汤健钊

高级客户顾问

jtang@acs-i.org

如何使用SciFinder获取医药信息

南方医科大学

2018.11.08

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（PatentPak）
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow
- 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——构建最高质量的化学数据库

arXiv.org

Aldrichimica Acta

ACS chemical biology

BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

division of polymer chemistry, inc American Chemical Society

JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

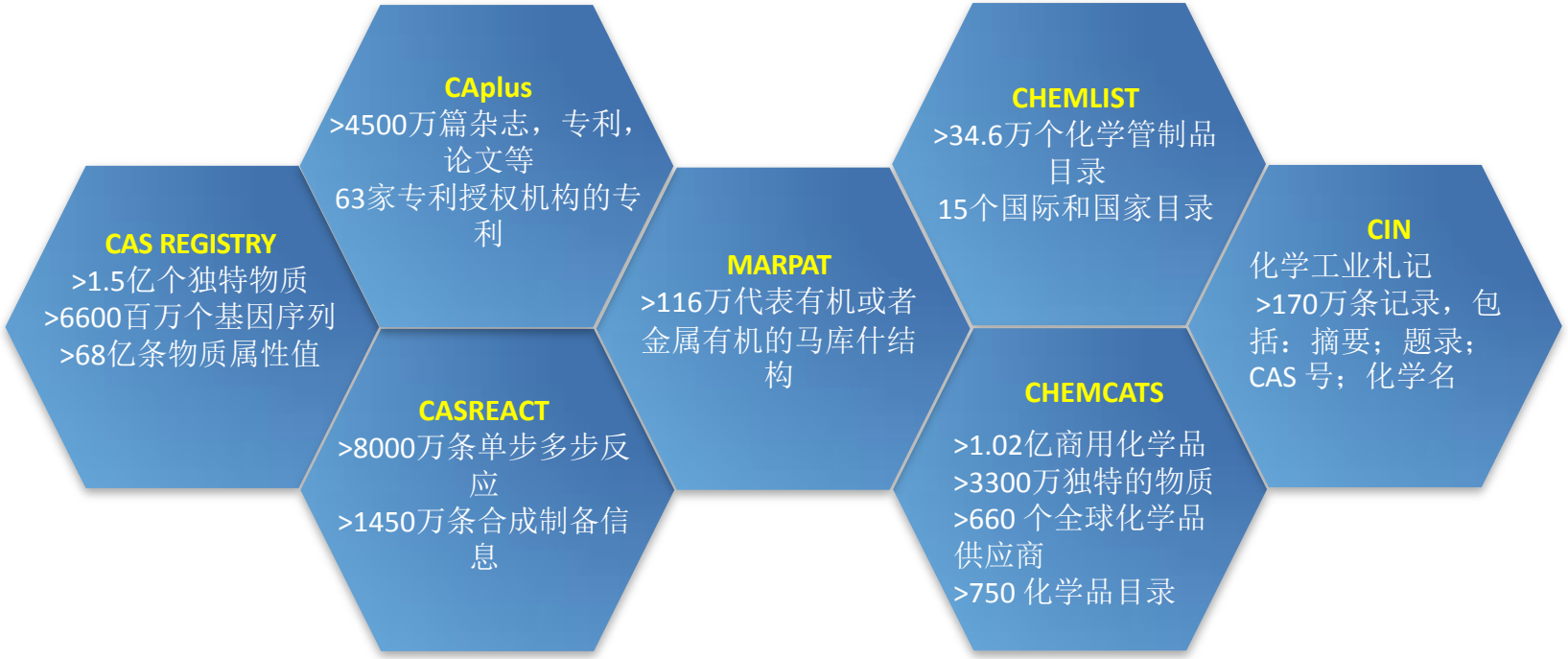
ACS Chemical Neuroscience

Cornell University Library

The Journal of Physical Chemistry Letters

SciFinder® A CAS SOLUTION

CAS——构建最高质量的化学数据库



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

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

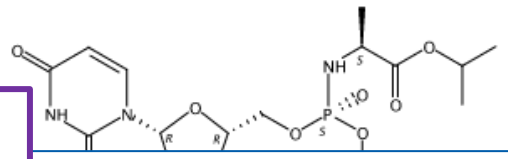
Concepts

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

CAS最新动向—解决方案

PatentPak™

NCI™ Global
A Solution Powered by CAS

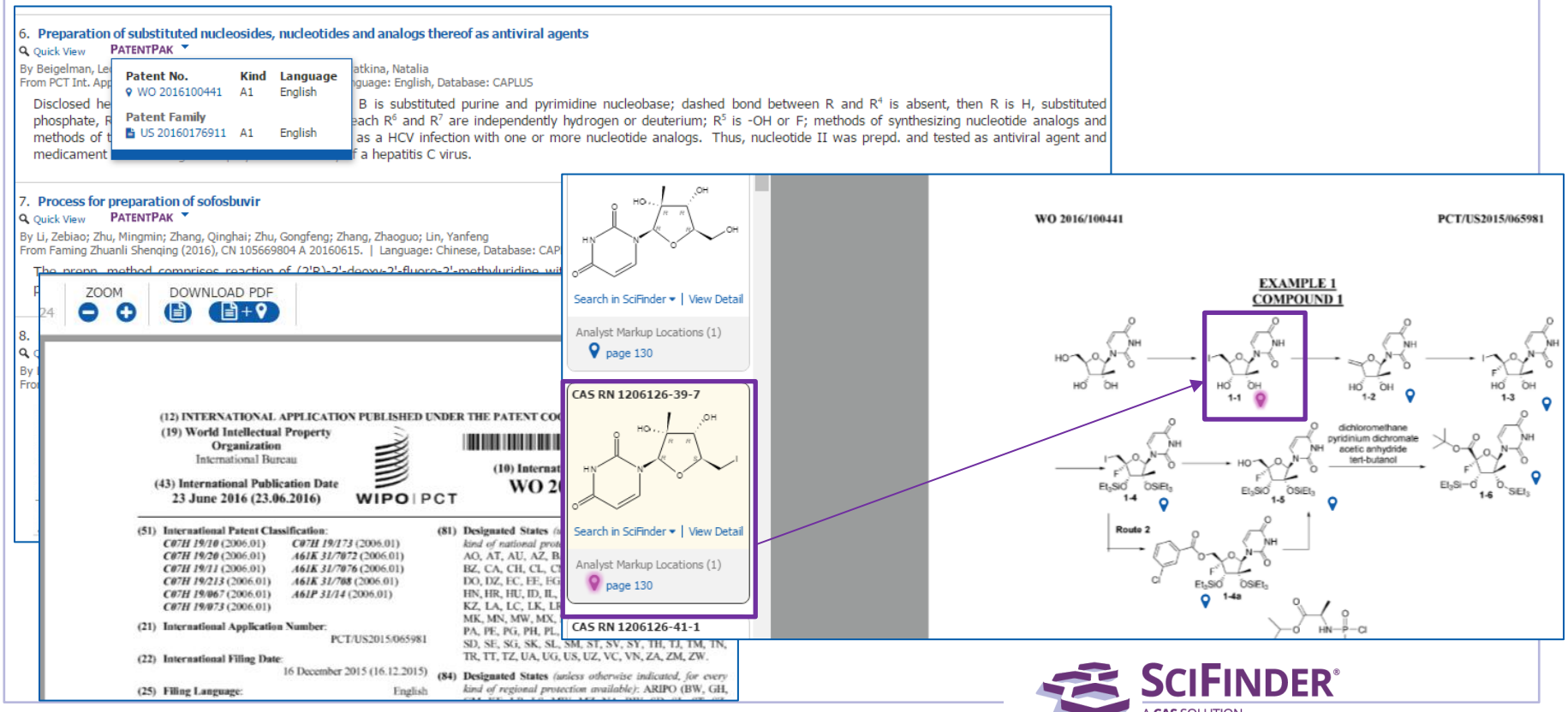
METHODSNOW™
A CAS SOLUTION

CHEMZENT™
A CAS SOLUTION

SCIFINDER®
A CAS SOLUTION

CAS最新动向—解决方案

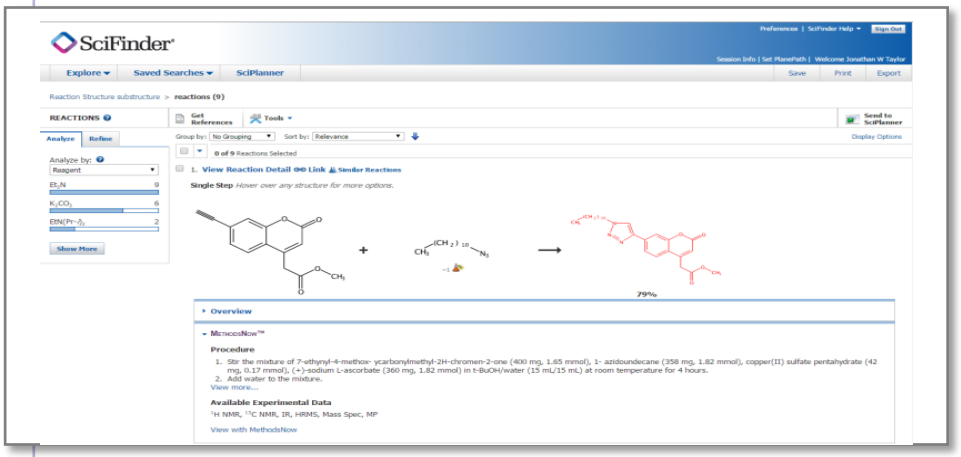
- CAS于2015年2月正式发布PatentPak™
- 专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息



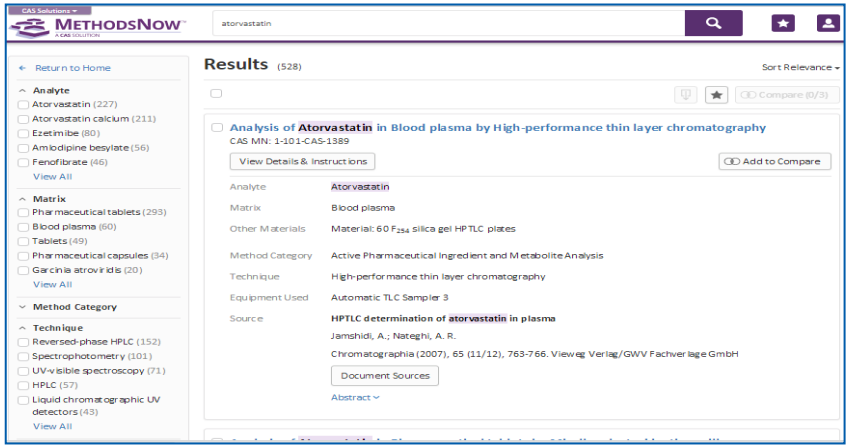
SciFinder® A CAS SOLUTION

CAS最新动向—解决方案

- CAS于2016年2月正式发布MethodsNowTM
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求



嵌在SciFinder中的合成模块



单独的分析界面

SCIFINDER®
A CAS SOLUTION

提纲

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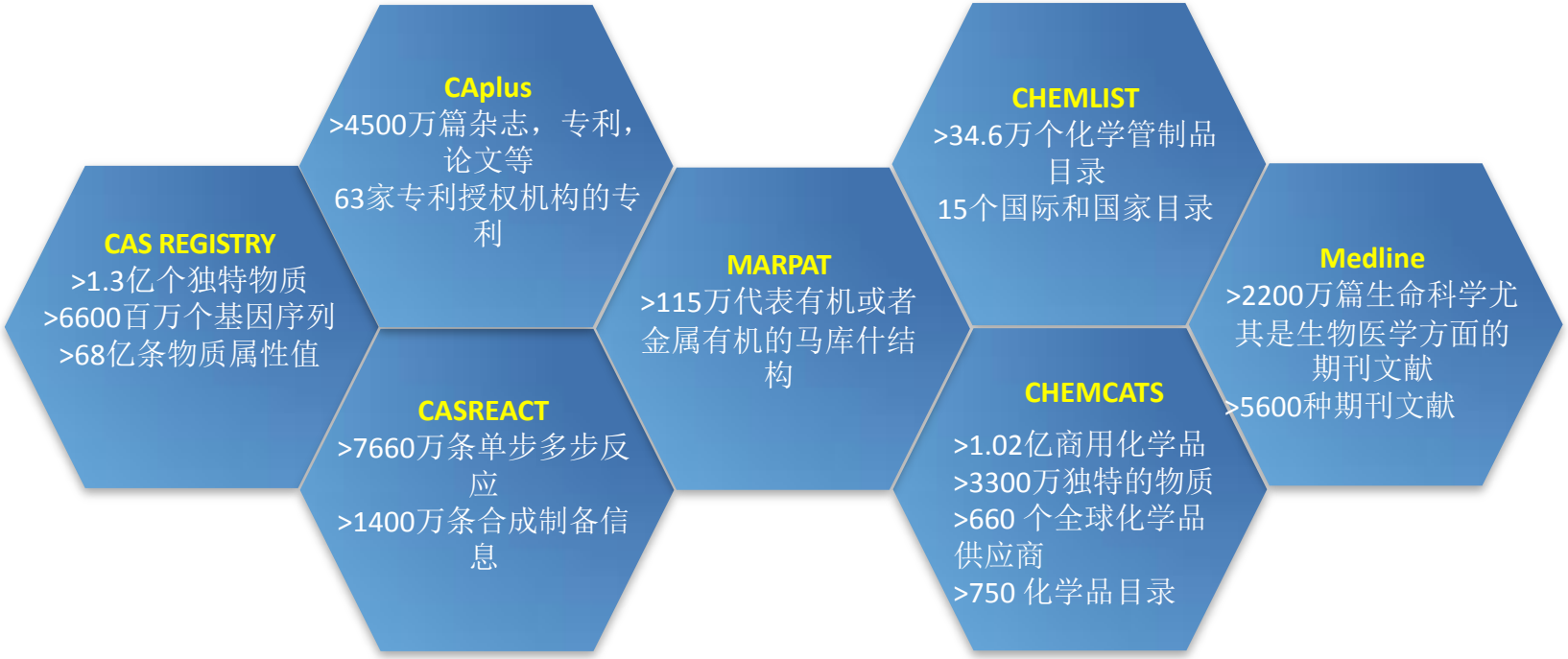
  - 物质检索
  - Markush检索
  - 反应检索（ MethodsNow Synthesis ）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

SciFinder覆盖的数据库



SciFinder® A CAS SOLUTION

SciFinder覆盖医学专家每日阅读的医学领域出版物

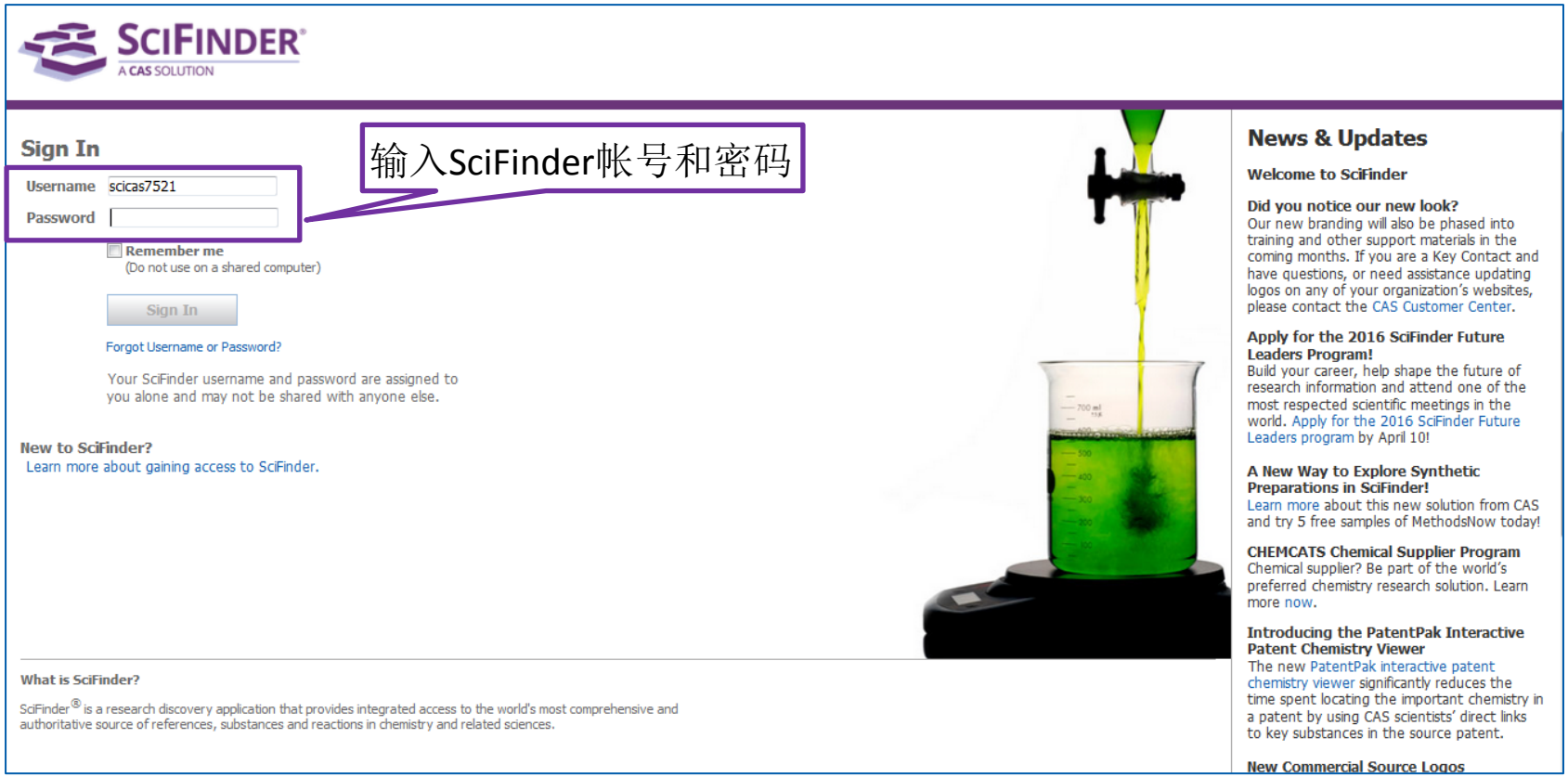
- Zhonghua Tangniaobing Zazhi
- Biomedical Chromatography
- Romanian Biotechnological Letters
- Pharmaceutical Patent Analyst
- Asian Pacific Journal of Tropical Biomedicine
- International Journal of Molecular Medicine
- Archives of Pharmacal Research
- BioMedical Research
- Journal of the Egyptian Medical Association
- European Journal of Medicinal Chemistry
- Klinische Wochenschrift

- ***ACS Synthetic Biology***
- ***Annual Review of Biochemistry***
- ***Biochemistry and Cell Biology***
- ***Cellular Physiology and Biochemistry***
- ***Journal of Biological Chemistry***
- ***Journal of Cellular Biochemistry***
- ***Molecular and Cellular Biochemistry***
- ***Preparative Biochemistry and Biotechnology***

- ***Advanced Drug Delivery Reviews***
- ***Annual Review of Pathology: Mechanisms of Disease***
- ***Anti-Inflammatory Anti-Allergy Agents in Medicinal Chemistry***
- ***Circulation Research***
- ***Immunity***
- ***Journal of the American Medical Association***
- ***Journal of Experimental Medicine***
- ***Nature Reviews Drug Discovery***
- ***Trends in Immunology***

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

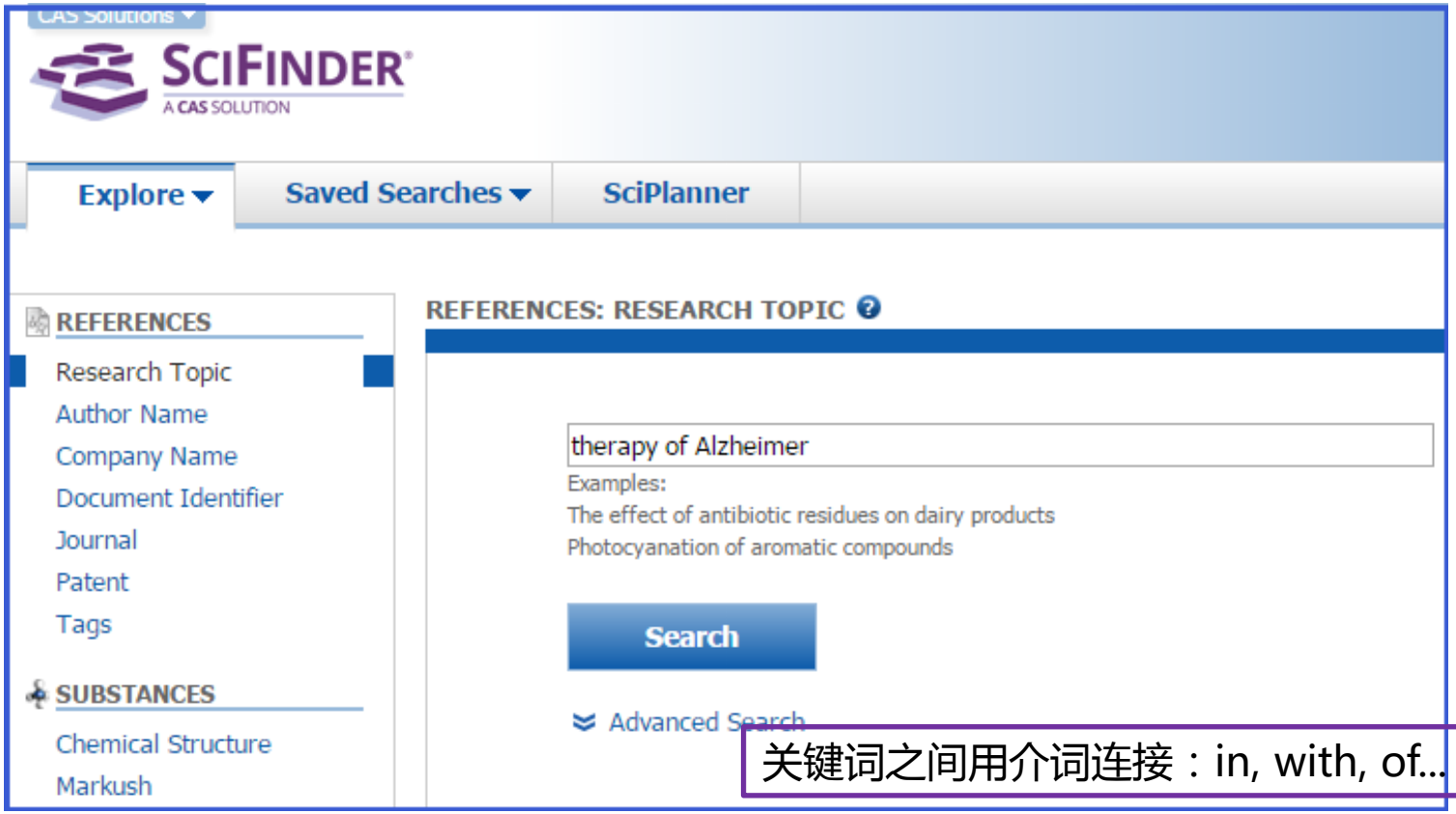
- 检索策略推荐
  - 关注某特定领域的文献：主题检索
  - 关注物质有关的文献：先获得物质，再获得文献
  - 关注某科研人员的文献：作者名检索
  - 关注某机构科研进展：机构名检索

SCIFINDER® A CAS SOLUTION

文献检索——主题

主题检索：阿尔茨海默症的治疗

检索式： therapy of Alzheimer



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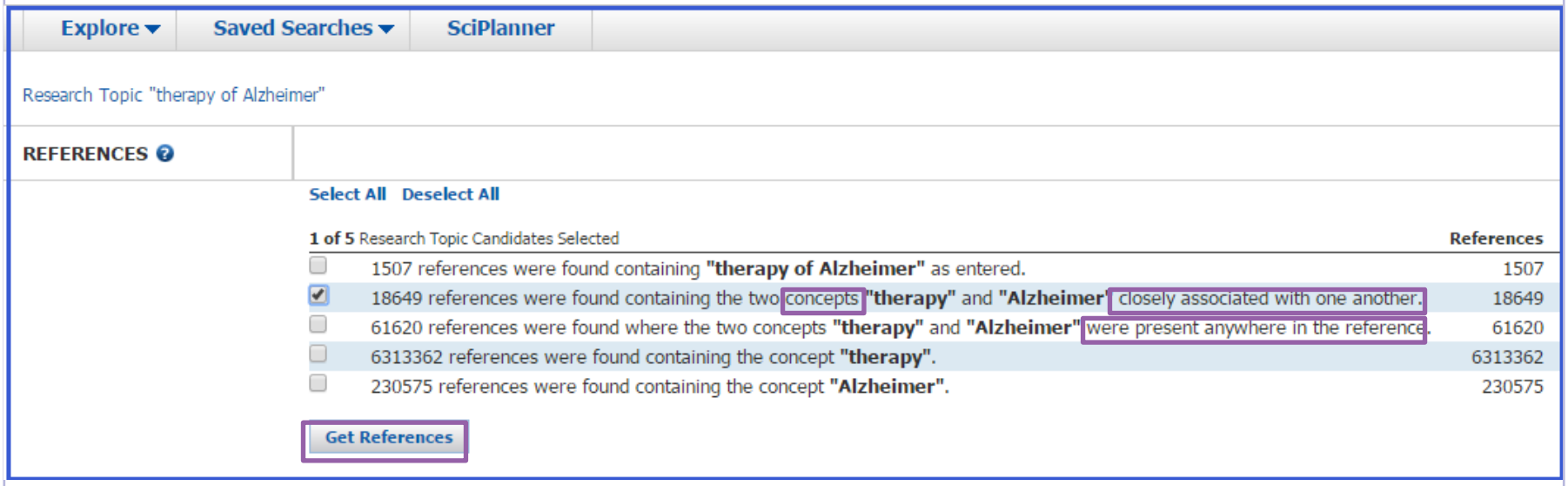
主题检索的候选项



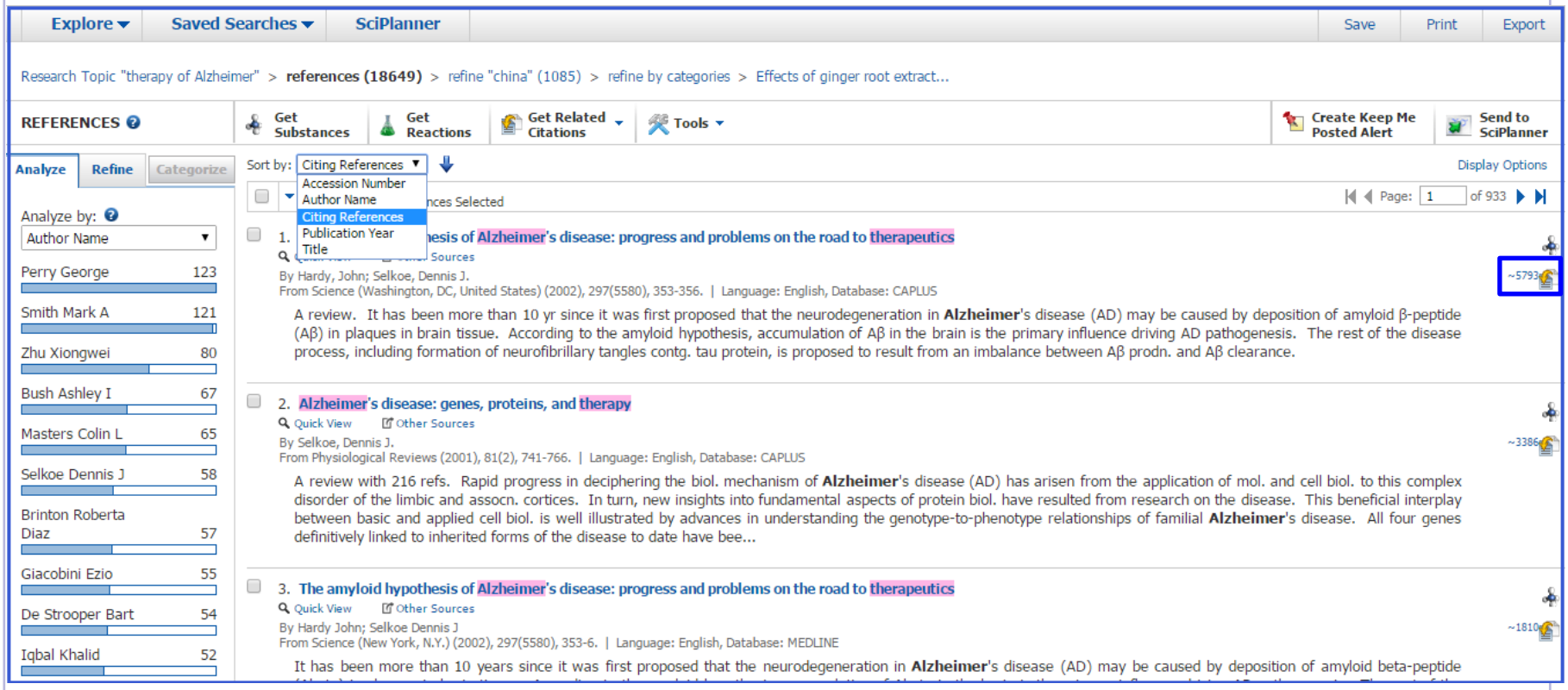
"Concepts"表示对主题词做了同义词的扩展；

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

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

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

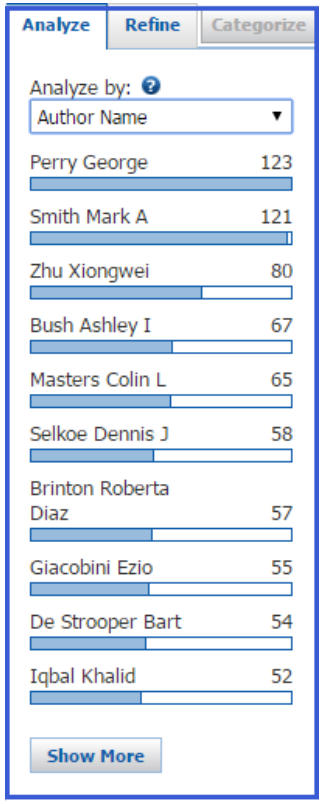
文献检索结果

SciFinder提供强大的文献处理工具，帮助处理文献

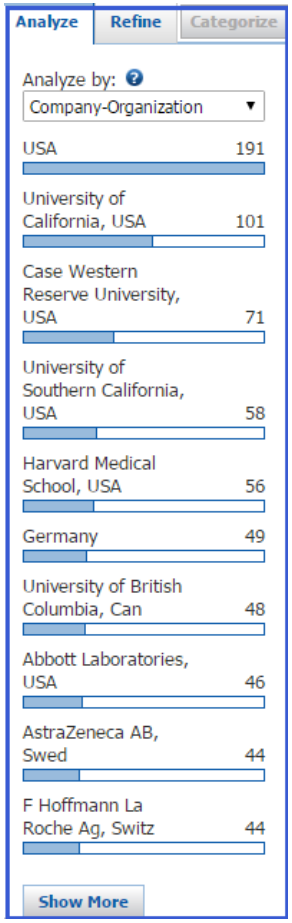
SCIFINDER® A CAS SOLUTION

文献检索结果的Analyze

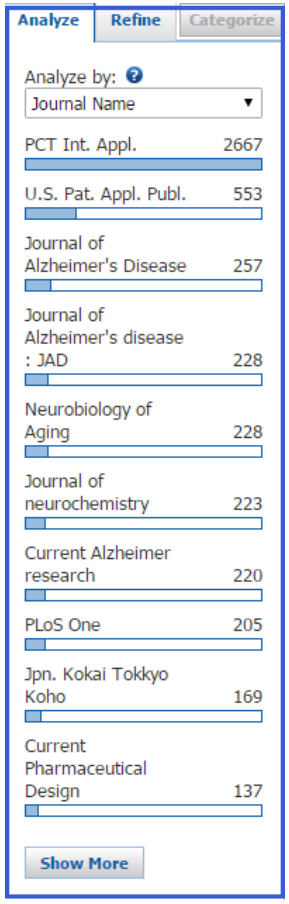
本领域研究人员



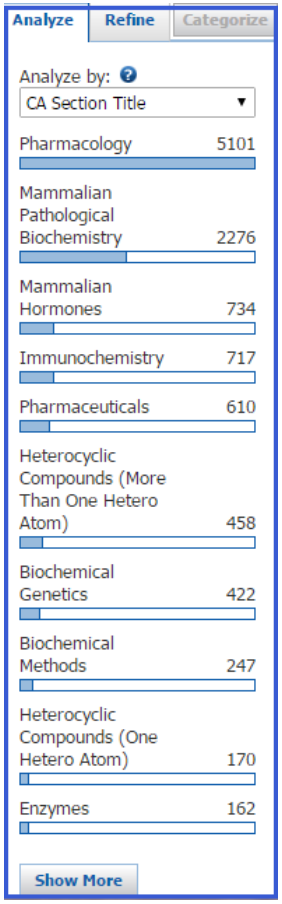
本领域研究机构、合作伙伴、竞争对手



期刊



涉及学科领域

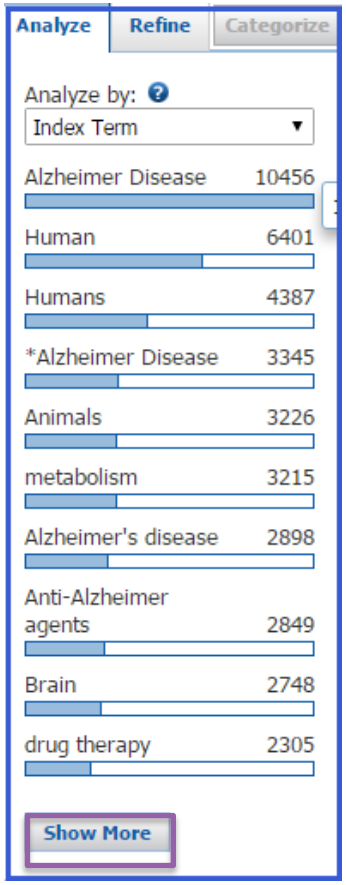


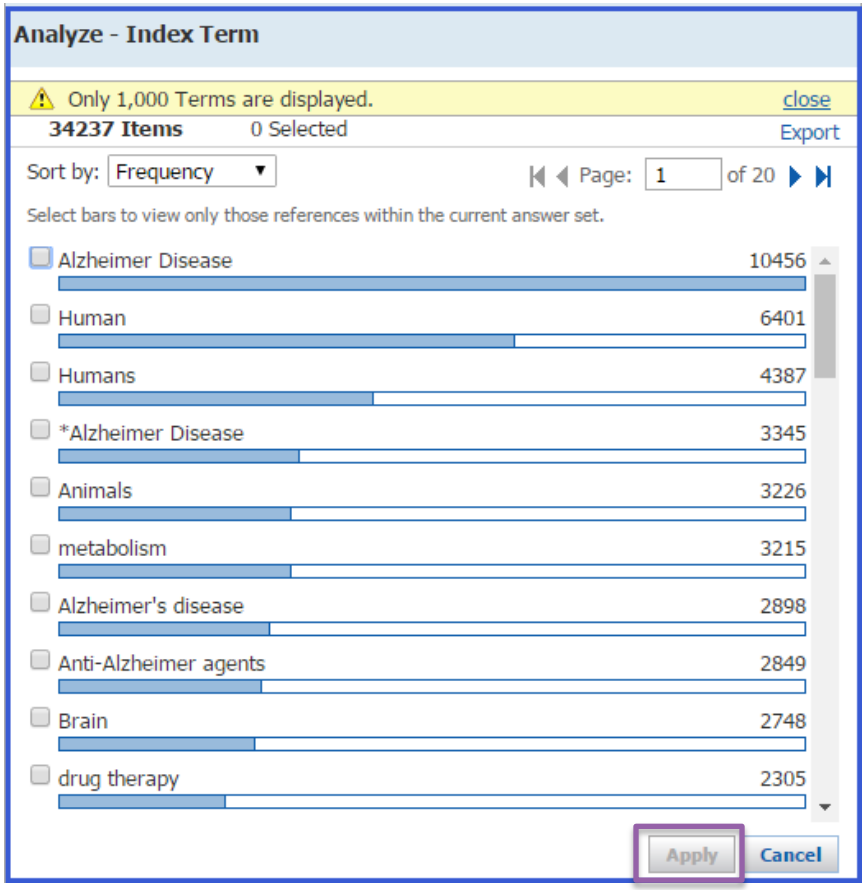
SCIFINDER® A CAS SOLUTION

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

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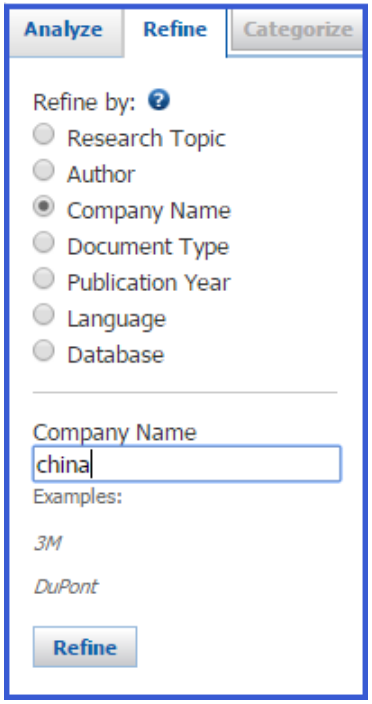
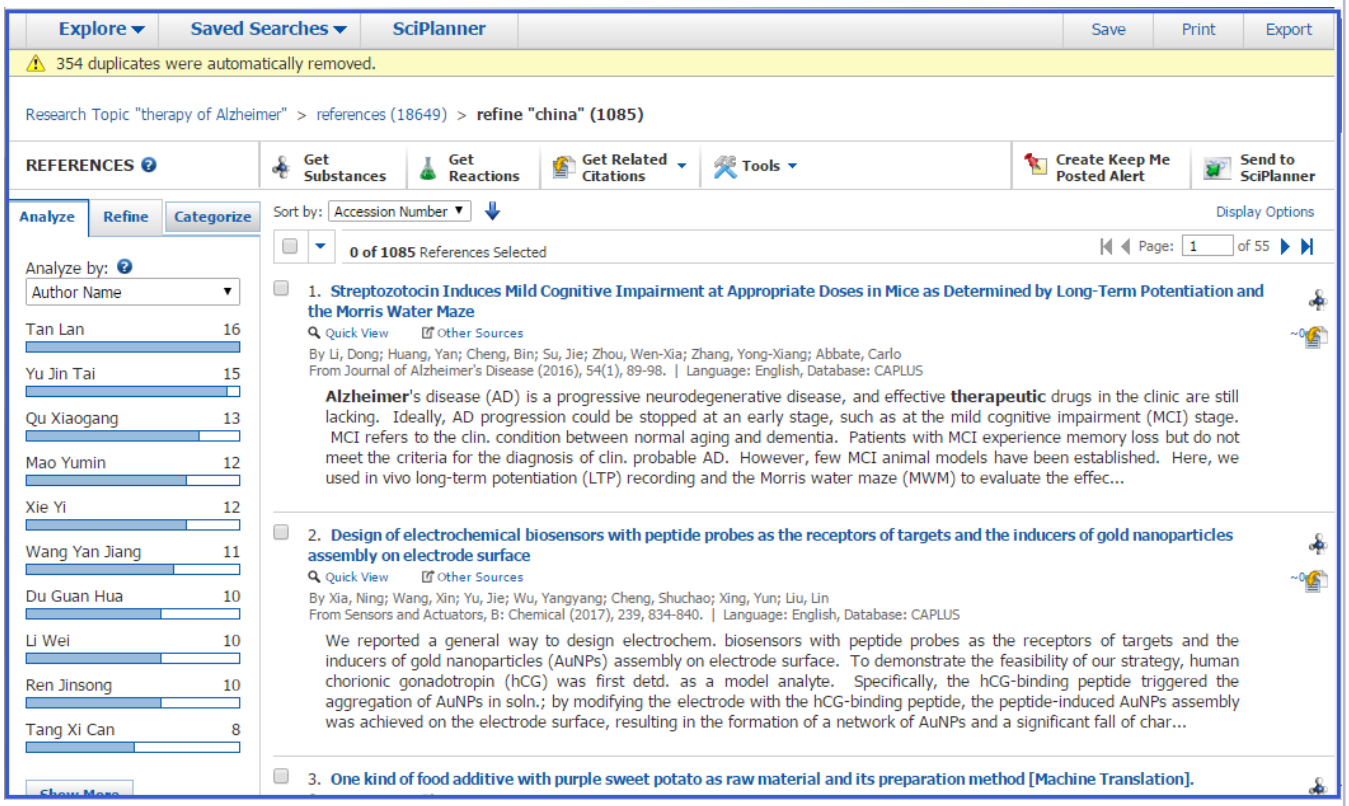
文献检索结果的Refine



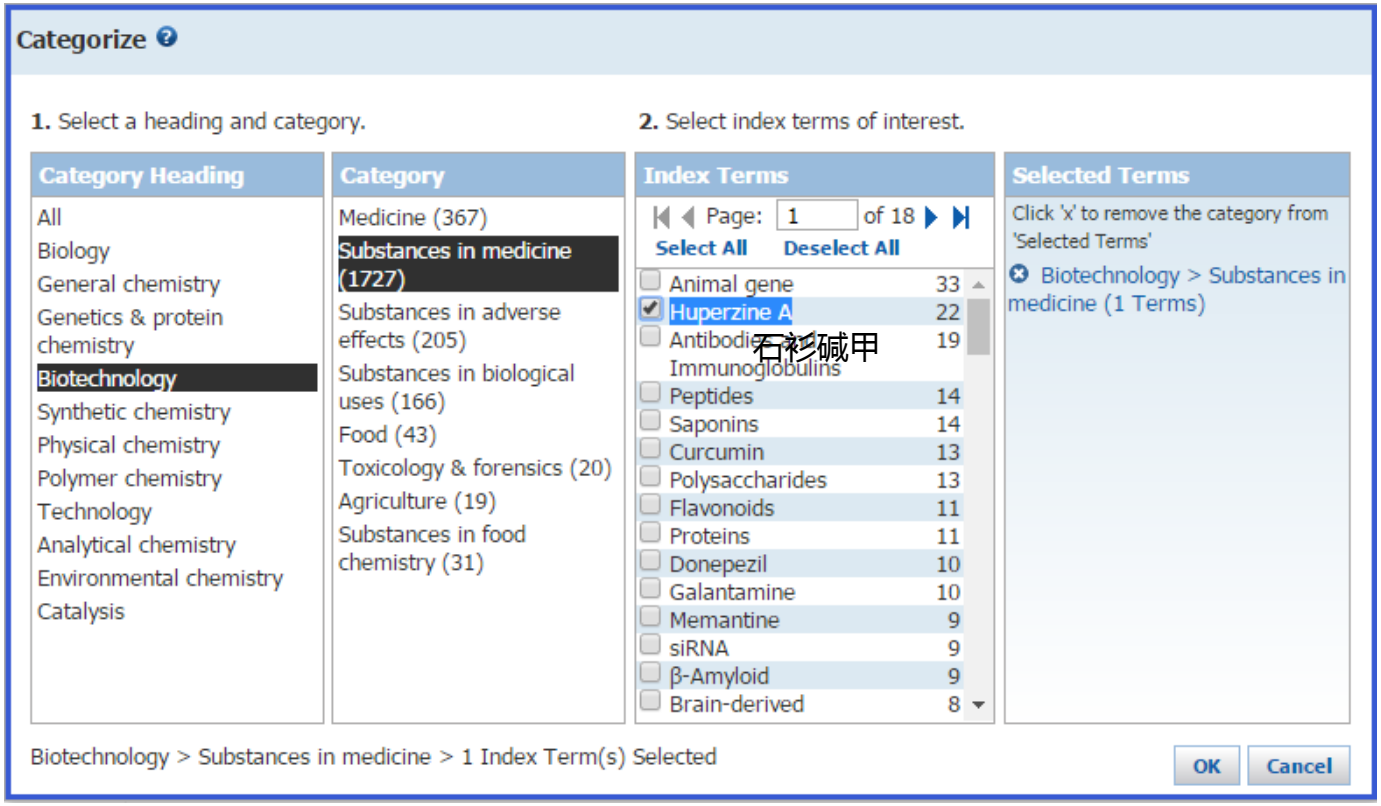


Refine：帮助用户迅速获得需要的文献

SciFinder® A CAS SOLUTION

文献检索结果的Categorize

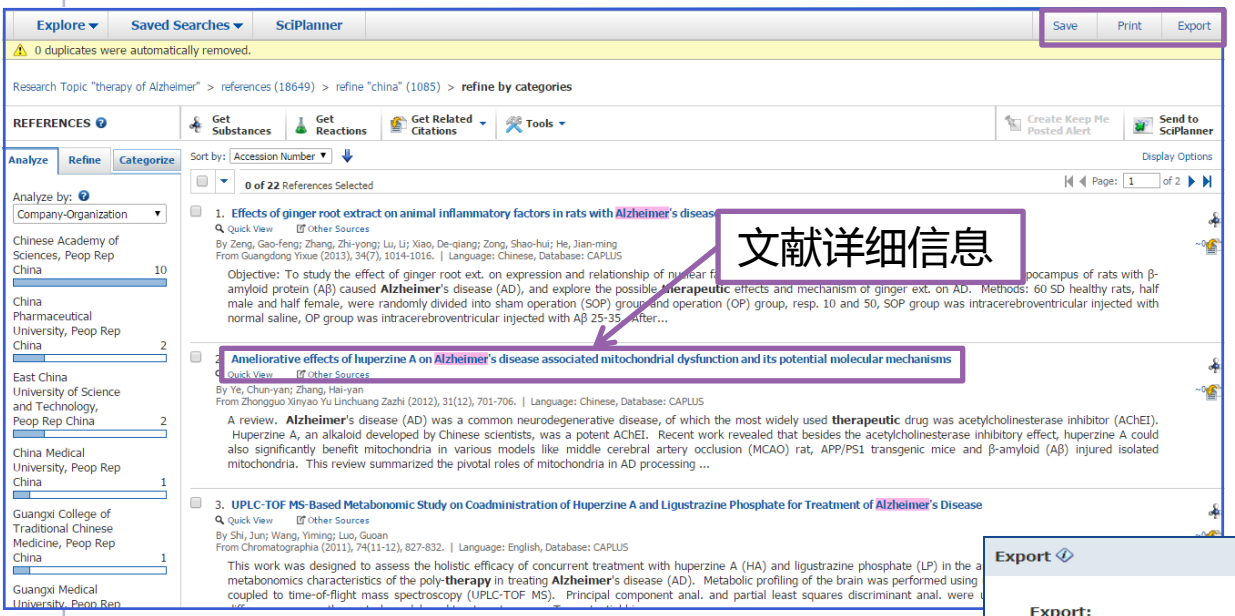
学科领域主分类　　学科领域副分类　　Index Term　　选中的Index Term



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

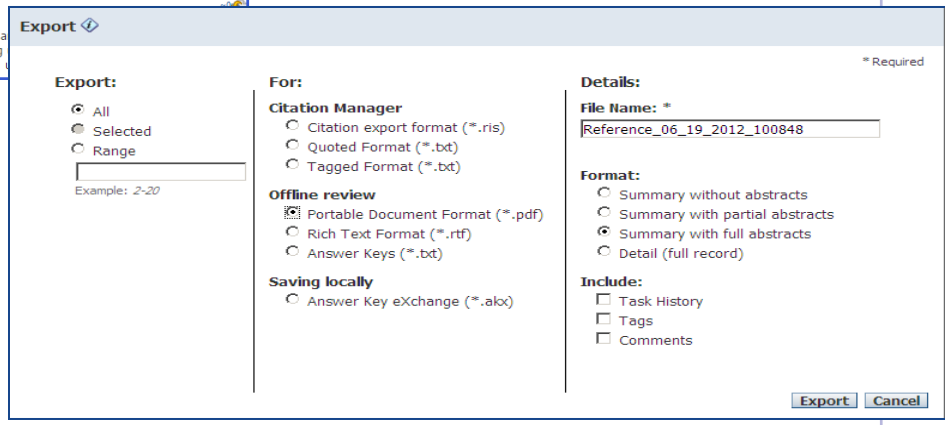
结果集的保存— Save, Print, Export



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

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

文献检索小结

- 主题检索时，使用介词 in, with, of 等作为连接词
- 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

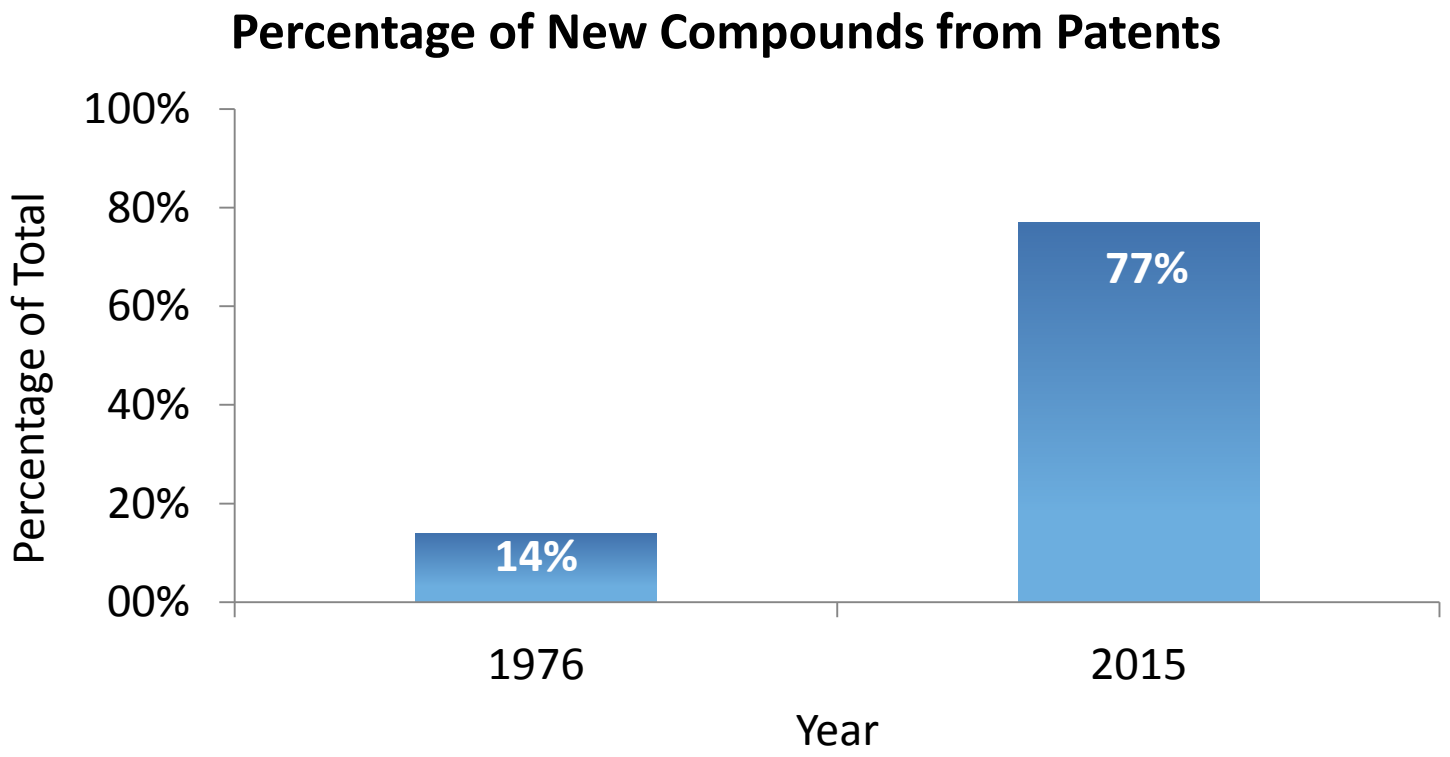
SCIFINDER® A CAS SOLUTION

PatentPak™

专利工作流程解决方案

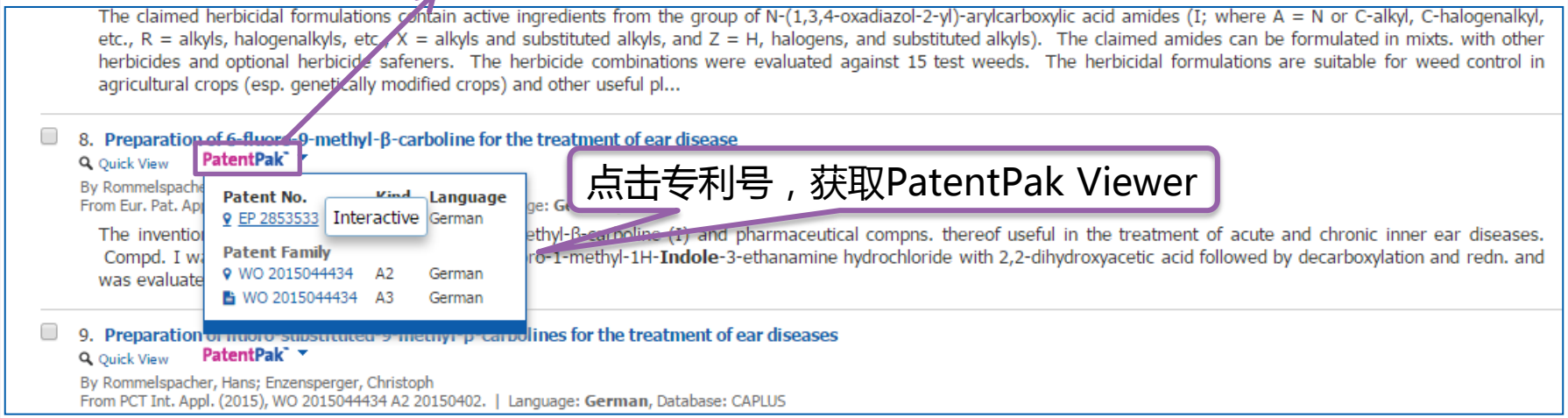
SciFinder® A CAS SOLUTION

越来越多的新化合物倾向于首先通过专利公布

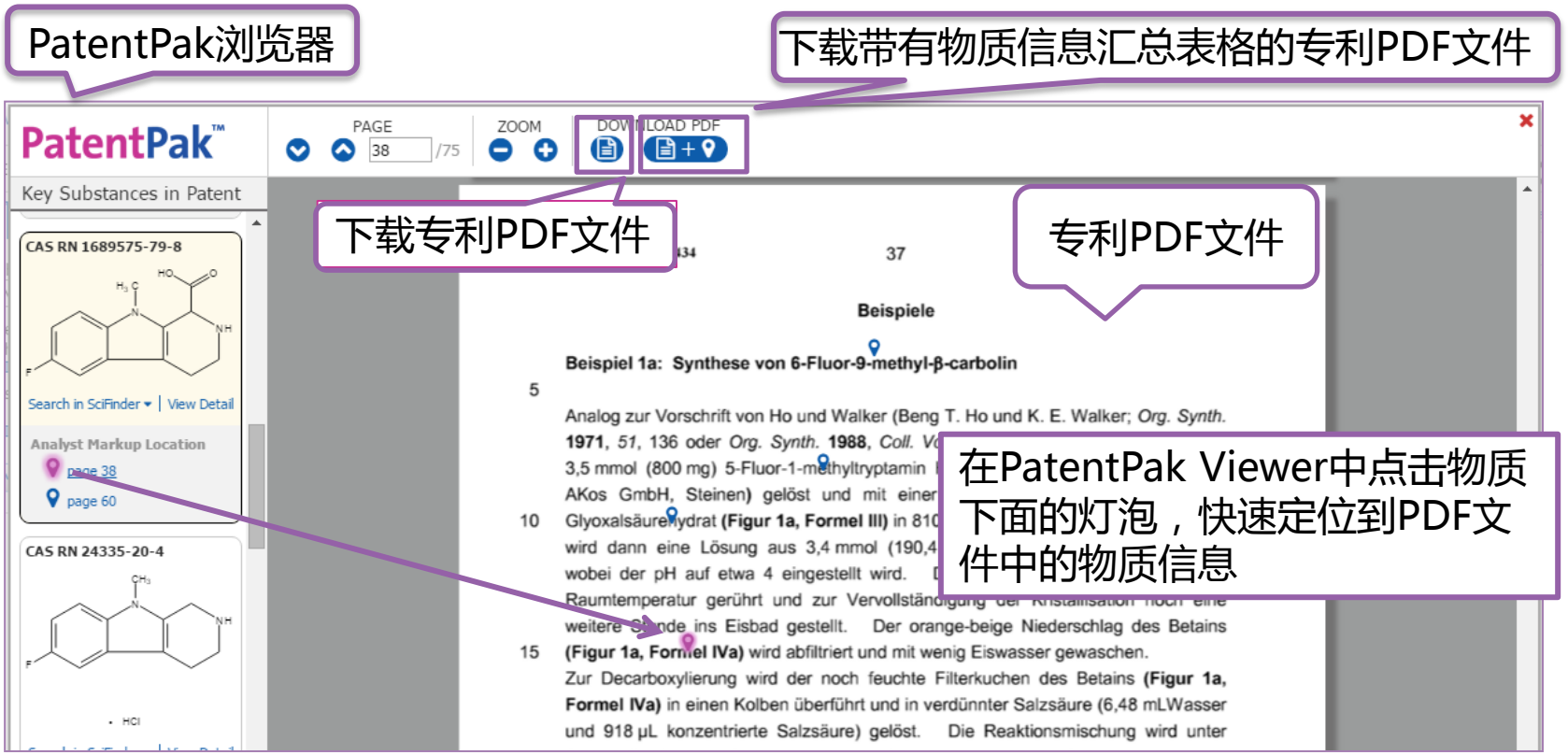


PatentPak——专利工作流程解决方案

在SciFinder检索结果中，看到PatentPak图标即可点击



PatentPak——专利工作流程解决方案



节省您最宝贵的资源——时间

- 即时获得来自世界上31家专利授权机构的逾900万份专利PDF文件，且数量持续增加
- 专利族涵盖了多种语言
- 通过CAS登记号获得物质在专利文献中的相关信息
- 专利研究安全保密
- 每日更新
- SciFinder检索功能中内置交互式浏览器

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  - 物质检索
  - Markush检索
  - 反应检索（ MethodsNow Synthesis ）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

SciFinder检索选项——物质检索

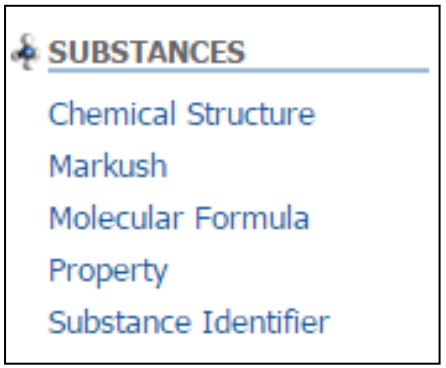
- 物质检索方法

  —结构式检索

  —分子式检索

  —理化性质检索

  —物质标识符检索：化学名称，CAS RN



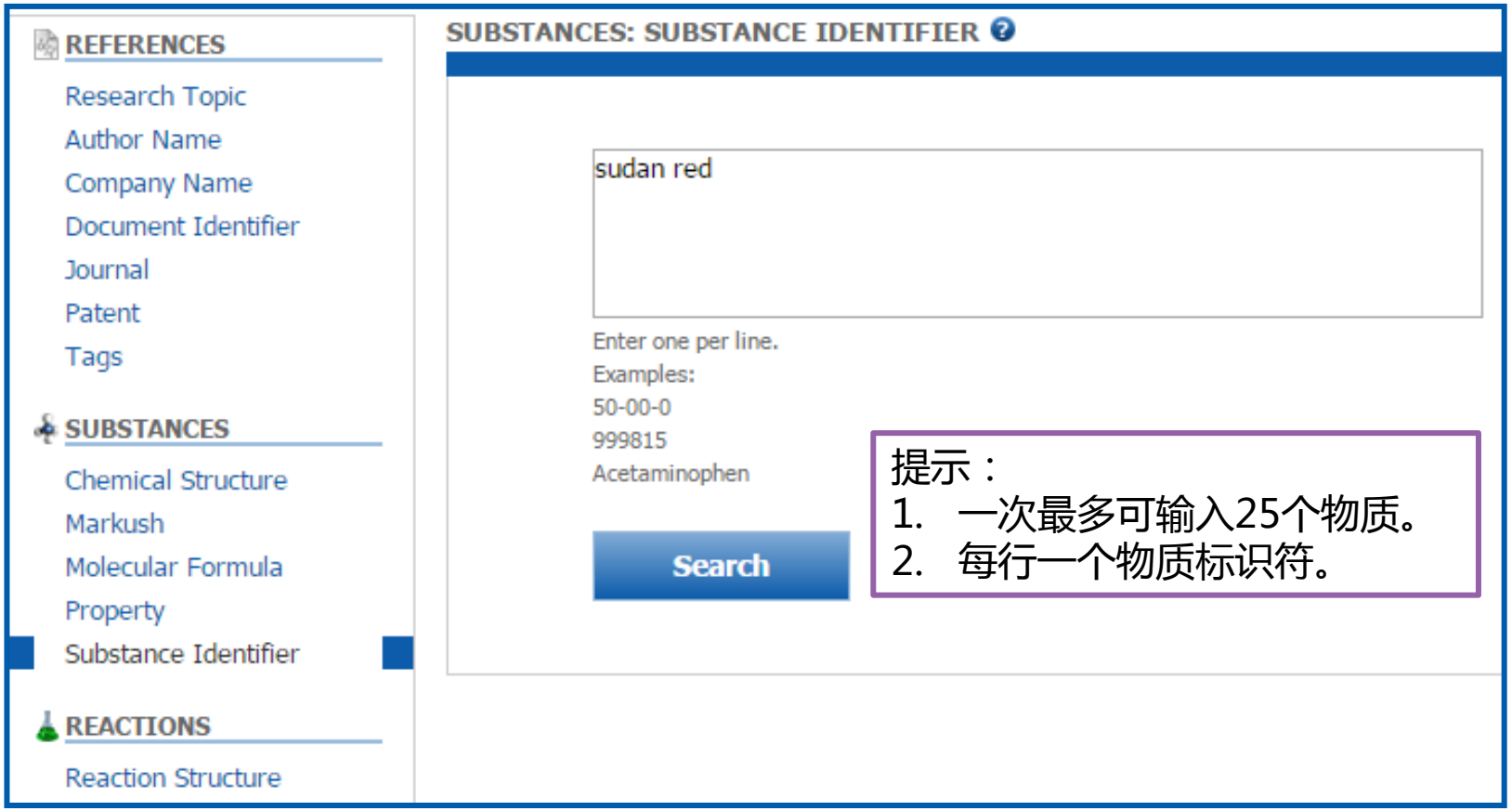
- 物质检索策略推荐

  —有机化合物，天然产物：结构检索

  —无机物，合金：分子式检索

  —高分子化合物：分子式检索和结构检索

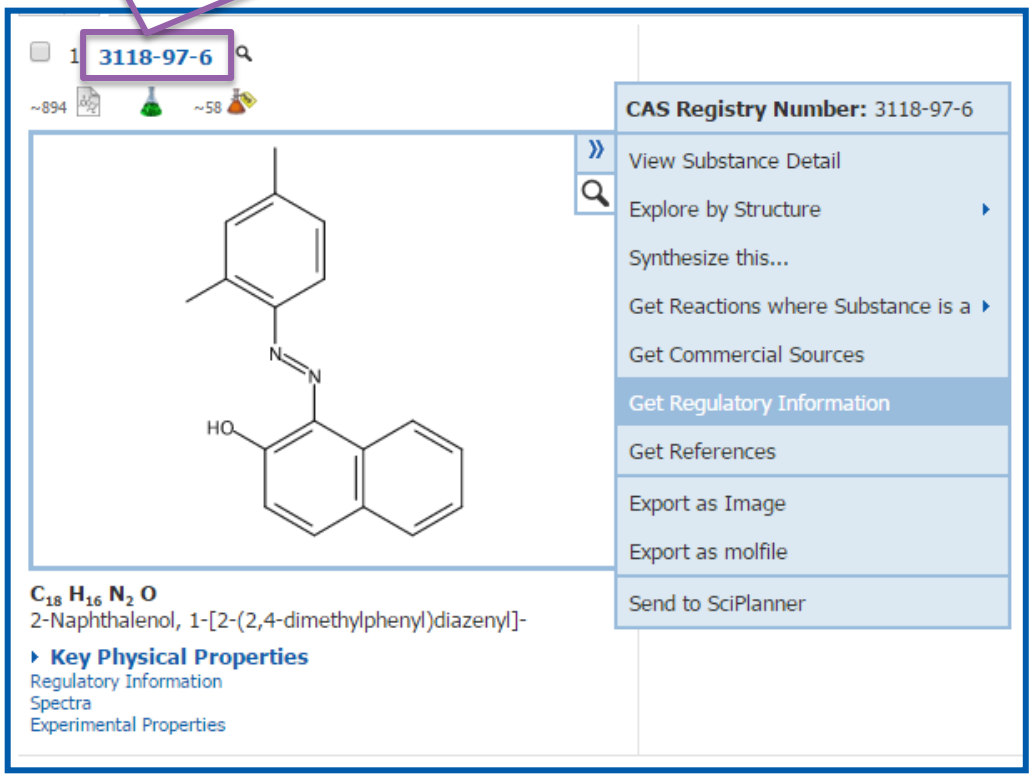
物质检索——标识符检索



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

SciFinder中的物质记录

点击CAS RN 获得物质详细信息



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

SciFinder中的物质记录

SUBSTANCE DETAIL

Get References | Get Reactions | Get Commercial Sources

Return

由物质获得文献，反应，供应商等信息

CAS Registry Number 3118-97-6

~894 ~58

$C_{18}H_{16}N_2O$

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

Molecular Weight
276.33

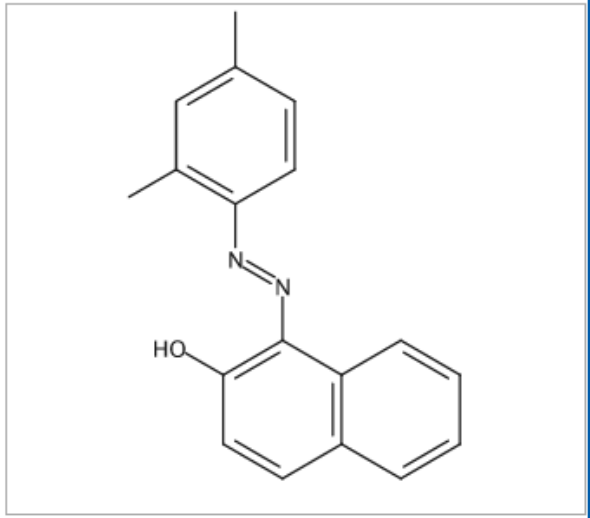
Melting Point (Experimental)
Value: 166 °C

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

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

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

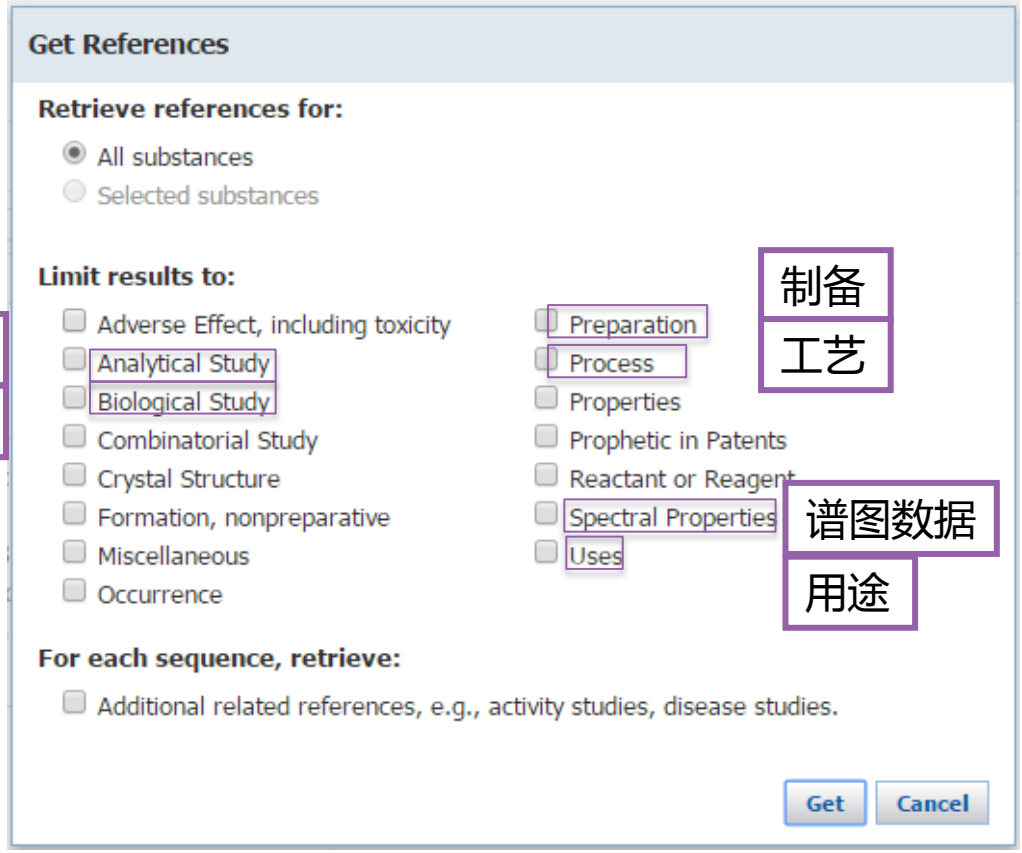
Other Names
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)
C.I. Solvent Orange 7 (7CI,8CI)
Sudan Red (6CI)
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol
AF Red No. 5
View more...



物质详情

SciFinder® A CAS SOLUTION

通过物质获得文献



分析化学

生物研究

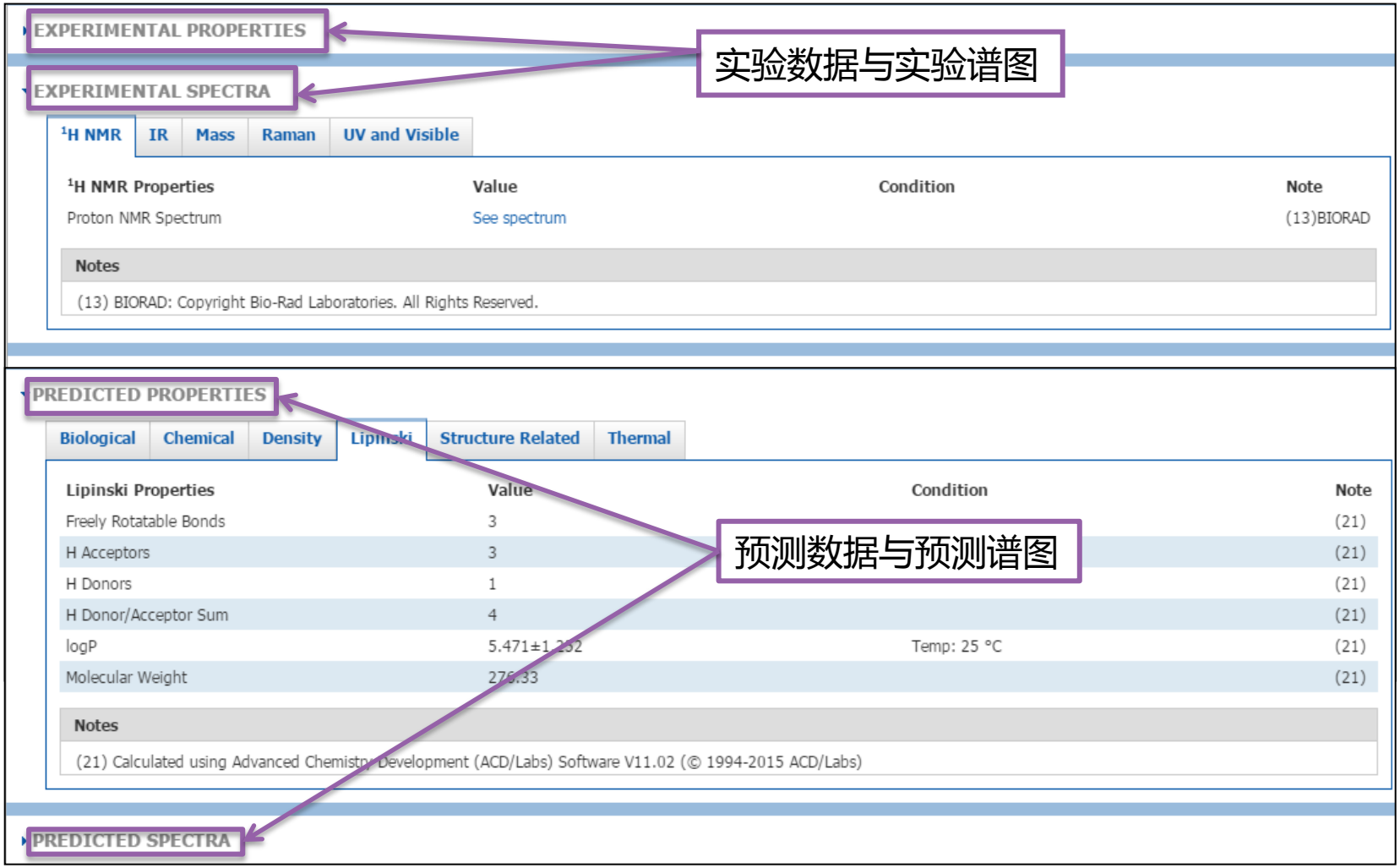
制备

工艺

谱图数据

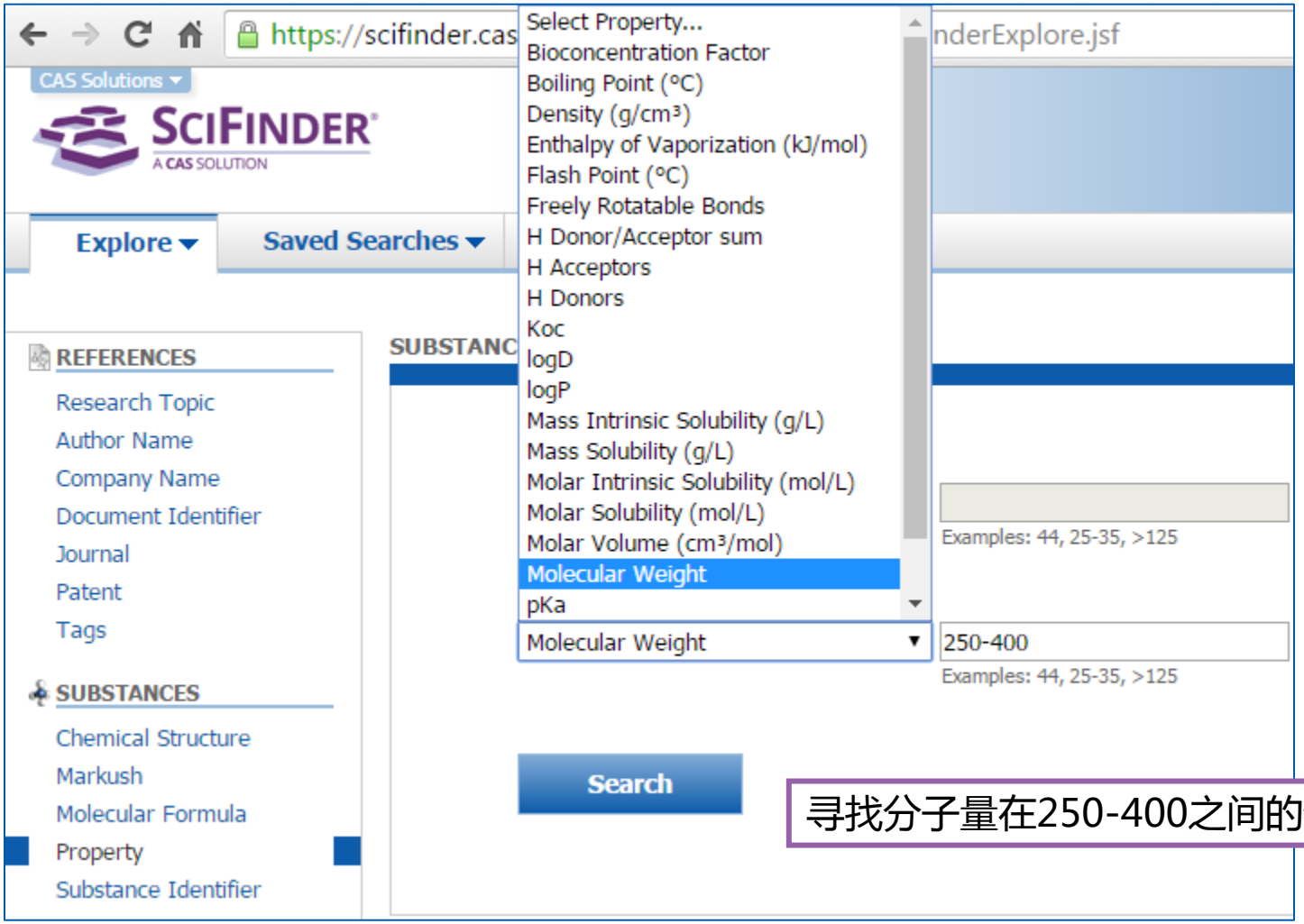
用途

SciFinder® A CAS SOLUTION



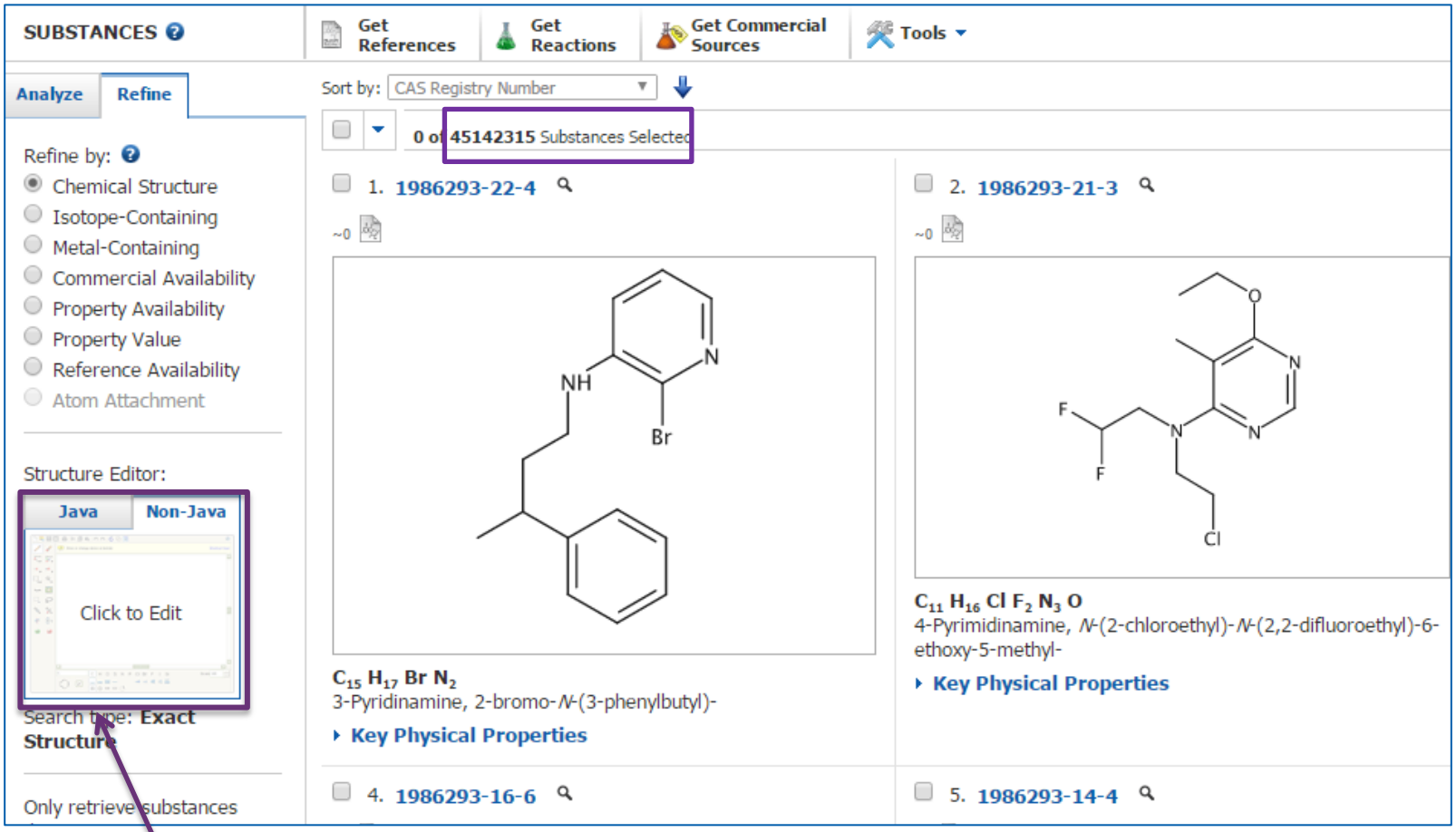
SciFinder® A CAS SOLUTION

物质检索——Property explore



寻找分子量在250-400之间的物质

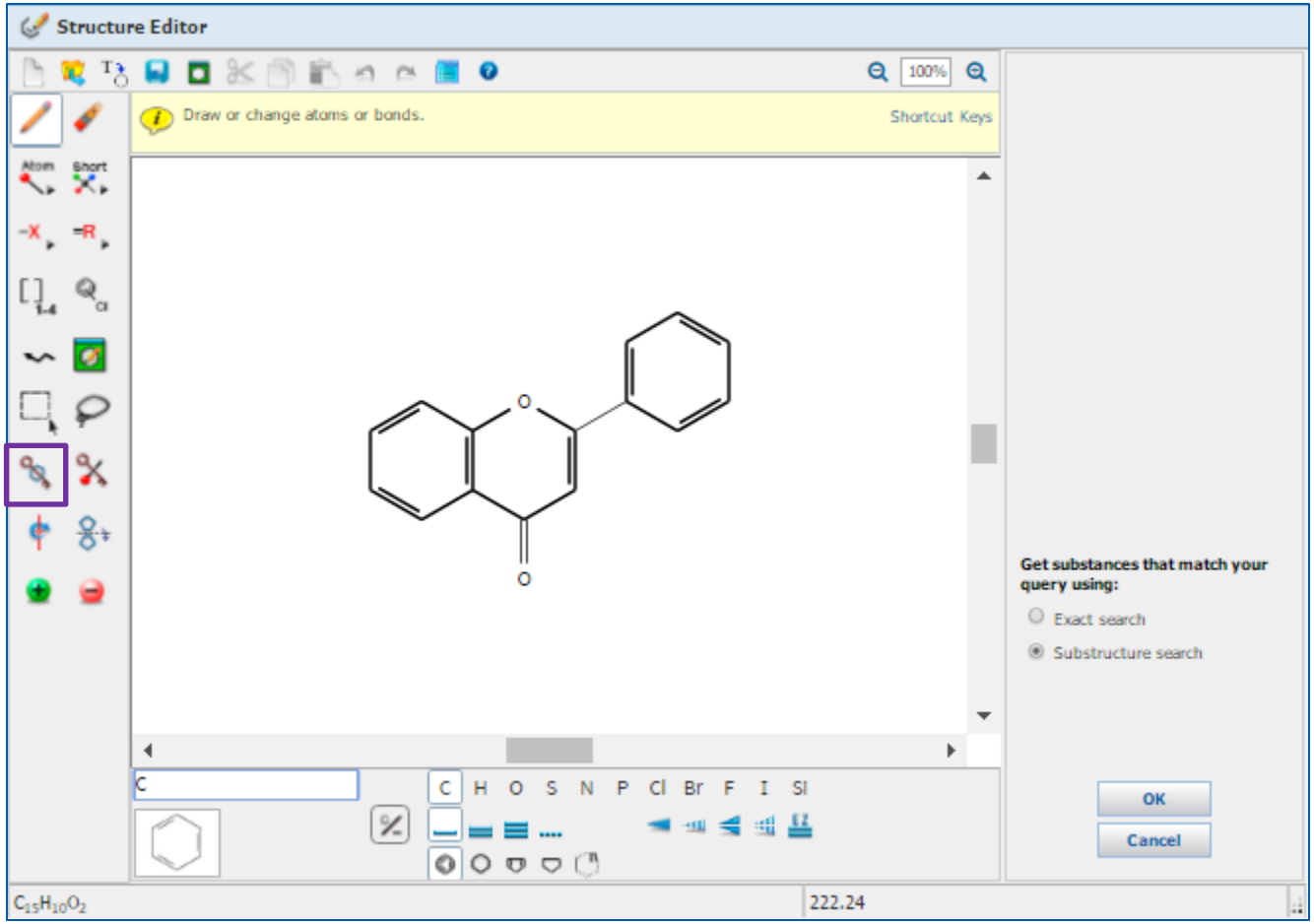
物质结果集的筛选——Refine

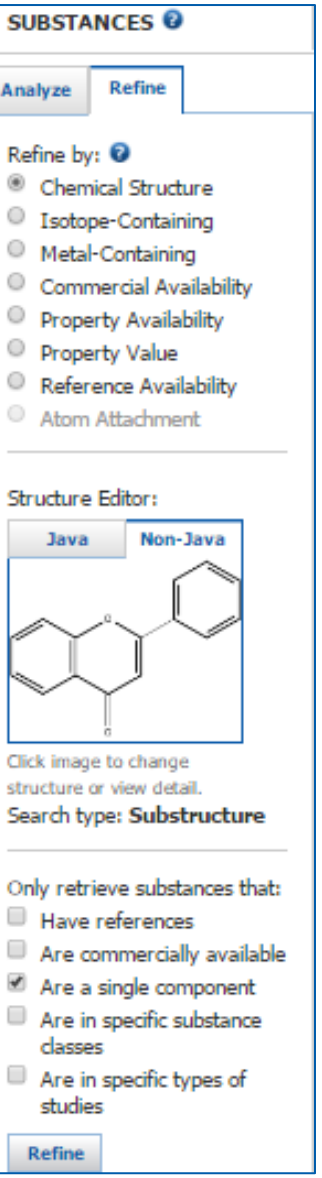


4500多万个结构，

如何筛选黄酮类物质？

物质结果集的筛选——Refine

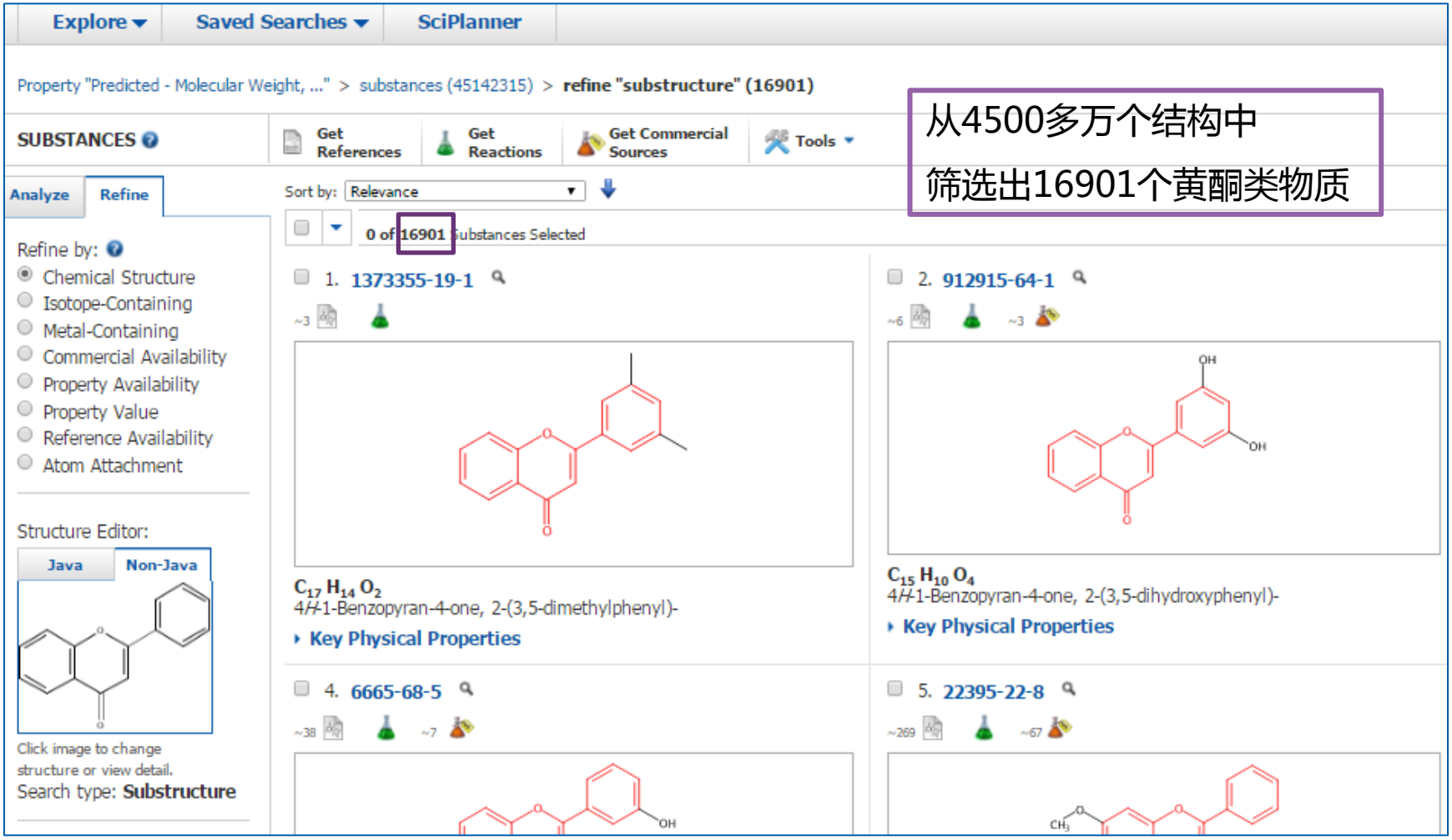




锁环工具：避免在被锁定的环结构上出现新的环结构

SciFinder® A CAS SOLUTION

物质检索结果集

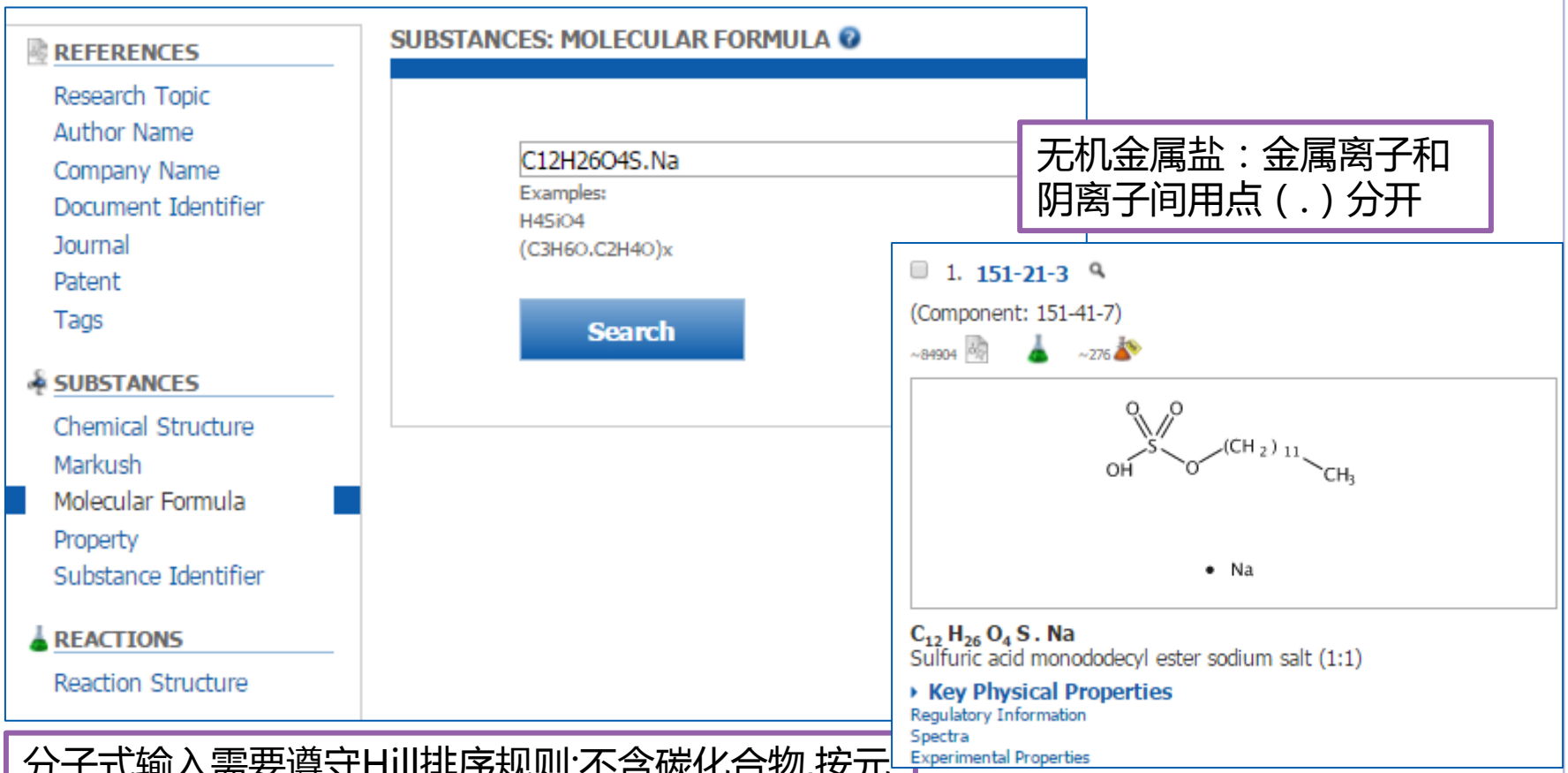


从4500多万个结构中

筛选出16901个黄酮类物质

SciFinder® A CAS SOLUTION

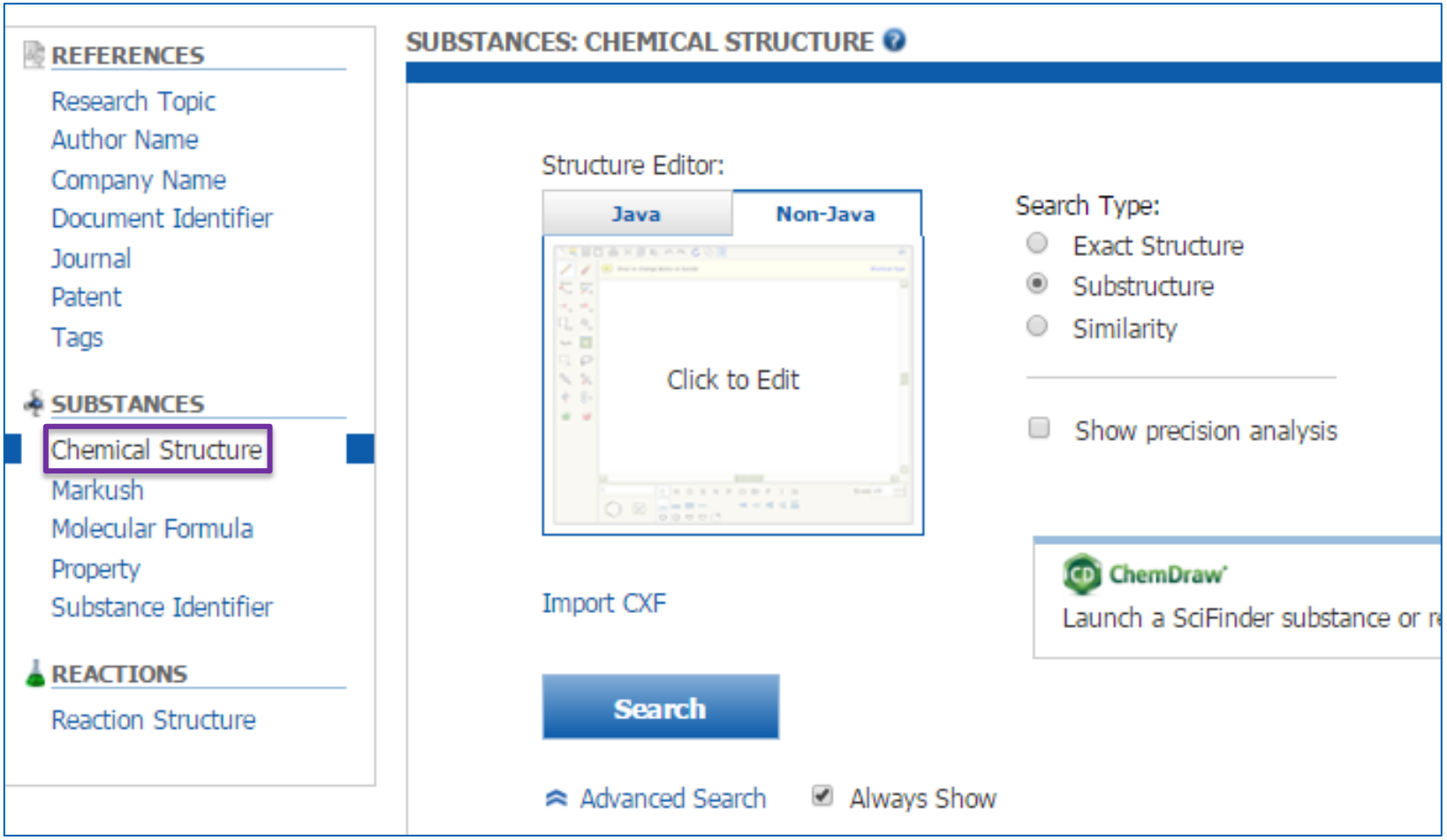
物质检索——分子式



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



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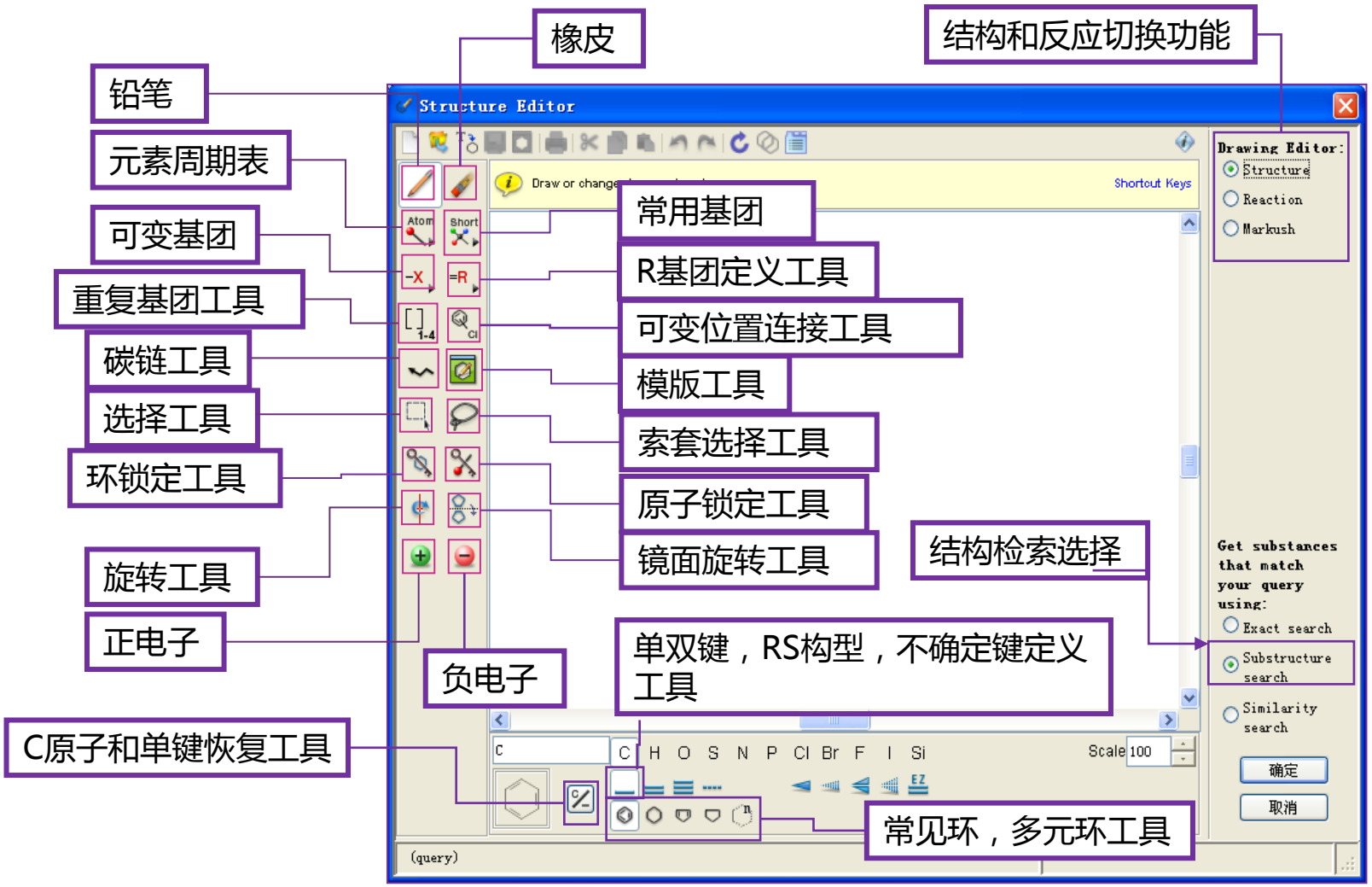
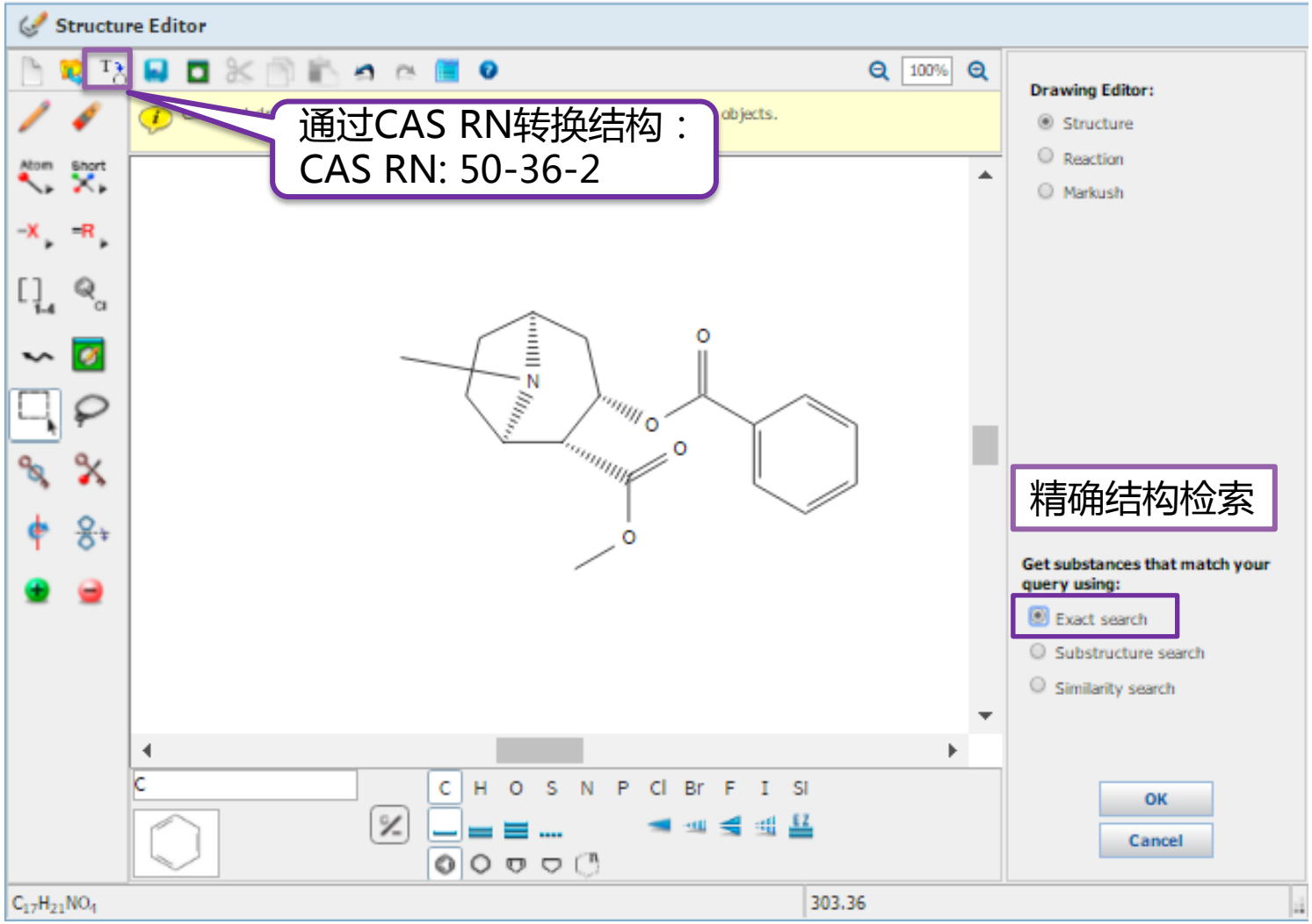
物质检索——结构


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

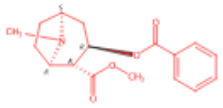
Get References | Get Reactions | Get Commercial Sources | Tools | Create Posted

Sort by: Relevance

0 of 6 Substances Selected

1. 668-19-9

~18 ~1



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

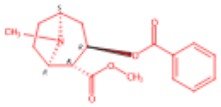
2. 114599-38-1

~5

可卡因组合物

668-19-9

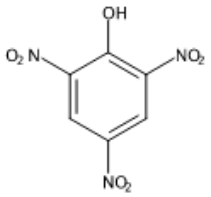
$C_{17}H_{21}NO_4$



Absolute stereochemistry.

88-89-1

$C_6H_3N_3O_7$



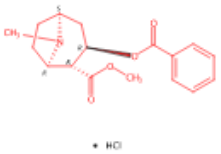
$C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$

Allococaine, picrate (6CI)

3. 109496-04-0

(Component: 668-19-9)

~1



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

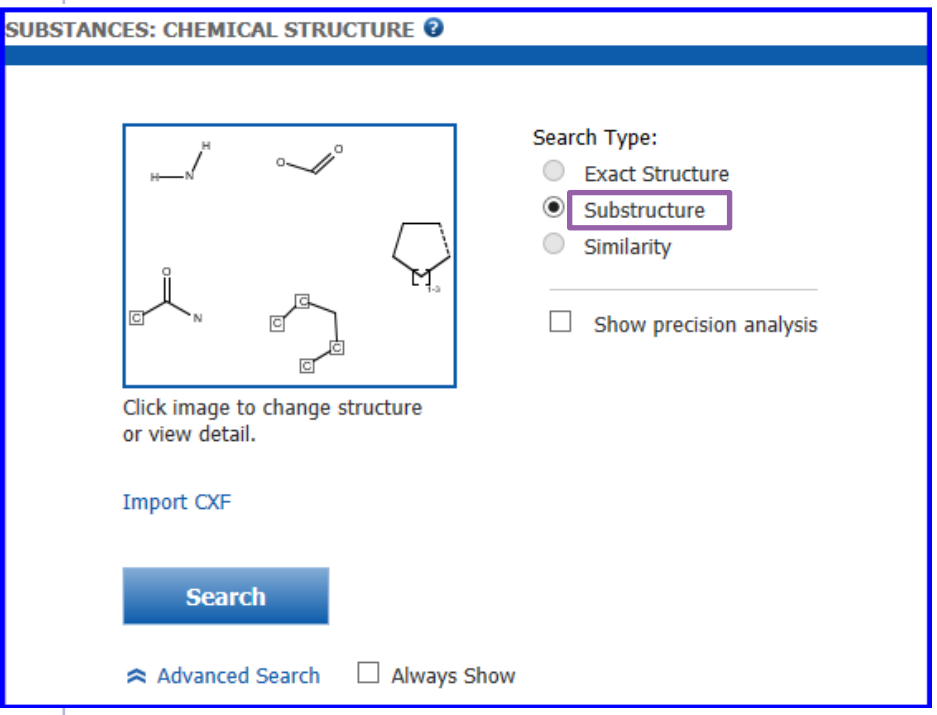
精确结构检索：

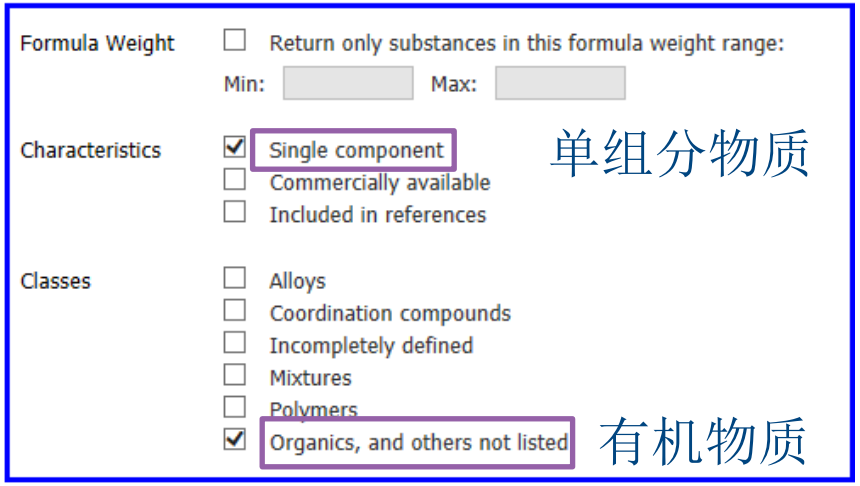
获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

作用机理 编辑本段

帕拉米韦是Babu等在分析唾液酸、扎那米韦、奥司他韦与NA的互相作用机制及构效关系的基础上设计并合成的环戊烷衍生物，与环连接的基团有亲水的羧基和胍基以及疏水的异戊基和乙酰氨基，4个极性不同的基团分别作用于流感病毒NA结构中不同的活性位点区域。羧基部分与NA活性位点的3个精氨酸残基Arg118，Arg292，





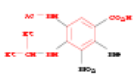
SciFinder® A CAS SOLUTION

物质检索——亚结构检索

0 of 704 Substances Selected

1. **Substance Detail**
127971-59-9

~1

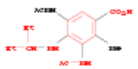


$C_{15}H_{21}N_3O_5$
Benzoic acid, 5-(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-3-nitro-

Experimental Properties

2. **Substance Detail**
127971-80-6

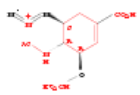
~1



$C_{17}H_{25}N_3O_4$
Benzoic acid, 3,5-bis(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-

3. **Substance Detail**
182367-45-9

~1

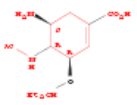


Relative stereochemistry.

$C_{14}H_{22}N_4O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-azido-3-(1-ethylpropoxy)-, (3α,4β,5α)-(9CI)

5. **Substance Detail**
182367-71-1

~2

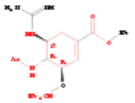


Relative stereochemistry.

$C_{14}H_{24}N_2O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, (3*R*,4*R*,5*S*)-*rel*-

6. **Substance Detail**
182367-73-3

~1



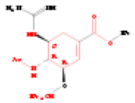
Relative stereochemistry.

$C_{17}H_{30}N_4O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-[(aminoiminomethyl)amino]-3-(1-ethylpropoxy)-, ethyl ester, (3*R*,4*R*,5*S*)-*rel*-

7. **Substance Detail**
182367-74-4

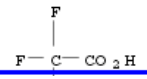
~1

182367-73-3
$C_{17}H_{30}N_4O_4$



Relative stereochemistry.

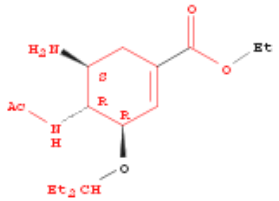
76-05-1
$C_2HF_3O_2$



4. **Substance Detail**
182367-47-1

达菲核心成分

~1



$C_{16}H_{28}N_2O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3α,4β,5α)-(9CI)

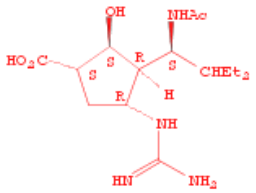
182368-47-4

~1

1. **Substance Detail**
330600-85-6

帕拉米韦

~286



$C_{15}H_{28}N_4O_4$
Cyclopentanecarboxylic acid, 3-[(1*S*)-1-(acetylamino)-2-ethylbutyl]-4-[(aminoiminomethyl)amino]-2-hydroxy-, (1*S*,2*S*,3*R*,4*R*)-

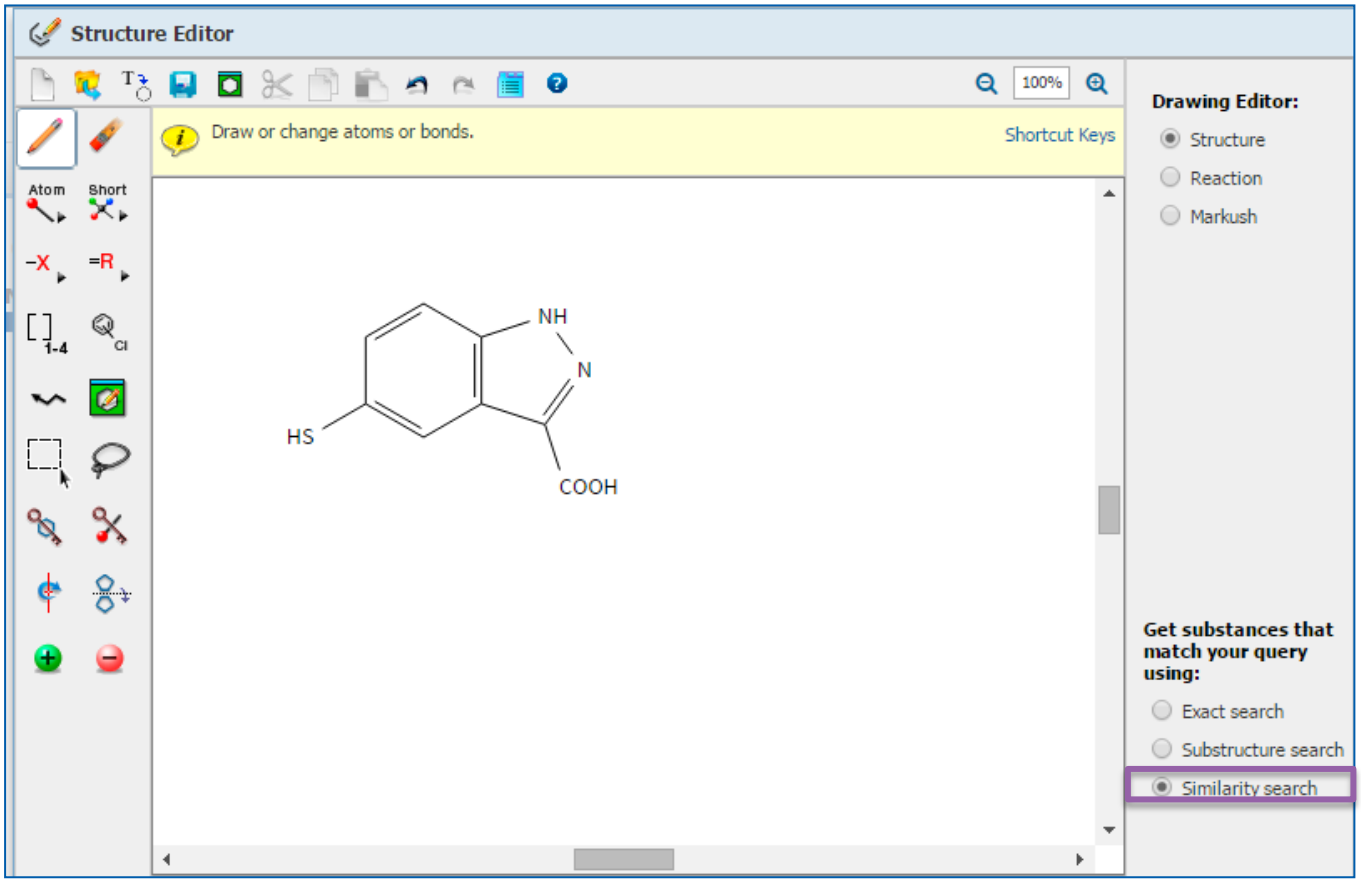
SciFinder® A CAS SOLUTION

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

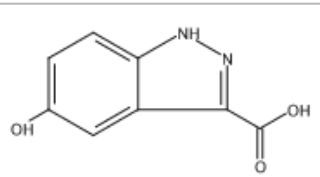
相似度越高，结构越相似

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-

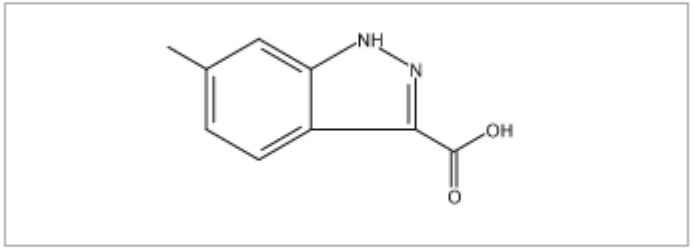
Key Physical Properties

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-

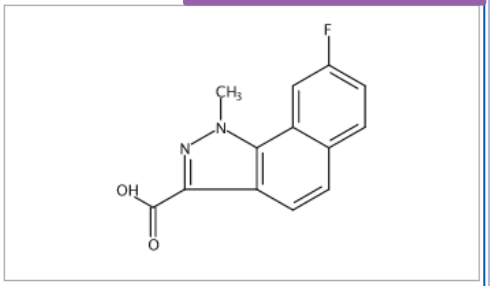
Key Physical Properties

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

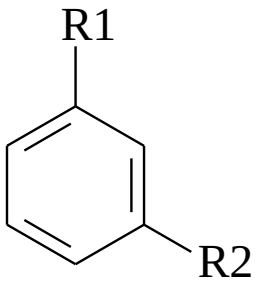
提纲

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

Markush检索

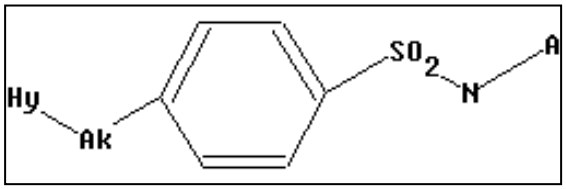
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 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

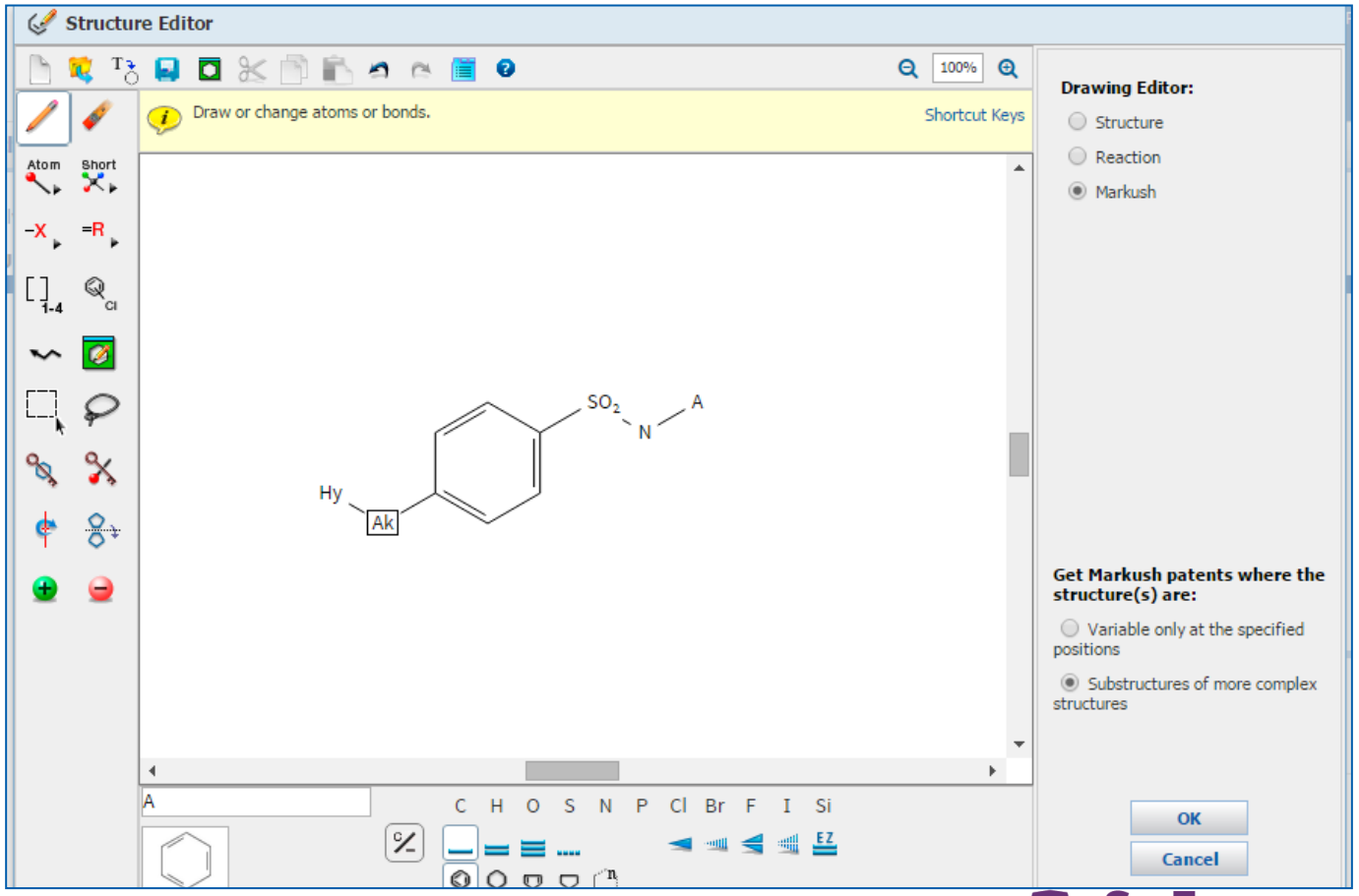


R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH_2–halogen, —CH(–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

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

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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 ▾

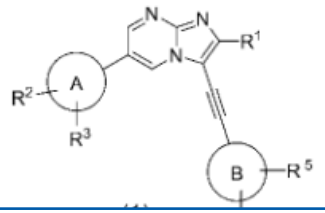
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

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^aR^b, SO_3H, $SO_2NR^aR^b$, SO_2R^b, or $NR^aSO_2R^b$; R^a, R^b (same...

全部是专利

SciFinder A CAS SOLUTION

提纲

- 美国化学文摘社简介
- 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 Synthesis）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

SciFinder检索选项——反应检索

- 反应检索方法

  结构式

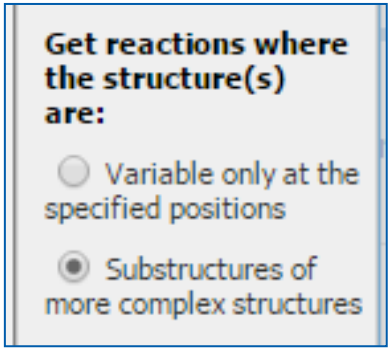
- 常用获取方法

  已知物质：由物质获取反应

  已知文献：从文献中获取反应

  精确结构反应检索

  亚结构反应检索



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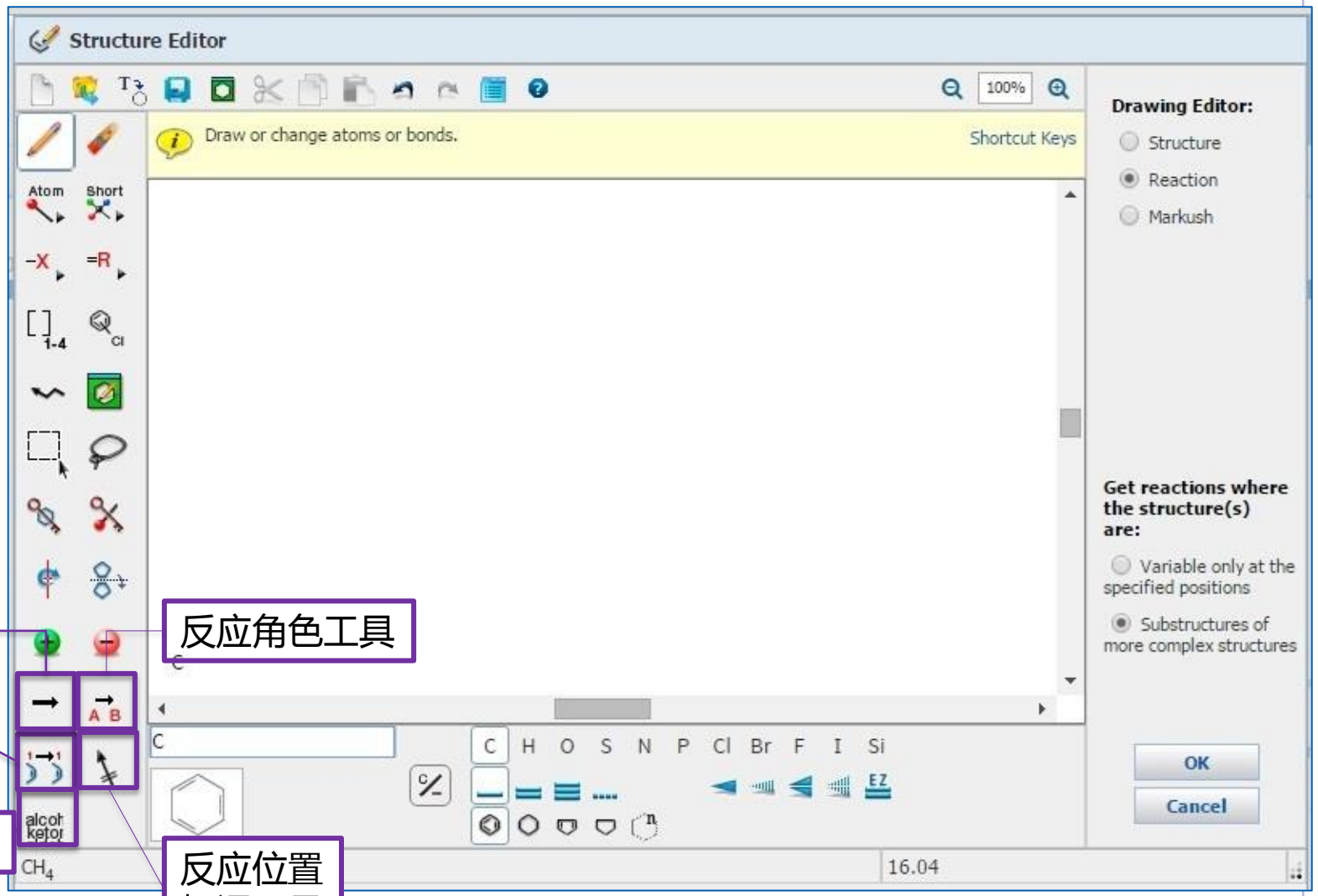
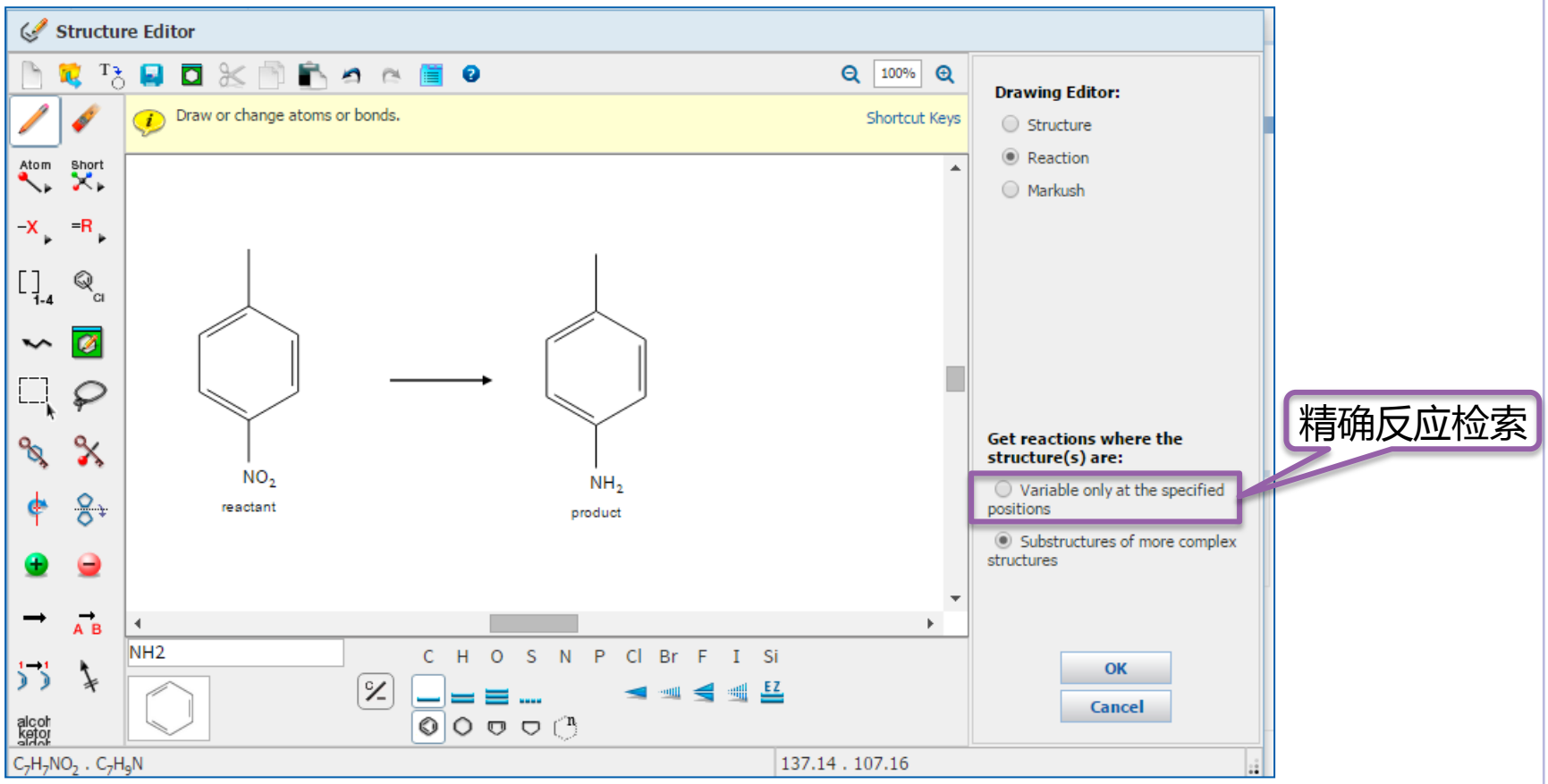
反应绘制工具

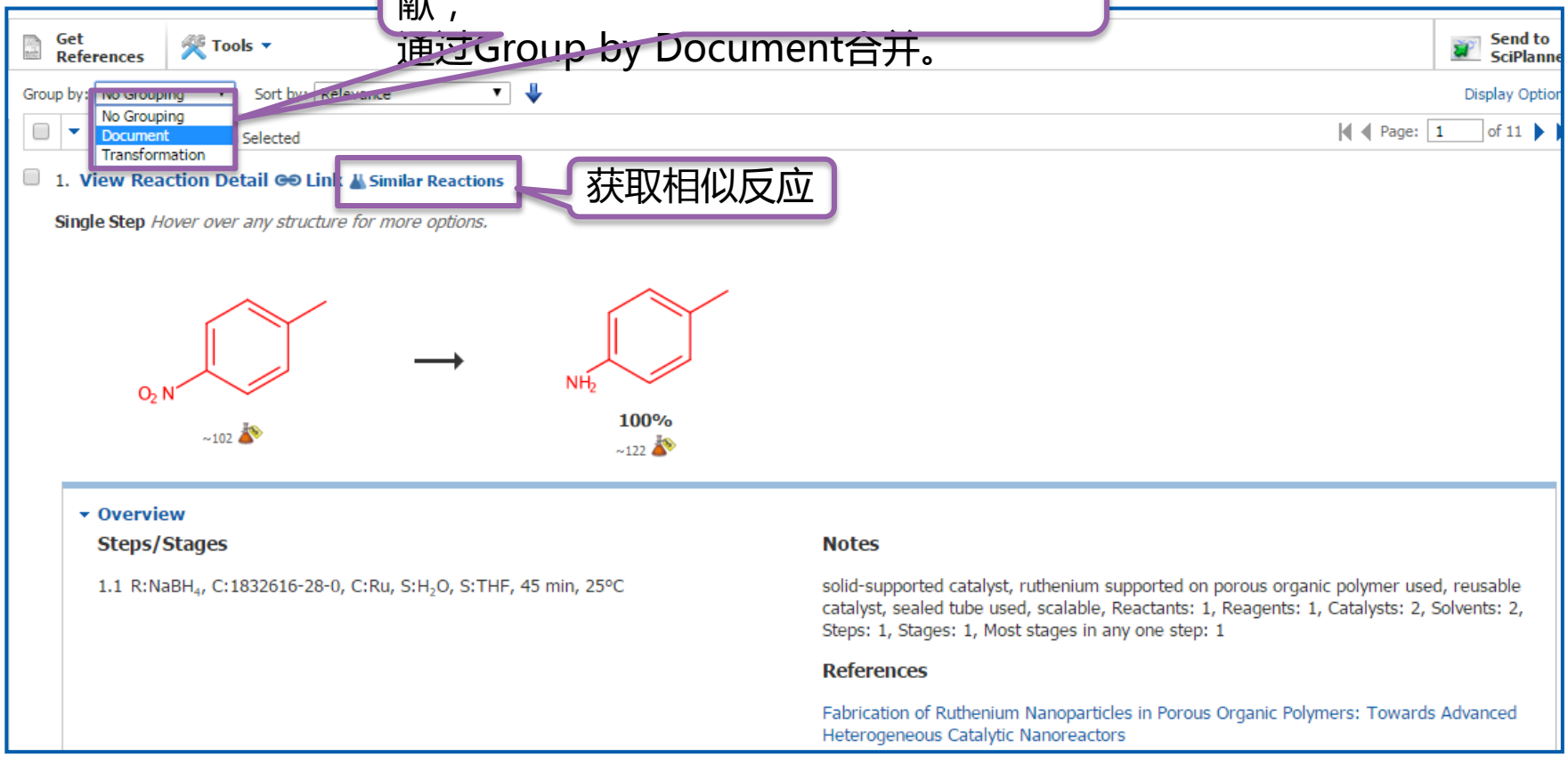

Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
C H O S N P Cl Br F I Si
CH4
16.04
反应箭头
反应角色工具
反应原子标记工具
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



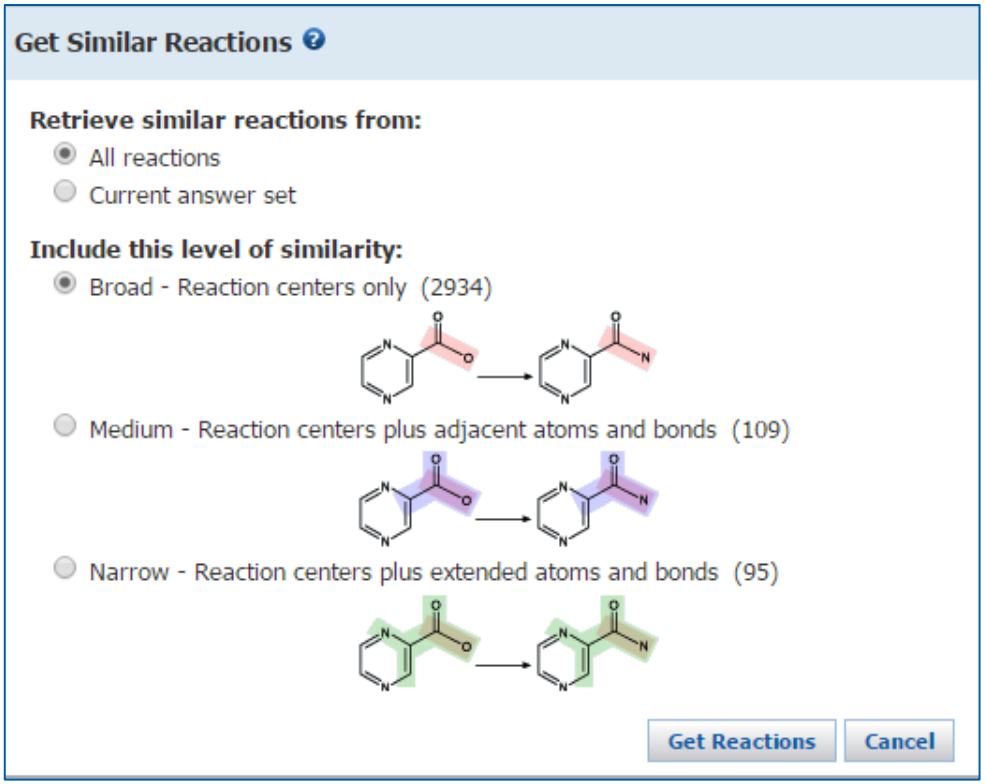
获取相似反应

选择相似反应的相似限制：

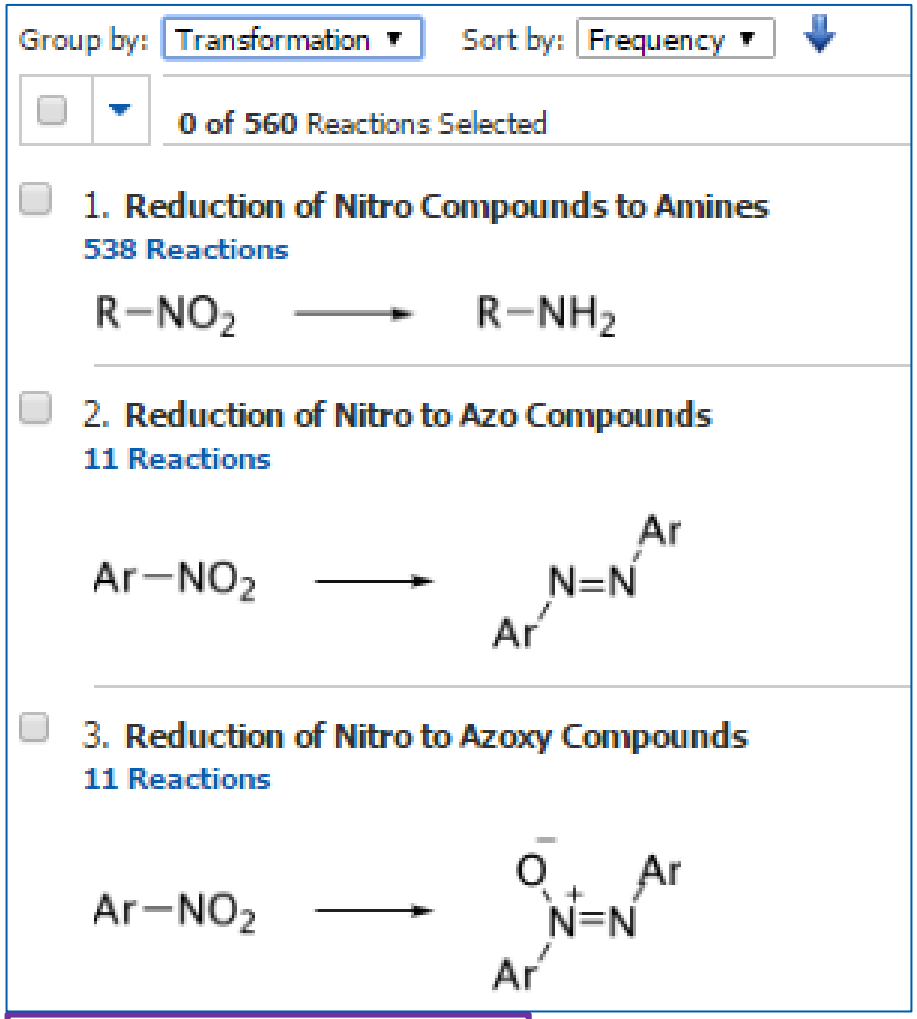
Broad：仅反应中心相似

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

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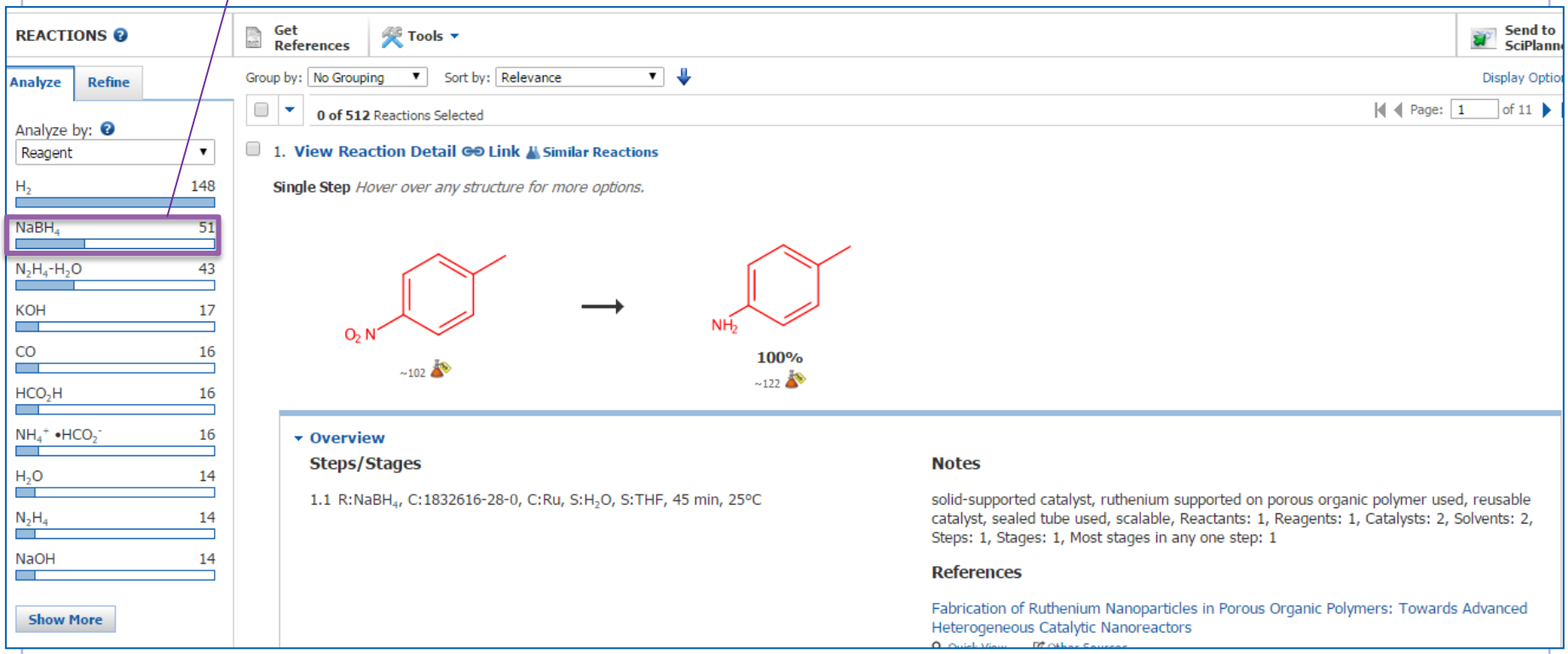
反应检索结果的筛选

获得特定物质做还原剂的反应



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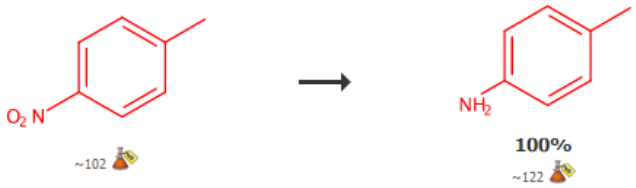
SciFinder囊括最大的反应实验过程合集

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



▾ **Overview**

Steps/Stages

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

Notes

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

References

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

Quick View Other Sources

By Sabater, Sara et al

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

▾ **Experimental Procedure**

ACS Catalysis

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

不用阅读全文，直接获得包含实验过程的反应记录

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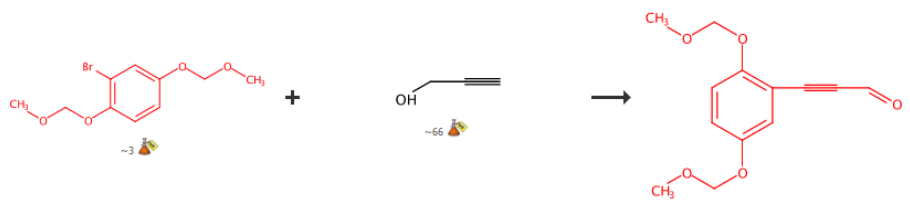
SciFinder囊括最大的反应实验过程合集

Experimental Procedure:

我们可以做得更好

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

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



Overview

Steps/Stages

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

Notes

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

Experimental Procedure

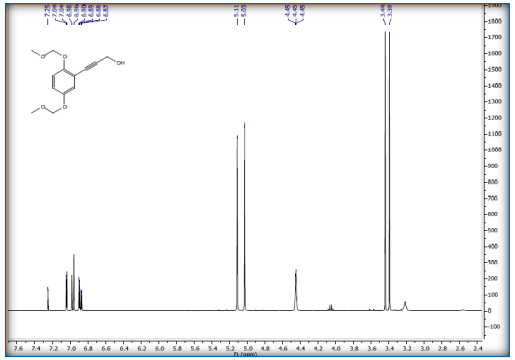
JOURNAL OF NATURAL PRODUCTS

Step 1

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

Step 2

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



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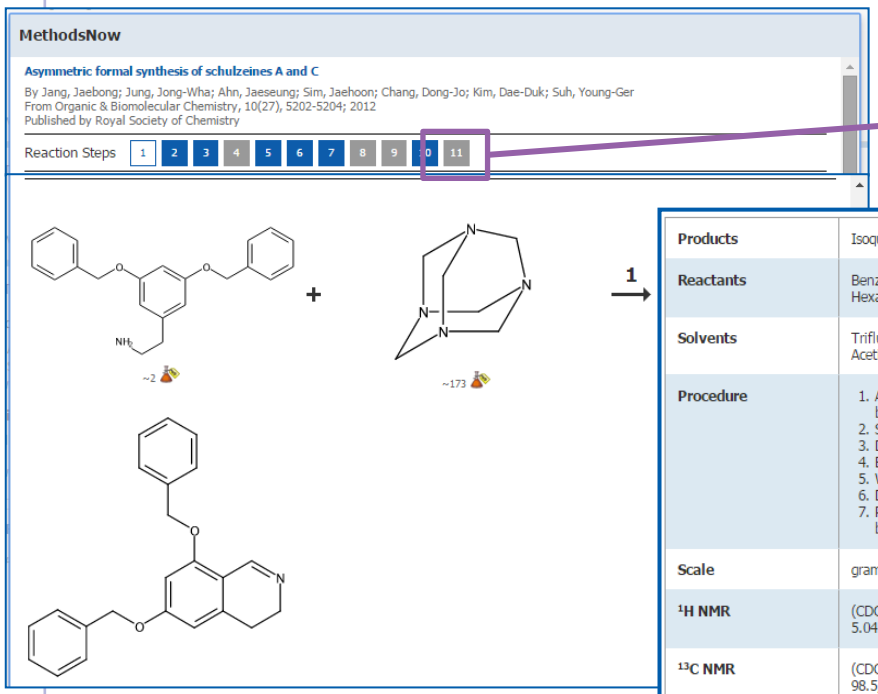
MethodsNow Synthesis



多步反应中，原文没有描述的实验过程以灰色标示

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

Print/Export Close

物质信息

实验过程

图谱信息

保存/导出方法

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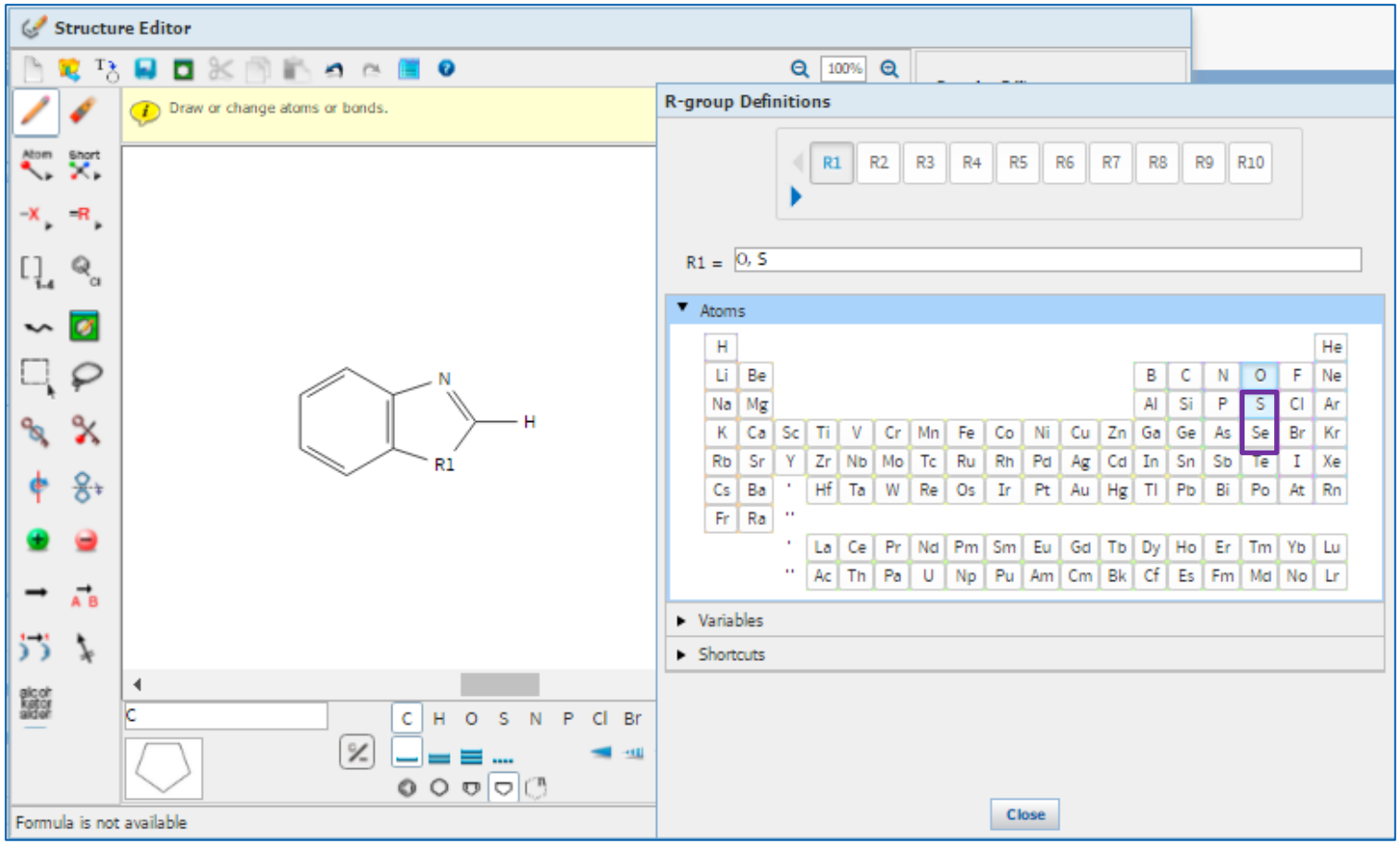
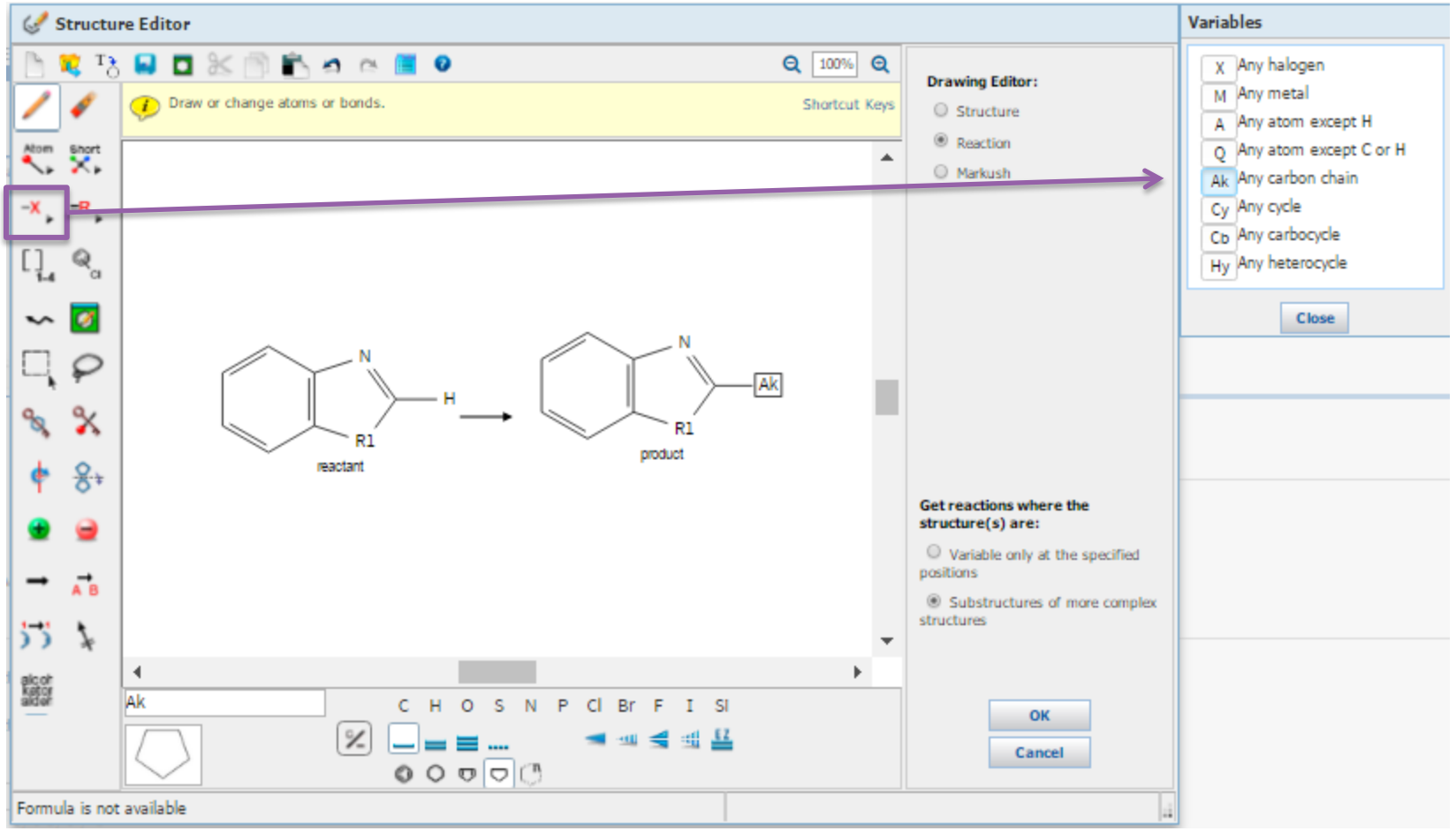
亚结构反应检索

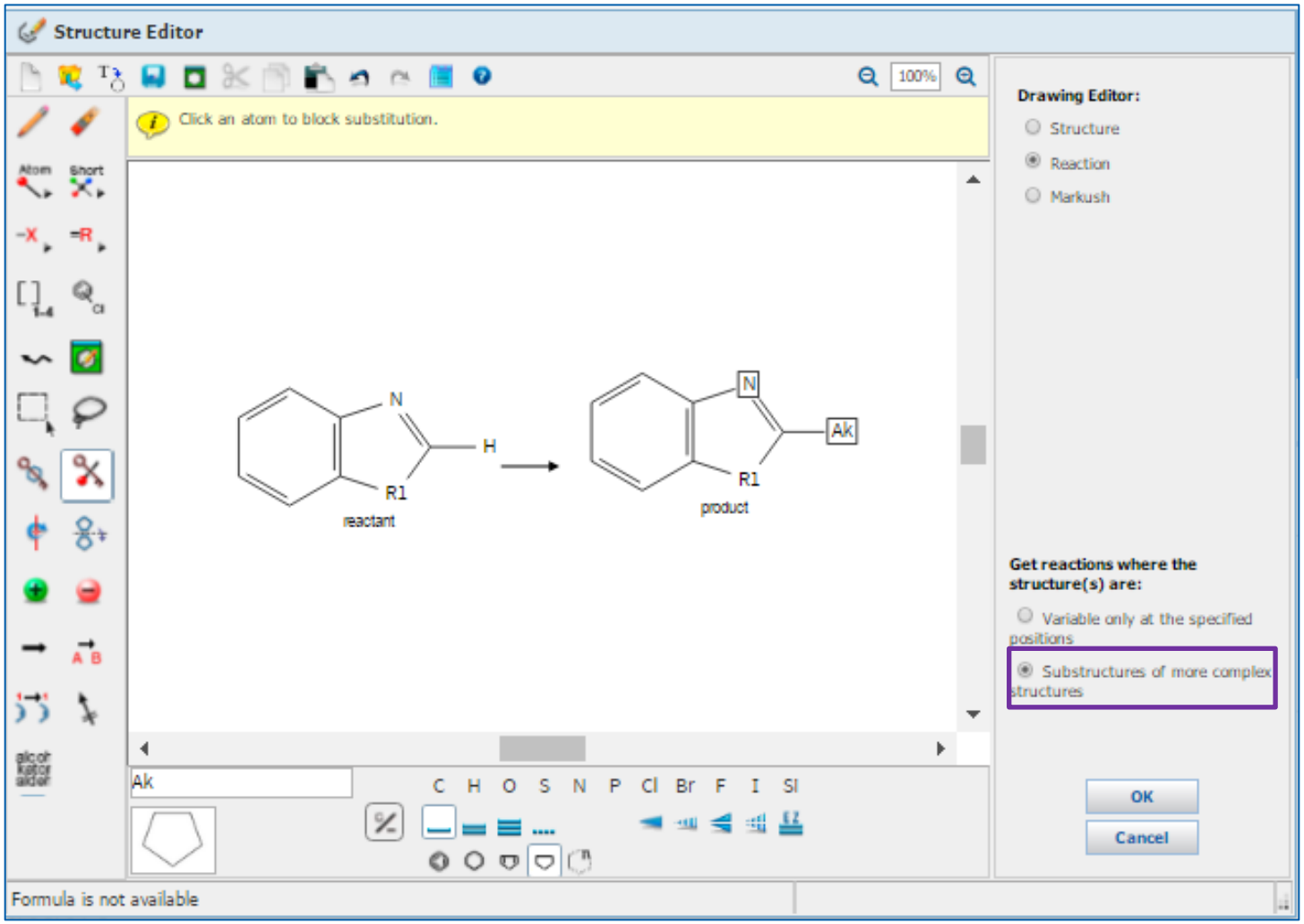
通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索


Structure Editor
Draw or change atoms or bonds.
Shortcut Keys
100%
Drawing Editor:
Structure
Reaction
Markush
N
H
R1
reactant
N
Ak
R1
product
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
Ak
C H O S N P Cl Br F I Si
OK
Cancel
Formula is not available
Variables
X Any halogen
M Any metal
A Any atom except H
Q Any atom except C or H
Ak Any carbon chain
Cy Any cycle
Cb Any carbocycle
Hy Any heterocycle
Close

亚结构反应检索



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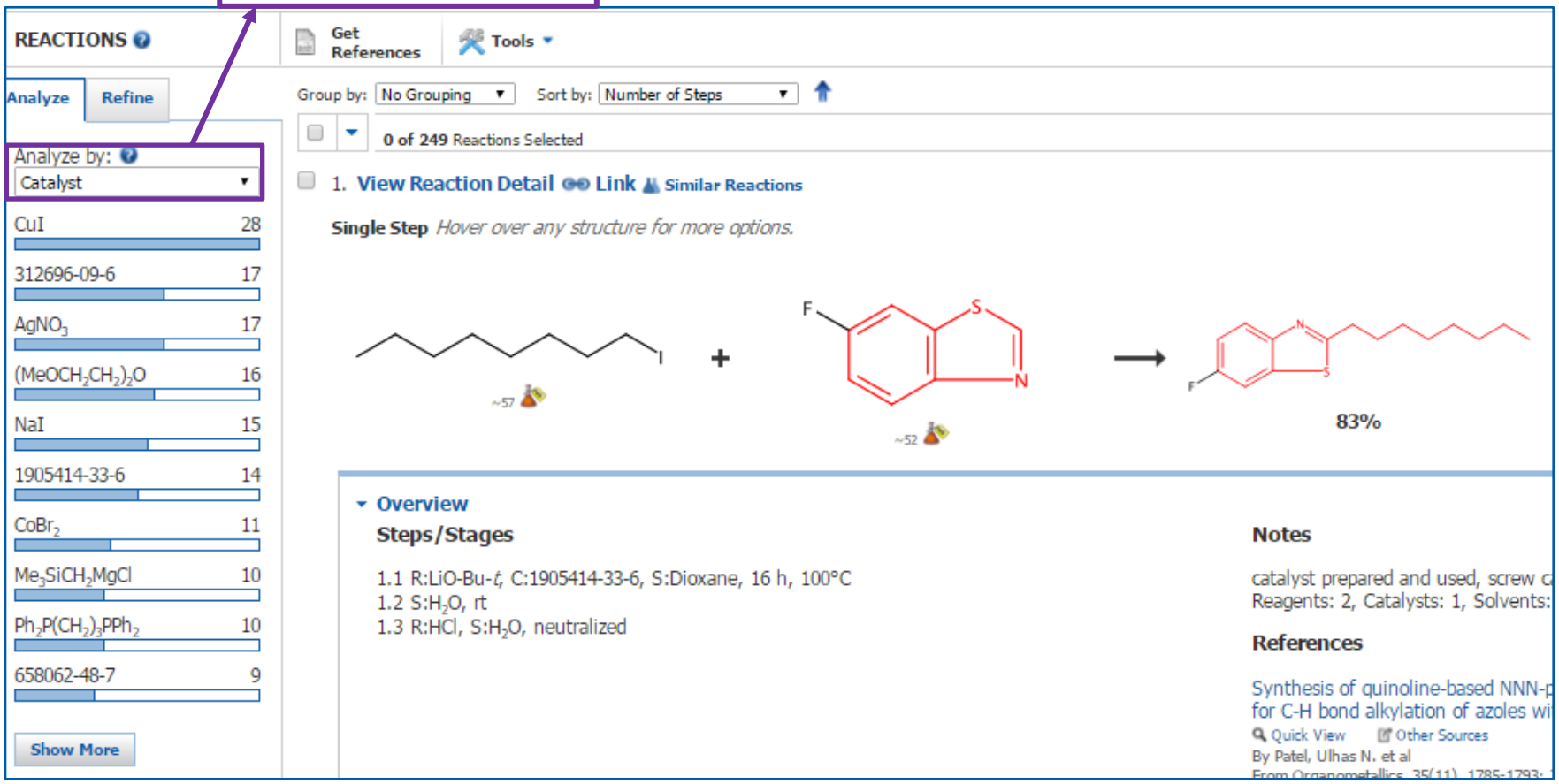
通过后处理工具筛选反应--Analyze

通过催化剂筛选反应



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  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

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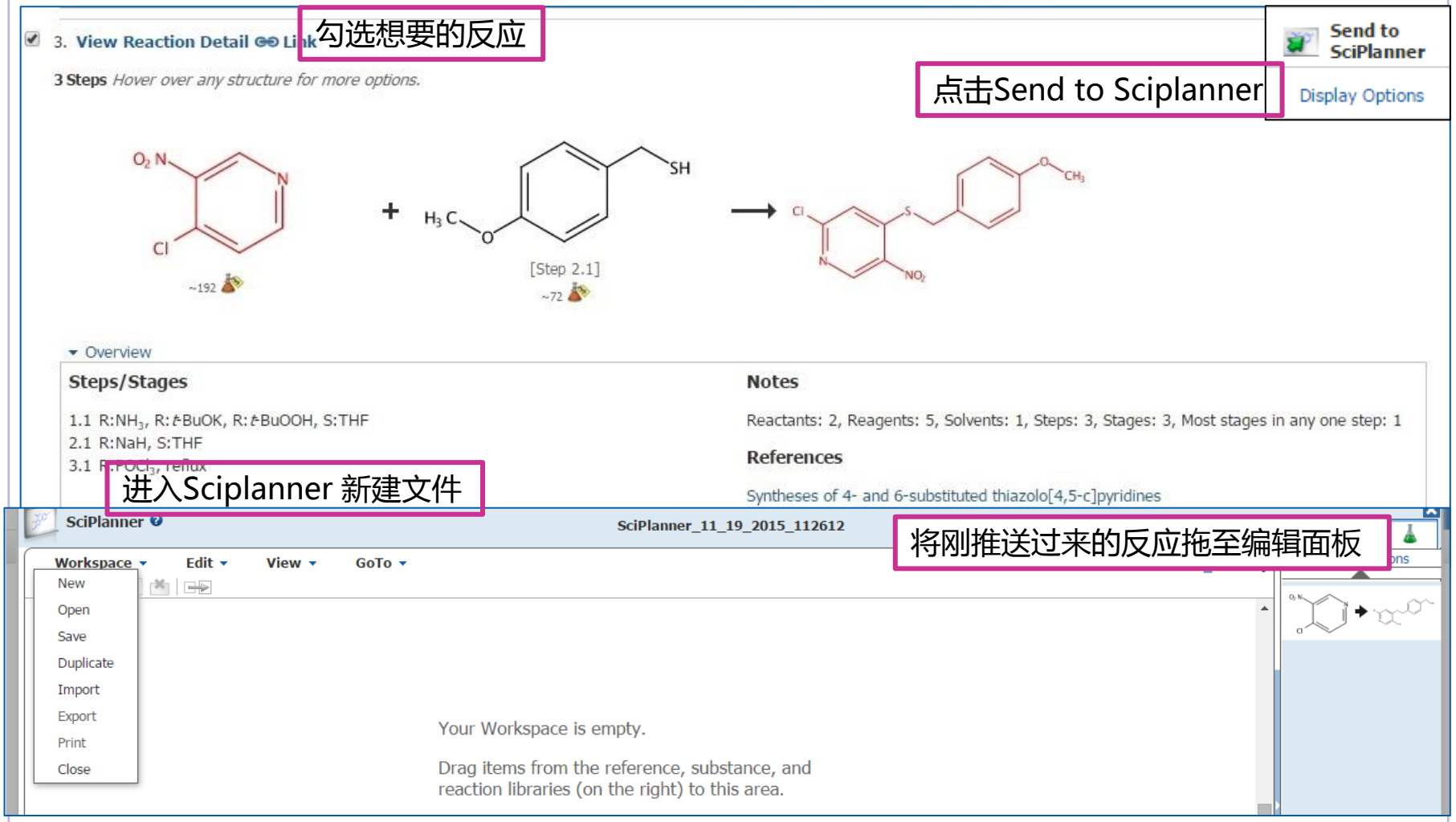
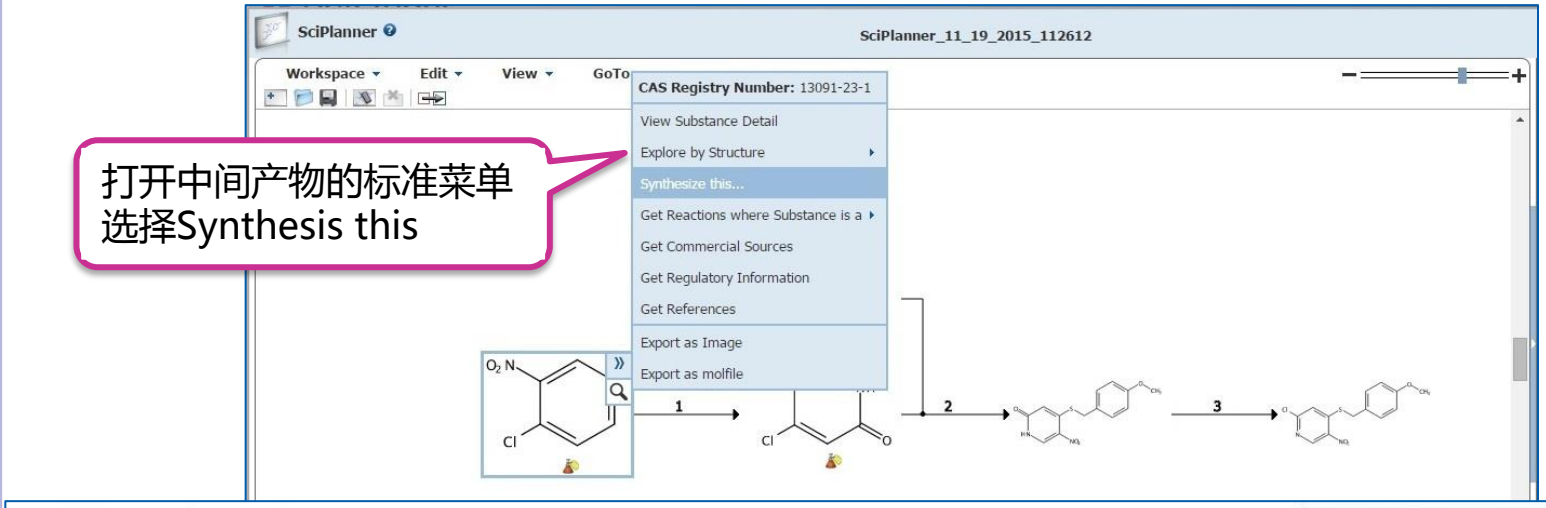
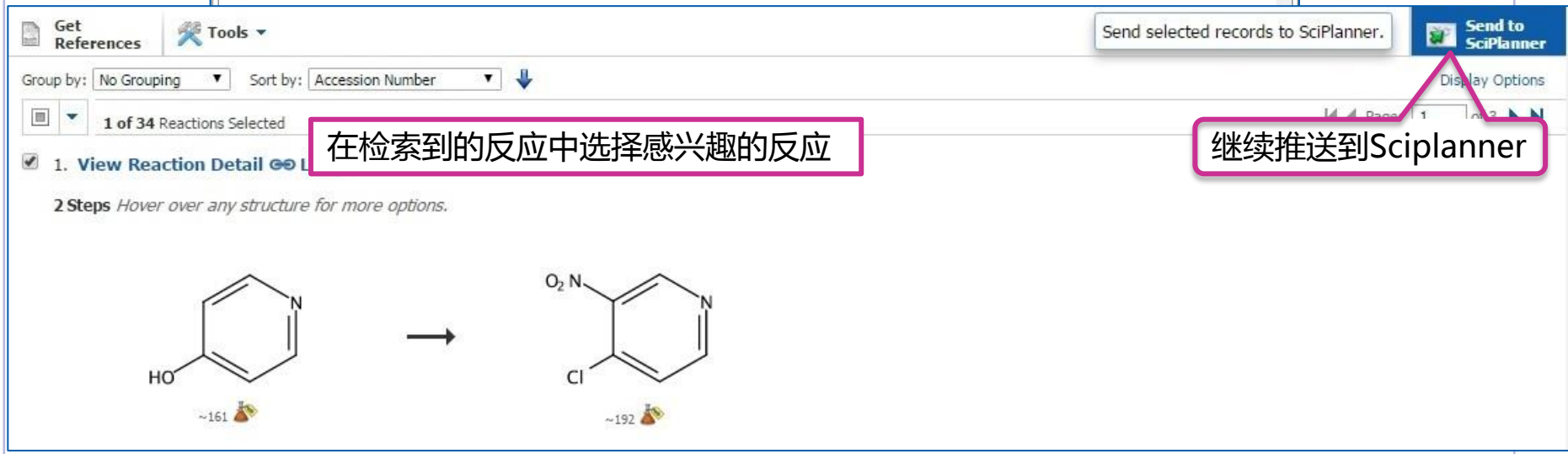
SciPlanner使用简介

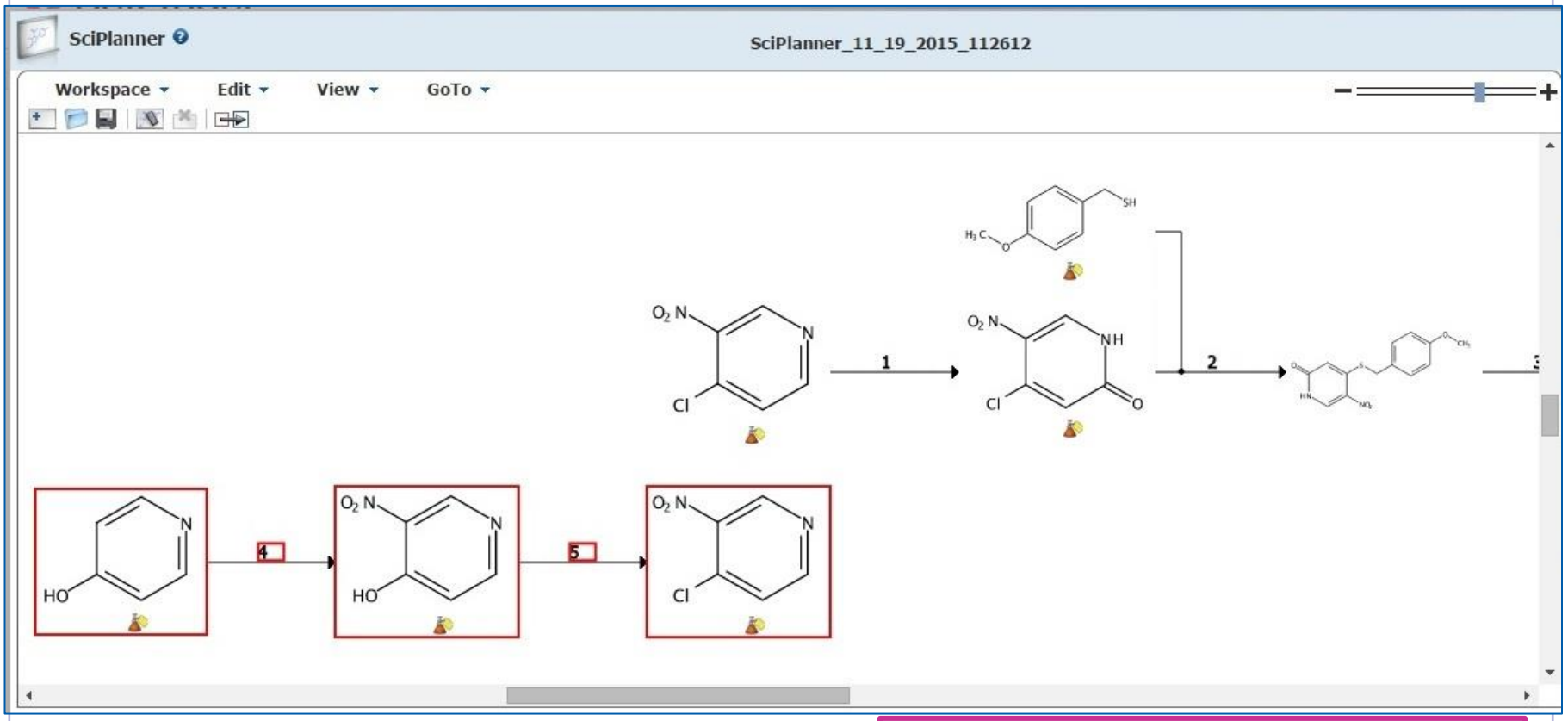


SciPlanner使用简介



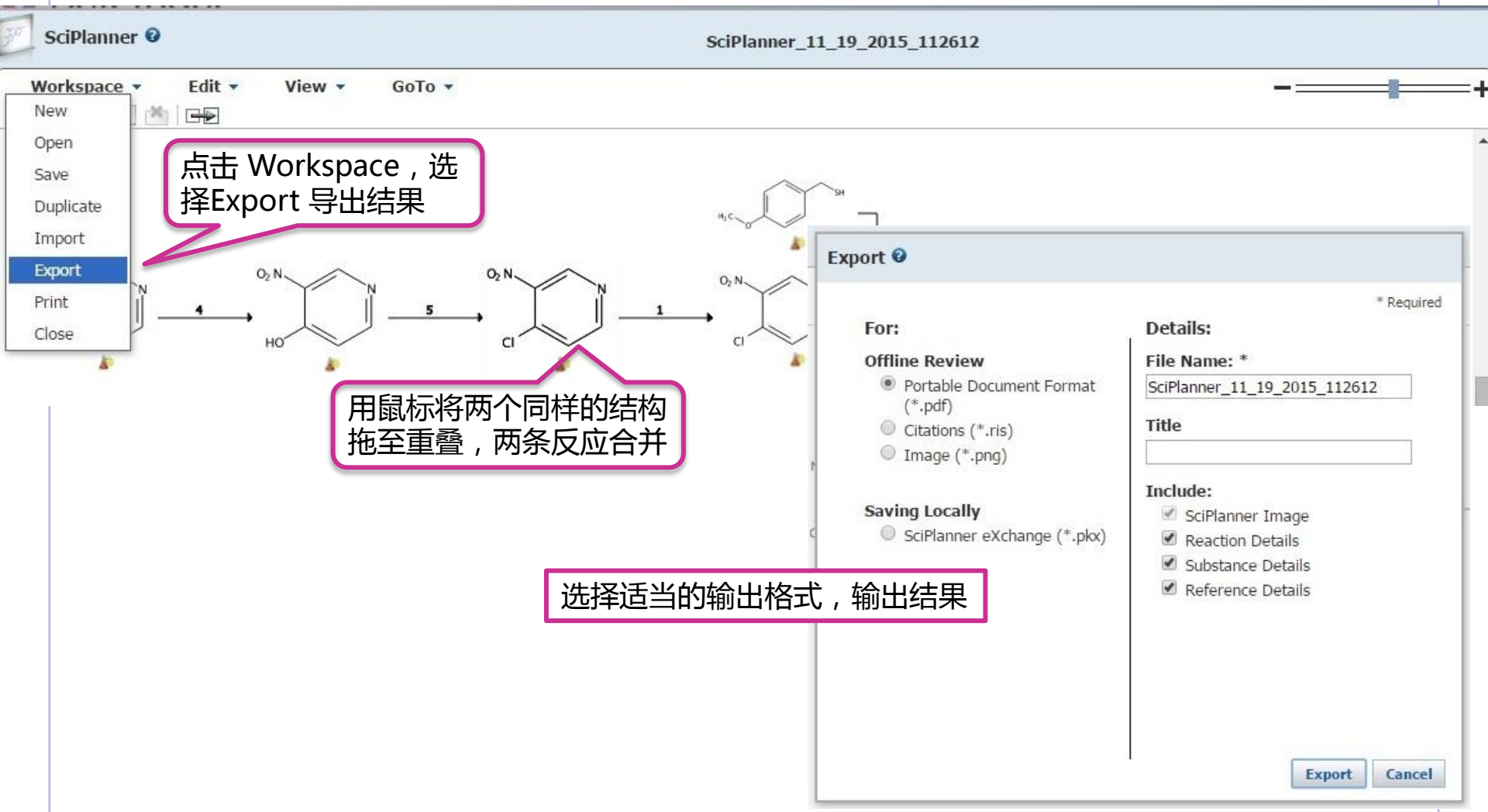


SciPlanner使用简介



步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介



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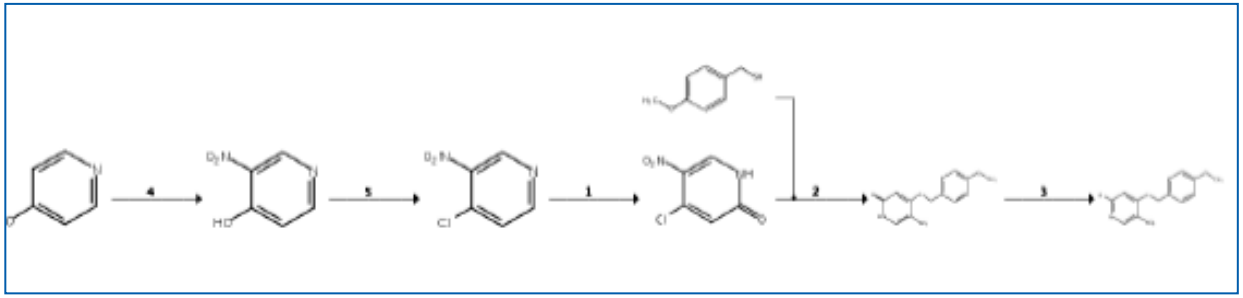
SciPlanner导出结果



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

References

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

By Poloek, Anurach et al

From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014

Substance Information

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

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提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索（PatentPak）
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow
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- 分析与合成两个模块
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- Pharmacology / Toxicology: 成瘾药物检测，有毒物检测…
- Bioassays: 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定…
- Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析…
- Historical Analysis / Dating: 考古分析，同位素分析
- Environmental Analysis: 土壤/空气/水分析，农药残留分析…
- Agricultural Applications / Analysis: 除草剂分析…
- Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析…
- Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工…
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目前有13个大类，45个小类。某些子项目属于多种方法分类

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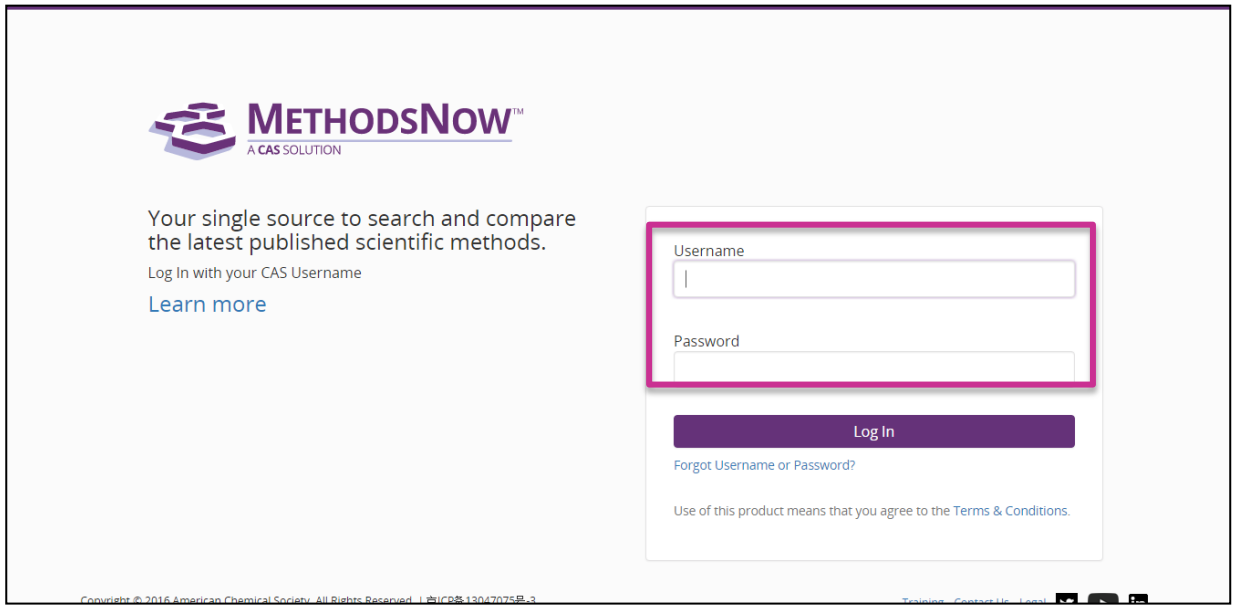

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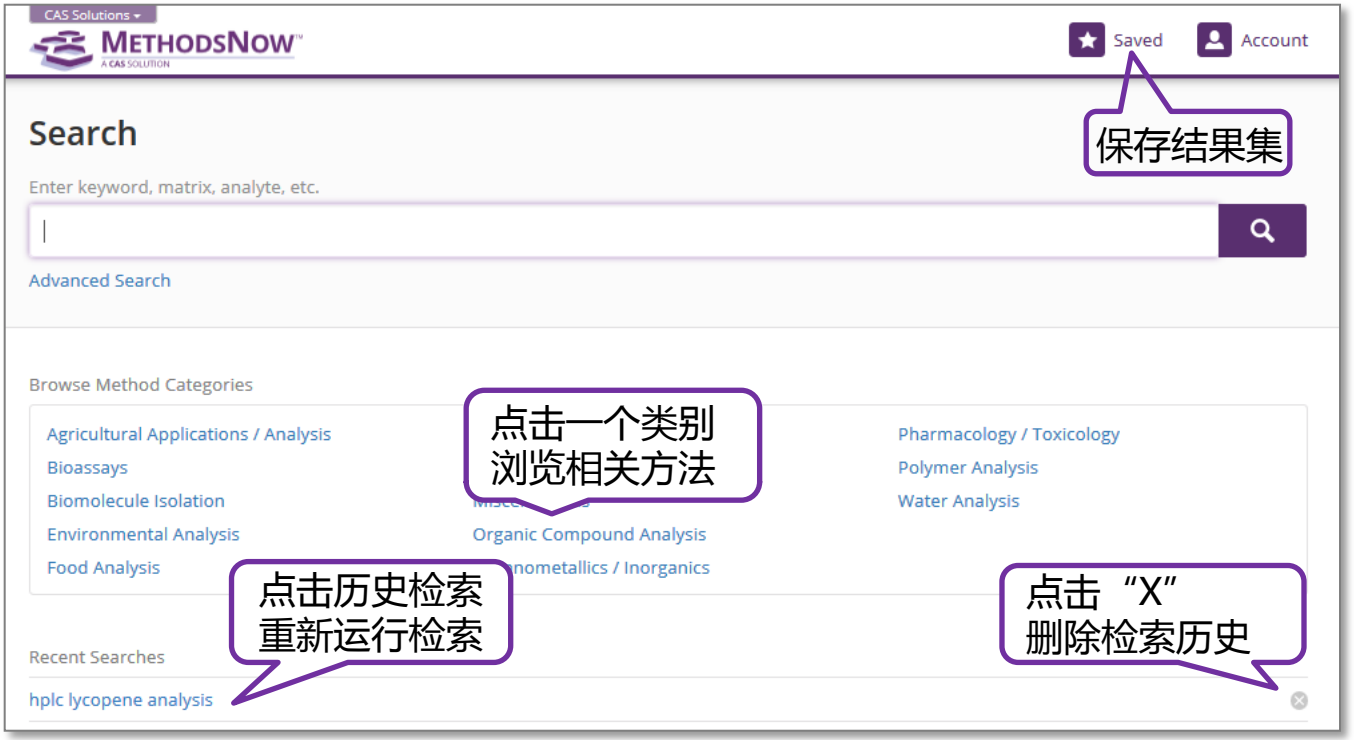
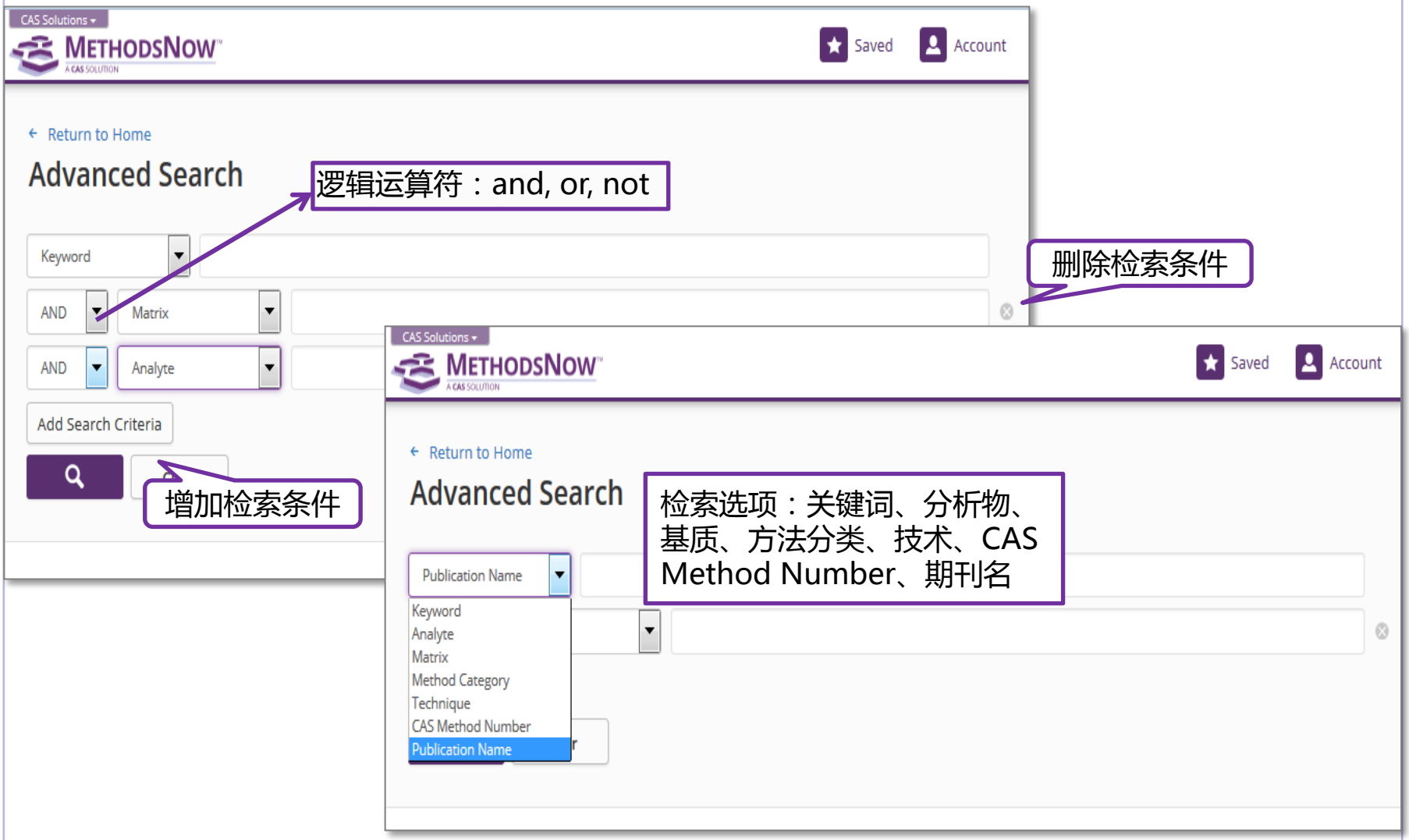
检索/高级检索

方法分类

历史检索



高级检索



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案例：氟比洛芬中的杂质分析

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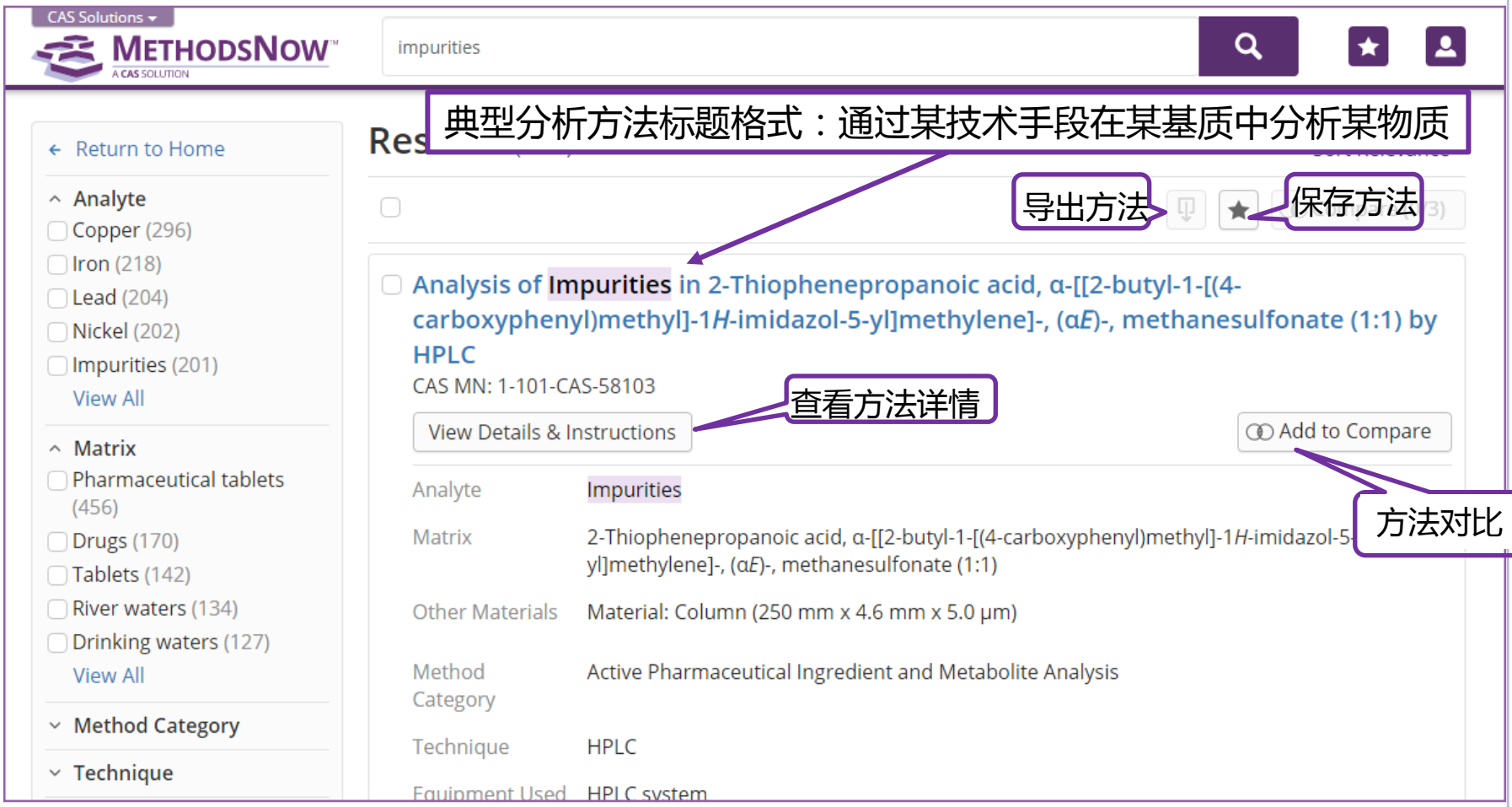
结果显示



限定分析物、基质、方法等条件

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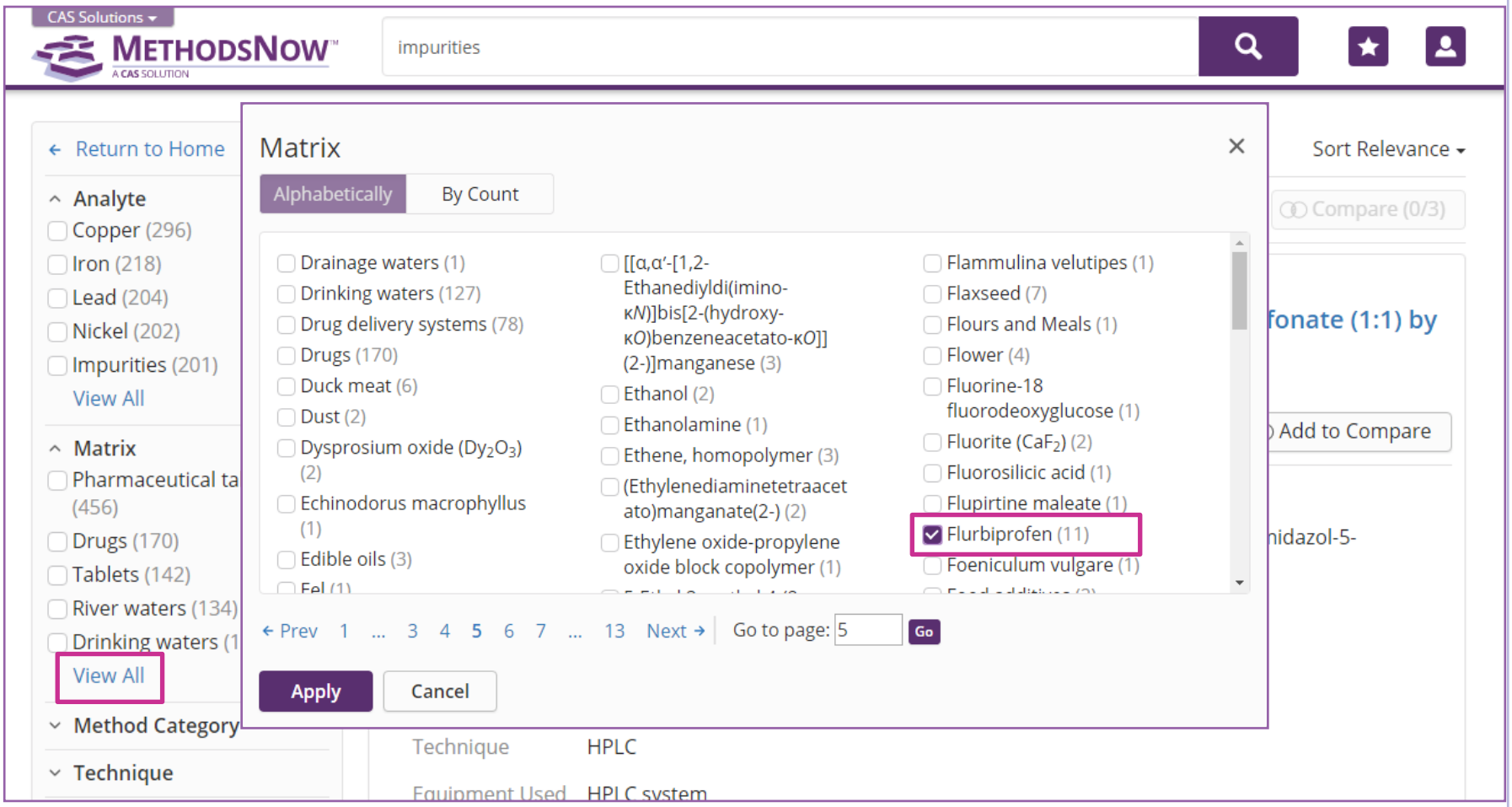
结果筛选



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结果显示

Analysis of (+)-Flurbiprofen in Tablets by Reversed-phase HPLC

CAS MN: 1-101-CAS-47394

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: Reversed-phase HPLC; UV-visible spectroscopy

Materials	Role	Image	CAS RN
(-)-Flurbiprofen	analyte	View Structure	51543-40-9
(-)-Ketoprofen	analyte	View Structure	56105-81-8
(+)-Ibuprofen	analyte	View Structure	51146-56-6
(+)-Pranoprofen	analyte	View Structure	103813-85-0
Naproxen	analyte	View Structure	22204-53-1
(-)-Pranoprofen	analyte	View Structure	132880-23-0
(+)-Ketoprofen	analyte	View Structure	22161-81-5
(+)-Flurbiprofen	analyte	View Structure	51543-39-[illegible]
(-)-Ibuprofen	analyte	View Structure	51146-57-7

实验材料

Source

High-performance enantiomer separation of nonsteroidal anti-inflammatory drugs (NSAIDs) by 3 μm reversed-phase chiral columns and application to the optical purity testing of naproxen drug substances and its formulations

Tanaka, Moe; Nagamatsu, Kumi; Nishi, Hiroyuki

Analytical Sciences (2014), 30 (3), 397 - 406. Japan Society for Analytical Chemistry

CODEN: ANSCEN | ISSN: 09106340 | DOI: 10.2116/analsci.30.397

Document Sources

Abstract

The enantiomer separation of 5 nonsteroidal anti-inflammatory drugs (NSAIDs), such as ibuprofen, ketoprofen (KP) and naproxen (NX), which are included in The Japanese Pharmacopoeia 16th edition (JP16), was investigated by employing 4 kinds of 3 μm reversed-phase chiral columns (AD-3R, AS-3R, OD-3R, and OJ-3R). Except for KP, the enantiomers of 4 NSAIDs were successfully separated by 1 of the 4 columns. Among 5 NSAIDs, only NX was used as a single enantiomer (S-form, active form) in the clin. field (JP16); therefore, optical purity testing method of NX is required for its quality evaluation. Among 4 CSPs, the method was developed by an AS-3R column, which showed good enantioselectivity for NX enantiomers. By optimizing the conditions, the resolution (Rs) of 2.55 was obtained for NX enantiomers within approx. 6 min. The minor enantiomer R-form eluted before the main active enantiomer S-form. Finally, the developed method was applied to the optical purity testing of NX active pharmaceutical ingredients (APIs), and its formulations (tablet and

文献信息

Instructions

Enantiomer separation by HPLC (water and ACN (3:2))

1. Prepare sample solutions of racemic NSAIDs (nonsteroidal anti-inflammatory drugs) with MeOH at a concentration of approximately 1 mg/mL.
2. Prepare a sample solution for NX, through mixing the active S(+)-form and the minor enantiomer R(-)-form at a ratio of approximately 1:1.
3. Prepare a solution of a paraben mixture by combining each 10 mL of a 100 mg/100 mL MeOH solution of uracil, Me (methyl p-hydroxybenzoate) paraben, Et (ethyl *p*-hyrdoxybenzoate) paraben, iPr (isopropyl *p*-hydroxybenzoate) paraben, nPr (*n*-propyl *p*-hydroxybenzoate) paraben, and Bu (*n*-butyl *p*-hydroxy-benzoate) paraben to a 100-mL volumetric flask.
4. Add water to the volume (10 mg each/100 mL).
5. Use uracil as a t_0 marker substance, because it was not retained under the applied HPLC conditions.
6. Investigate HPLC separations of enantiomers of five NSAIDs a mixture of paraben by employing four kinds of the 3 μm reversed-phase chiral columns (AD-3R) under the following conditions: column temperature, 25°C (room temperature); flow rate, 1.0 mL/min; detection, UV 254 nm (210 nm for IB).
7. Employ a mixture of water and ACN (3:2) as mobile phase.
8. Inject a constant volume (2-5 μL) of the sample solution manually through a Rheodyne 7725i injector (20 μL loop).

Validation

Retention Time	4.36 (enantiomer-1 pranoprofen), 4.76 (enantiomer-2 pranoprofen) (t_{R1}/min, t_{R2}/min respectively)
	7.77 (enantiomer-1 naproxen), 8.70 (enantiomer-2 naproxen) (t_{R1}/min, t_{R2}/min respectively)
	11.2 (enantiomer-1 ibuprofen), 12.3 (enantiomer-2 ibuprofen) (t_{R1}/min, t_{R2}/min respectively)

实验步骤及数据有效性

Equipment Used

HPLC apparatus, Kyoto, Japan

HPLC system, Shimadzu

UV/VIS spectrophotometer, UV-2550, Shimadzu, Japan

Injector, Rheodyne 7725i

设备条件

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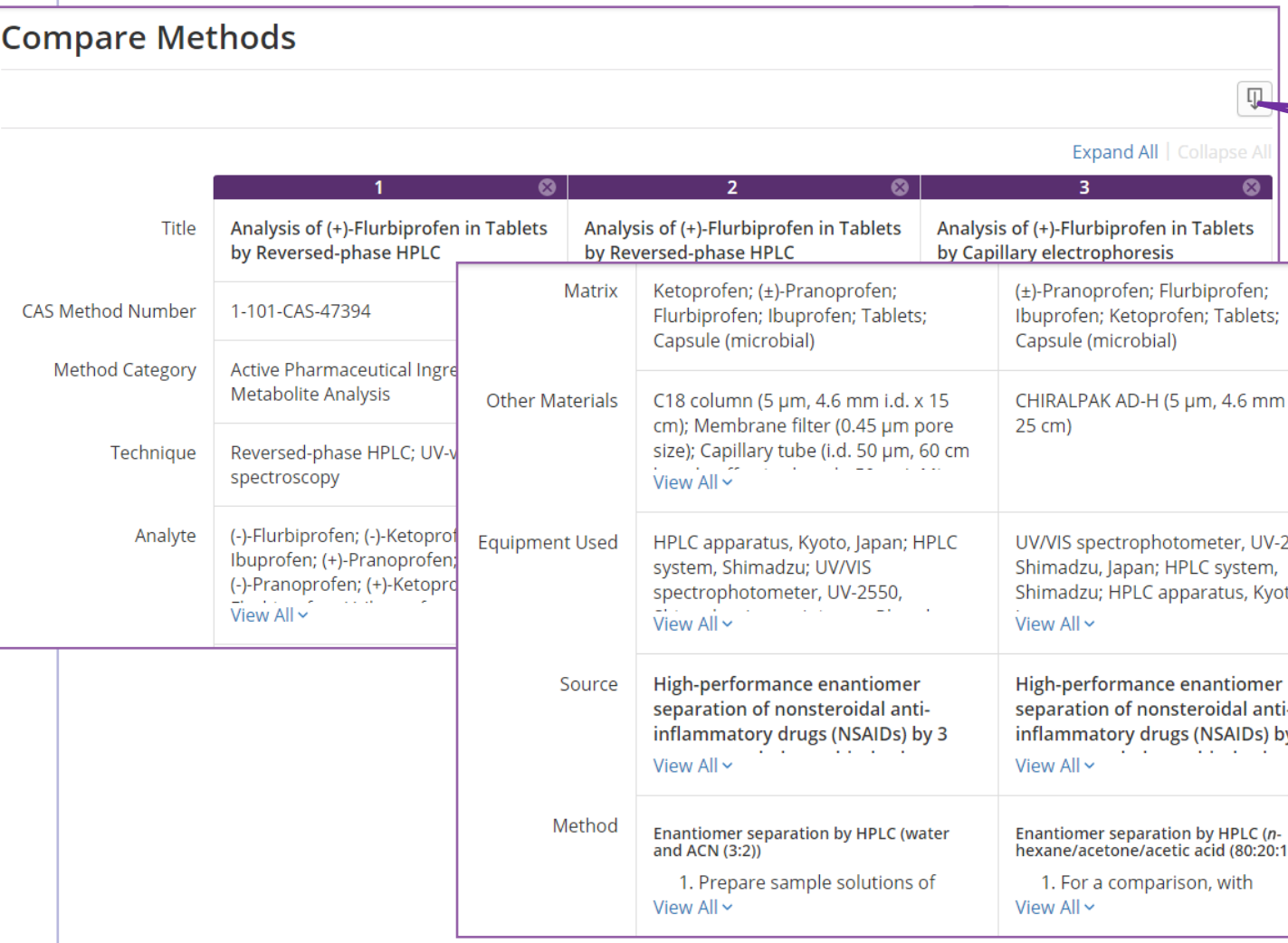
对比不同分析方法



导出对比PDF文件

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提纲

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

SciFinder浏览器选择建议

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- 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

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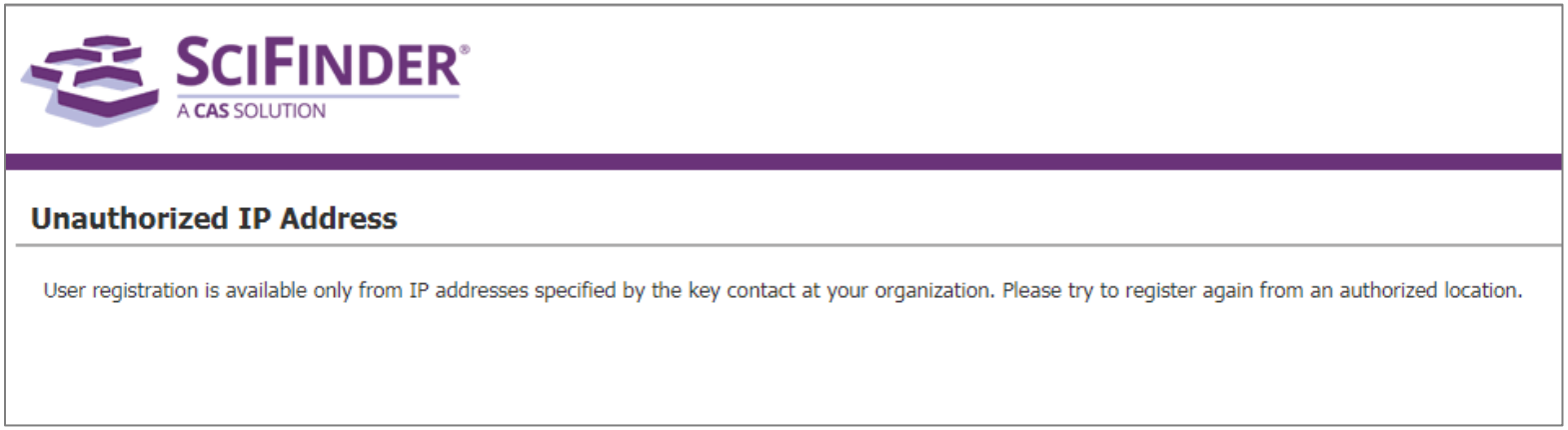

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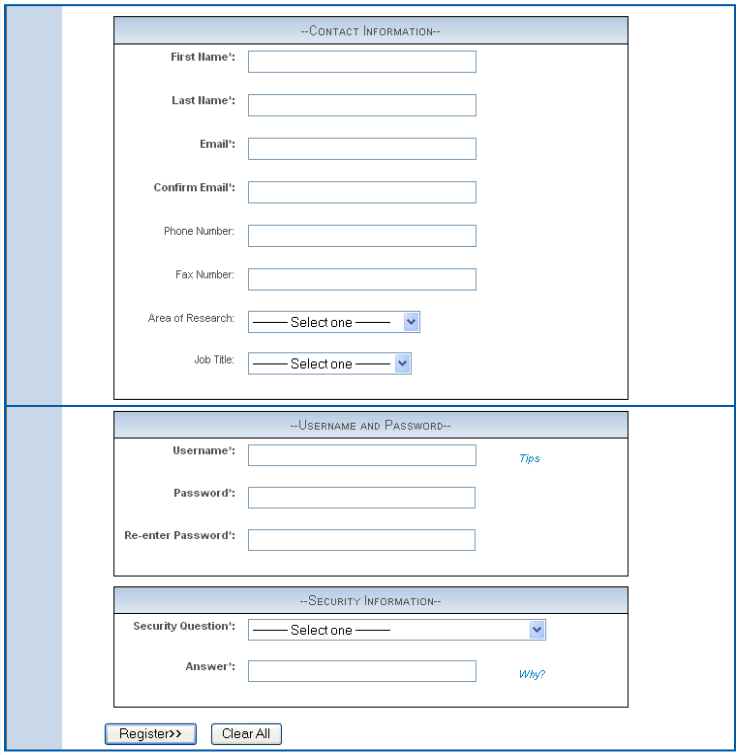

请注意：
1.必须输入真实姓名和自己邮箱。
2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- -（破折号）
- _（下划线）
- .(句点）
- @（表示“at”的符号）

3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：

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

例：abc@123
4.从下拉列表中选择一个密码提示问题并给出答案。
单击 Register（注册）。

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- 严禁账号分享
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