匡金海

客户顾问

jkuang@acs-i.org

如何使用SciFinder获取科技信息

东北大学

2018.05.22

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 Analysis
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

美国化学文摘社—Chemical Abstracts Service

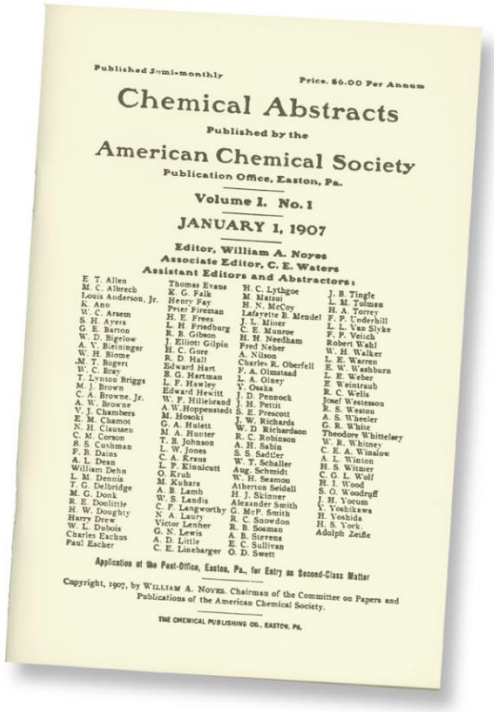
- ACS的分支机构
- 创建于1907年，简称”CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市

SciFinder® A CAS SOLUTION

1907年，信息的汇集、管理发生了重大的变化

威廉•诺伊斯
(William A. Noyes)

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



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American Chemical Society

Publication Office, Easton, Pa.

Volume I. No. 1

JANUARY 1, 1907

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Application at the Post-Office, Easton, Pa., for Entry as Second-Class Matter

The Chemical Publishing Co., Easton, Pa.

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CAS——构建最高质量的化学数据库

arXiv.org

Aldrichimica ACTA

ACS chemical biology

BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

division of polymer chemistry, inc American Chemical Society

JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical Neuroscience

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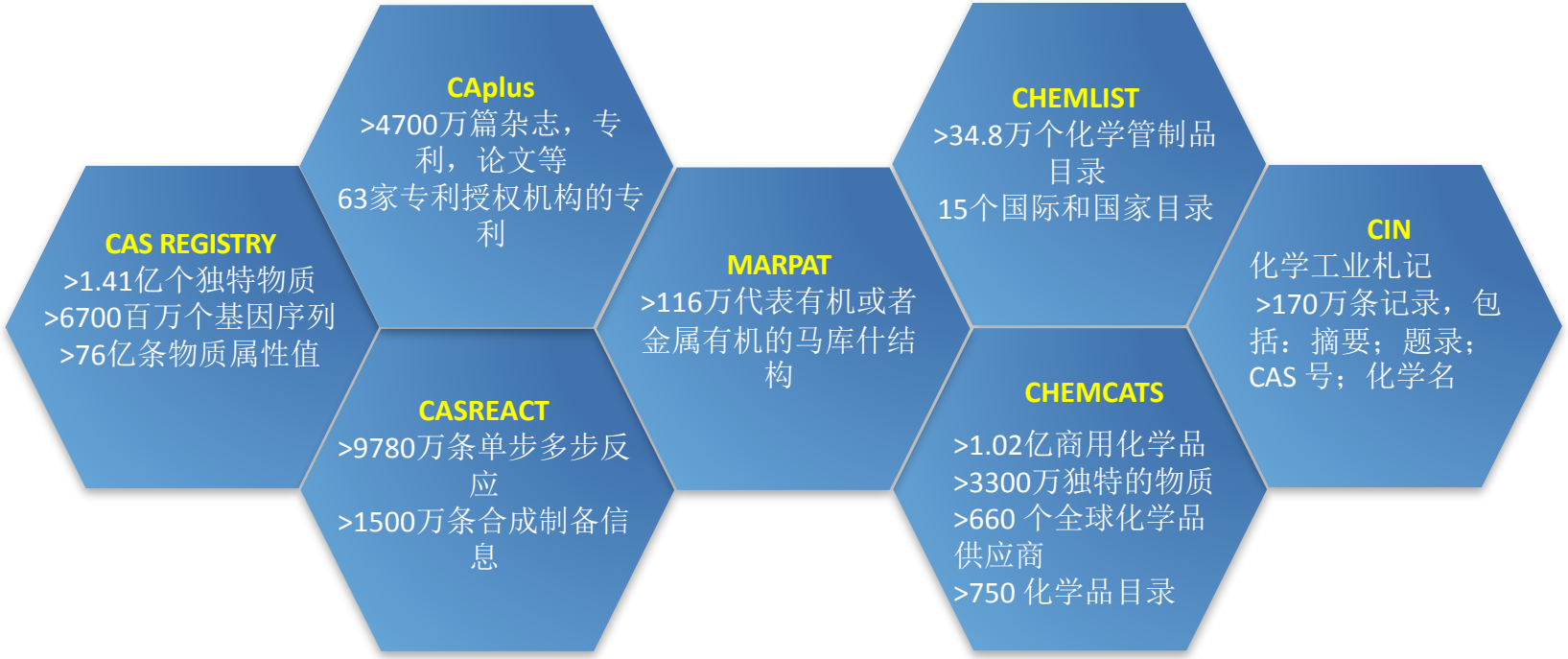
CAS——构建最高质量的化学数据库



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CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

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

应用化学各领域 ：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学

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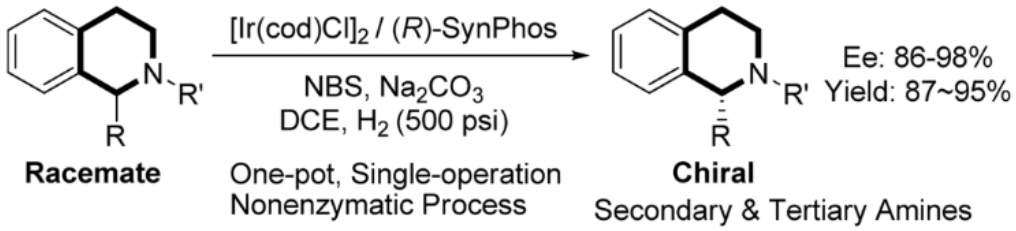
CAS数据库最具价值的内容——人工标引

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

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

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



Indexing

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

Concepts

Enantioselective synthesis
Hydrogenation catalysts
Oxidation

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

Chiral ligands

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

Substances

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

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

Catalyst use; Uses

QUICK LINKS
0 Tags, 0 Comments

SOURCE
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CAPLUS

PUBLISHER
American Chemical Society

LANGUAGE
English

Tips:
98%以上的文献，都经过人工标引
用Index Term标引文献中的重要技术术语
用CAS RN标引出文献中的重要物质
用CAS Role标引文献中重要物质的研究领域

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CAS人工标引解决的问题

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

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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®
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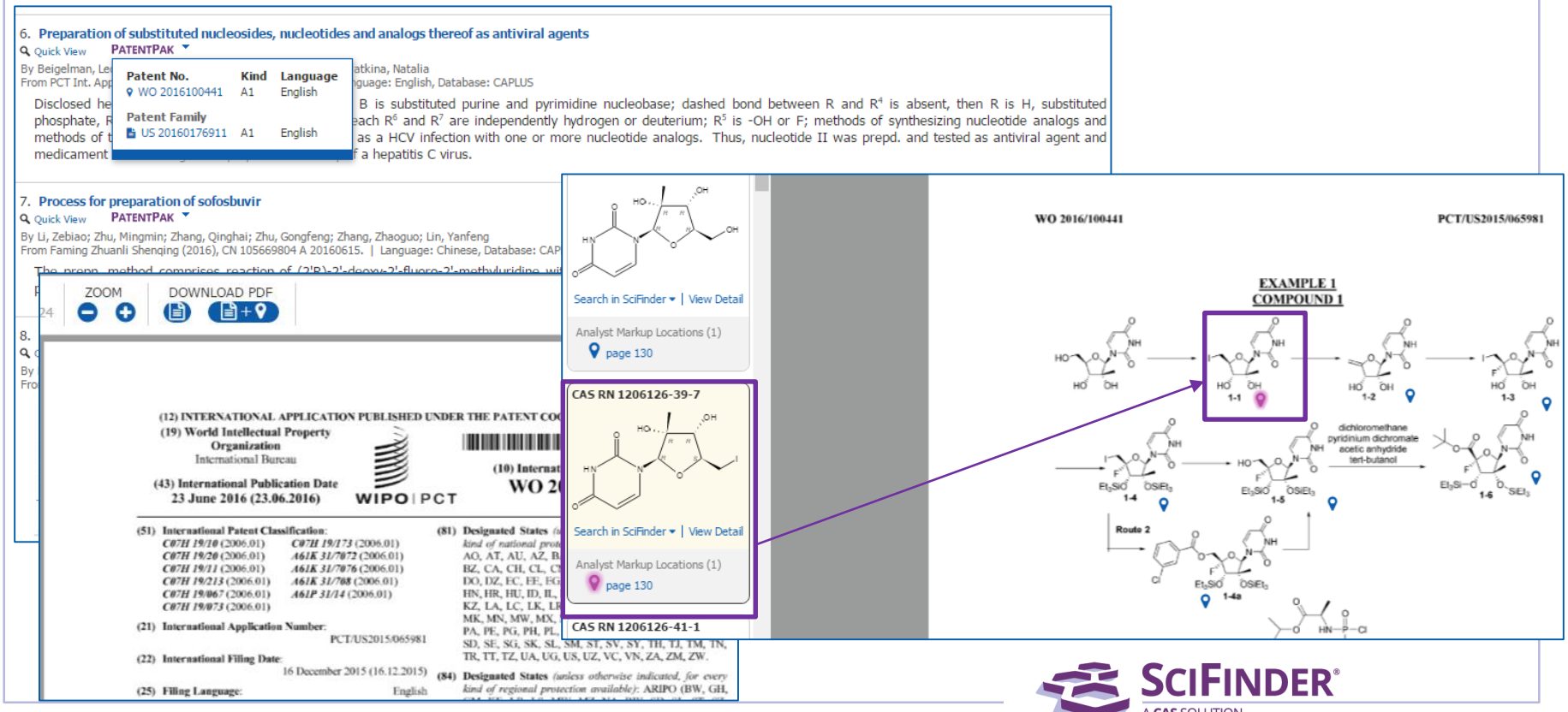
CAS最新动向—解决方案

- 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



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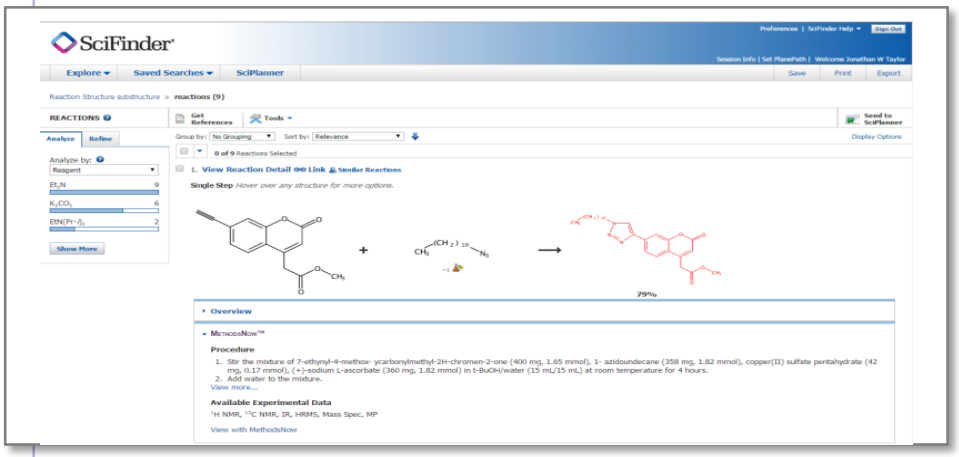
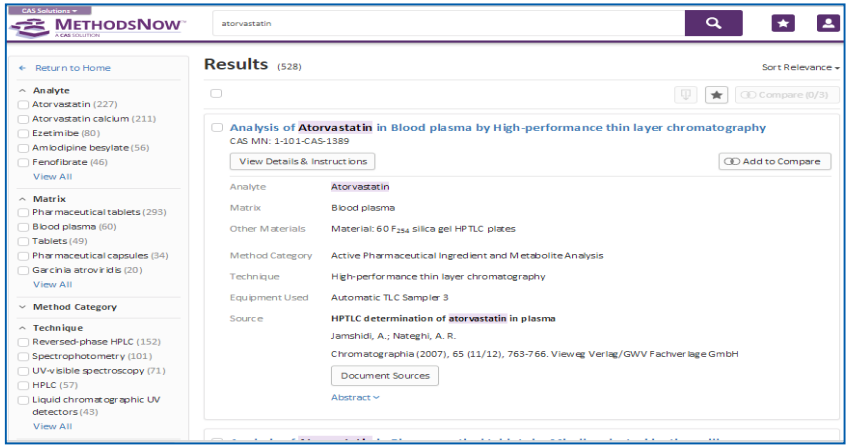
CAS最新动向—解决方案

- 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

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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 Analysis
- SciFinder常见问题及解决

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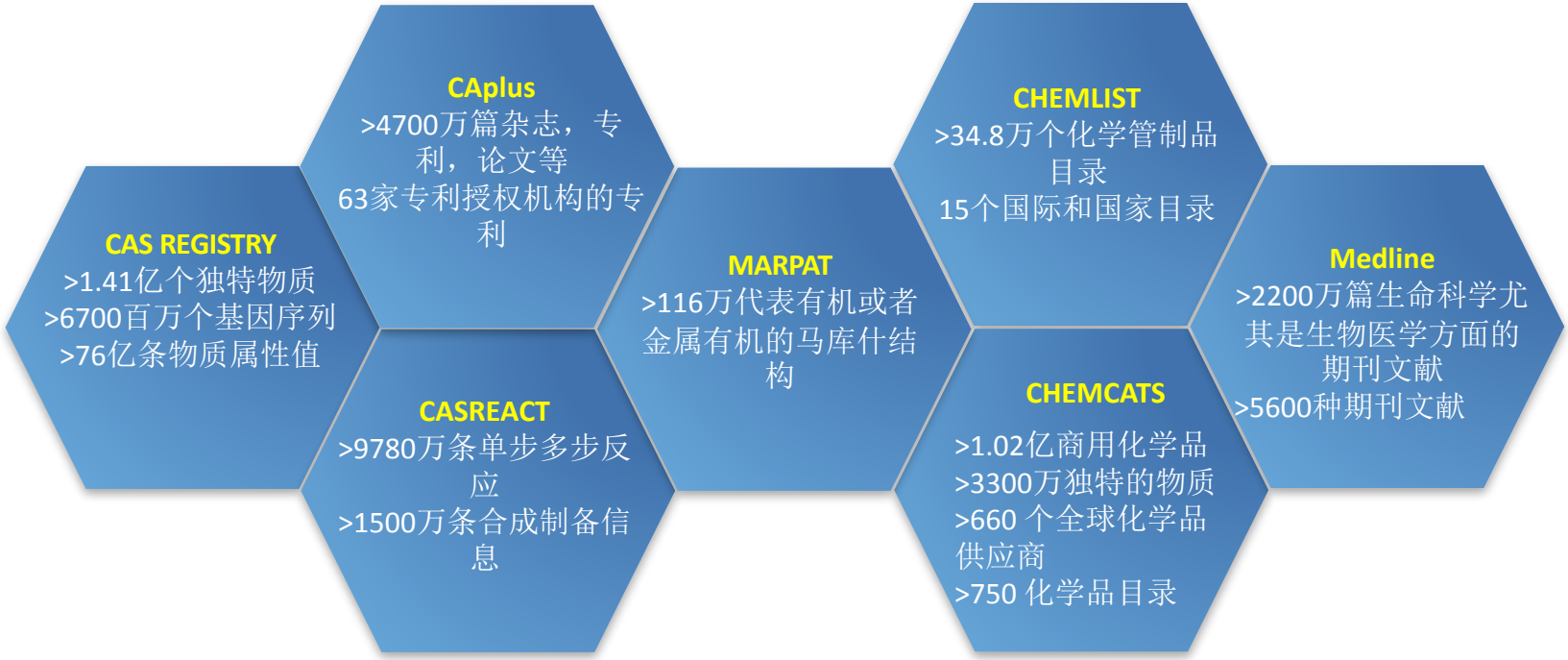
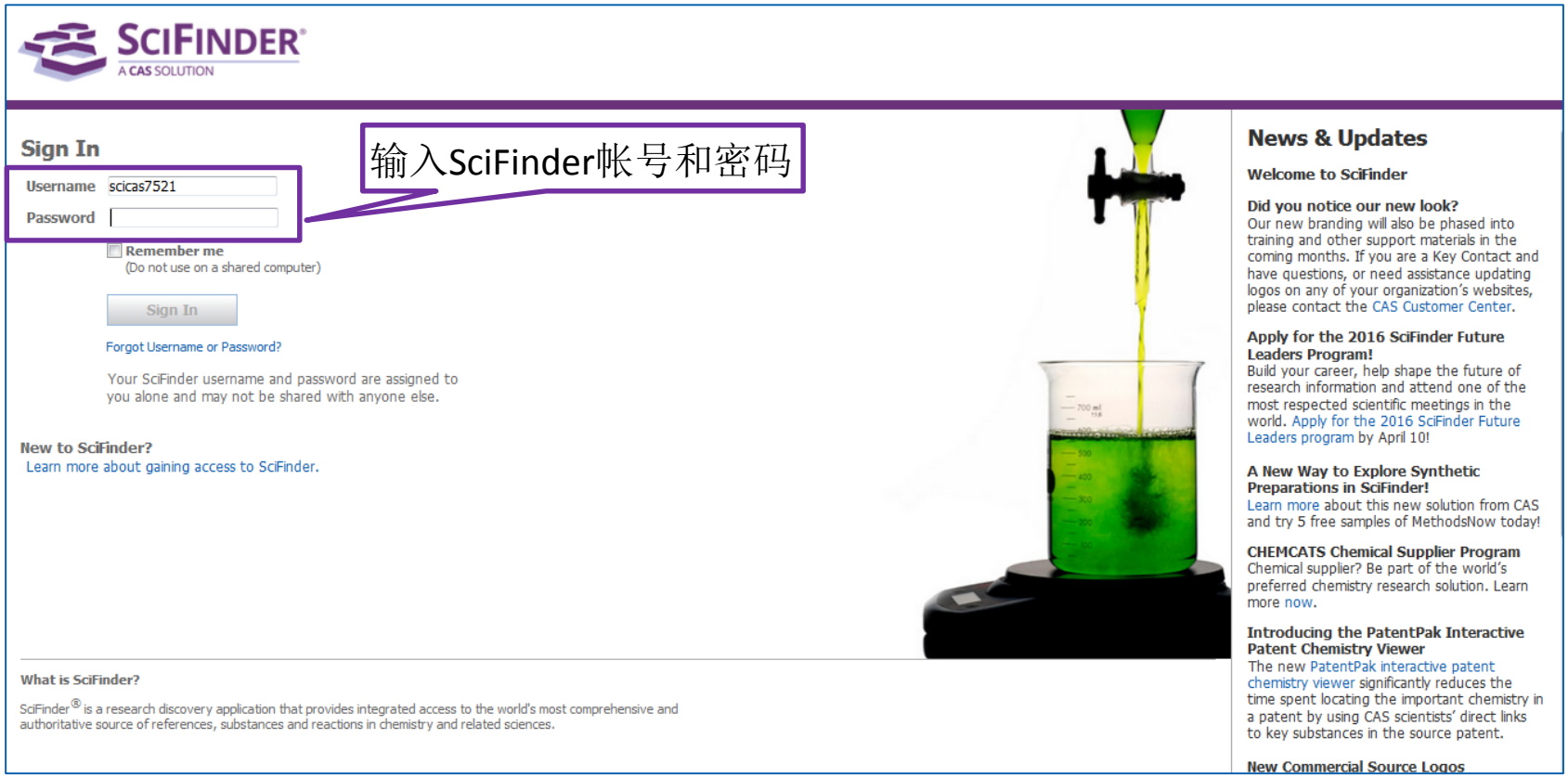
SciFinder覆盖的数据库



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



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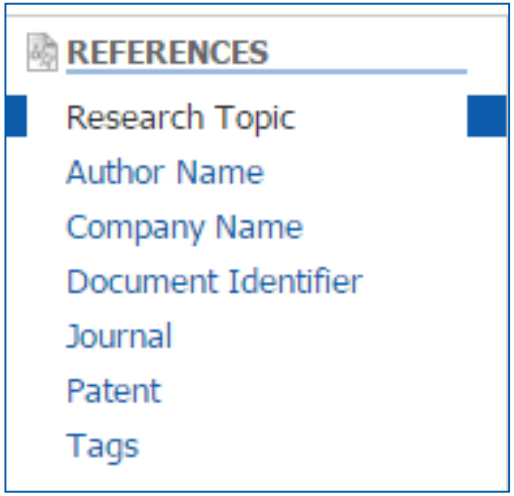
A CAS SOLUTION

SciFinder主界面

SciFinder检索——文献检索

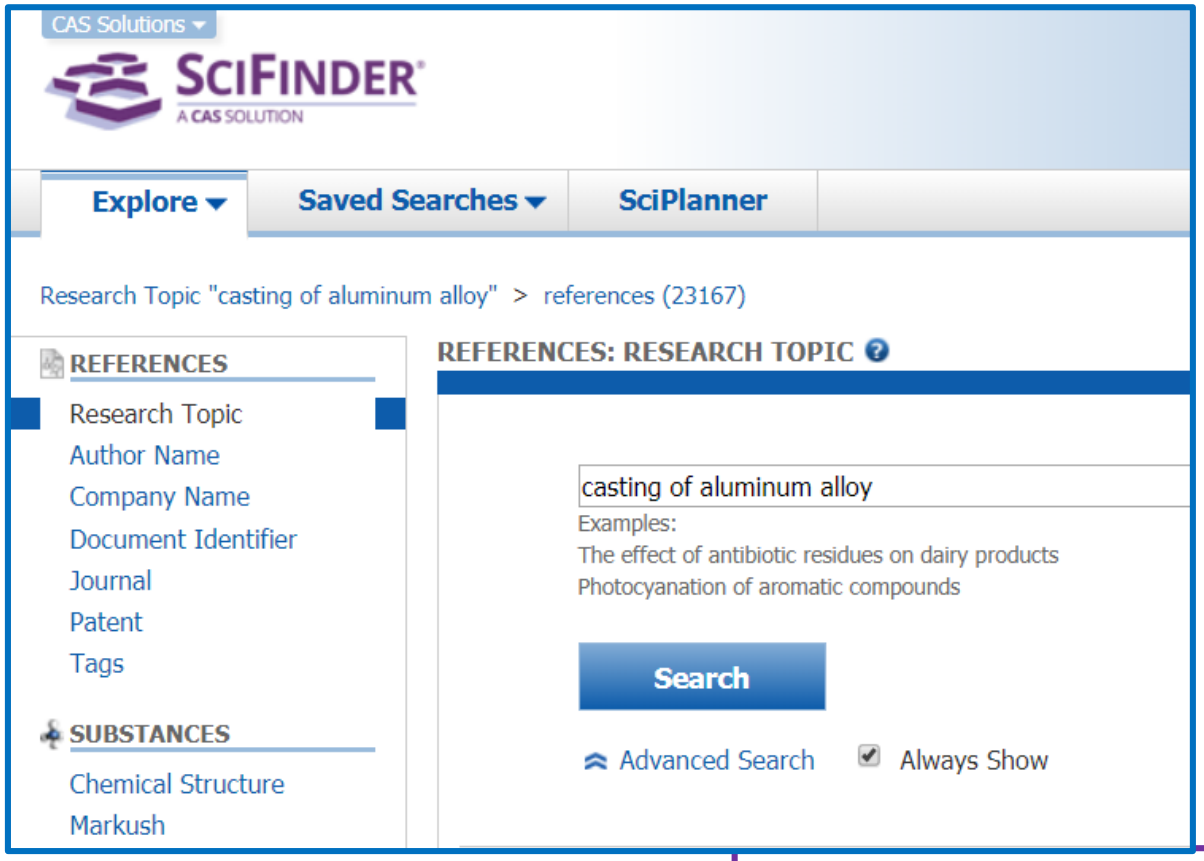
- 文献检索方法
  - 主题检索
  - 作者名检索
  - 机构名检索
  - 文献标识符检索
  - 期刊名称和专利信息（公开号，申请号等）
  - 从物质，反应获得文献



- 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

文献检索——主题: 铝合金铸造

- 检索词：铝合金 铸造
- 检索式： casting of aluminum alloy



关键词之间可用介词连接：in, with, of…

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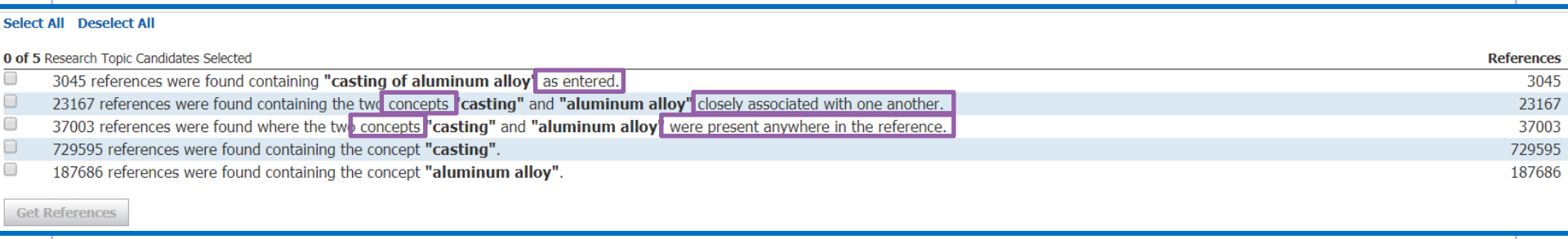
主题检索的候选项



"Concepts"表示对主题词做了同义词的扩展；

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

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

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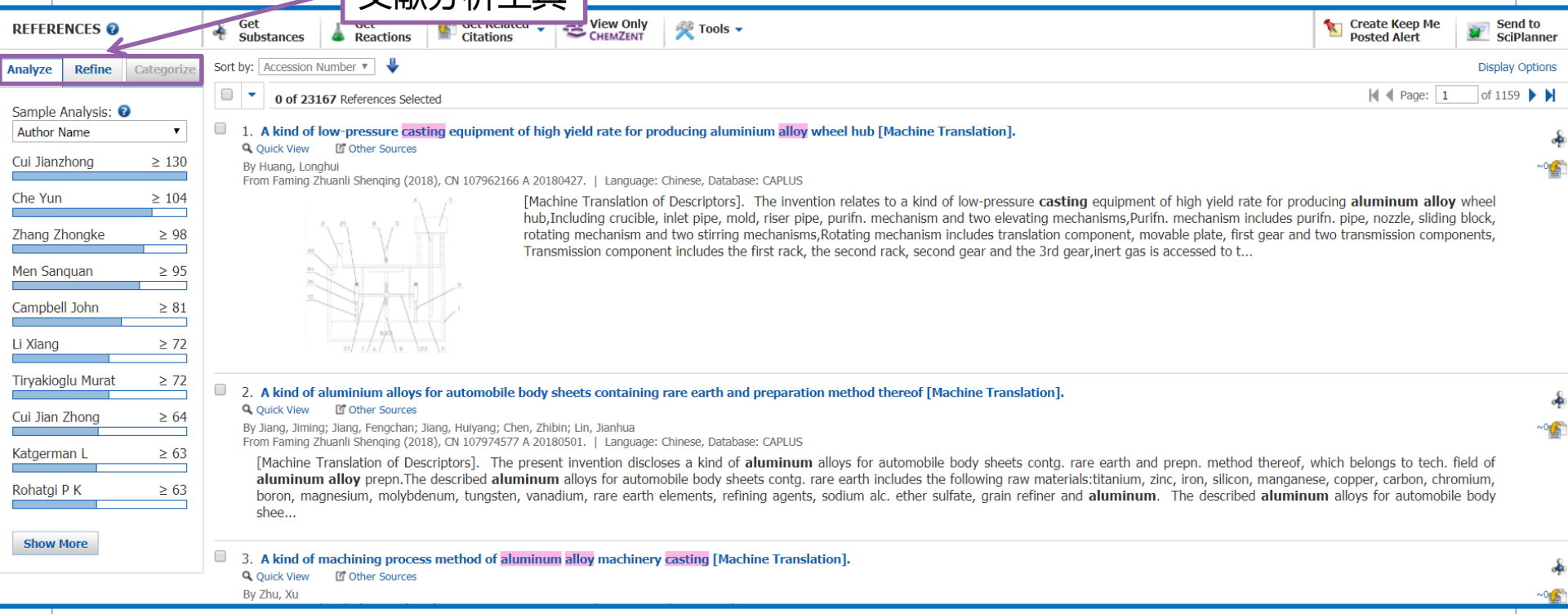
文献检索结果



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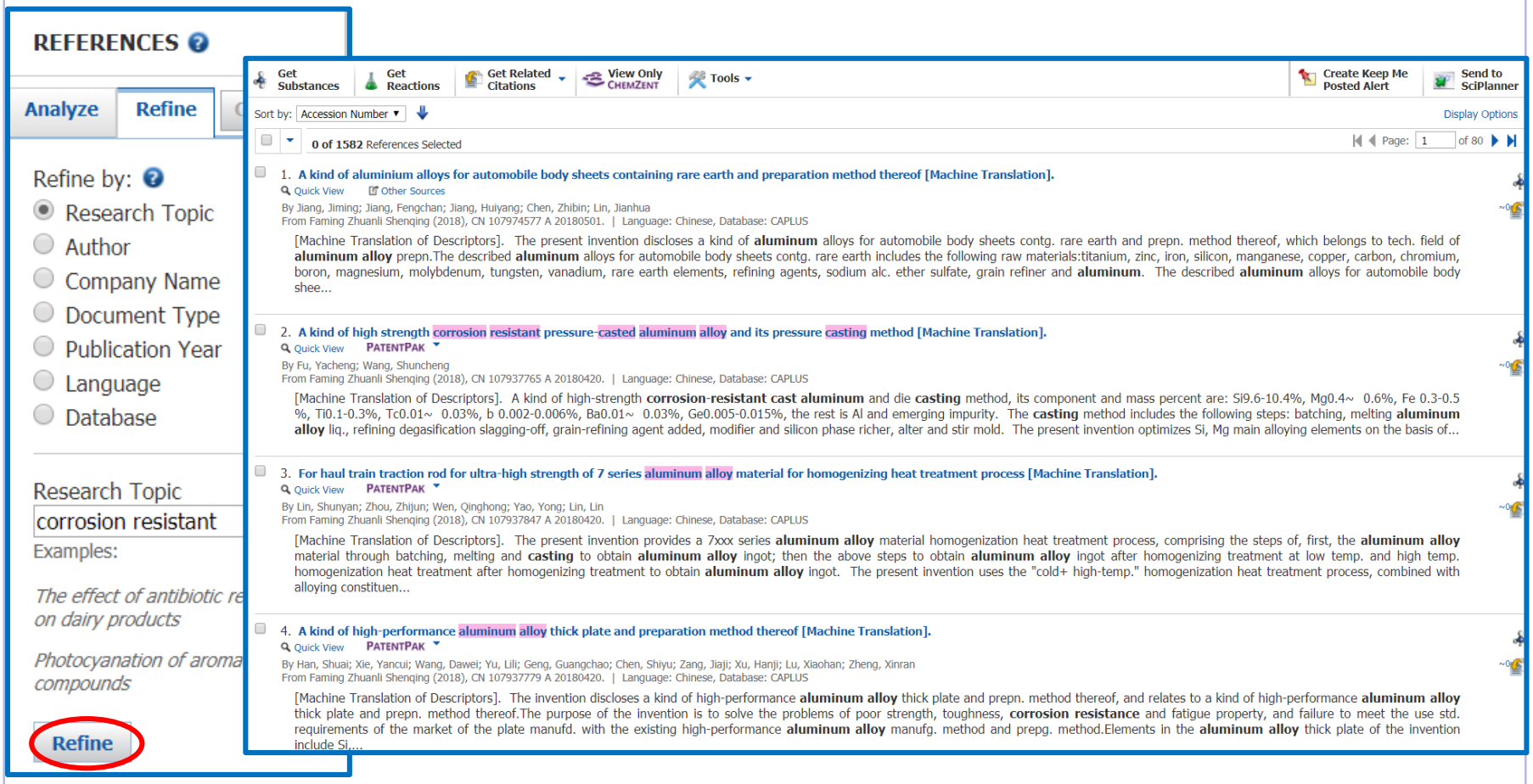
文献检索结果：Refine



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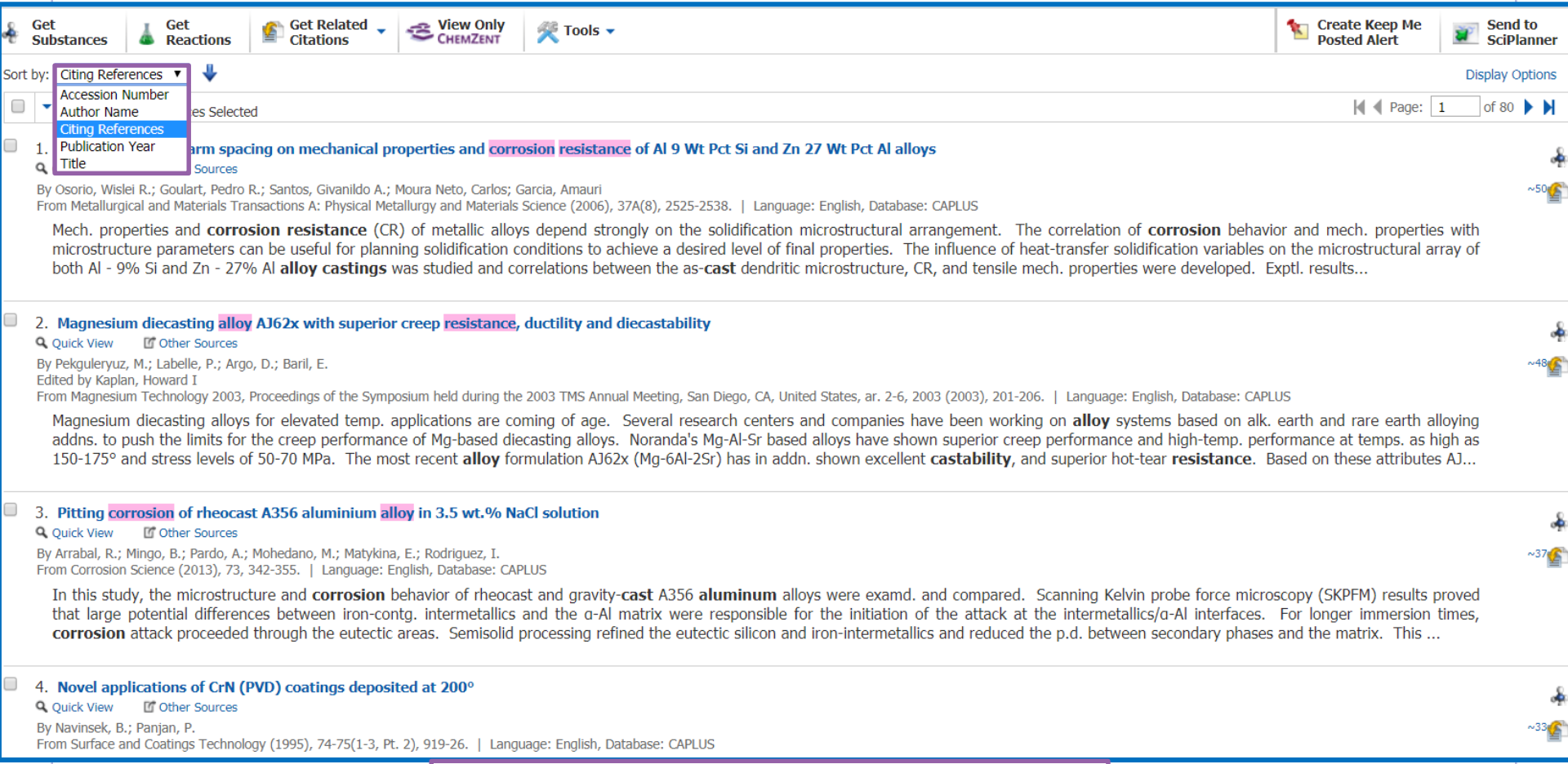
按被引次数排序— Citing References



Citing Reference: 帮助找到最重要的文献

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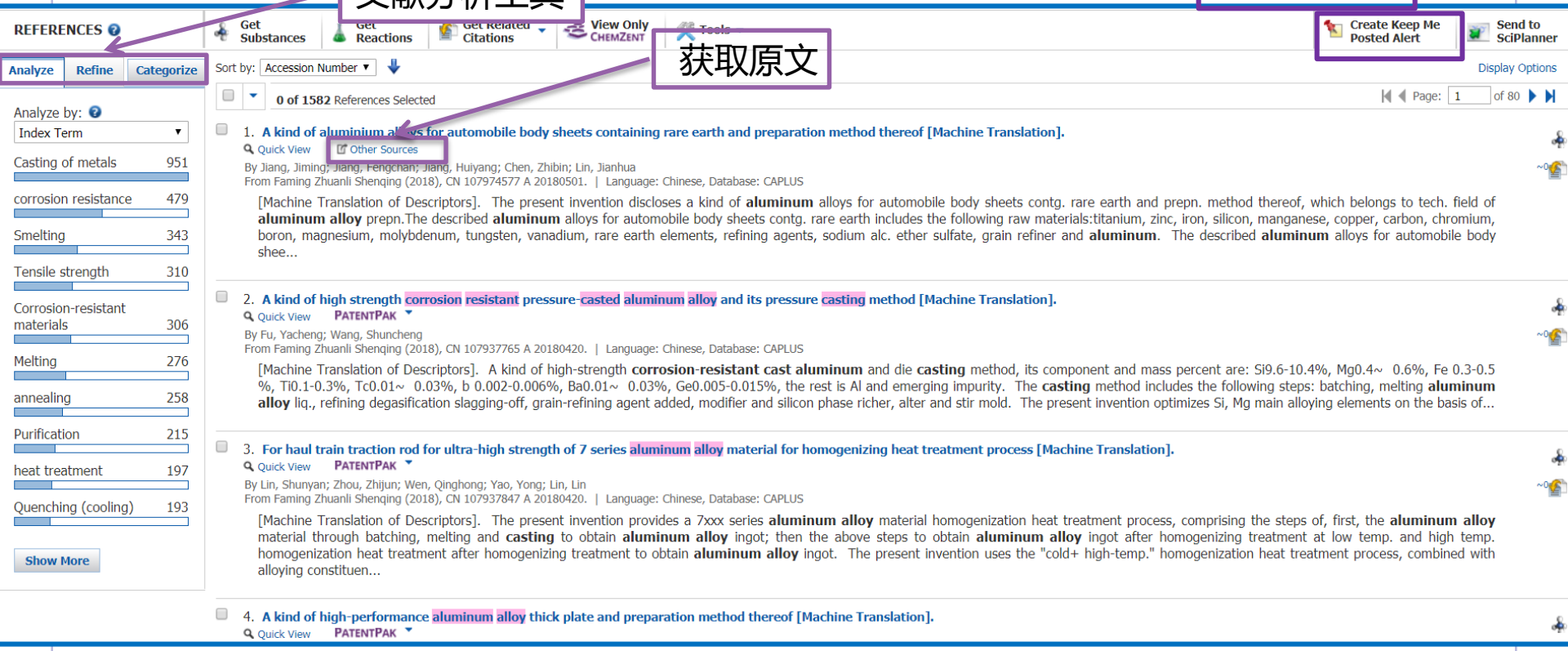
文献检索结果



SciFinder提供强大的文献处理工具，帮助处理文献

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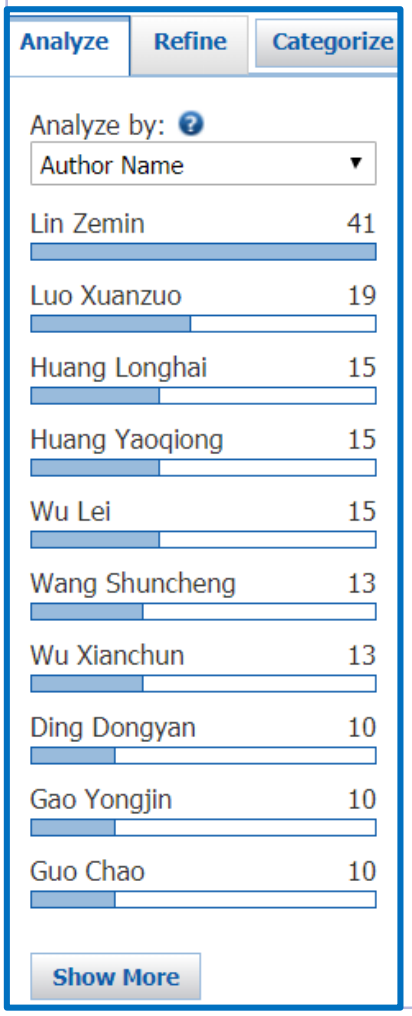
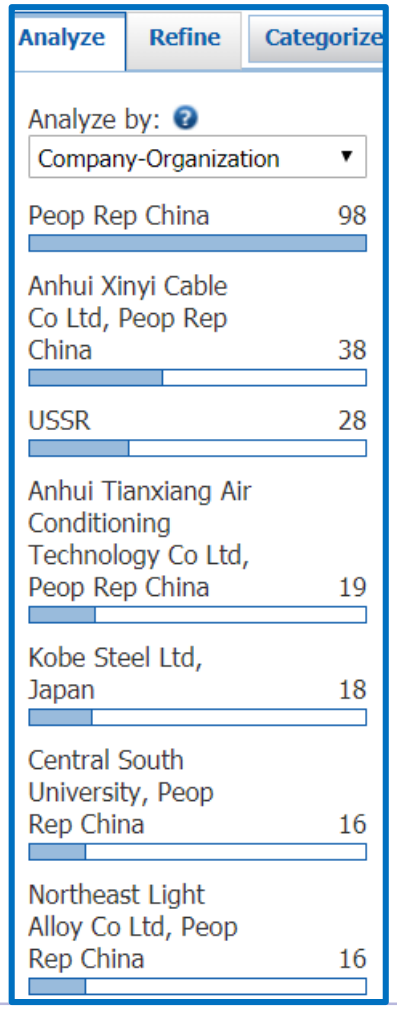
文献检索结果的Analyze

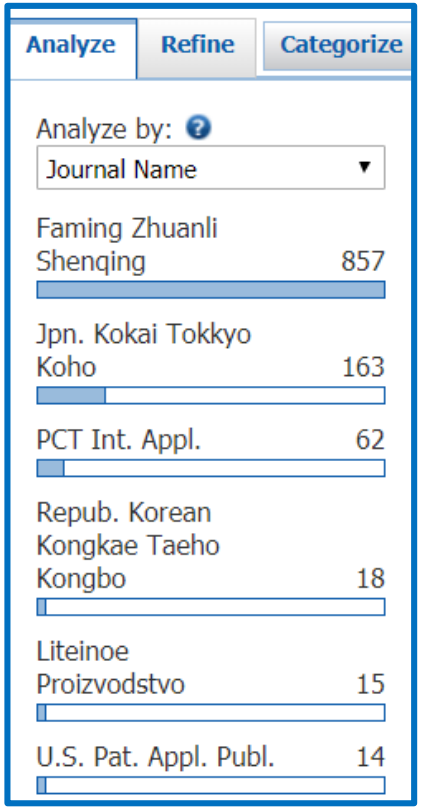
本领域研究人员



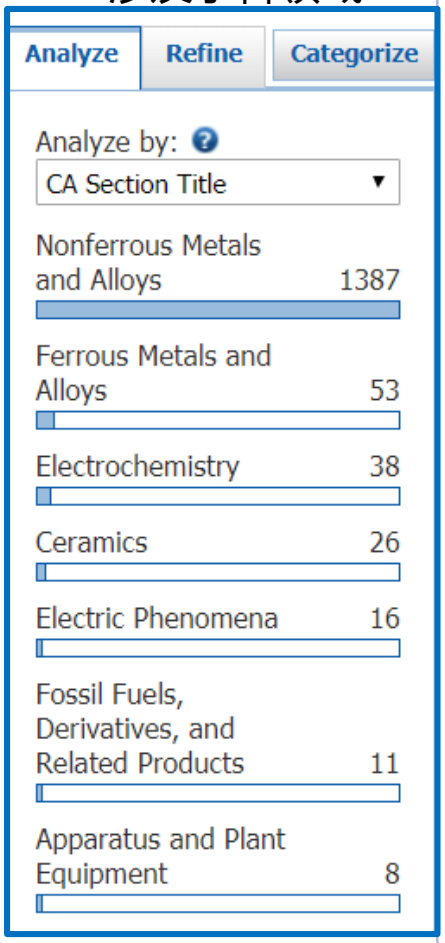
本领域研究机构、合作伙伴、竞争对手



期刊



涉及学科领域



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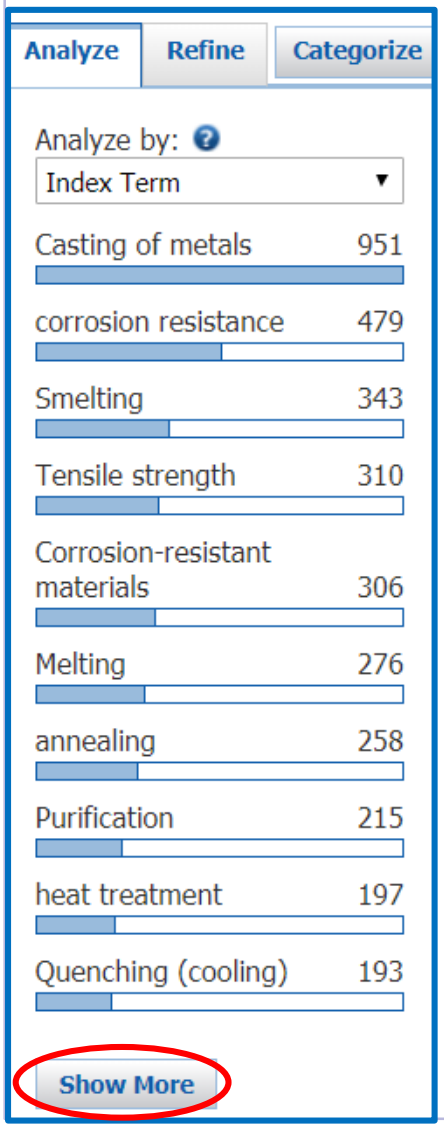
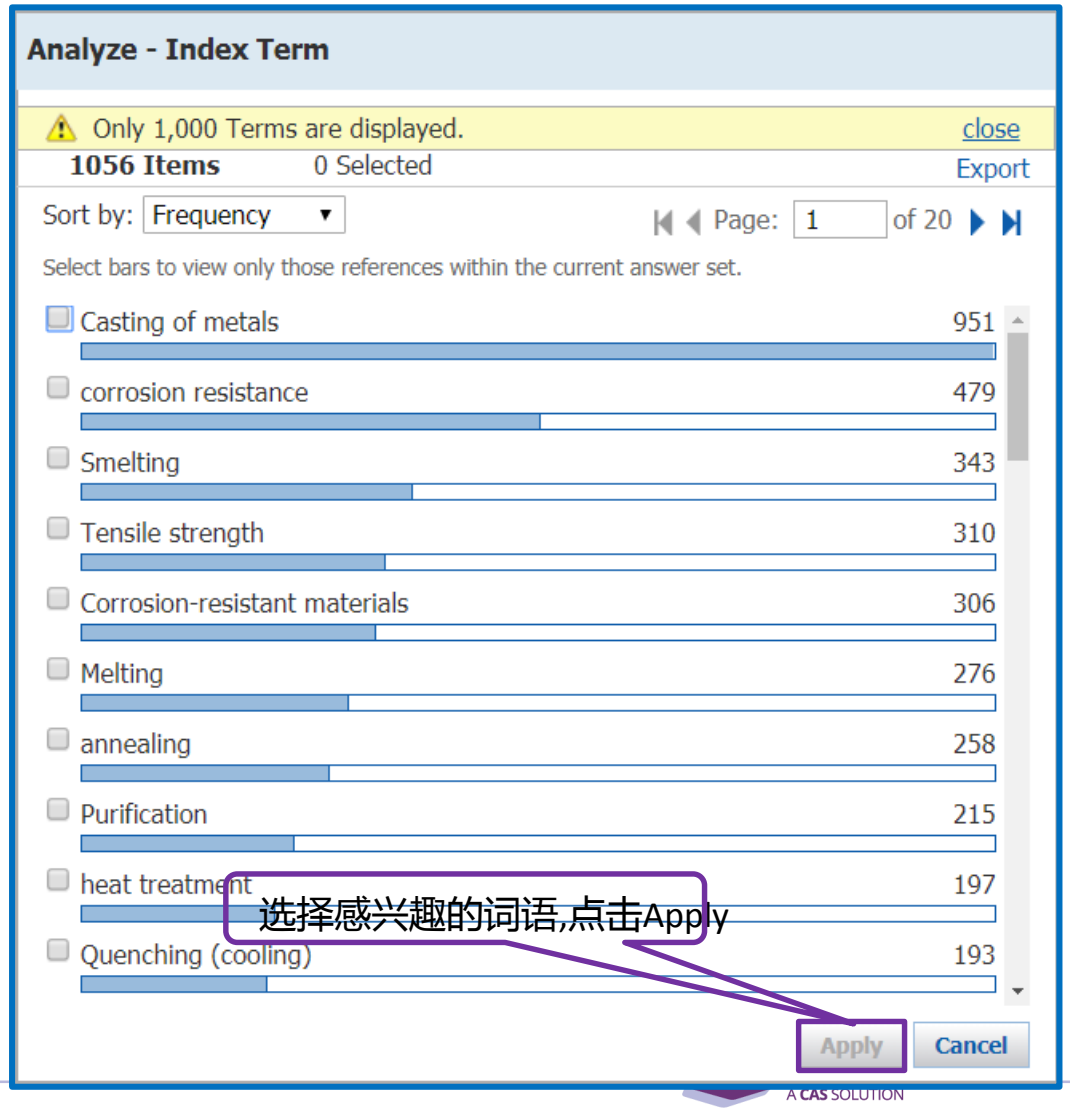
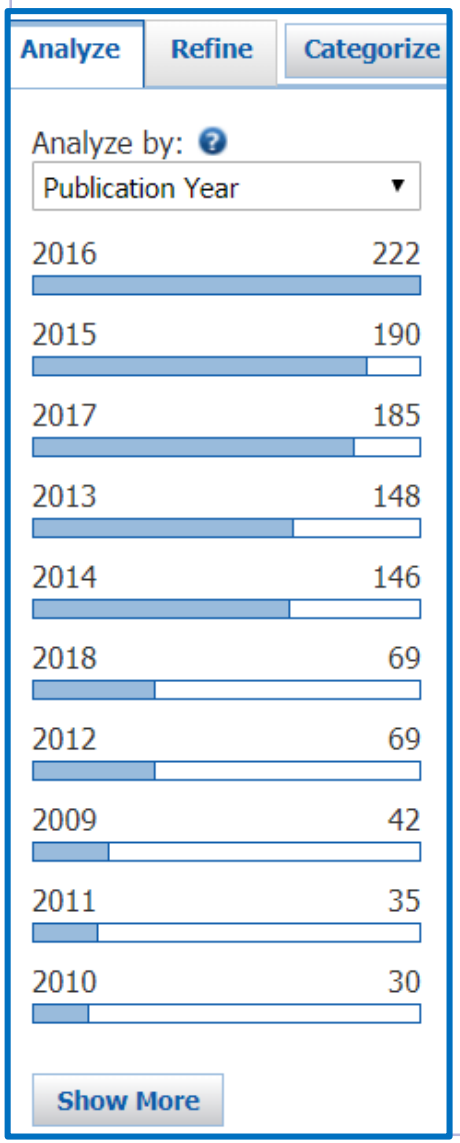
文献检索结果：Analyze

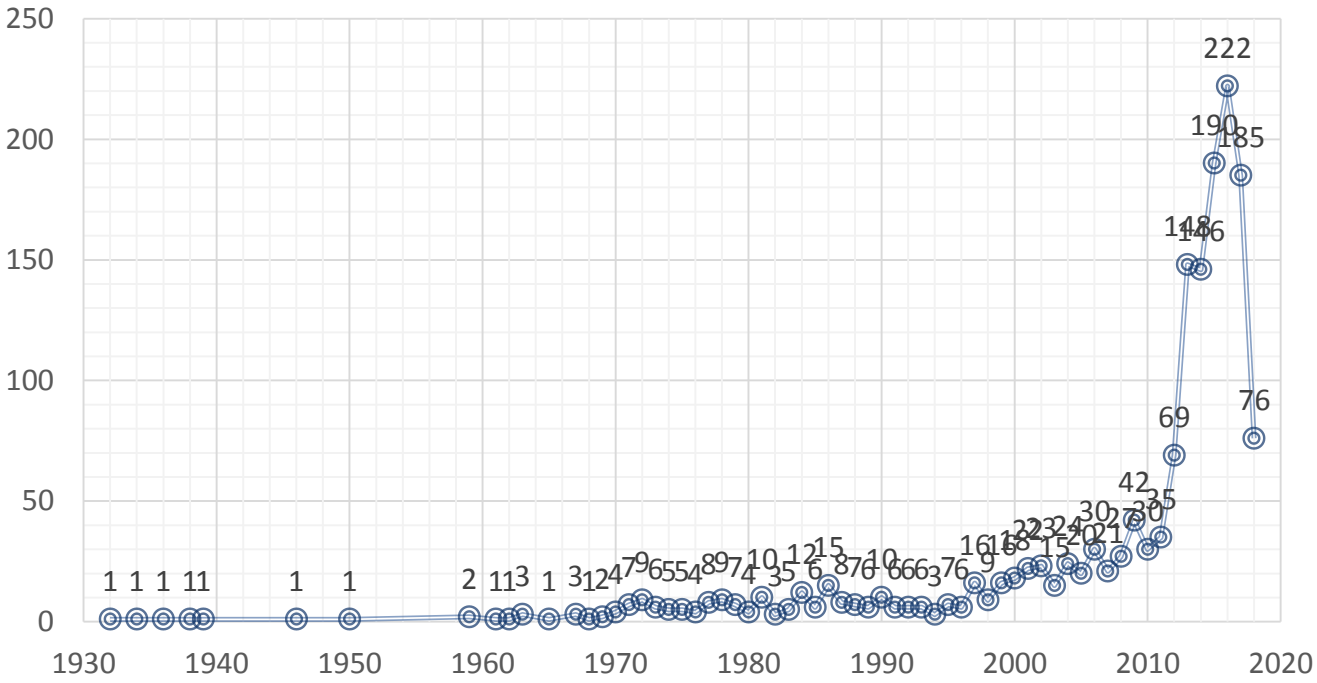
Index Term:帮助用户全景了解本领域涉及的重要技术术语，精选文献





文献检索结果的Analyze

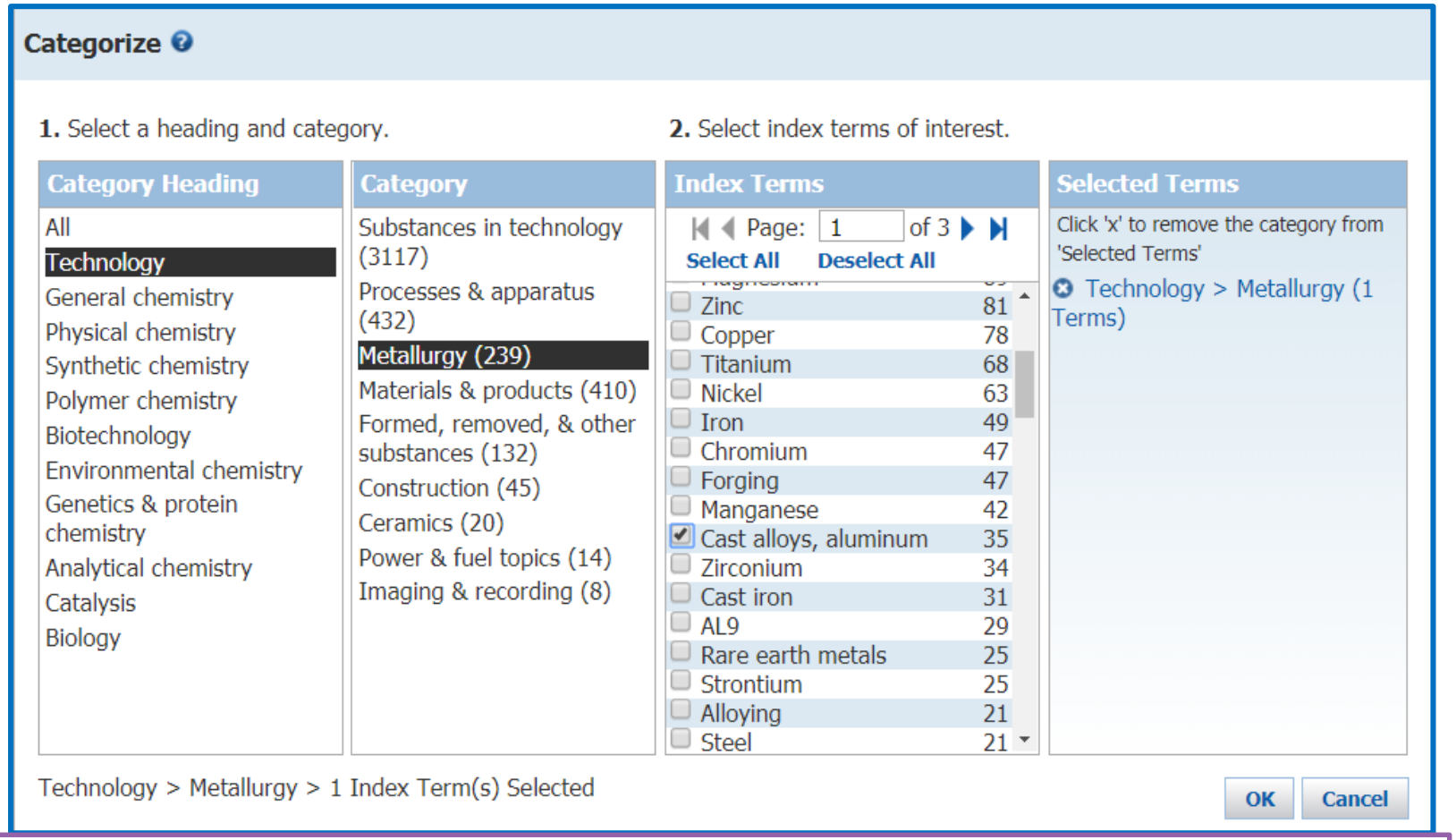




Publication Year: 分析领域发展趋势

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



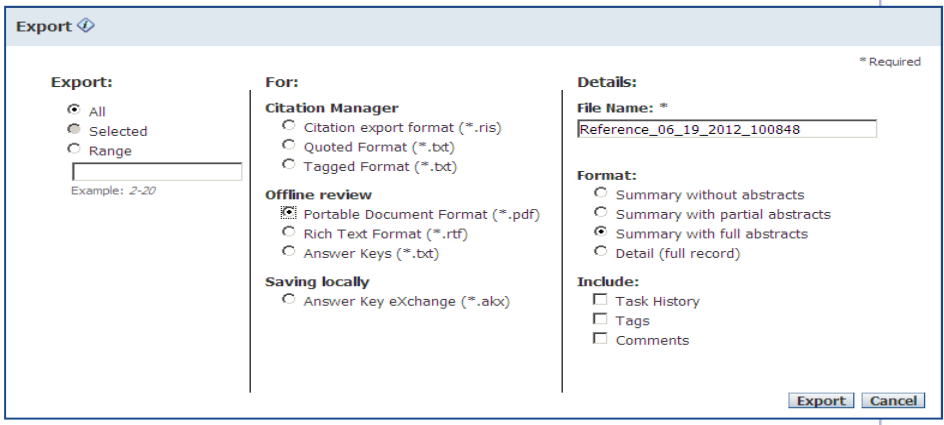
Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

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

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

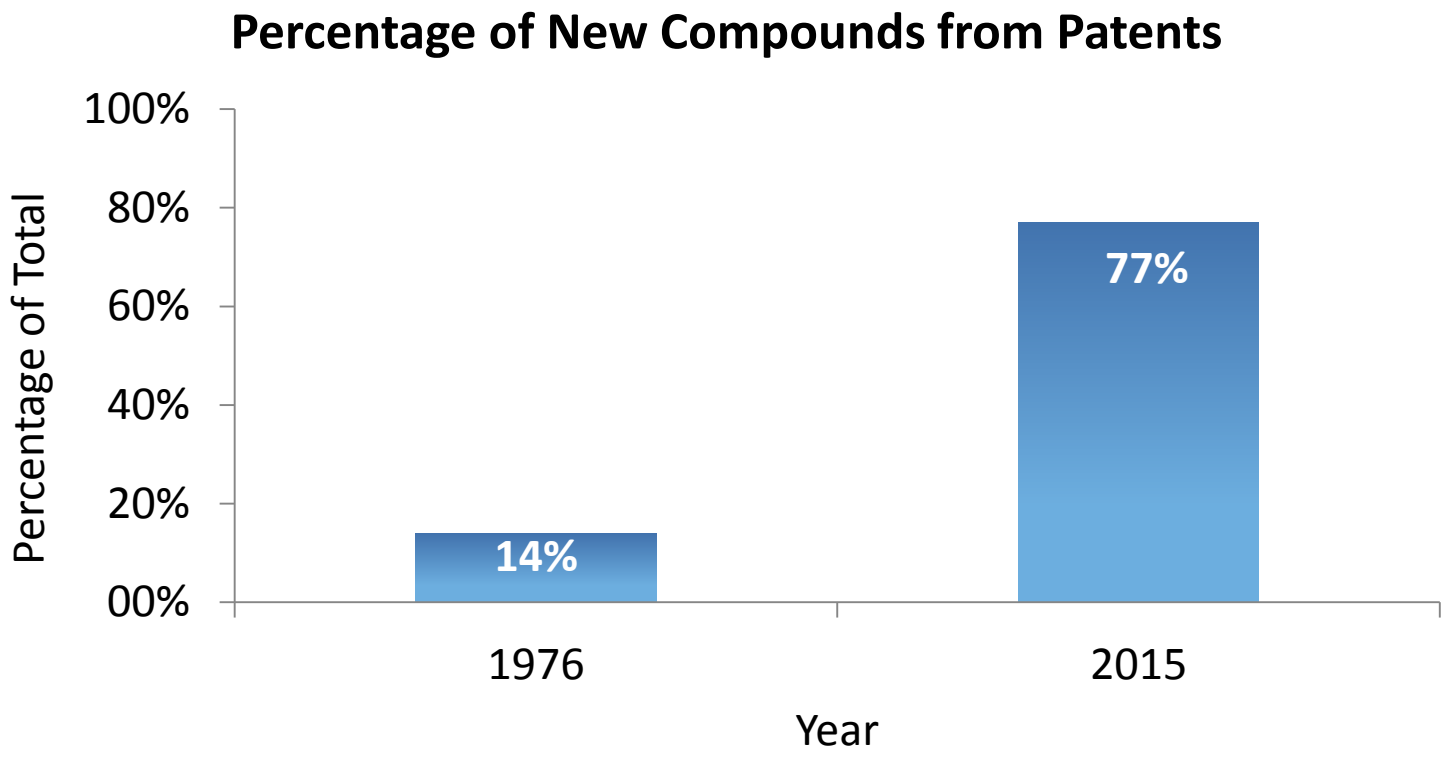
SCIFINDER® A CAS SOLUTION

PatentPak™

专利工作流程解决方案

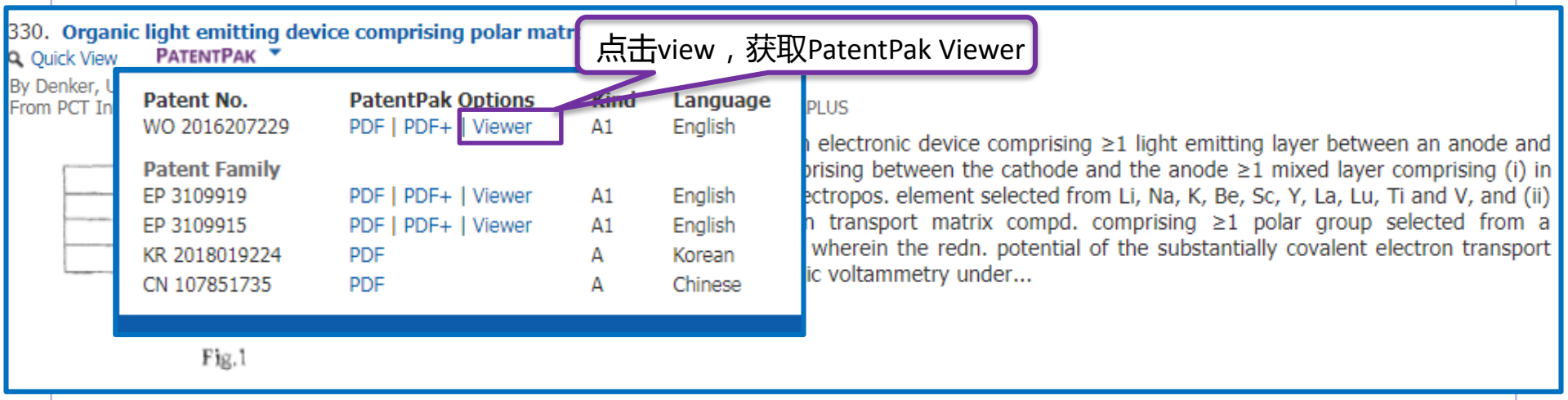
SciFinder®
A CAS SOLUTION

越来越多的新化合物倾向于首先通过专利公布



SciFinder® A CAS SOLUTION

PatentPak——专利工作流程解决方案：



PatentPak——专利工作流程解决方案

PatentPak浏览器

专利PDF文件

PATENTPAK A CAS SOLUTION

PAGE 51 /69 ZOOM DOWNLOAD PDF

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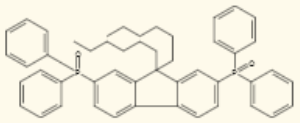
Key Substances in Patent

page 23
page 40

CAS RN 1798388-23-4



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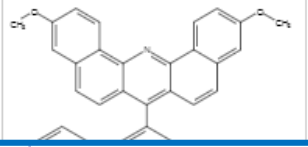
Analyst Markup Locations (3)
page 23
page 40
page 50

CAS RN 1441062-80-1



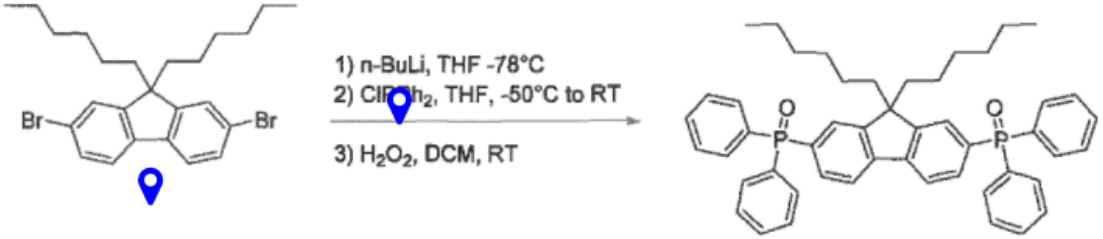
followed by [illegible] acetate (50 mL) [illegible] desired compound was obtained in 70 % yield (5.71 g). Finally, the [illegible]

The pure sublimed compound was amorphous, with no detectable melting peak on the DSC curve, glass transition onset at 86 °C, and started to decompose at 490 °C.

Synthesis example 2

在PatentPak Viewer中点击物质下面的灯泡，快速定位到PDF文件中的物质信息

(9,9-dihexyl-9H-fluorene-2,7-diyl)bis-diphenylphosphine oxide (E8)



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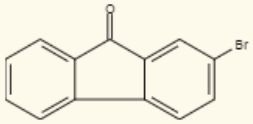
PatentPak——专利工作流程解决方案

PATENTPAK A CAS SOLUTION

PAGE 52 /69 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 3096-56-8



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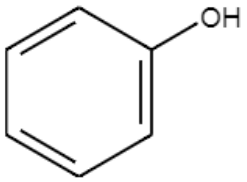
Analyst Markup Locations (2)

page 51

page 51

CAS RN 108-95-2



Search in SciFinder | View Detail

Analyst Markup Locations (2)

page 51

Synthesis of 2-bromospiro[fluorene-9,9'-xanthene]

Chemical Formula: $C_{13}H_7BrO$
Molecular Weight: 259,10

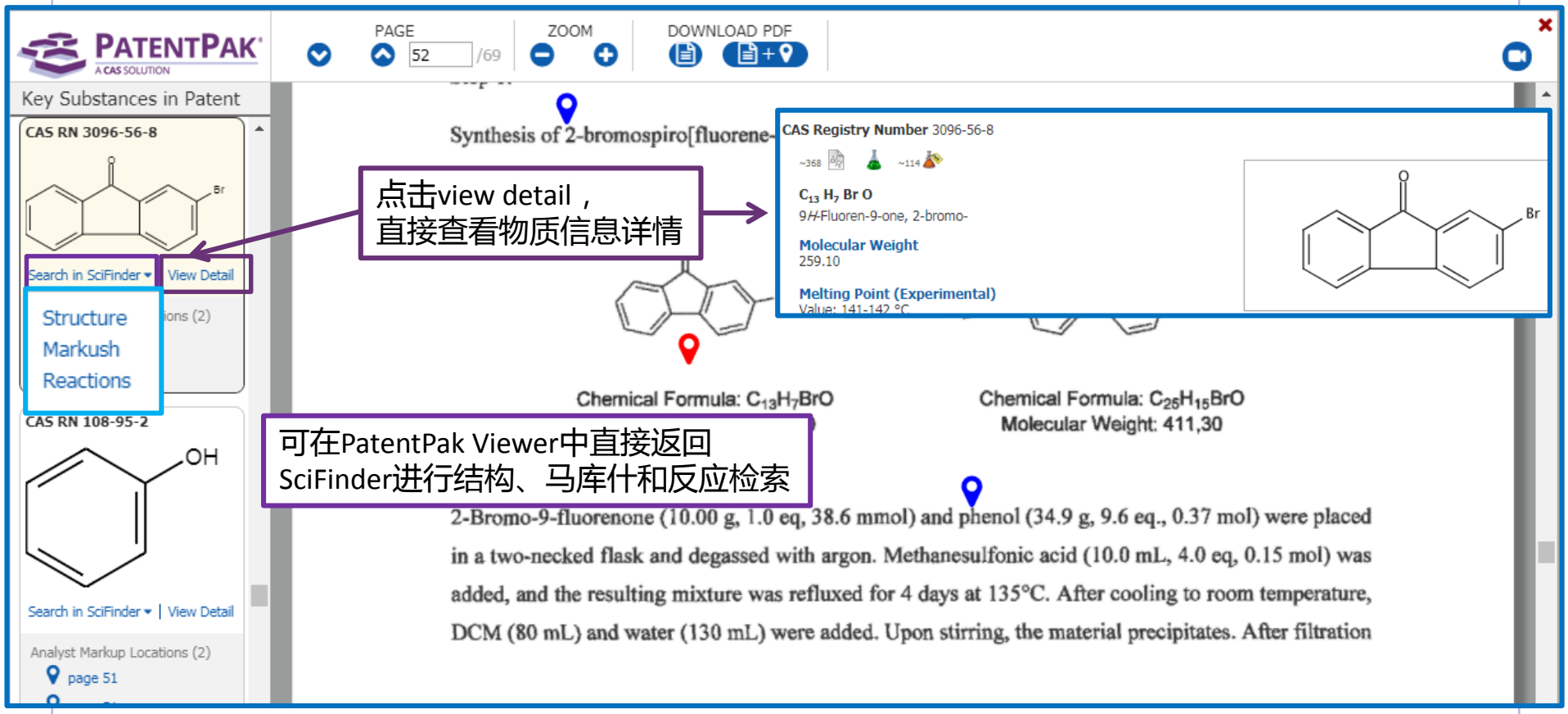
Chemical Formula: C
Molecular Weight

也可实现PDF文件与PatentPak Viewer互动

2-Bromo-9-fluorenone (10.00 g, 1.0 eq, 38.6 mmol) and phenol (34.9 g, 9.6 eq., 0.37 mol) were placed in a two-necked flask and degassed with argon. Methanesulfonic acid (10.0 mL, 4.0 eq, 0.15 mol) was added, and the resulting mixture was refluxed for 4 days at 135°C. After cooling to room temperature, DCM (80 mL) and water (130 mL) were added. Upon stirring, the material precipitates. After filtration

SCIFINDER A CAS SOLUTION

PatentPak——专利工作流程解决方案



SCIFINDER
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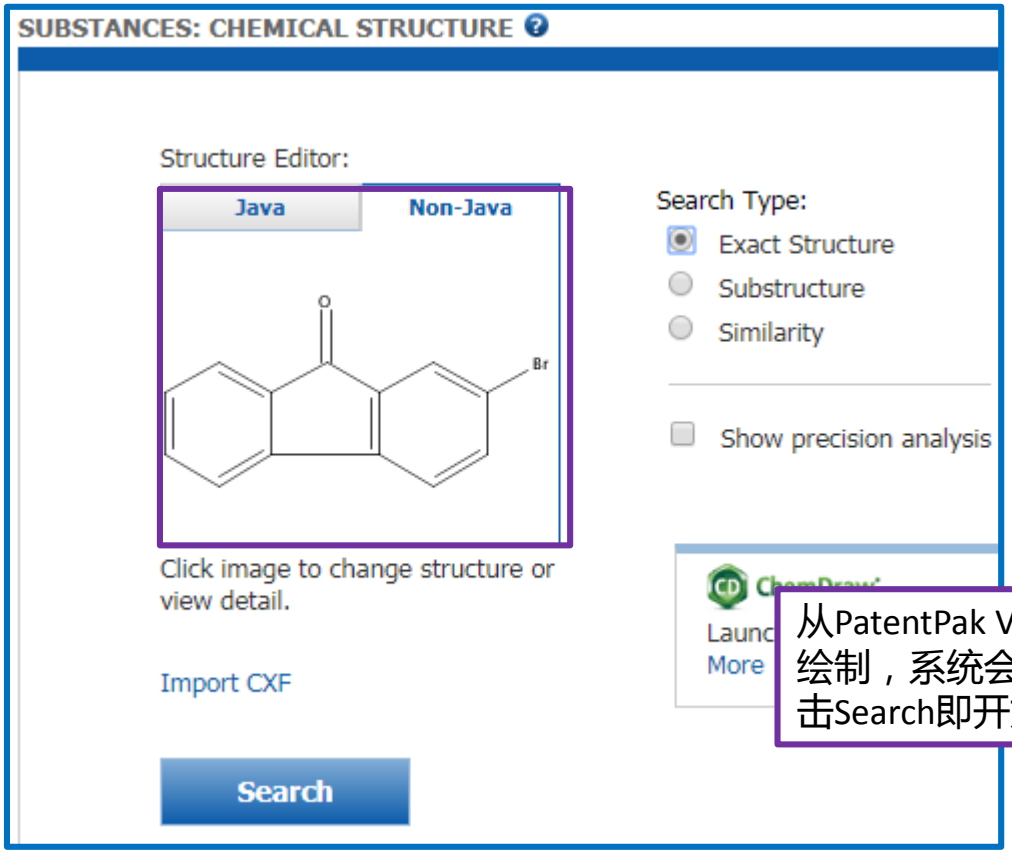
PatentPak——专利工作流程解决方案



从PatentPak Viewer直接跳转到结构检索界面，同时无需绘制，系统会自动将相应的结构直接导入到绘图面板，点击Search即开始SciFinder检索，拓展新的研究方向

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1200万份专利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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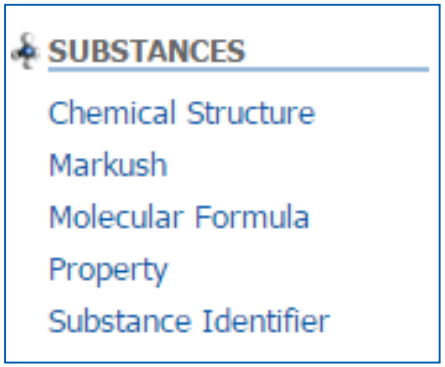
提纲

- 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 Analysis
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

SciFinder检索选项——物质检索

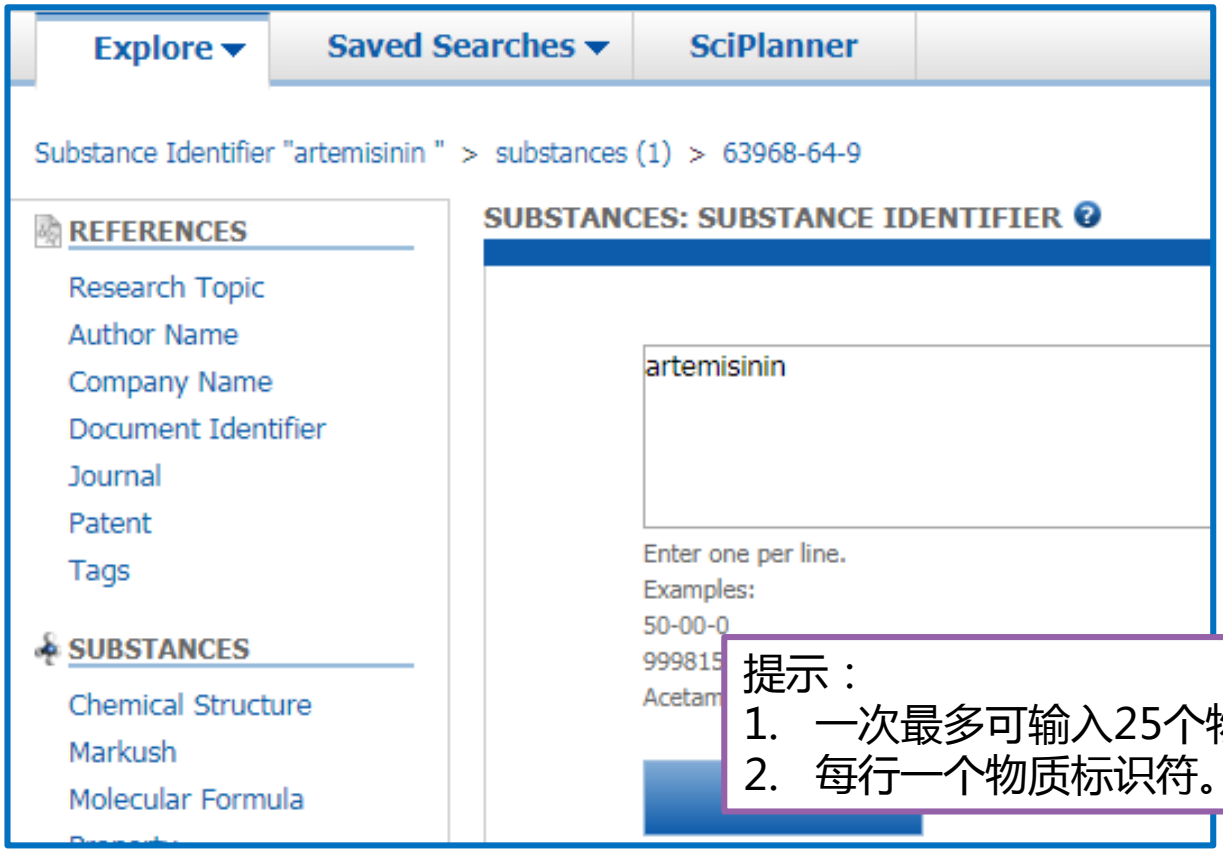
- 物质检索方法
  - —结构式检索
  - —分子式检索
  - —理化性质检索
  - —物质标识符检索：化学名称，CAS RN



- 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

SciFinder® A CAS SOLUTION

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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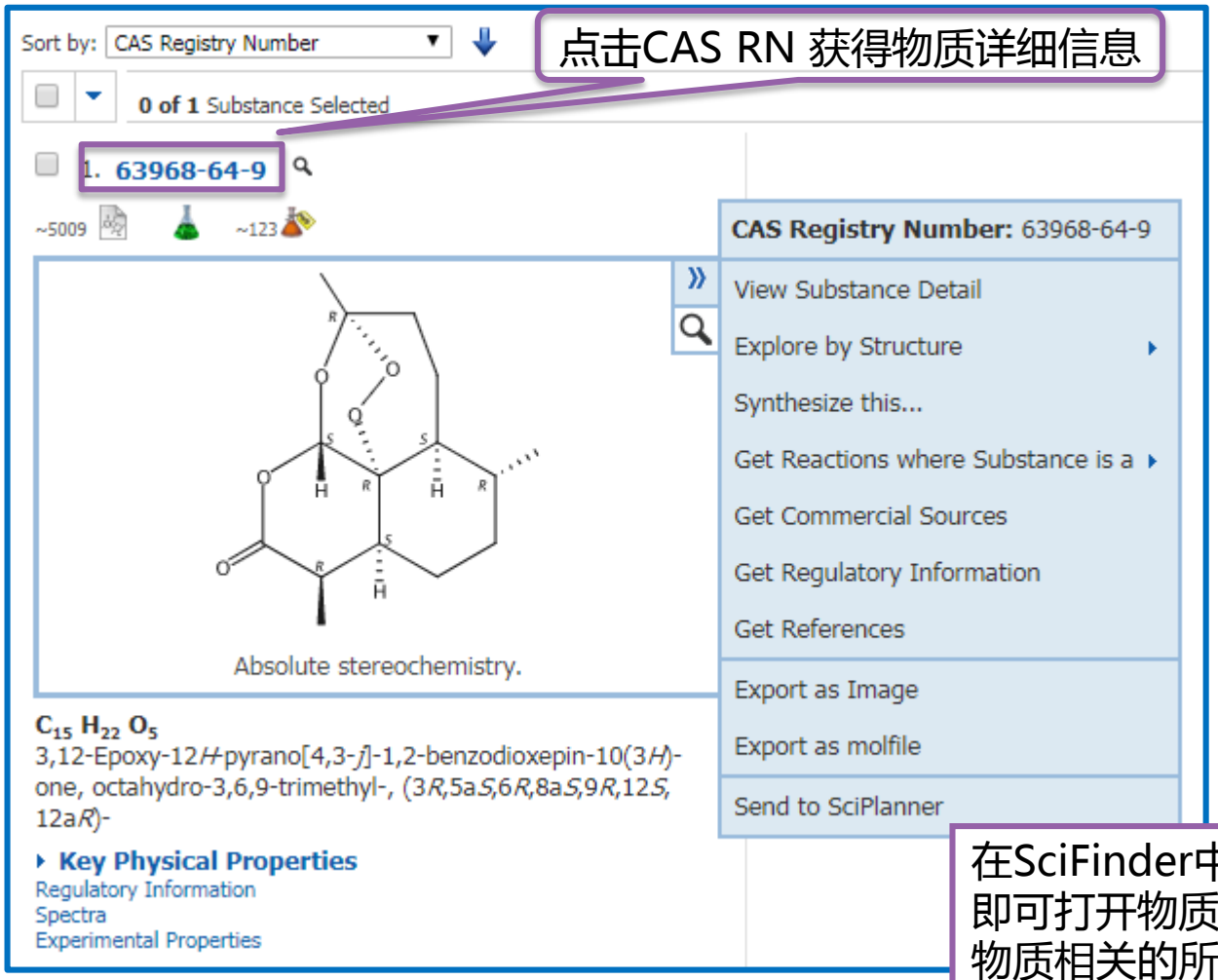
SciFinder中的物质记录



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

SCIFINDER® A CAS SOLUTION

SciFinder中的物质记录

SUBSTANCE DETAIL

Get References | Get Reactions | Get Commercial Sources

由物质获得文献，反应，供应商等信息

Return

CAS Registry Number 63968-64-9

~5,009 ~123

$C_{15}H_{22}O_5$

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*)-

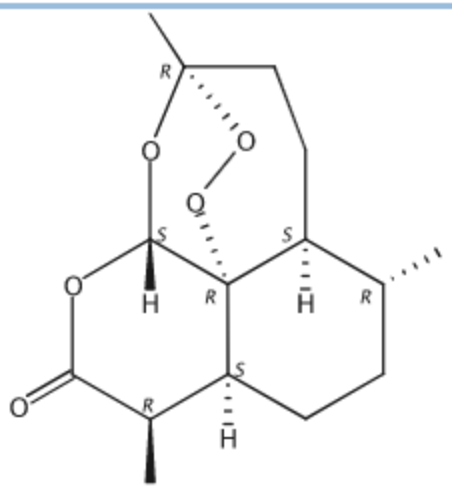
Molecular Weight
282.33

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...

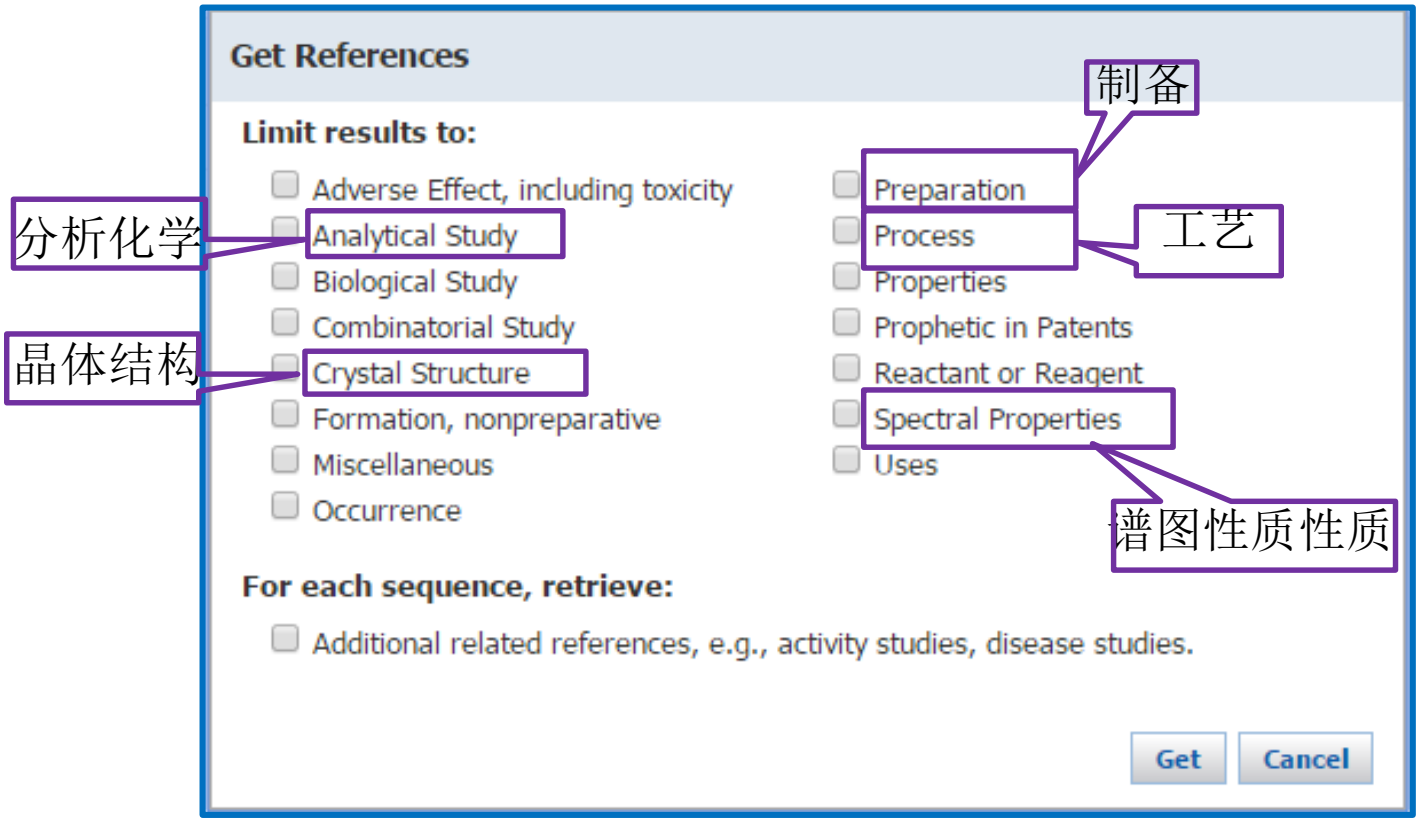


Absolute stereochemistry.

物质详情

SCIFINDER® A CAS SOLUTION

通过物质获得文献


Get References
Limit results to:
Adverse Effect, including toxicity
Analytical Study
Biological Study
Combinatorial Study
Crystal Structure
Formation, nonpreparative
Miscellaneous
Occurrence
Preparation
Process
Properties
Prophetic in Patents
Reactant or Reagent
Spectral Properties
Uses
For each sequence, retrieve:
Additional related references, e.g., activity studies, disease studies.
Get
Cancel
制备
工艺
分析化学
晶体结构
谱图性质性质

EXPERIMENTAL PROPERTIES

Biological | Chemical | Density | Flow and Diffusion | Lipinski | Optical and Scattering | Structure Related | Thermal

Structure Related Properties	Value	Note
Bond Angle	See full text	(2)CAS
Bond Length	See full text	(2)CAS
Permeability	See full text	
X-Ray Diffraction Pattern	See full text	

Notes

(2) Galasso, V.; Chemical Physics 2007, V335(2-3), P141-154 CAPLUS

(23) Du-Cuny, Lei; Bioorganic & Medicinal Chemistry 2009, V17(19), P

(25) Sahoo, Nanda Gopal; Journal of Pharmaceutical Sciences 2009, V

实验数据与实验谱图

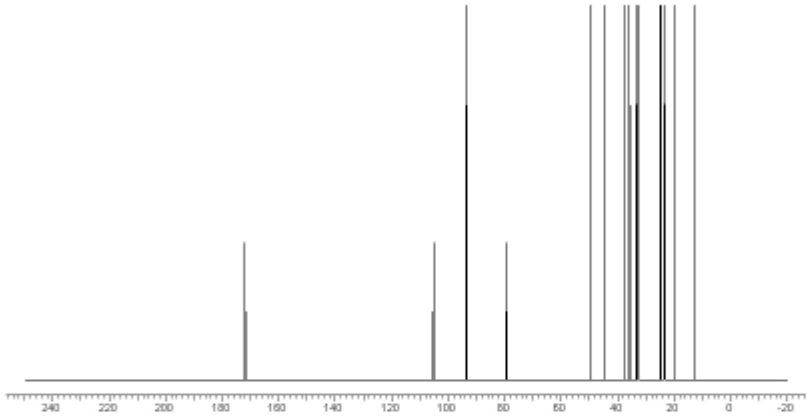
EXPERIMENTAL SPECTRA

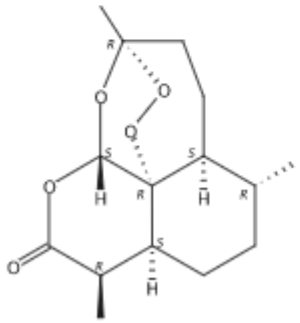
^{1}H NMR | ^{13}C NMR | Hetero NMR | IR | Mass | Raman

^{13}C NMR Properties	Value
Carbon-13 NMR Spectrum	See spectru
Carbon-13 NMR Spectrum	See spectru
Carbon-13 NMR Spectrum	See full tex

1 of 4

Carbon-13 NMR Spectrum





FORMULA

$C_{15}H_{22}O_5$

CAS INDEX NAME

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*)-

NUCLEUS

13C

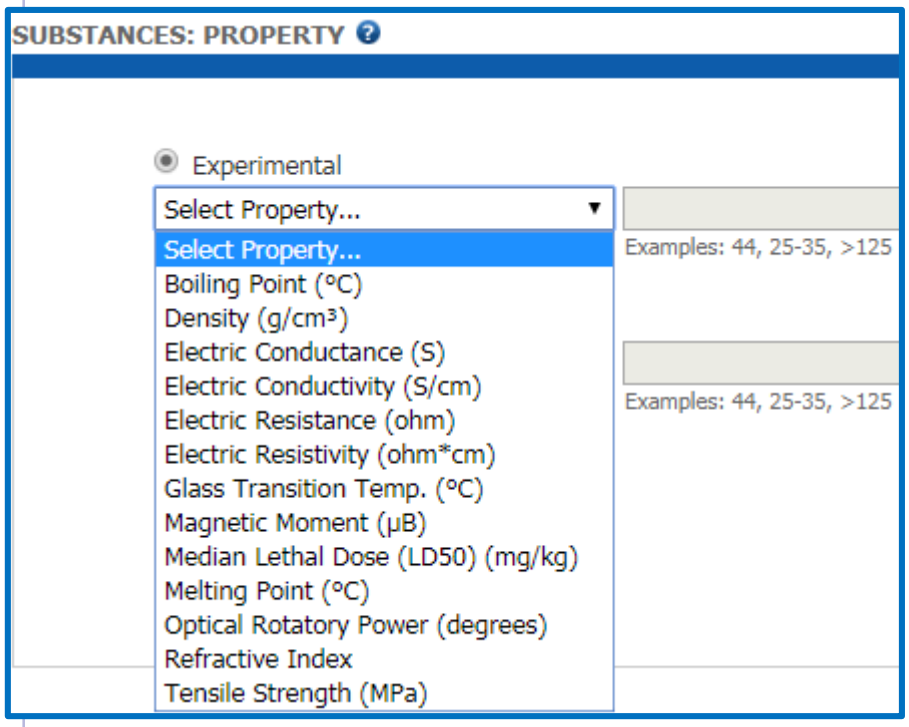
SOURCE

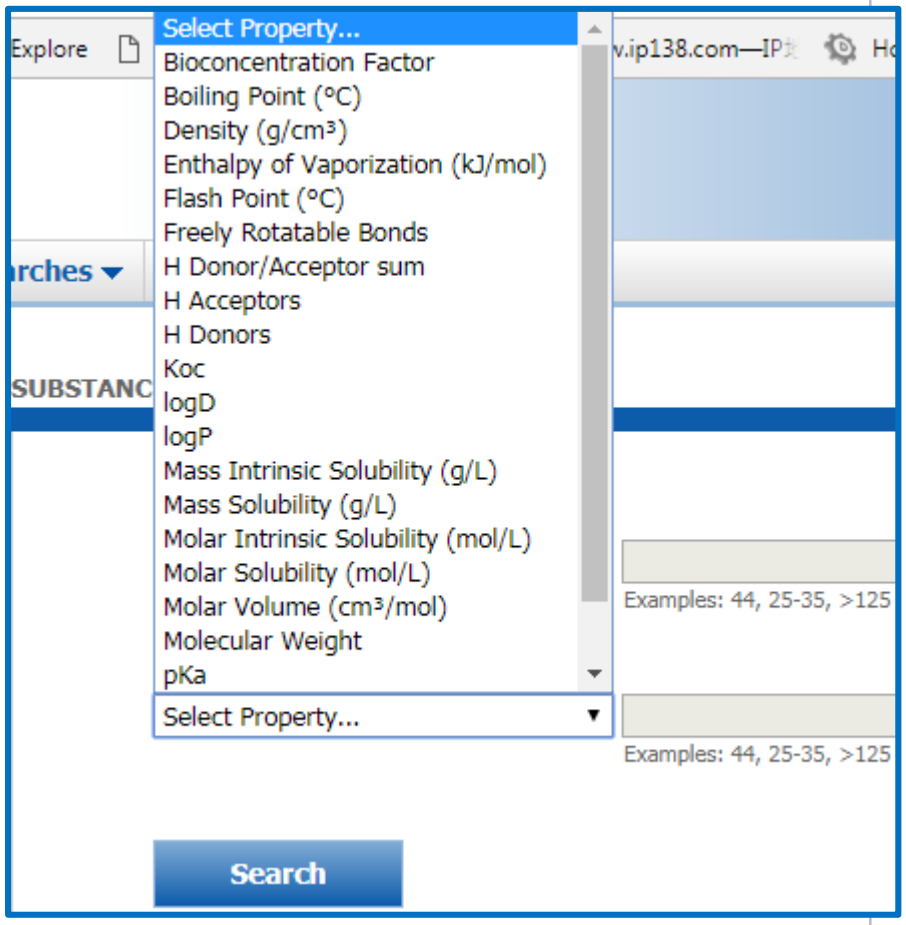
Spectral data were obtained from Advanced Chemistry Development, Inc.

Absolute stereochemistry

SciFinder® A CAS SOLUTION

物质检索——理化性质性质检索





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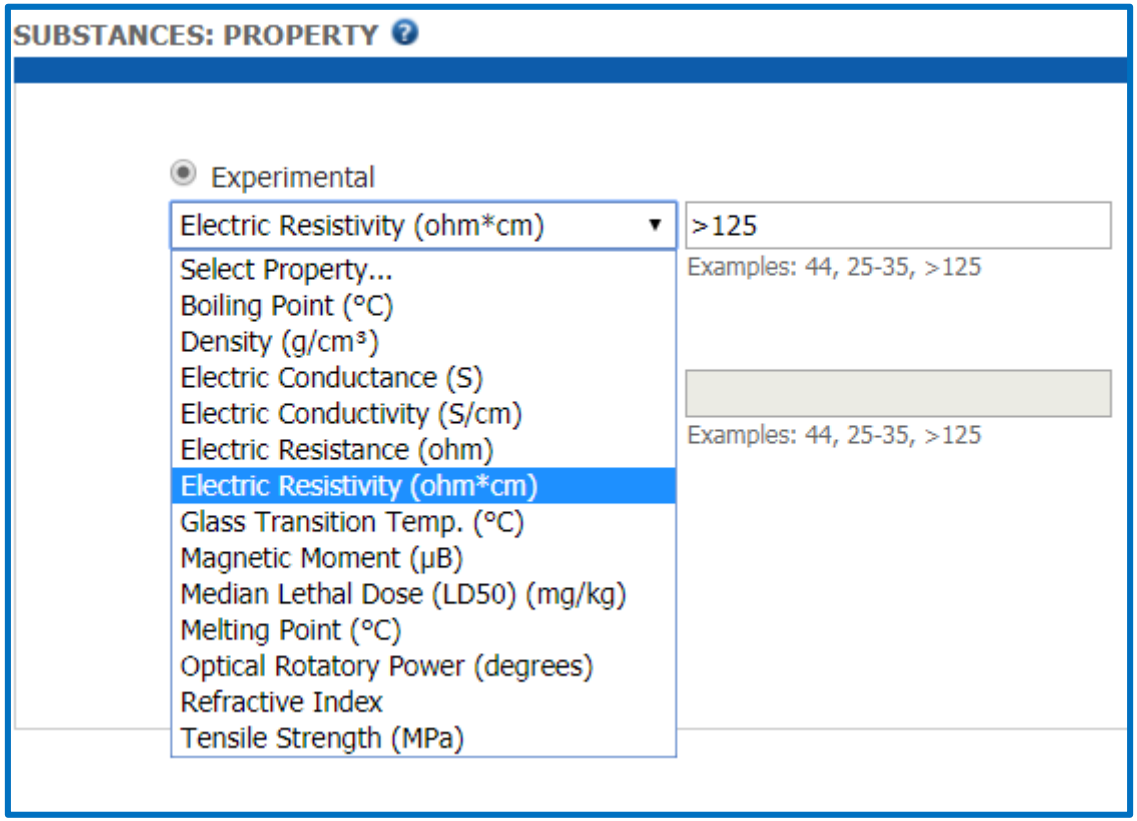
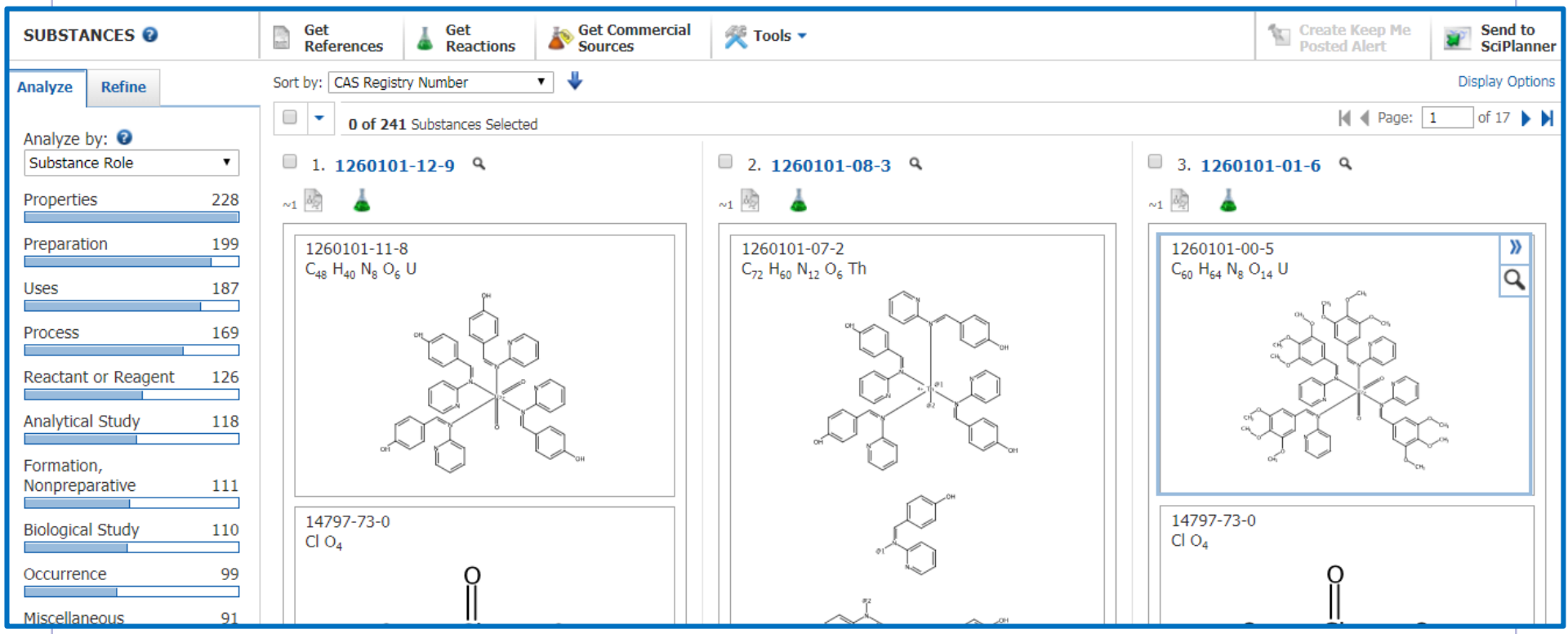
物质检索——理化性质检索：寻找电阻率大于125ohm的含铁物质



SciFinder物质检索结果



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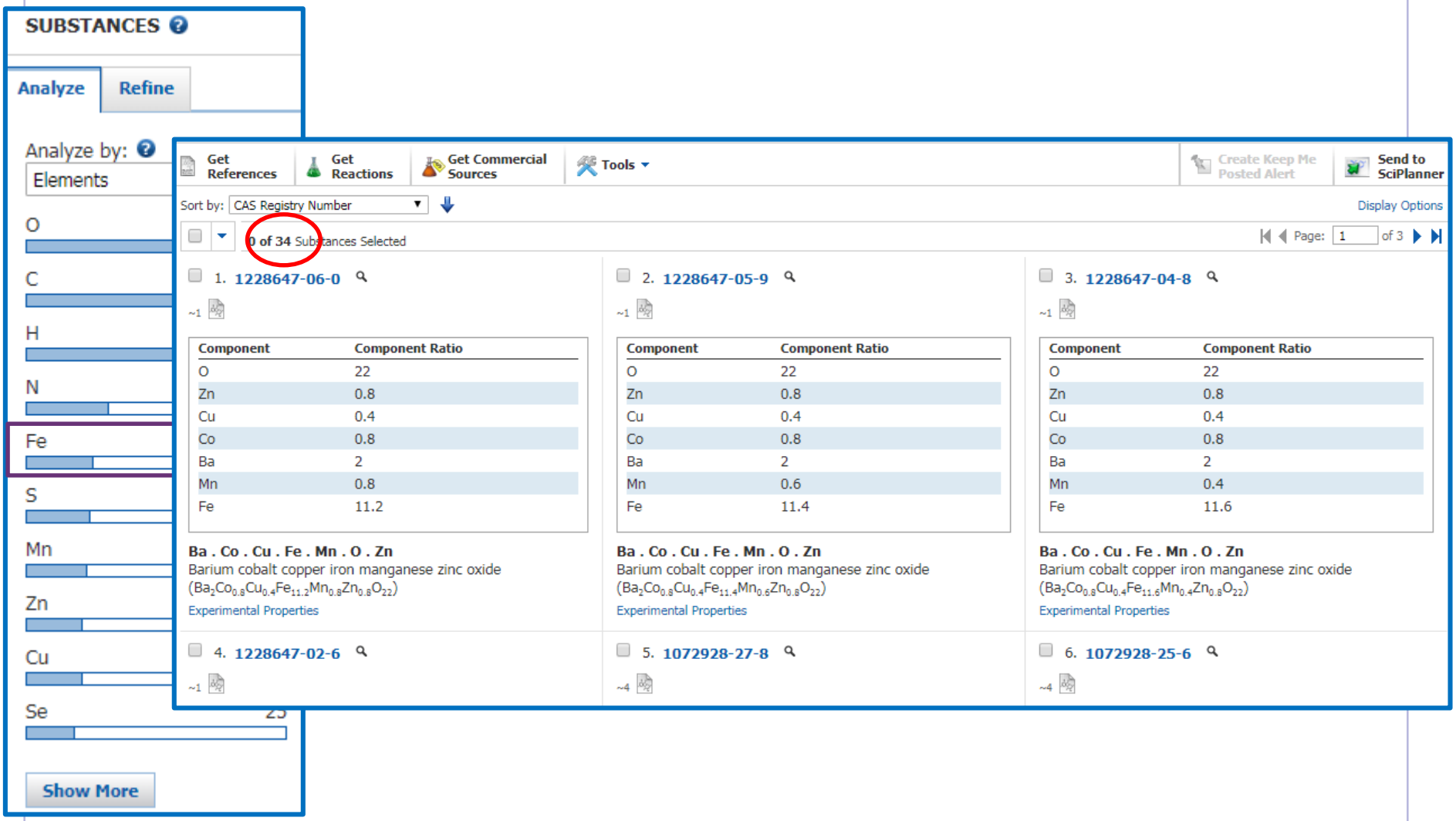
通过分析/限定工具筛选结果



SciFinder® A CAS SOLUTION

分子式检索


CAS Solutions
SciFinder
A CAS SOLUTION
Explore
Saved Searches
SciPlanner
REFERENCES
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier
REACTIONS
Reaction Structure
SUBSTANCES: MOLECULAR FORMULA
Examples:
H4SiO4
(C3H6O.C2H4O)x
Search

分子式书写规则—Hill 规则

- 单一组分物质：
  - 对于不含C的物质，按照字母顺序排序
  - 对于含C的物质，C、H写在前面，其他的按照字母顺序排列
  - 相邻的两个元素之间必须有区分号，即数字或者空格，倘若数字为1，那么可以用空格来区分
  - 区分大小写

- 多组分物质：
  - 每一组分必须遵照单一组分物质的分子式来书写。
  - 不同组分之间的排序按照各组分的首元素的字母顺序排序，但是含C组分的一定排在不含C的组分前面。用点将不同的组分分开
  - 倘若不同组分的首元素相同，则看元素数量多少，数量多的排在前面，若元素数量一样，则按次元素的顺序排列。

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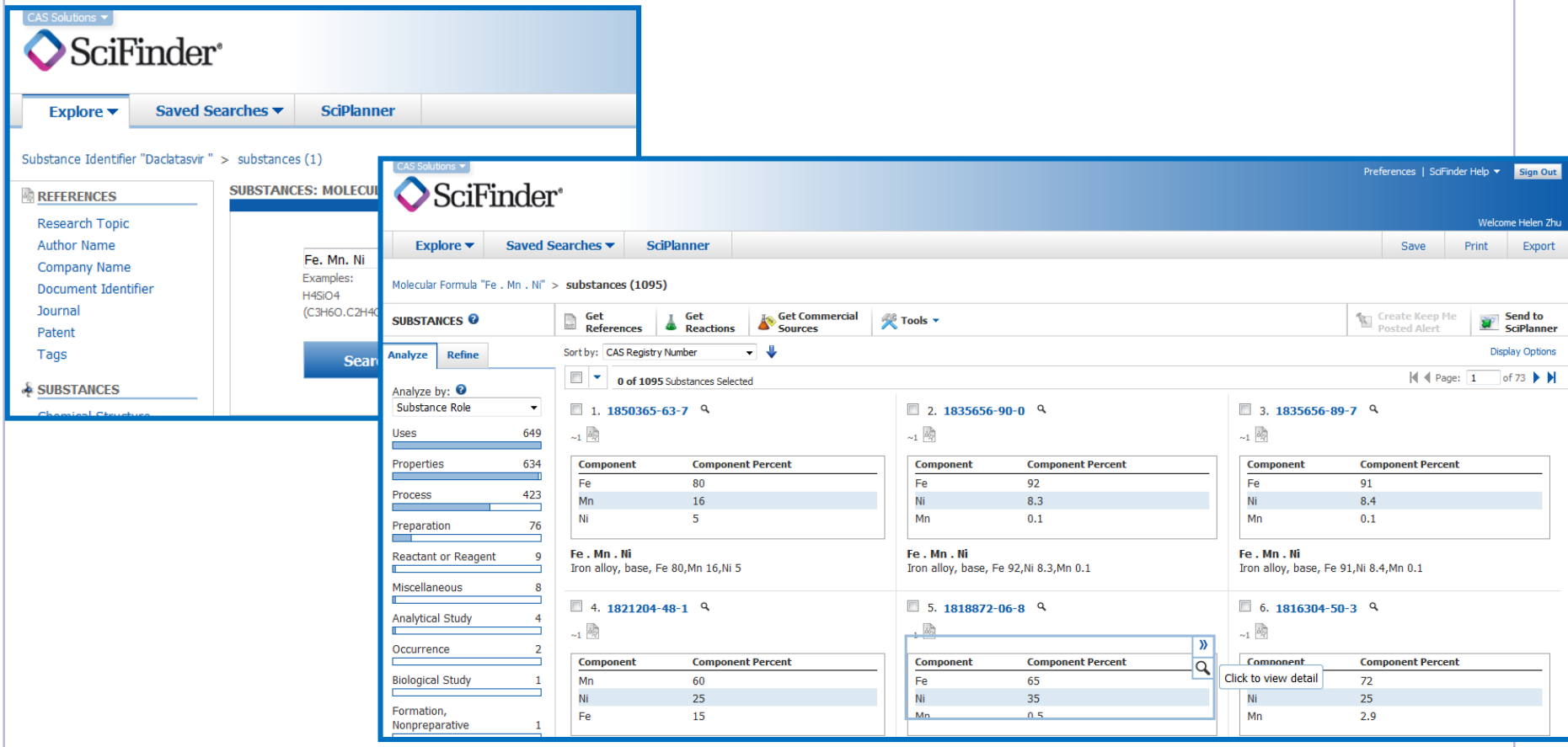
合金的检索

检索铁、锰、镍合金



合金物质以列表形式呈现

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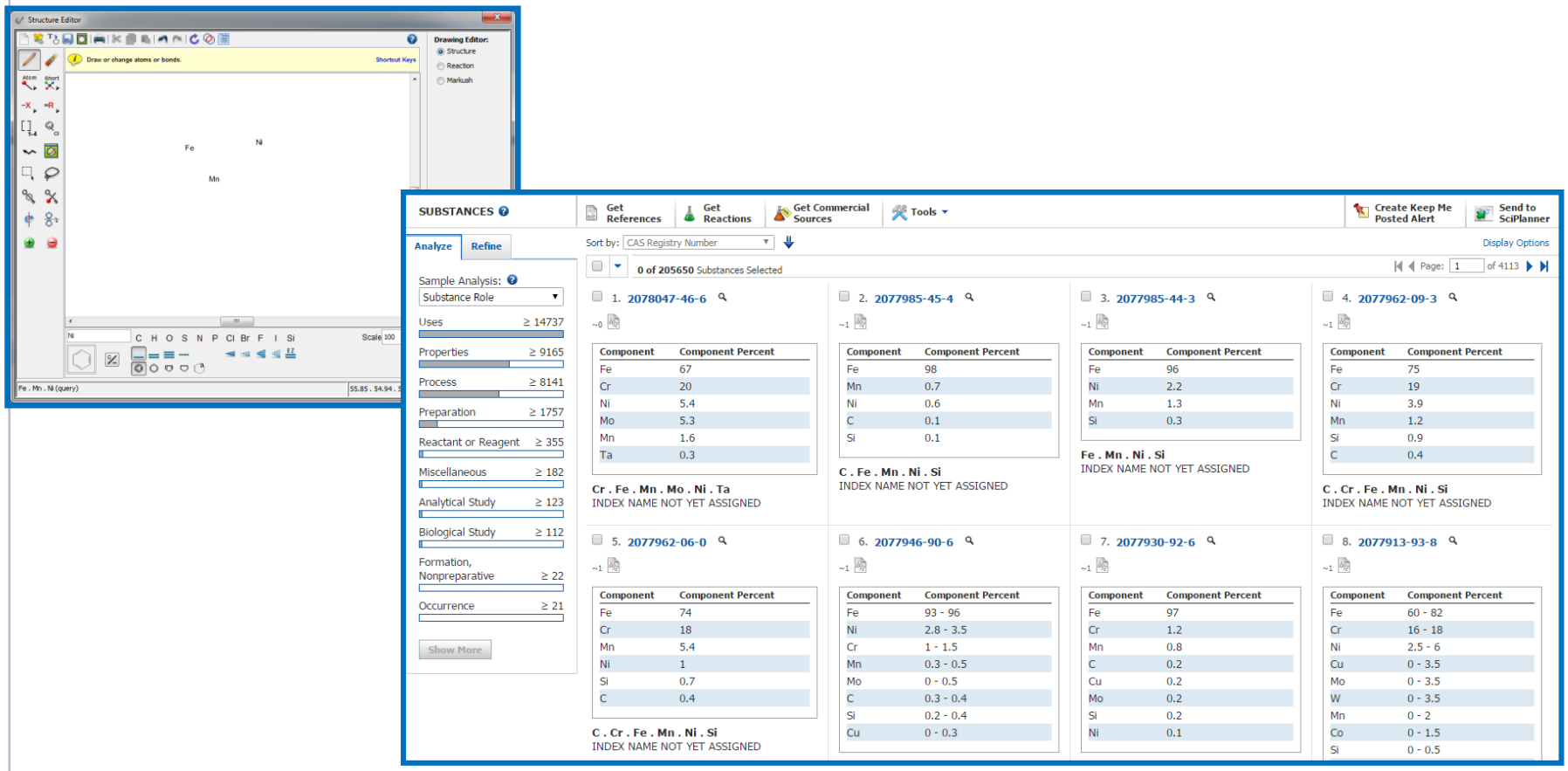
合金的检索

检索参杂铁、锰、镍原子的合金



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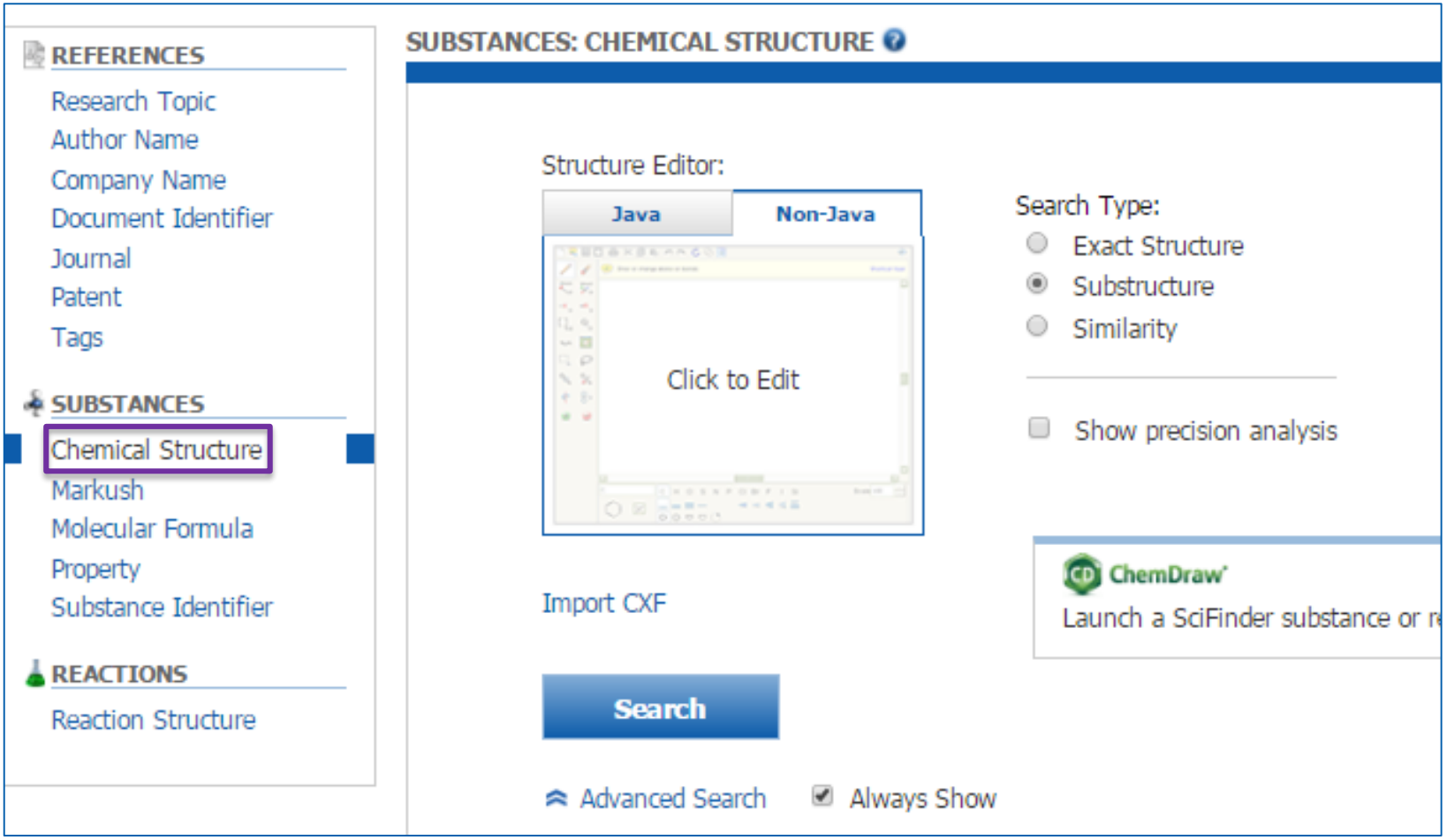
物质检索——结构



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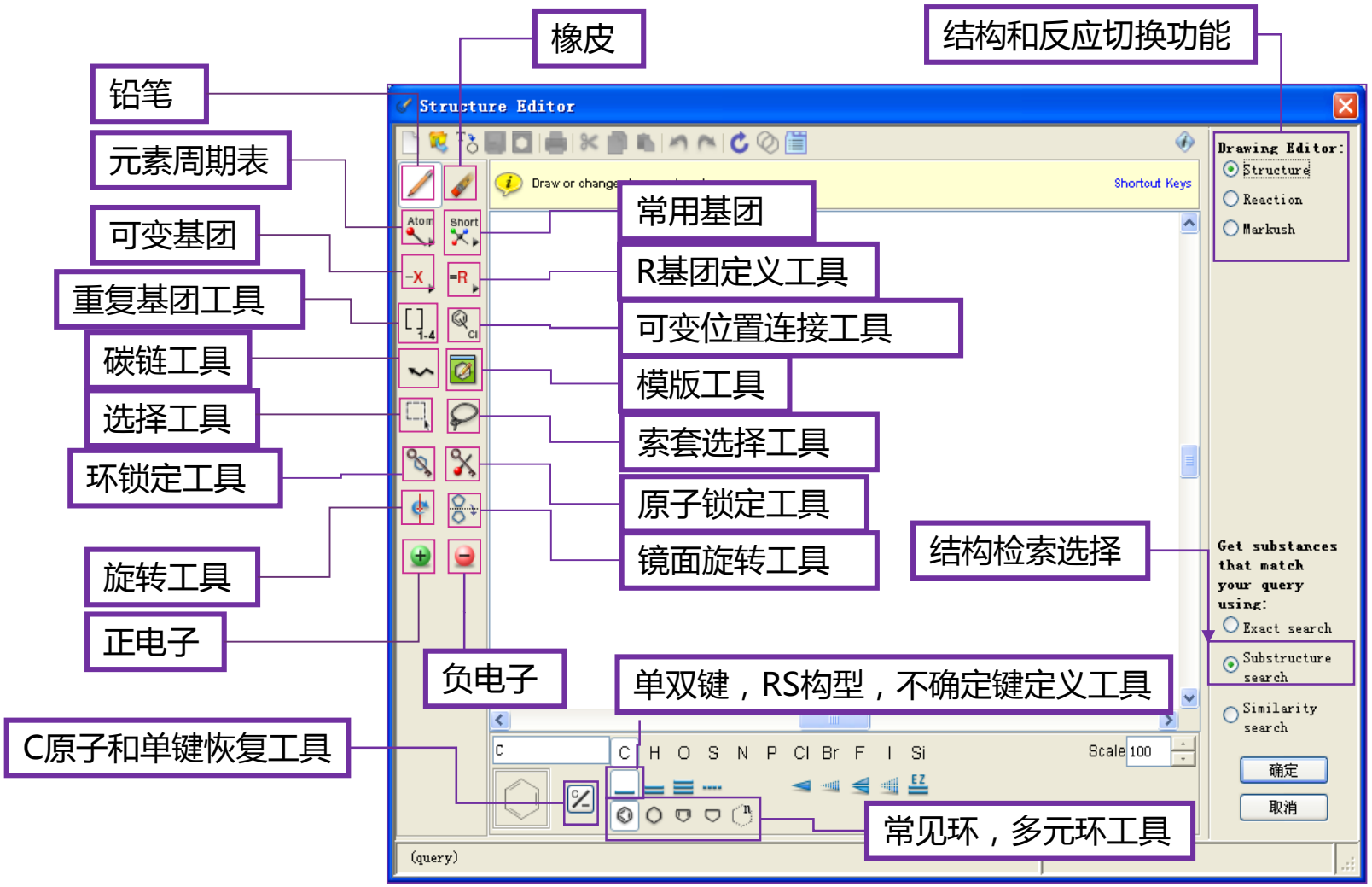
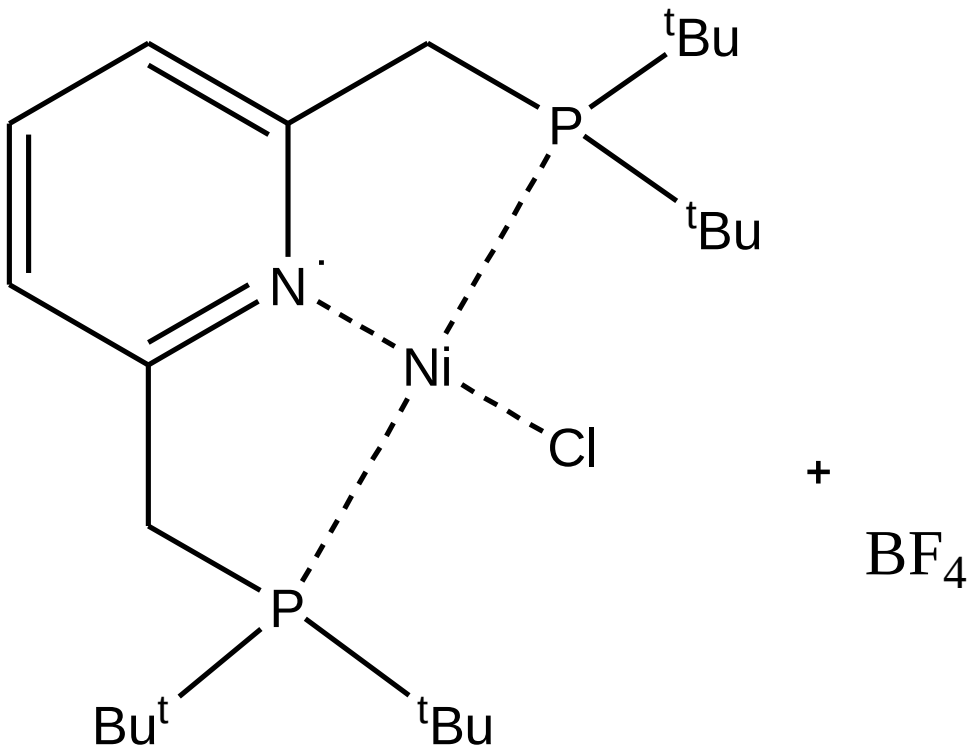
物质检索——结构


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
常用基团
R基团定义工具
可变位置连接工具
模版工具
索套选择工具
原子锁定工具
镜面旋转工具
结构检索选择
负电子
单双键，RS构型，不确定键定义工具
常见环，多元环工具
Structure Editor
Drawing Editor:
Structure
Reaction
Markush
Shortcut Keys
Get substances that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
(query)

物质检索——精确结构检索

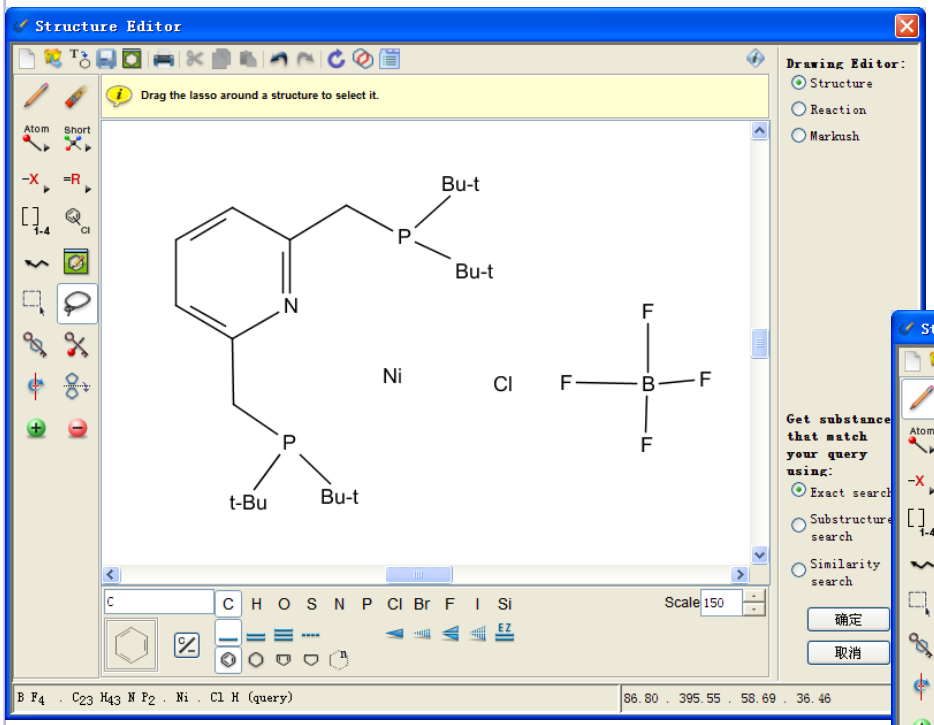


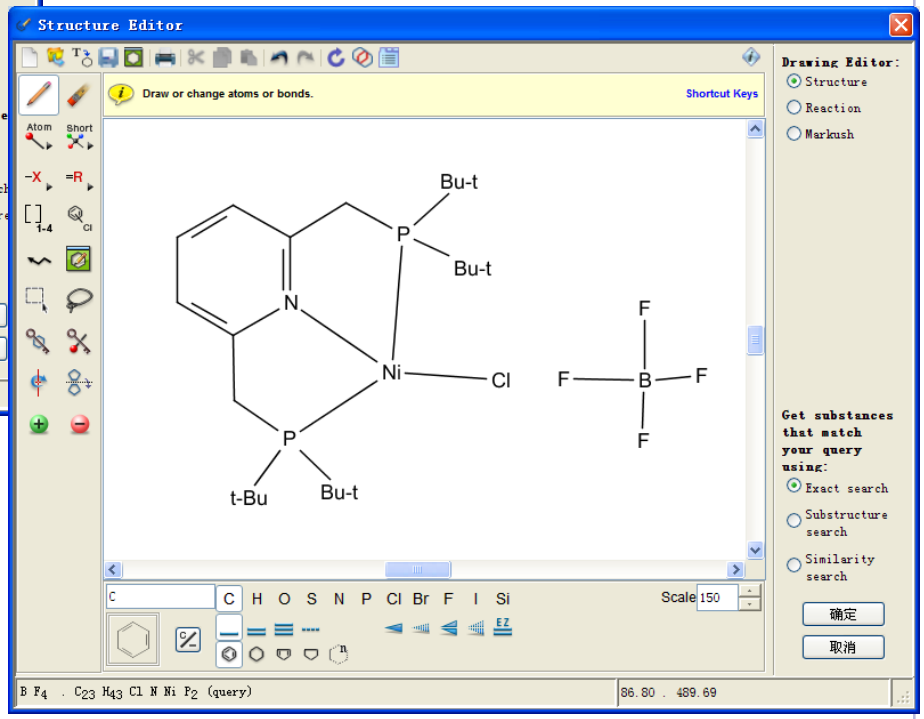
+ BF_4

该结构中包含：

配体
金属
阳离子
阴离子

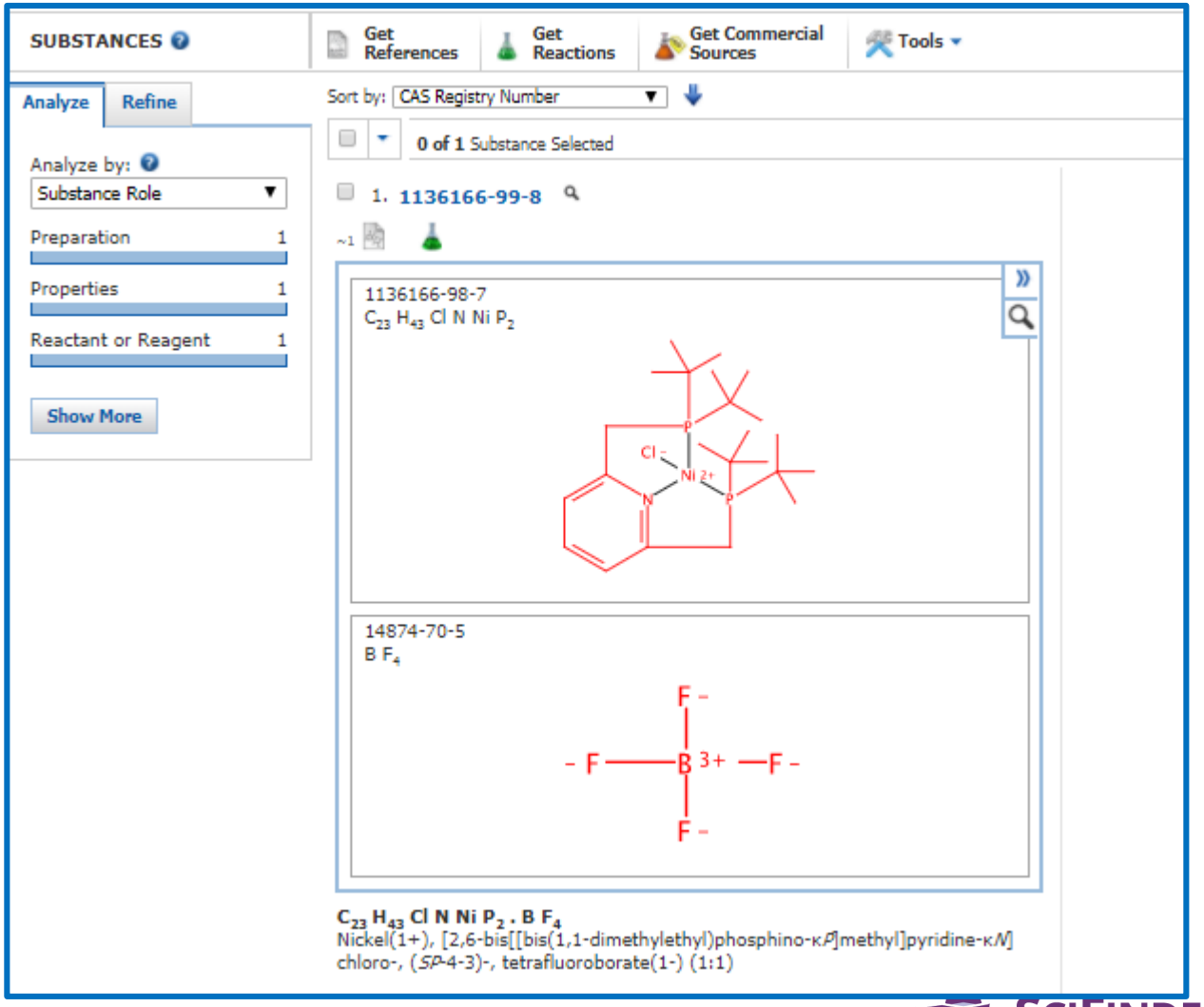
物质检索——精确结构检索





任何一种结构,使用精确结构都可以检索到

精确结构检索结果

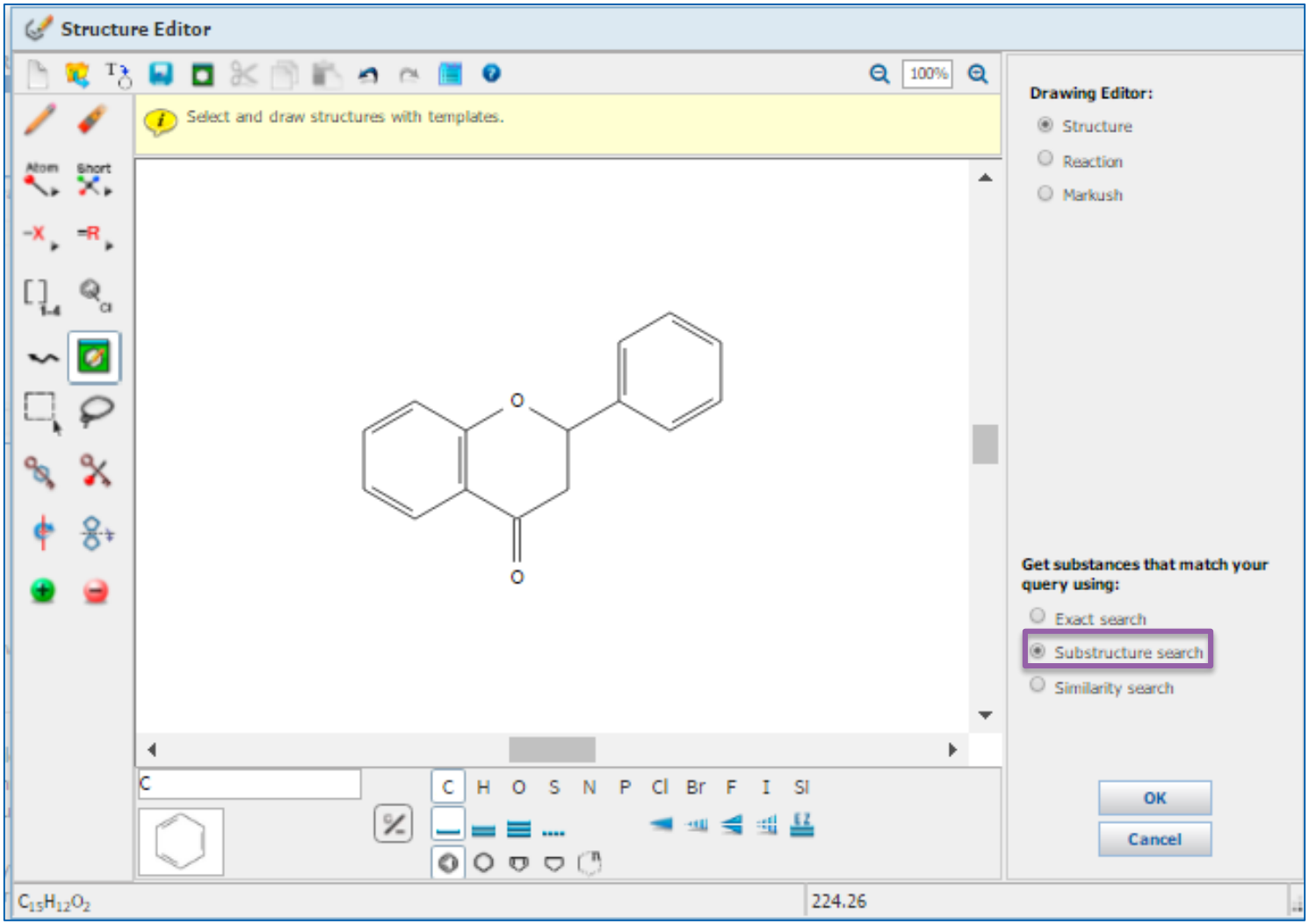

SUBSTANCES
Get References
Get Reactions
Get Commercial Sources
Tools
Analyze
Refine
Sort by: CAS Registry Number
Analyze by:
Substance Role
Preparation 1
Properties 1
Reactant or Reagent 1
Show More
0 of 1 Substance Selected
1. 1136166-99-8
1136166-98-7
$C_{23}H_{43}ClNNiP_2$
14874-70-5
BF_4
$C_{23}H_{43}ClNNiP_2 . BF_4$
Nickel(1+), [2,6-bis[[bis(1,1-dimethylethyl)phosphino-κP]methyl]pyridine-κN]chloro-, (SP-4-3)-, tetrafluoroborate(1-) (1:1)

物质检索——精确结构检索

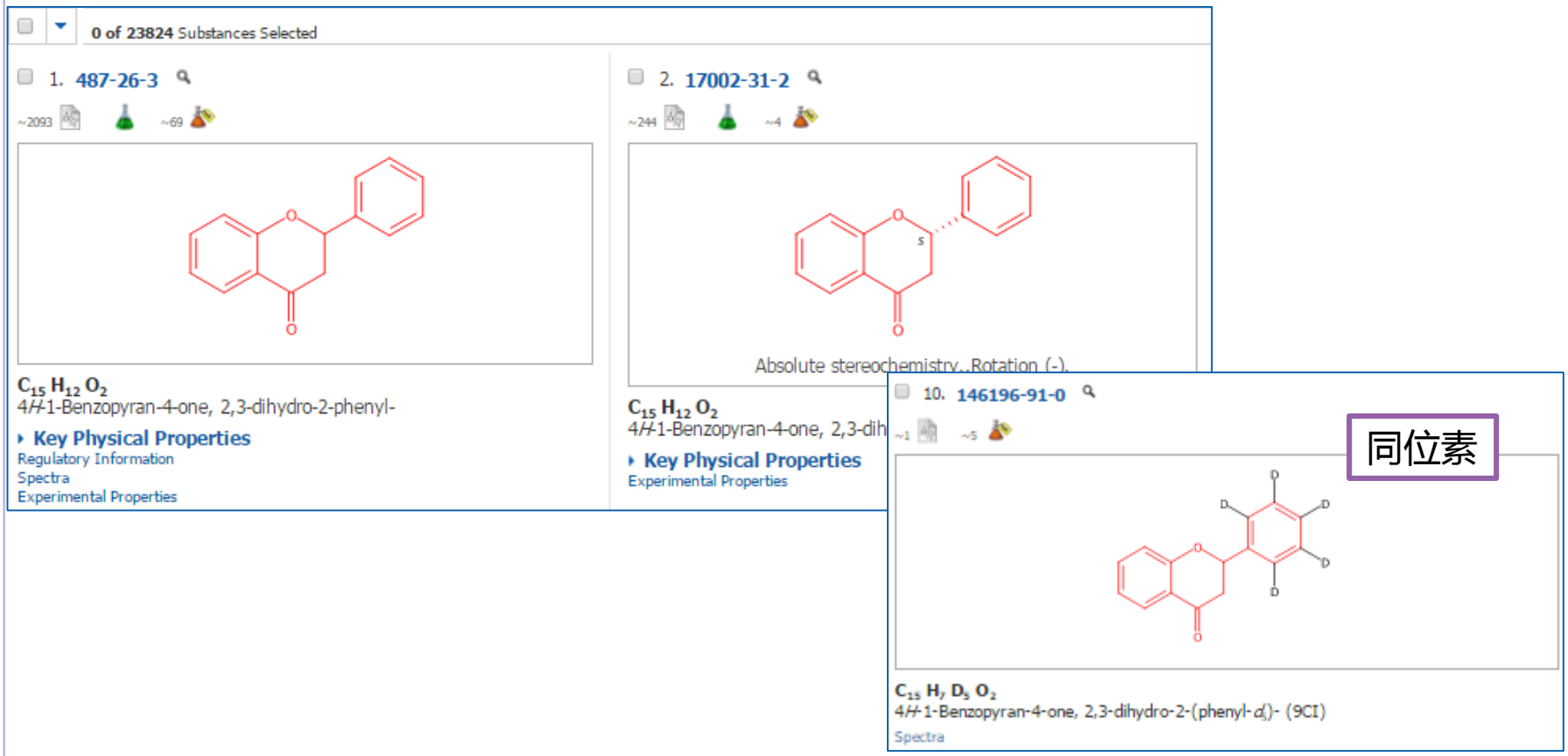
- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索


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

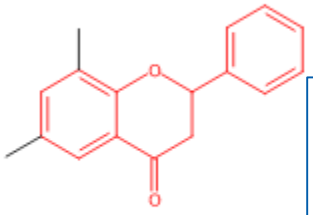
物质检索——亚结构检索


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

亚结构检索结果

281. 123251-10-5

取代物

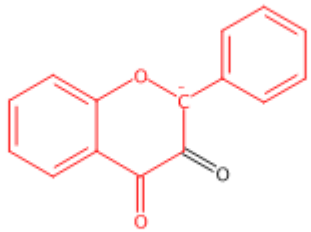


$C_{17}H_{16}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl

Key Physical Properties
Experimental Properties

295. 780723-19-5

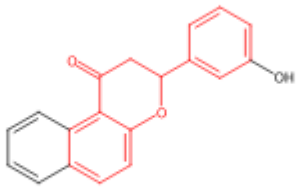
离子



$C_{15}H_9O_3$
2*H*-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

284. 136116-23-9

稠环物质

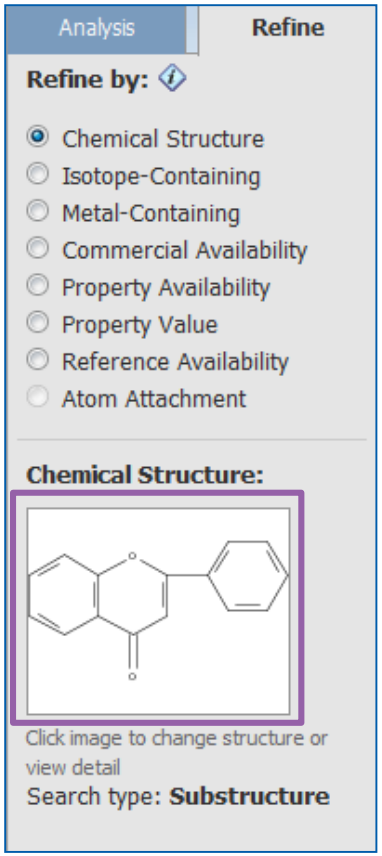


$C_{19}H_{14}O_3$
1*H*-Naphtho[2,1-*b*]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

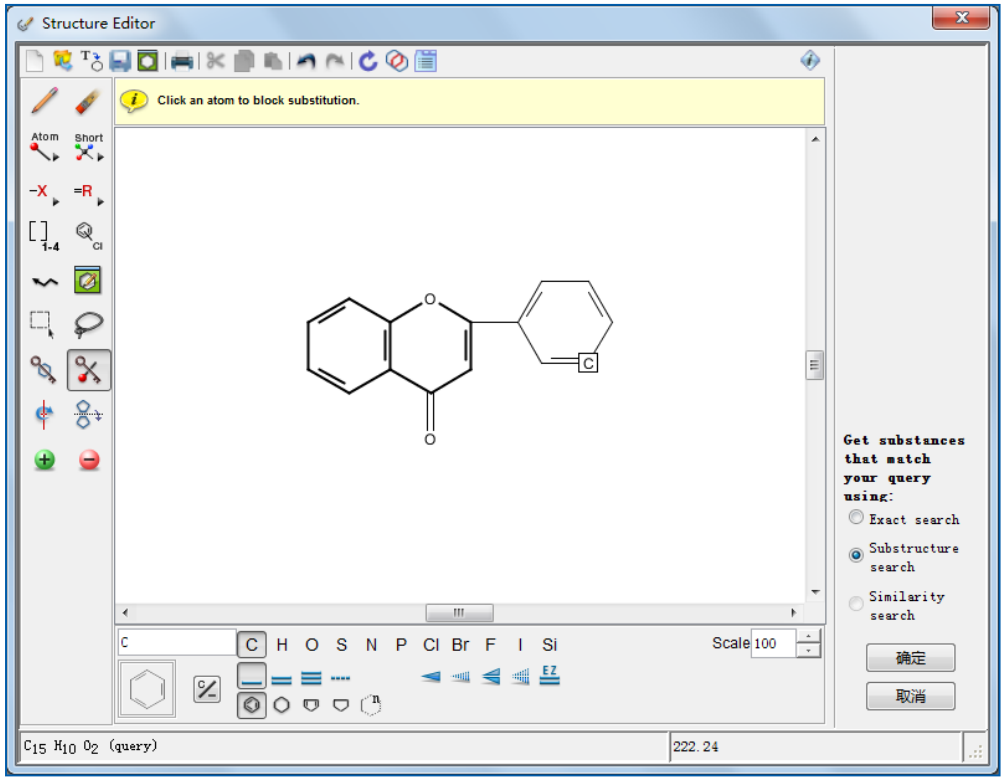
Key Physical Properties

SciFinder® A CAS SOLUTION

亚结构检索结果的限定



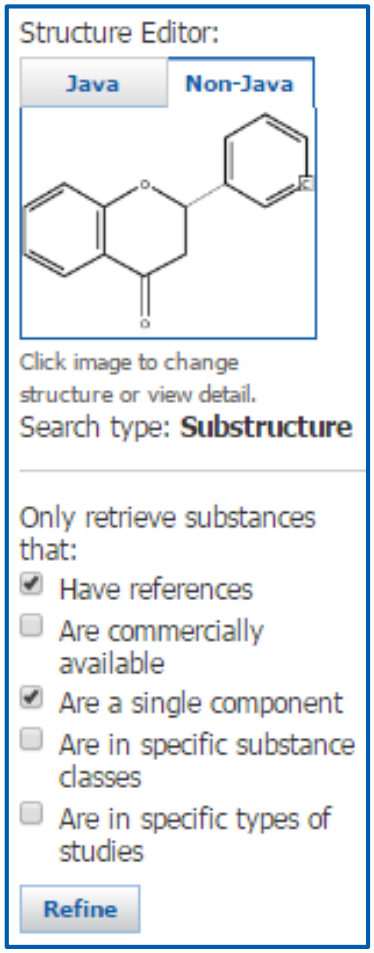
化学结构的再次限定

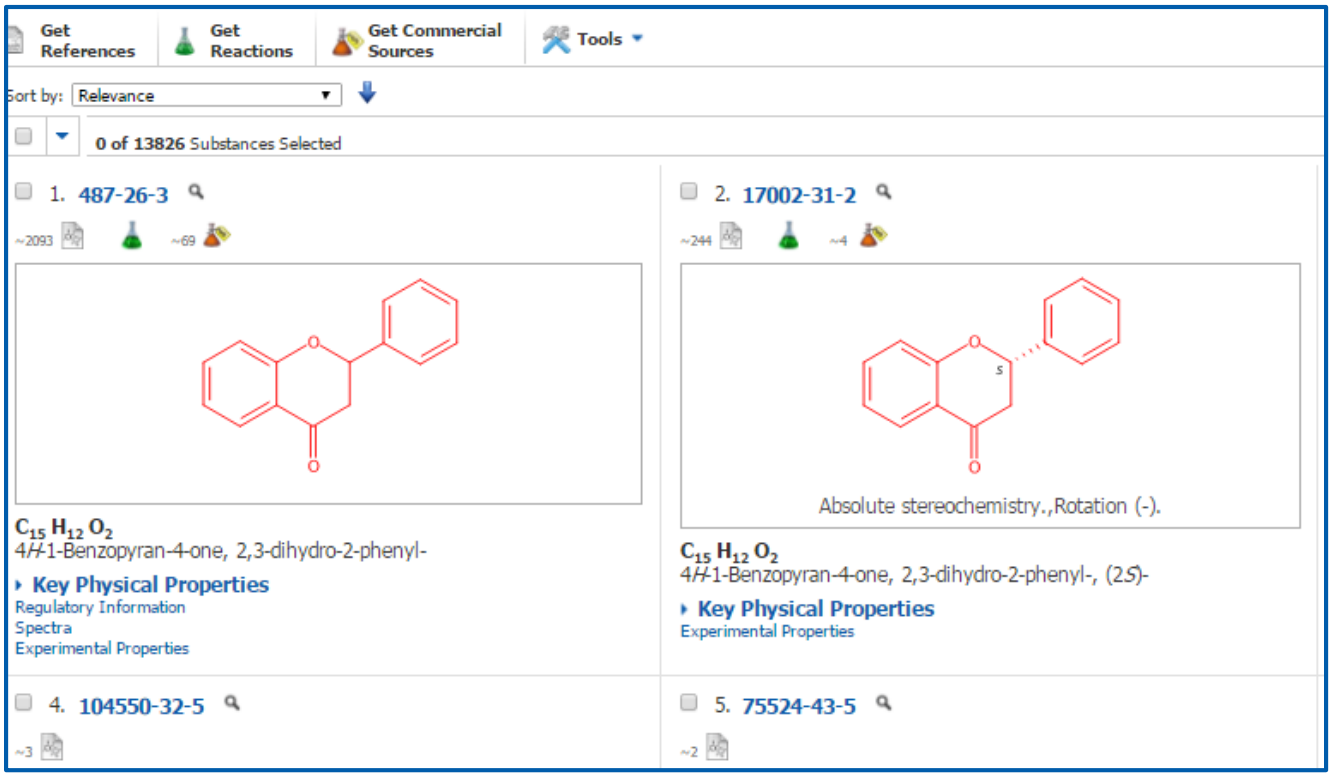


环锁定

原子锁定

亚结构检索结果的限定





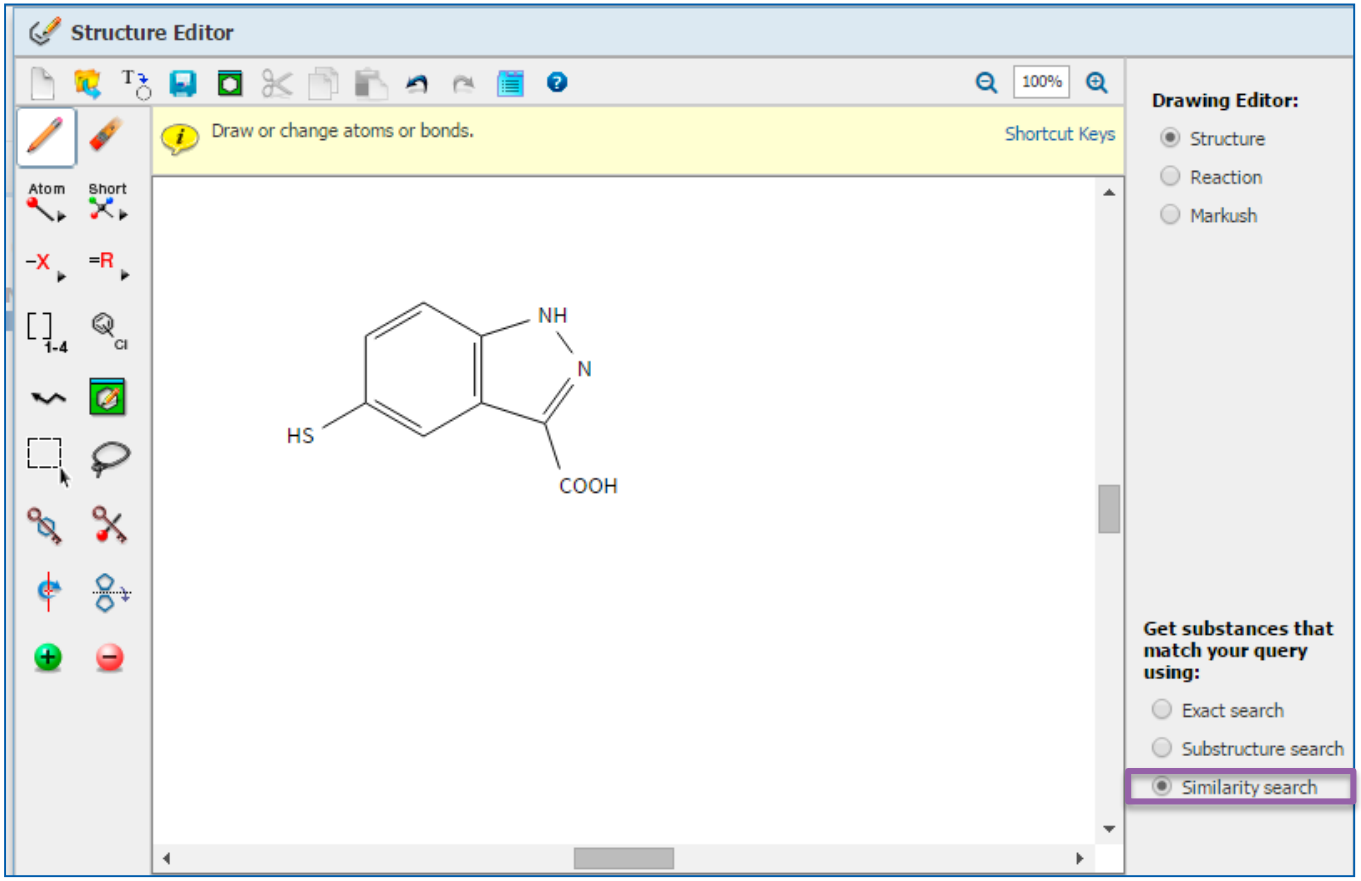
SciFinder® A CAS SOLUTION

物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索——相似结构检索


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

相似结构检索结果

Select All Deselect All

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

Get Substances

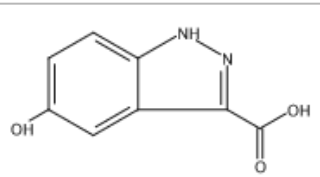
评分越高，相似度越高，结构越相似

Score: 88

1. **885518-94-5**

~1 ~35

取代基变化



$C_8H_6N_2O_3$

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

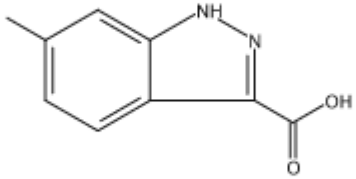
Key Physical Properties

Score: 86

5. **858227-12-0**

~7 ~41

取代基位置变化



$C_9H_8N_2O_2$

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

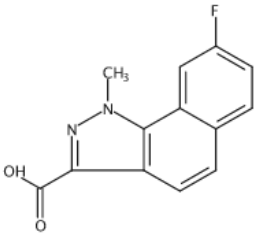
Key Physical Properties

Score: 65

541. **1100422-**

~1

母体结构变化



$C_{13}H_9FN_2O_2$

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

Key Physical Properties

SciFinder® A CAS SOLUTION

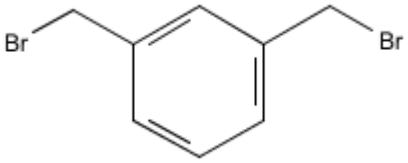
物质检索——相似结构检索

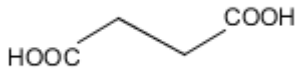
- 相似结构检索：

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

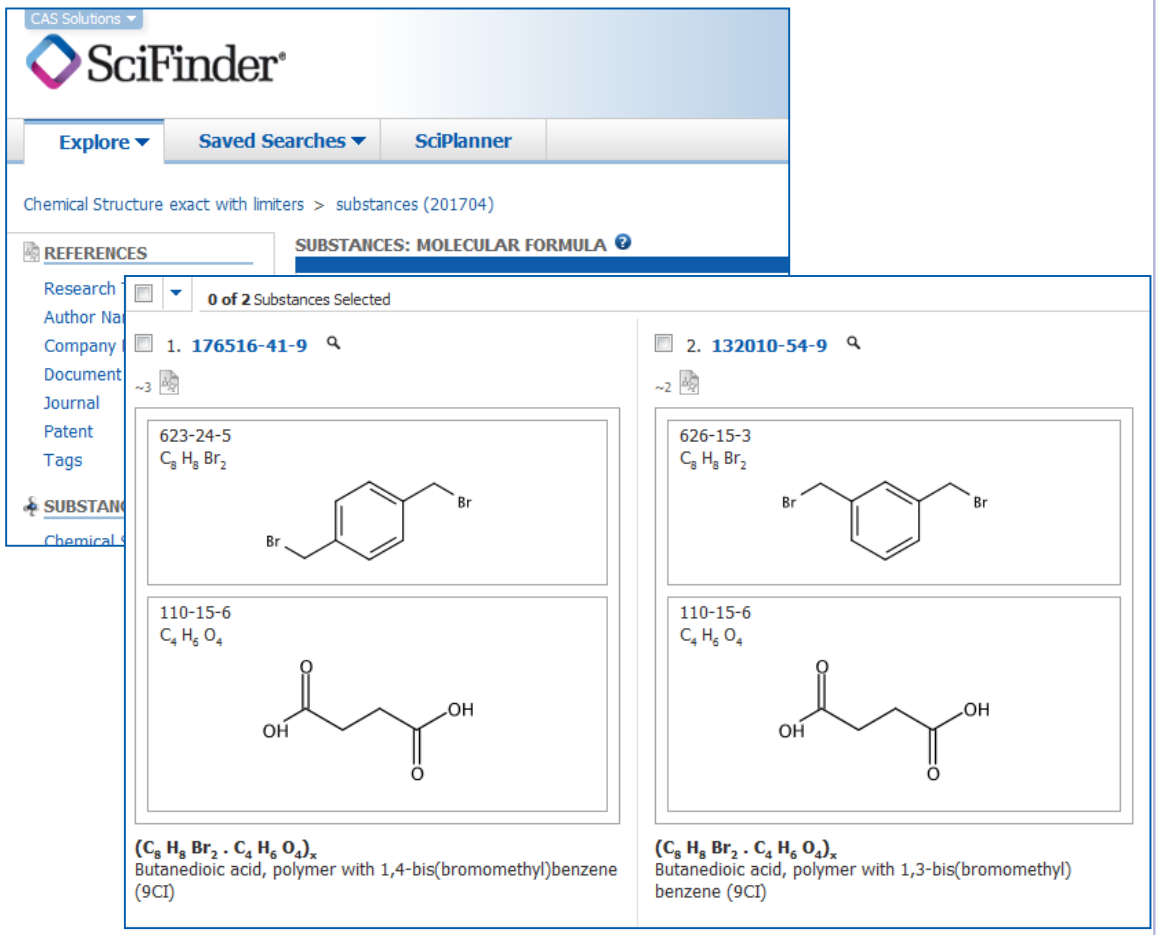
聚合物的检索

已知起始原料的聚合物





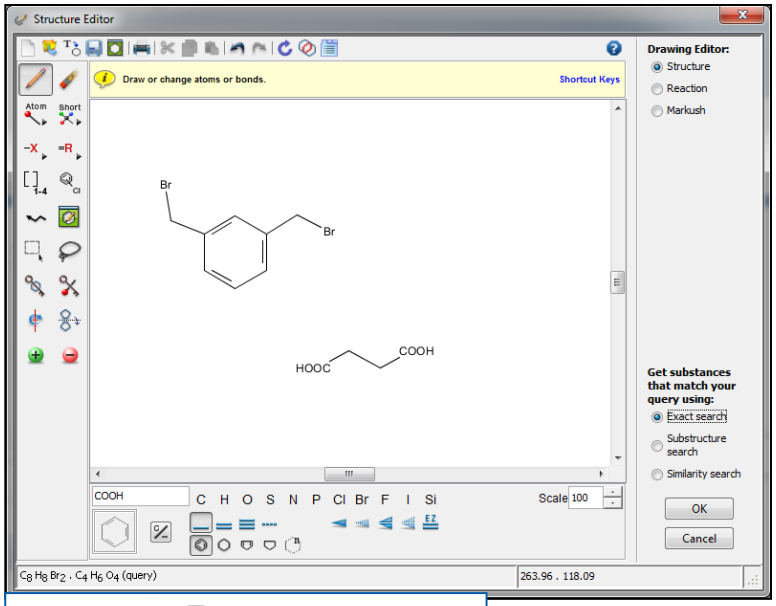
（C8 H8 Br2 . C4 H6 O4）x

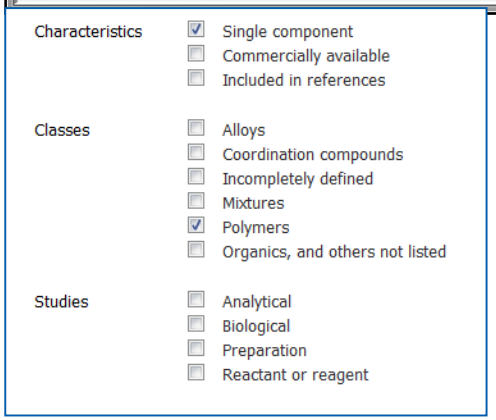


分子式检索后会得到同分异构体

SCIFINDER® A CAS SOLUTION

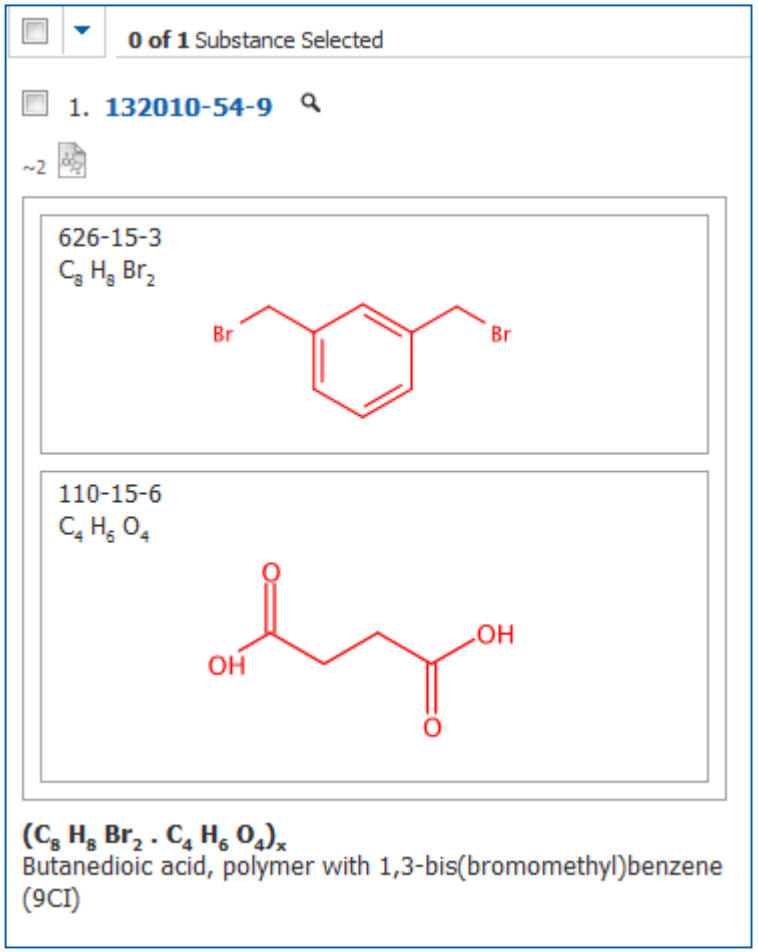
聚合物的检索





单一组分

聚合物



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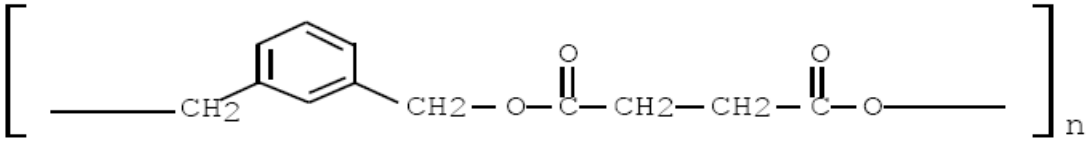
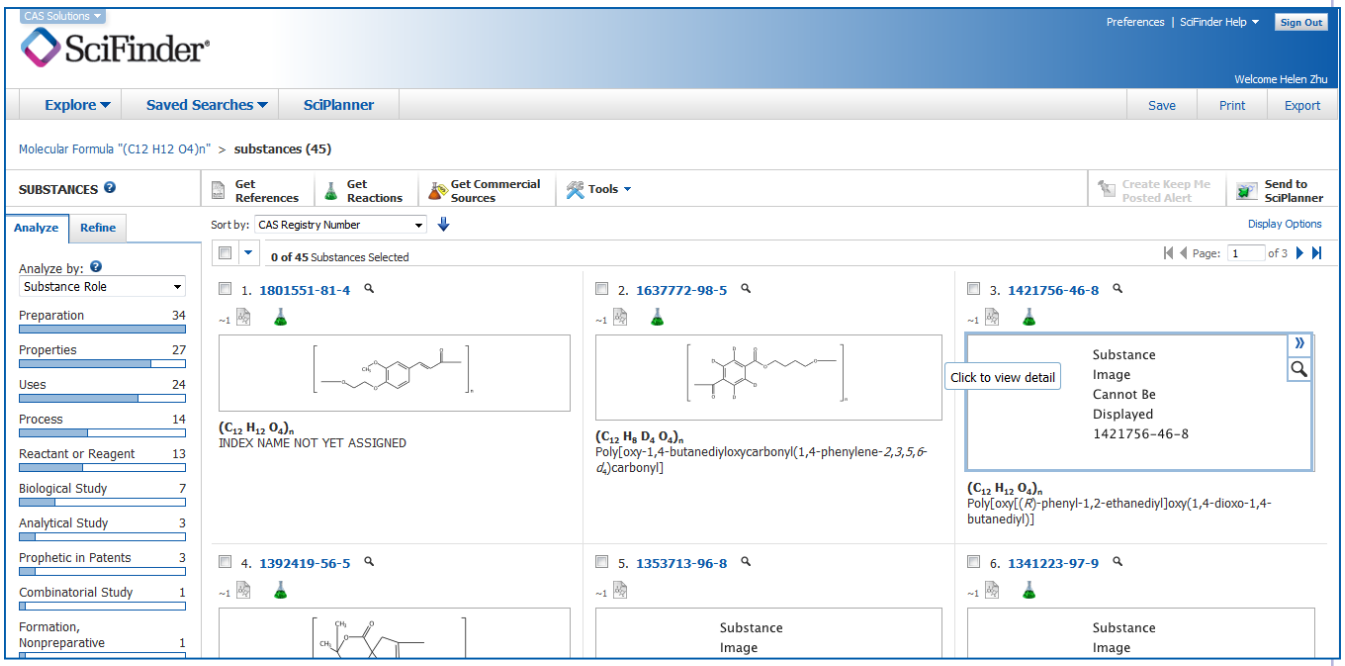
聚合物的检索

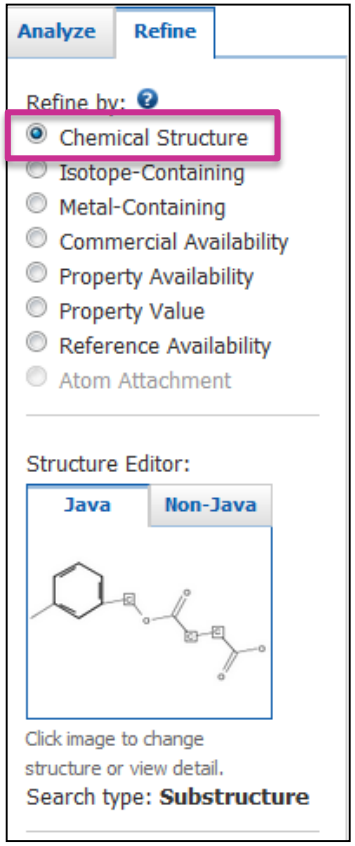
已知重复单元的聚合物

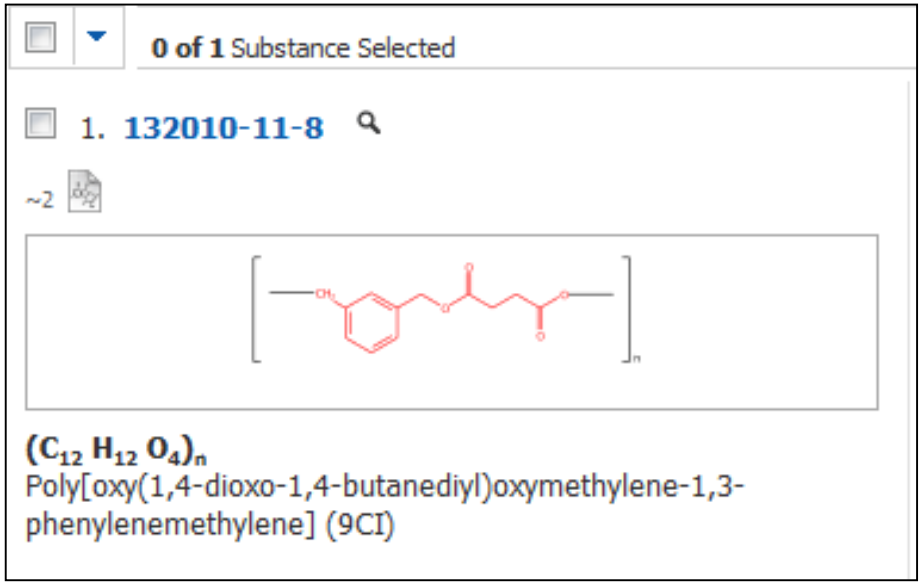


(C12 H12 O4)n



聚合物的检索

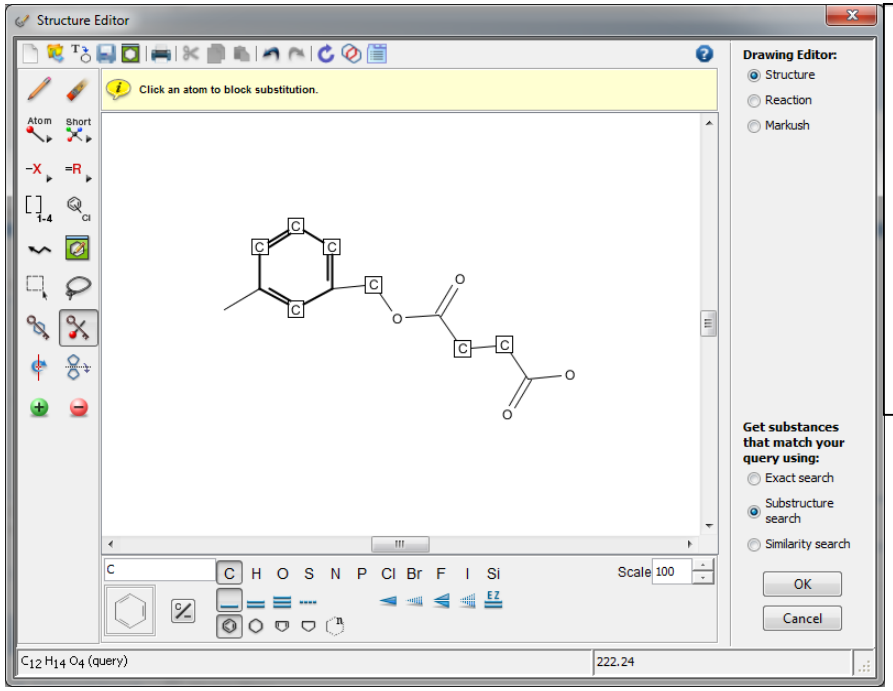




利用结构特征进行Refine，迅速查找需要的物质

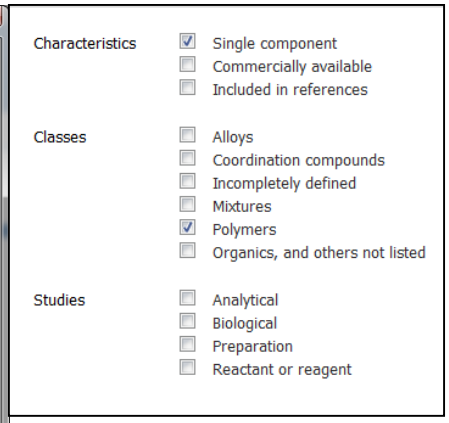
SciFinder® A CAS SOLUTION

聚合物检索



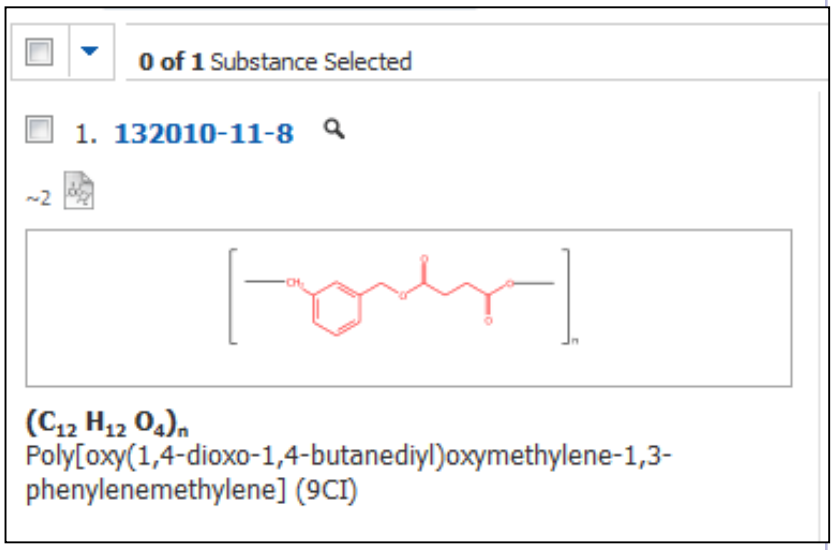
绘制好SRU后用亚结构检索

因为两段为开放状态



单一组分

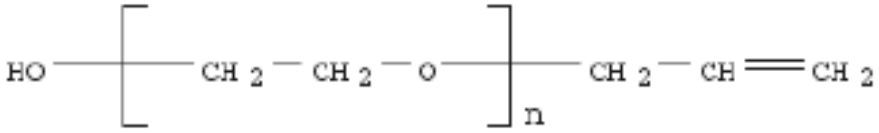
聚合物

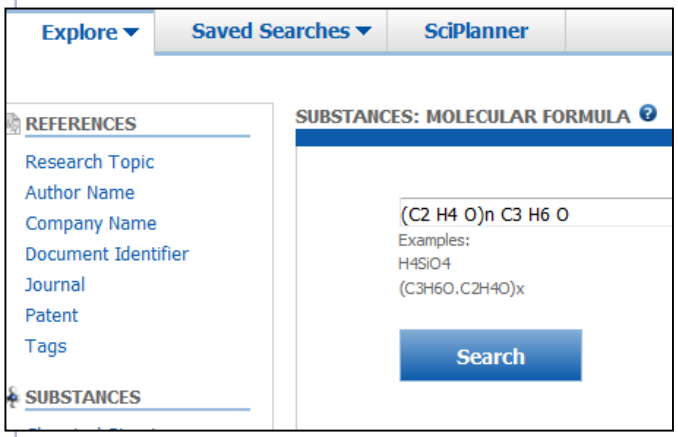


SciFinder® A CAS SOLUTION

聚合物的检索

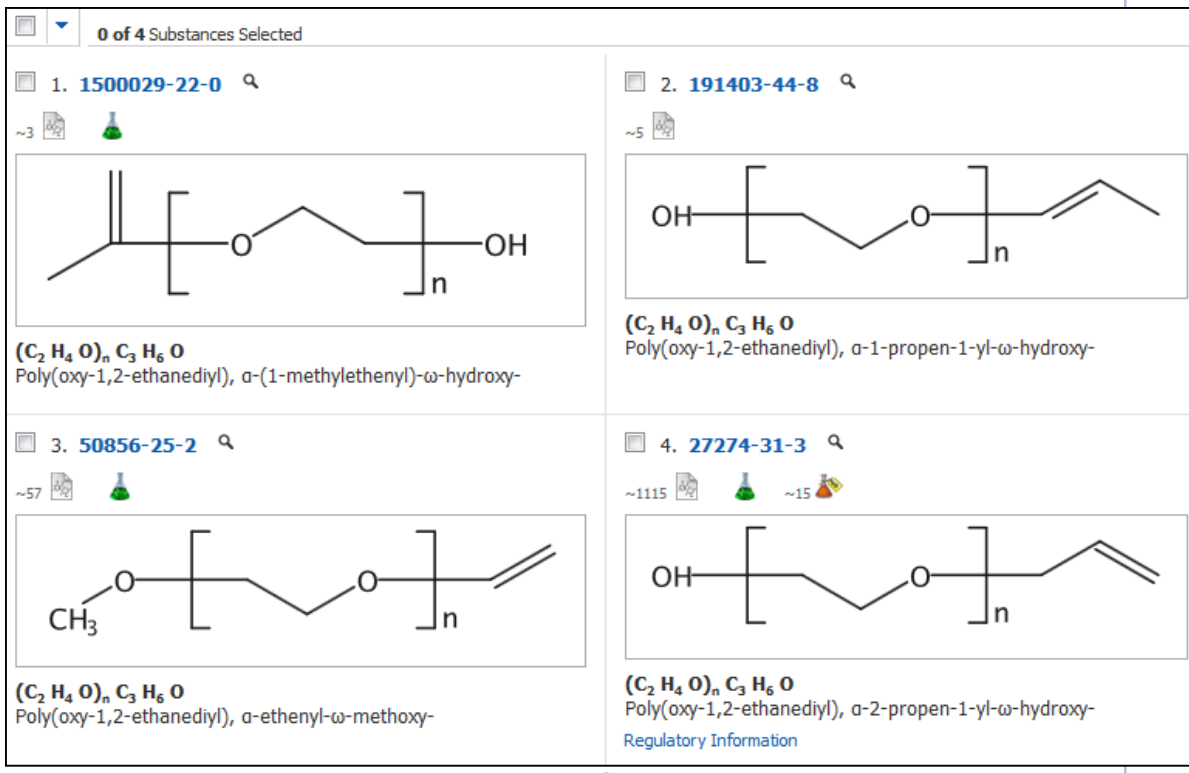
含端基和SRUs的聚合物





(C2 H4 O)n C3 H6 O

SRU部分　　两端部分



SciFinder® A CAS SOLUTION

提纲

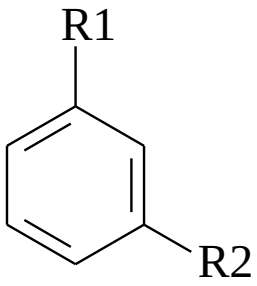
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索（PatentPak）
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow Analysis
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

Markush检索

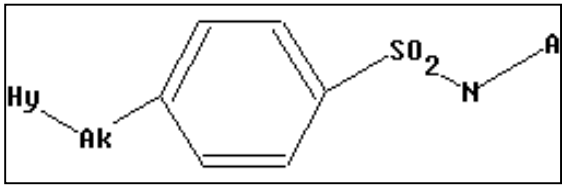
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 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

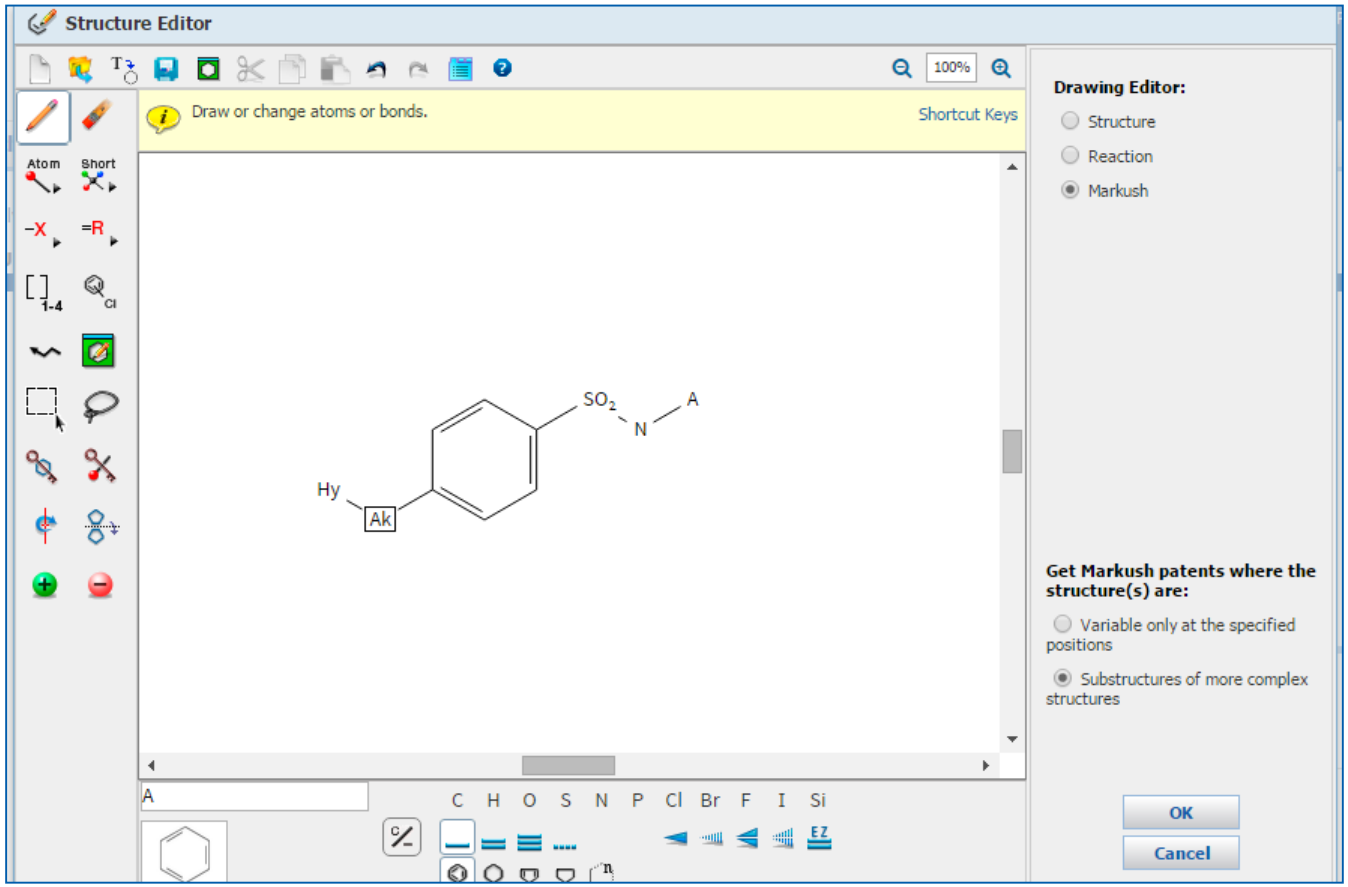


R1 = H, Br, Cl, I

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

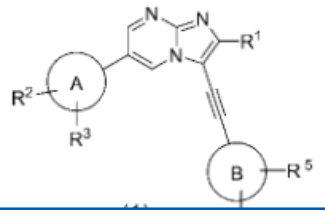
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

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

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 Analysis
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

SciFinder检索选项——反应检索

- 反应检索方法

  结构式

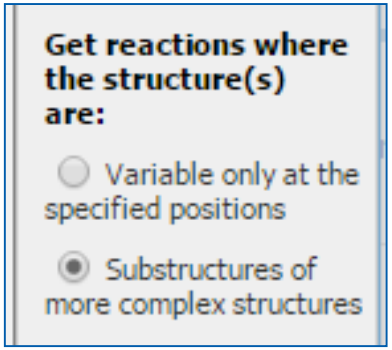
- 常用获取方法

  已知物质：由物质获取反应

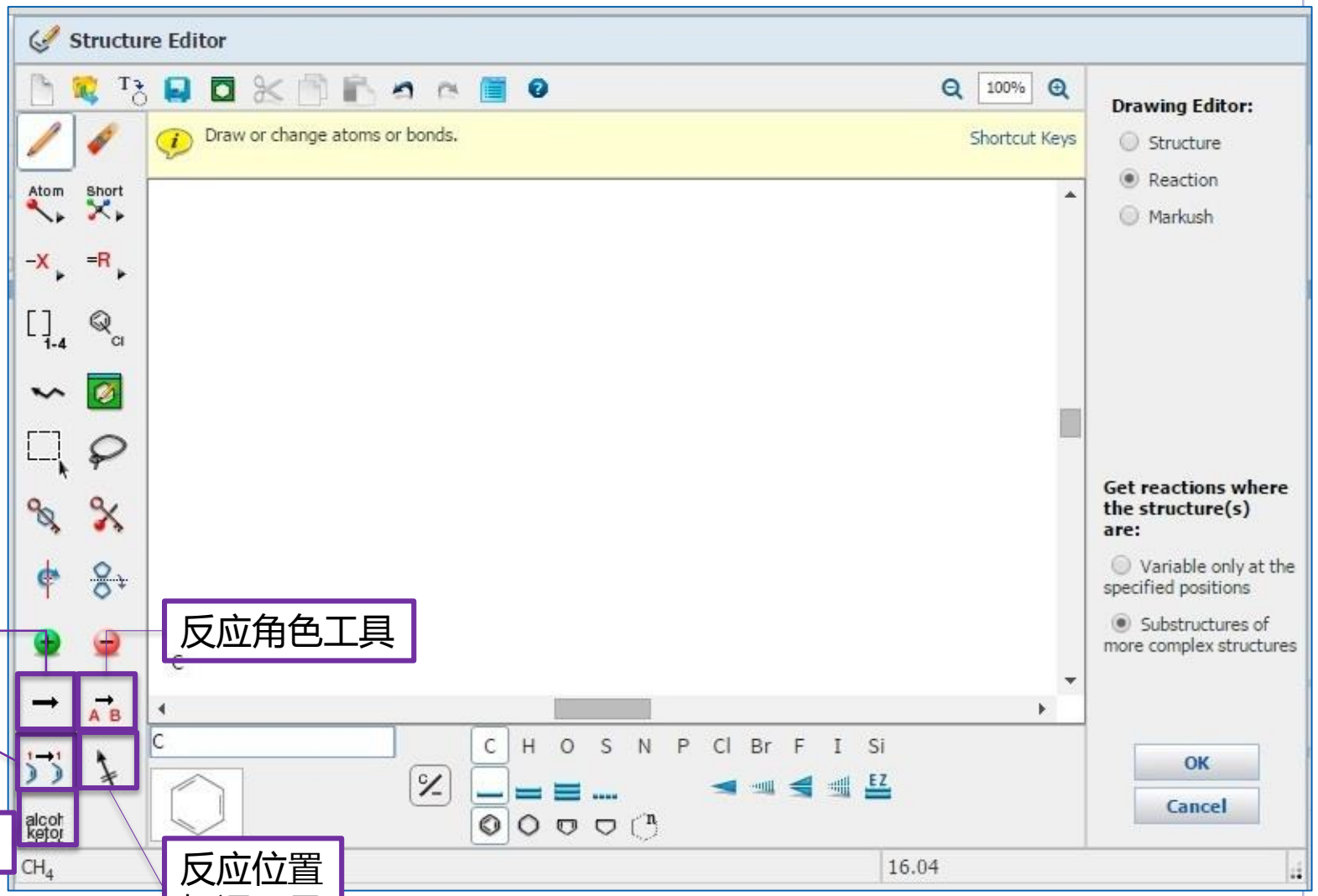
  已知文献：从文献中获取反应

  精确结构反应检索

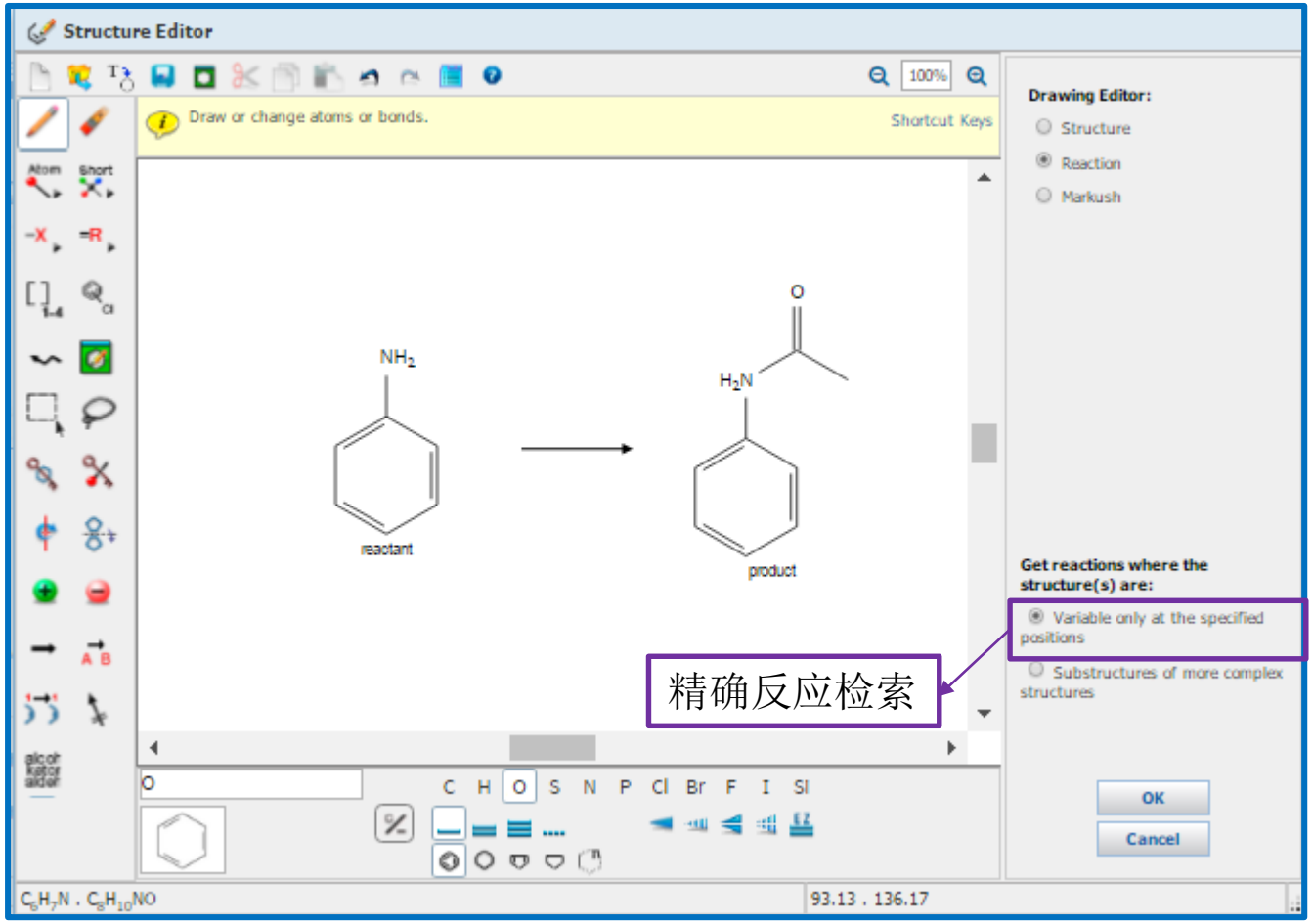
  亚结构反应检索



反应绘制工具

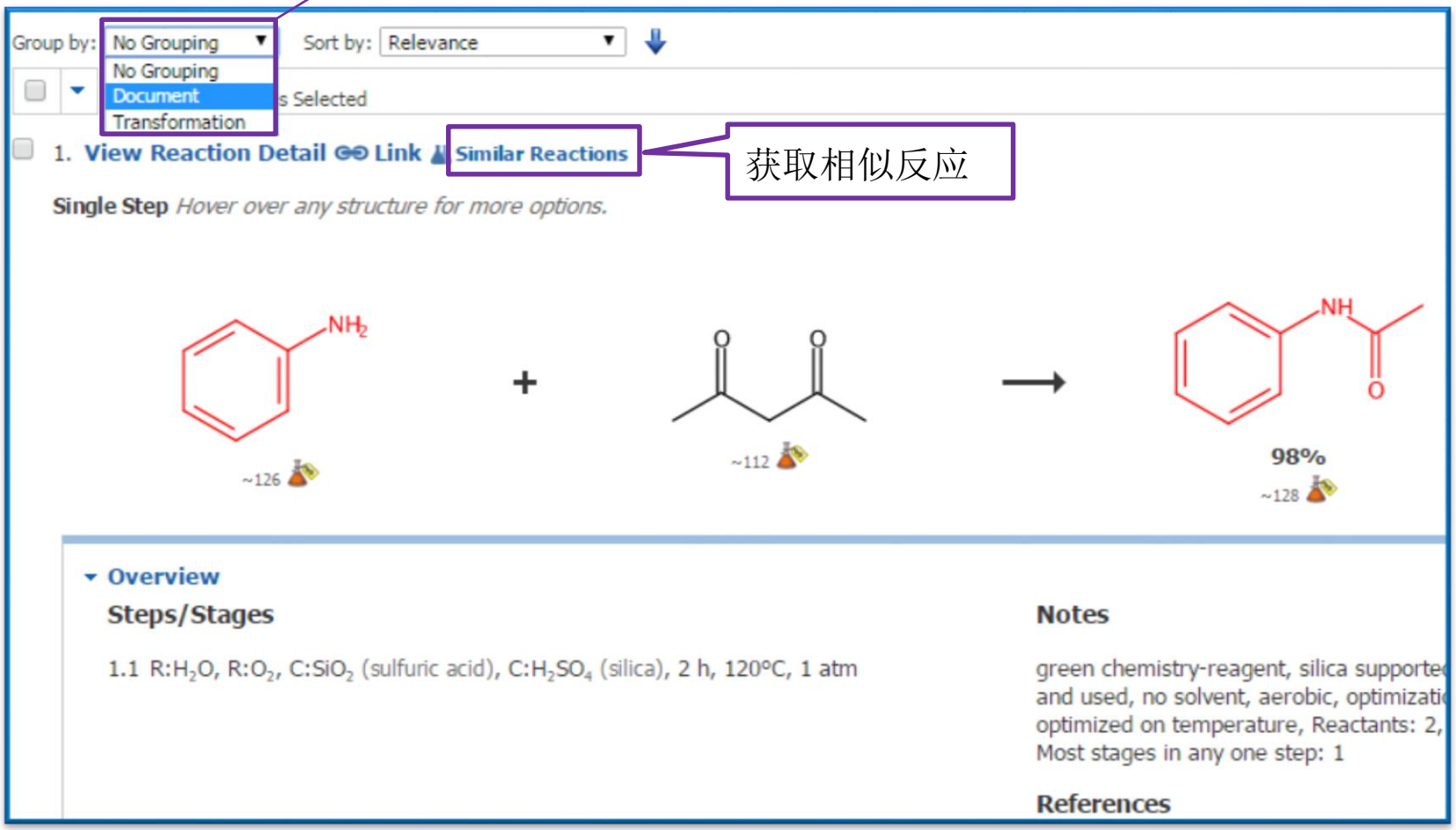

Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
C H O S N P Cl Br F I Si
CH4
16.04
反应箭头
反应角色工具
反应原子标记工具
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

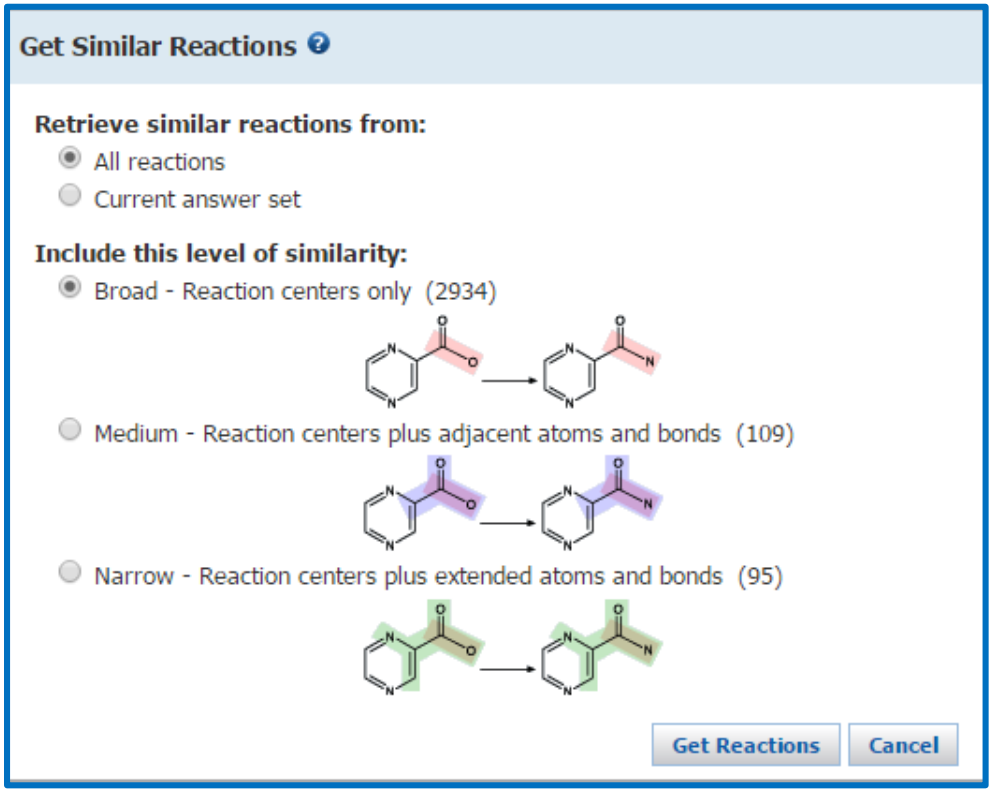
浏览记录，发现很多反应来自同一篇文献，通过Group by Document合并。



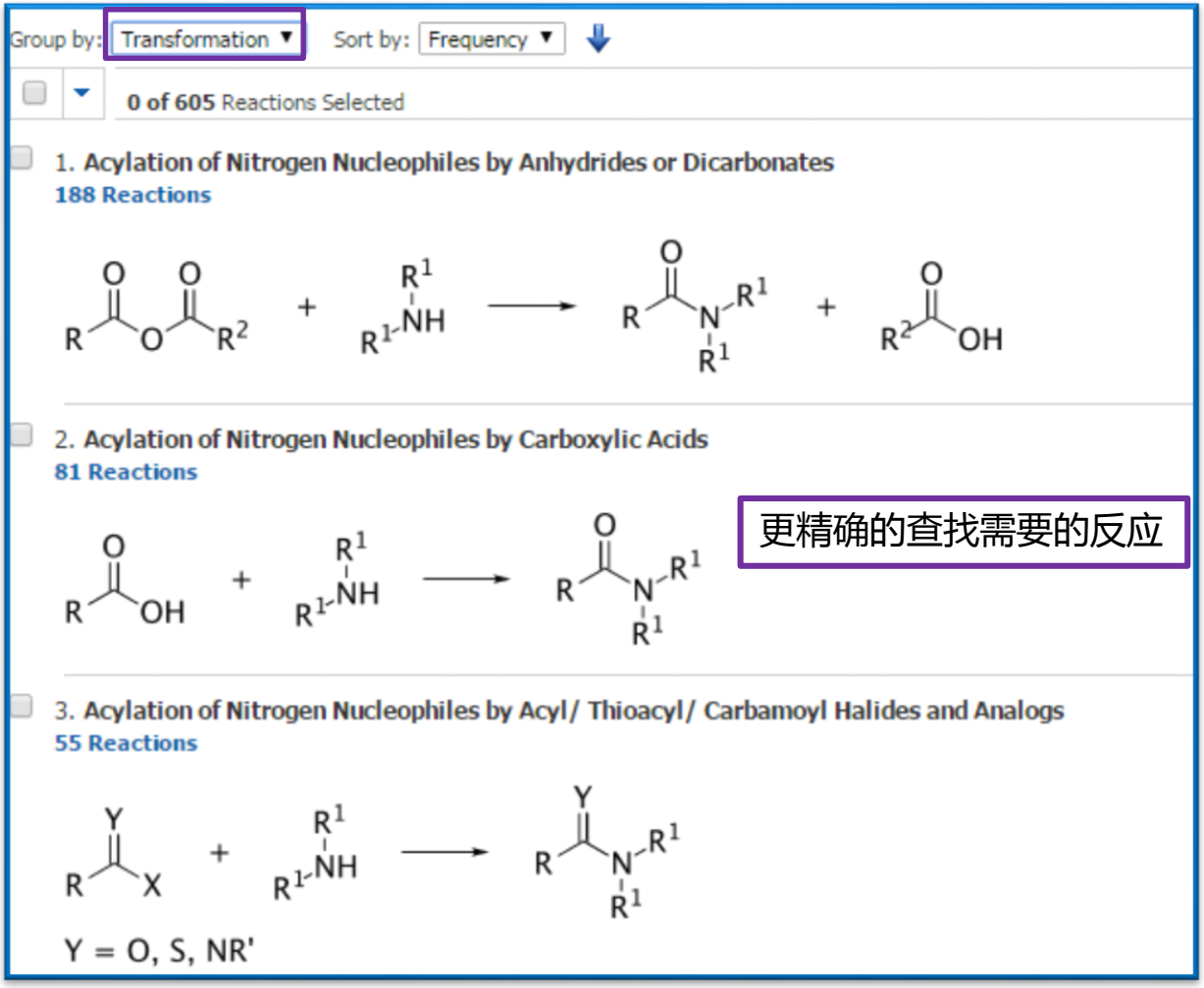
获取相似反应

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

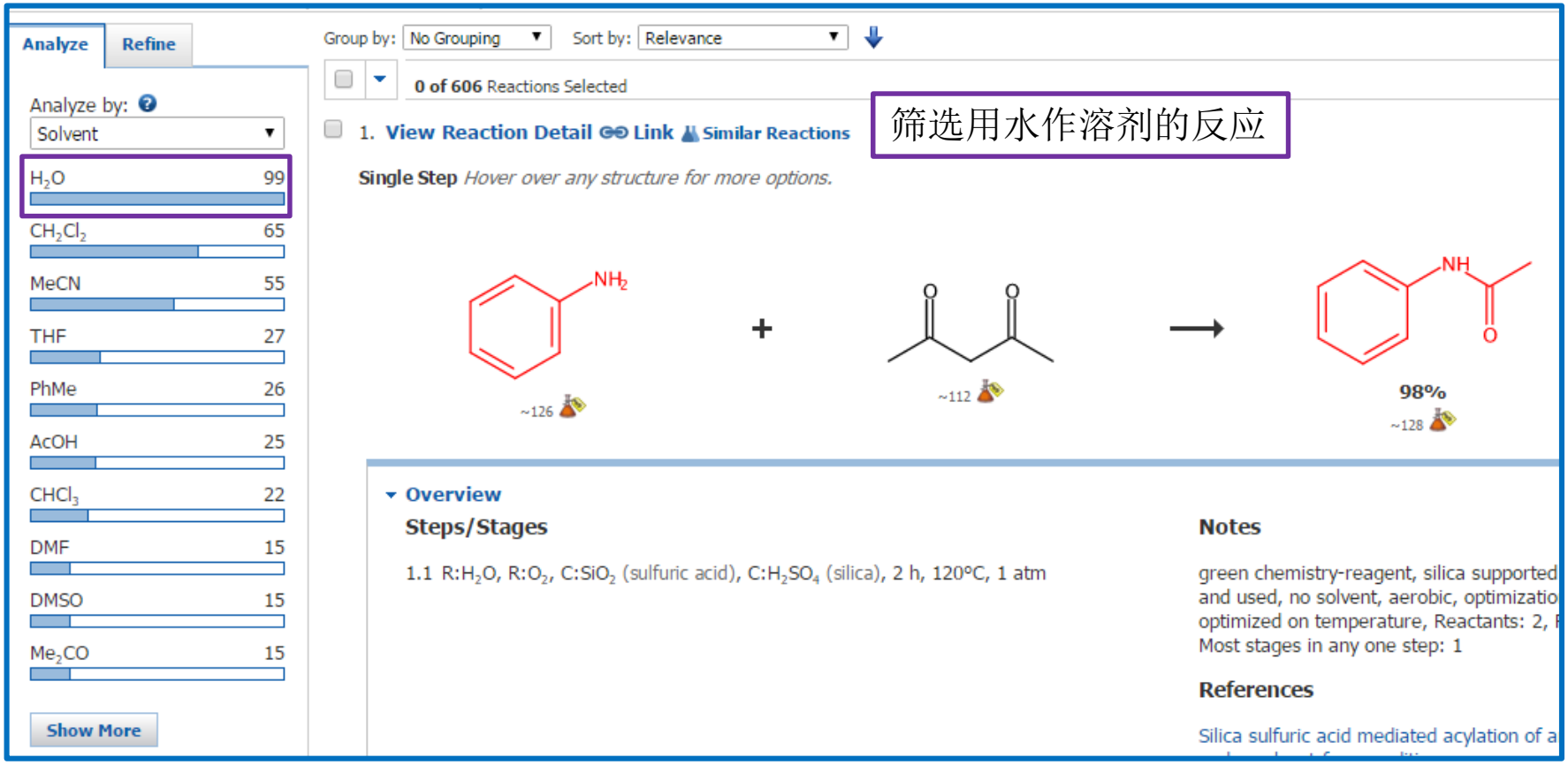


按照反应类型排序

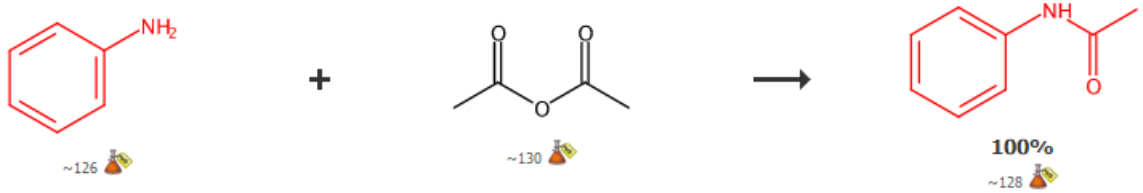


更精确的查找需要的反应

反应检索结果的筛选


Analyze
Refine
Group by: No Grouping
Sort by: Relevance
Analyze by:
Solvent
H2O 99
CH2Cl2 65
MeCN 55
THF 27
PhMe 26
AcOH 25
CHCl3 22
DMF 15
DMSO 15
Me2CO 15
Show More
0 of 606 Reactions Selected
1. View Reaction Detail Link Similar Reactions
筛选用水作溶剂的反应
Single Step Hover over any structure for more options.
NH2
~126
~112
NH
O
98%
~128
Overview
Steps/Stages
1.1 R:H2O, R:O2, C:SiO2 (sulfuric acid), C:H2SO4 (silica), 2 h, 120°C, 1 atm
Notes
green chemistry-reagent, silica supported
and used, no solvent, aerobic, optimizatio
optimized on temperature, Reactants: 2,
Most stages in any one step: 1
References
Silica sulfuric acid mediated acylation of a

SciFinder囊括最大的反应实验过程合集



▾ **Overview**

Steps/Stages

1.1 S:CH_2Cl_2, 20-120 min, rt

Notes

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

References

Indole Synthesis via Rhodium Catalyzed Oxidative Coupling of Acetanilides and Internal Alkynes

Quick View Other Sources

By Stuart, David R. et al

From Journal of the American Chemical Society, 130(49), 16474-16475; 2008

不用阅读全文，直接获得包含实验过程的反应记录

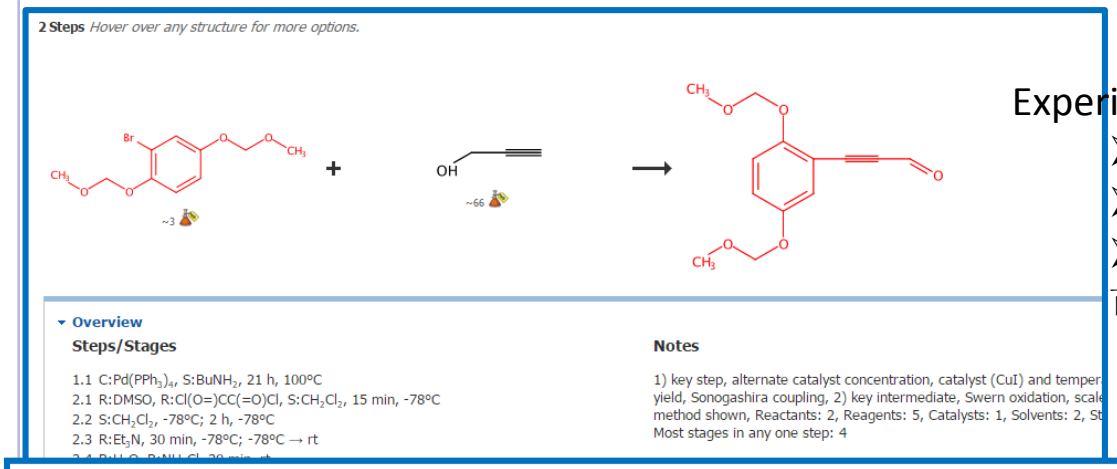
▾ **Experimental Procedure**

J|A|C|S

Represenative procedure for the preparation of acetanilides: Aniline (10.1 mL, 109.7 mmol, 1 eq) was added to a round-bottom flask via syringe and fitted with a rubber septum. The flask was purged with argon and dry DCM (300 mL, 0.4 M) was added. Acetic anhydride (12.5 mL, 132.2 mmol, 1.2 eq) was added and the reaction was stirred at room temperature and monitored by TLC. Upon completion (generally a couple of hours, but as short as 20 minutes) the reaction mixture was washed with a saturated solution of sodium carbonate, the organic layers dried with $MgSO_4$ and the solvent removed under reduced pressure. The product was obtained in quantitative yield (14.8 g). In most cases analytically pure acetanilides can be obtained after extraction however if necessary purification by flash chromatography with ethyl acetate/pet. ether was used (see below for specific conditions). **Acetanilide (1a):** The above procedure was followed to afford the product in quantitative yield. This compound can also be purchased from commercial sources (CAS: 103-84-4). **^{1}H NMR (400 MHz, $CDCl_3$, 293 K):** δ 7.50 (d, J = 7.8 Hz, 2H), 7.32 (t, J = 7.9 Hz, 2H), 7.10 (t, J = 7.4 Hz, 1H), 2.17 (s, 3H). The signal for the exchangeable NH does not appear in the spectrum.

SCIFINDER® A CAS SOLUTION

SciFinder囊括最大的反应实验过程合集



Experimental Procedure: 我们可以做得更好

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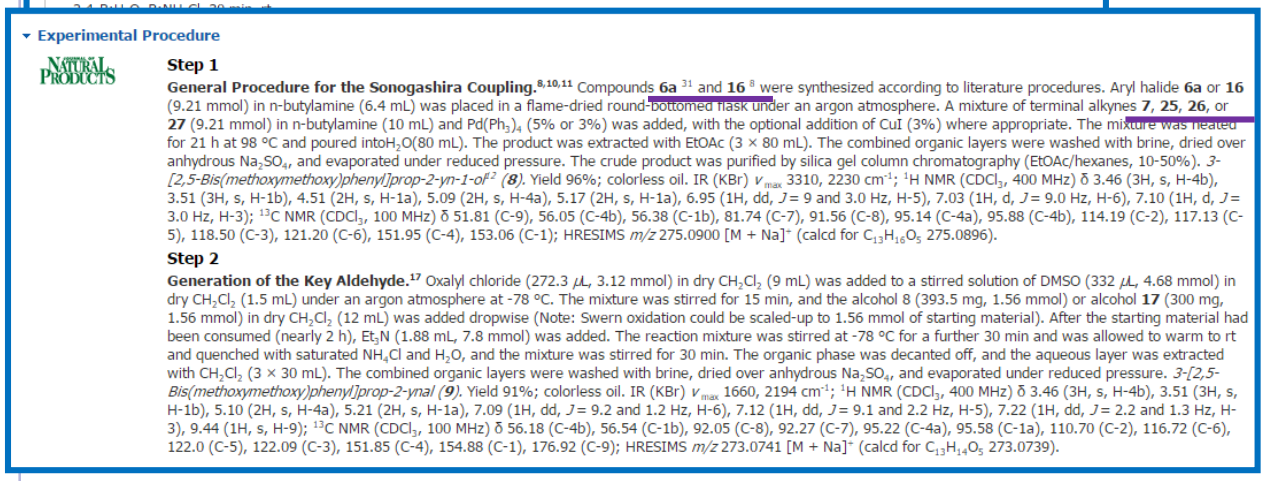
- 这些数字代表什么？
- 去免费的Supporting Information查？

可能只有图谱。



Experimental Procedure

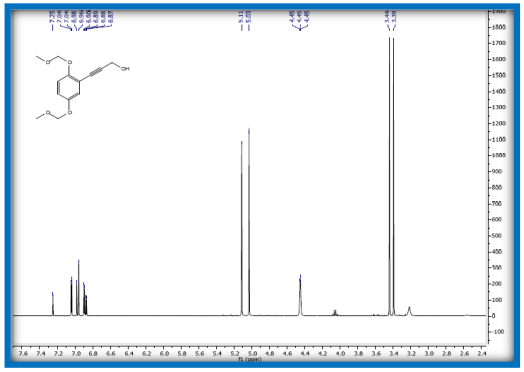
JOURNAL OF NATURAL PRODUCTS

Step 1

General Procedure for the Sonogashira Coupling.[8,10,11] Compounds **6a** [31] and **16** [8] were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in n-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in n-butylamine (10 mL) and $Pd(Ph_3)_4$ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured into H_2O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10-50%). *3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol*[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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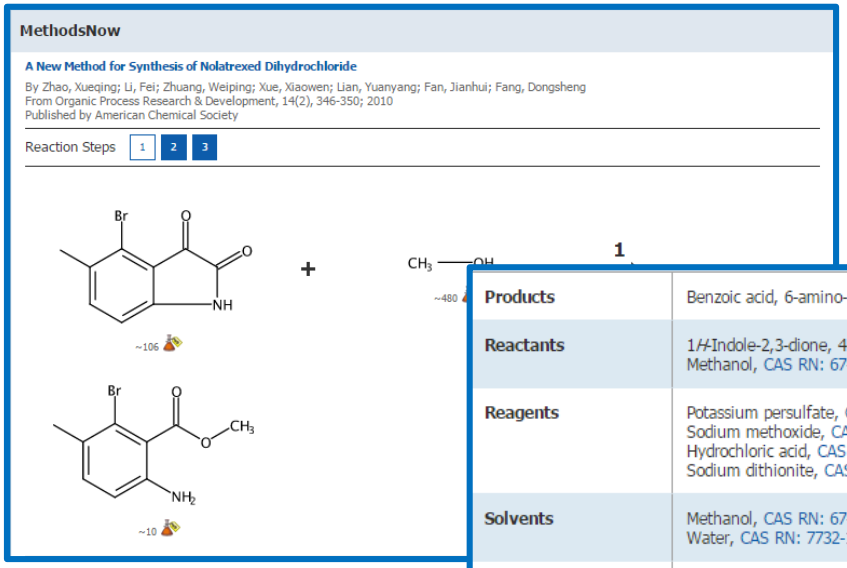
MethodsNow Synthesis



Products	Benzoic acid, 6-amino-2-bromo-3-methyl-, methyl ester, 84%, CAS RN: 147149-88-0
Reactants	1*H*-Indole-2,3-dione, 4-bromo-5-methyl-, CAS RN: 147149-84-6 Methanol, CAS RN: 67-56-1
Reagents	Potassium persulfate, CAS RN: 7727-21-1 Sodium methoxide, CAS RN: 124-41-4 Hydrochloric acid, CAS RN: 7647-01-0 Sodium dithionite, CAS RN: 7775-14-6
Solvents	Methanol, CAS RN: 67-56-1 Water, CAS RN: 7732-18-5
Procedure	1. Add sodium methoxide (22.6%, 4.80 kg, 20.1 mol) to a mixture of 4-bromo-5-methylisatin (6.67 mol) and anhydrous methanol (6.70 L). 2. Add $K_2S_2O_8$ (1.90 kg, 7.03 mol) to the mixture in parts 10°C with an ice-water bath. 3. After addition the reactant mixture turns yellow, continue the stirring for 1 hour at room temperature. 4. Adjust the reaction mixture to pH 8-9 with aqueous 36% HCl (1.24 L) 15 °C. 5. Destroy the excessive $K_2S_2O_8$ by aqueous 5% $Na_2S_2O_4$ solution (450 mL). 6. After rotary evaporation under a reduced pressure at 55 °C, Leave a brown liquid. 7. Mix the mixture with CH_2Cl_2 (6 L) and H_2O (4 L). 8. Separate the organic phase. 9. Extract the aqueous phase with CH_2Cl_2 (4 L). 10. Dry the combined organic phases over Na_2SO_4. 11. Concentrate the combined organic phases with a rotavapor. 12. Distill the resulted brown liquid under high vacuum.
Scale	milligram
^{1}H NMR	$CDCl_3$: δ2.28 (s, 3 H, Ar-C*H*$_3$), 3.91 (s, 3 H, -OCH$_3$), 4.26 (br s, 2 H, NH$_2$), 6.54 (d, *J*= 8.2 Hz, 1 H, Ar-H), 7.00 (d, *J*= 8.2 Hz, 1 H, Ar-H).
IR	KBr cm^{-1}: υ3472, 3382, 2953, 2924, 1716, 1622, 1480, 1277, 816.

物质信息

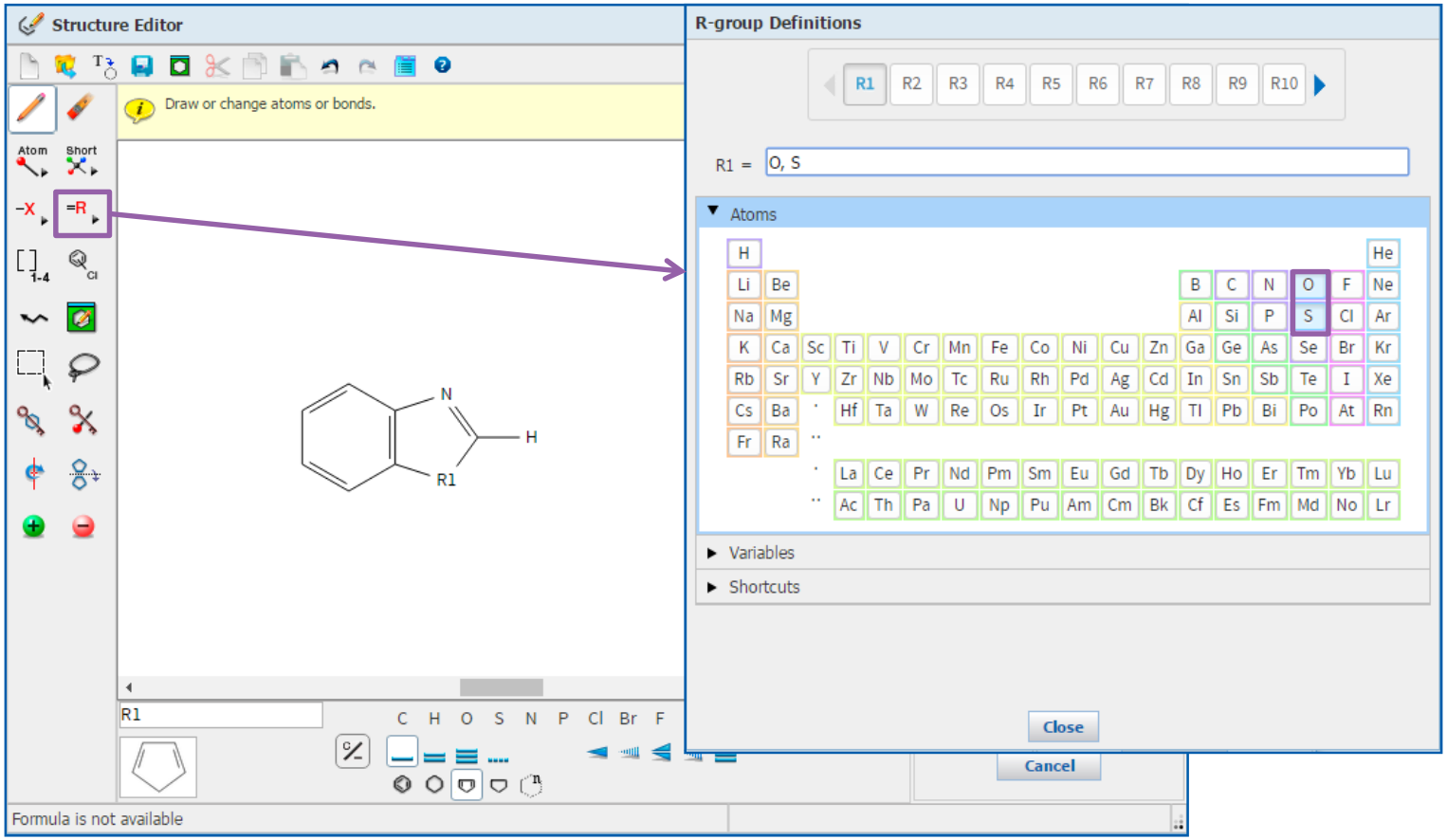
实验过程

图谱信息

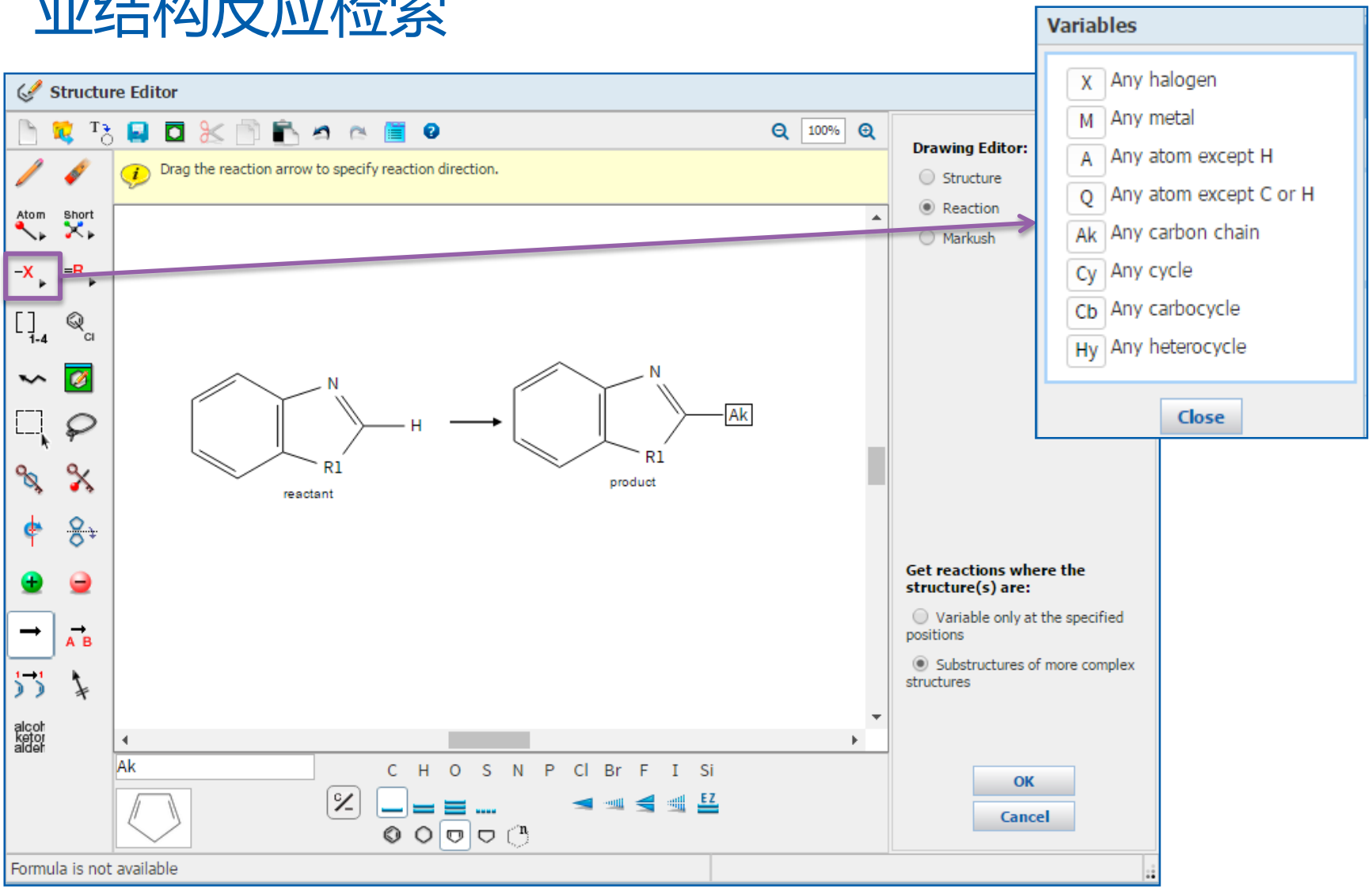
SciFinder® A CAS SOLUTION

亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索


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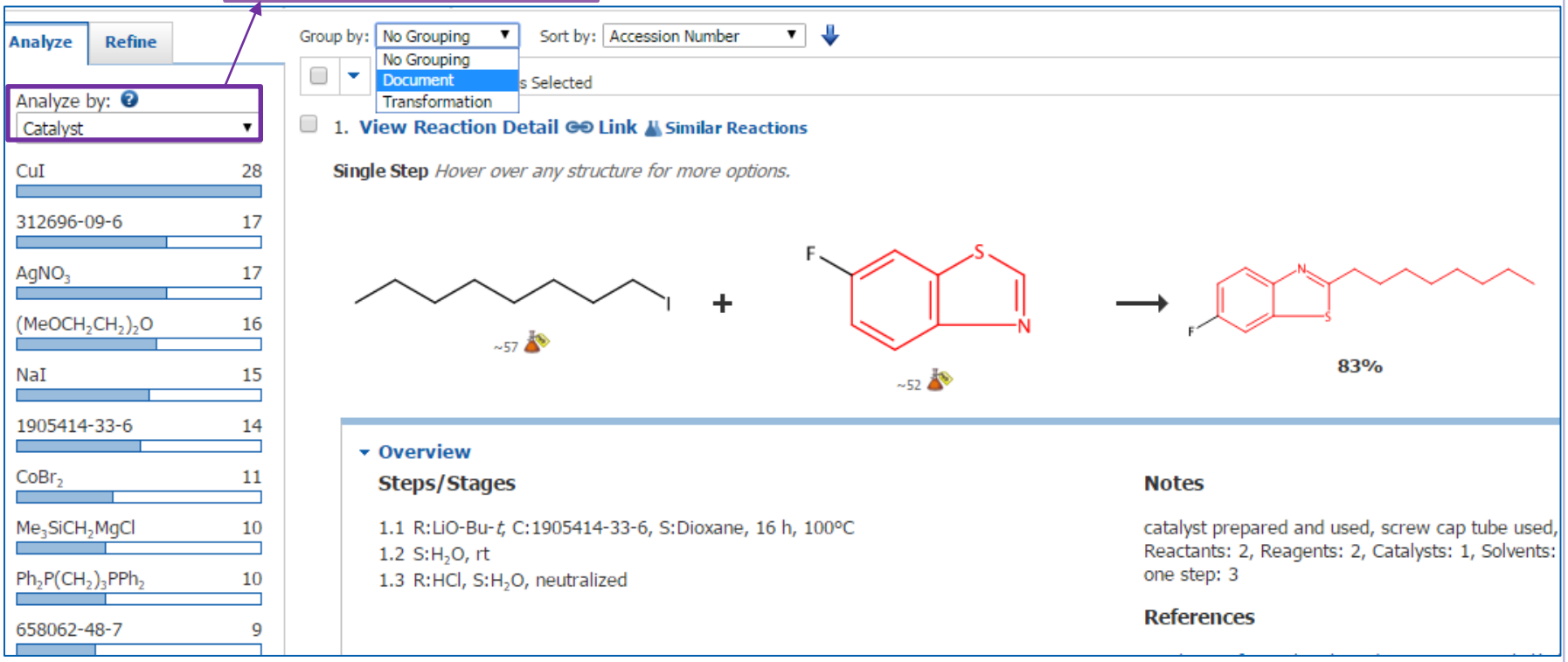
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
Ak
C H O S N P Cl Br F I Si
Formula is not available
Variables
X Any halogen
M Any metal
A Any atom except H
Q Any atom except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

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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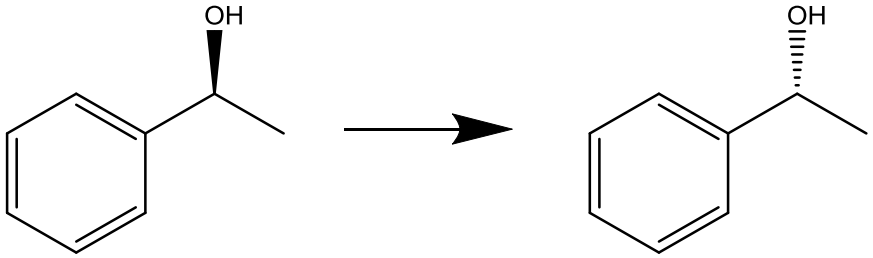
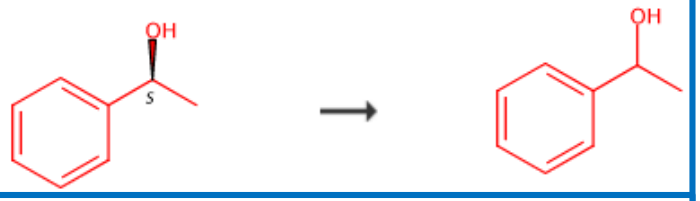
案例：如何获取手性翻转反应



1. View Reaction Detail Link

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



4. View Reaction Detail Link

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

6. View Reaction Detail Link

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

94. View Reaction Detail Link

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

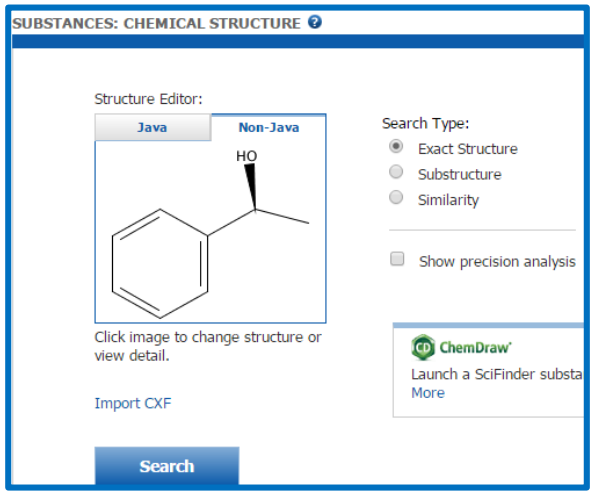
案例：如何获取手性翻转反应

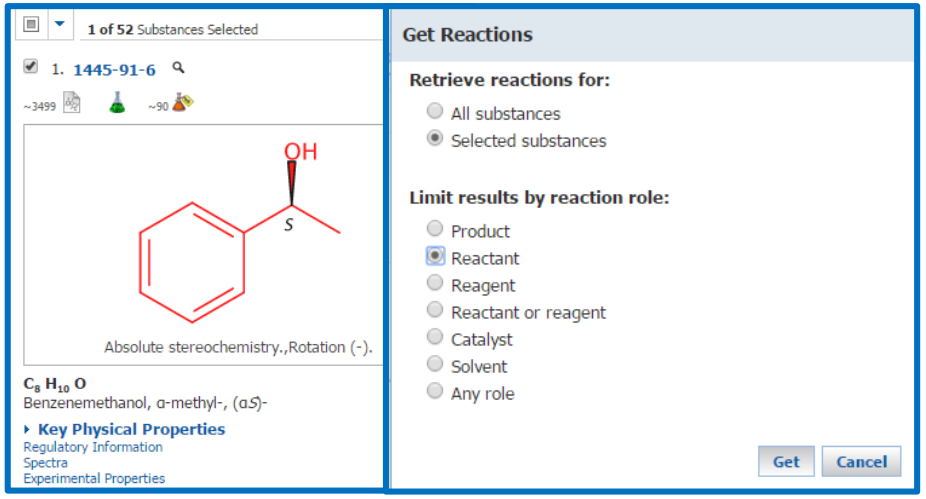
检索思路：

1). 先获取反应物物质，然后再获取其作为反应物的反应，得到检索结果集1。

2). 先获取产物物质，然后再获取其作为产物的反应，得到检索结果集2。

3). 两个结果集取交集。





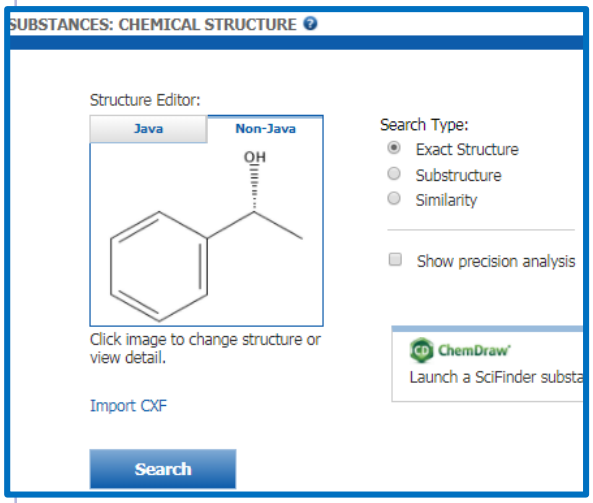
案例：如何获取手性翻转反应

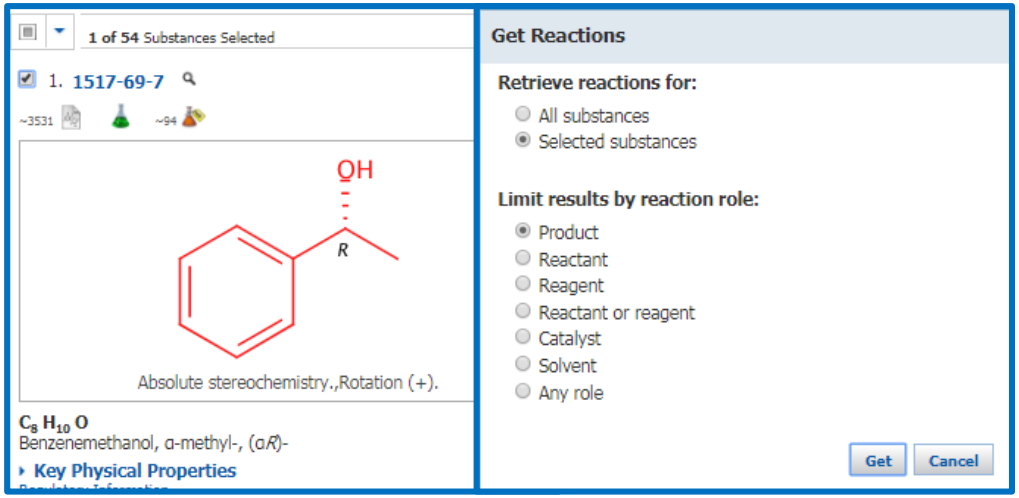
检索思路：

1). 先获取反应物物质，然后再获取其作为反应物的反应，得到检索结果集1。

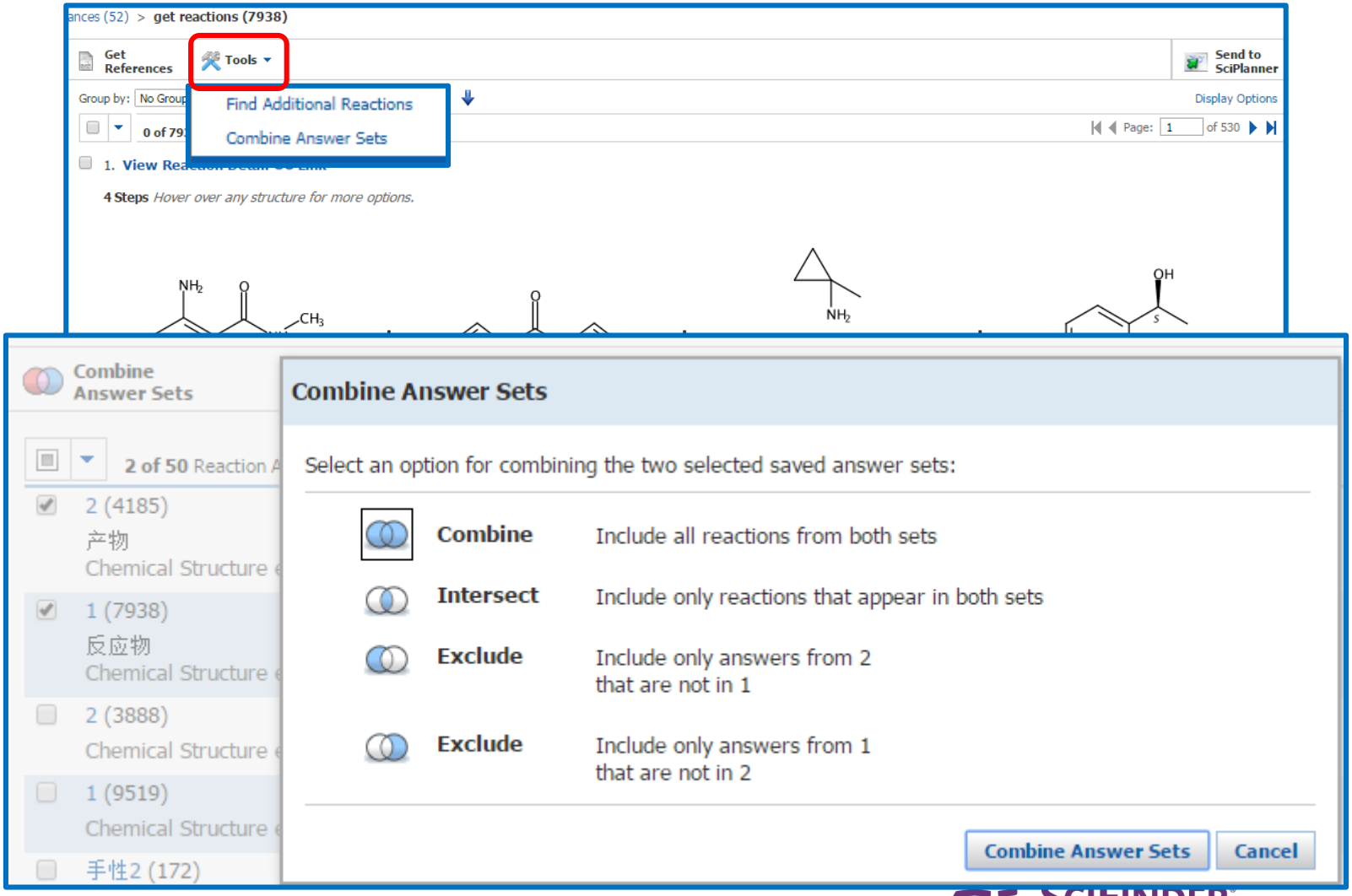
2). 先获取产物物质，然后再获取其作为产物的反应，得到检索结果集2。

3). 两个结果集取交集。





案例：如何获取手性翻转反应



反应检索结果集

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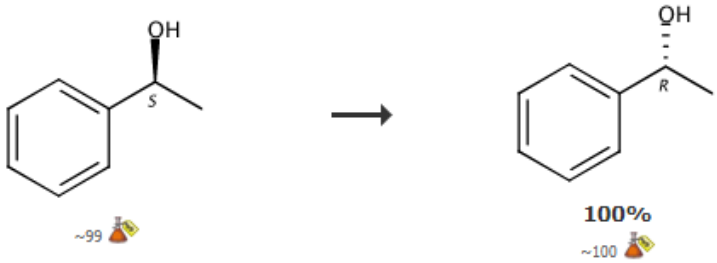
1. View Reaction Detail Link

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



~99 ~100

Overview

Steps/Stages

1.1 $S:H_2O$, S:M, 360 h, 30°C

Notes

biotransformation, ee=92%, resting cells of the yeast C. albicans used, stereoselective, Reactants: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Deracemization of 1-phenylethanol via tandem biocatalytic oxidation and reduction

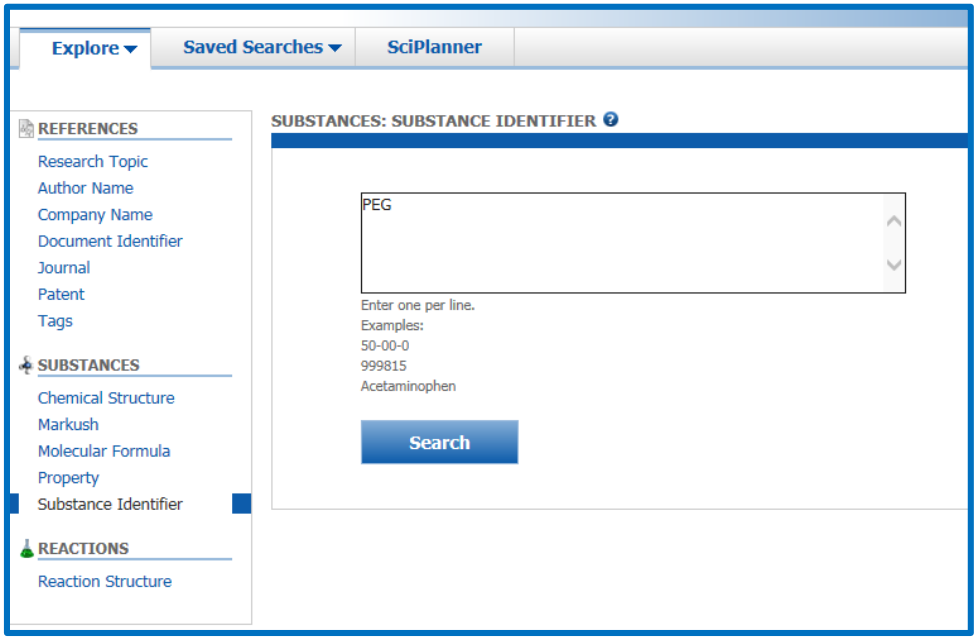
SciFinder® A CAS SOLUTION

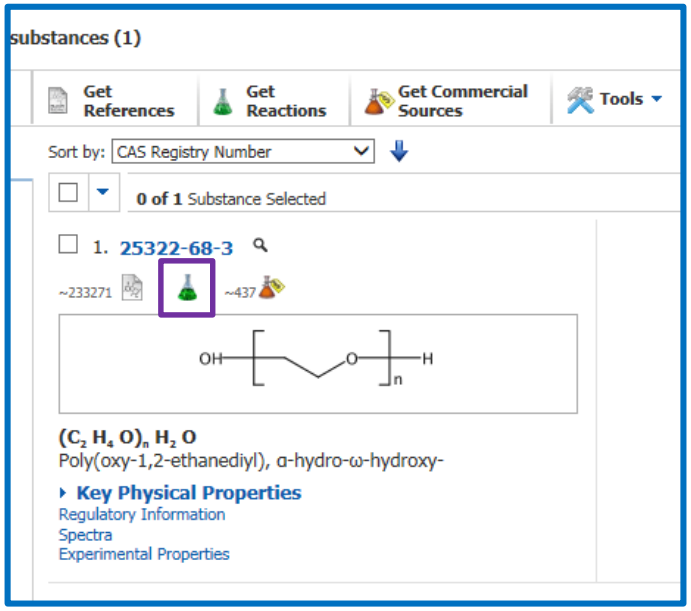
聚合物改性案例：甲基丙烯酸甲酯对聚乙二醇的改性反应

思路：

1. 从物质检索出发，先检索到聚乙二醇的物质信息
2. 从物质获取反应，获得聚乙二醇参与的反应信息
3. 限定反应，通过接枝物质的结构（甲基丙烯酸甲酯）来限定反应
4. 获得聚合物的改性反应

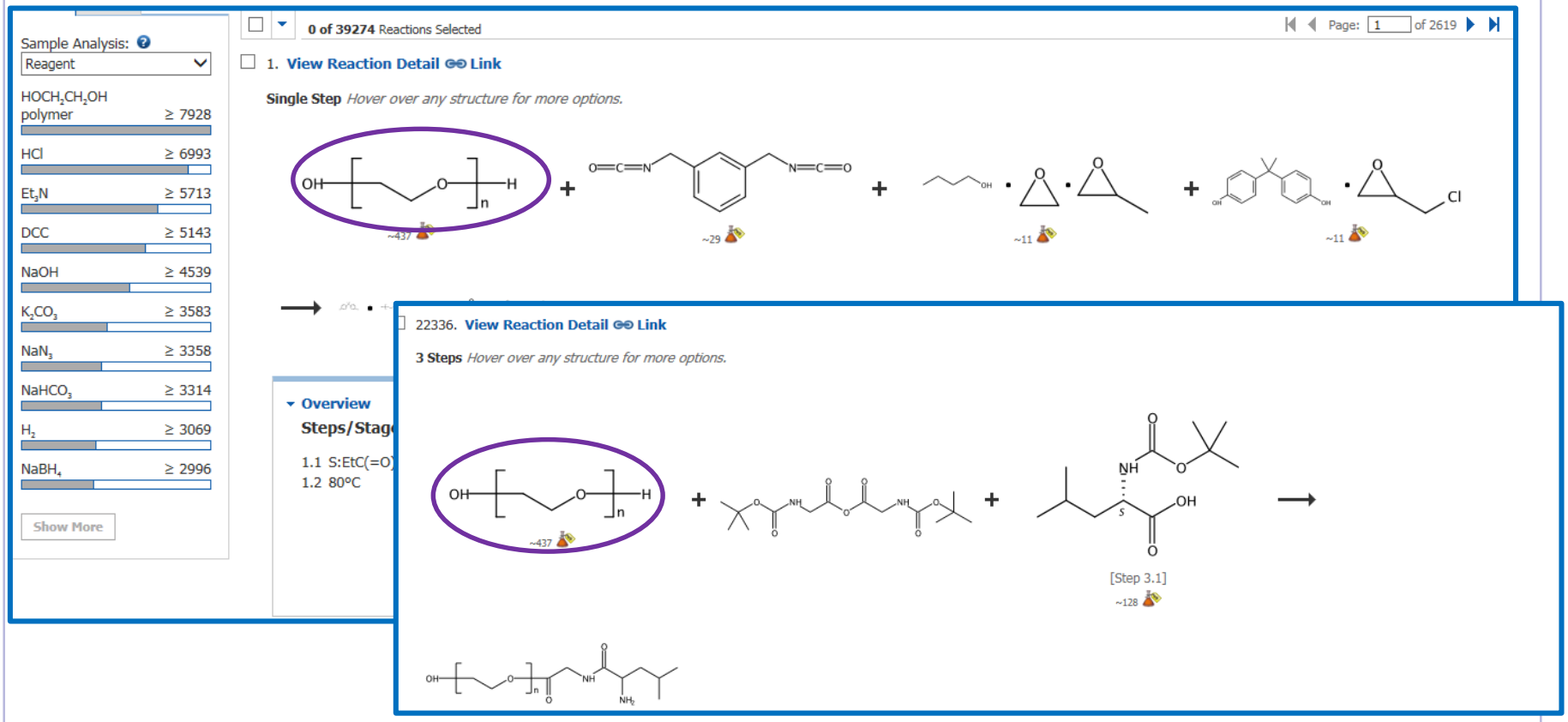
检索聚乙二醇物质信息：物质识别号检索





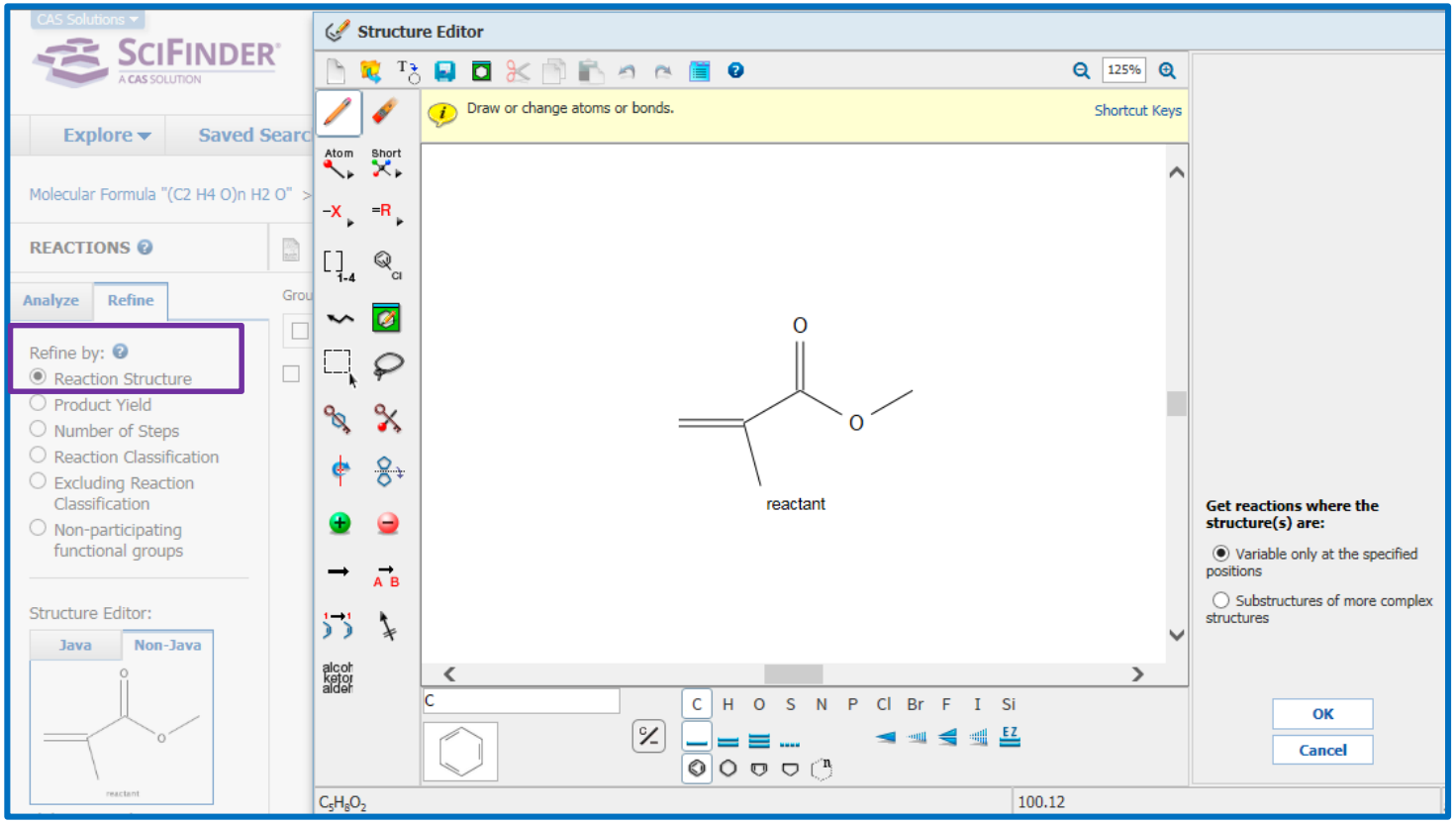
SciFinder® A CAS SOLUTION

从物质获取反应信息：获取聚乙二醇作为反应物的反应



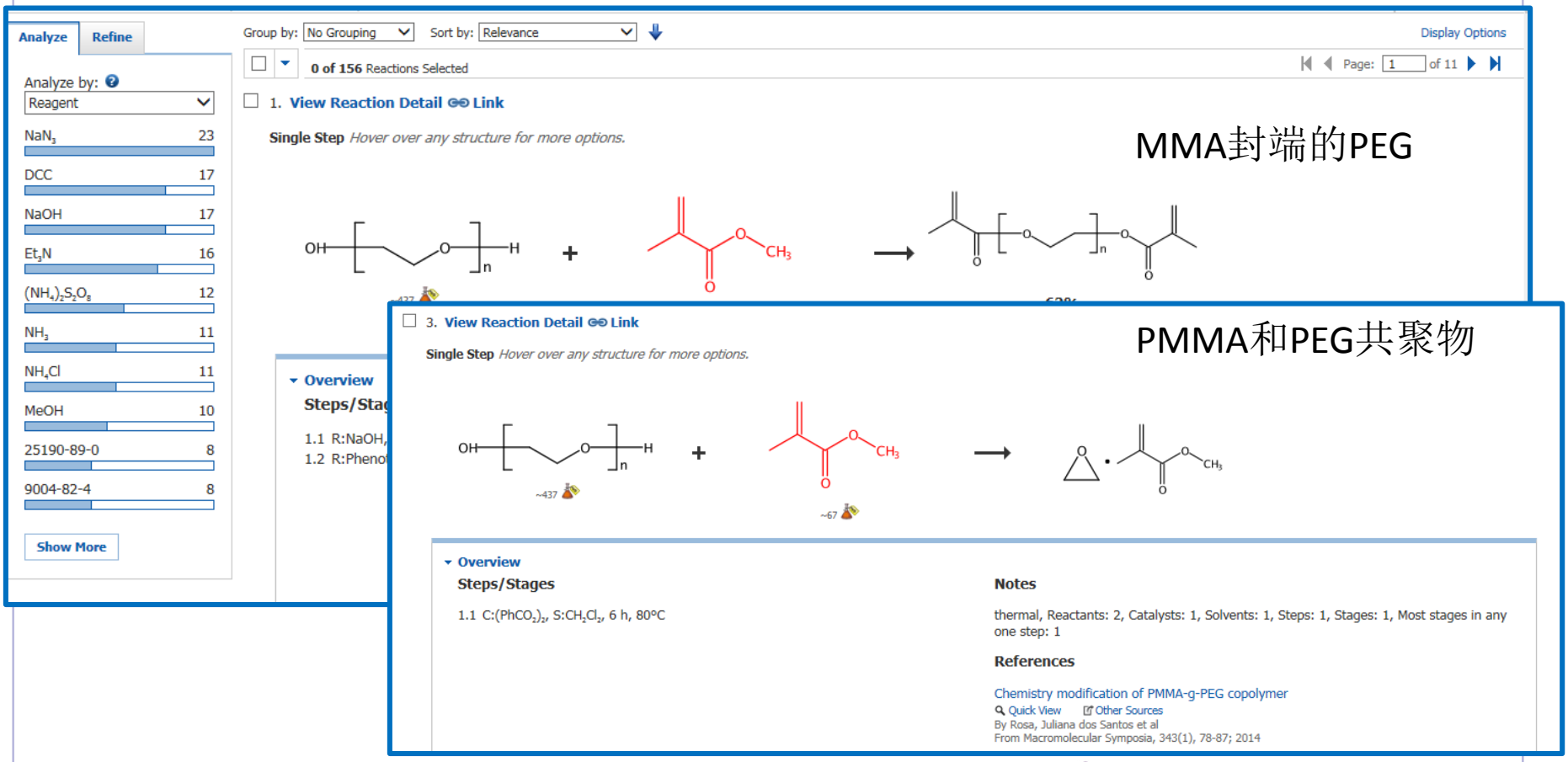
SciFinder® A CAS SOLUTION

限定反应：根据参与反应的甲基丙烯酸甲酯，限定反应结构



SciFinder® A CAS SOLUTION

获得改性后的聚合物：获得甲基丙烯酸甲酯（MMA）接枝的PEG



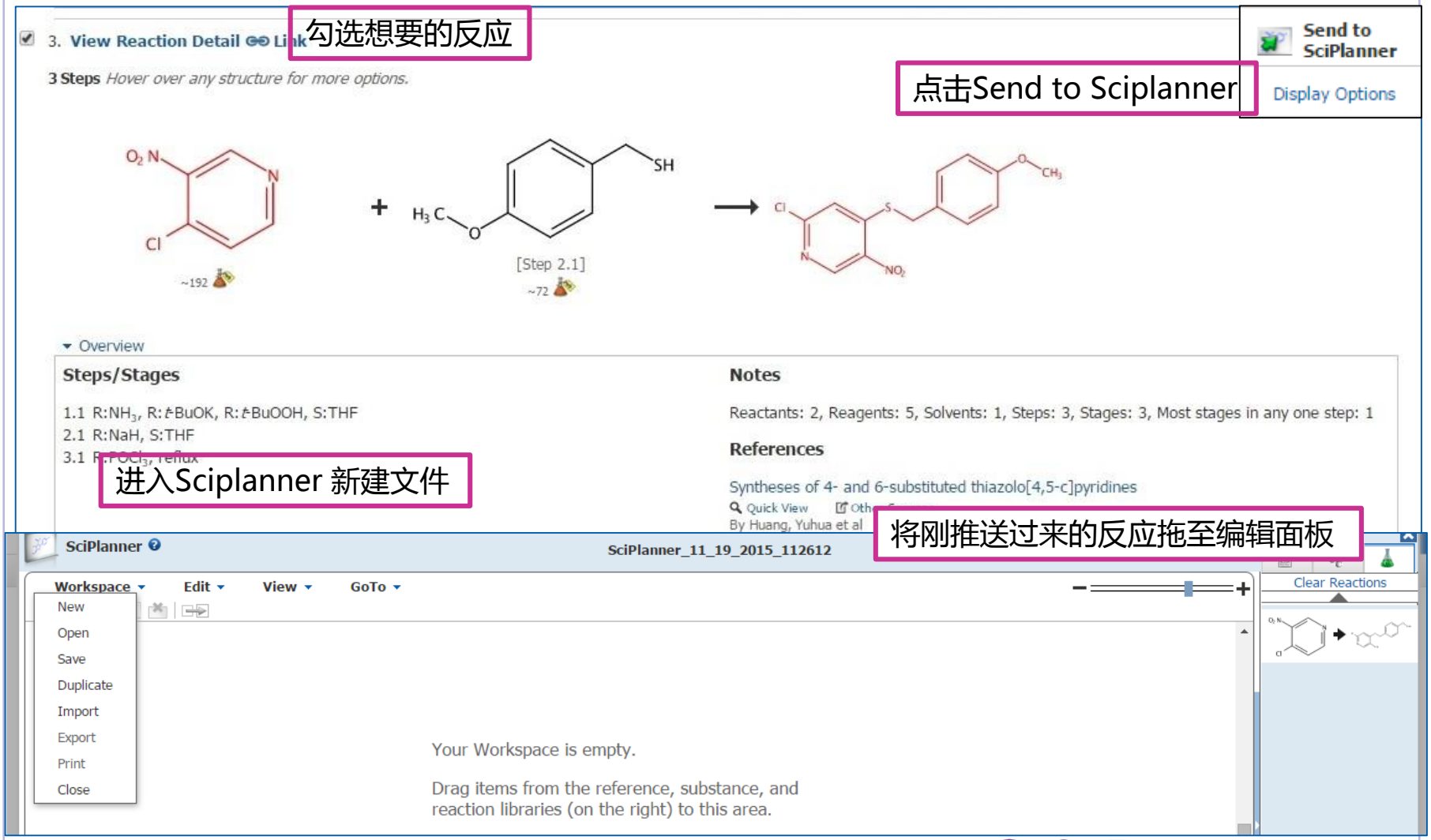
SciFinder® A CAS SOLUTION

提纲

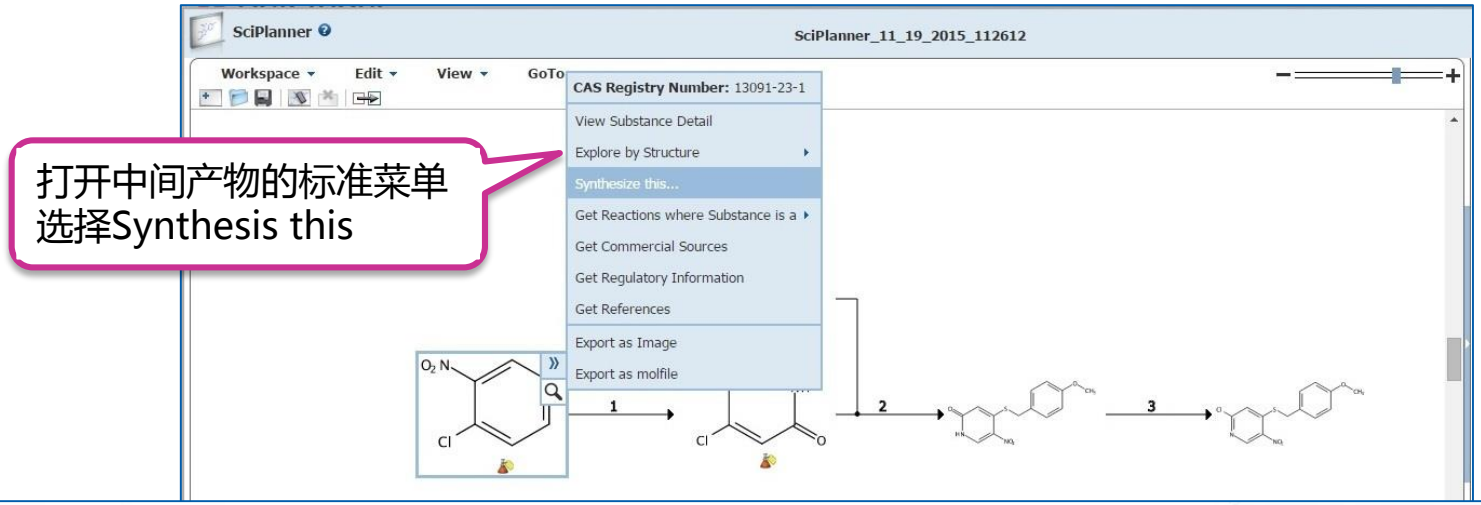
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索（PatentPak）
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow Analysis
- SciFinder常见问题及解决

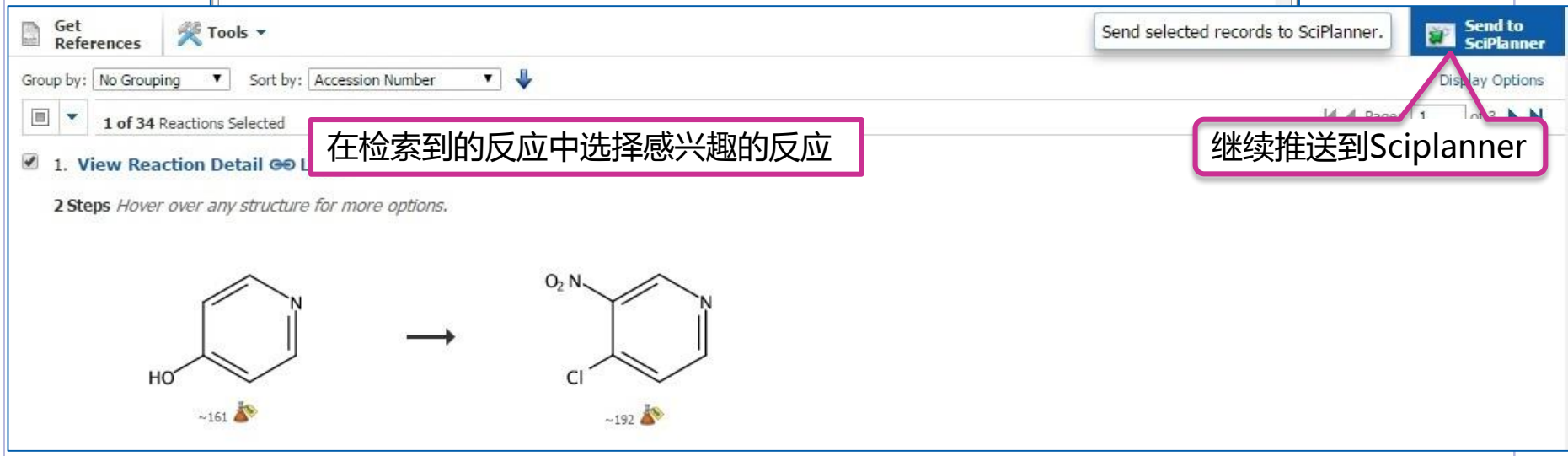
SCIFINDER® A CAS SOLUTION

SciPlanner使用简介



SciPlanner使用简介





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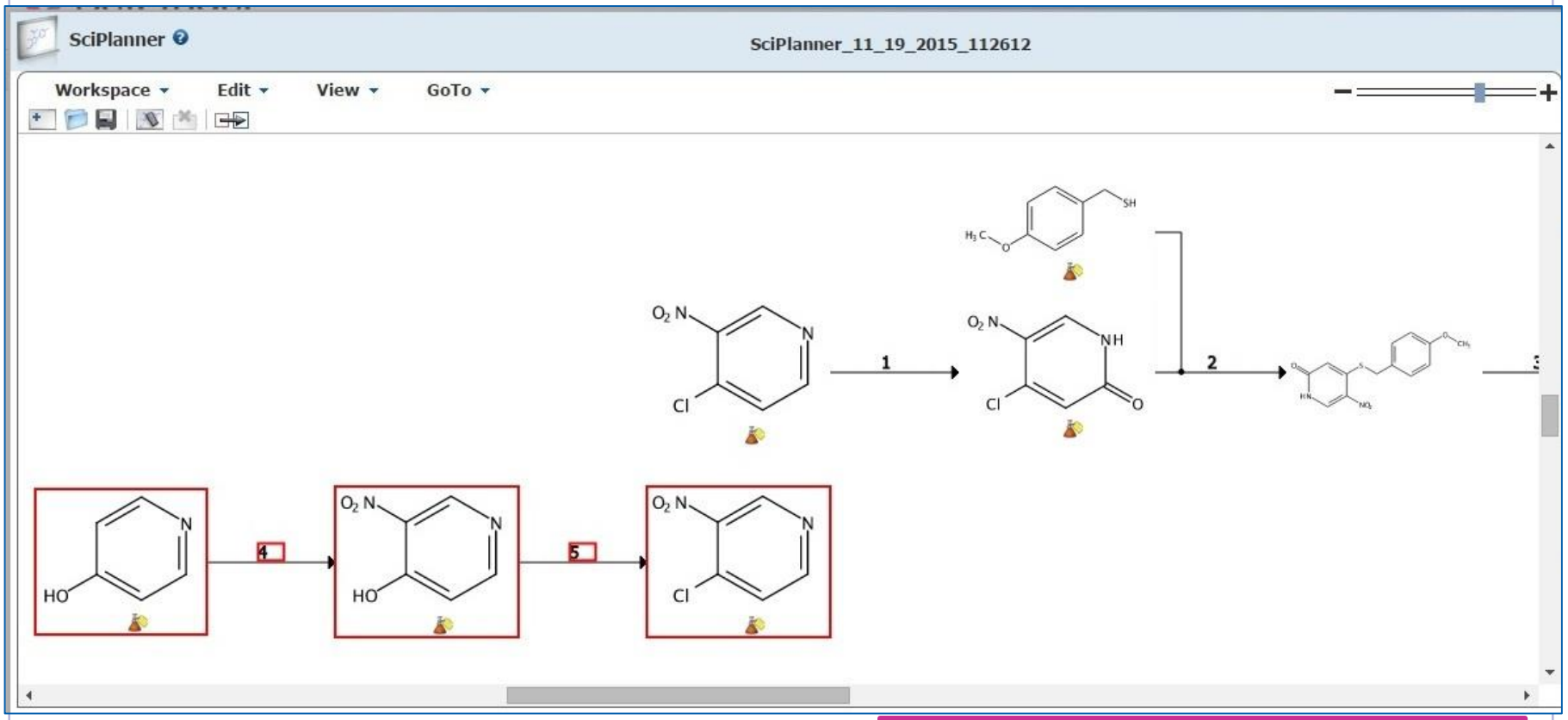
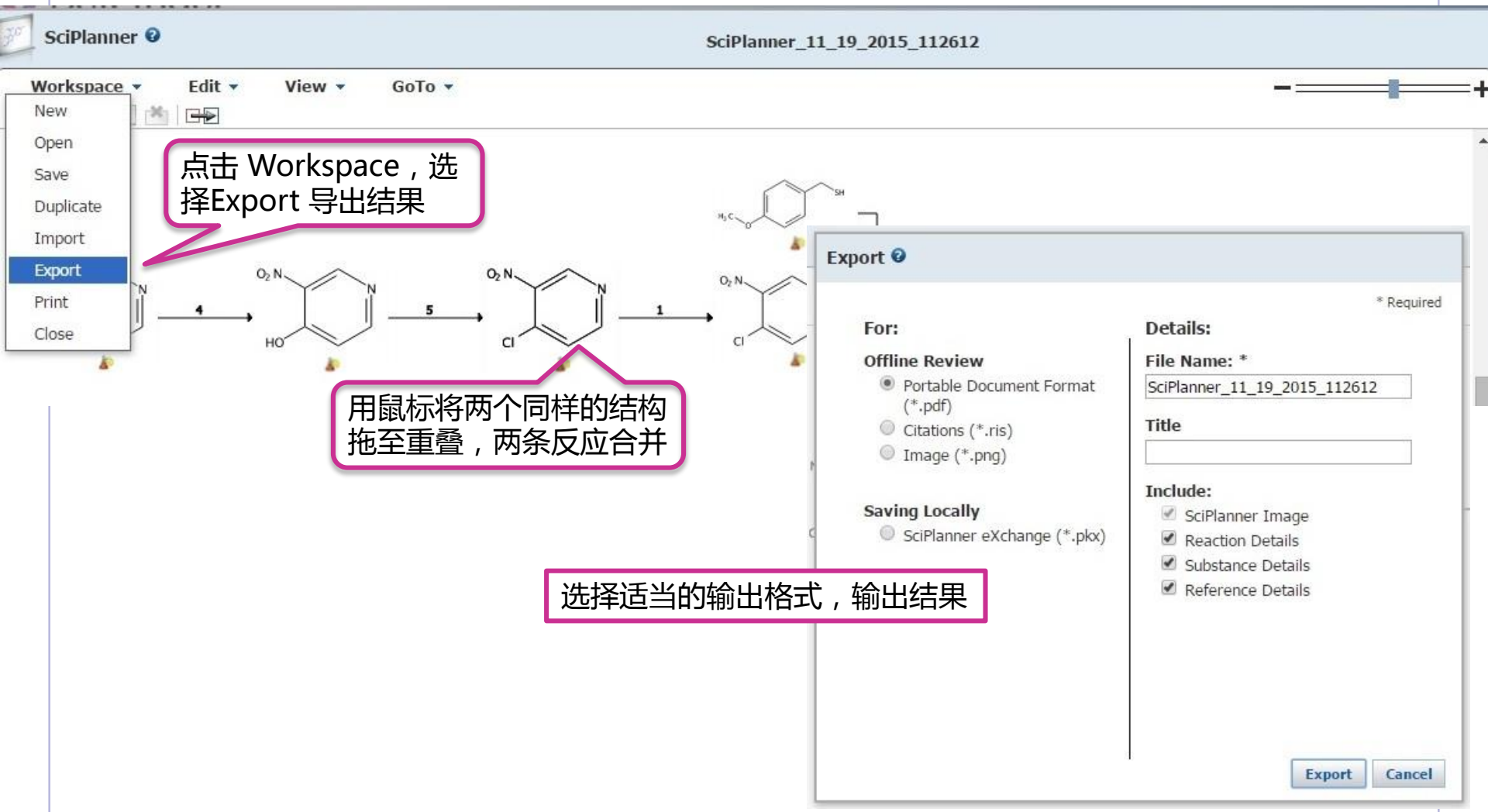
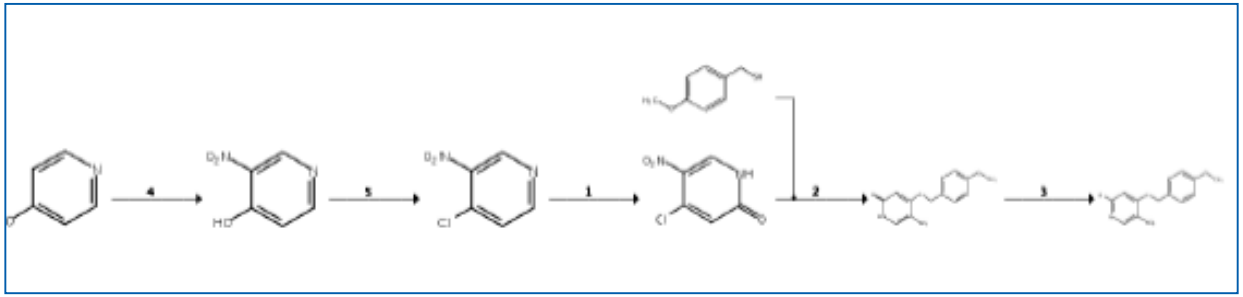


步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

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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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 Analysis
- SciFinder常见问题及解决

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MethodsNowTM 是一个完整的 CAS 解决方案

- 最大的方法信息合集，聚焦核心化学市场
- 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
- 分析与合成两个模块
- 逾百万的合成和分析方法合集——数量持续增加!

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MethodsNow – Analysis(www.methodsnow.com)

- Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…
- Organometallics / Inorganics: 地质分析，无机物分析，金属有机化合物分析
- 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…
- Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析…

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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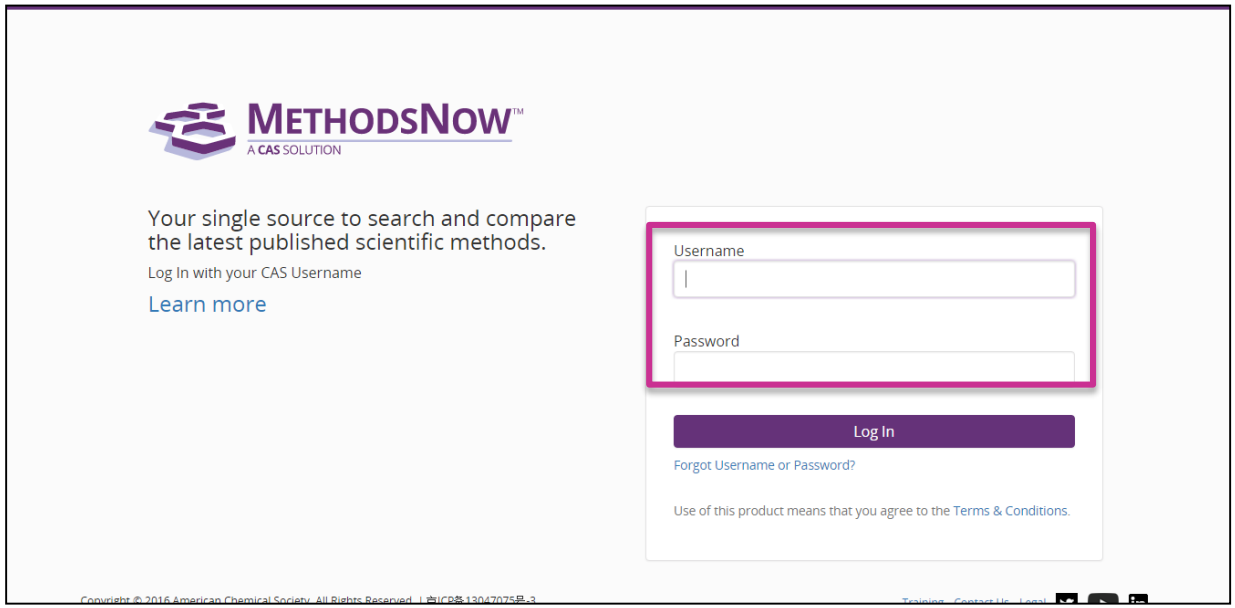

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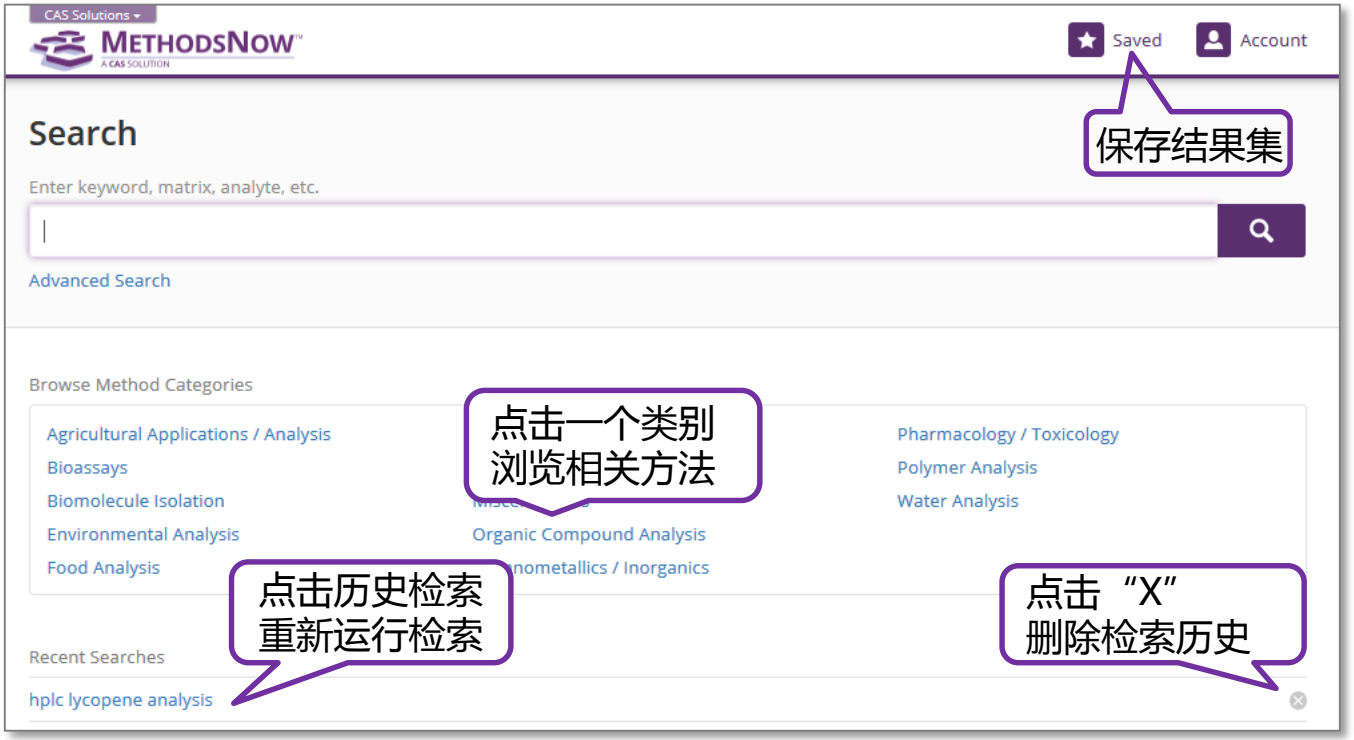
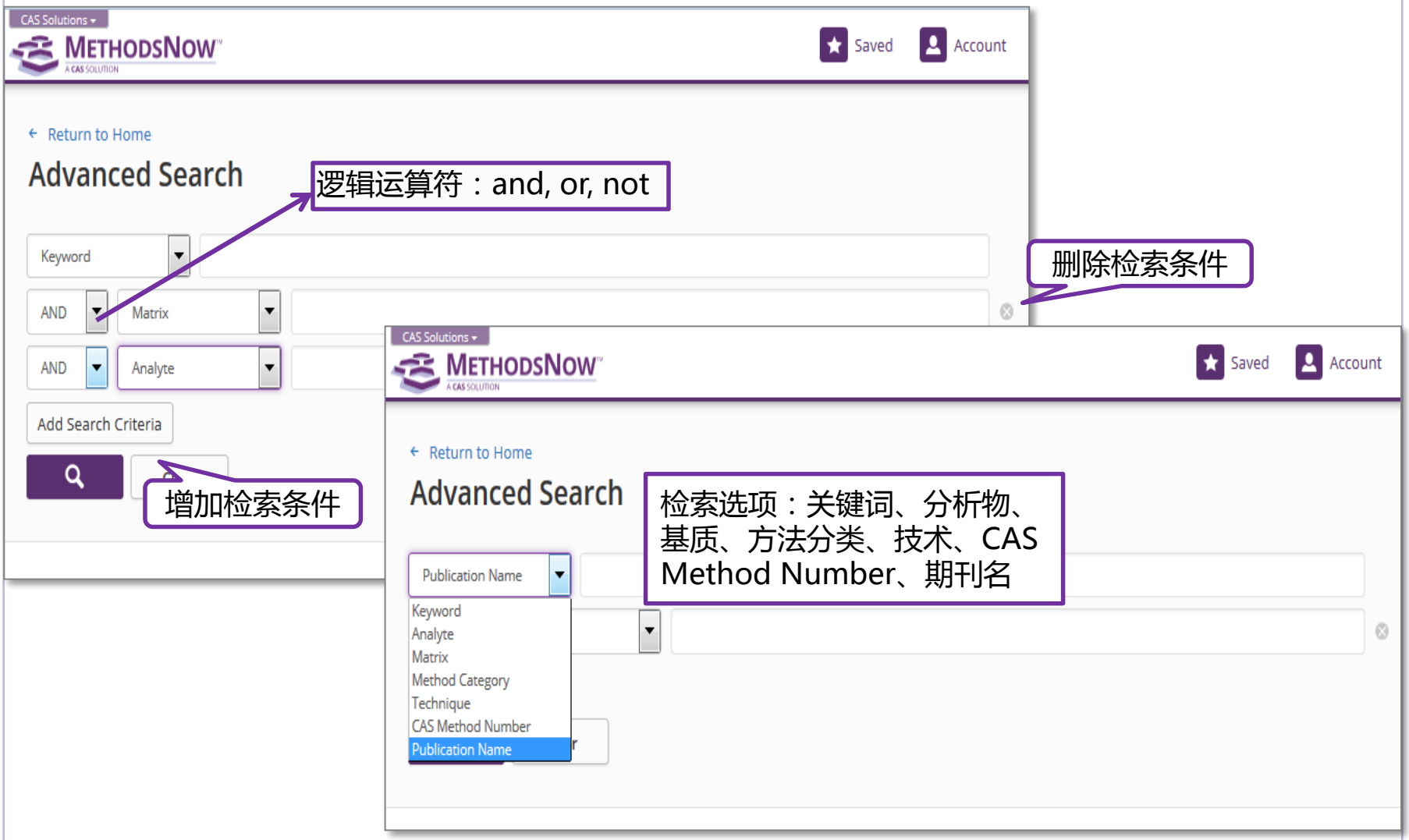
检索/高级检索

方法分类

历史检索



高级检索



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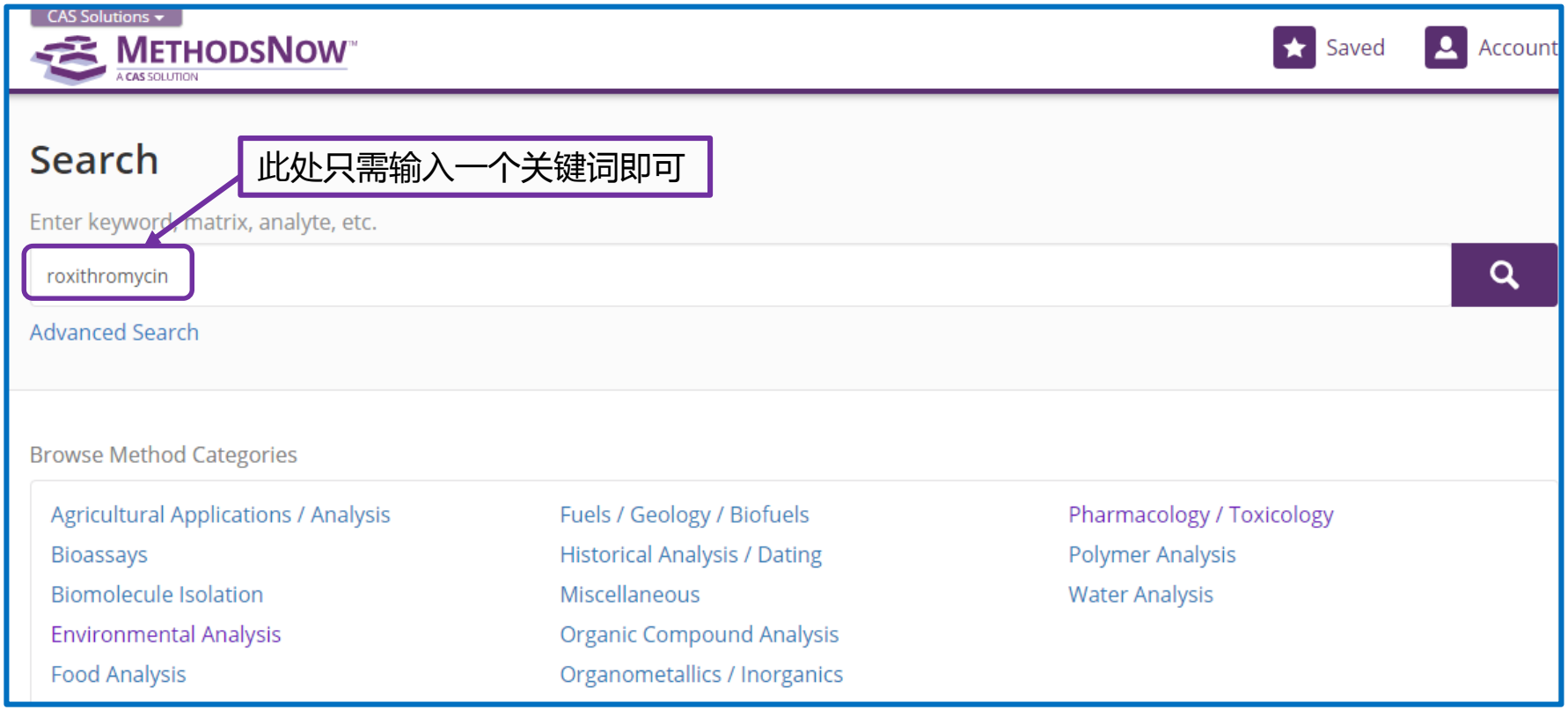
案例：高效液相色谱法测定血液中罗红霉素的含量



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结果显示

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结果显示

Method Detail (2 of 5)

实验材料

Analysis of Roxithromycin in Blood plasma by HPLC

CAS MN: 1-101-CAS-67878

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: Fluorescence; HPLC

Materials	Role
Roxithromycin	analyte
Blood plasma	matrix
Column, 125 x 4.6 mm i.d. LiChrospher RP-18e	material
SPE Bakerbond cartridges, C18	material

文献信息

Source

Determination of roxithromycin in human plasma by HPLC with fluorescence and UV absorbance detection: Application to a pharmacokinetic study

Glowka, Franciszek K.; Karazniewicz-Lada, Marta

Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2007), 852 (1-2), 669 - 673. Elsevier B.V.

CODEN: JCBAAI | ISSN: 15700232 | DOI: 10.1016/j.jchromb.2007.02.022

Document Sources

Abstract

A selective HPLC method with fluorescence detection for the determination of roxithromycin (ROX) in human plasma was described. After solid-phase extraction (SPE), ROX and erythromycin (internal standard, I.S.) were derivatized by treatment with 9-fluorenylmethyl chloroformate (FMOC-Cl). Optimal resolution of fluorescence derivatives of ROX and I.S. was obtained during one anal. run using reversed phase, C_{18} column. The mobile phase was composed of potassium dihydrogenphosphate solution, pH 7.5 and acetonitrile. Fluorescence of the compounds was measured at the maximum excitation, 255 nm and emission, 313 nm, of ROX derivatives Validation parameters of the method were also established. After SPE, differences in recoveries of ROX and erythromycin from human plasma were observed The linear range of the standard curve of ROX in plasma was 0.5-10.0 mg/l. The validated method was successfully applied for pharmacokinetic studies of ROX after administration of a single tablet of ROX.

设备条件

Equipment Used

HPLC system, HP 1100, Hewlett-Packard, Waldbronn, Germany

Autosampler, G1313A

Conditions

Chromatographic

HPLC : mobile phase : 700 ml of acetonitrile + 300 ml of a 0.05 mol/L
column oven : at 40 °C, fluorescence detector excitation wavelength

Instructions

Standards Preparation

1. Prepare stock solutions of roxithromycin (ROX) and erythromycin (I.S.) with 1 g/L, each in methanol.
2. Prepare standard solutions: 5.0, 7.5,15.0, 20.0, 50.0, 75.0 and 100.0 mg/L of ROX and 200.0 mg/L of I.S. in methanol.
3. Transfer the volume of 50 µL aliquots of the sample to a glass vial containing 0.5 mL blank human plasma.

Solid phase extraction procedure

1. Process the resulting plasma samples containing: 0.5, 0.75, 1.5, 2.0, 5.0, 7.5 and 10.0 mg/l of ROX and 20.0 mg/l of I.S.according to the SPE.
2. Add the volume of 0.5 ml of a phosphate buffer, pH 7.5 (prepared as a mixture of 85.2 ml of 1/15 M Na_2HP0_4 and 14.8 ml 1/15 M KH_2PO_4).
3. Transfer the samples into C18 SPE Bakerbond cartridges (J.T. Baker Mallinckrodt Deventer, Holland).
4. Wash the absorbed analytes with water and elute with methanol.
5. Evaporate the organic liquid to dryness at 40 °C.

Derivatization

1. Dissolve the residue in 200 µL aliquots of acetonitrile and transfer the sample to a glass reaction vial.
2. Add a 100 µL aliquots of a 2.5 mg/L 9-fluorenylmethyl chloroformate (FMOC-Cl) in acetonitrile and 100 µL aliquots of a phosphate buffer, pH 7.5.
3. Incubate the sample at 40 °C for 40 min.
4. Inject an aliquot 100 µL after derivatization, onto the chromatographic system.

HPLC

1. Prepare the mobile phase by mixing 700 mL of acetonitrile with 300 ml of a 0.05 mol/L solution of potassium dihydrogenphosphate in water, adjust to pH 7.5 with a 10% sodium hydroxide solution.
2. Determine ROX and I.S. in human plasma in a chromatograph model HP 1100 (Hewlett-Packard, Waldbronn, Germany).
3. Set at a flow rate of quaternary pump at 2 mL/min, a column oven at 40 °C and a fluorescence detector model HP 1046A and G13 21 A-1100, at an excitation wavelength (Ex) of 255 nm and emission wavelength (Em) of 315 nm.
4. Inject the samples (100 µL) using autosampler model G1313A.
5. Perform the separation on a 125 x 4.6 mm i.d. LiChrospher RP-18e column packed with 5 µm particles, with a guard column (LiChrospher RP-18e), both from Merck.

实验步骤

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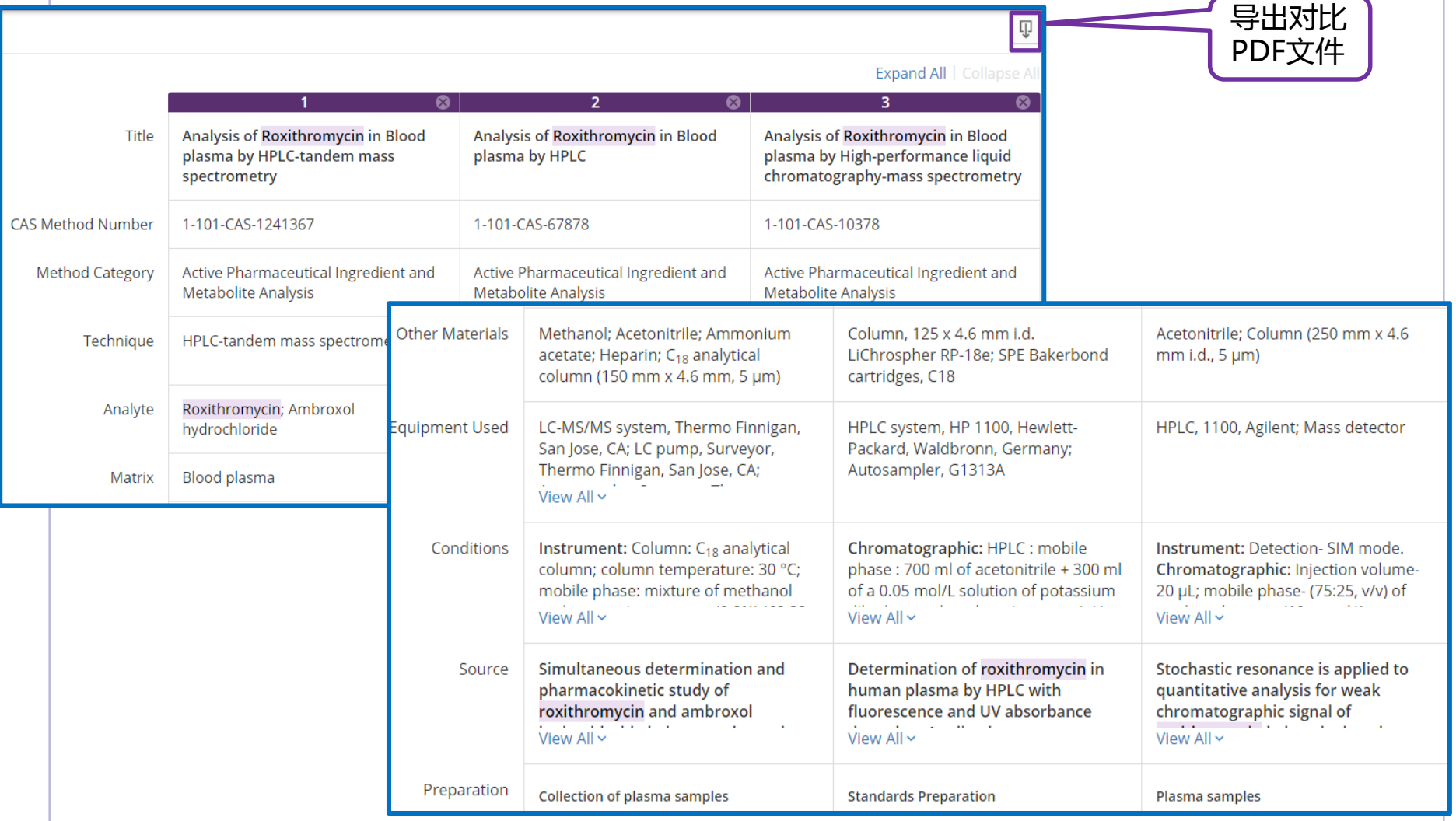
对比不同分析方法


导出对比
PDF文件
Expand All | Collapse All
1
2
3
Title
Analysis of Roxithromycin in Blood plasma by HPLC-tandem mass spectrometry
Analysis of Roxithromycin in Blood plasma by HPLC
Analysis of Roxithromycin in Blood plasma by High-performance liquid chromatography-mass spectrometry
CAS Method Number
1-101-CAS-1241367
1-101-CAS-67878
1-101-CAS-10378
Method Category
Active Pharmaceutical Ingredient and Metabolite Analysis
Active Pharmaceutical Ingredient and Metabolite Analysis
Active Pharmaceutical Ingredient and Metabolite Analysis
Technique
HPLC-tandem mass spectrome
Analyte
Roxithromycin; Ambroxol hydrochloride
Matrix
Blood plasma
Other Materials
Methanol; Acetonitrile; Ammonium acetate; Heparin; C18 analytical column (150 mm x 4.6 mm, 5 µm)
Column, 125 x 4.6 mm i.d. LiChrospher RP-18e; SPE Bakerbond cartridges, C18
Acetonitrile; Column (250 mm x 4.6 mm i.d., 5 µm)
Equipment Used
LC-MS/MS system, Thermo Finnigan, San Jose, CA; LC pump, Surveyor, Thermo Finnigan, San Jose, CA;
View All
HPLC system, HP 1100, Hewlett-Packard, Waldbronn, Germany; Autosampler, G1313A
HPLC, 1100, Agilent; Mass detector
Conditions
Instrument: Column: C18 analytical column; column temperature: 30 °C; mobile phase: mixture of methanol
View All
Chromatographic: HPLC : mobile phase : 700 ml of acetonitrile + 300 ml of a 0.05 mol/L solution of potassium
View All
Instrument: Detection- SIM mode. Chromatographic: Injection volume- 20 µL; mobile phase- (75:25, v/v) of
View All
Source
Simultaneous determination and pharmacokinetic study of roxithromycin and ambroxol
View All
Determination of roxithromycin in human plasma by HPLC with fluorescence and UV absorbance
View All
Stochastic resonance is applied to quantitative analysis for weak chromatographic signal of
View All
Preparation
Collection of plasma samples
Standards Preparation
Plasma samples

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 Analysis
- SciFinder常见问题及解决

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SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
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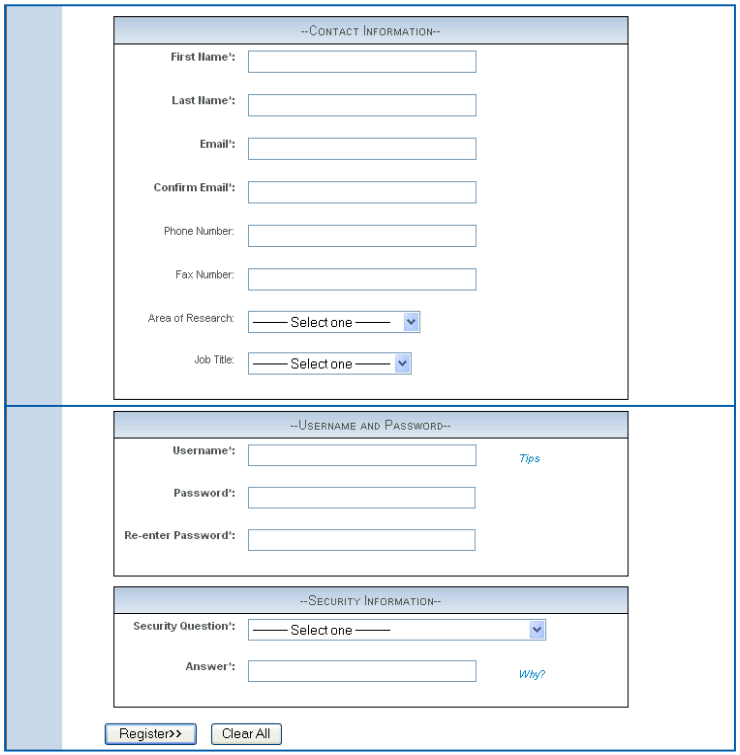

请注意：
1.必须输入真实姓名和学校域名邮箱。
2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

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

3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：

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

例：abc@123
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单击 Register（注册）。

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