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如何使用SciFinder获取科技信息

郑州轻工业大学

2018.11.28

SCIFINDER®
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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
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

美国化学文摘社—Chemical Abstracts Service

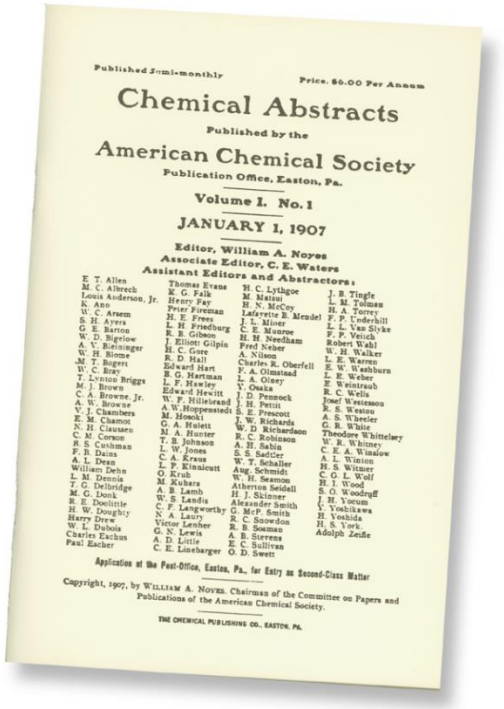
- ACS的分支机构
- 创建于1907年，简称”CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市

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



Published Semi-monthly Price, $6.00 Per Annum

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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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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

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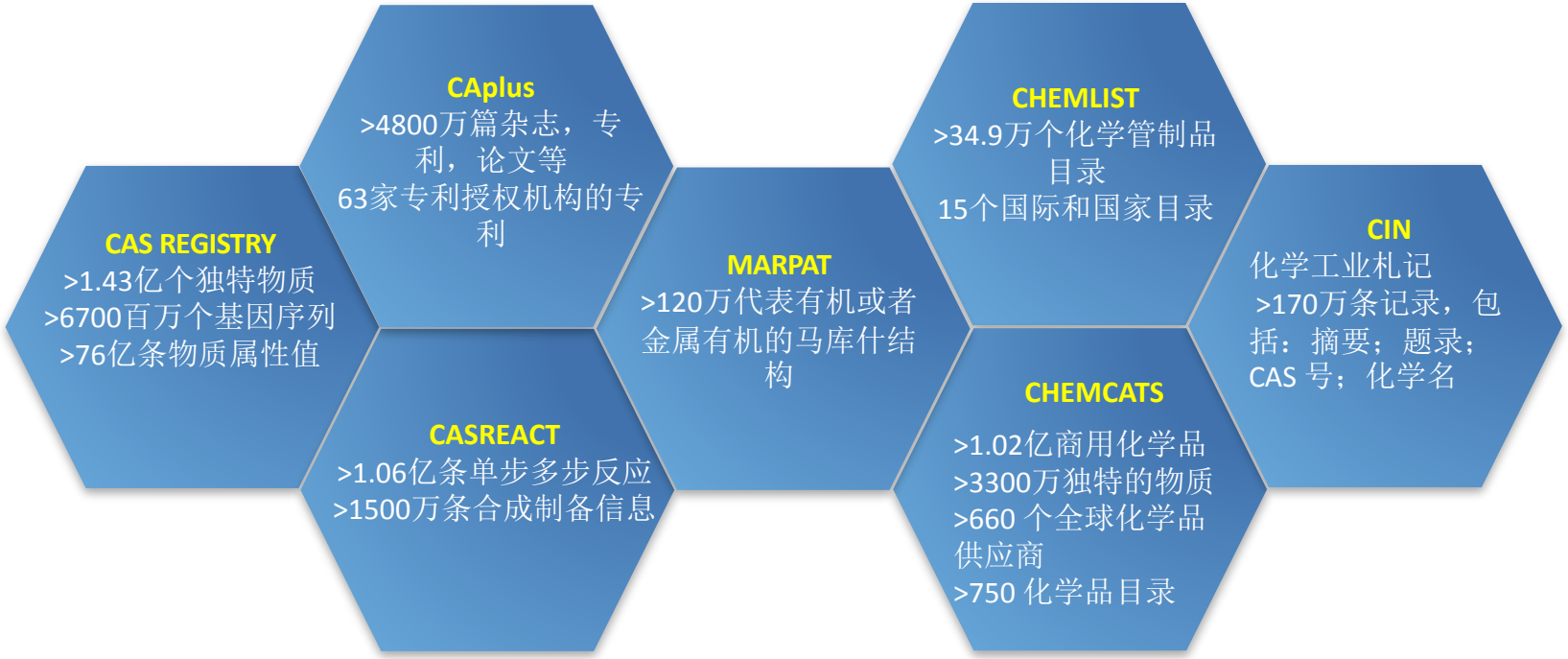

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CAS数据库——源于化学，超越化学

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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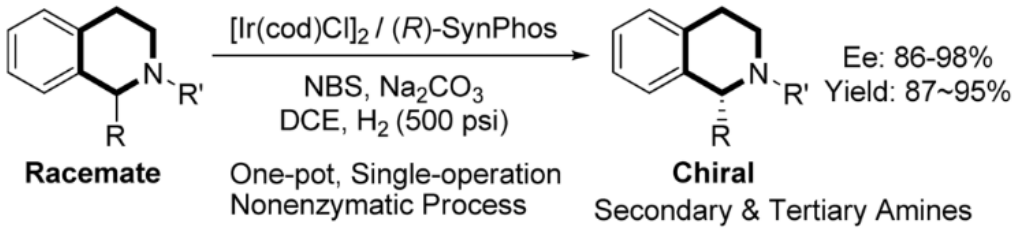
CAS数据库最具价值的内容——人工标引

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

Substances

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

Chiral ligands

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

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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Chinese Academy of Sciences
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116023

ACCESSION NUMBER
2015:1340032
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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

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。

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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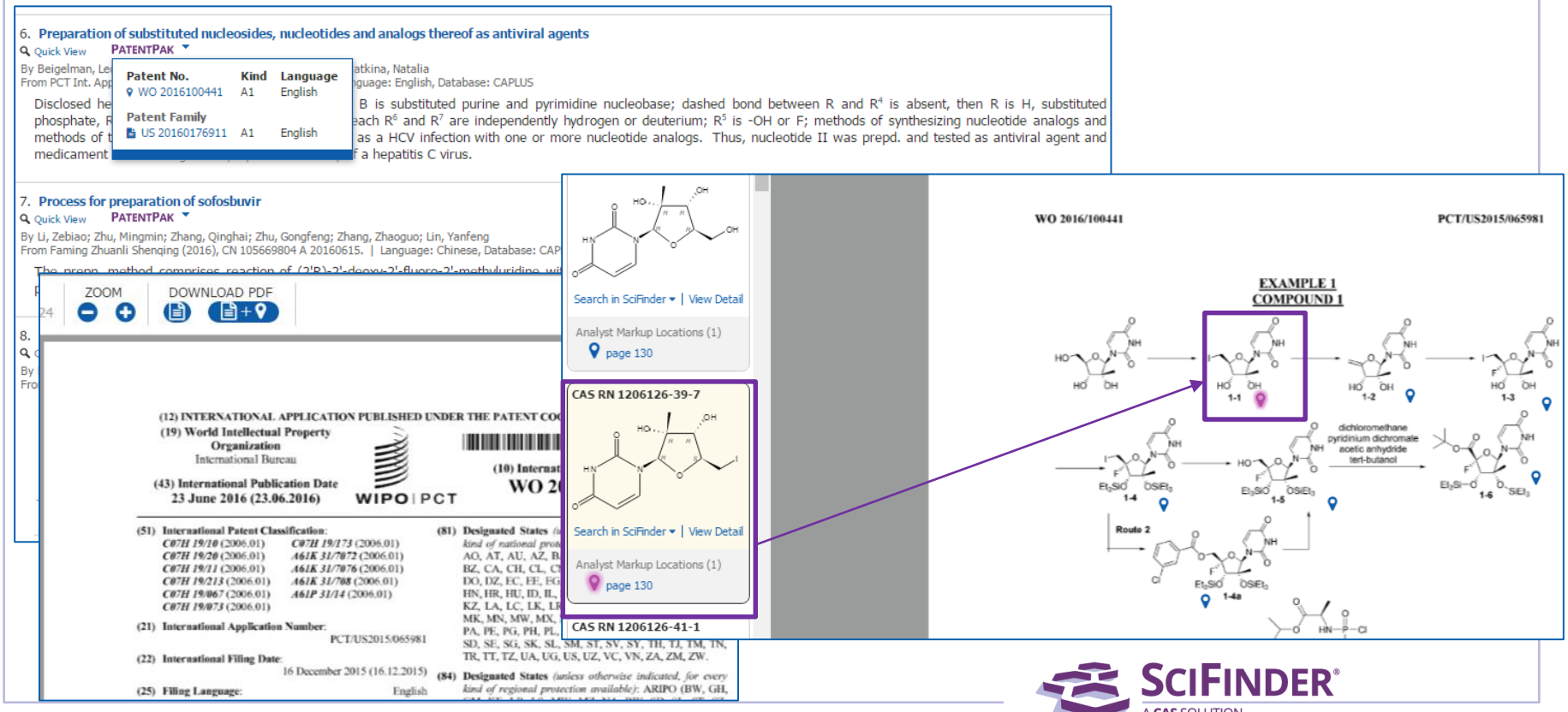
CAS最新动向—解决方案

- 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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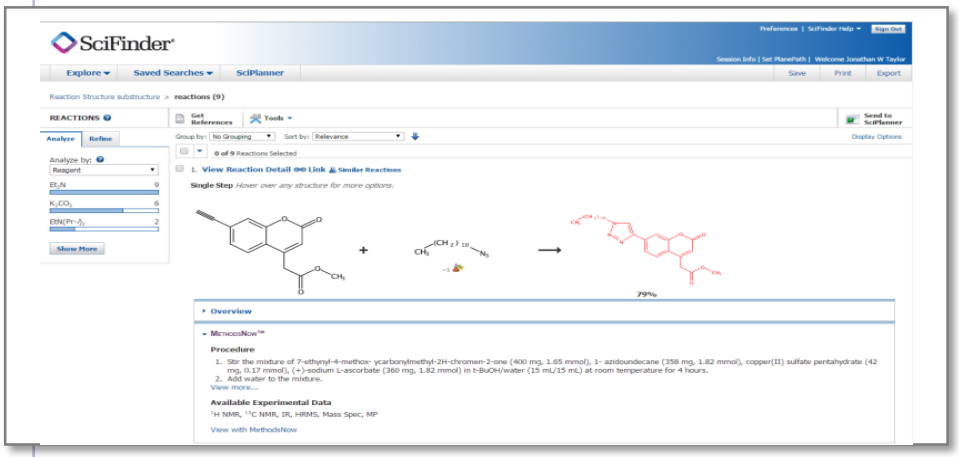
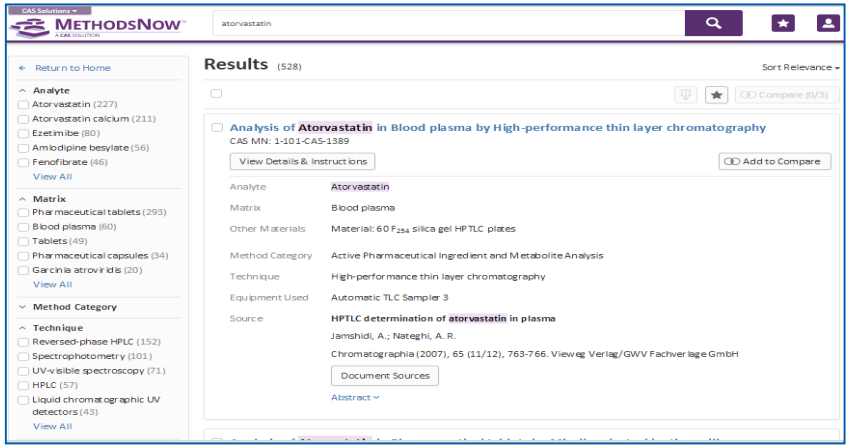
CAS最新动向—解决方案

- 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

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
- SciFinder常见问题及解决

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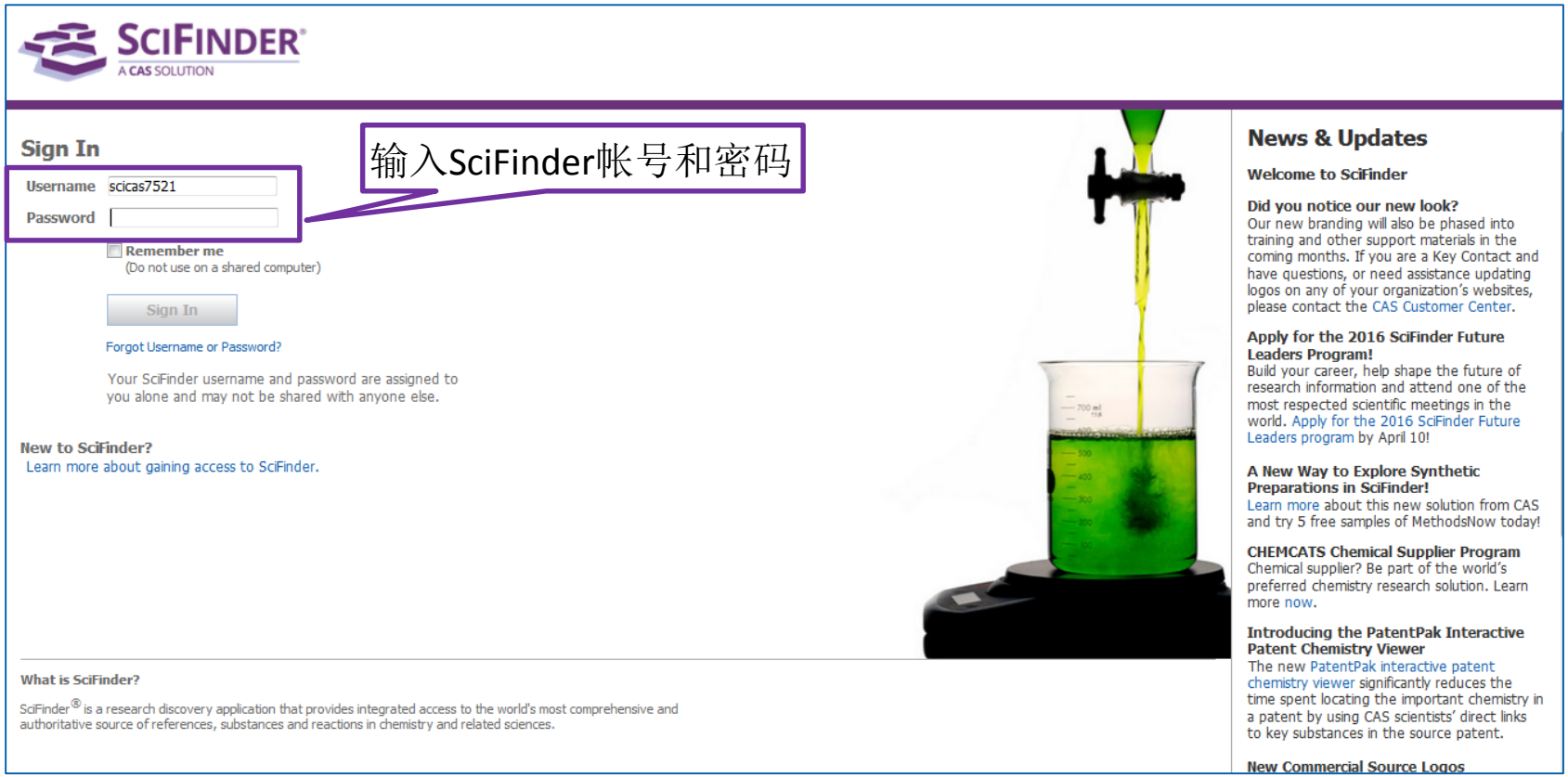
SciFinder覆盖的数据库

SciFinder® A CAS SOLUTION

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



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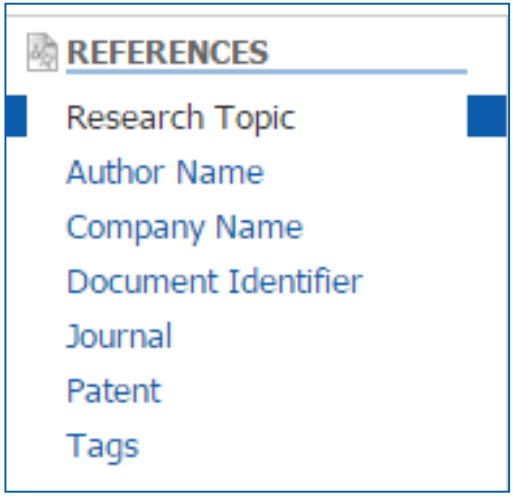
SciFinder主界面

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

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文献检索——主题

主题检索：催化剂的制备及在热分解反应中的应用

关键词：制备、催化剂、热分解反应

检索式： prepare of catalyst

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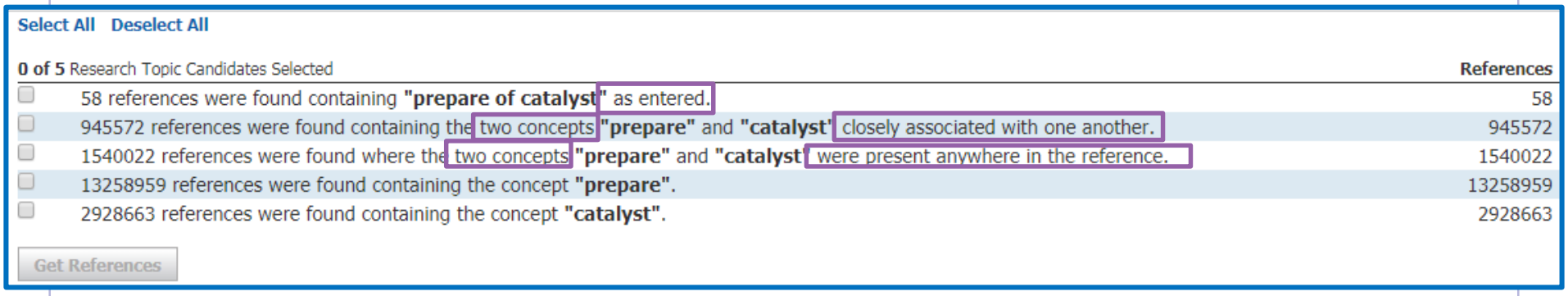
主题检索的候选项



"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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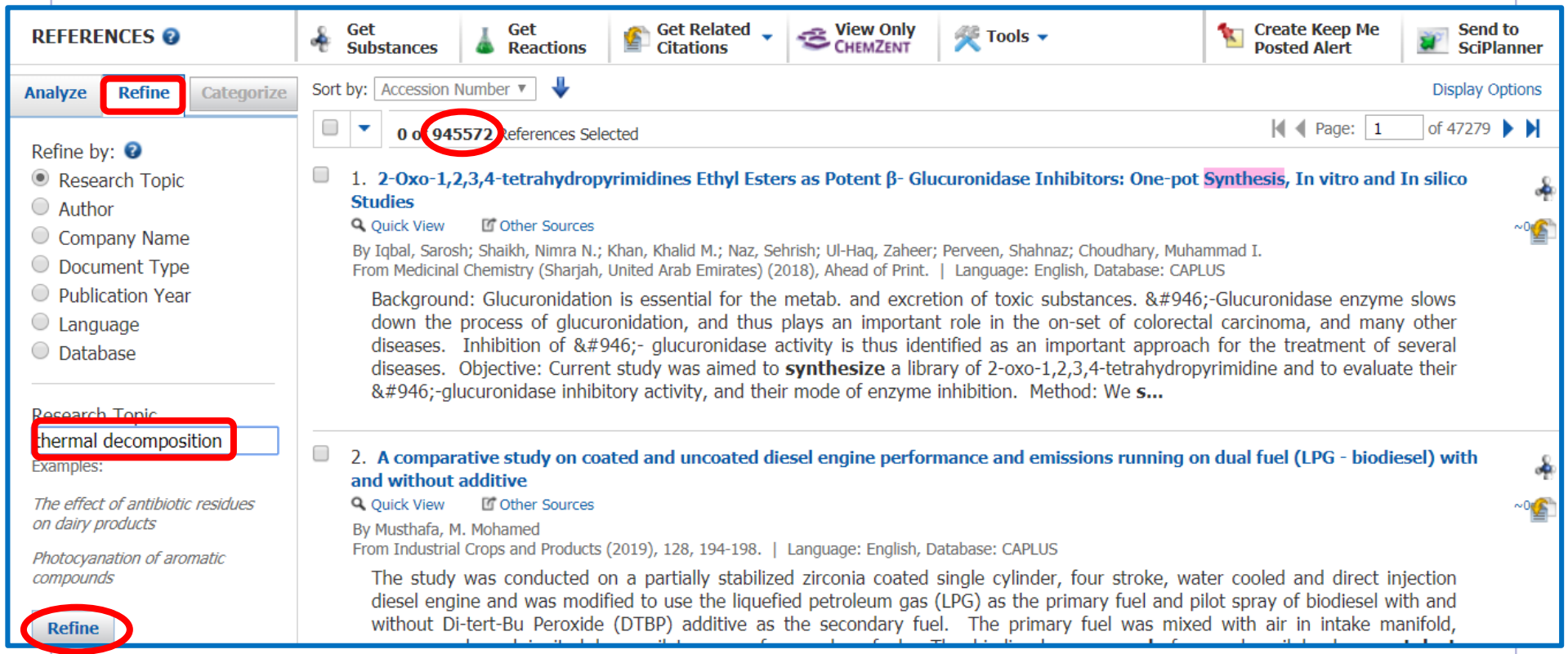
文献检索集



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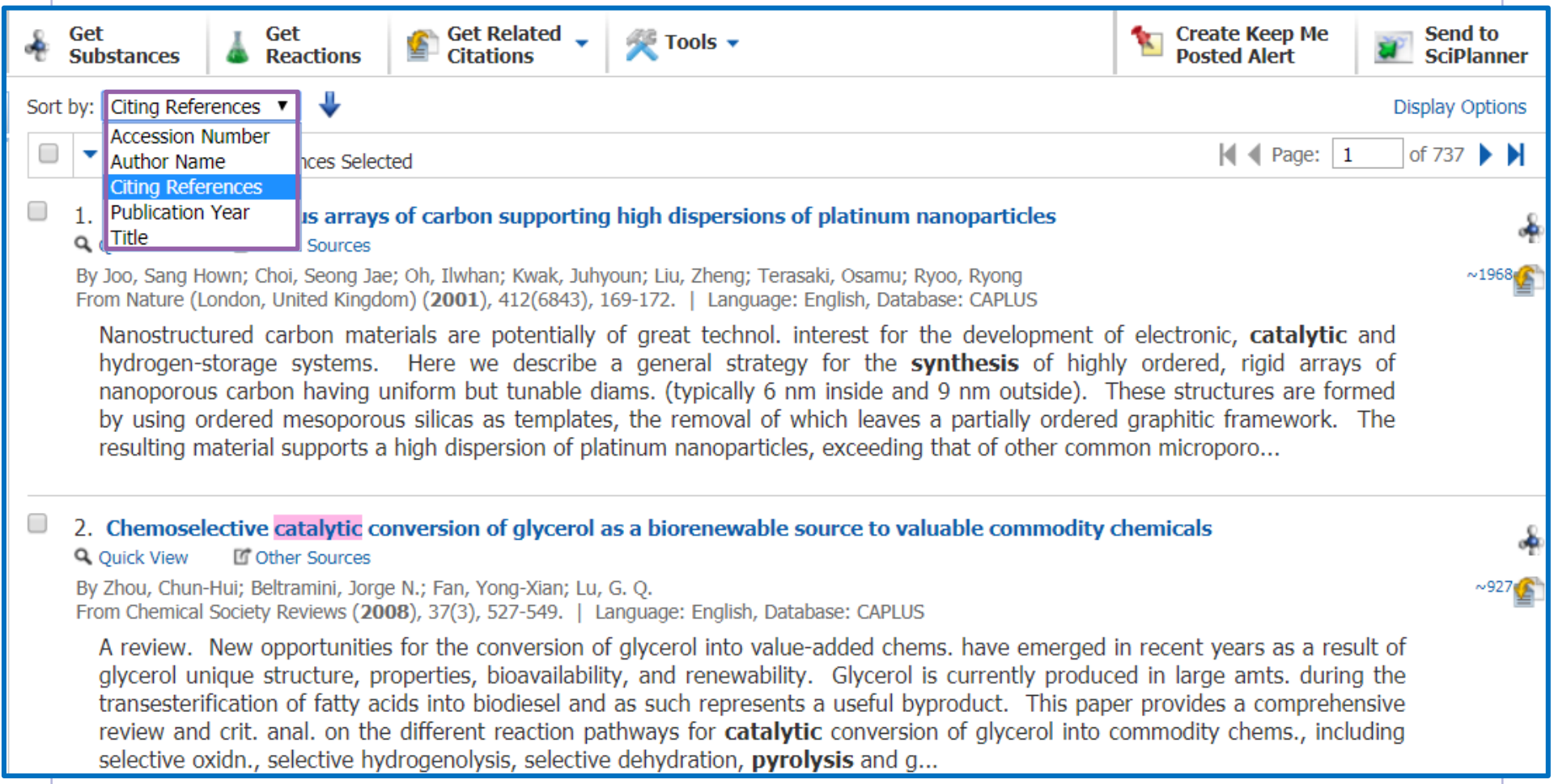
按被引次数排序— Citing References



Citing Reference: 帮助找到最重要的文献

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文献检索结果

创建Alert，追踪最新文献

文献后处理工具

获取原文

SciFinder提供强大的文献处理工具，帮助处理文献

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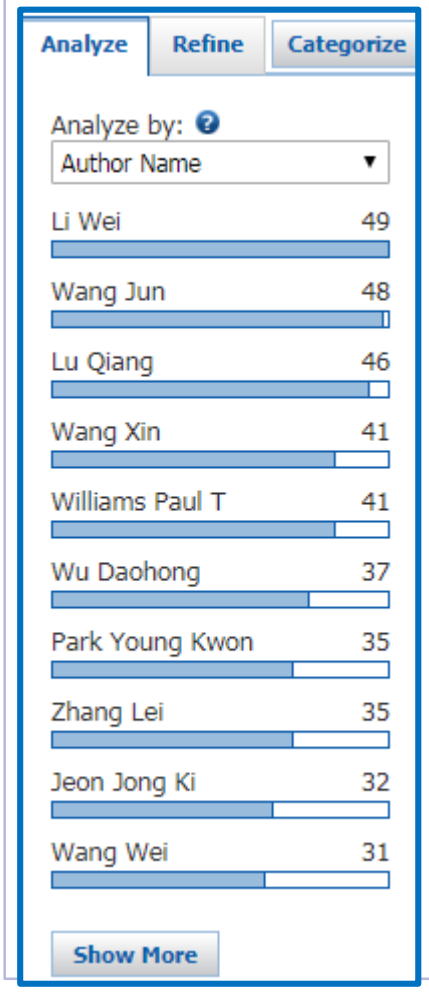
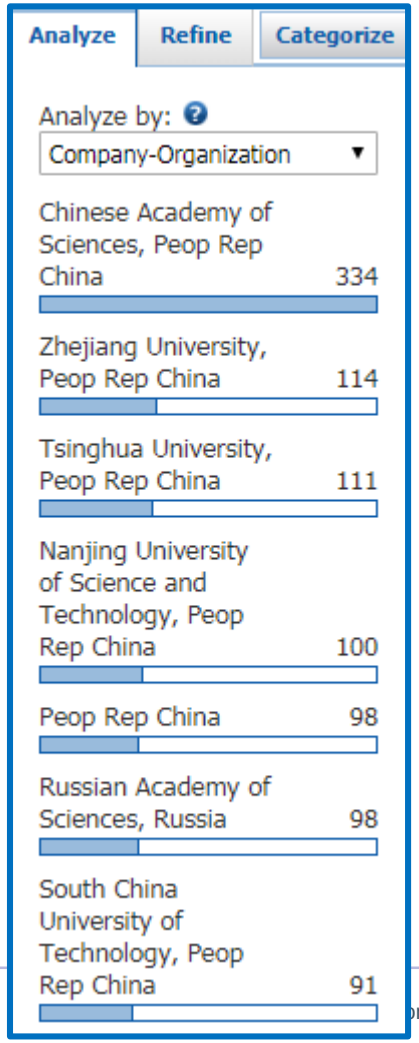
文献检索结果的Analyze

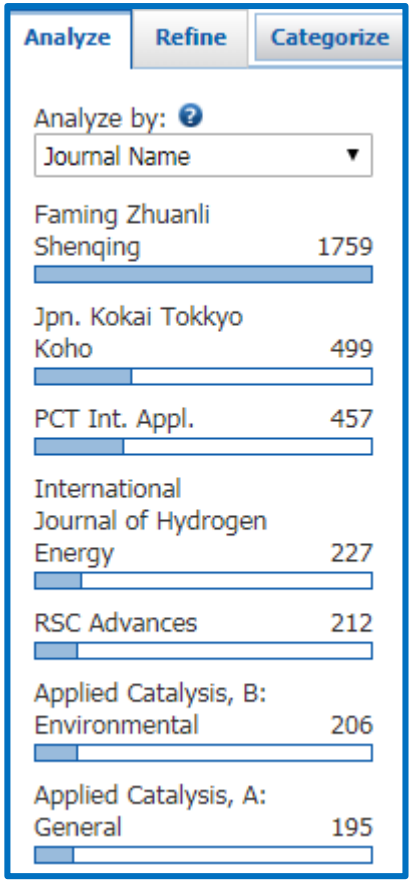
本领域研究人员



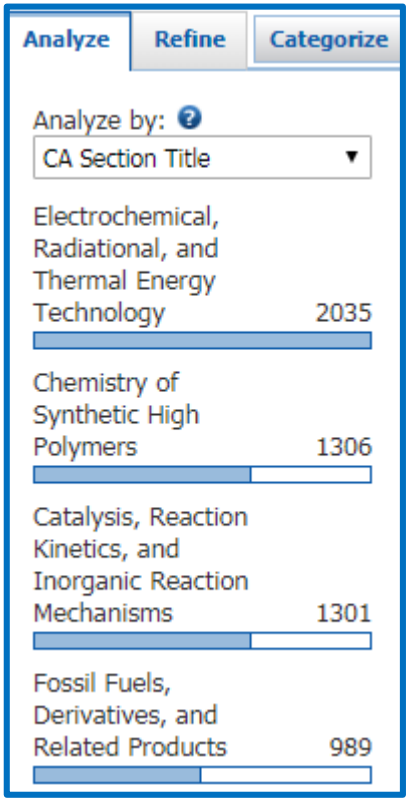
本领域研究机构、合作伙伴、竞争对手



期刊



涉及学科领域



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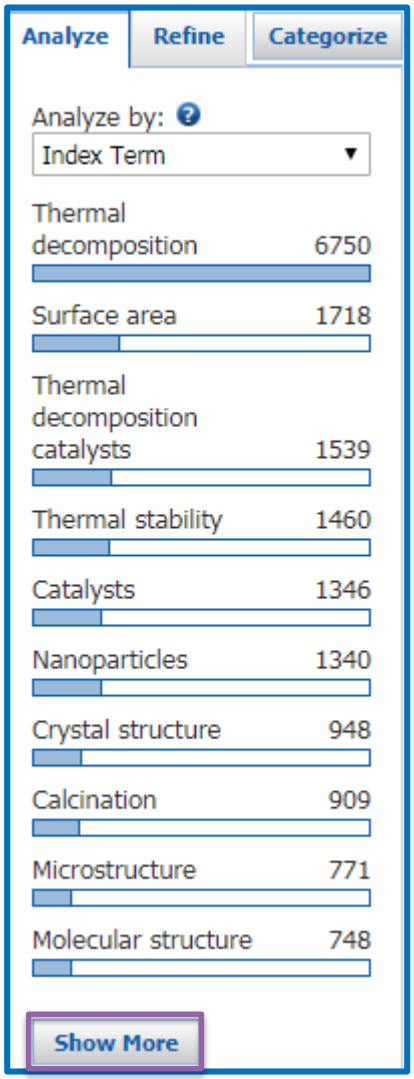
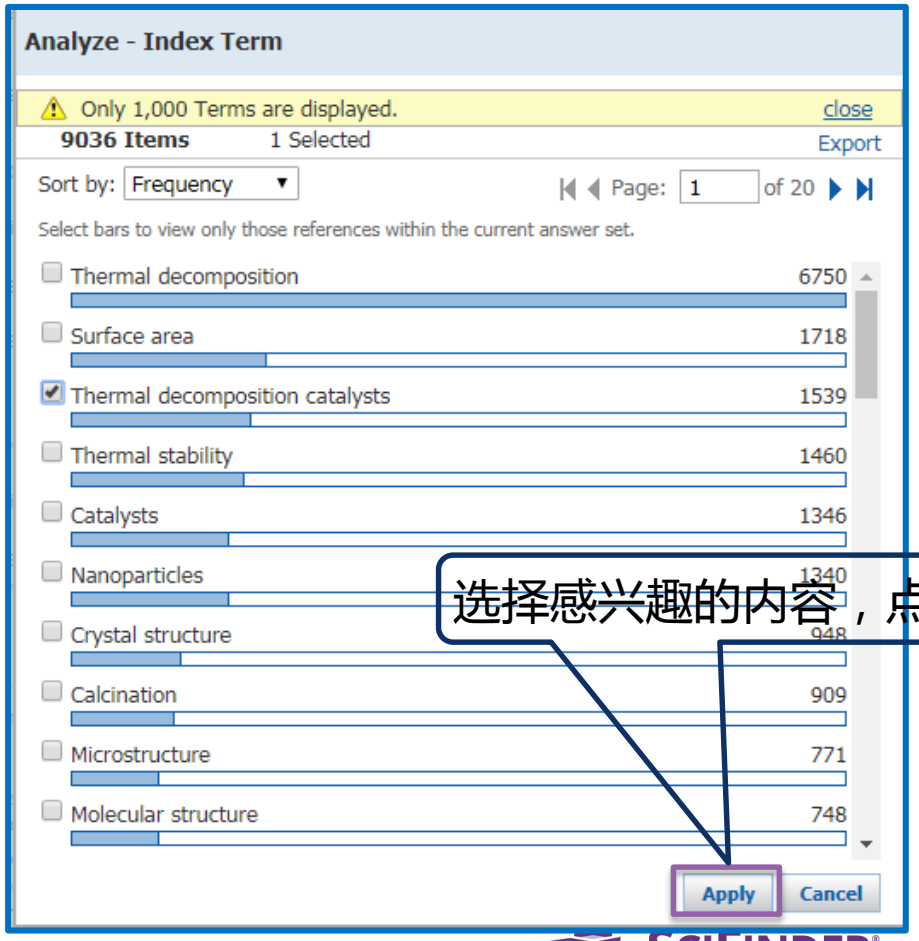
文献检索结果的Analyze



Index Term：

帮助用户了解涉及到的重要技术术语，并修正检索词



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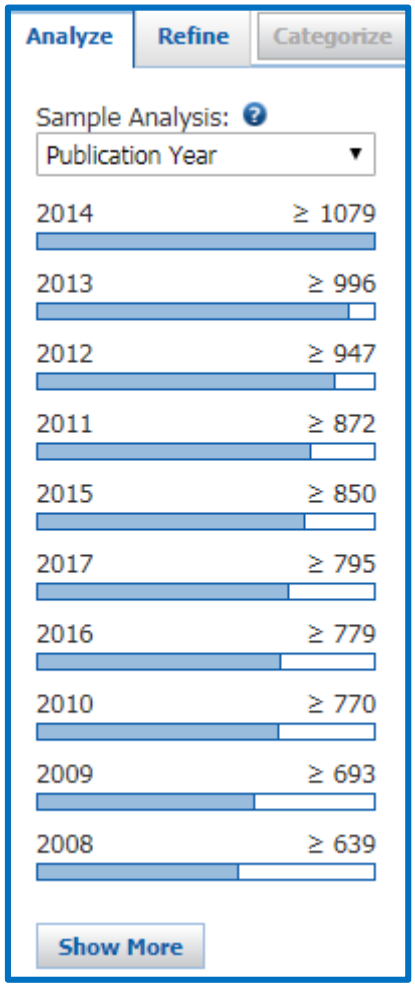
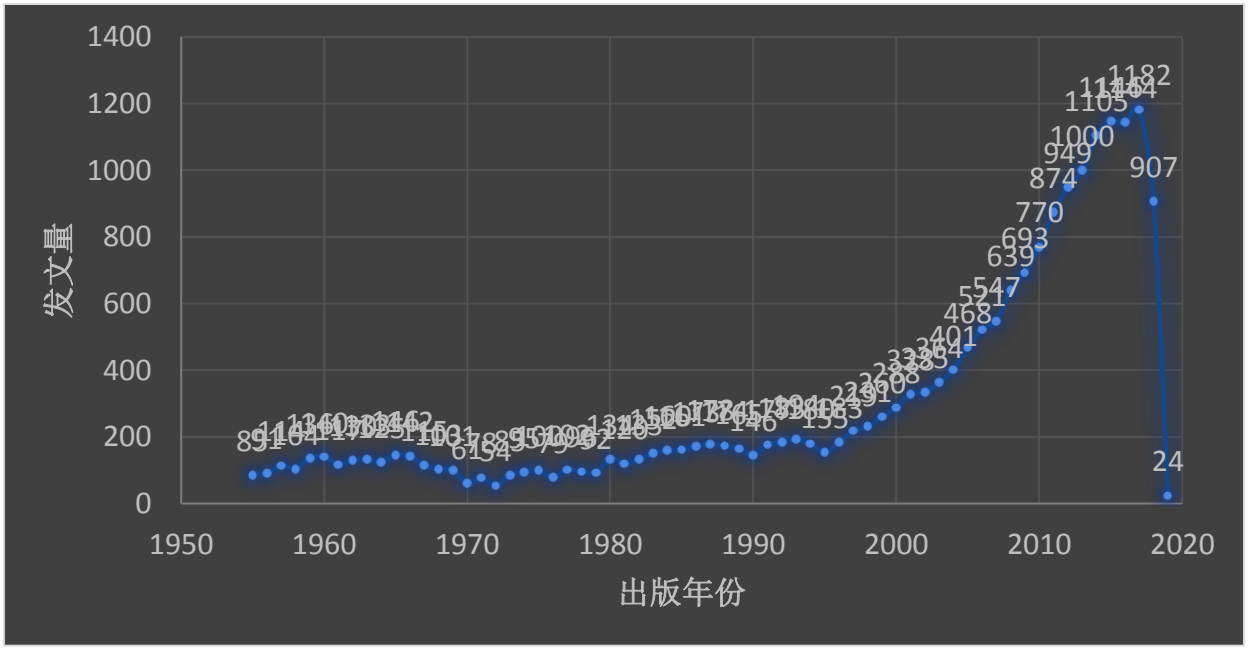
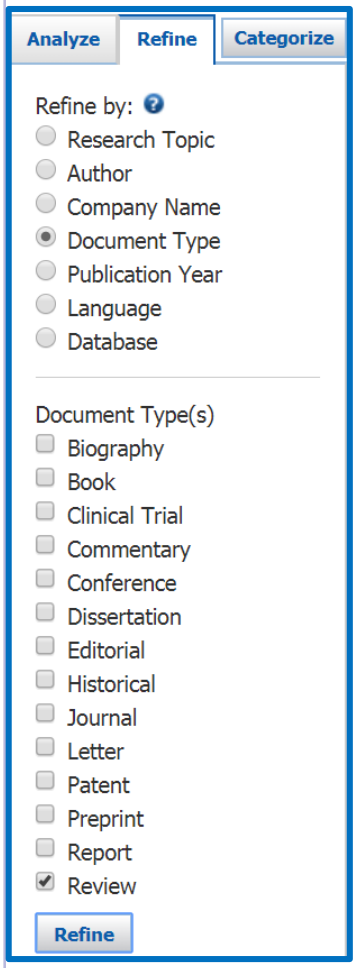
文献检索结果的Analyze

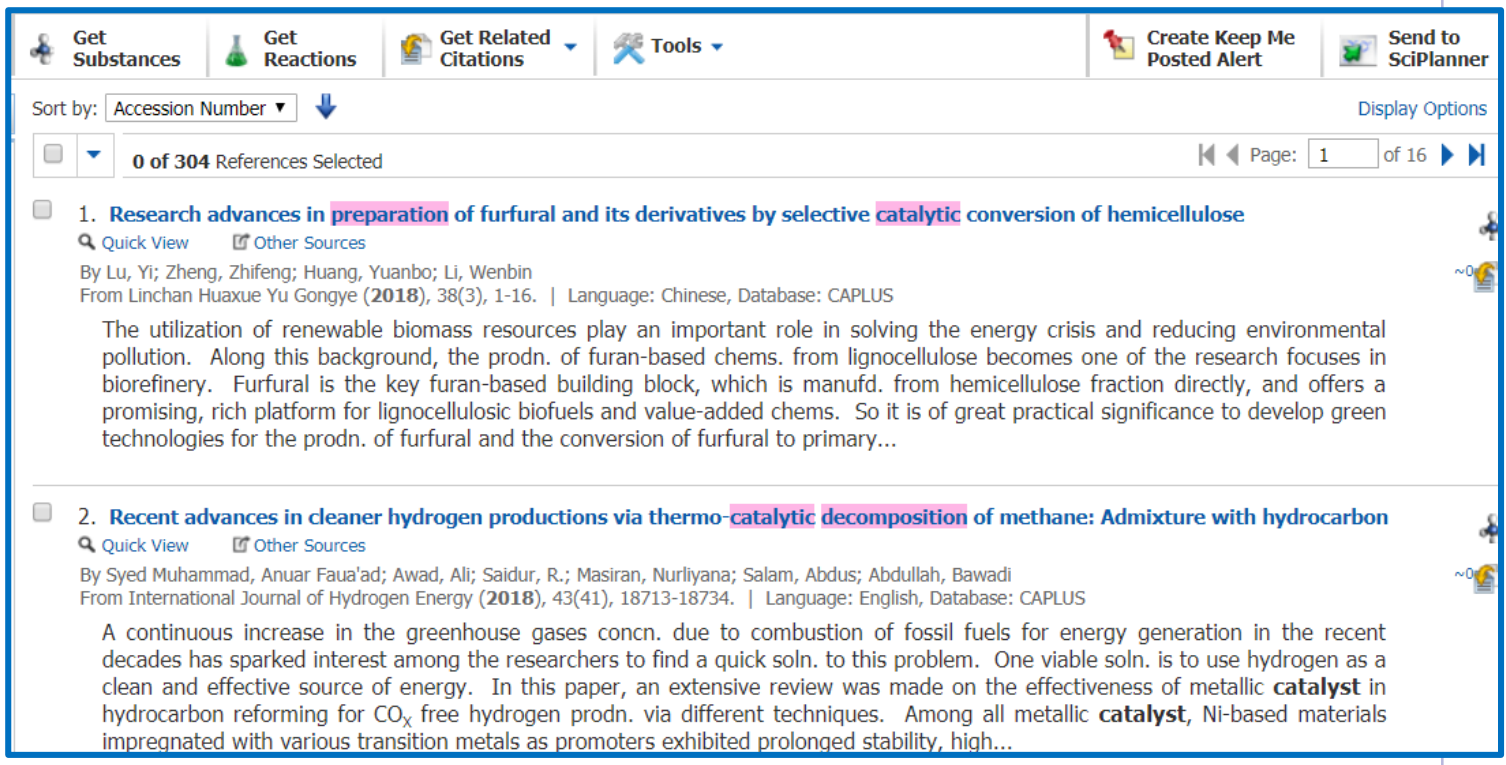




Publication Year: 分析领域发展趋势

文献检索结果的Refine





Refine：帮助用户迅速获得需要的文献

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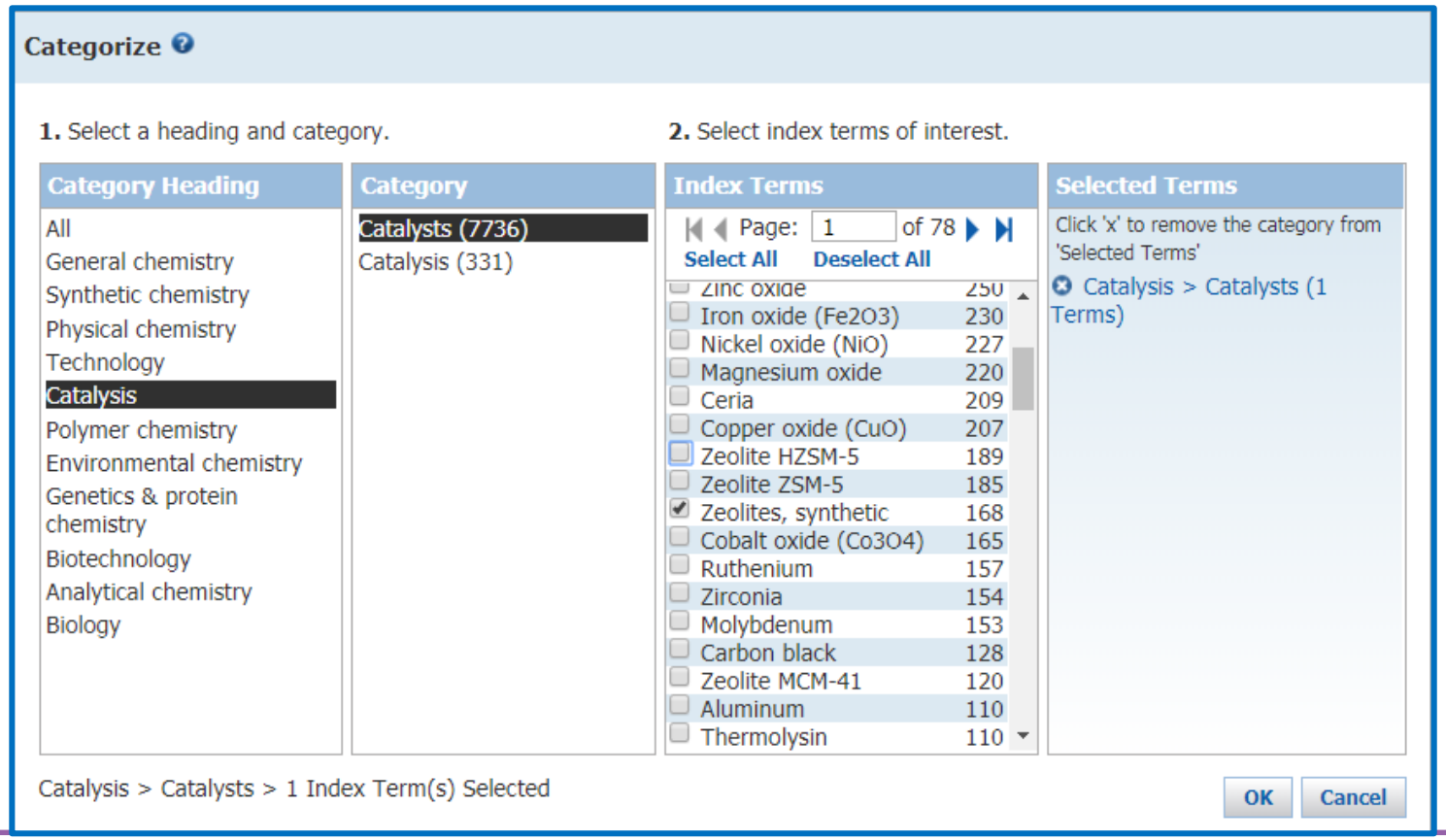
文献检索结果的Categorize

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。

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结果集的保存— Save, Print, Export

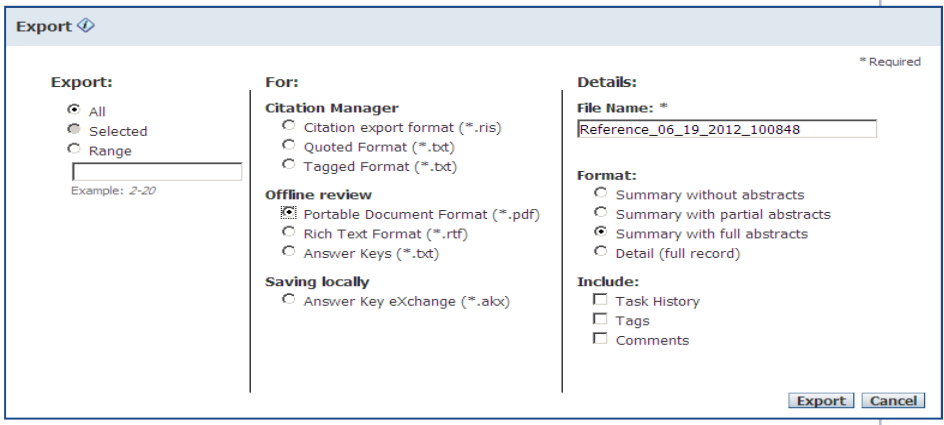
Save：保存在服务器上，方便以后登陆查看，每次可存1万条记录。

Export：导出至本地电脑。

Print：打印成PDF格式

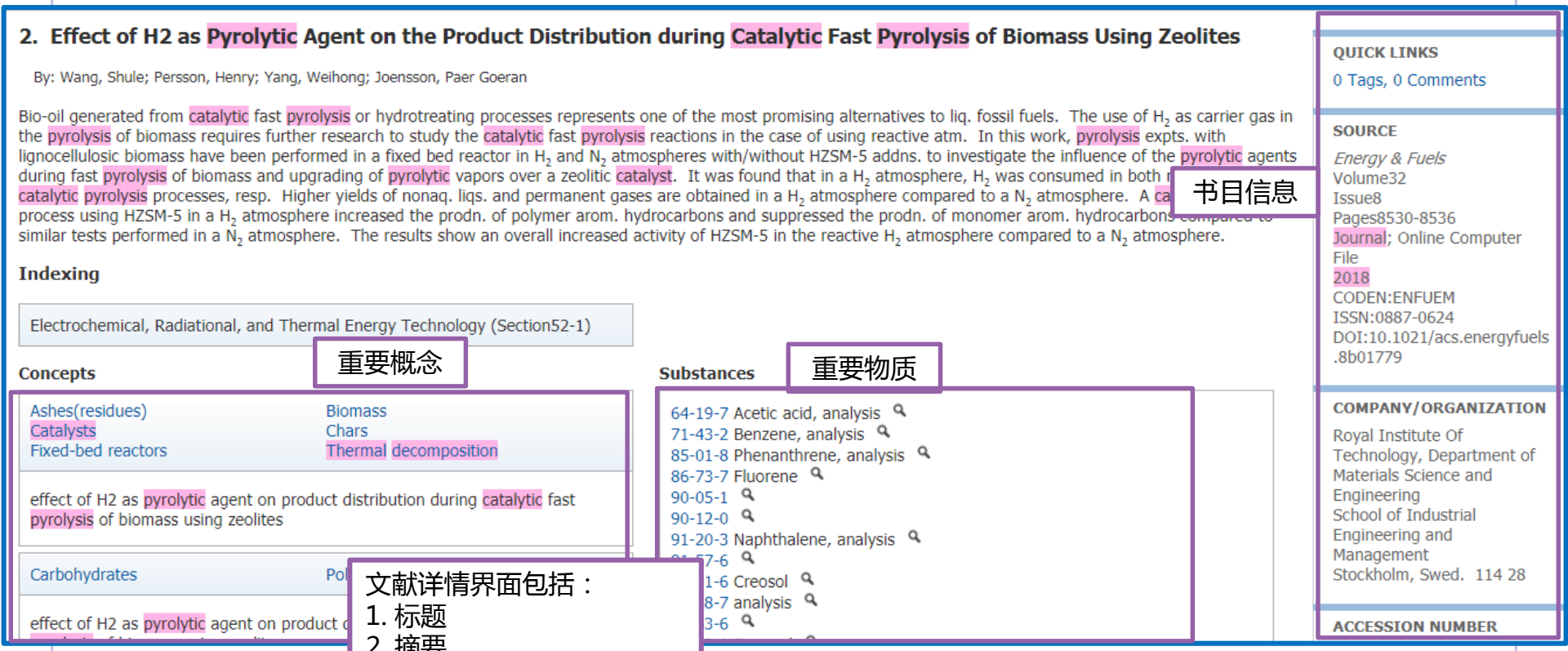
Citation manager: 保存成RIS等格式，可导入EndNote 等文献管理工具

Offline Review：保存成PDF，RTF等格式，用于脱机浏览



SciFinder® A CAS SOLUTION

文献信息—题录、摘要、索引



2. Effect of H2 as Pyrolytic Agent on the Product Distribution during Catalytic Fast Pyrolysis of Biomass Using Zeolites

By: Wang, Shule; Persson, Henry; Yang, Weihong; Joensson, Paer Goeran

Bio-oil generated from catalytic fast pyrolysis or hydrotreating processes represents one of the most promising alternatives to liq. fossil fuels. The use of H_2 as carrier gas in the pyrolysis of biomass requires further research to study the catalytic fast pyrolysis reactions in the case of using reactive atm. In this work, pyrolysis expts. with lignocellulosic biomass have been performed in a fixed bed reactor in H_2 and N_2 atmospheres with/without HZSM-5 addns. to investigate the influence of the pyrolytic agents during fast pyrolysis of biomass and upgrading of pyrolytic vapors over a zeolitic catalyst. It was found that in a H_2 atmosphere, H_2 was consumed in both n catalytic pyrolysis processes, resp. Higher yields of nonaq. liqs. and permanent gases are obtained in a H_2 atmosphere compared to a N_2 atmosphere. A ca process using HZSM-5 in a H_2 atmosphere increased the prodn. of polymer arom. hydrocarbons and suppressed the prodn. of monomer arom. hydrocarbons compared to similar tests performed in a N_2 atmosphere. The results show an overall increased activity of HZSM-5 in the reactive H_2 atmosphere compared to a N_2 atmosphere.

书目信息

Indexing

Electrochemical, Radiational, and Thermal Energy Technology (Section52-1)

重要概念

Concepts

Ashes(residues) Biomass
Catalysts Chars
Fixed-bed reactors Thermal decomposition

effect of H2 as pyrolytic agent on product distribution during catalytic fast pyrolysis of biomass using zeolites

Carbohydrates Pol

effect of H2 as pyrolytic agent on product d

重要物质

Substances

64-19-7 Acetic acid, analysis
71-43-2 Benzene, analysis
85-01-8 Phenanthrene, analysis
86-73-7 Fluorene
90-05-1
90-12-0
91-20-3 Naphthalene, analysis
1-6 Creosol
8-7 analysis
3-6

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Energy & Fuels
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2018
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ISSN:0887-0624
DOI:10.1021/acs.energyfuels.8b01779

COMPANY/ORGANIZATION

Royal Institute Of Technology, Department of Materials Science and Engineering
School of Industrial Engineering and Management
Stockholm, Swed. 114 28

ACCESSION NUMBER

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

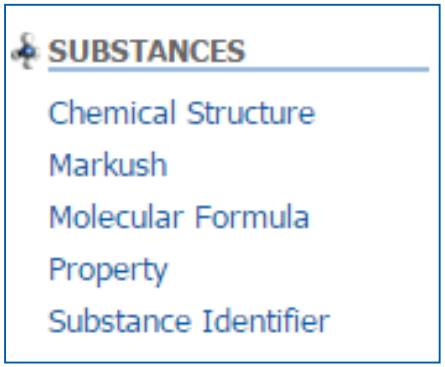
SCIFINDER®
A CAS SOLUTION

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
- SciFinder常见问题及解决

SciFinder检索选项——物质检索

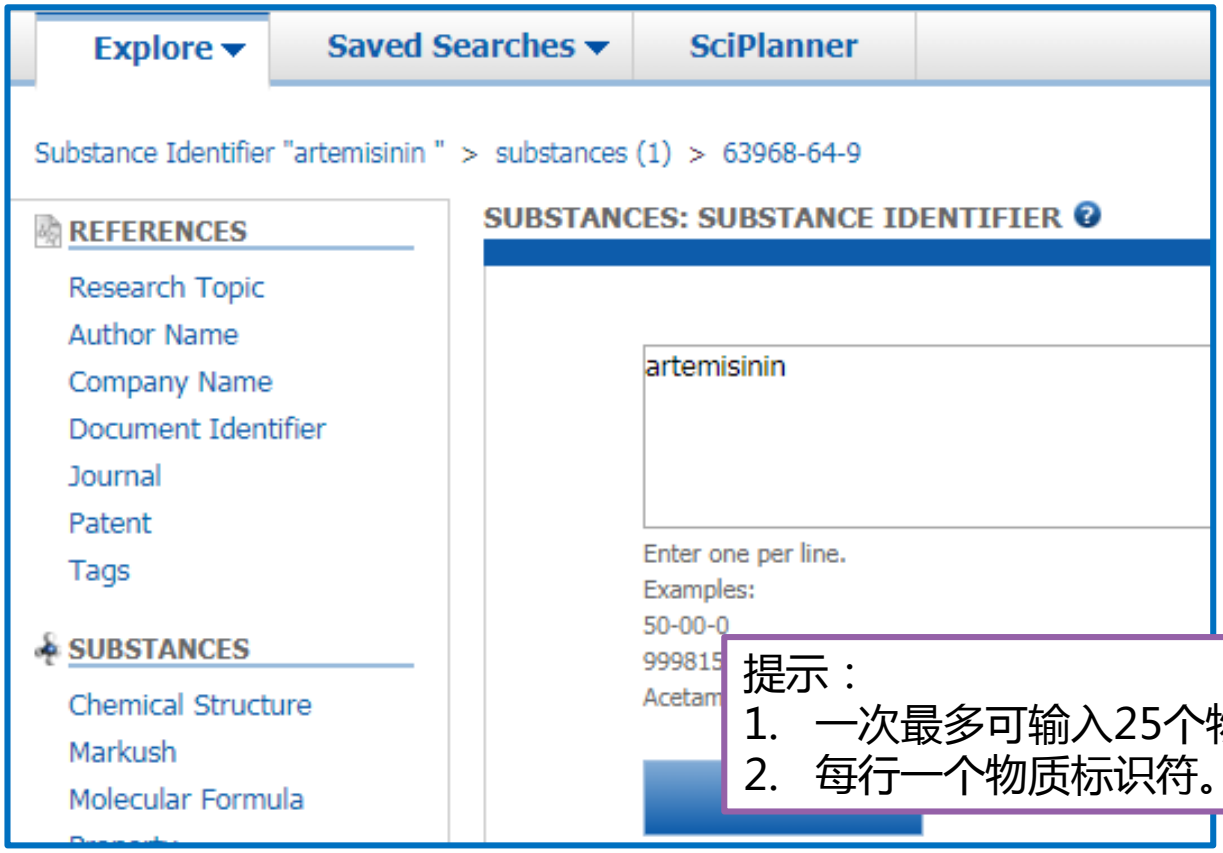
- 物质检索方法
  - —结构式检索
  - —分子式检索
  - —理化性质检索
  - —物质标识符检索：化学名称，CAS RN



- 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

SciFinder® A CAS SOLUTION

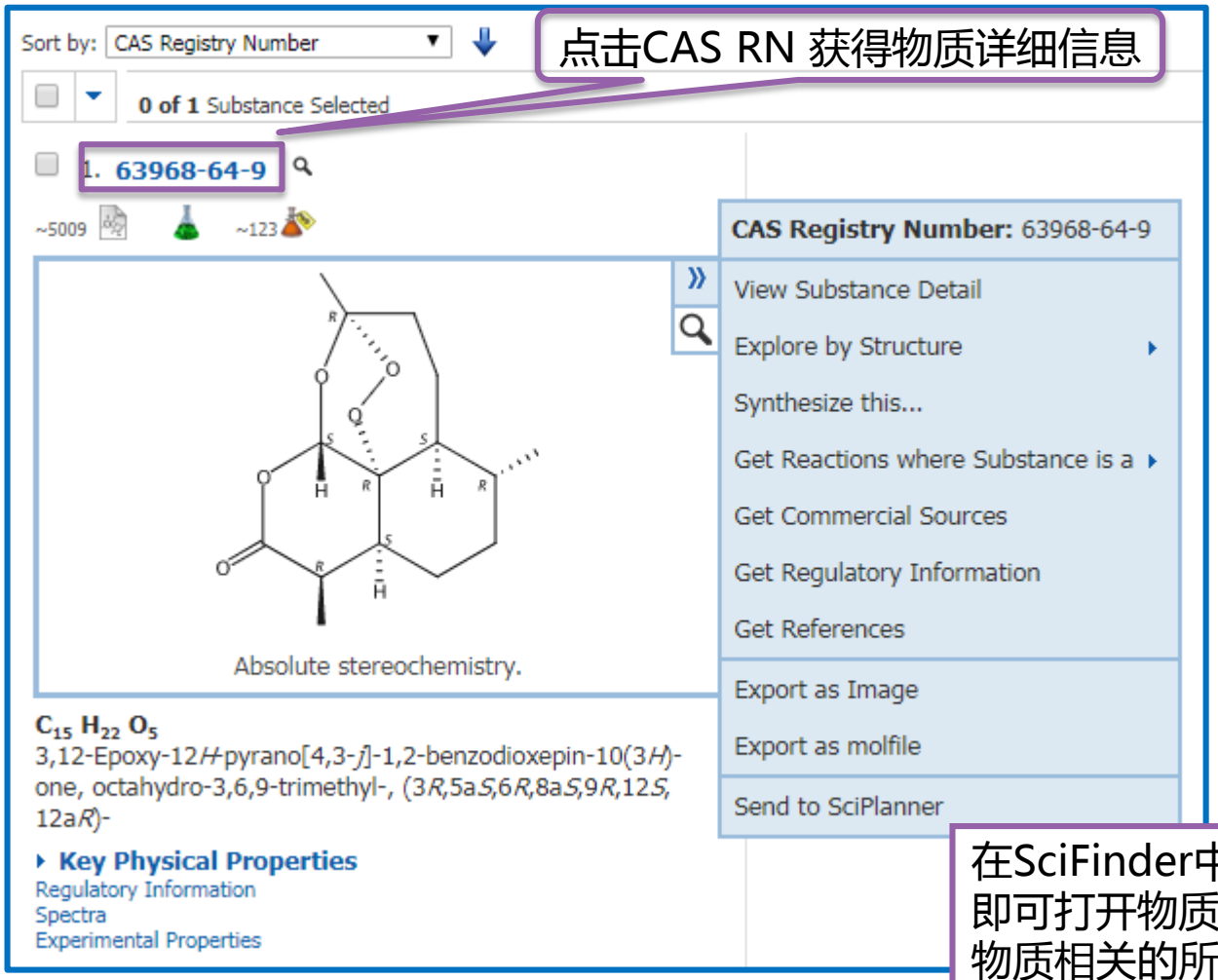
物质检索——标识符检索



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® A CAS SOLUTION

SciFinder中的物质记录



点击CAS RN 获得物质详细信息

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

SCIFINDER® A CAS SOLUTION

SciFinder中的物质记录

SUBSTANCE DETAIL | Get References | Get Reactions | Get Commercial Sources

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*)-

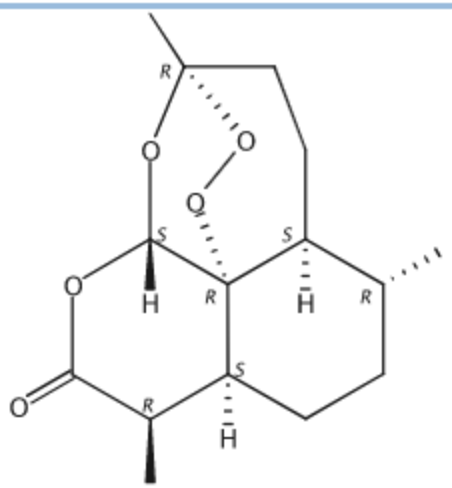
Molecular Weight
282.33

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...

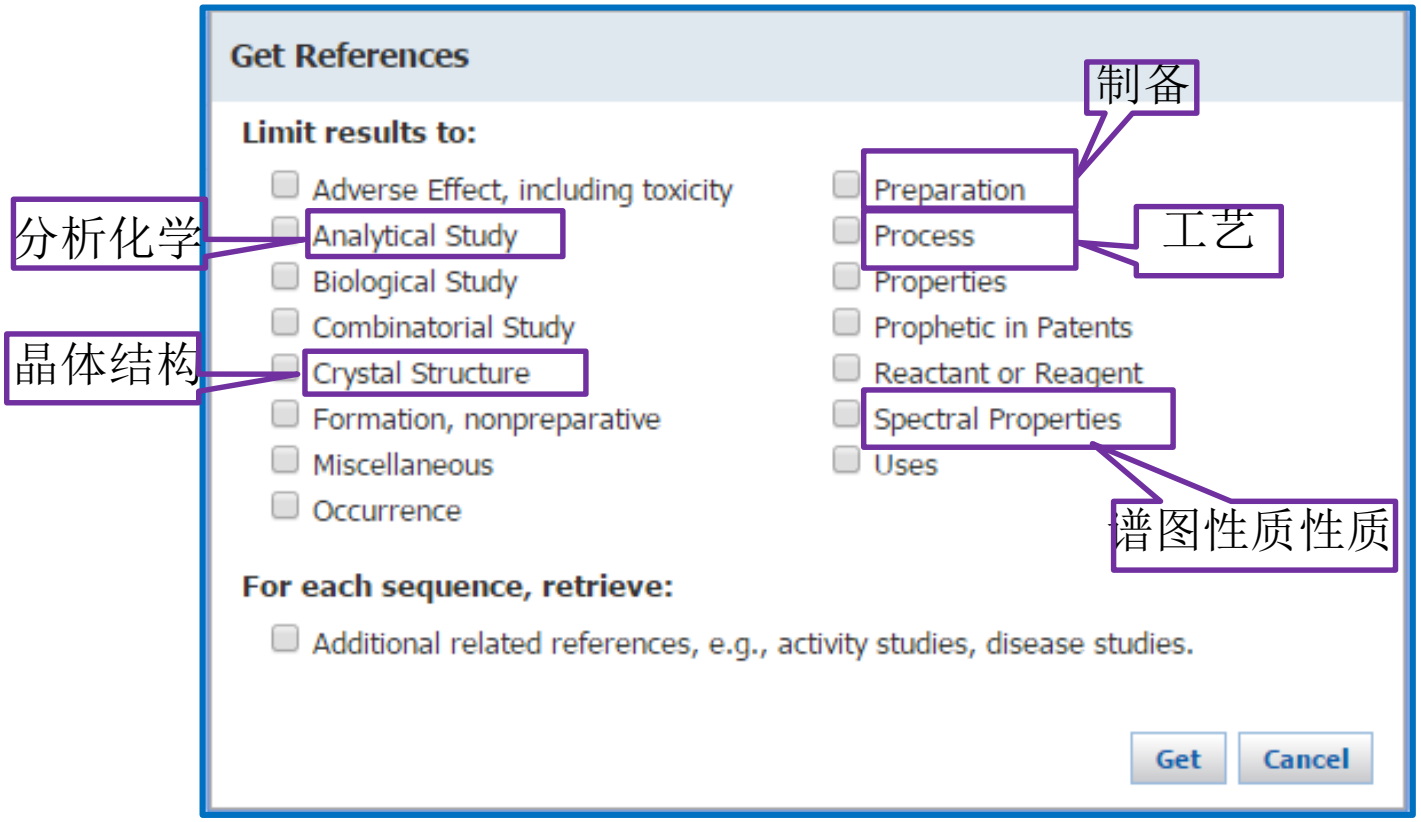


Absolute stereochemistry.

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

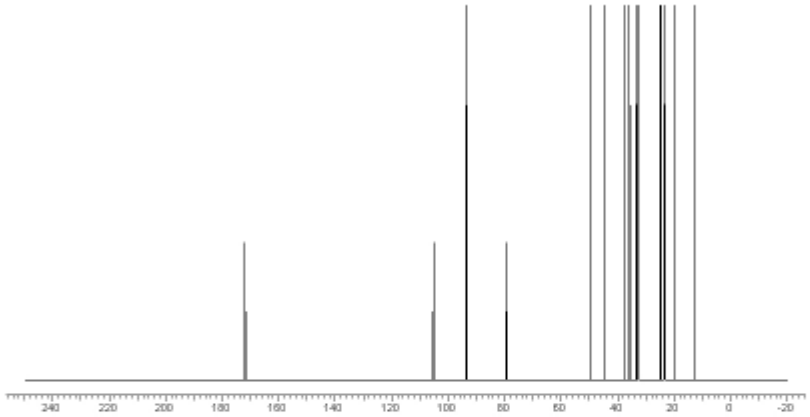
EXPERIMENTAL SPECTRA

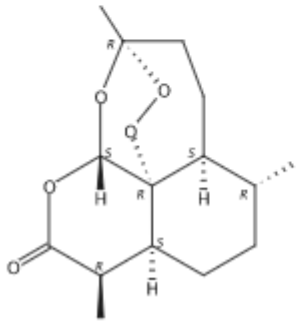
^{1}H NMR | ^{13}C NMR | Hetero NMR | IR | Mass | Raman

^{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

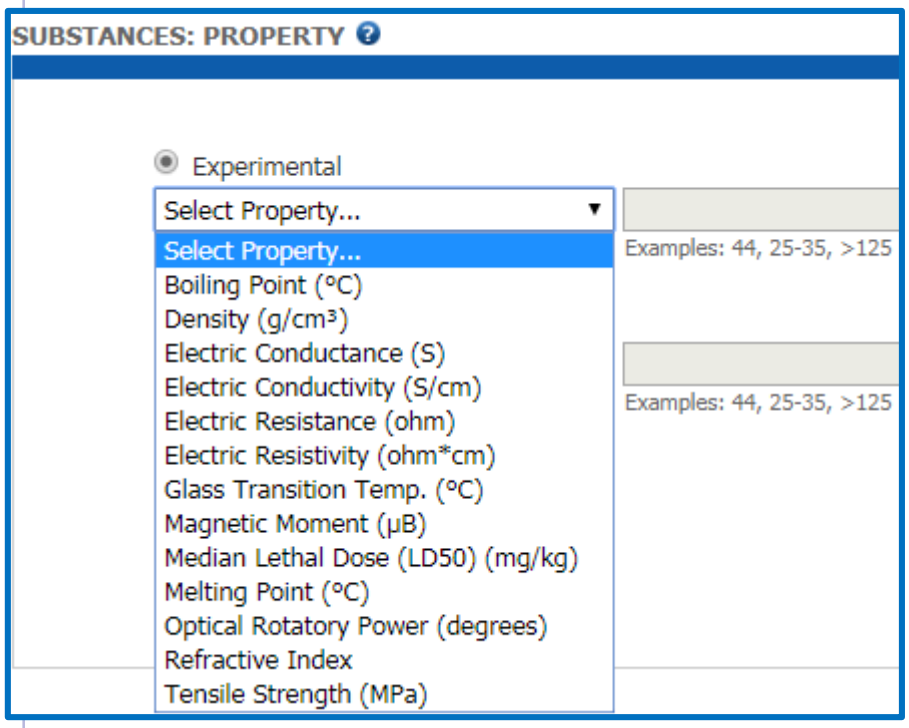
SOURCE

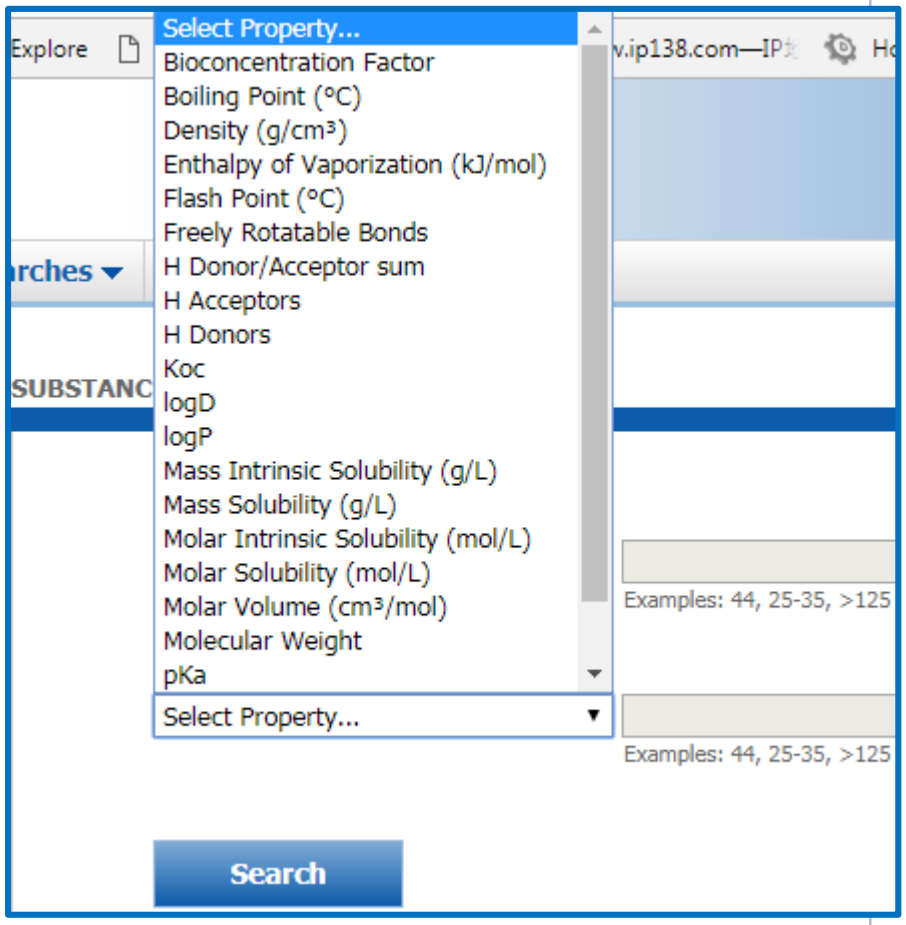
Spectral data were obtained from Advanced Chemistry Development, Inc.

Absolute stereochemistry

SciFinder® A CAS SOLUTION

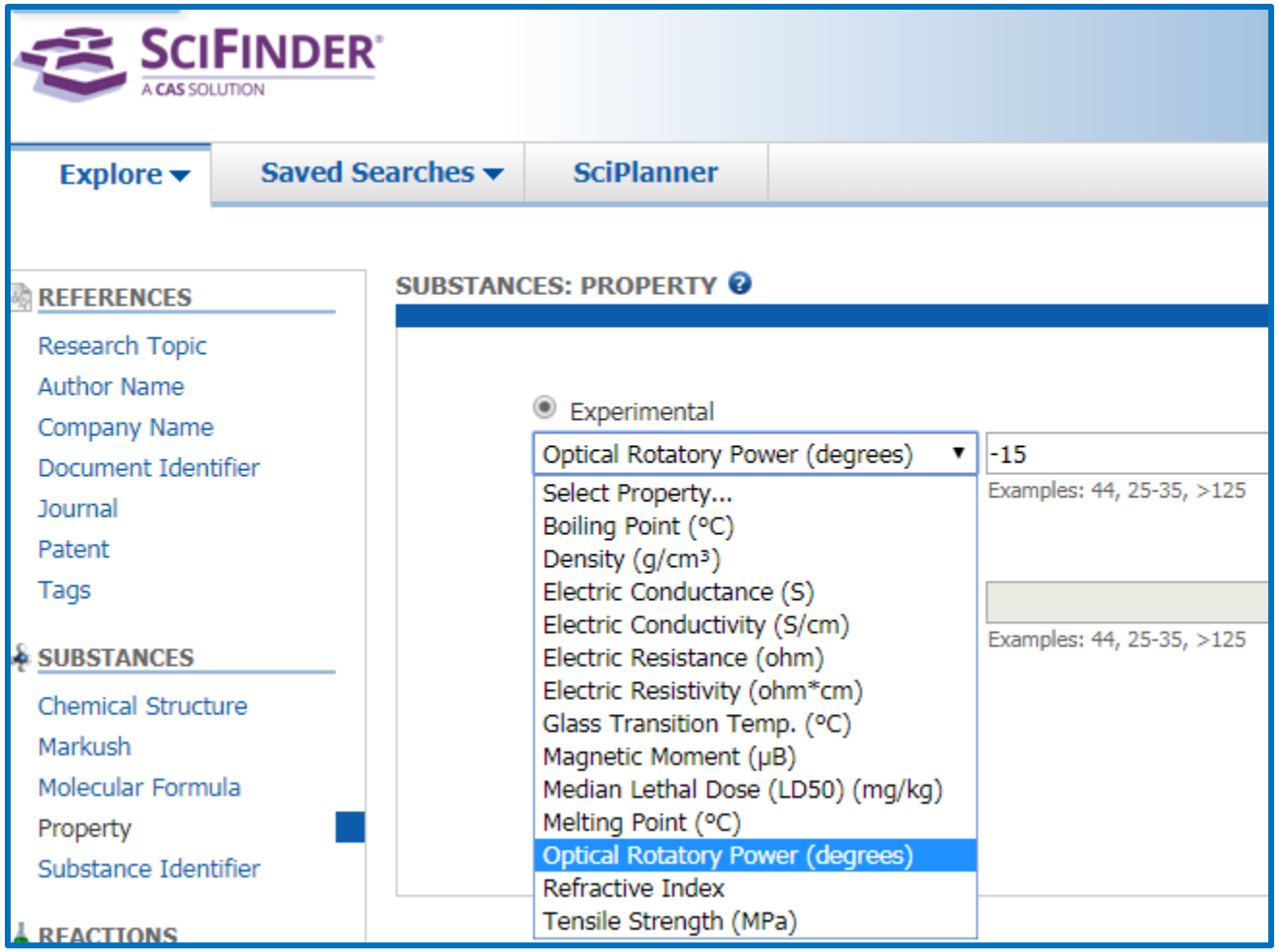
物质检索——理化性质性质检索





SciFinder® A CAS SOLUTION

物质检索——理化性质检索：寻找旋光值为-15°的物质



SciFinder物质检索结果

SUBSTANCES | Get References | Get Reactions | Get Commercial Sources | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine

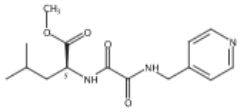
Sort by: CAS Registry Number | Display Options

0 of 1193 Substances Selected | Page: 1 of 80

Analyze by: Substance Role

Preparation	1081
Reactant or Reagent	658
Properties	362
Biological Study	361
Uses	237
Occurrence	140
Process	140
Analytical Study	132
Formation, Nonpreparative	92
Prophetic in Patents	39

1. 1433200-70-4

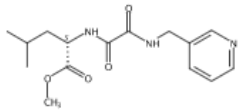


Absolute stereochemistry.

$C_{15}H_{21}N_3O_4$
L-Leucine, *N*-[2-oxo-2-[(4-pyridinylmethyl)amino]acetyl]-, methyl ester

Key Physical Properties
Experimental Properties

2. 1433200-67-9

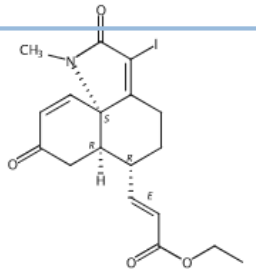


Absolute stereochemistry.

$C_{15}H_{21}N_3O_4$
L-Leucine, *N*-[2-oxo-2-[(3-pyridinylmethyl)amino]acetyl]-, methyl ester

Key Physical Properties
Experimental Properties

3. 1346255-54-6



Double bond geometry as shown.,Relative stereochemistry.

$C_{18}H_{20}INO_4$
2-Propenoic acid, 3-[(6*R*,6a*R*,10a*S*)-1,2,4,5,6,6a,7,8-octahydro-3-iodo-1-methyl-2,8-dioxobenz[*h*]indol-6-yl]-, ethyl ester, (2*E*)-*rel*-

Key Physical Properties
Experimental Properties

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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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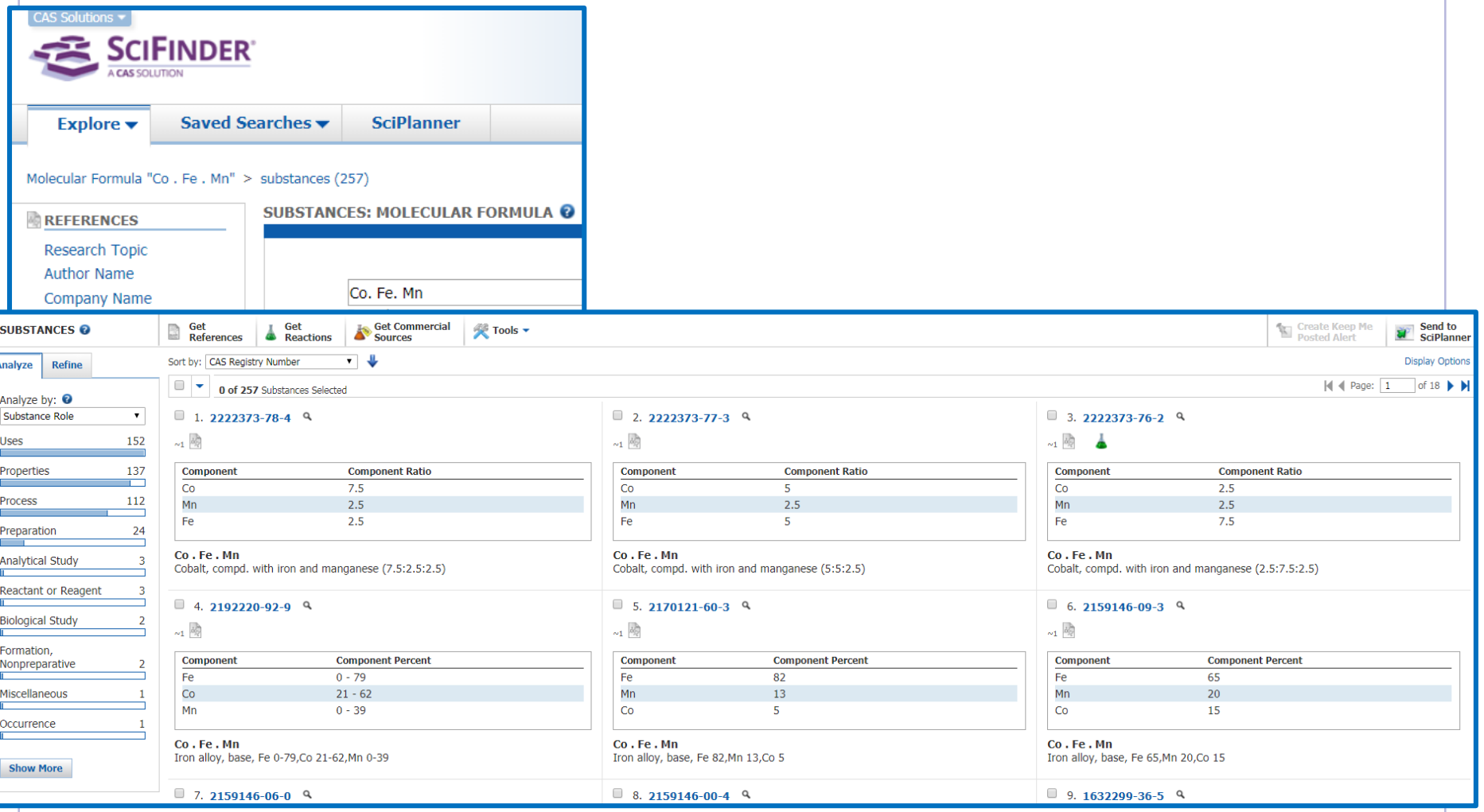
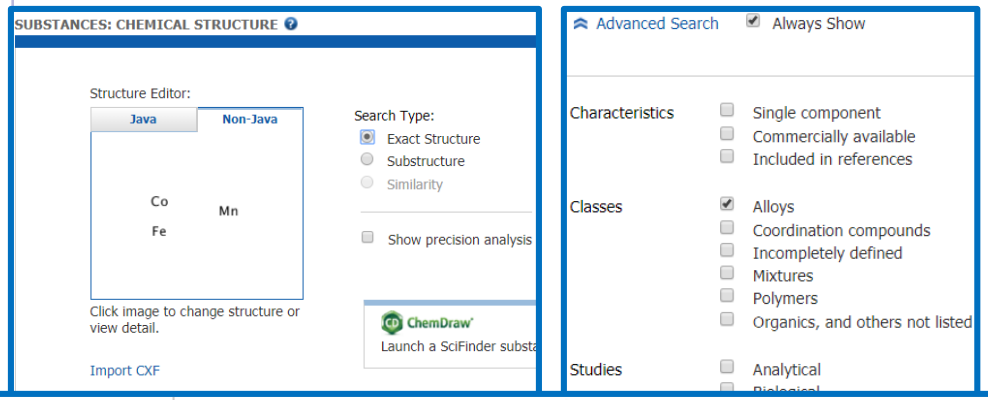
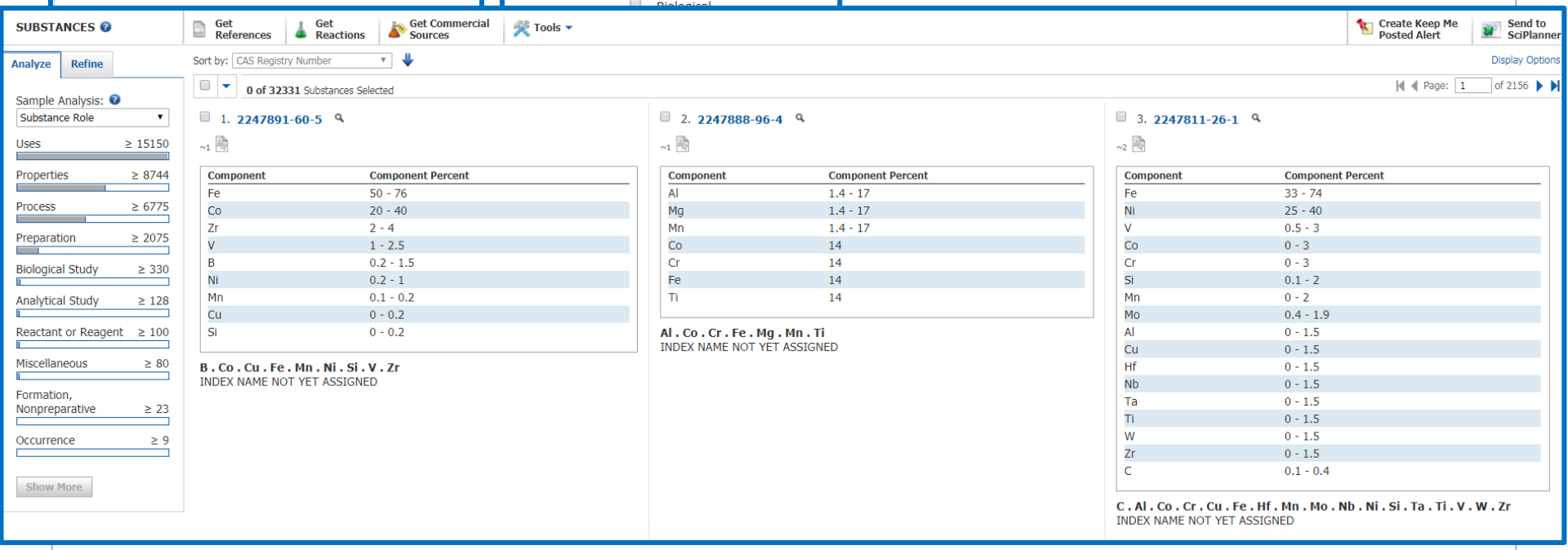
合金的检索——钴铁锰合金

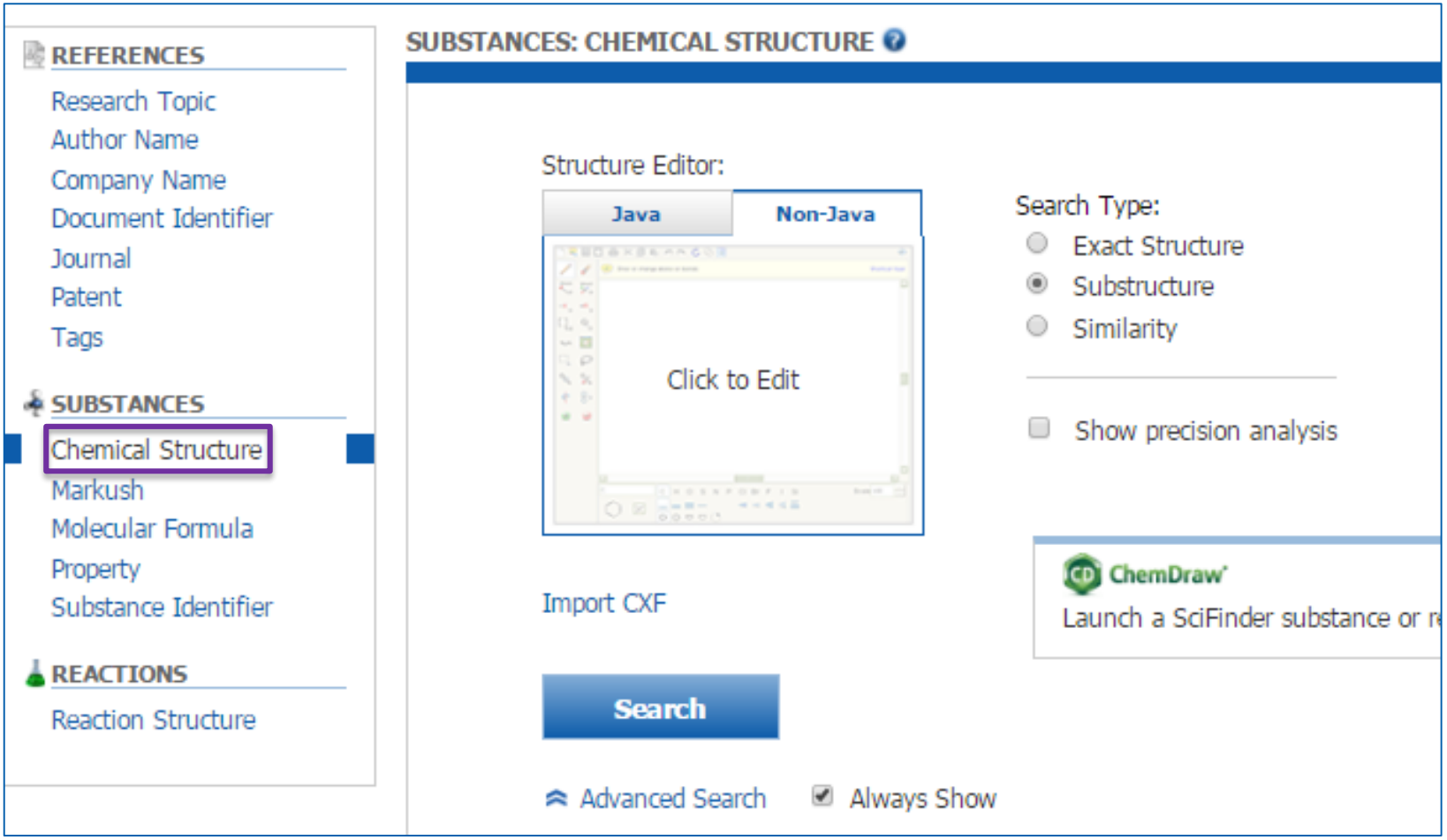

CAS Solutions
SciFinder
A CAS SOLUTION
Explore
Saved Searches
SciPlanner
Molecular Formula "Co . Fe . Mn" > substances (257)
REFERENCES
Research Topic
Author Name
Company Name
SUBSTANCES: MOLECULAR FORMULA
Co. Fe. Mn
SUBSTANCES
Get References
Get Reactions
Get Commercial Sources
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Analyze by:
Substance Role
Uses 152
Properties 137
Process 112
Preparation 24
Analytical Study 3
Reactant or Reagent 3
Biological Study 2
Formation, Nonpreparative 2
Miscellaneous 1
Occurrence 1
Show More
Sort by: CAS Registry Number
Display Options
0 of 257 Substances Selected
Page: 1 of 18
1. 2222373-78-4
Component | Component Ratio
Co | 7.5
Mn | 2.5
Fe | 2.5
Co . Fe . Mn
Cobalt, compd. with iron and manganese (7.5:2.5:2.5)
2. 2222373-77-3
Component | Component Ratio
Co | 5
Mn | 2.5
Fe | 5
Co . Fe . Mn
Cobalt, compd. with iron and manganese (5:5:2.5)
3. 2222373-76-2
Component | Component Ratio
Co | 2.5
Mn | 2.5
Fe | 7.5
Co . Fe . Mn
Cobalt, compd. with iron and manganese (2.5:7.5:2.5)
4. 2192220-92-9
Component | Component Percent
Fe | 0 - 79
Co | 21 - 62
Mn | 0 - 39
Co . Fe . Mn
Iron alloy, base, Fe 0-79,Co 21-62,Mn 0-39
5. 2170121-60-3
Component | Component Percent
Fe | 82
Mn | 13
Co | 5
Co . Fe . Mn
Iron alloy, base, Fe 82,Mn 13,Co 5
6. 2159146-09-3
Component | Component Percent
Fe | 65
Mn | 20
Co | 15
Co . Fe . Mn
Iron alloy, base, Fe 65,Mn 20,Co 15
7. 2159146-06-0
8. 2159146-00-4
9. 1632299-36-5

合金的检索——掺杂钴铁锰的合金





物质检索——结构



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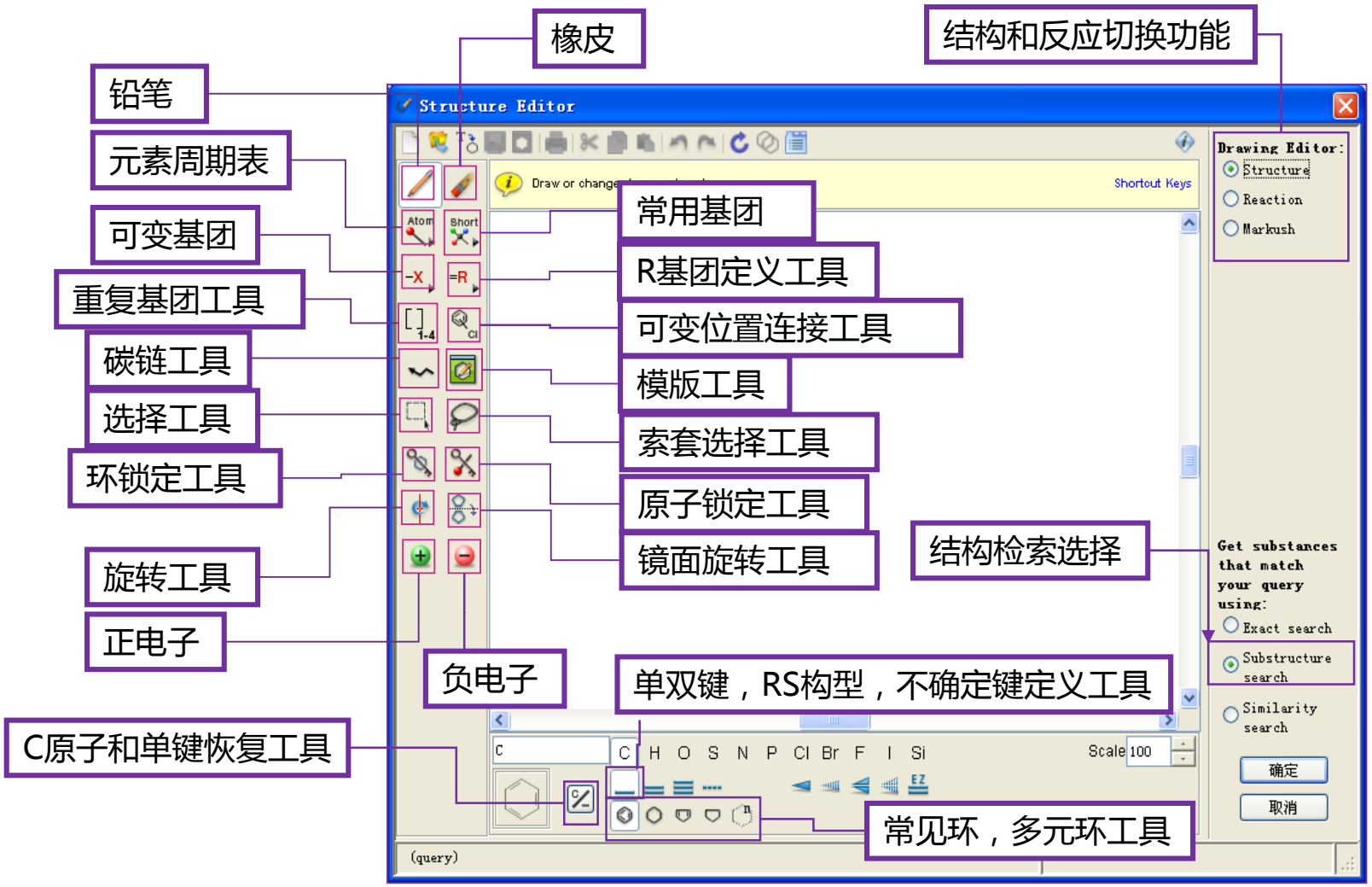
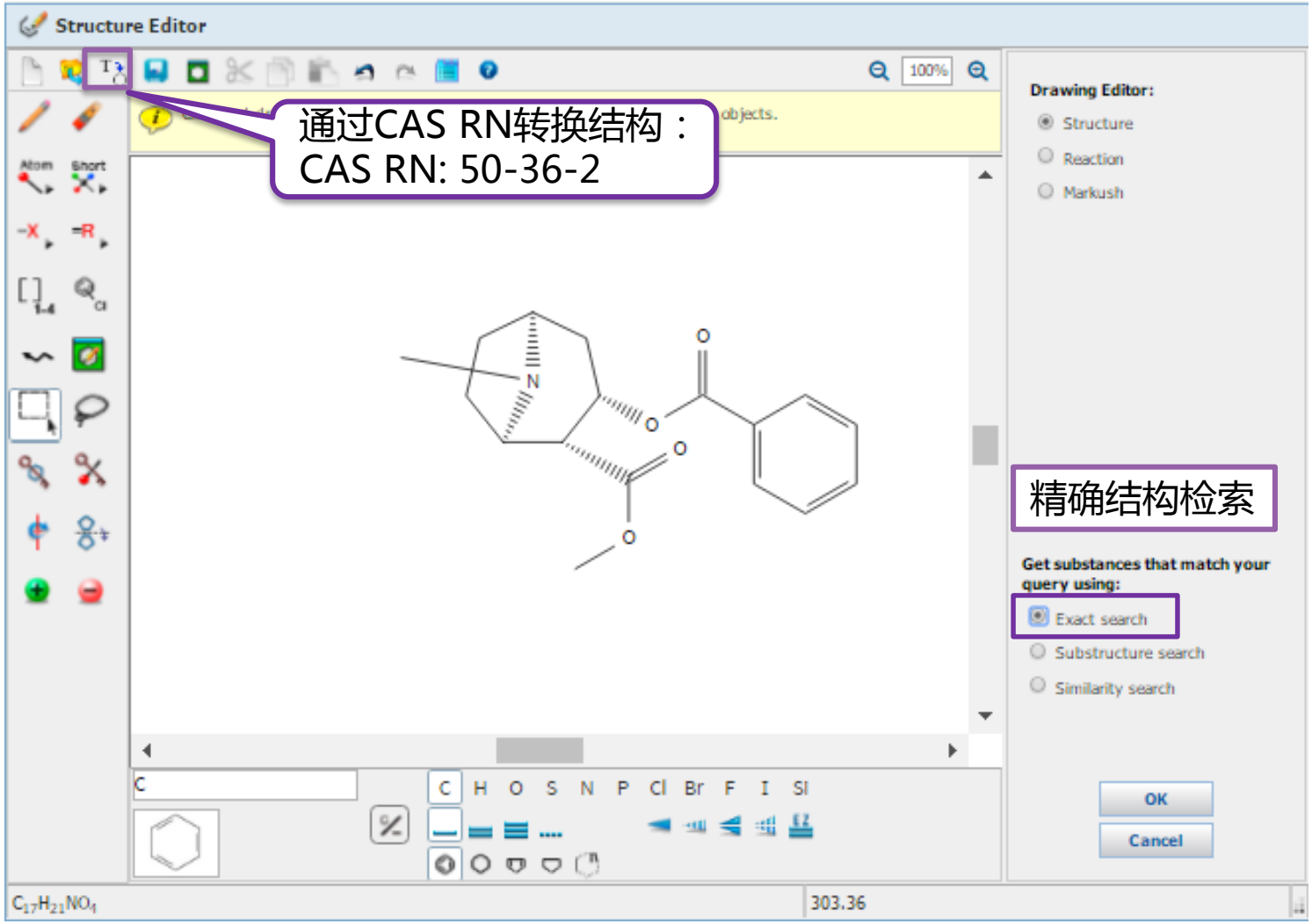
物质检索——结构


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

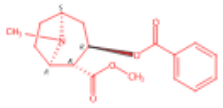
精确结构检索结果

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

Sort by: Relevance

0 of 6 Substances Selected

1. 668-19-9



Absolute stereochemistry.

$C_{17}H_{21}NO_4$

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

Key Physical Properties

Spectra

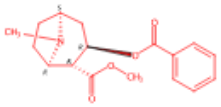
可卡因

2. 114599-38-1

可卡因组合物

668-19-9

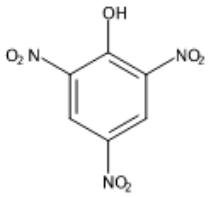
$C_{17}H_{21}NO_4$



Absolute stereochemistry.

88-89-1

$C_6H_3N_3O_7$

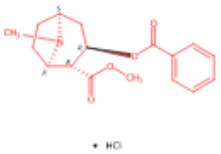


$C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$

Allococaine, picrate (6CI)

3. 109496-04-0

(Component: 668-19-9)



Absolute stereochemistry.

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

Allococaine, hydrochloride (6CI)

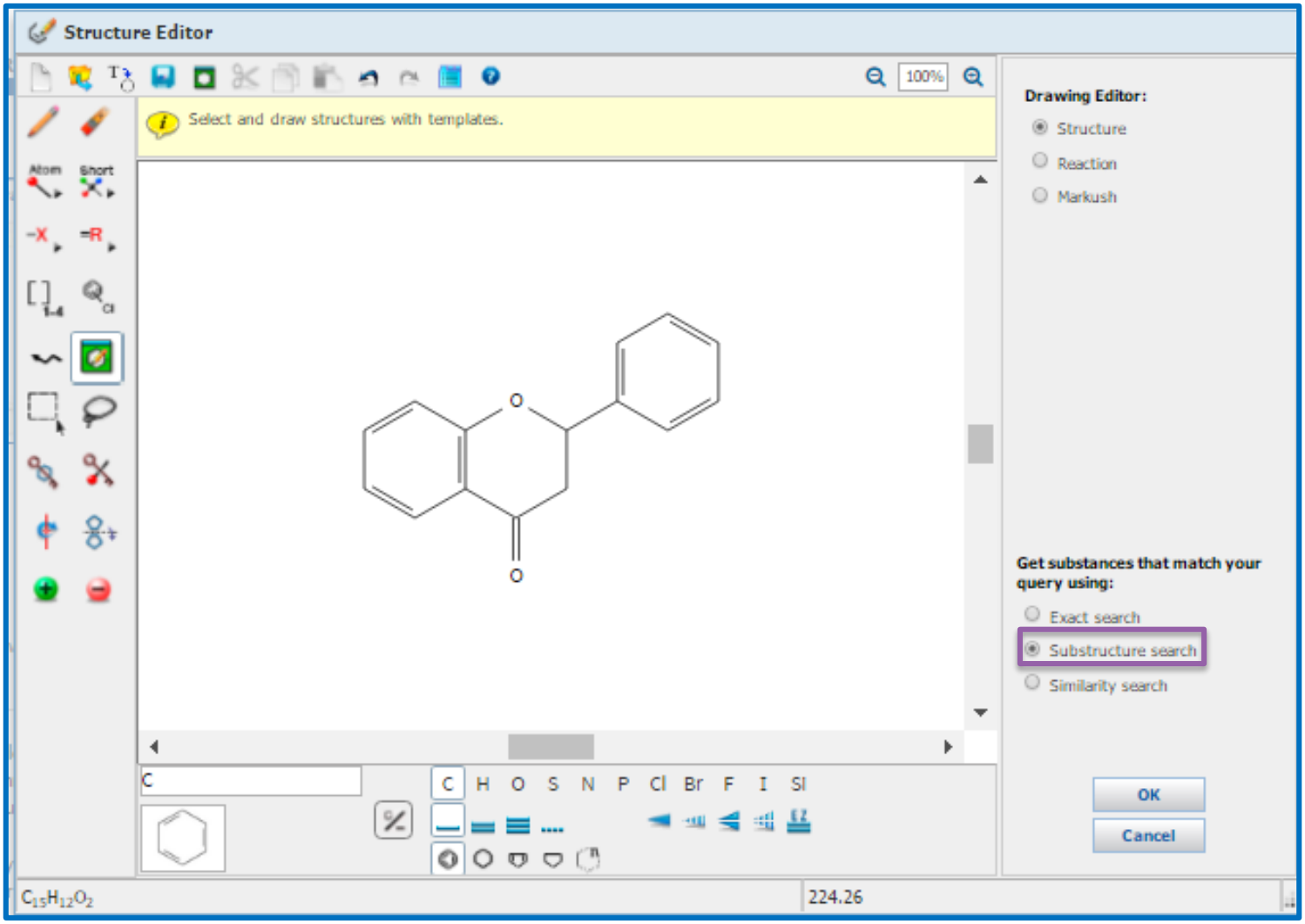
盐酸可卡因

物质检索——精确结构检索

- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索



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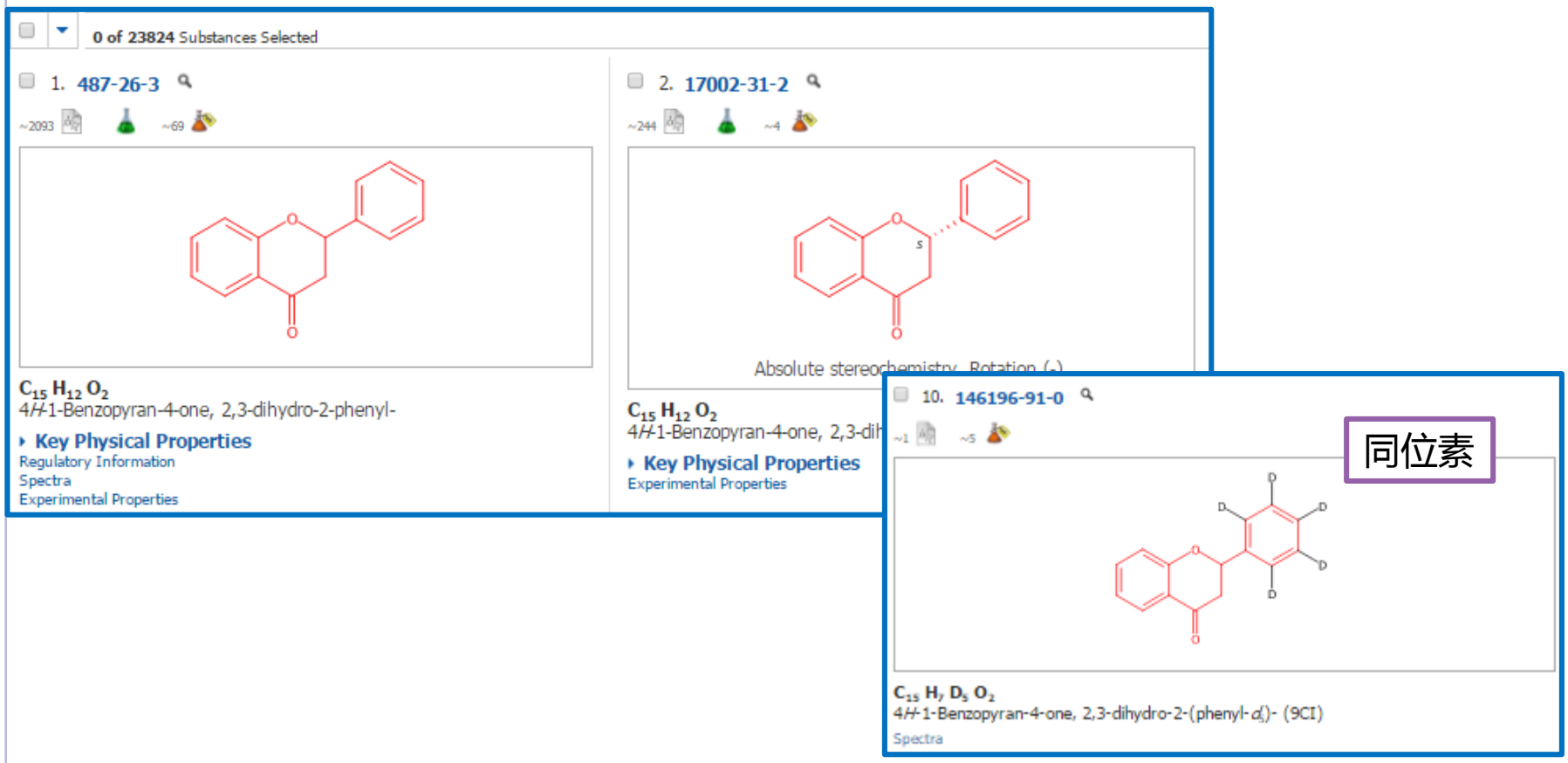
物质检索——亚结构检索

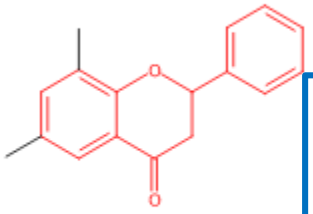


SciFinder® A CAS SOLUTION

亚结构检索结果

281. 123251-10-5

取代物



$C_{17}H_{16}O_2$

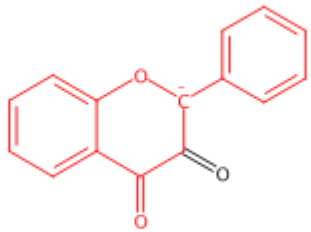
4*H*-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethy

Key Physical Properties

Experimental Properties

295. 780723-19-5

离子

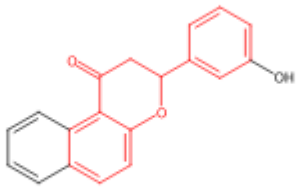


$C_{15}H_9O_3$

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

284. 136116-23-9

稠环物质



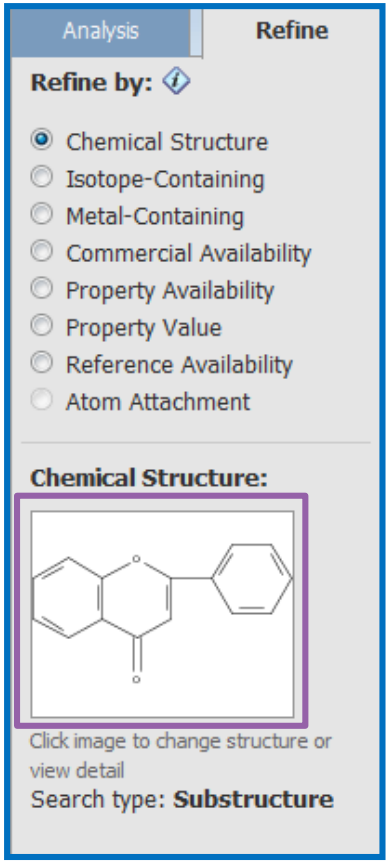
$C_{19}H_{14}O_3$

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

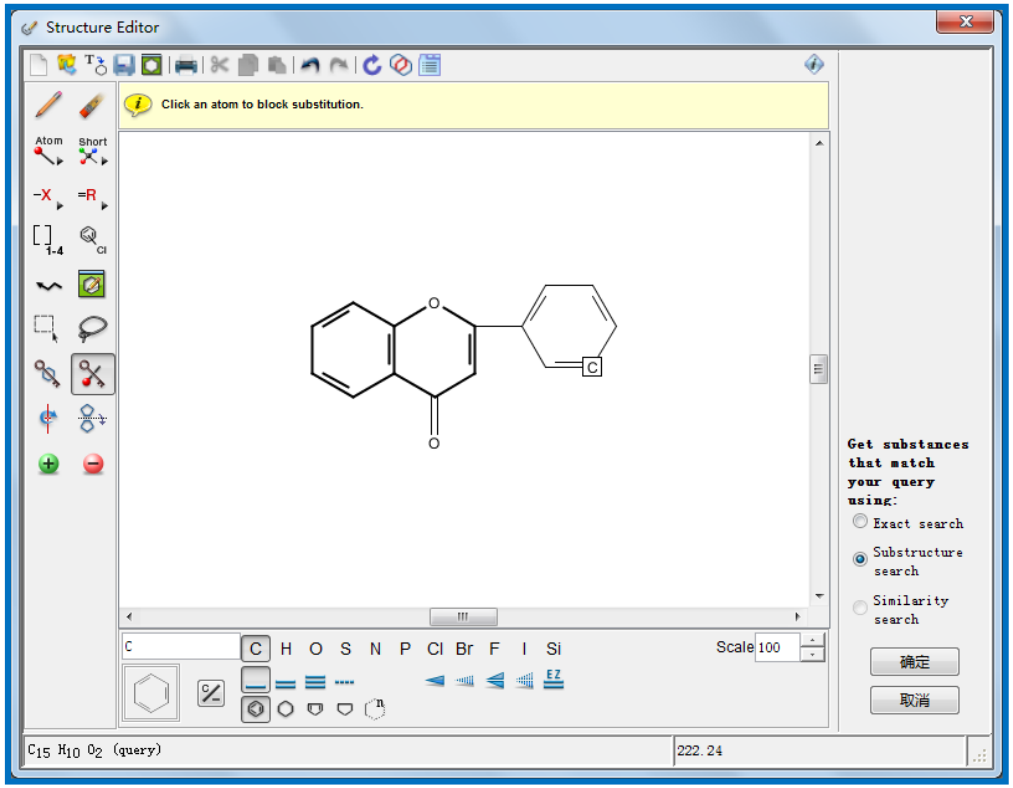
Key Physical Properties

SciFinder® A CAS SOLUTION

亚结构检索结果的限定



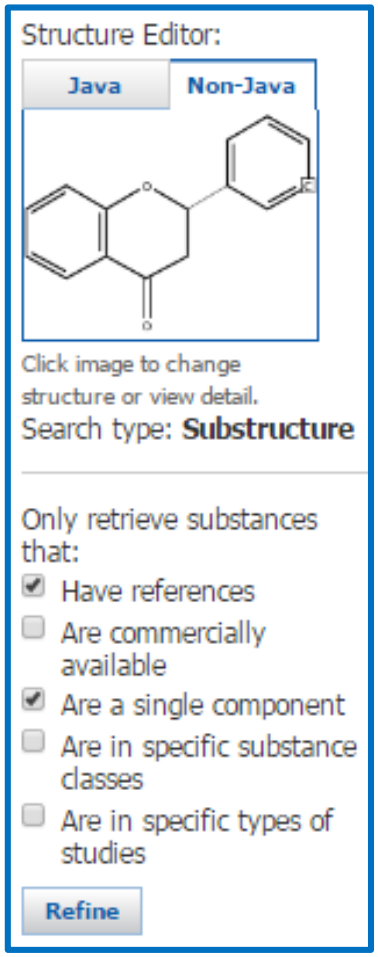
化学结构的再次限定

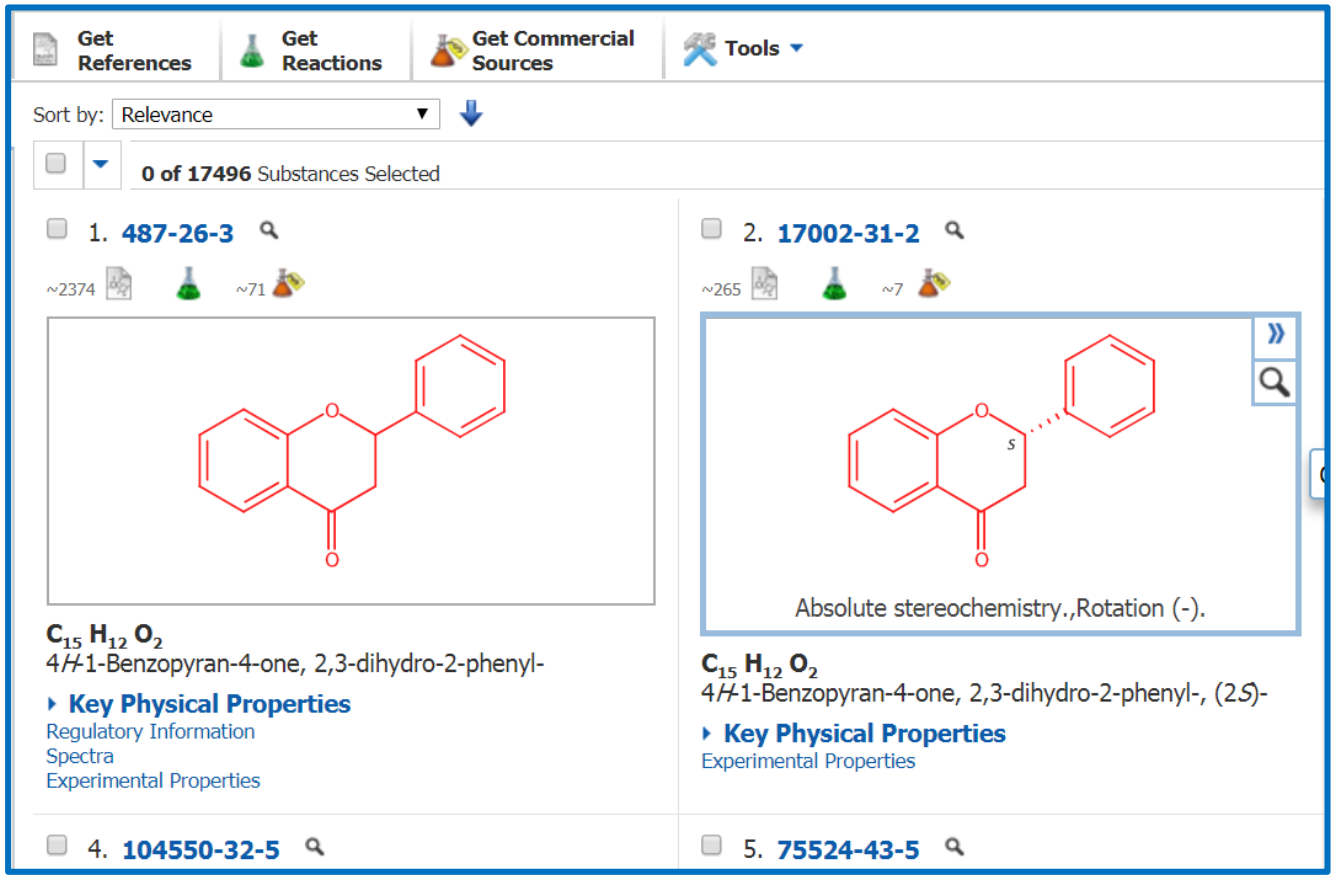


环锁定

原子锁定

亚结构检索结果的限定





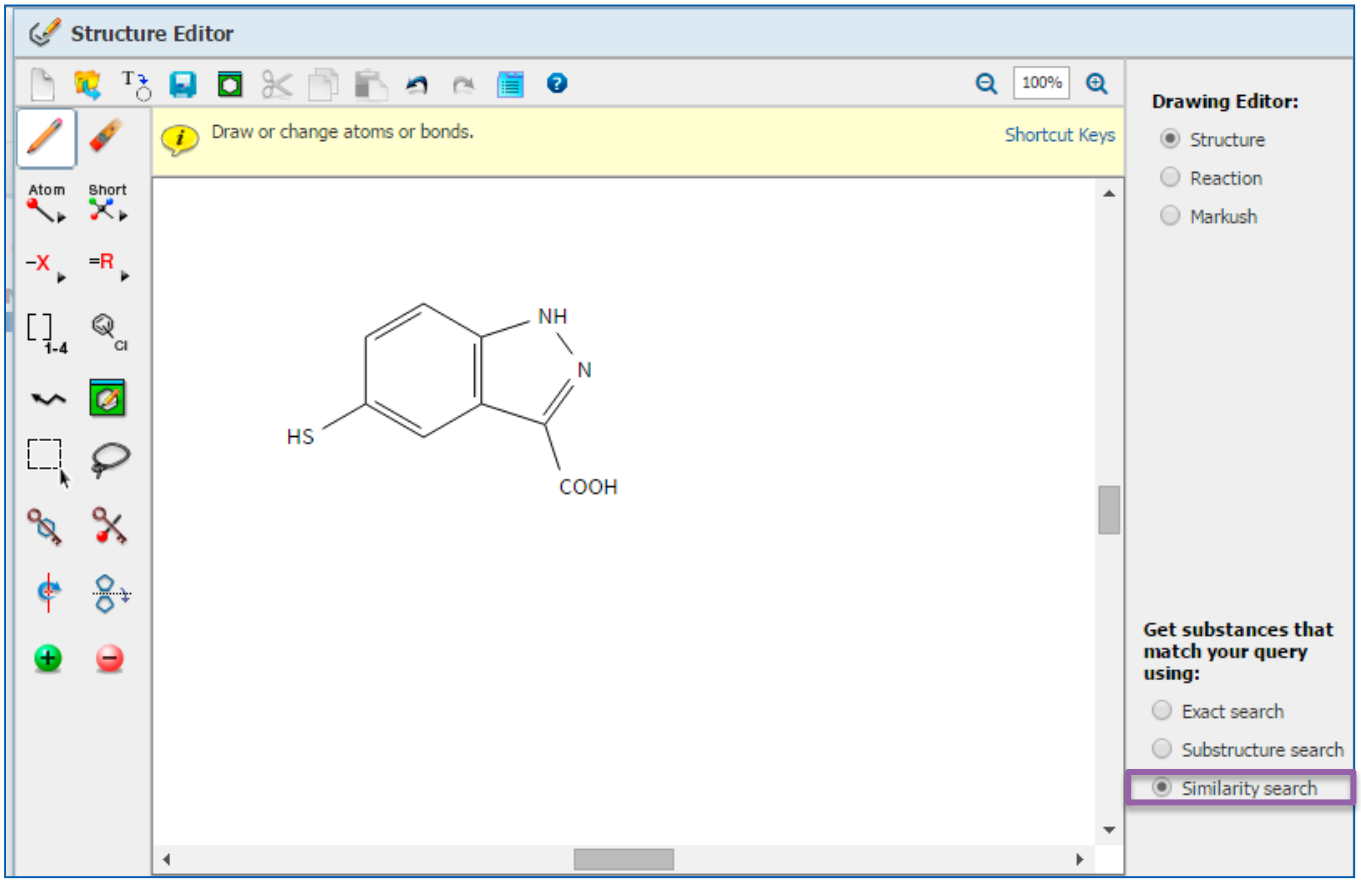
SciFinder® A CAS SOLUTION

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

相似结构检索结果

Select All Deselect All

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

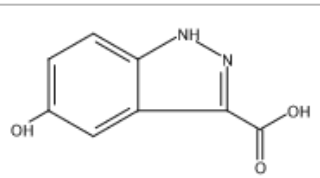
Get Substances

评分越高，相似度越高，结构越相似

Score: 88

1. **885518-94-5**

~1 ~35



取代基变化

$C_8H_6N_2O_3$

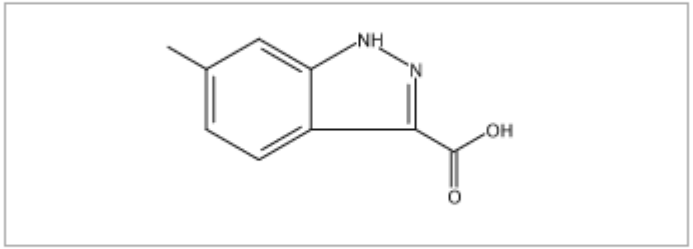
1*H*-Indazole-3-carboxylic acid, 5-hydroxy-

Key Physical Properties

Score: 86

5. **858227-12-0**

~7 ~41



取代基位置变化

$C_9H_8N_2O_2$

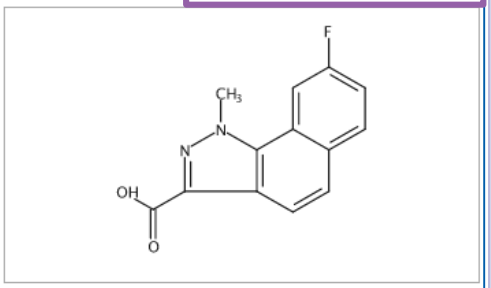
1*H*-Indazole-3-carboxylic acid, 6-methyl-

Key Physical Properties

Score: 65

541. **1100422-**

~1



母体结构变化

$C_{13}H_9FN_2O_2$

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

Key Physical Properties

SciFinder® A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

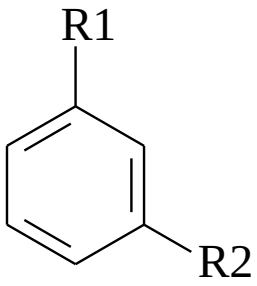
提纲

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

Markush检索

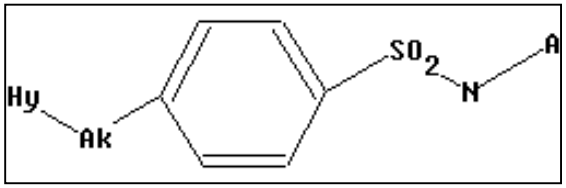
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 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

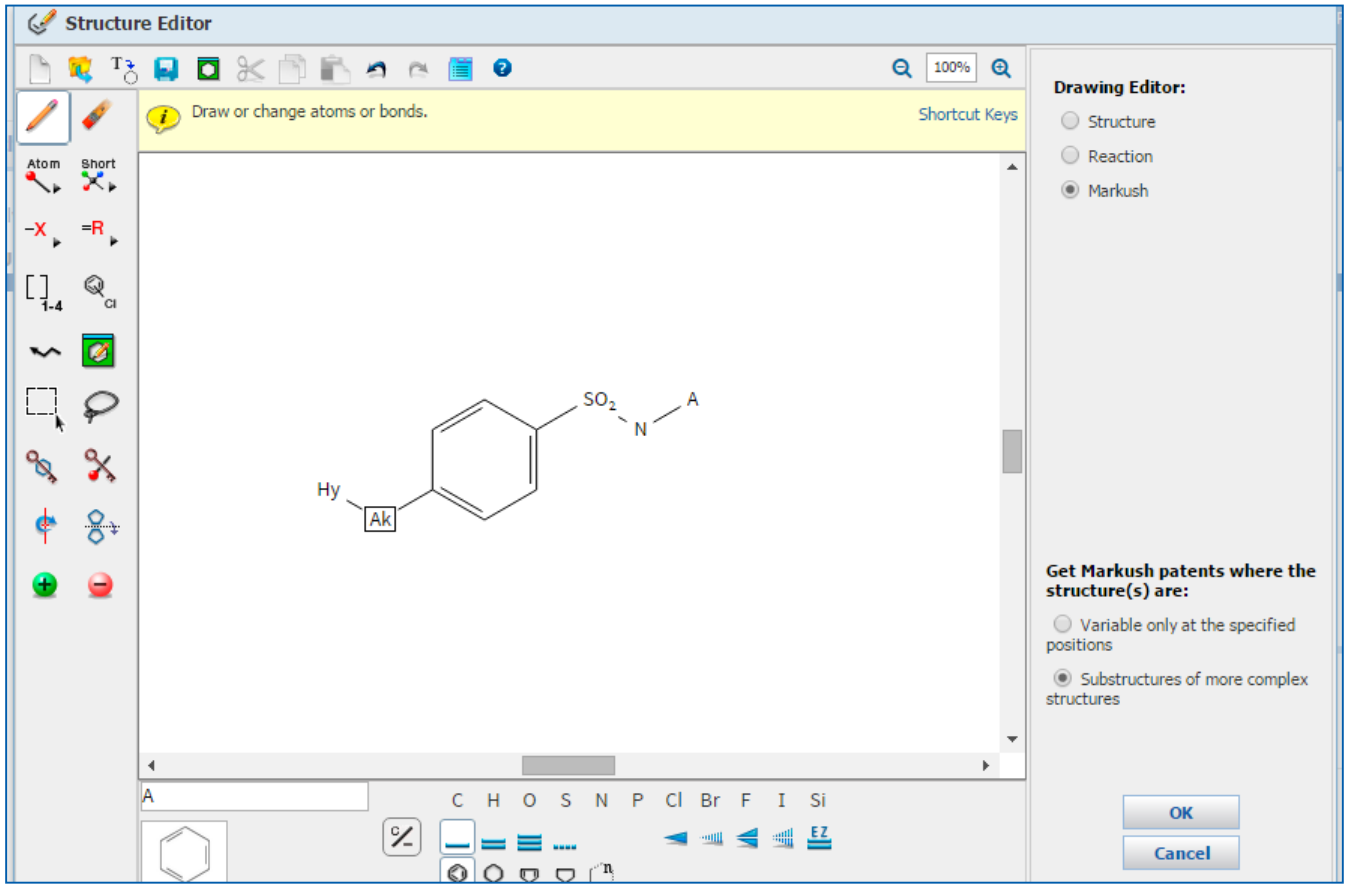


R1 = H, Br, Cl, I

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

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

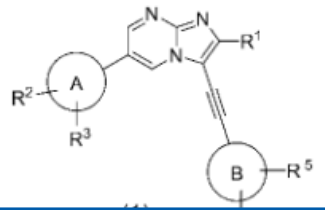
The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat 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^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
- 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

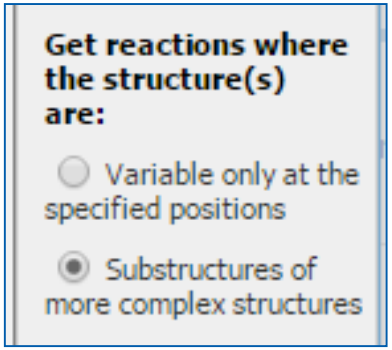
- 常用获取方法

  已知物质：由物质获取反应

  已知文献：从文献中获取反应

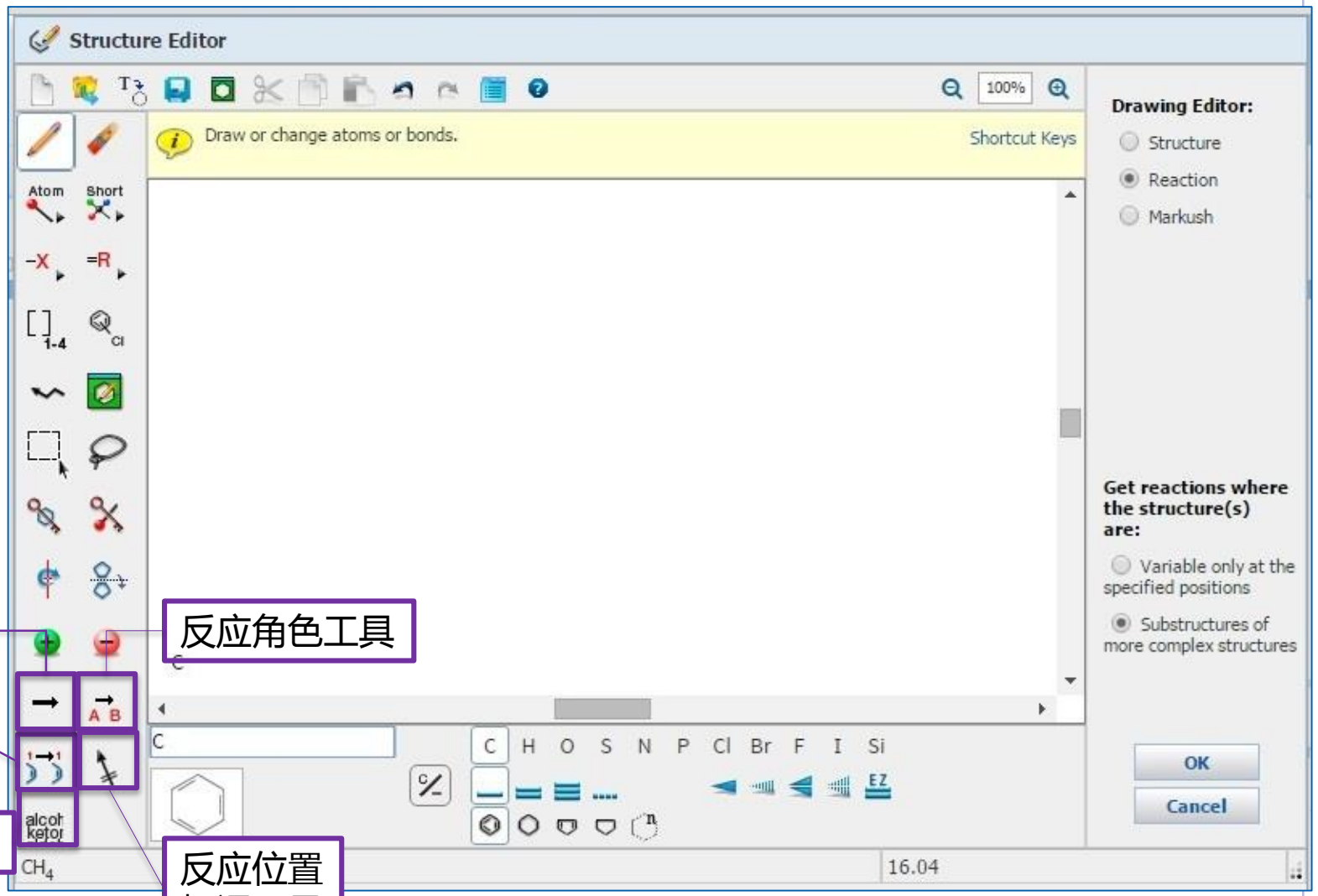
  精确结构反应检索

  亚结构反应检索

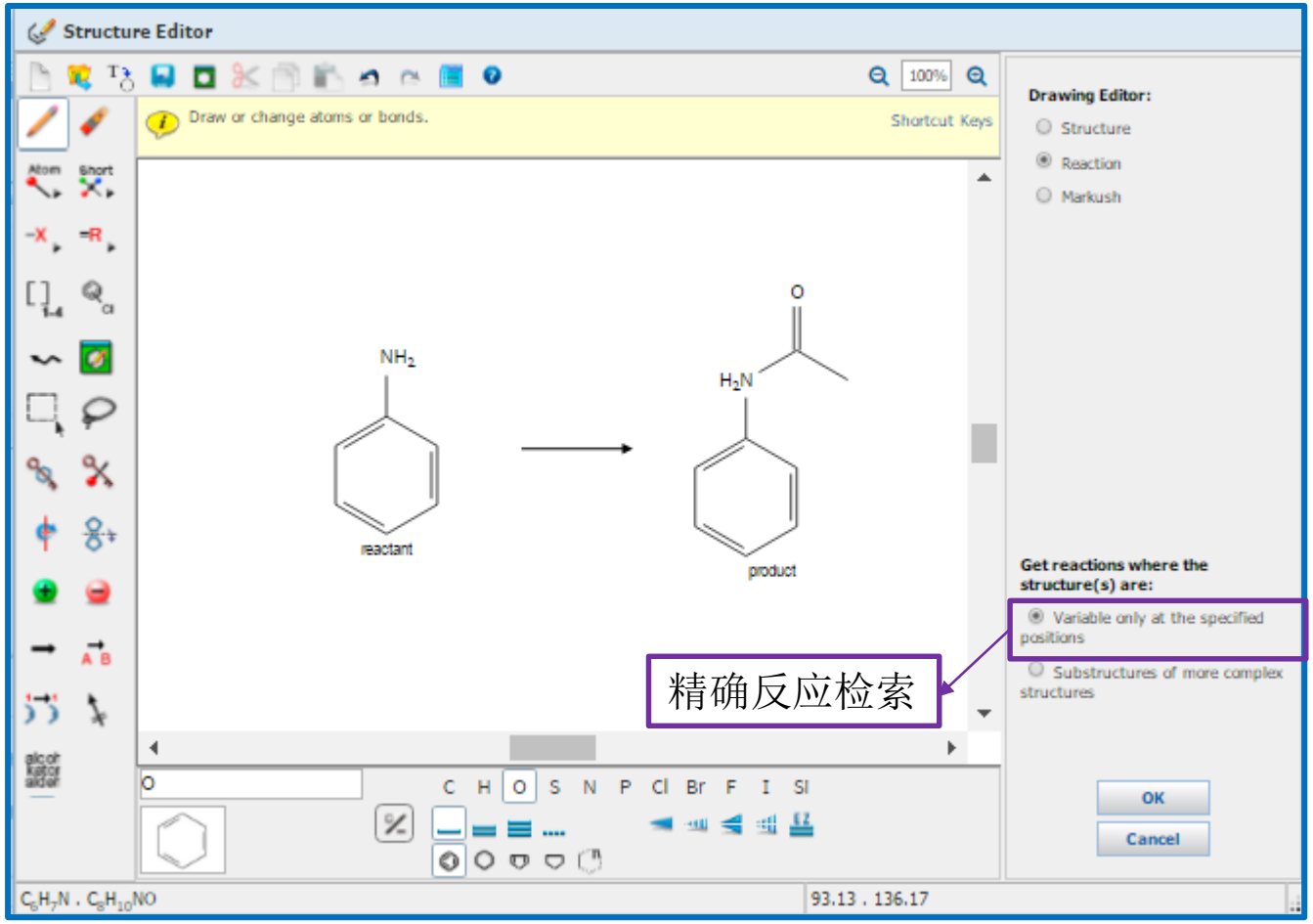


SciFinder® A CAS SOLUTION

反应绘制工具

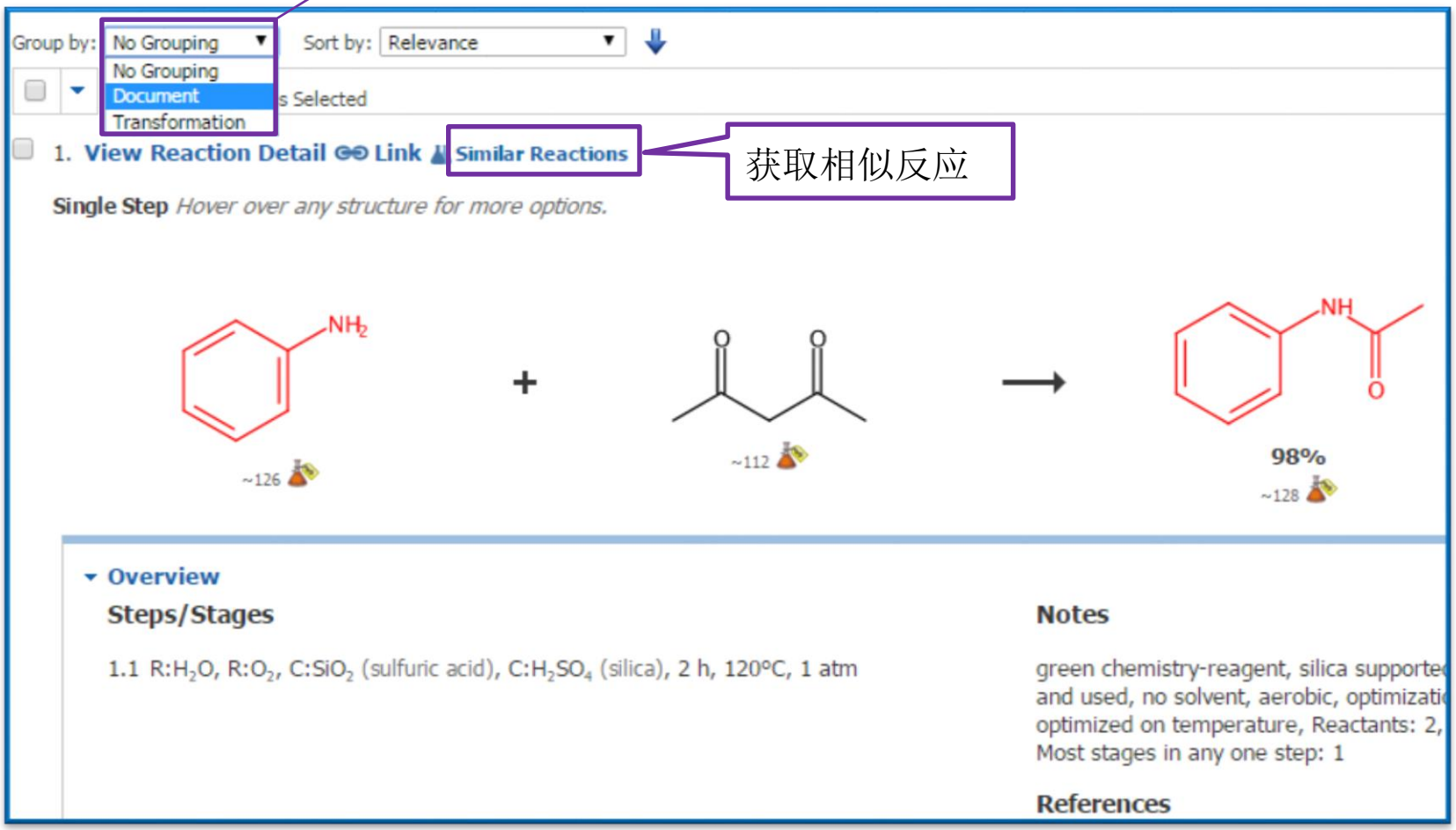

Structure Editor
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
C H O S N P Cl Br F I Si
CH4
16.04
反应箭头
反应角色工具
反应原子标记工具
官能团列表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

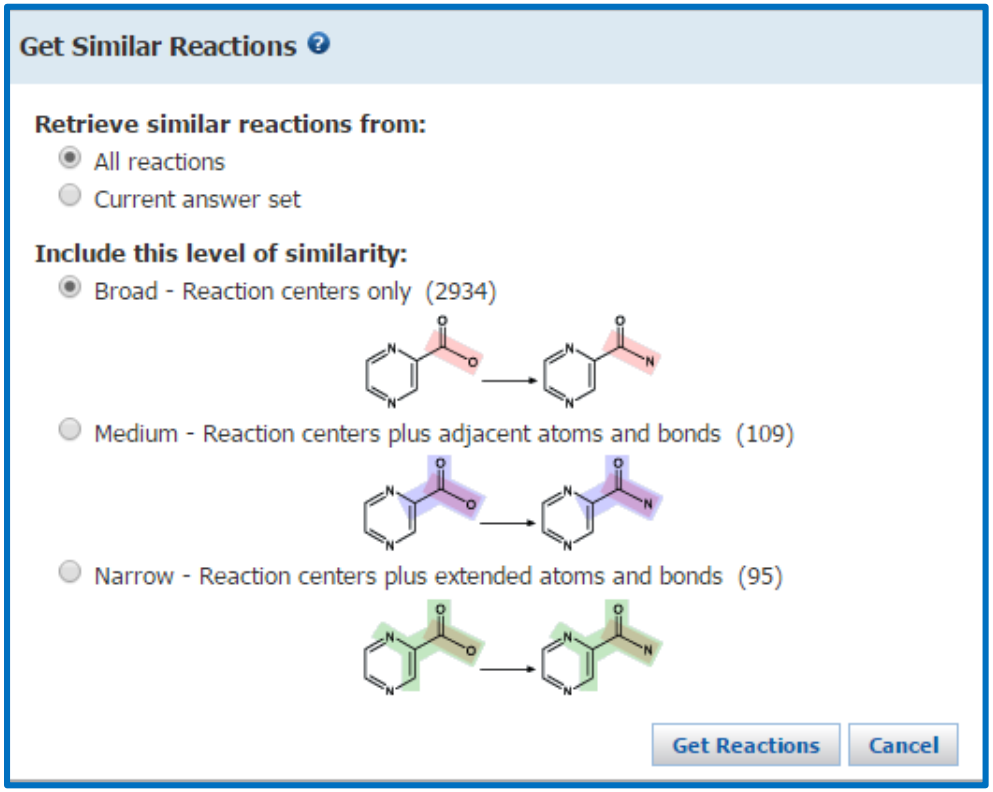
浏览记录，发现很多反应来自同一篇文献，通过Group by Document合并。



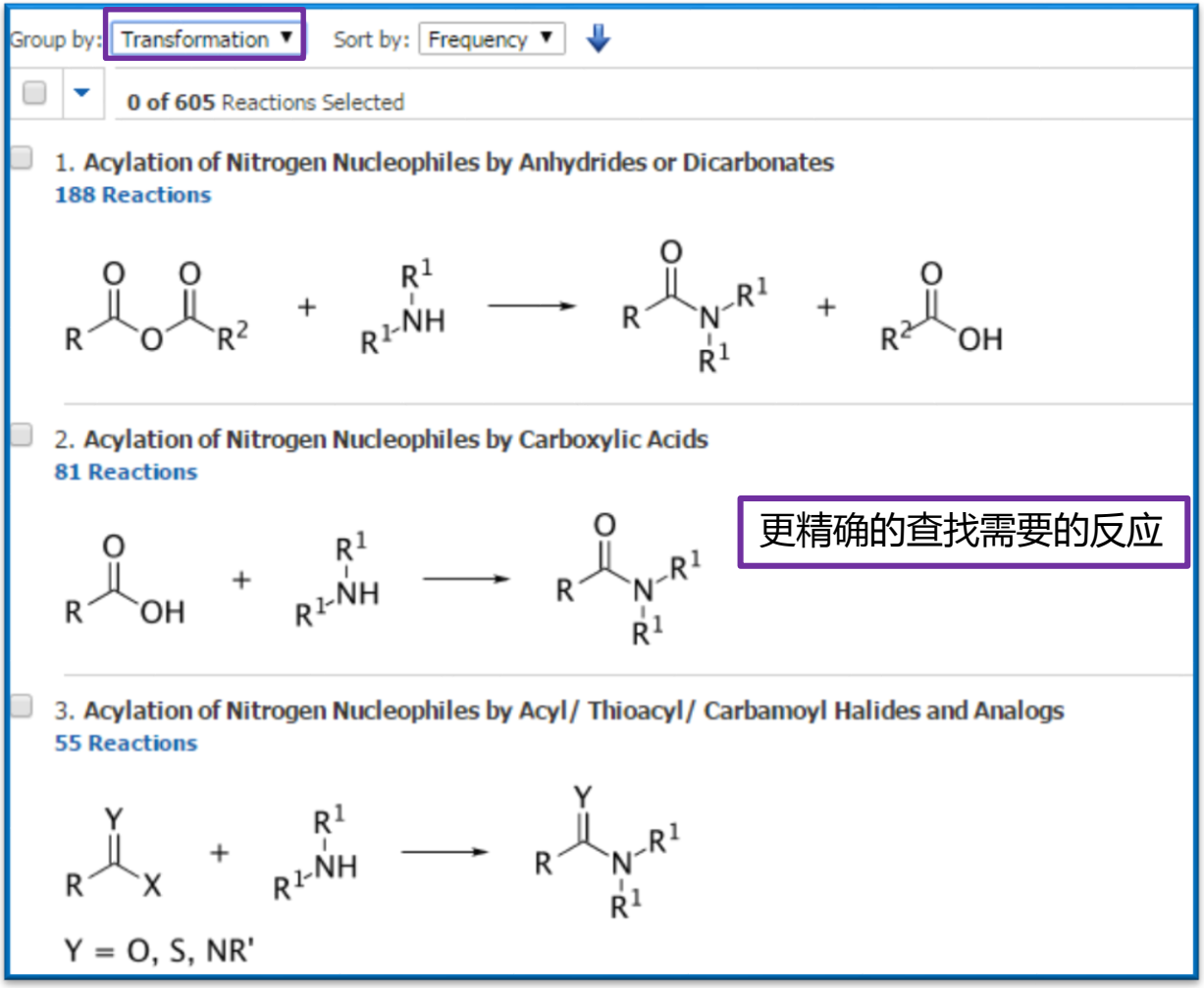
获取相似反应

选择相似反应的相似限制：

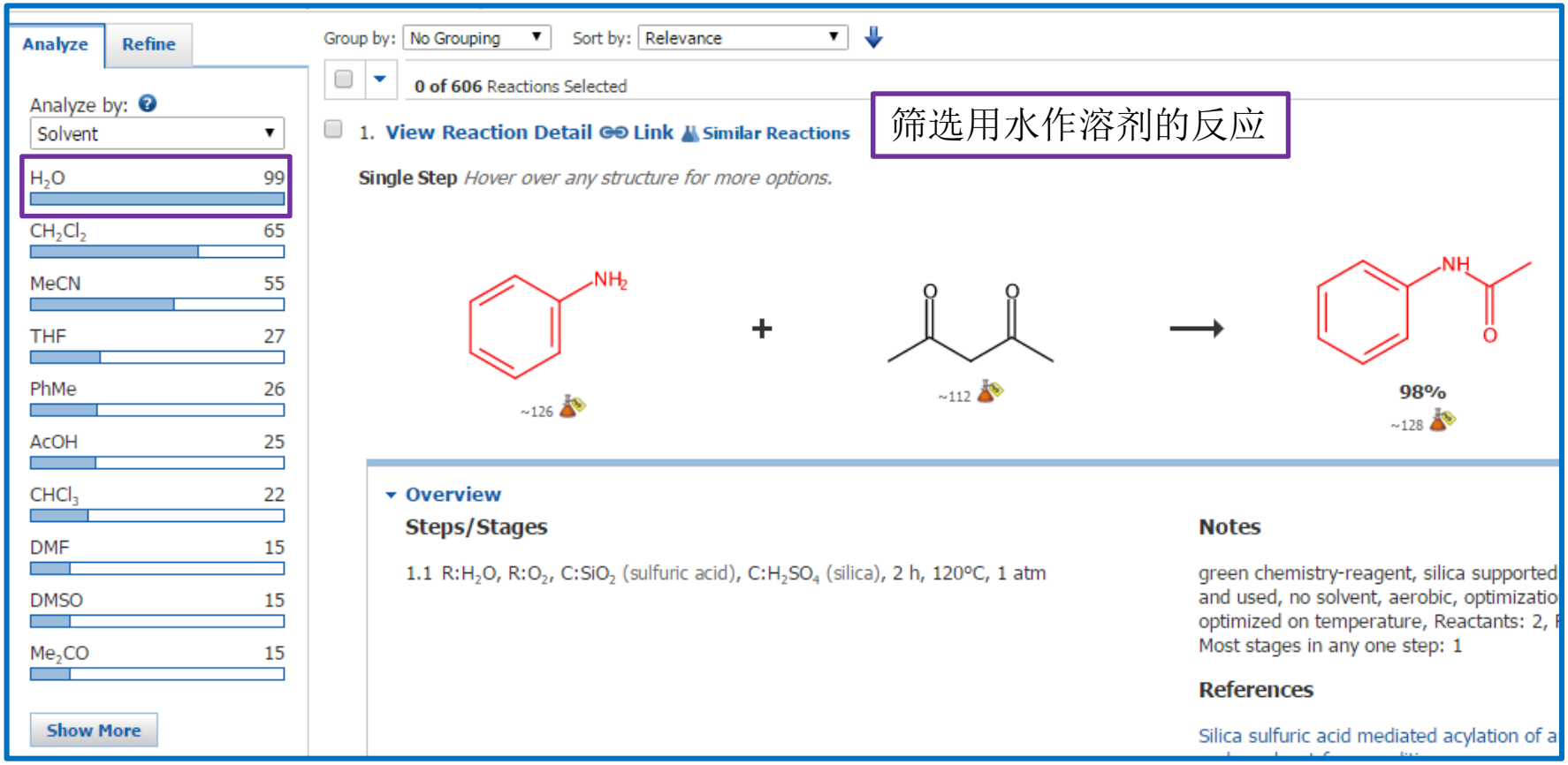
- Broad：仅反应中心相似
- Miedum：反应中心及附属原子和键
- Narrow：反应中心及扩展的原子和键



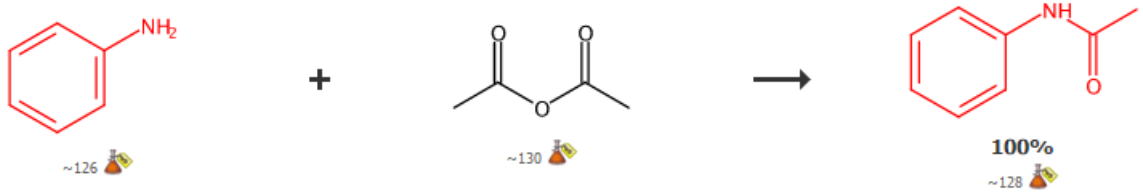
按照反应类型排序


Group by: Transformation
Sort by: Frequency
0 of 605 Reactions Selected
1. Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarbonates
188 Reactions
2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids
81 Reactions
3. Acylation of Nitrogen Nucleophiles by Acyl/ Thioacyl/ Carbamoyl Halides and Analogs
55 Reactions
Y = O, S, NR'
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

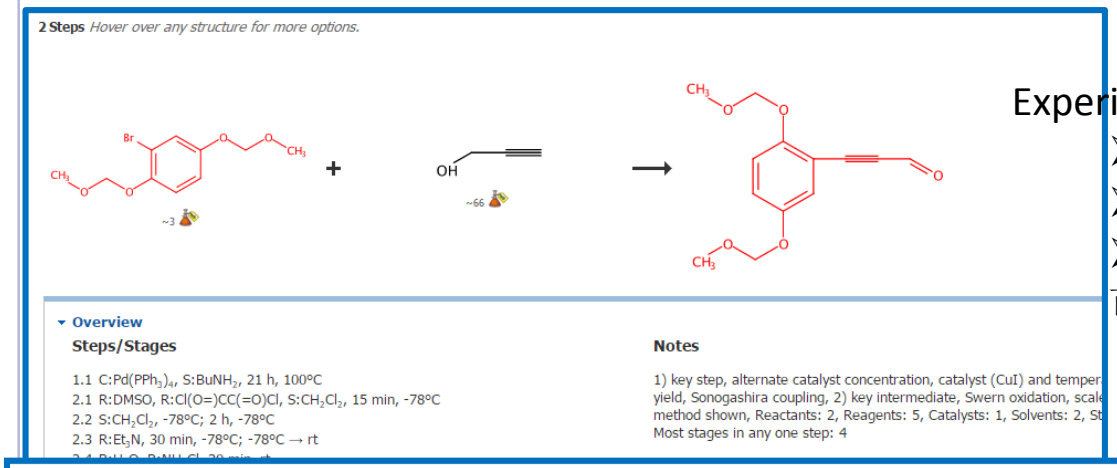
▾ **Experimental Procedure**

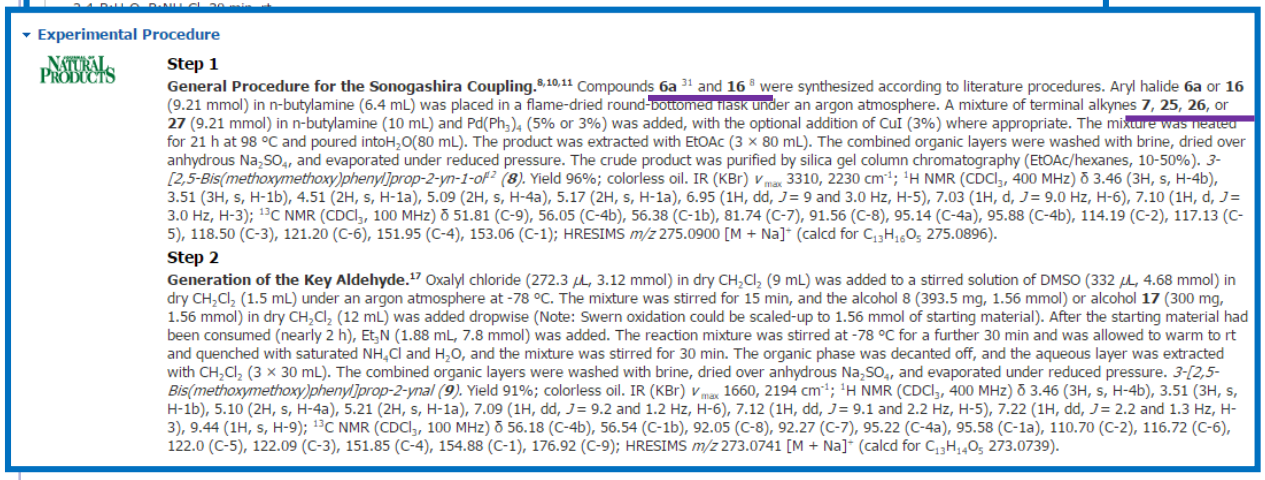
JACS

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

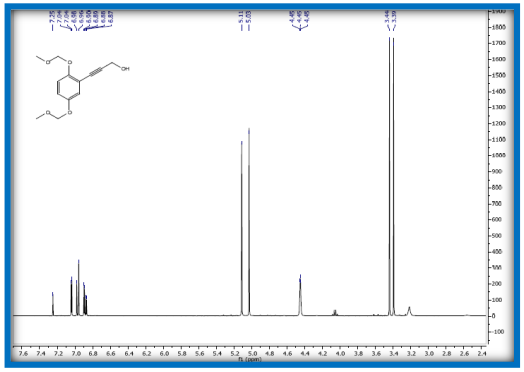




Experimental Procedure: 我们可以做得更好

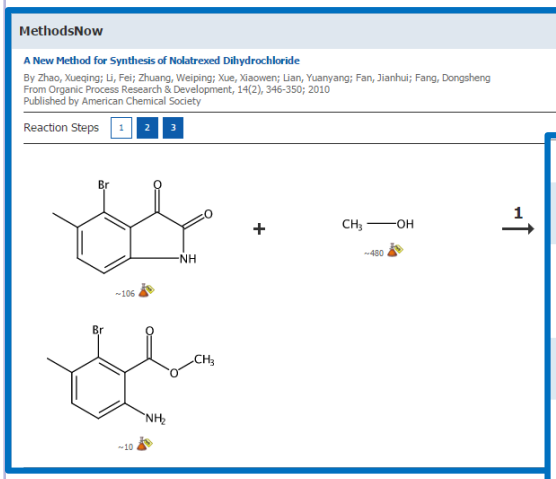
- 更好的阅读体验?
- 这些数字代表什么？
- 去免费的Supporting Information查？

可能只有图谱。



SciFinder® A CAS SOLUTION

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}: ν3472, 3382, 2953, 2924, 1716, 1622, 1480, 1277, 816.

物质信息

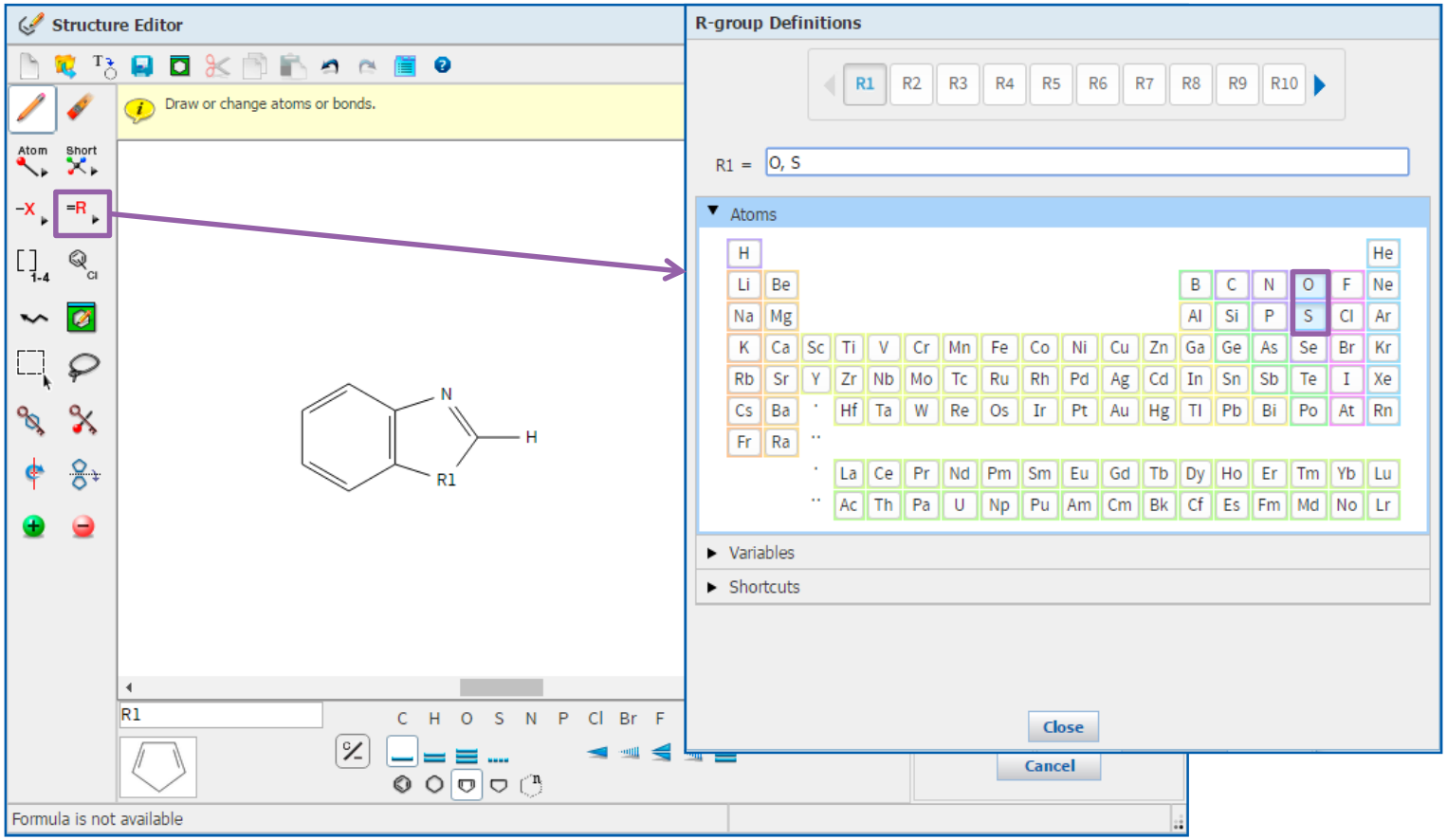
实验过程

图谱信息

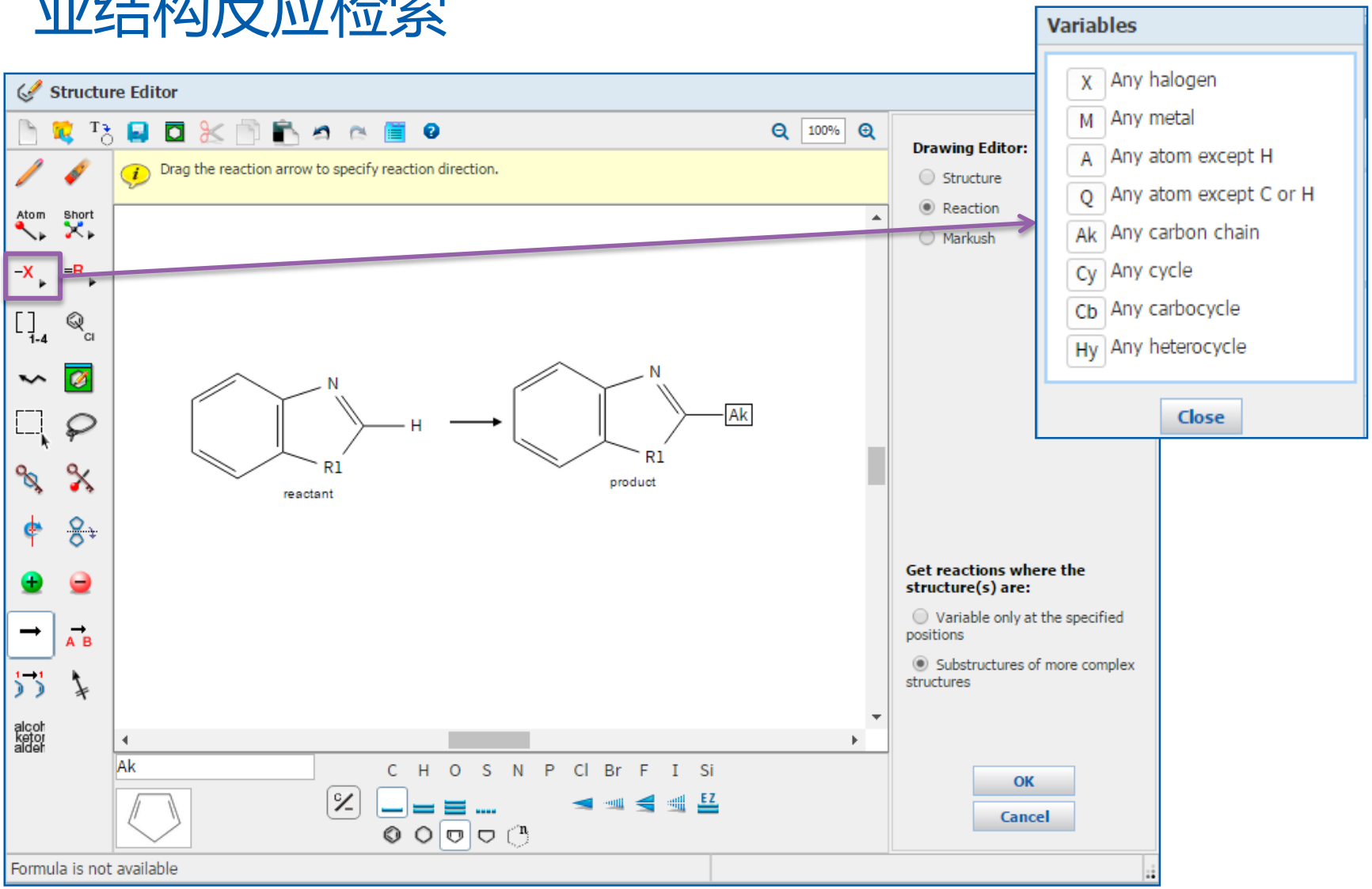
SciFinder® A CAS SOLUTION

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

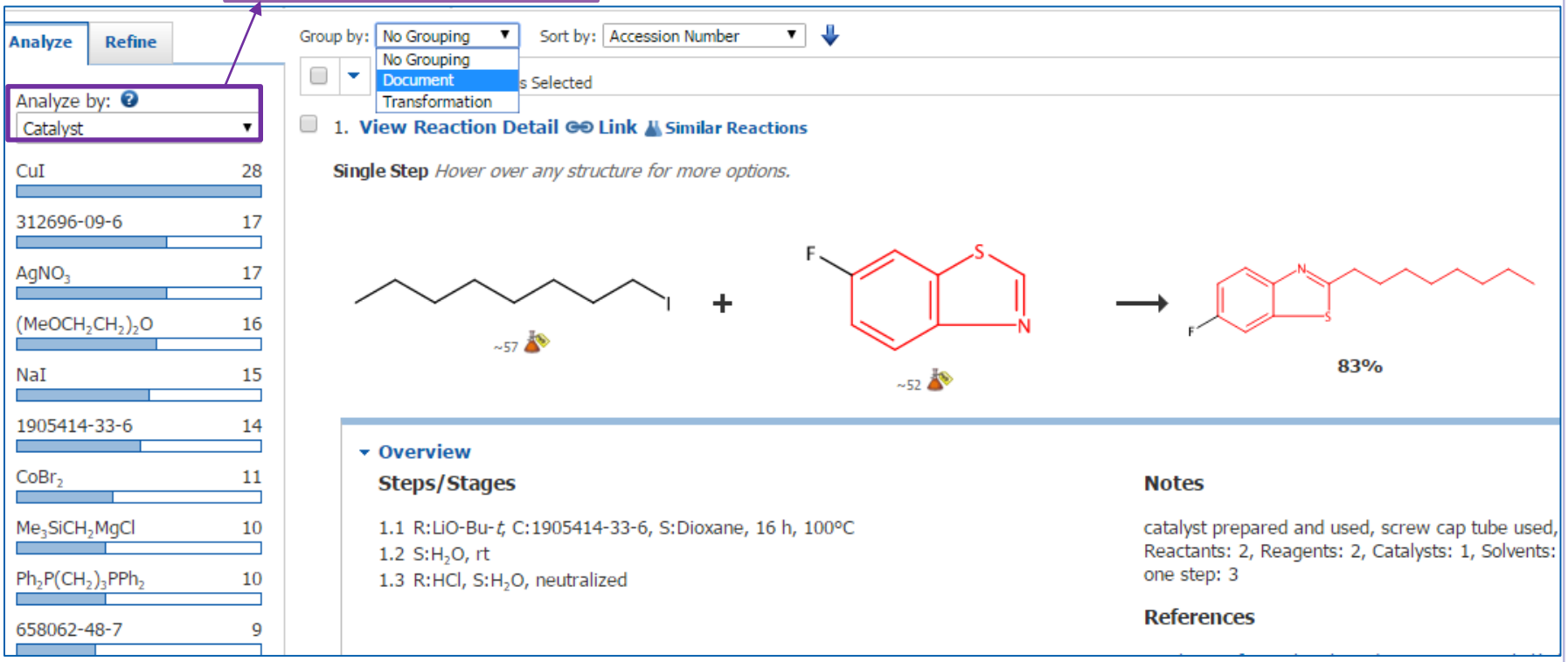


亚结构反应检索


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

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应



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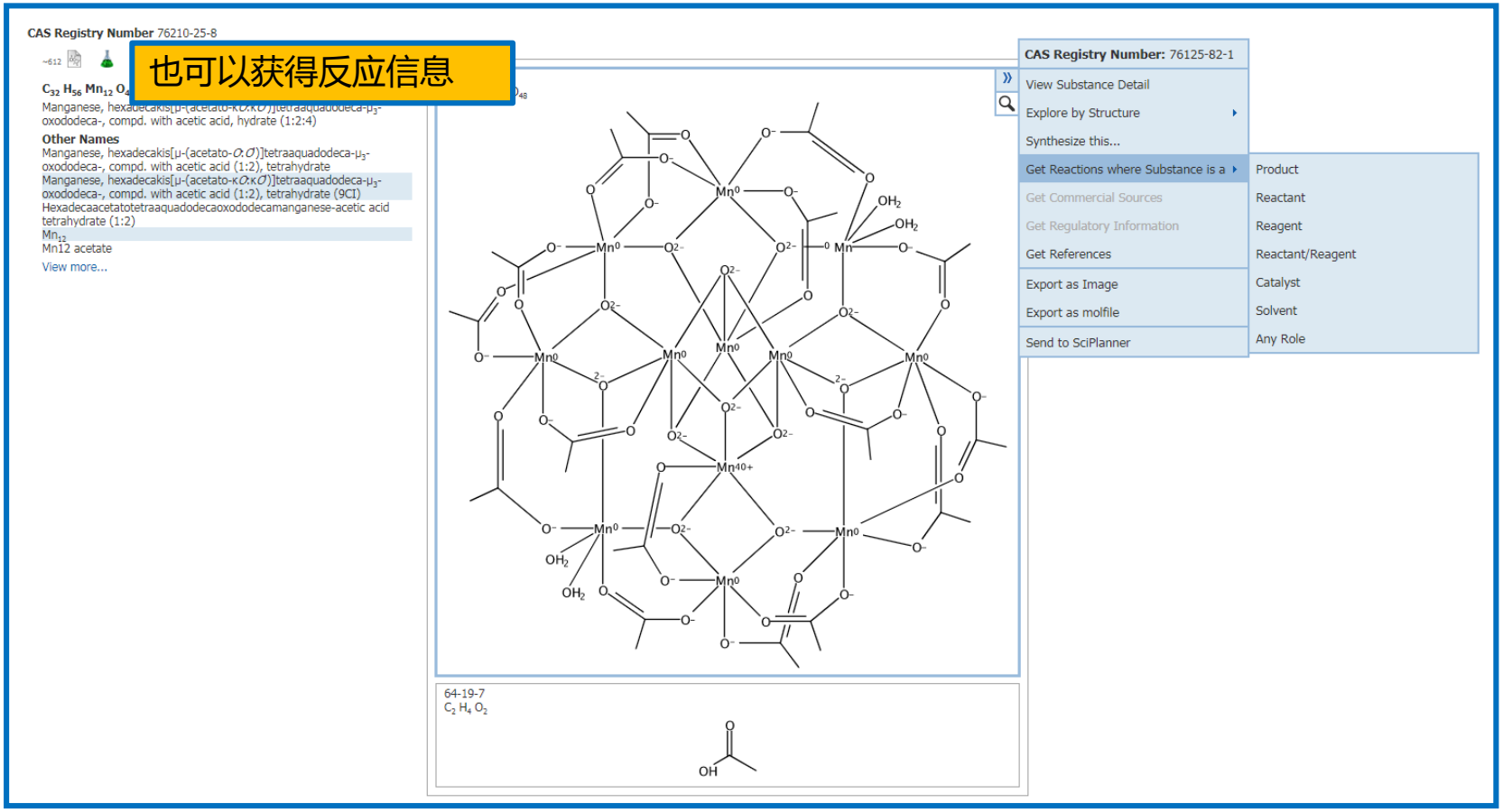
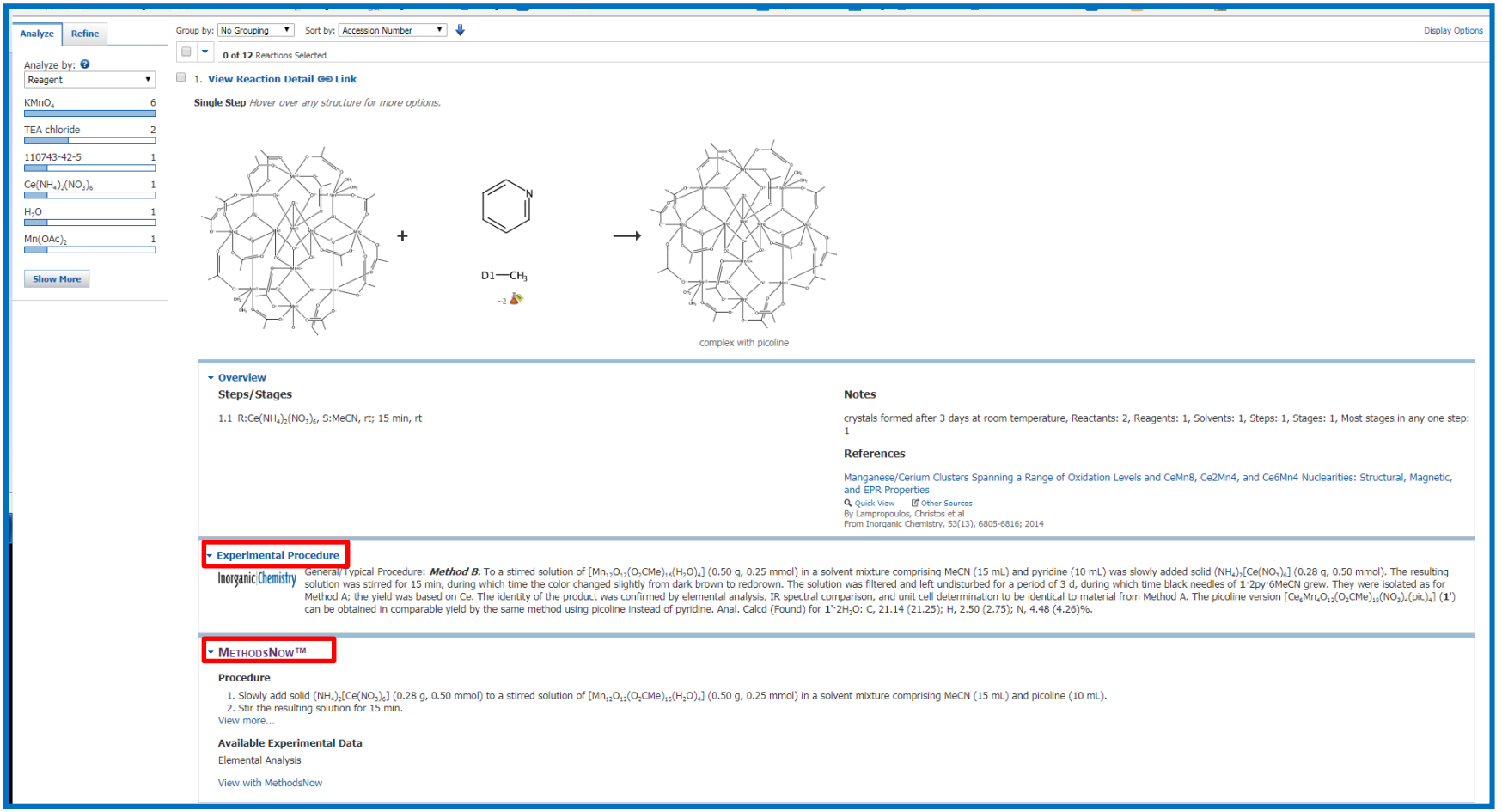
案例一：查找多氧族金属的反应信息



查看反应信息详情



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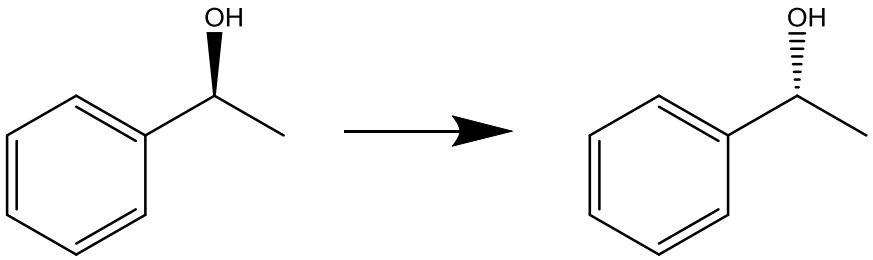
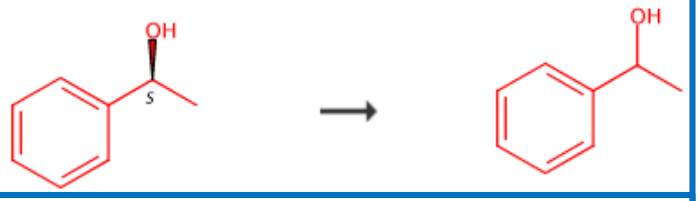
案例二：如何获取手性翻转反应



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.*

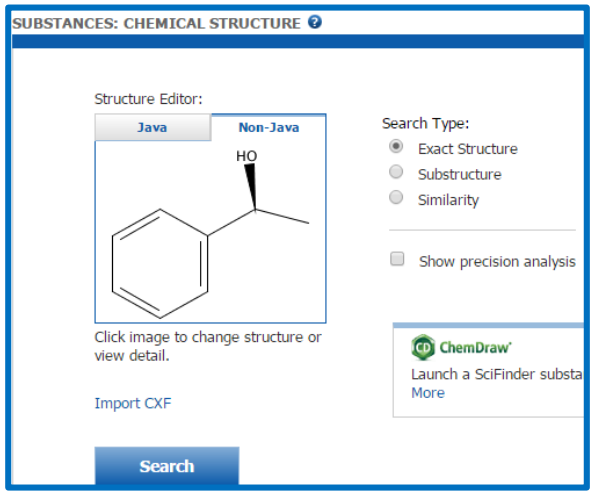
案例：如何获取手性翻转反应

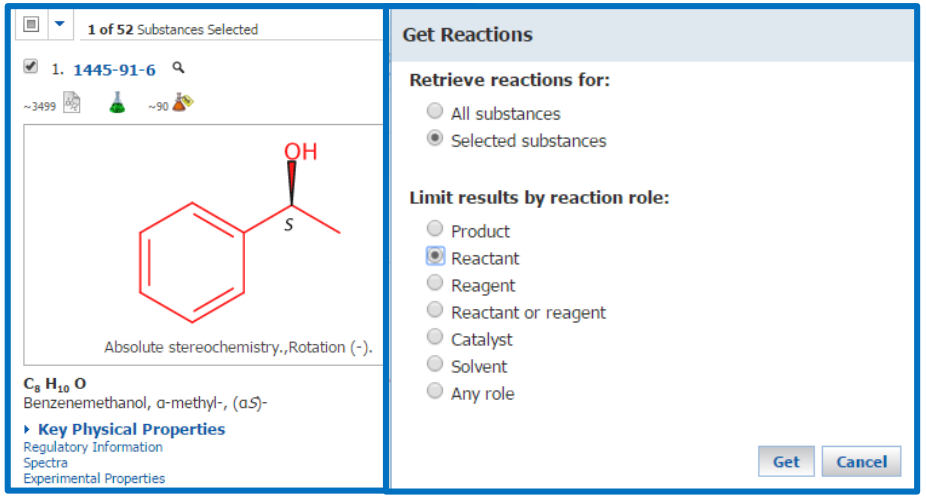
检索思路：

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。





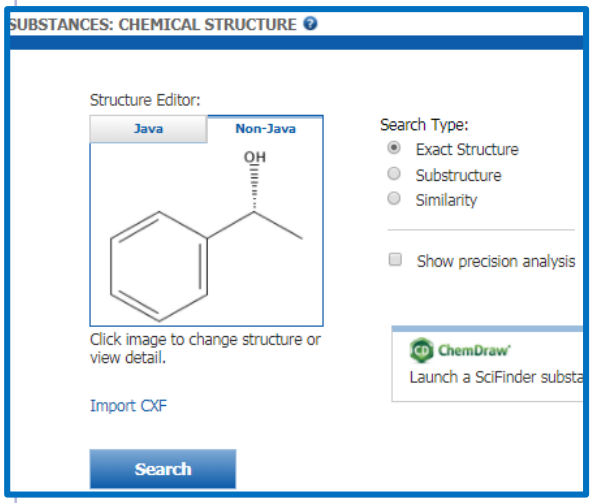
案例：如何获取手性翻转反应

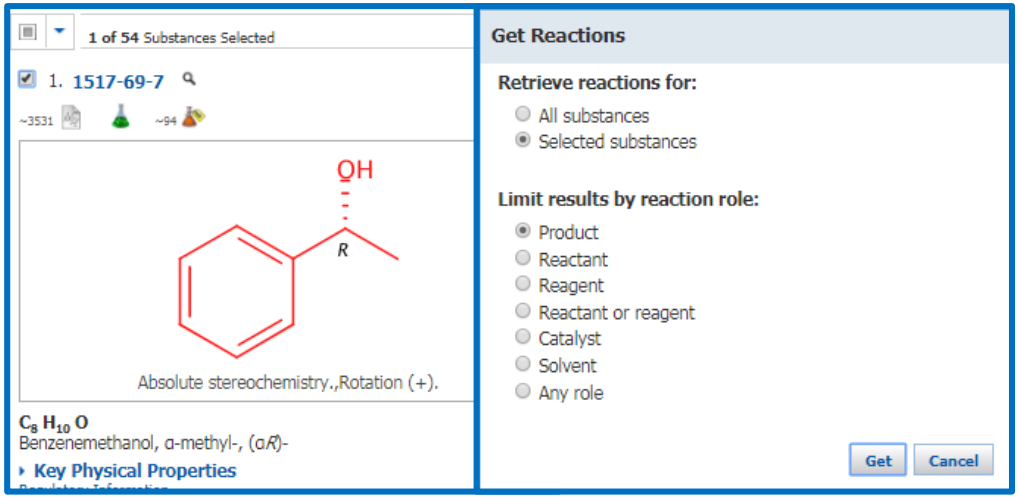
检索思路：

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。

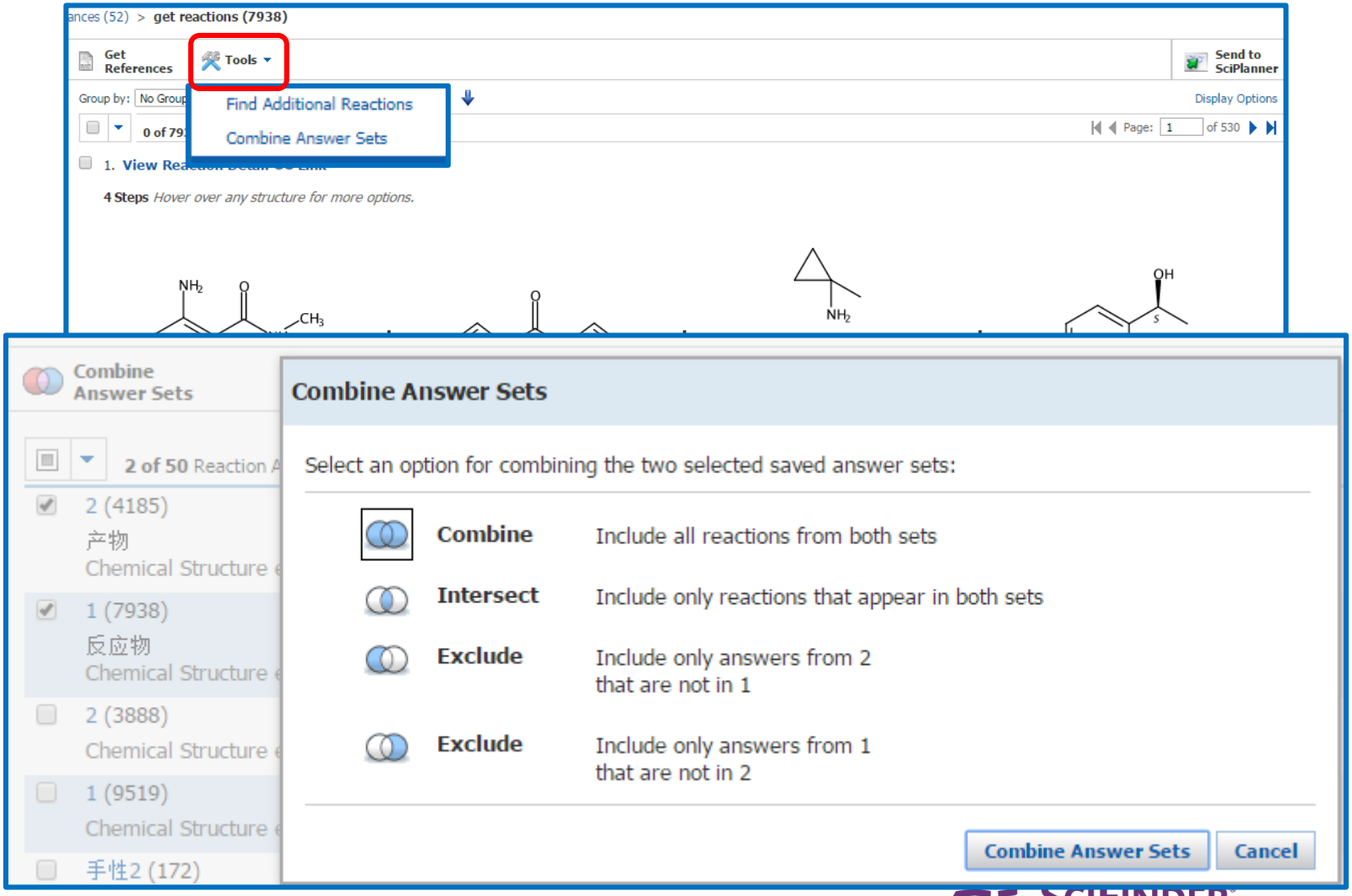
2). 先获取产物物质，然后再获取其作为产物的反应，得到检索结果集2。

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

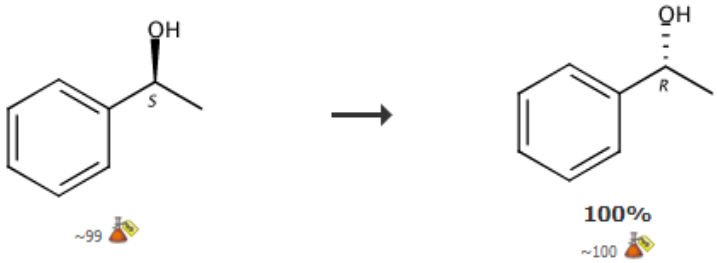
Get References | Tools | Send to SciPlanner

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

0 of 27 Reactions Selected | Page: 1 of 2

1. View Reaction Detail Link

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



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

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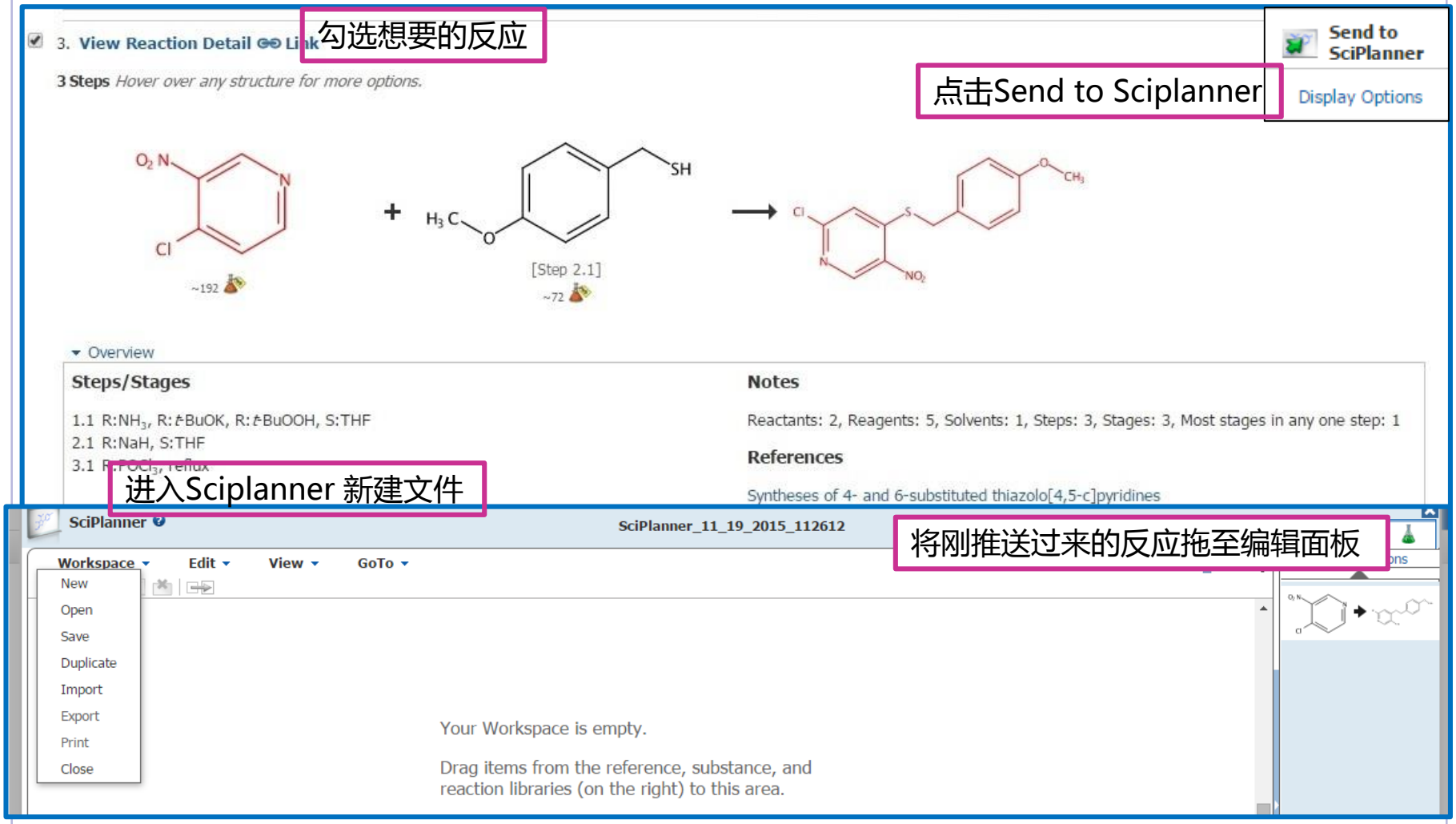
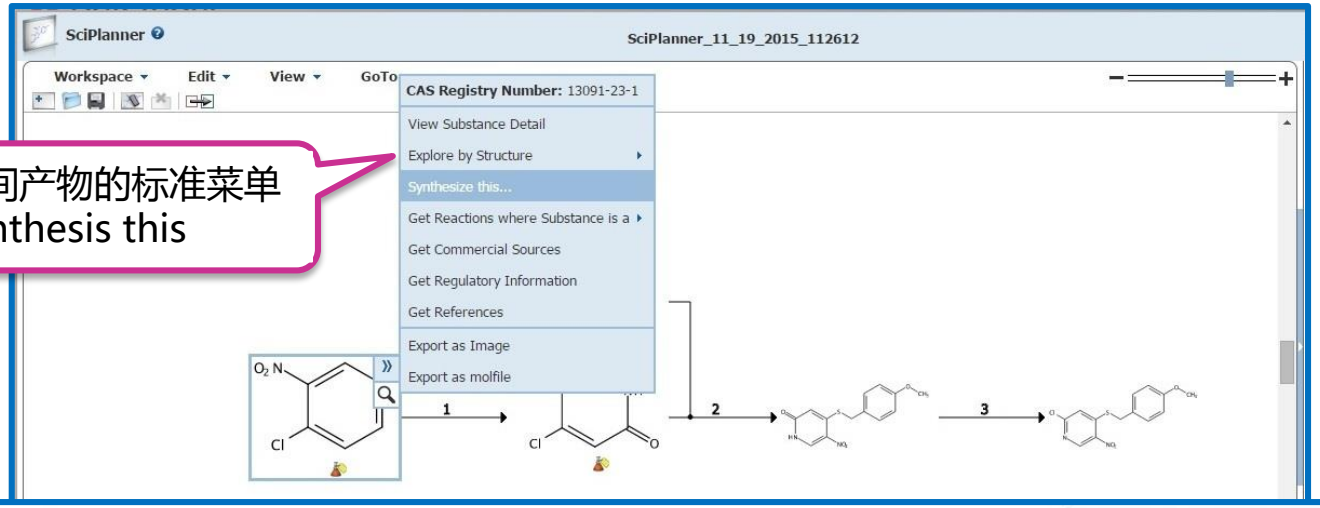
提纲

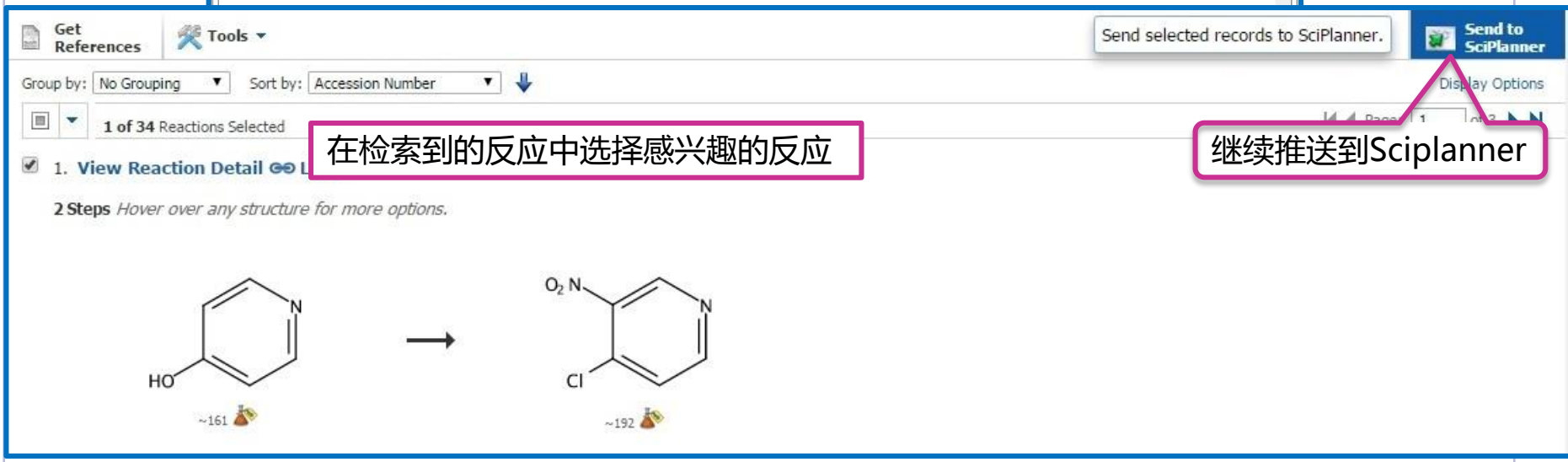
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索（PatentPak）
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
- SciFinder常见问题及解决

SciPlanner使用简介

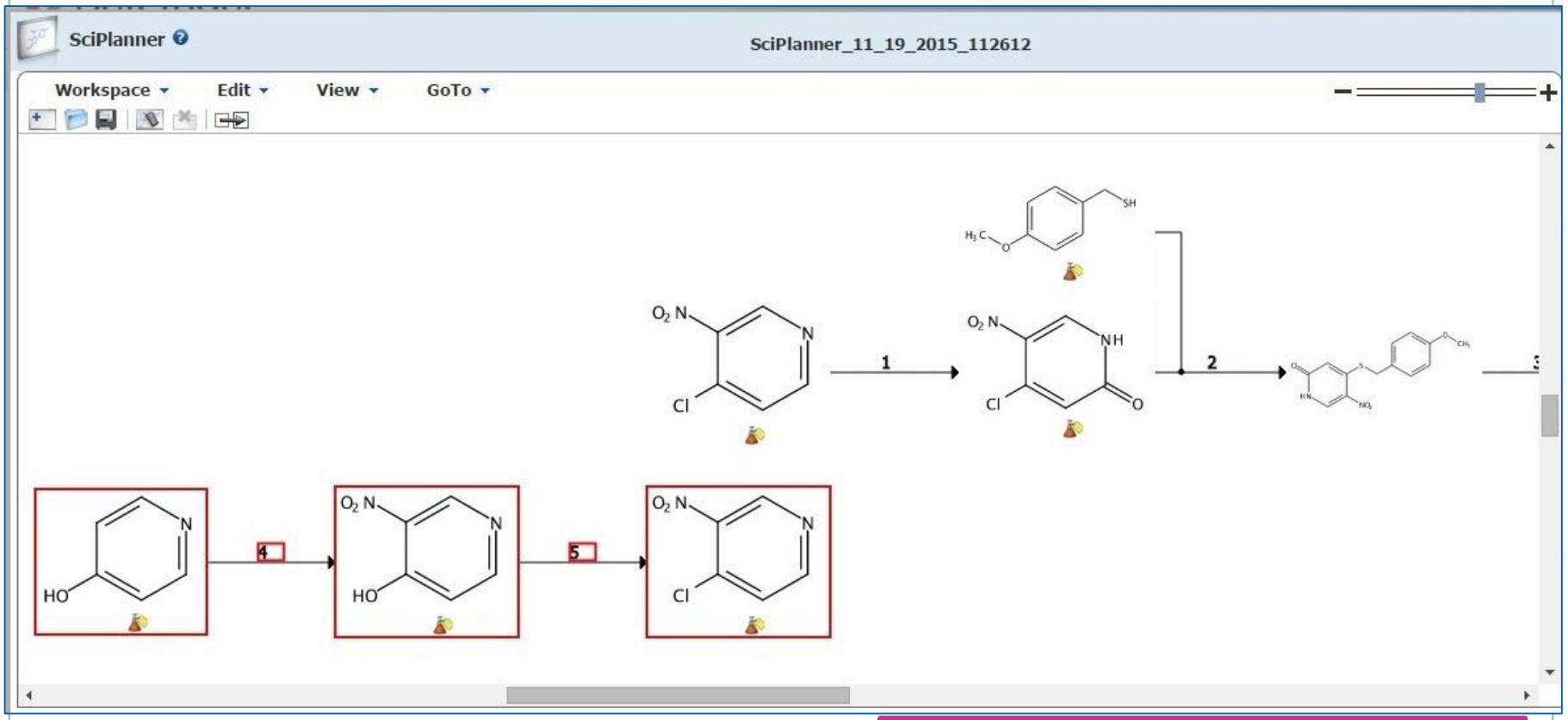


SciPlanner使用简介



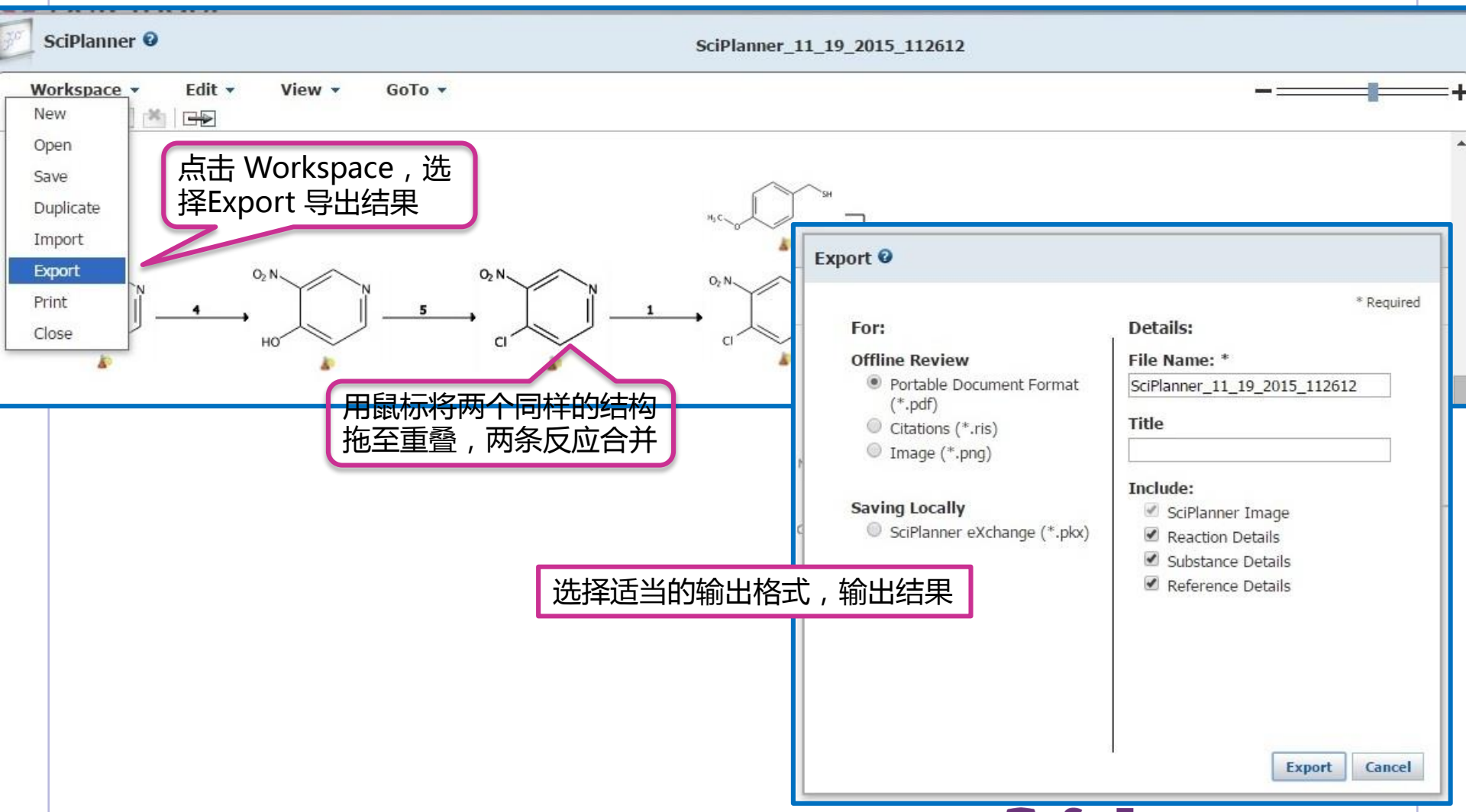


SciPlanner使用简介

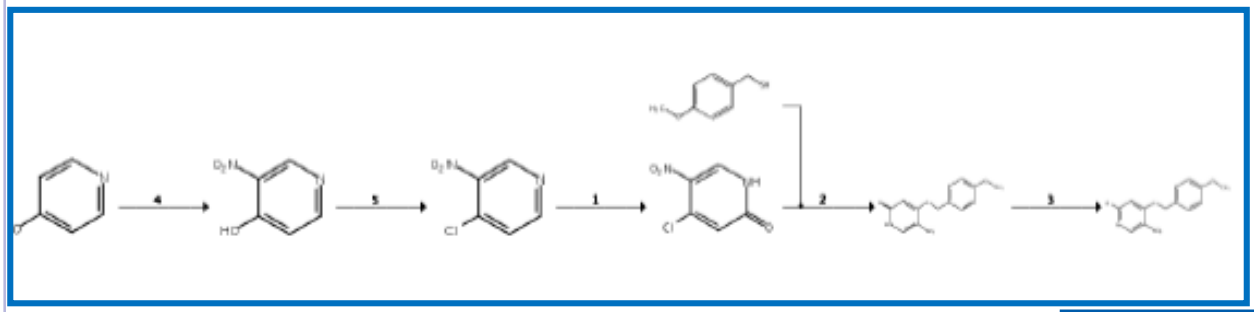


步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介



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

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

SCIFINDER® A CAS SOLUTION

SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

SCIFINDER® A CAS SOLUTION

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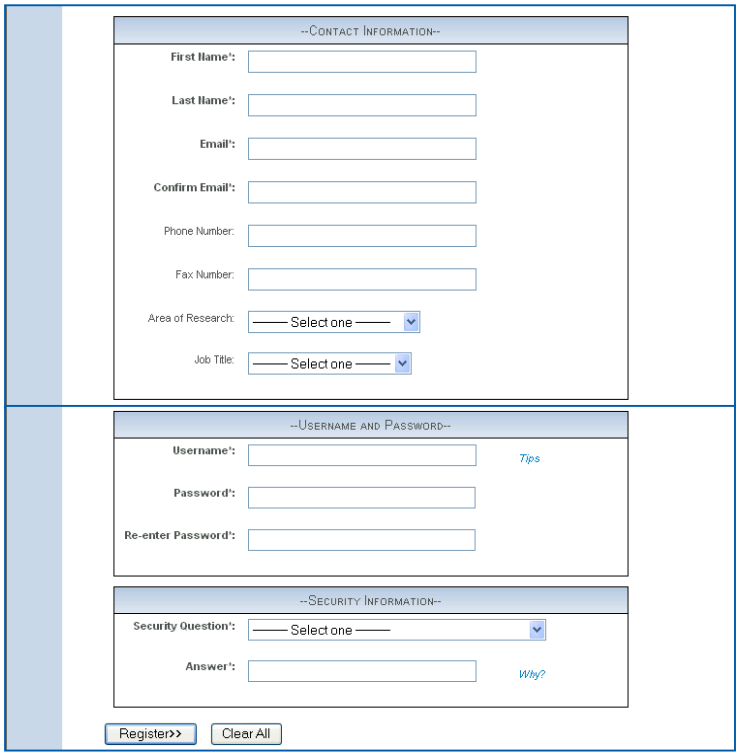

请注意：
1.必须输入真实姓名和学校域名邮箱。
2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- -（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
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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