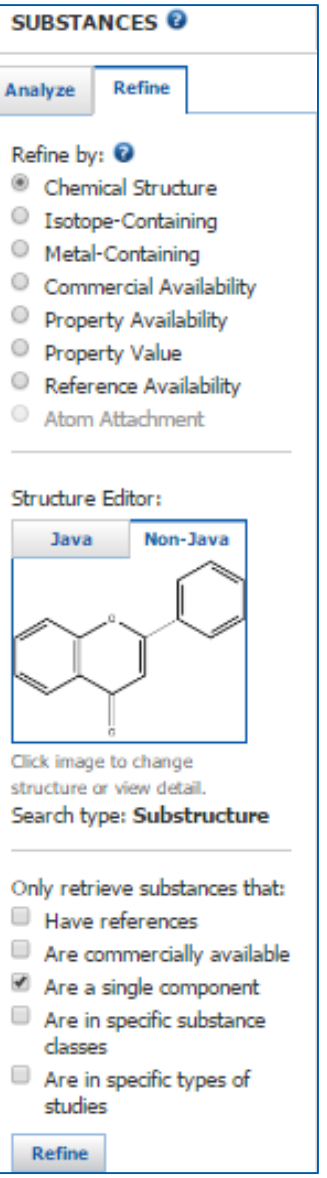


4500多万个结构，

如何筛选黄酮类物质?

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

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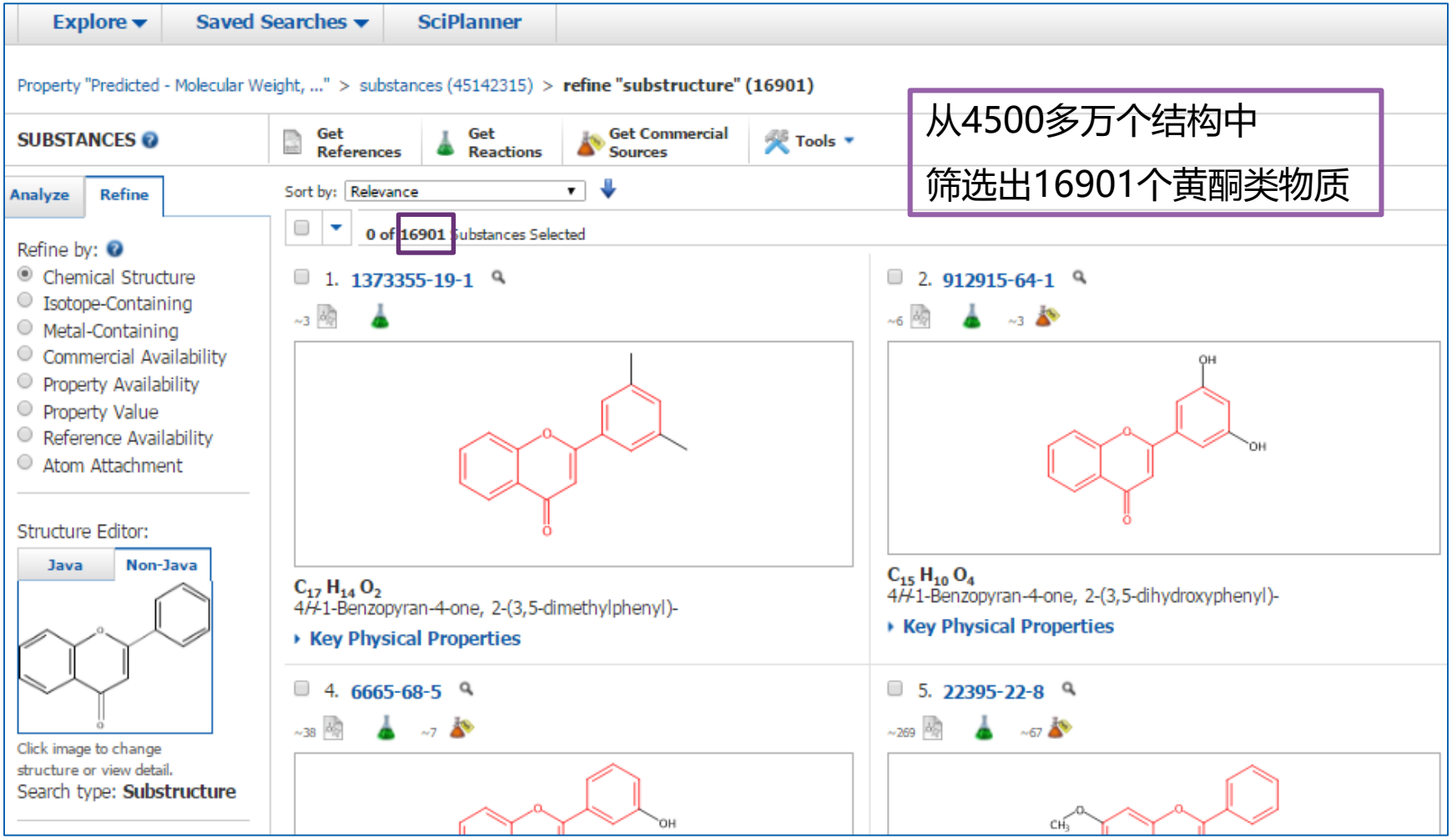
物质检索结果集

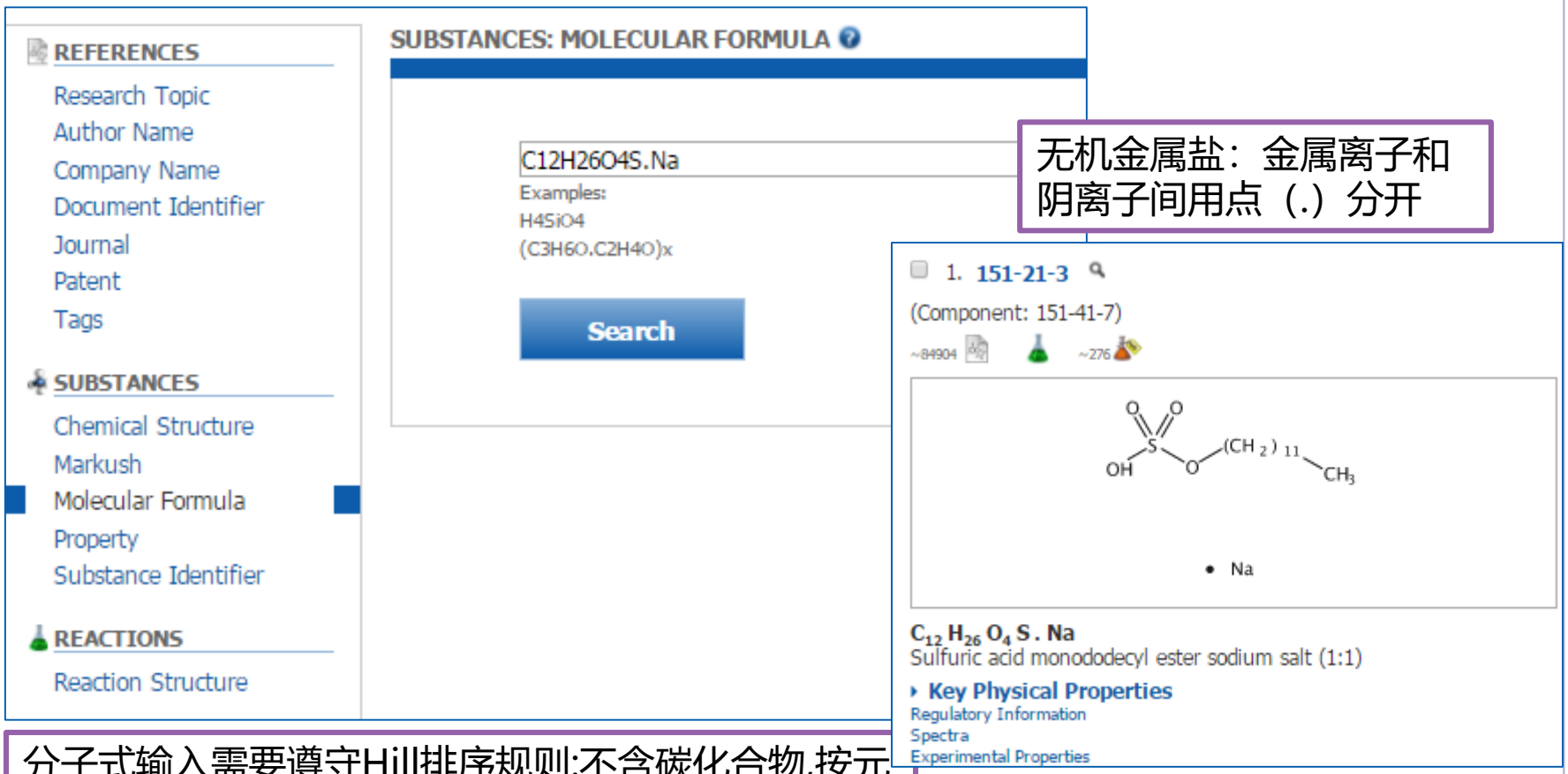


从4500多万个结构中

筛选出16901个黄酮类物质

SciFinder® A CAS SOLUTION

物质检索——分子式

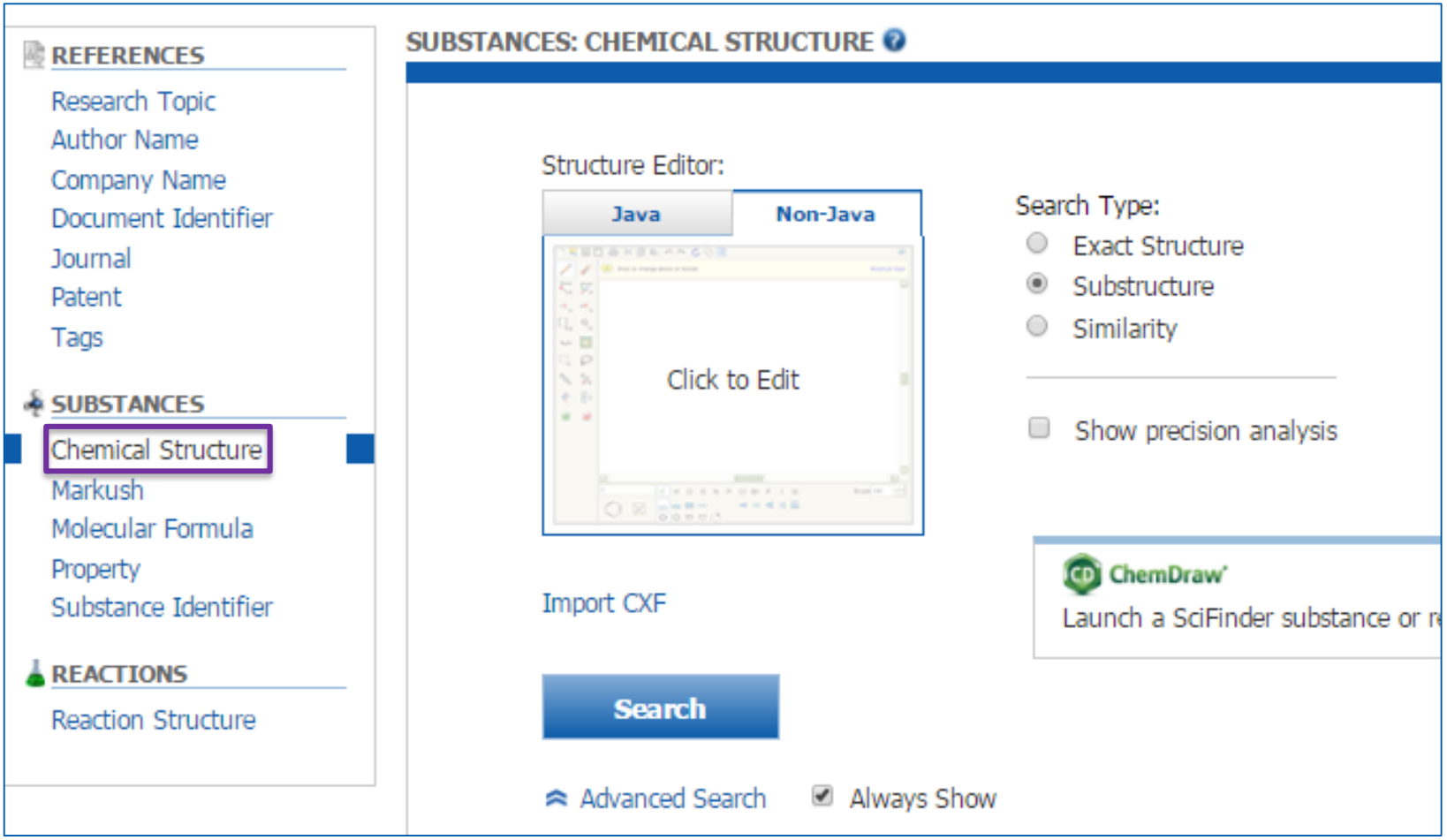


无机金属盐：金属离子和阴离子间用点（.）分开

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

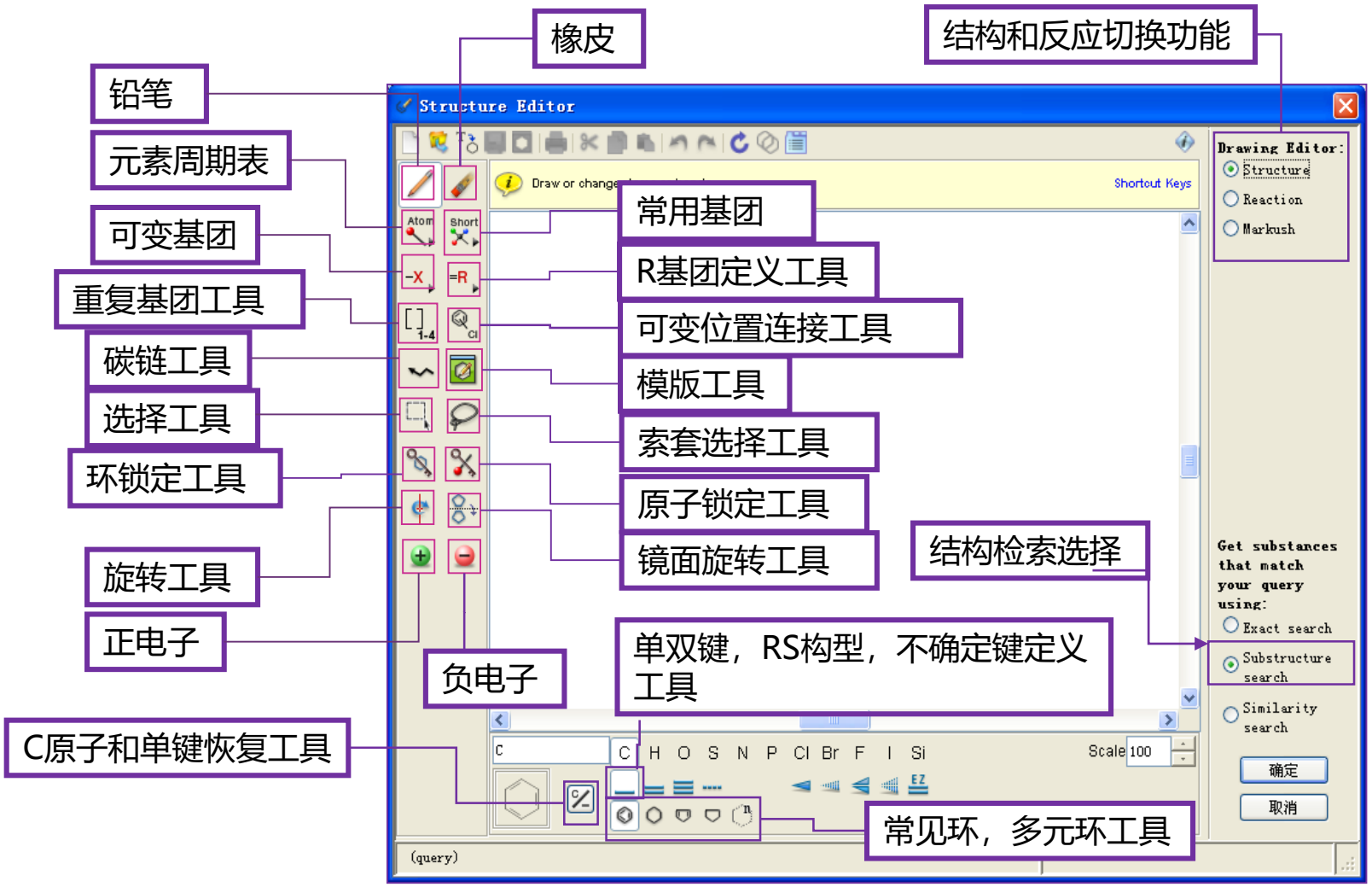
SciFinder® A CAS SOLUTION

物质检索——结构

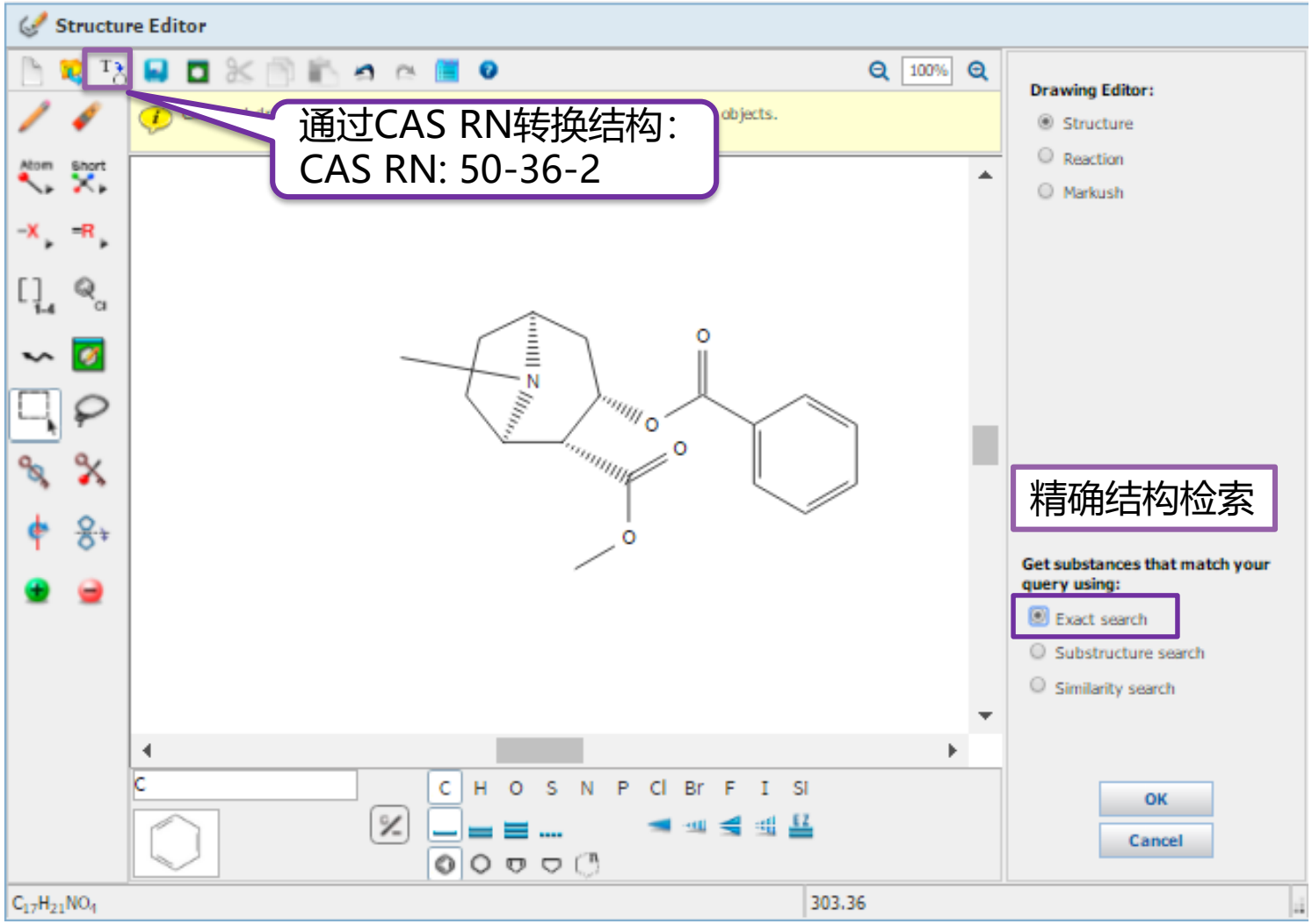


SciFinder® A CAS SOLUTION

物质检索——结构


橡皮
结构和反应切换功能
铅笔
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



SciFinder® A CAS SOLUTION

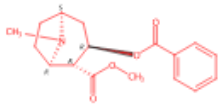
精确结构检索结果

Get References | Get Reactions | Get Commercial Sources | Tools | Create Posted

Sort by: Relevance

0 of 6 Substances Selected

1. 668-19-9



Absolute stereochemistry.

$C_{17}H_{21}NO_4$

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

Key Physical Properties

Spectra

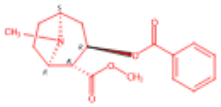
可卡因

2. 114599-38-1

可卡因组合物

668-19-9

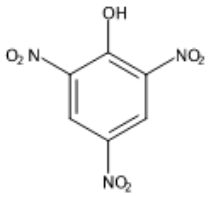
$C_{17}H_{21}NO_4$



Absolute stereochemistry.

88-89-1

$C_6H_3N_3O_7$

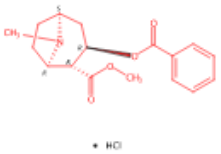


$C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$

Allococaine, picrate (6CI)

3. 109496-04-0

(Component: 668-19-9)



Absolute stereochemistry.

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

Allococaine, hydrochloride (6CI)

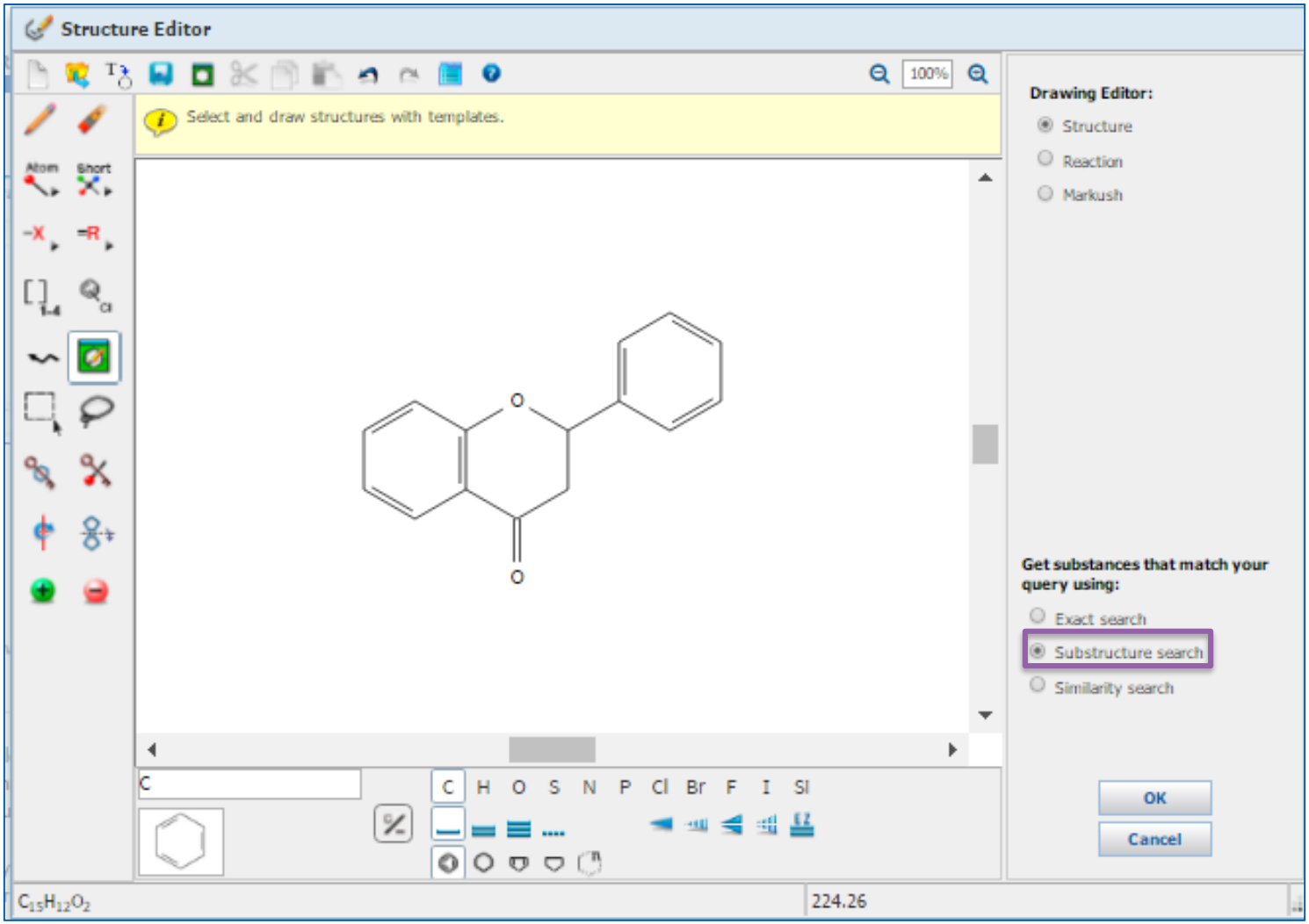
盐酸可卡因

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

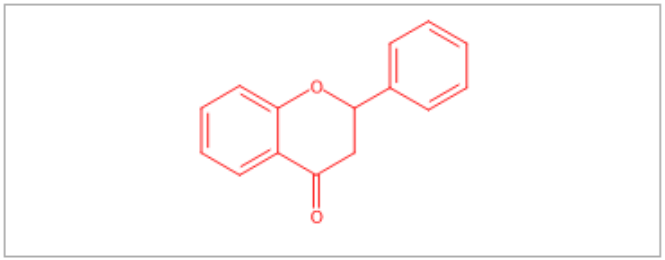
物质检索——亚结构检索


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

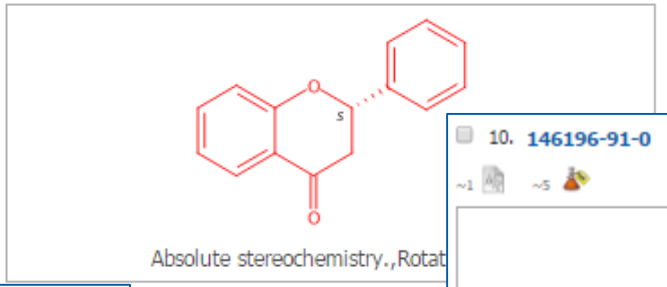
物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3



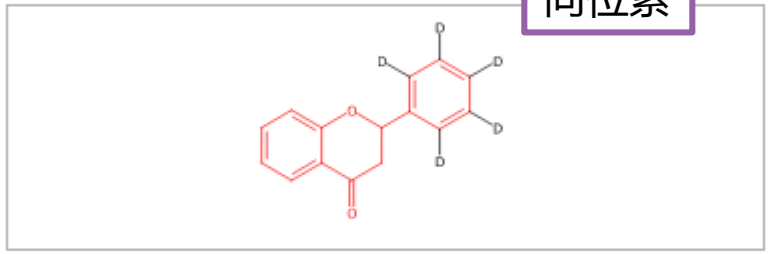
2. 17002-31-2



Absolute stereochemistry.,Rotat

10. 146196-91-0

同位素

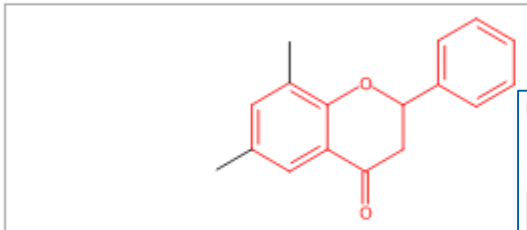


$C_{15}H_7D_5O_2$

e, 2,3-dihydro-2-(phenyl-d_5)- (9CI)

281. 123251-10-5

取代物



$C_{17}H_{16}O_2$

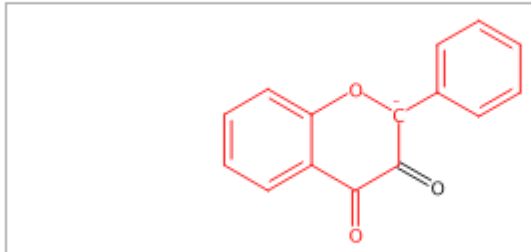
4*H*-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl

Key Physical Properties

Experimental Properties

295. 780723-19-5

离子

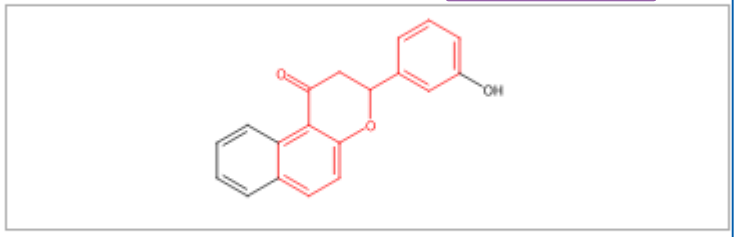


$C_{15}H_9O_3$

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

284. 136116-23-9

稠环物质

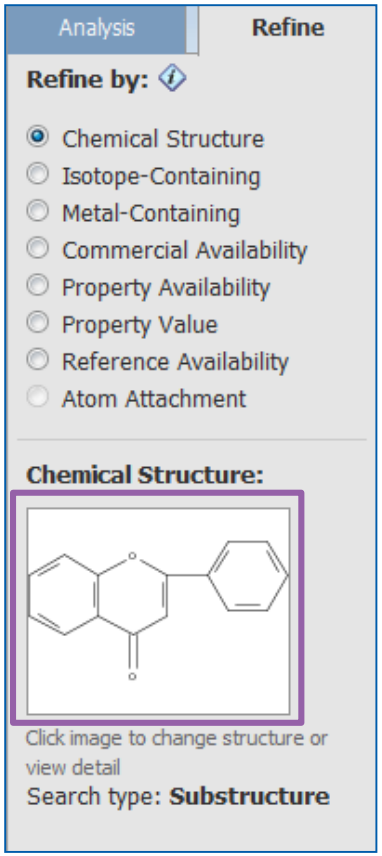


$C_{19}H_{14}O_3$

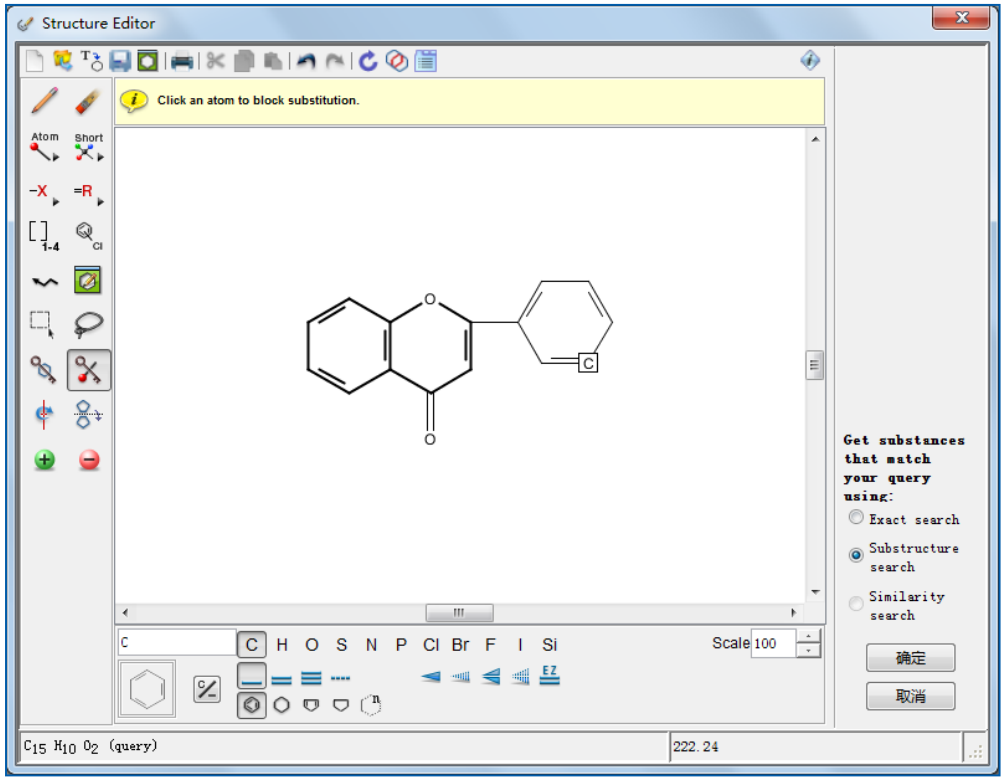
1*H*-Naphtho[2,1-*b*]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

Key Physical Properties

亚结构检索结果的限定



化学结构的再次限定



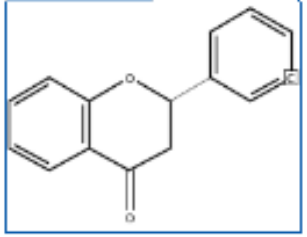
环锁定

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

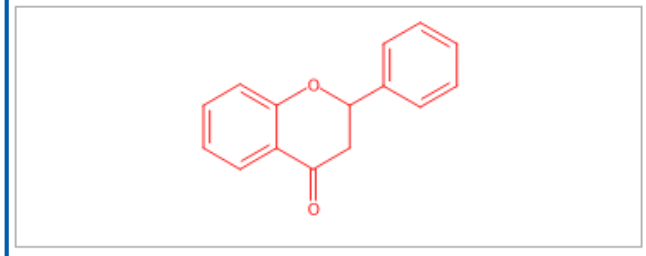
Get References | Get Reactions | Get Commercial Sources | Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. **487-26-3**

~2093 ~69

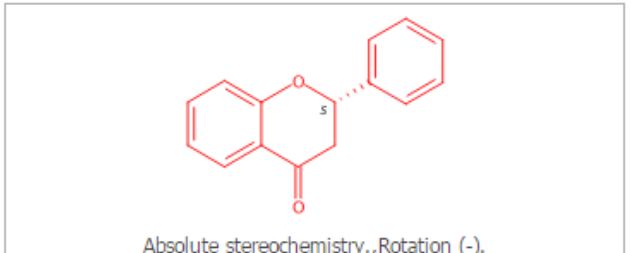


$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

▸ **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

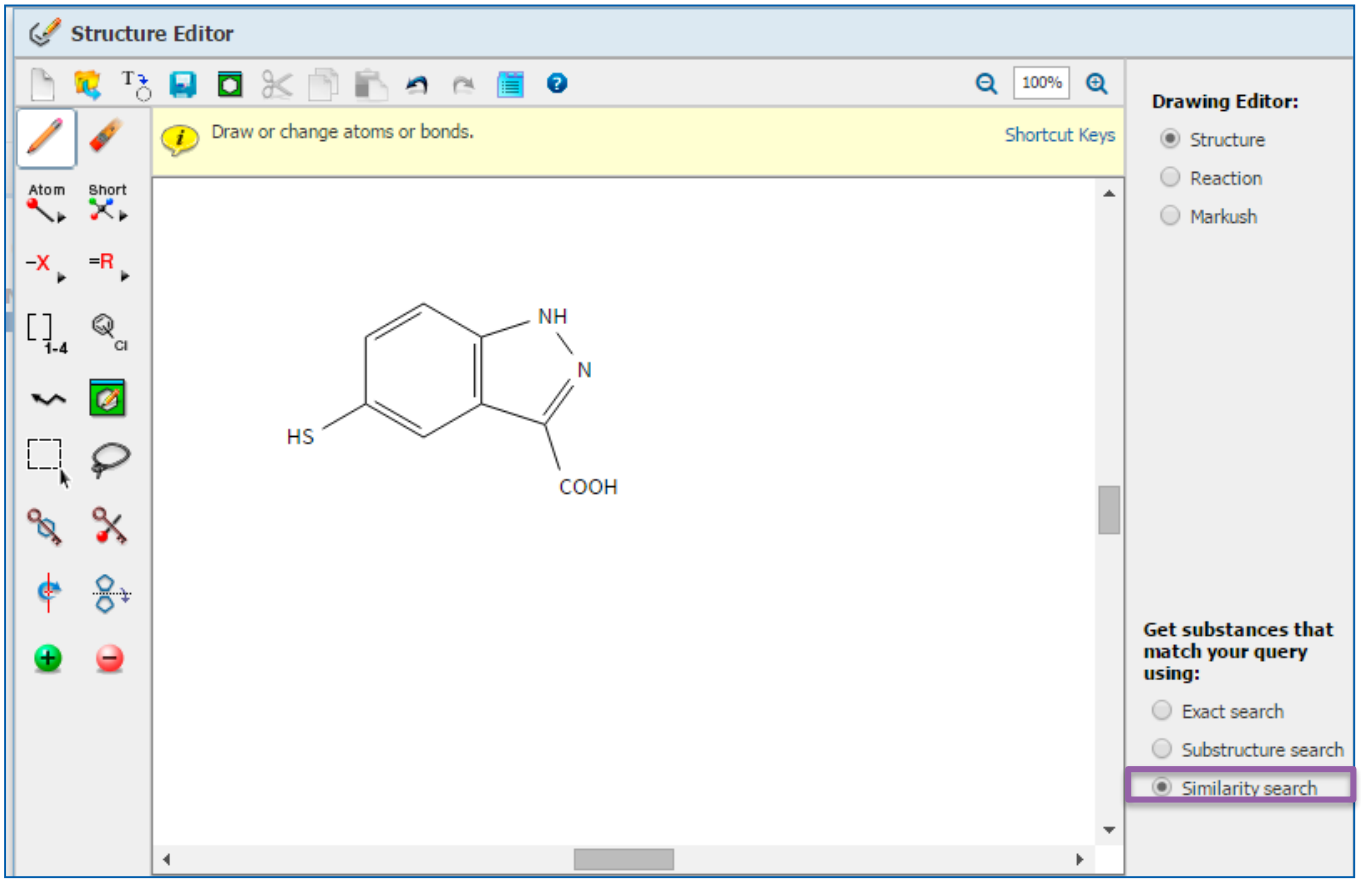
SciFinder® A CAS SOLUTION

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

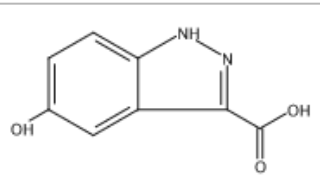
相似度越高，结构越相似

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-

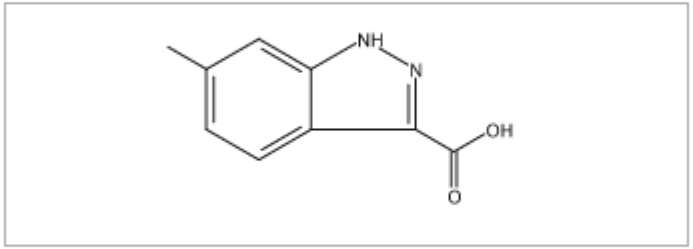
Key Physical Properties

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-

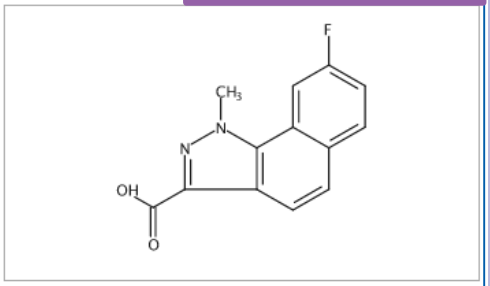
Key Physical Properties

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

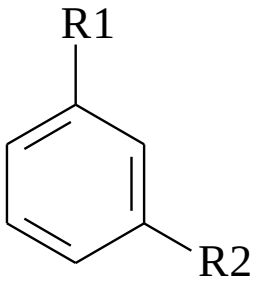
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

Markush检索

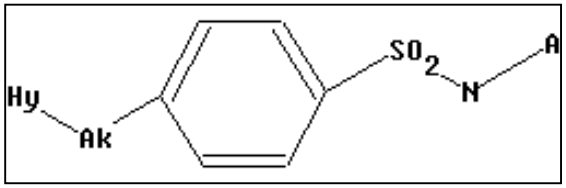
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 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

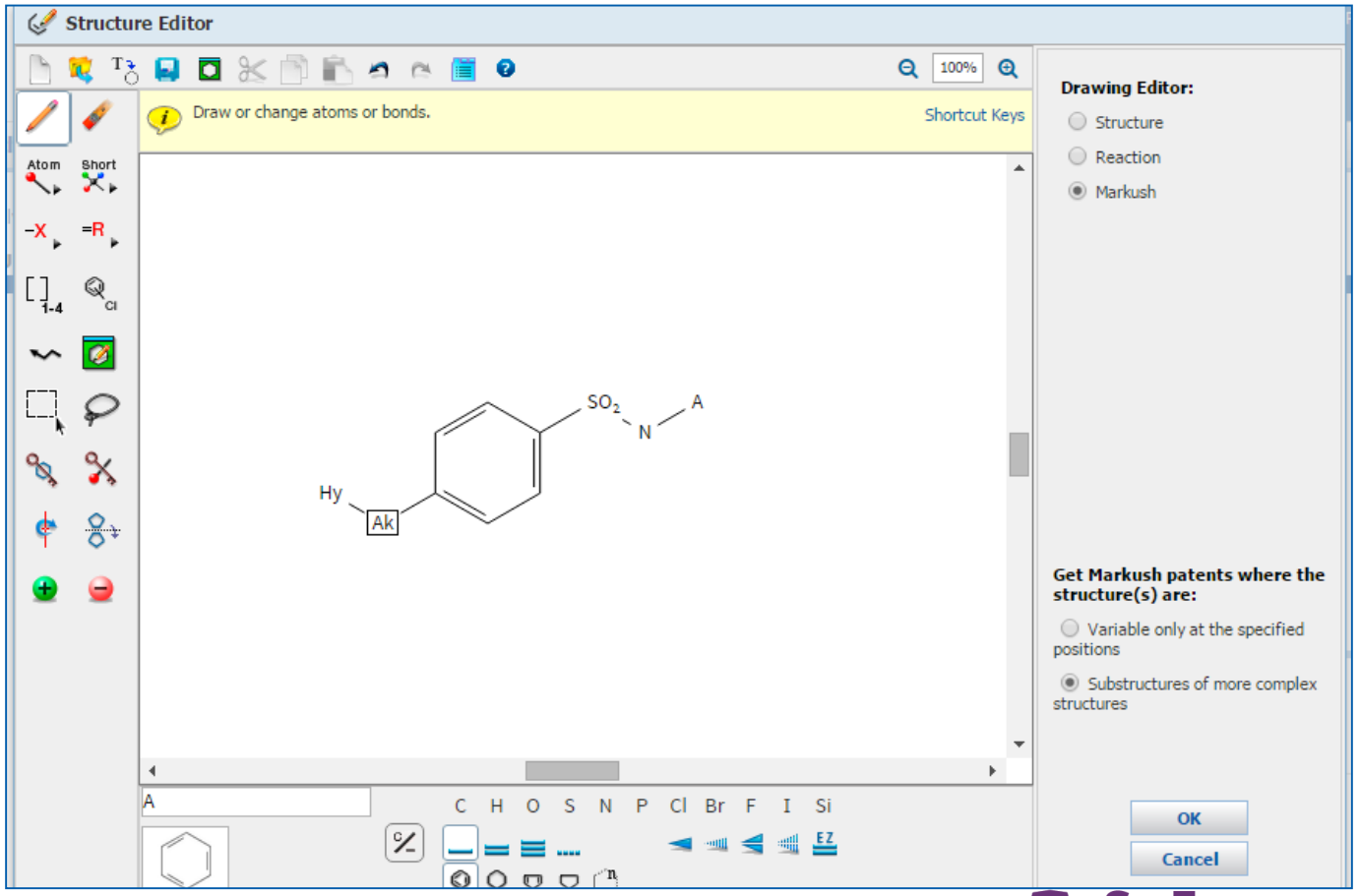


R1 = H, Br, Cl, I

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



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

Welcome Helen Zhu

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

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

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Analyze by: Document Type

Patent 1969

Journal 1

Show More

Sort by: Accession Number | Display Options

0 of 1969 References Selected | Page: 1 of 99

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

Quick View | PATENTPAK

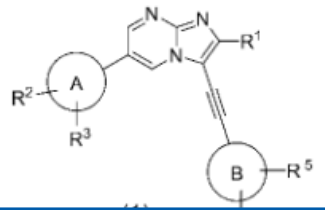
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

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^{a}R^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

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SciFinder检索选项——反应检索

- 反应检索方法

  结构式

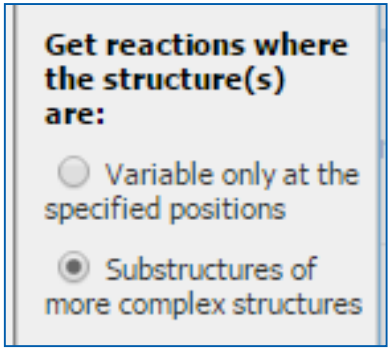
- 常用获取方法

  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



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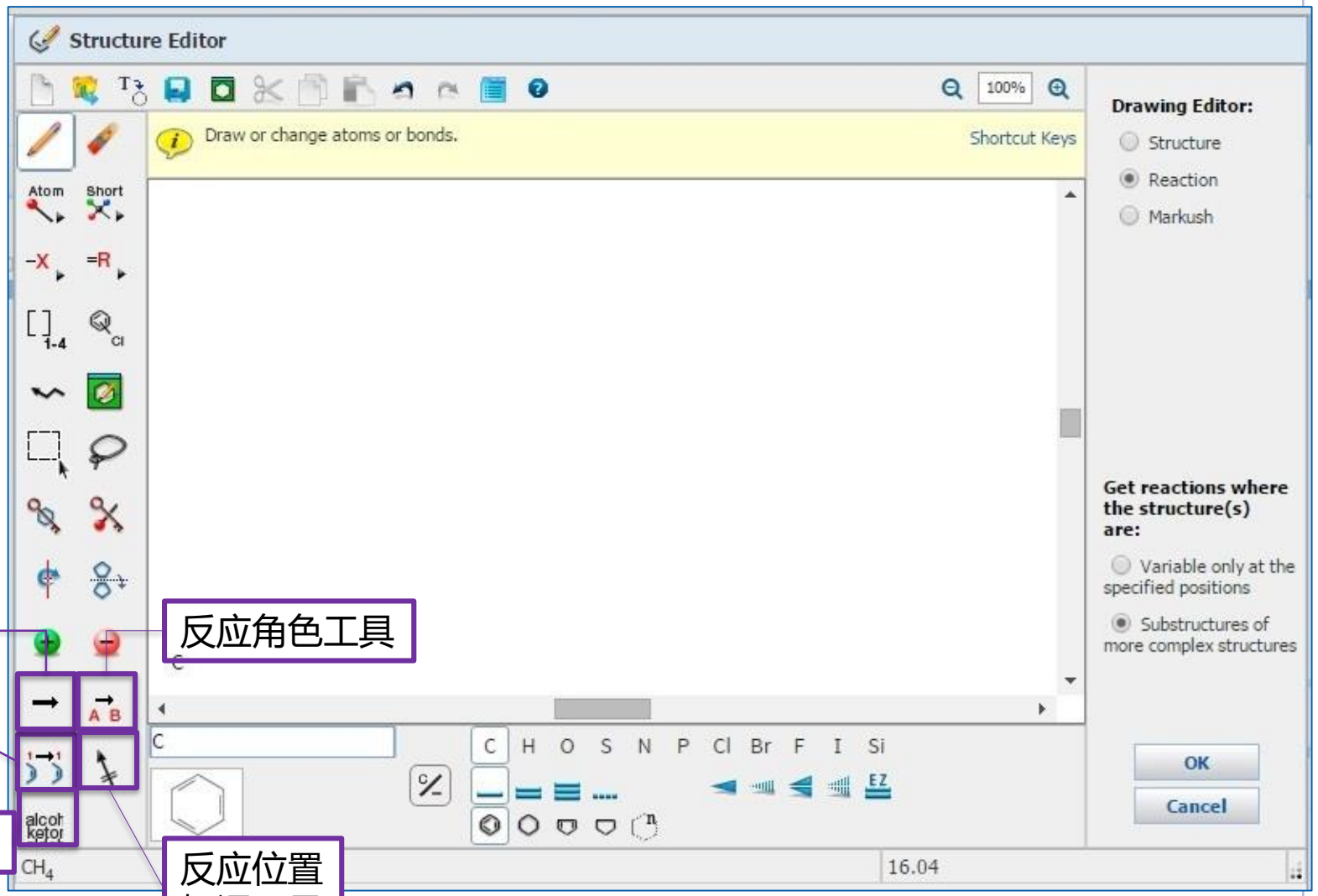
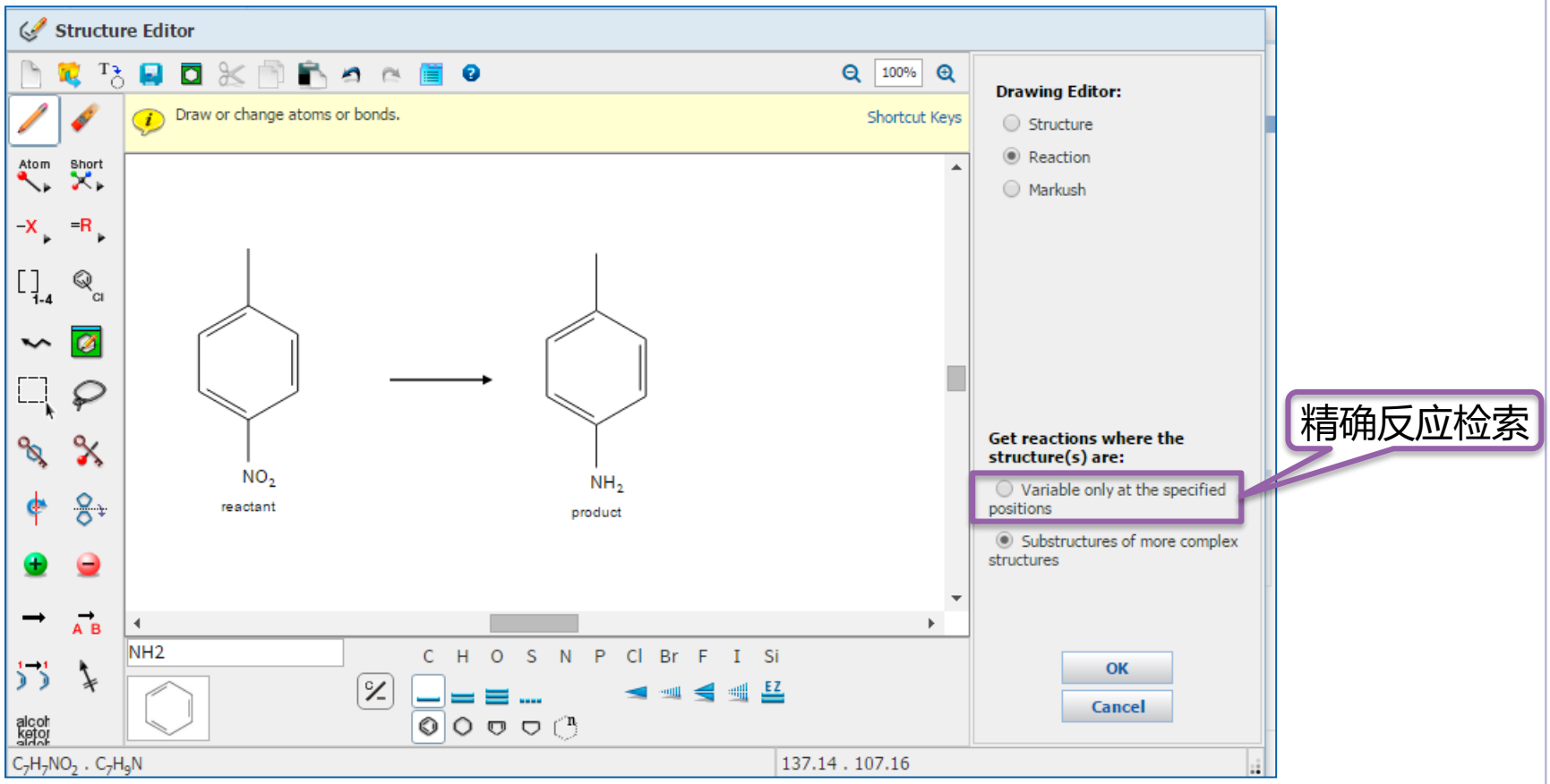
反应绘制工具

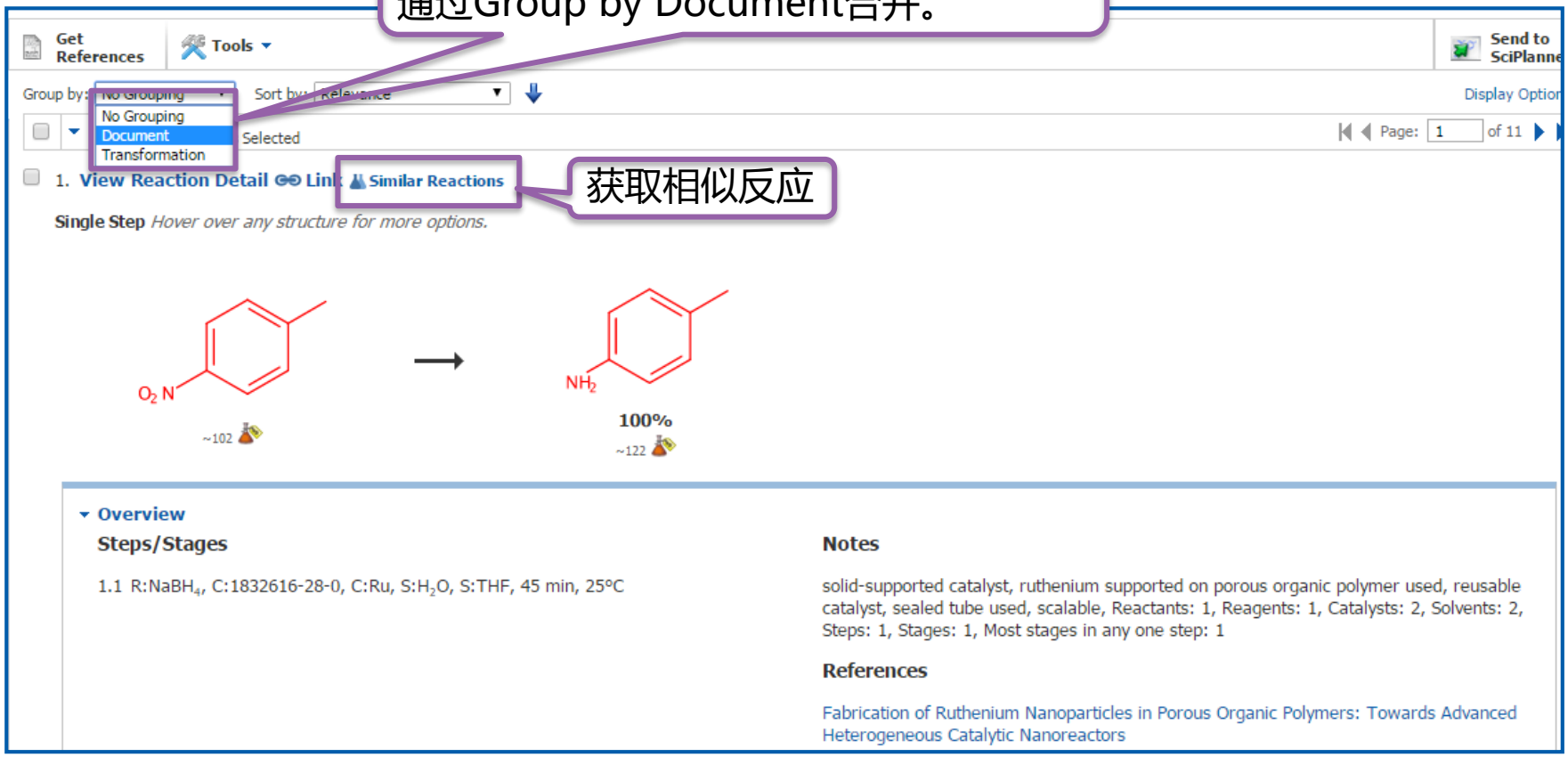

Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
C H O S N P Cl Br F I Si
CH4
16.04
反应箭头
反应角色工具
反应原子标记工具
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



SciFinder® A CAS SOLUTION

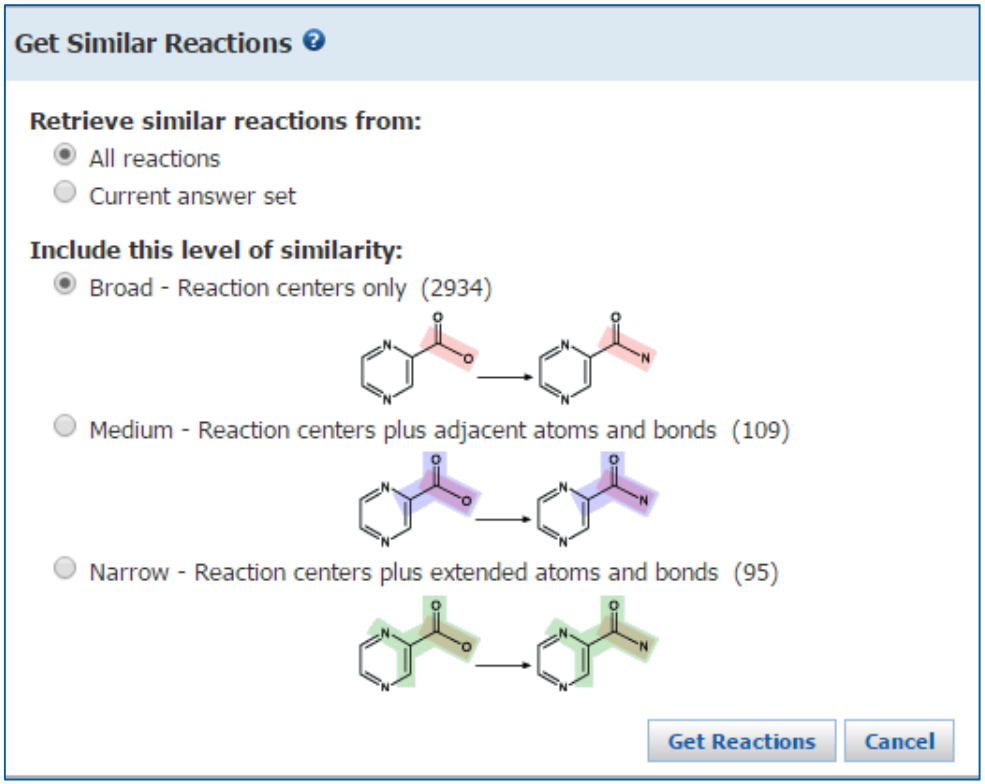
获取相似反应

选择相似反应的相似限制：

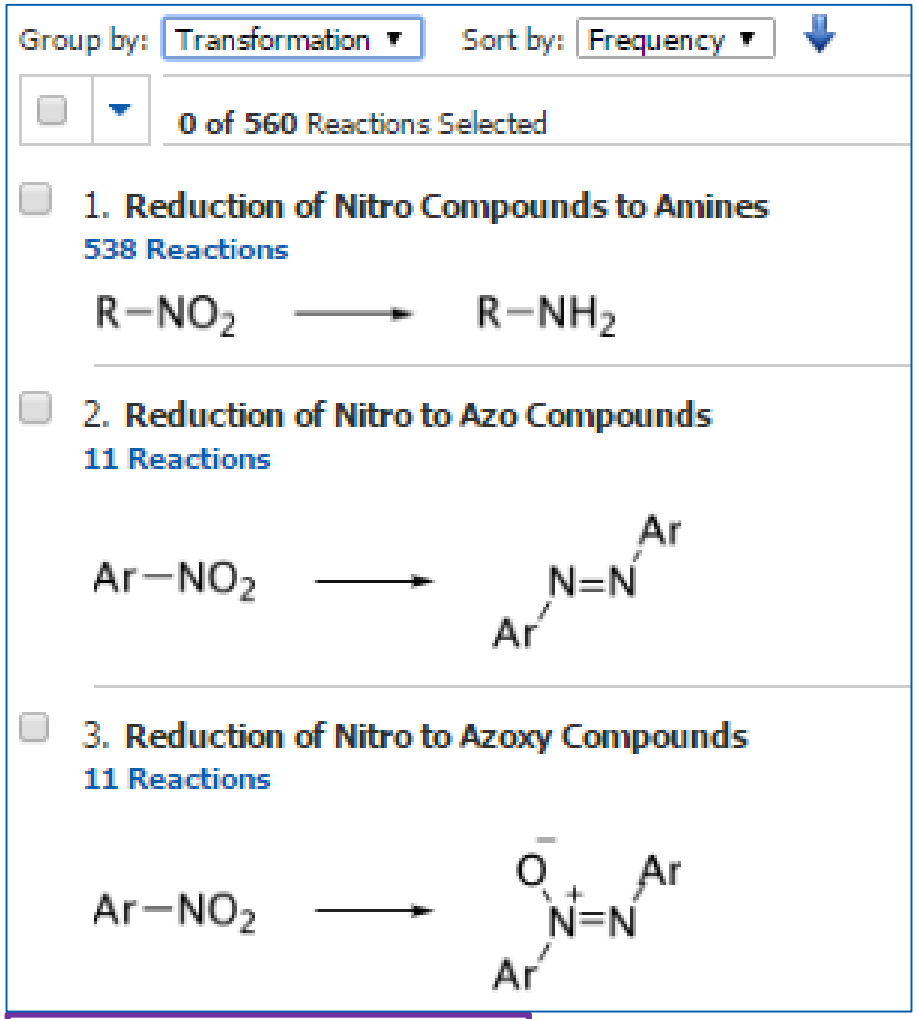
Broad：仅反应中心相似

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

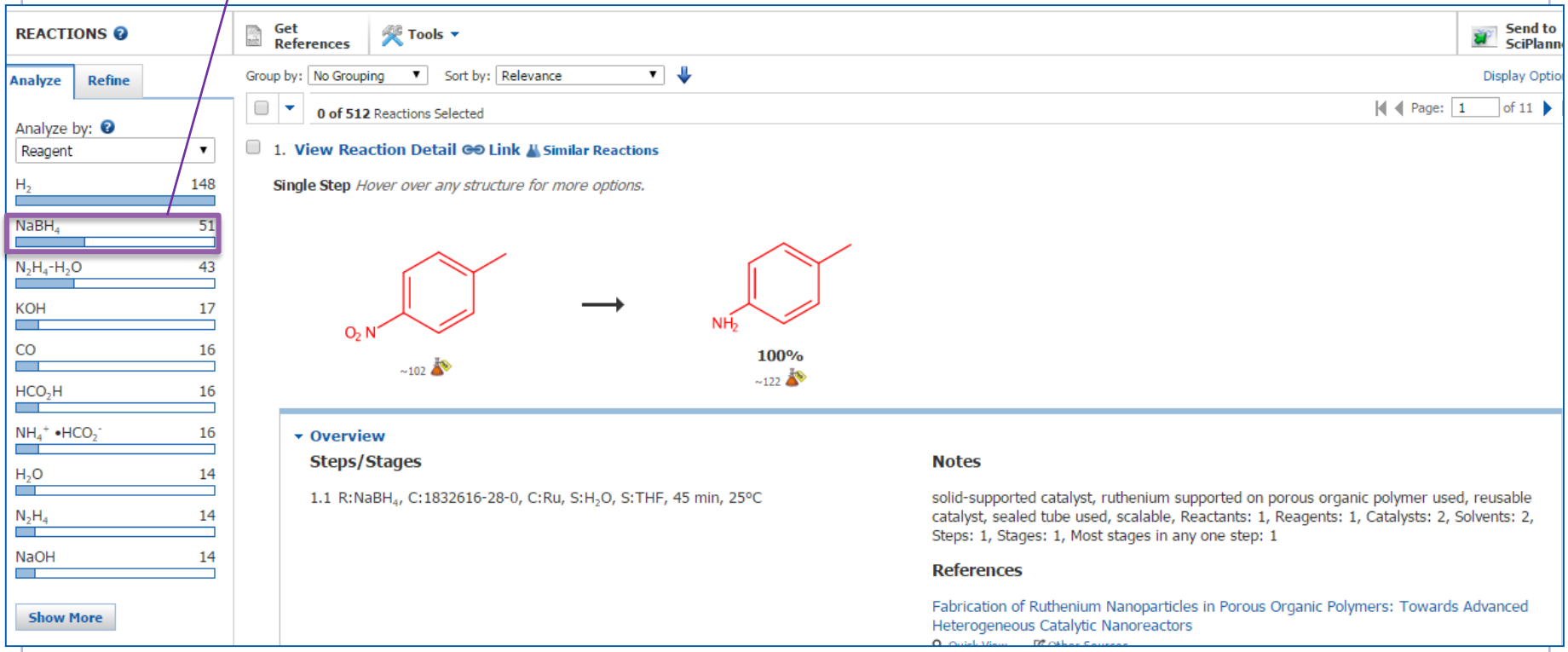


更精确的查找需要的反应

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

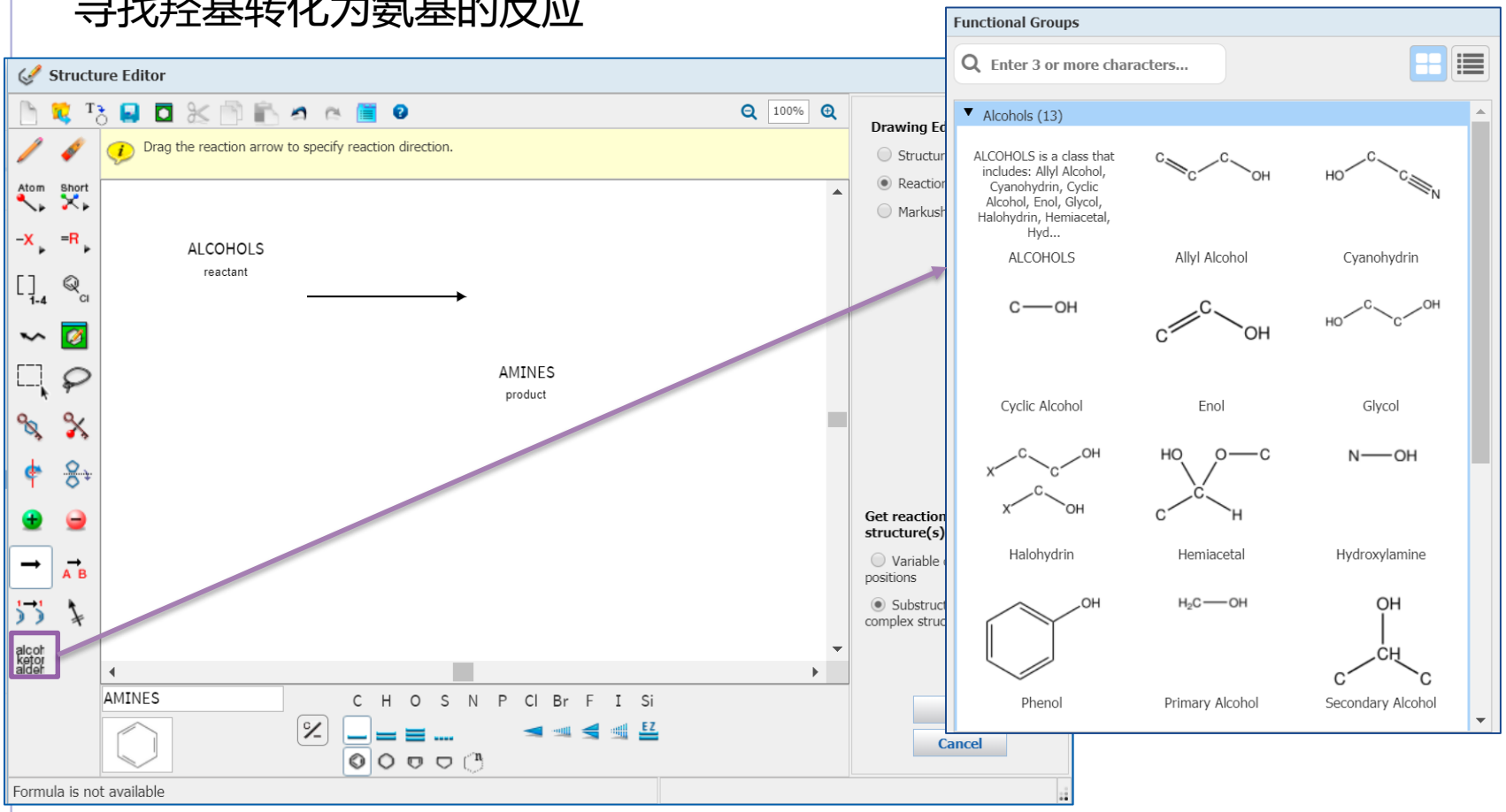
General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H_2 to a mixture of nitroarene (0.3 mmol), Cs_2CO_3 (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6×10^{-3} mmol, based on metal) in toluene (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

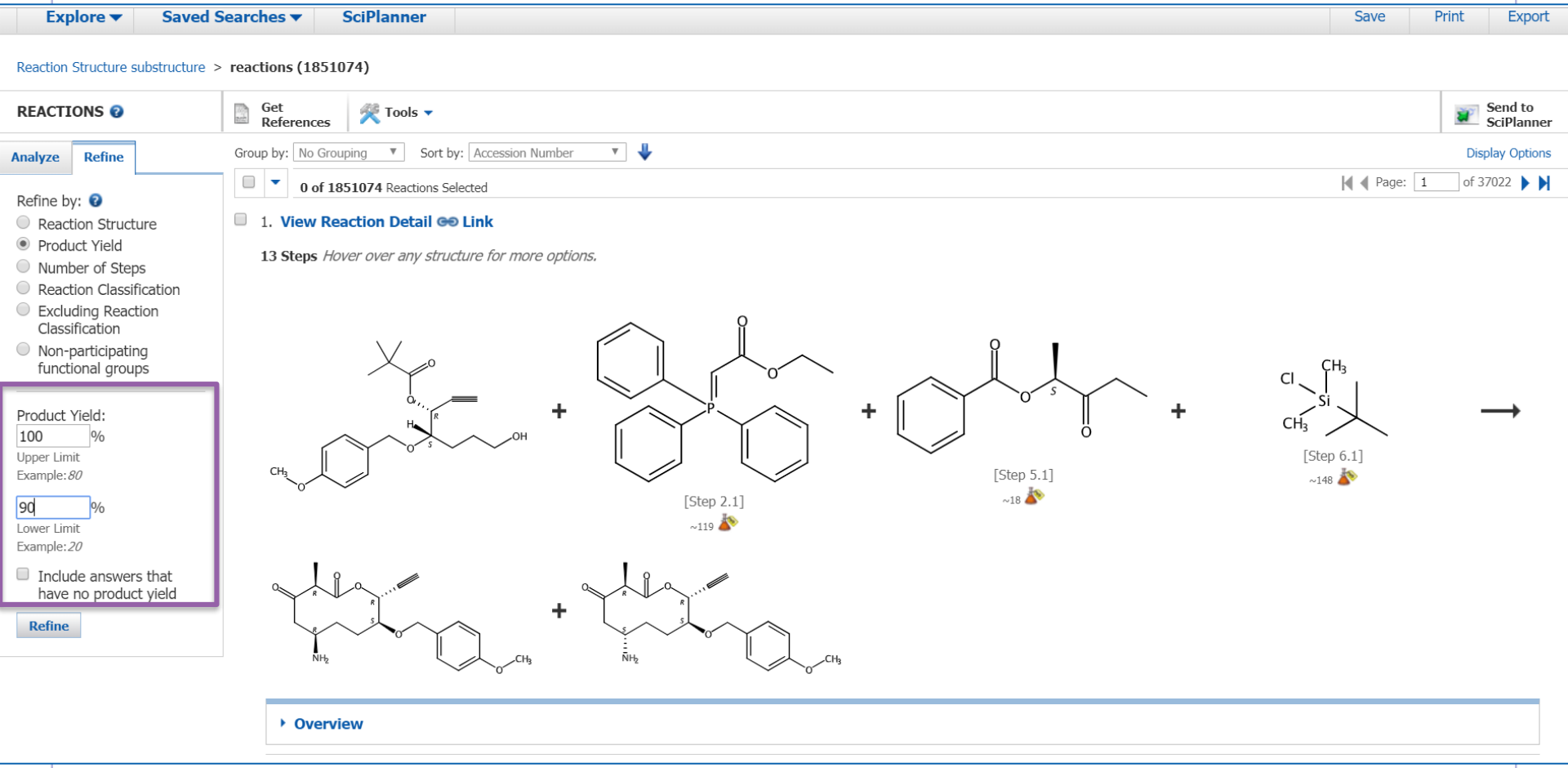
SciFinder® A CAS SOLUTION

官能团反应检索

寻找羟基转化为氨基的反应



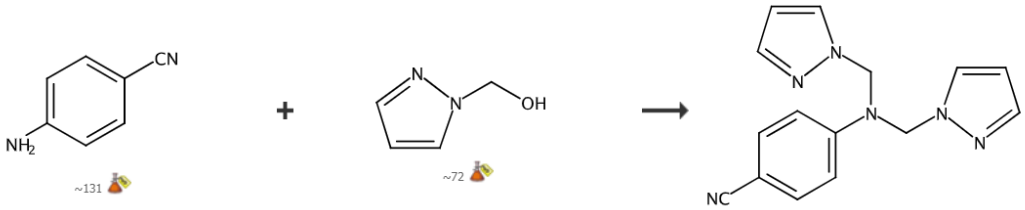
通过后处理工具筛选反应—Refine



通过后处理工具筛选反应—Refine

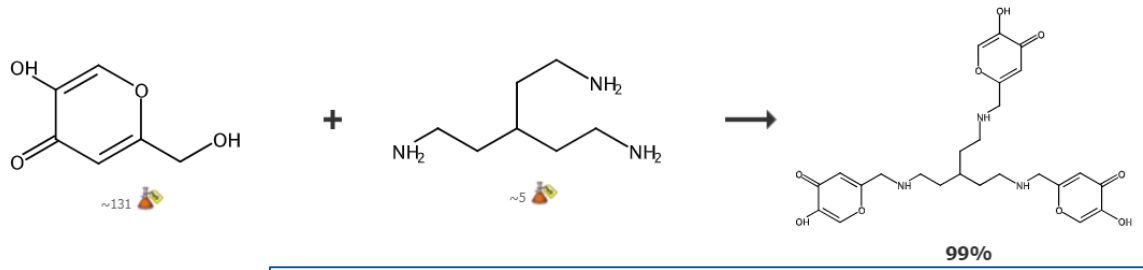
1. View Reaction Detail Link Similar Reactions

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



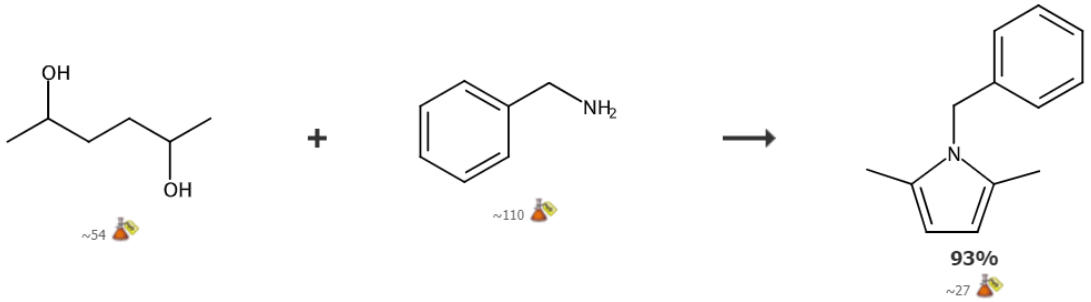
3. View Reaction Detail Link Similar Reactions

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



5. View Reaction Detail Link Similar Reactions

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



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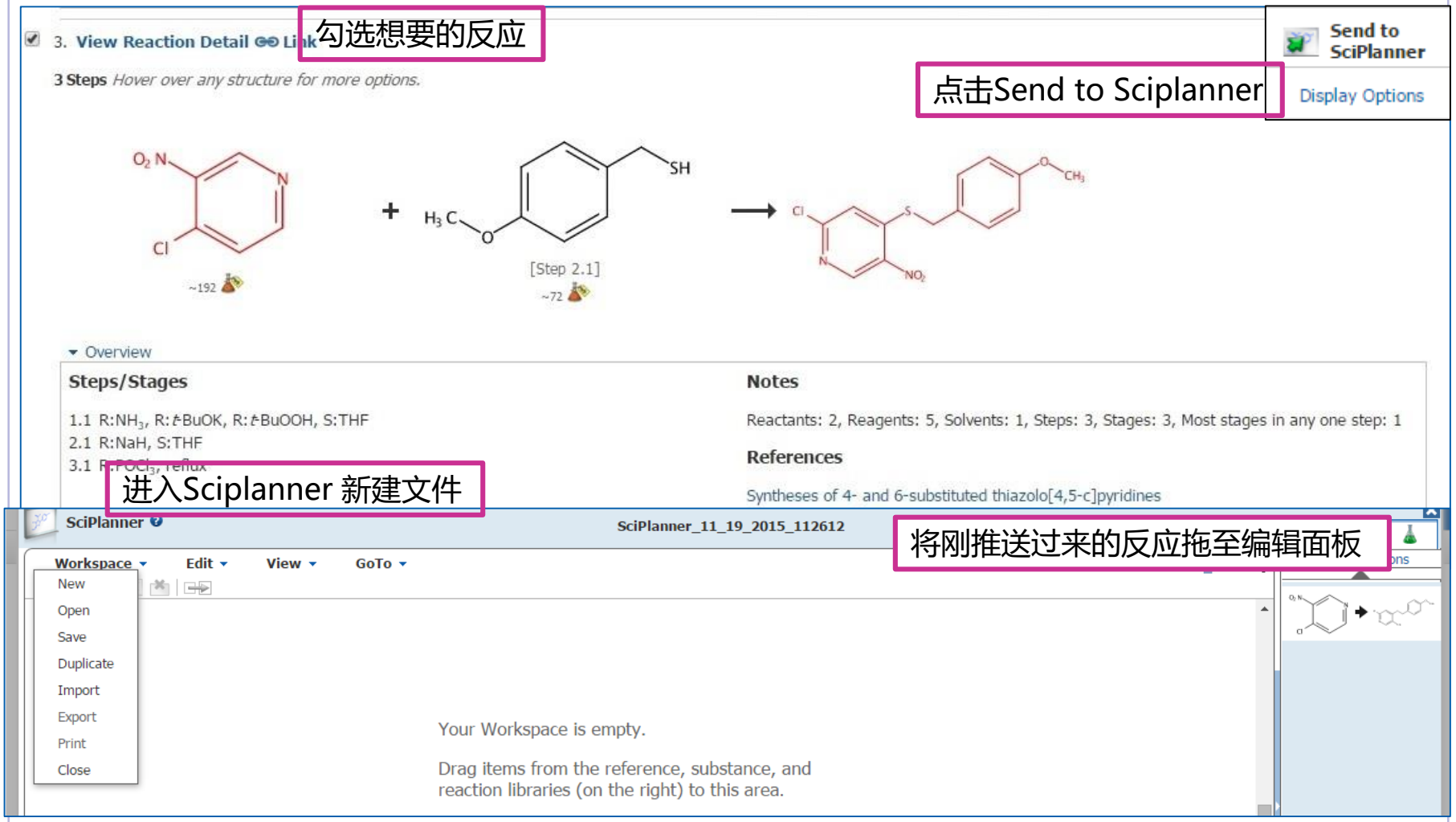
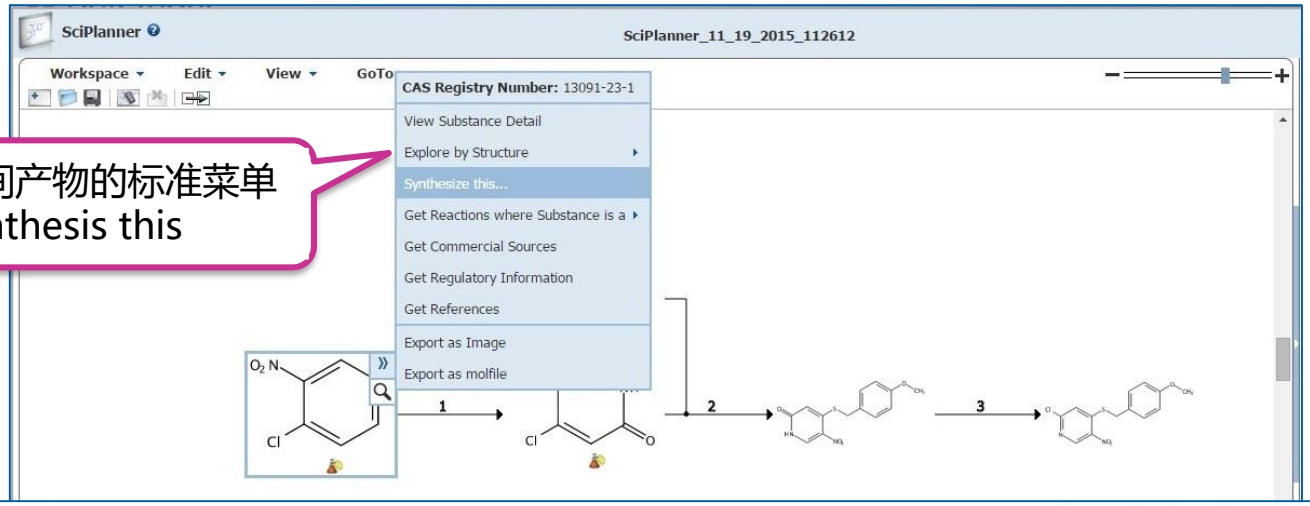
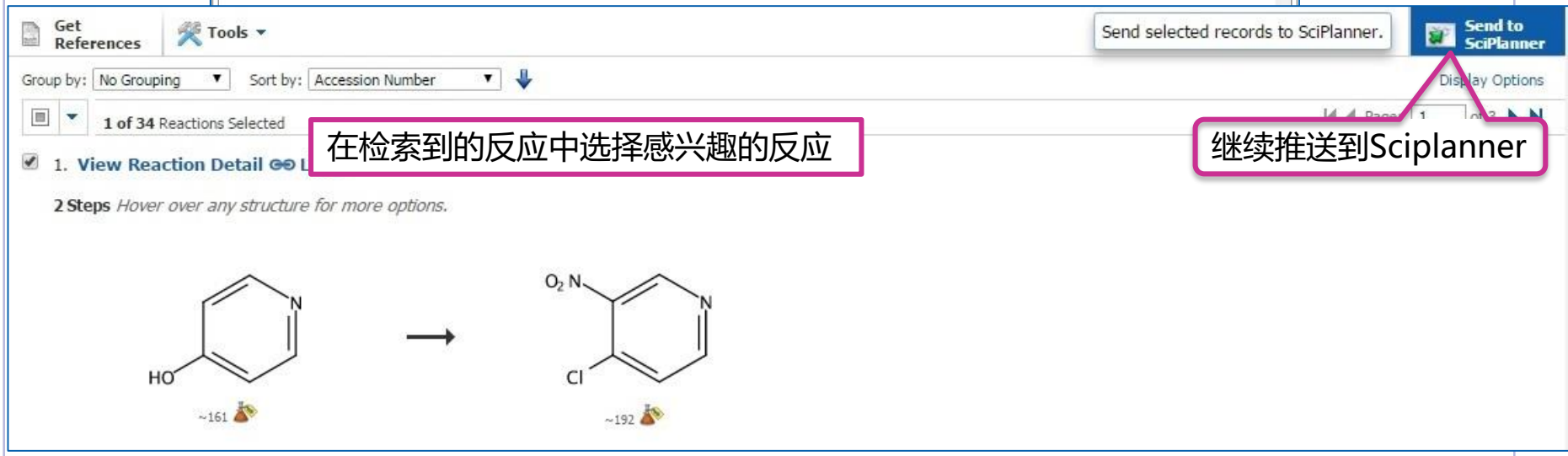
SciPlanner使用简介



SciPlanner使用简介



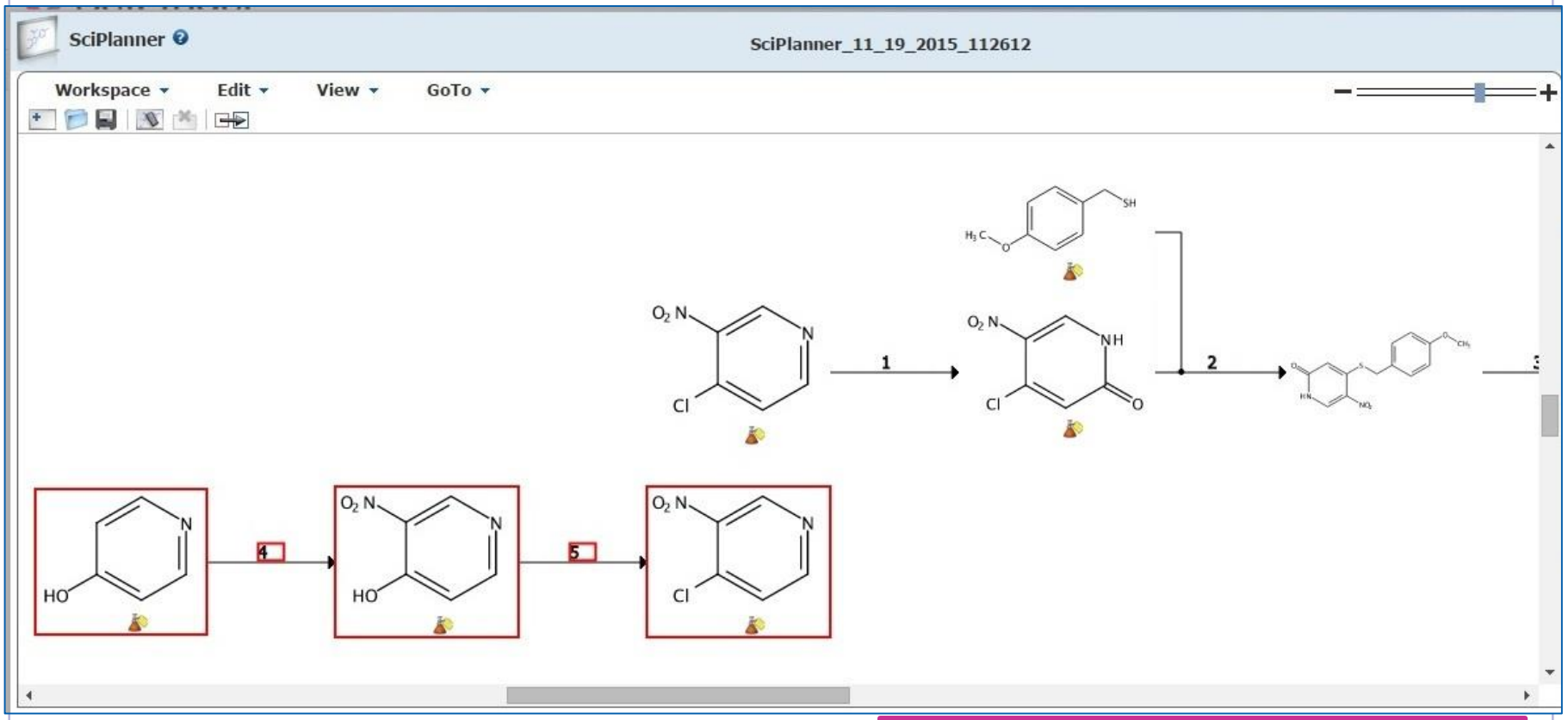
打开中间产物的标准菜单
选择Synthesis this



在检索到的反应中选择感兴趣的反应

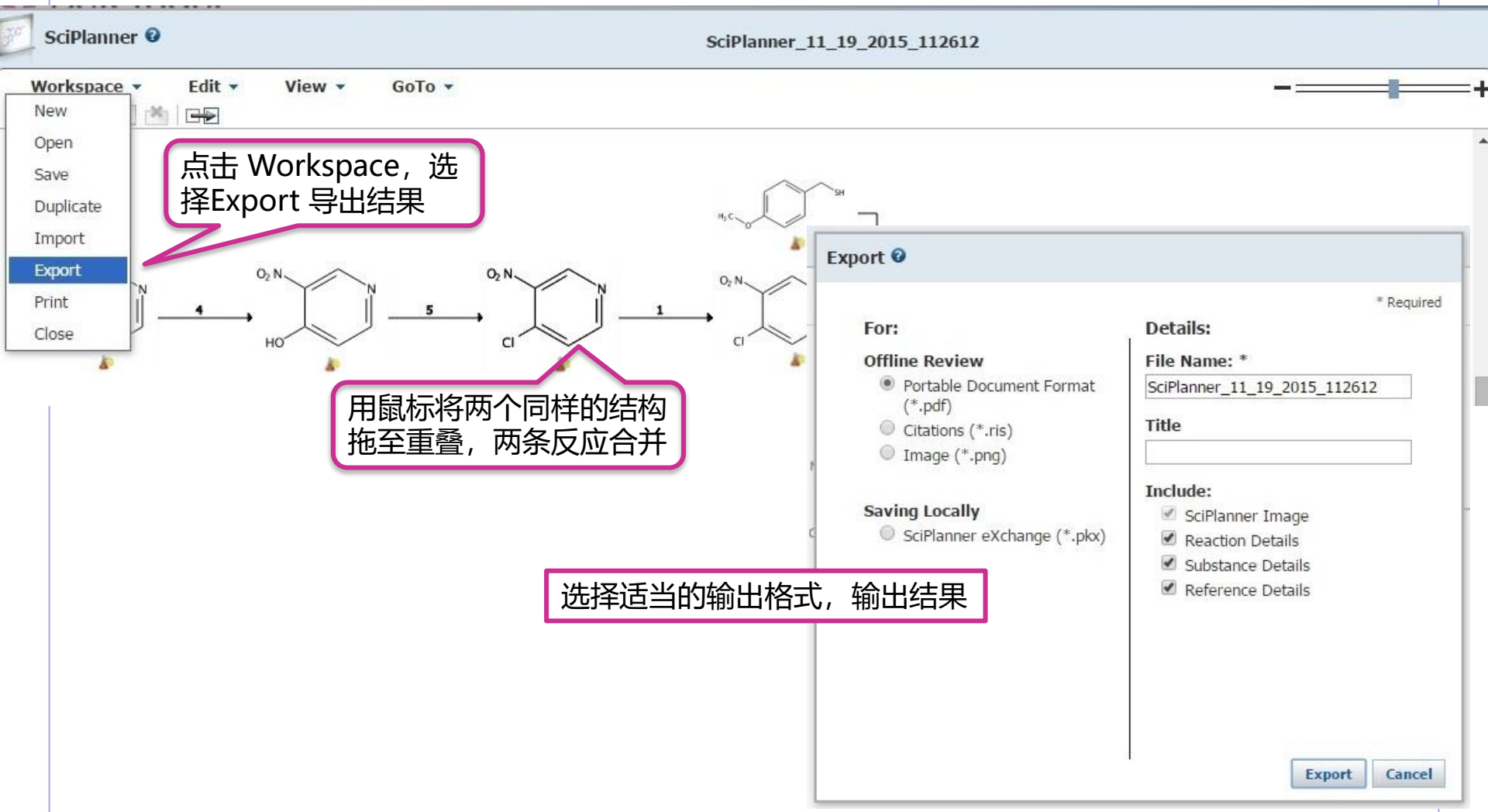
继续推送到Sciplanner

SciPlanner使用简介

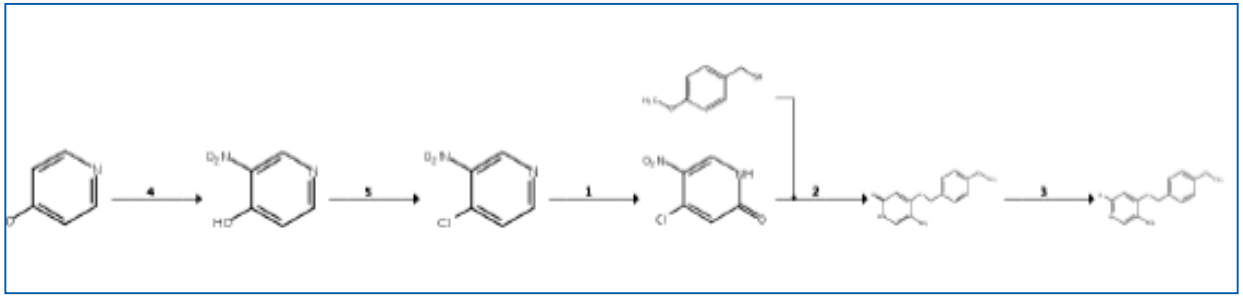


步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介



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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SCIFINDER® A CAS SOLUTION

SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上，不支持IE7、 IE8
- 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

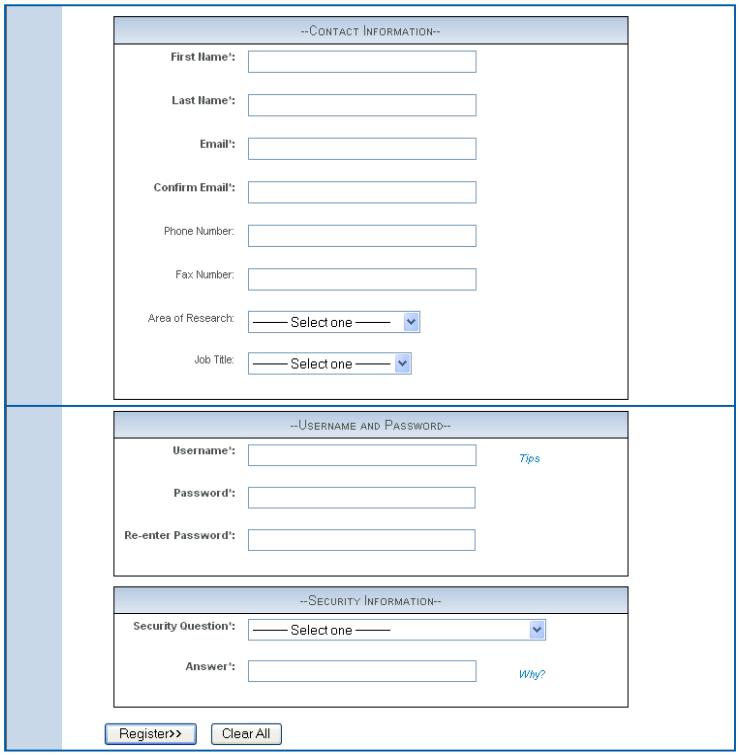
SciFinder

发布日期：2019年05月07日 来源： 点击：[140]

数据库名称	SciFinder
数据库链接	读者注册地址： https://scifinder.cas.org/registration/index.html?corpKey=6BE07969X86F35040X3C9C945423CF0CF467 SciFinder检索网址： https://scifinder.cas.org/ （试用至2019年5月31日）

SCIFINDER® A CAS SOLUTION

如何获取SciFinder账号



请注意：
1.必须输入真实姓名和邮箱。
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）

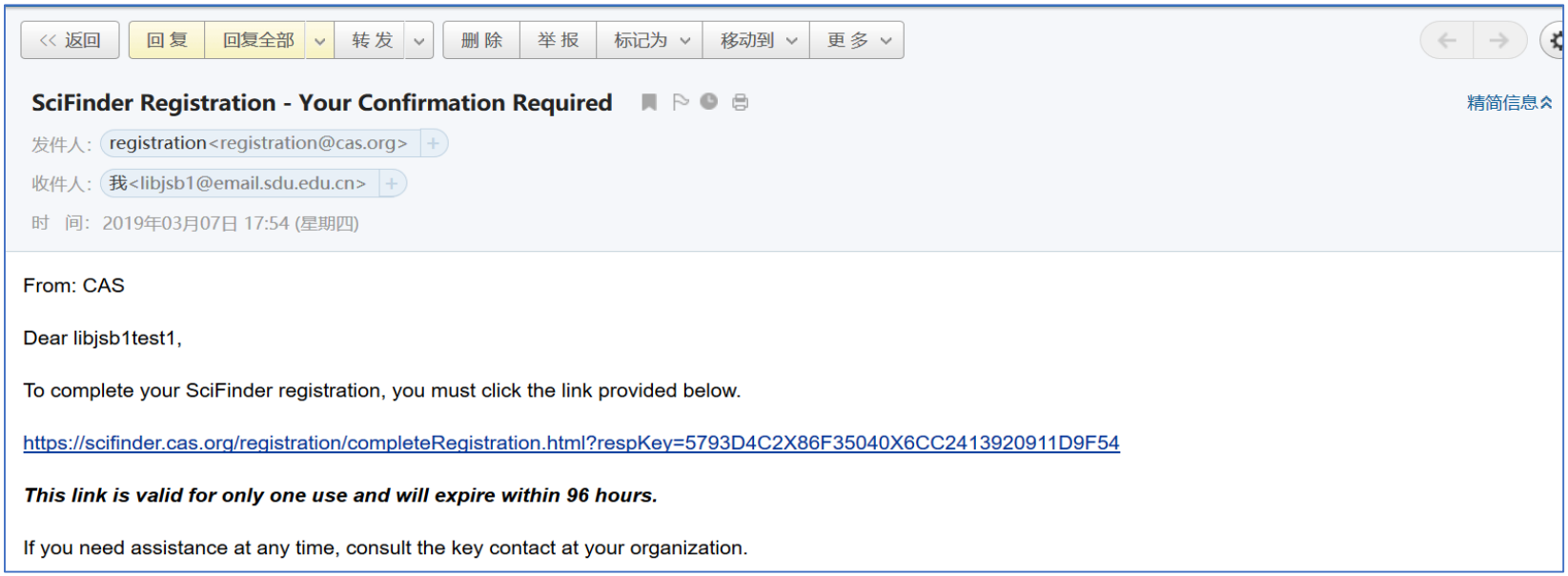
3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：

- 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）。

SciFinder® A CAS SOLUTION

如何获取SciFinder账号

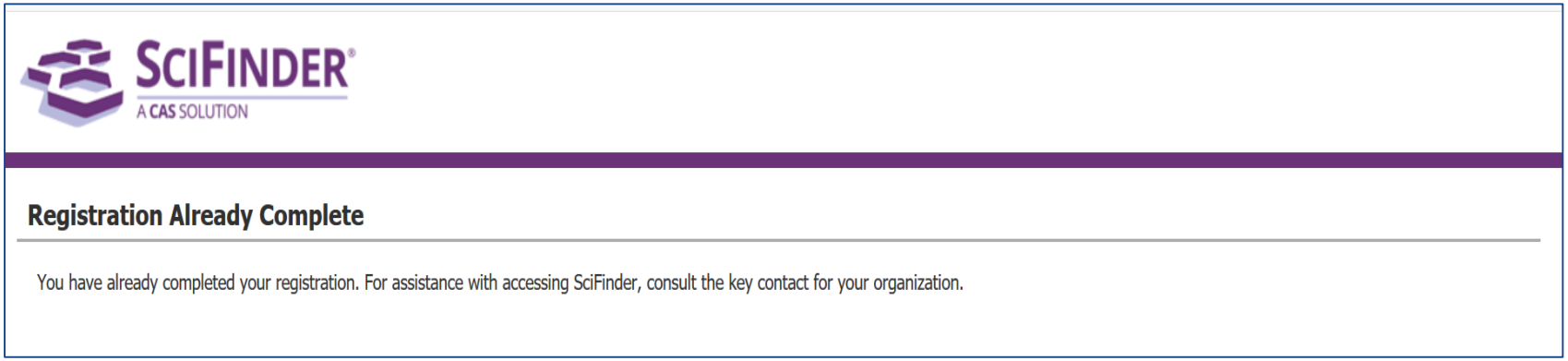


打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件

SciFinder® A CAS SOLUTION

如何获取SciFinder账号



注册成功后直接点击https://SciFinder.cas.org即可访问SciFinder数据库

SCIFINDER
A CAS SOLUTION

SciFinder使用注意事项

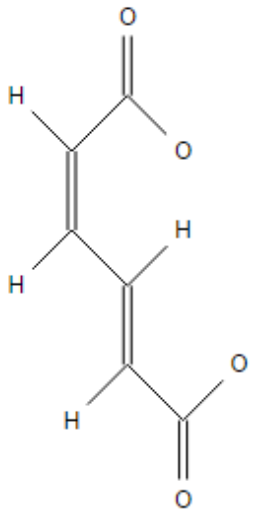
- 一人注册一个帐号
- 请提供真实姓名信息
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

更多培训资料请访问

www.cas-china.org

上机练习

- 检索“中药在帕金森病（Parkinson’s disease）治疗中的应用”的文献。被引次数最高的文献来自哪份期刊？发文最多的研究机构是哪家？该研究领域专利多还是期刊多？
- 找出分析五味子素（ Schisandrin）的相关文献？用TLC方法做分析的文献？
- 检索环系上含有以下结构片段的天然产物



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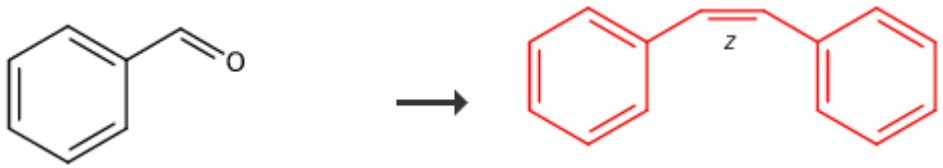
上机练习

1. 检索以下反应：



2. 检索保护吲哚环上N原子而环上的羟基不受影响的反应？

美国化学文摘社北京代表处

010-62508026

china@acs-i.org

SciFinder®
A CAS SOLUTION