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江南大学
2019.11.7

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  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

美国化学文摘社—Chemical Abstracts Service

- ACS的分支机构
- 创建于1907年，简称”CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
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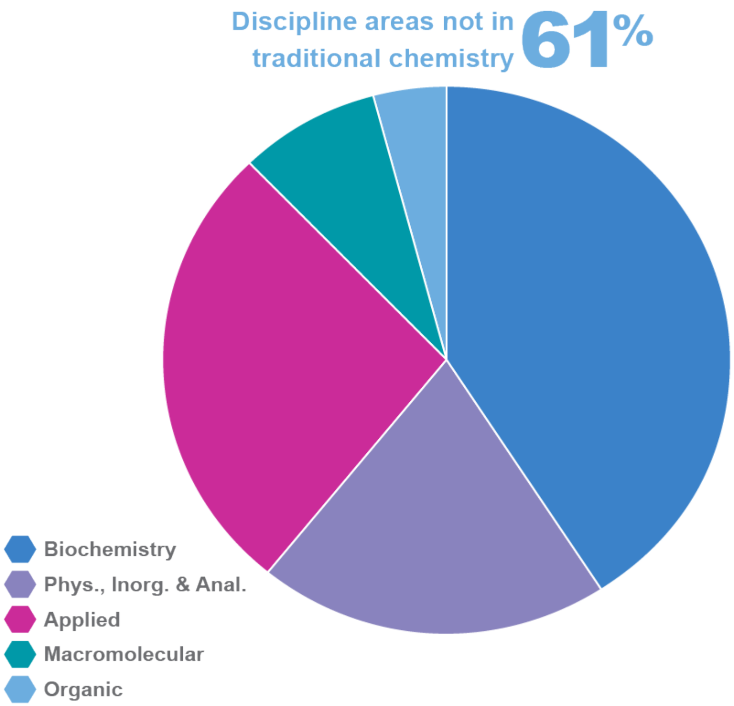

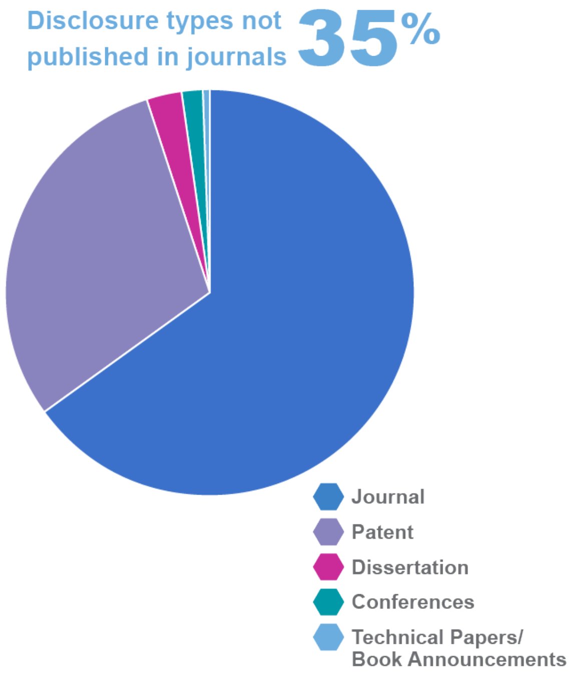

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人工标引----精准揭示关键技术信息

- 数千名科学家组成的编辑团队深刻理解客户的实际需求
- 审阅、筛选、摘要、标引以覆盖并揭示全球所有已公开的化学及相关信息
- CAS登记号——物质的黄金标准
- CAS Roles (CAS物质角色)——生物研究、性能用途、分析检测、合成制备
- CAS Index Terms (CAS技术词语标准)——揭示技术词语相互间的关联
- CA Sections (CAS学科分类，80个类别)——精准定位具体研究领域

Proprietary, standardized indexing in CAS databases ensures consistent, comprehensive search results.

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>1.18亿个独特物质
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>750 化学品目录

Medline
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>5600种期刊文献

人工标引——CAS数据库最具价值的内容

4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia
Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751 PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014

Indexing

Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

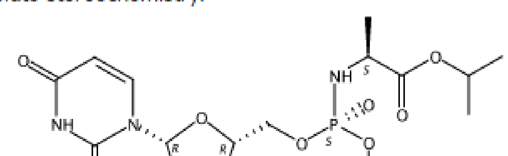
Concepts

Crystallization
Drug bioavailability
Hepatitis C
Hepatitis C virus
Homo sapiens
Human
Pharmaceutical coated tablets

prepn. of novel sofosbuvir crystal

Substances

1190307-88-0P Sofosbuvir   Page 2 in PATENTPAK
Absolute stereochemistry.



Tips:
1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域

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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提纲

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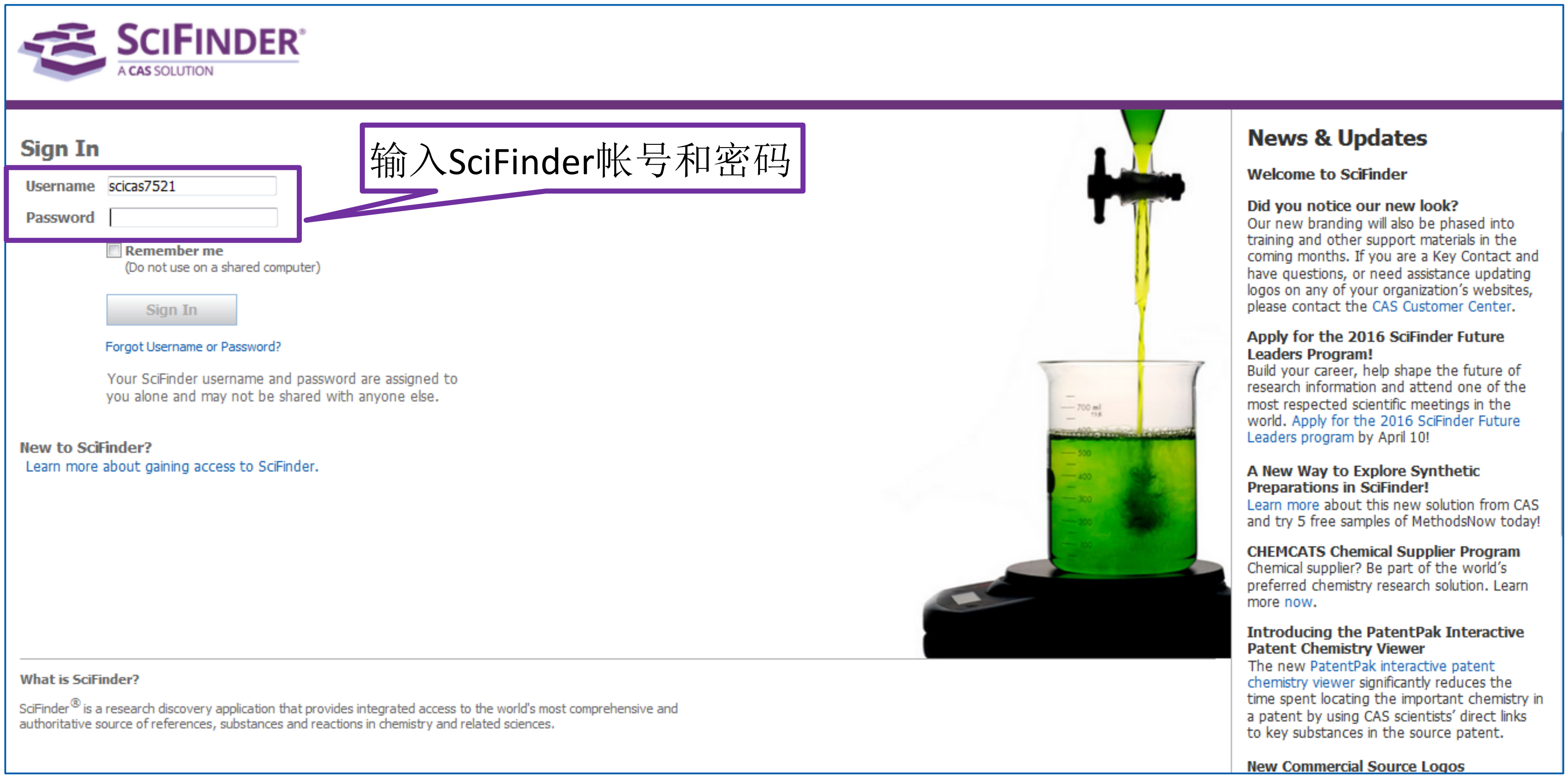

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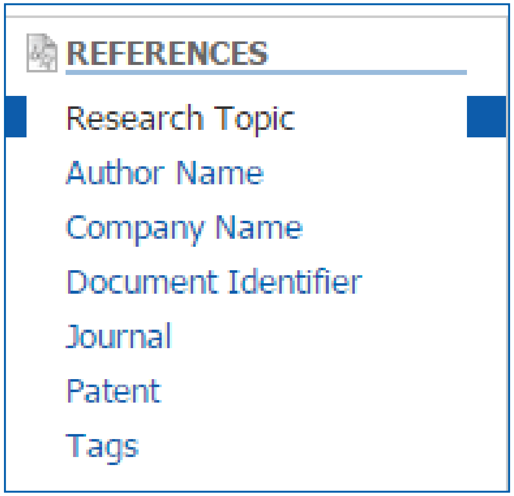

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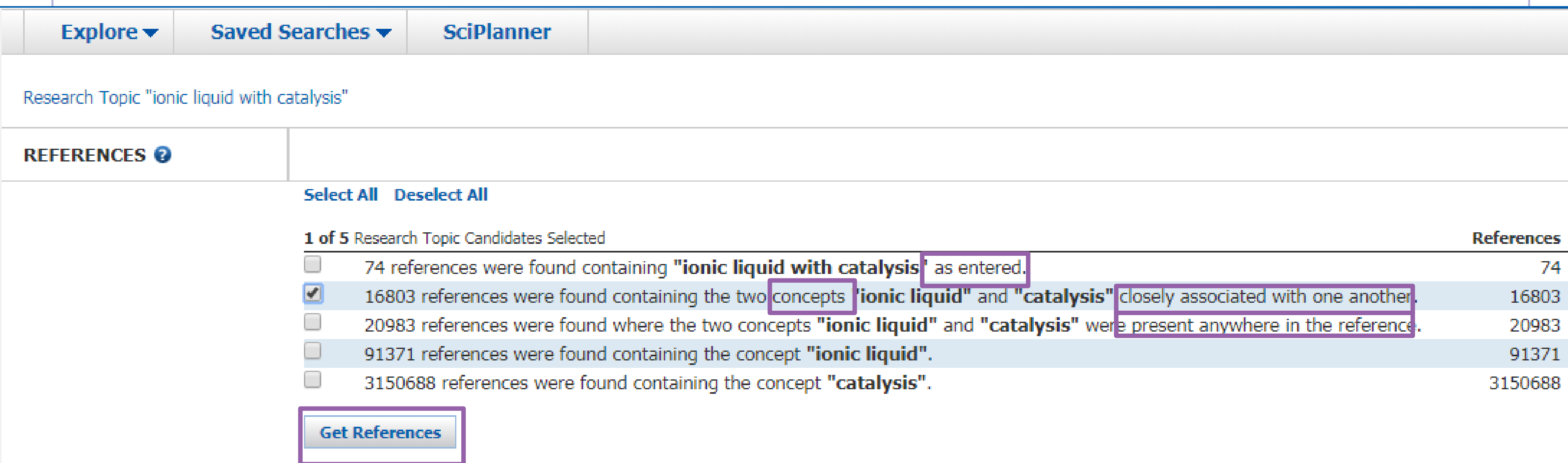
文献检索——主题

主题检索：离子液体催化剂

检索式： ionic liquid with catalysis

关键词之间用介词连接：in, with, of...

主题检索的候选项



"As entered"表示对检索式做精确文本检索；

"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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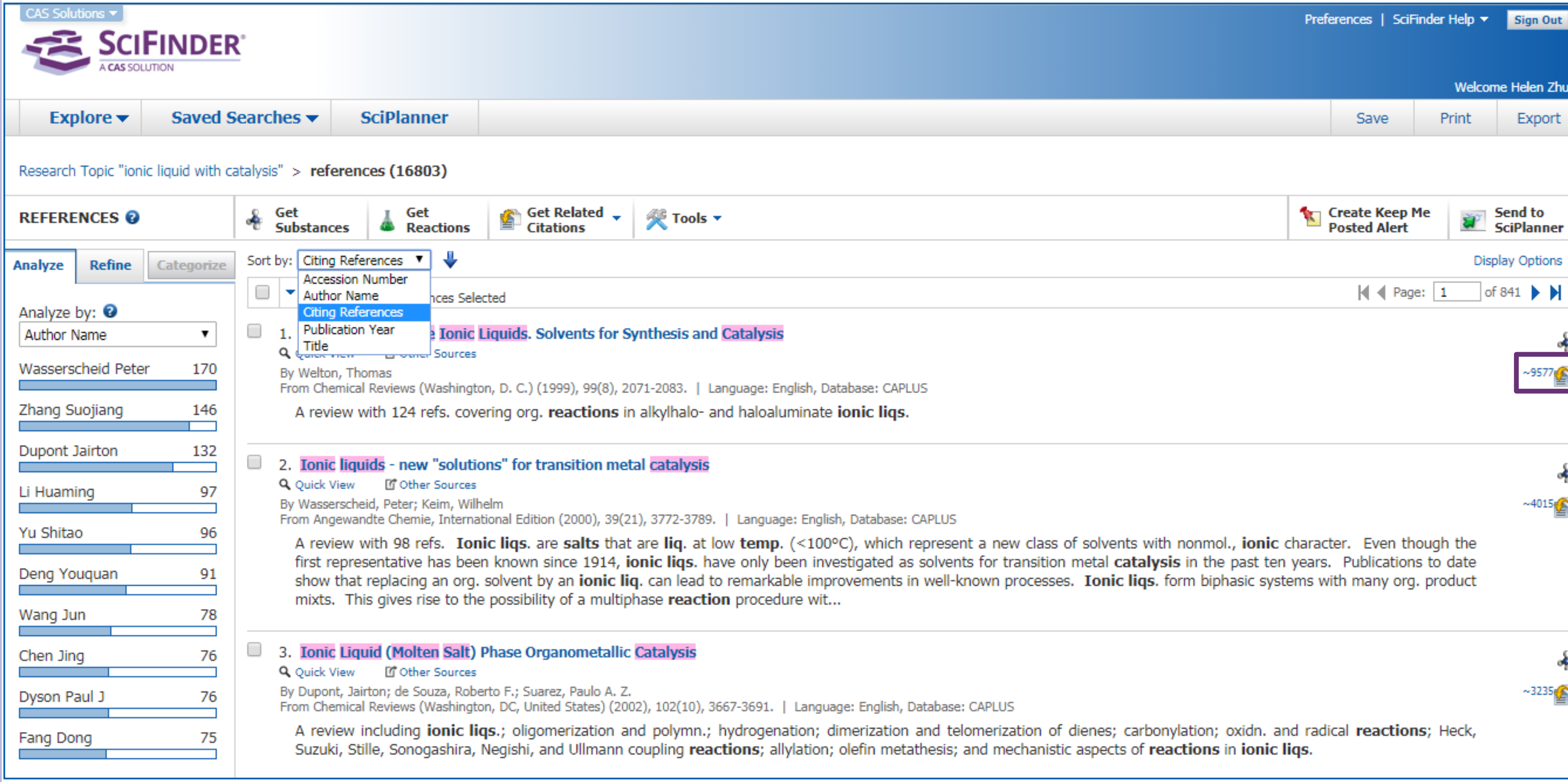
按被引次数排序— Citing References



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文献检索结果的Analyze

本领域研究人员

Analyze | Refine | Categorize

Analyze by: Author Name

Wasserscheid Peter	170
Zhang Suojiang	146
Dupont Jairton	132
Li Huaming	97
Yu Shitao	96
Deng Youquan	91
Wang Jun	78
Chen Jing	76
Dyson Paul J	76
Fang Dong	75

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Analyze by: Company-Organization

Chinese Academy of Sciences, Peop Rep China	446
East China Normal University, Peop Rep China	200
Qingdao University of Science and Technology, Peop Rep China	196
South China University of Technology, Peop Rep China	182
Chevron U S A Inc, USA	178
Jiangsu University, Peop Rep China	167
Zhejiang University, Peop Rep China	164
Zhejiang University of Technology, Peop Rep China	151

期刊

Analyze | Refine | Categorize

Analyze by: Journal Name

Faming Zhuanli Shenqing	2078
PCT Int. Appl.	490
RSC Advances	380
Green Chemistry	360
U.S. Pat. Appl. Publ.	319
Tetrahedron Letters	312
Journal of Molecular Catalysis A: Chemical	255
Catalysis Communications	189
Chemical Communications (Cambridge, United Kingdom)	186
ChemSusChem	160

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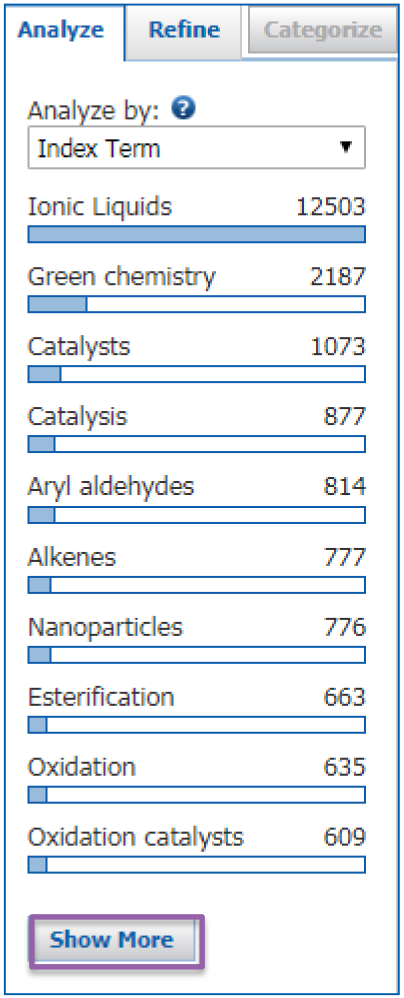
涉及学科领域

Analyze | Refine | Categorize

Analyze by: CA Section Title

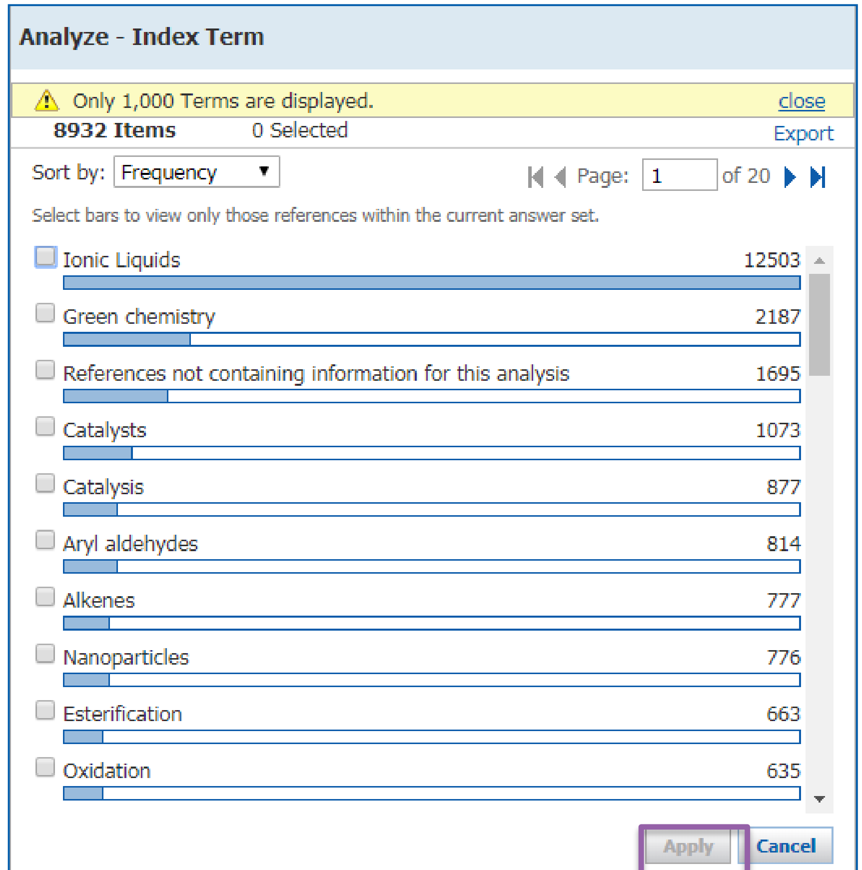
Industrial Organic Chemicals, Leather, Fats, and Waxes	2516
Heterocyclic Compounds (More Than One Hetero Atom)	1297
Benzene, Its Derivatives, and Condensed Benzenoid Compounds	1246
Heterocyclic Compounds (One Hetero Atom)	928
Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms	892
General Organic Chemistry	872
Fossil Fuels, Derivatives, and Related Products	831

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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- Research Topic
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Document Type(s)

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- [ ] Book
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- [ ] Report
- [x] Review

Refine

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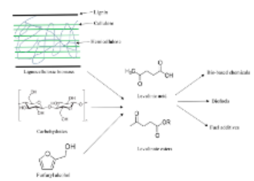
Sort by: Accession Number | Display Options

0 of 1224 References Selected | Page: 1 of 62

1. **Conversion of Biomass and Its Derivatives to Levulinic Acid and Levulinate Esters via Ionic Liquids**
Quick View | Other Sources
By Tiong, Yong Wei; Yap, Chiew Lin; Gan, Suyin; Yap, Winnie Soo Ping
From Industrial & Engineering Chemistry Research (2018), 57(14), 4749-4766. | Language: English, Database: CAPLUS



A review. Biomass has emerged as an abundant and relatively low cost carbon resource alternative to fossil fuel resources in the sustainable prodn. of specialty chems. and biofuel. Levulinic acid is an attractive platform chem. Upgrading of levulinic acid produces levulinate esters, which serve as a transportation fuel and fuel additive. The present review focuses on the development of sustainable conversion of biomass into levulinic acid and levulinate esters via **ionic liqs**. dual solvent-**catalysts**. The synthesis routes of levulinic acid and levulinate esters and the corresponding **ionic l...**

2. **Recent Advances in Pd-Catalyzed Cross-Coupling Reaction in Ionic Liquids**
Quick View | Other Sources
By Li, Jianxiao; Yang, Shaorong; Wu, Wanqing; Jiang, Huanfeng
From European Journal of Organic Chemistry (2018), 2018(11), 1284-1306. | Language: English, Database: CAPLUS

A review. **Ionic liqs**. (**ILs**) can behave as green solvents in comparison with conventional org. solvents, but more often they also act as ligands, co-**catalysts**, and stabilizing agents both for metal active species and for intermediates of **catalytic** systems. In this review we have mainly summarized the recent achievements (2013 to the present) in Pd-**catalyzed** cross-coupling in **ILs** for the assembly of structurally diverse and highly functionalized org. mols., with the focus on cascade **reactions** triggered by nucleopalladation, Suzuki coupling, Sonogashira coupling, allylic functionalization, and ...

3. **Acid-Catalyzed Conversion of Carbohydrates into Value-Added Small Molecules in Aqueous Media and Ionic Liquids**
Quick View | Other Sources
By Bodachivskyi, Iurii; Kuzhiumparambil, Unnikrishnan; Williams, D. Bradley G.
From ChemSusChem (2018), 11(4), 642-660. | Language: English, Database: CAPLUS

A review. Biomass is the only realistic major alternative source (to crude oil) of hydrocarbon substrates for the com. synthesis of bulk and fine chems. Within biomass, terrestrial sources are the most accessible, and therein lignocellulosic materials are most abundant. Although lignin shows promise for the delivery of certain types of org. mols., cellulose is a biopolymer with significant potential for conversion into high-vol. and high-value chems. This review covers the acid-**catalyzed** conversion of lower value (poly) carbohydrates into valorized org. building-block chems. (platform mols....

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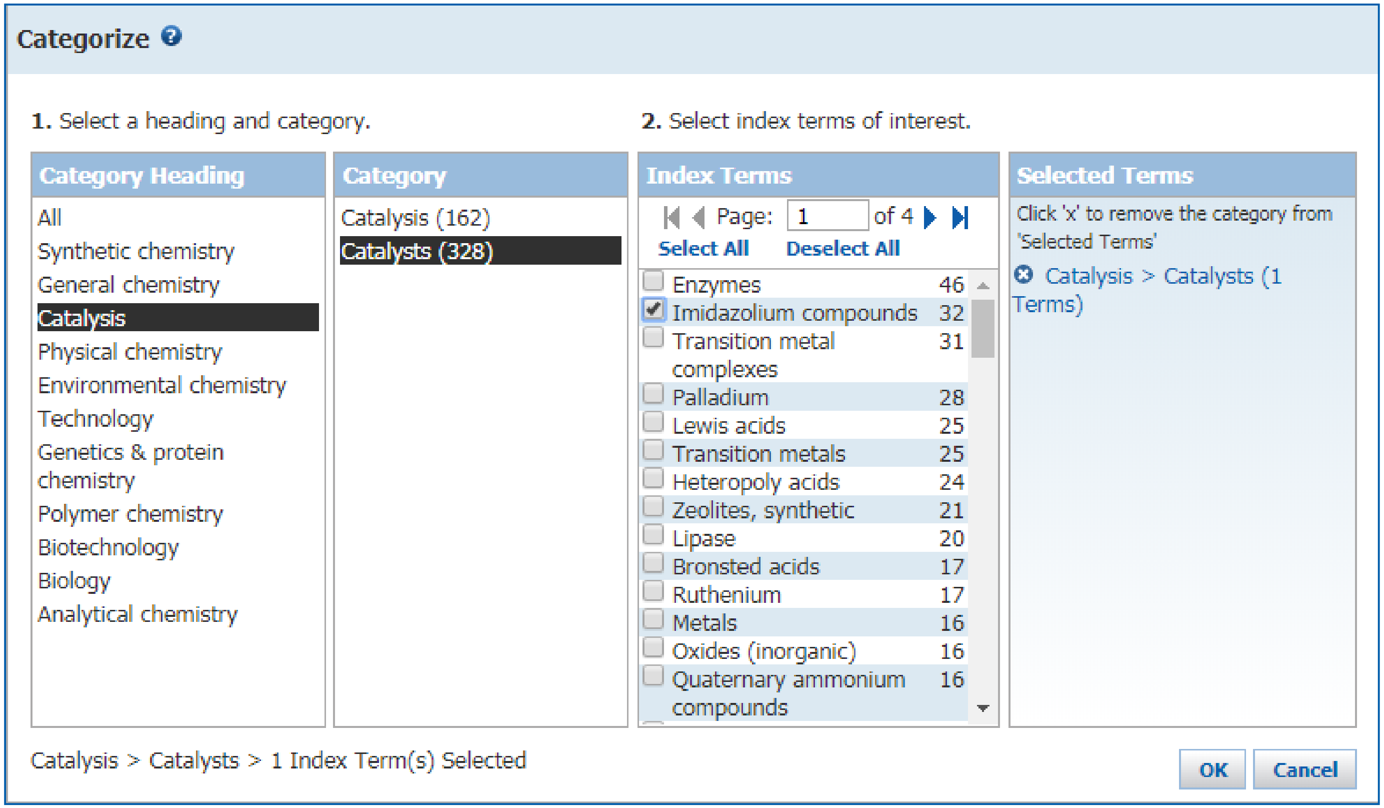
学科领域主分类 | 学科领域副分类 | Index Term | 选中的Index Term



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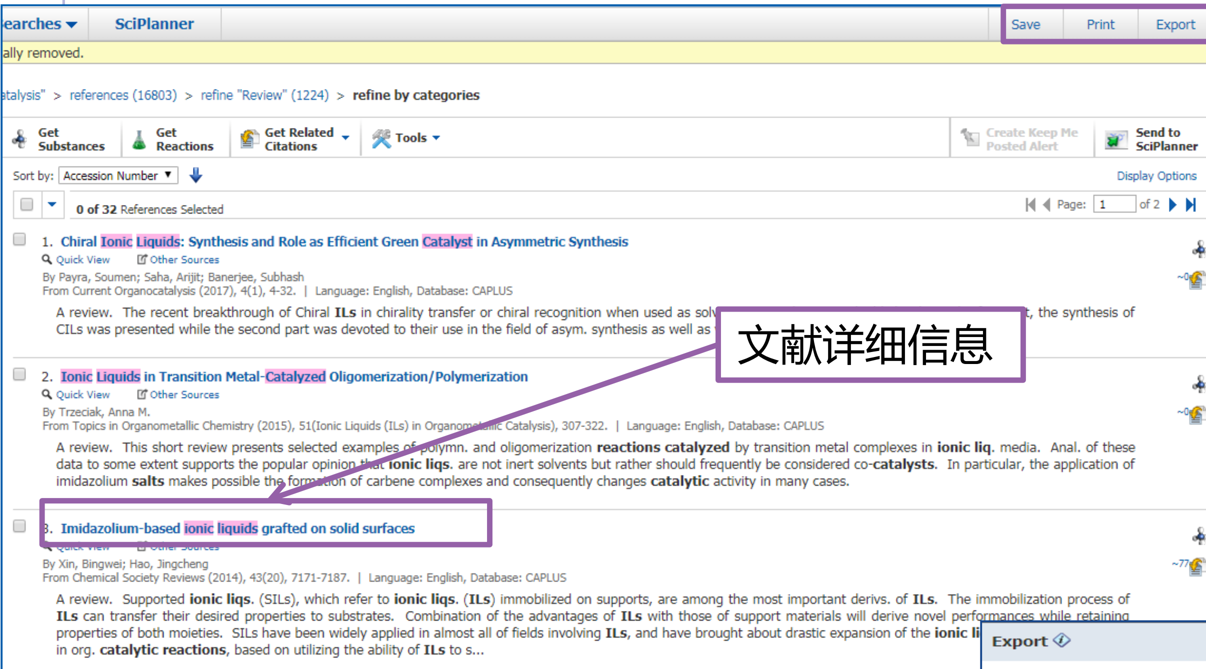

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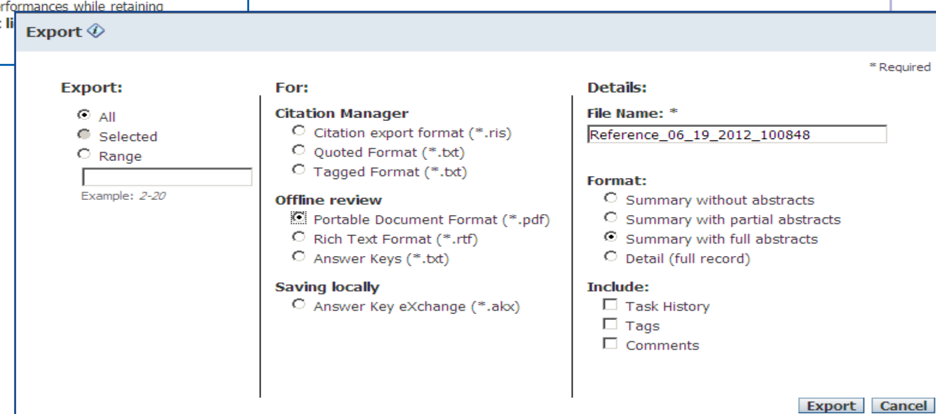

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4. The Partial Hydrogenation of 1,3-Dienes Catalyzed by Soluble Transition-Metal Nanoparticles

By: Luza, Leandro; Gual, Aitor; Dupont, Jairton

A review. The partial hydrogenation of a 1,3-dienes is a structure sensitive reaction that is typically catalyzed by classical heterogeneous (heterotopic) or homogeneous (homotopic) catalysts. Recently, sol. transition-metal nanoparticles (M-NPs), particularly palladium and gold-based systems, have emerged as an efficient alternative. Here, the authors review the current state of the techniques for the partial hydrogenation of 1,3-dienes by M-NPs and conclude that, from the reactivity point of view, these materials possess heterotopic-like and homotopic-like characteristics. They are heterotopic-like because the relative concn. of the monoalkene with respect to the diene does not affect the product selectivity and their catalytic performance is affected by their phys. properties (such as size and shape). Furthermore, they are easily recoverable, with long catalytic lifetimes. Addnl., as homotopic systems, their reactivity can be tuned by using an appropriate org. stabilizer, which displays substrate-selective levels that are not obsd. for classical heterotopic catalysts.

Indexing

General Organic Chemistry (Section21-0)

Concepts 重要概念

Hydrogenation
Ionic liquids
Polymer-supported catalysts
Hydrogenation catalysts
Nanoparticles
Surfactants

advances in developm...
catalyst hydrogenatio...

Dendrimers
Transition metals

advances in developm...
catalyst hydrogenatio...

Catalyst use; Uses

Group 10 elements

Substances 重要物质

7439-89-6 Iron (nanoparticles), uses
7440-05-3 Palladium (nanoparticles), uses
7440-16-6 Rhodium (nanoparticles), uses
7440-18-8 Ruthenium (nanoparticles), uses

advances in development of methods for synthesis of alkene derivs. by transition-metal catalyst hydrogenation of alkadienes

Catalyst use; Uses

592-57-4 1,3-Cyclohexadiene

advances in development of methods for synthesis of alkene derivs. by transition-metal catalyst hydrogenation of alkadienes

Reactant; Reactant or reagent

QUICK LINKS

0 Tags, 0 Comments

SOURCE

ChemCatChem
Volume6
Issue3
Pages702-710
Journal; General Review;
Online Computer File
2014
CODEN:CHEMK3
ISSN:1867-3880
DOI:10.1002/cctc.201300673

COMPANY/ORGANIZATION

UFRGS, Avenida Bento Goncalves
Institute of Chemistry
Porto Alegre, Brazil 91501-970 RS

ACCESSION NUMBER

2013:1749284
CAN160:412993
CAPLUS

PUBLISHER

Wiley-VCH Verlag GmbH & Co. KGaA

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1. 标题
2. 摘要
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- 主题检索时，使用介词 in, with, of 等作为连接词
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- 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，精准定位文献

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  - 文献检索
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- SciFinder常见问题及解决

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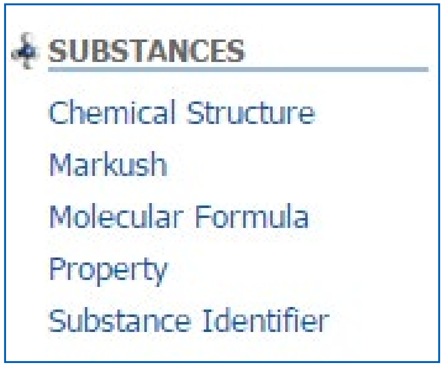
—结构式检索

—分子式检索

—理化性质检索

—物质标识符检索：化学名称，CAS RN



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—有机化合物，天然产物：结构检索

—无机物，合金：分子式检索

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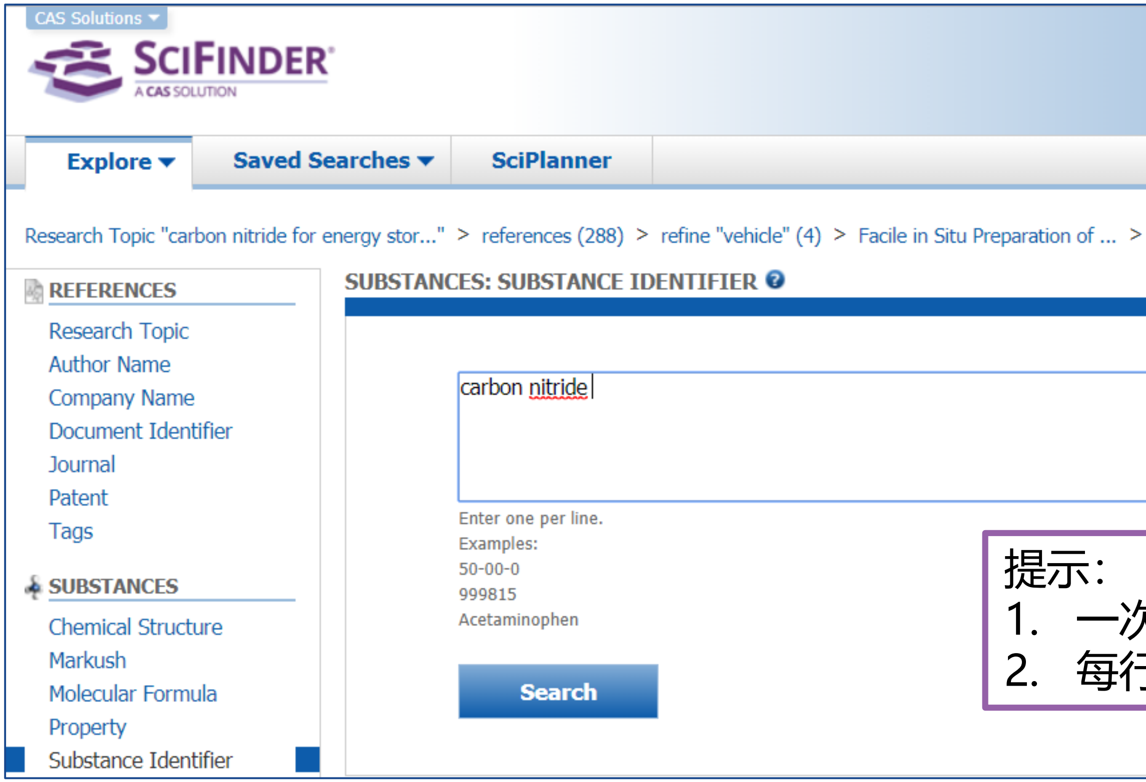

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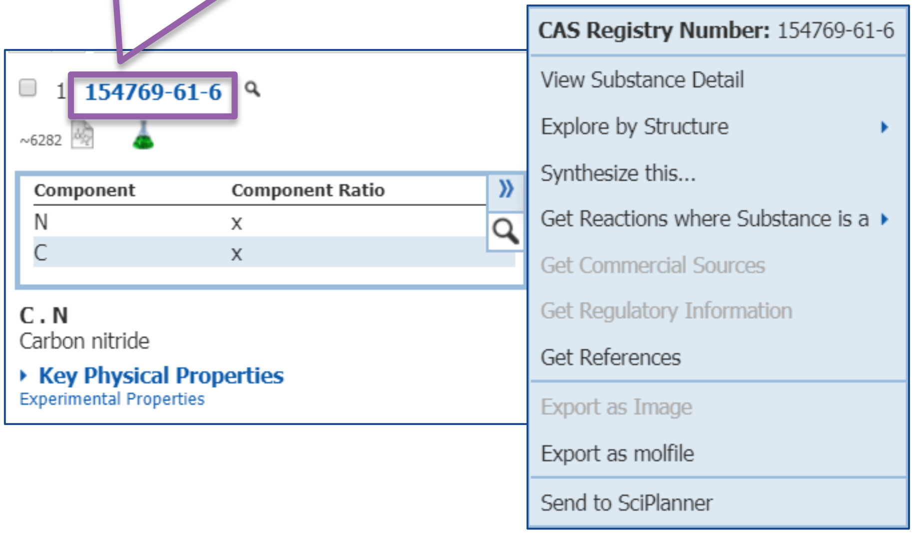

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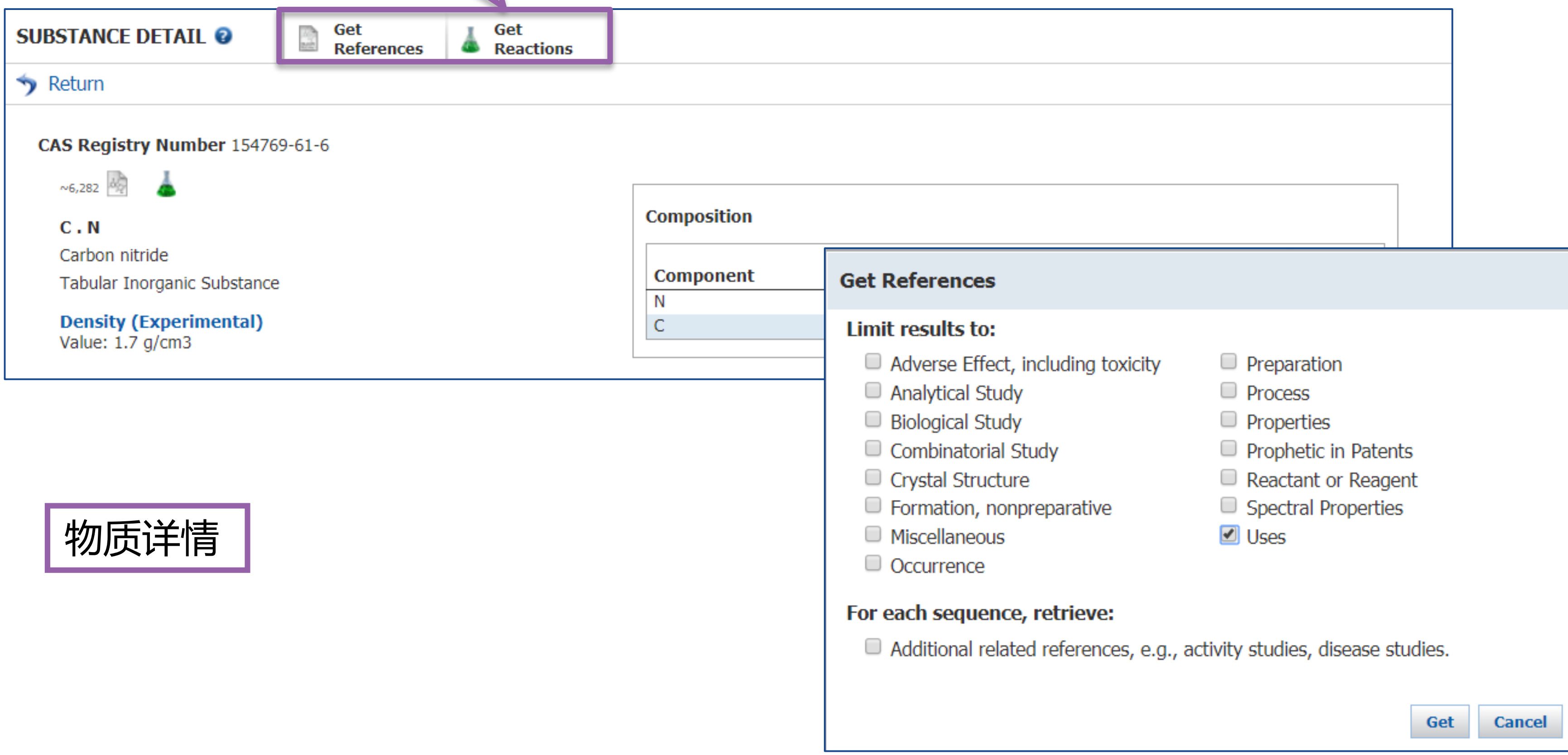

物质详情

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▾ EXPERIMENTAL PROPERTIES

Density | Electrical | Electronic | Interface | Mechanical | Optical and Scattering | Structure Related | Thermal

Structure Related Properties	Value	Condition	Note
Crystal Lattice Parameters	See full text	1 of 4	(6)CAS
Crystal Structure	See full text		(7)CAS
Particle Size	See full text	1 of 5	(25)CAS
Pore Size	See full text	1 of 9	(16)CAS
Porosity	See full text	1 of 2	(28)CAS
Specific Surface Area	See full text	1 of 9	(16)CAS
X-Ray Diffraction Pattern	See full text	1 of 50	(13)CAS

Notes

(6) Mengucci, P.; Recent Research Developments in Applied Physics 2002, V5(Pt. 1), P69-87 CAPLUS

(7) Kojima, Yohei; Diamond and Related Materials 2013, V39, P1-7 CAPLUS

(13) Abd El-kader, F. H.; Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy 2012, V97, P1115-1119 CAPLUS

(16) Yang, Zhuxian; Studies in Surface Science and Catalysis 2005, V156(Nanoporous Materials IV), P573-580 CAPLUS

(25) Bai, Xinjiao; Applied Surface Science 2010, V256(8), P2327-2331 CAPLUS

(28) Mane, Gurudas P.; Journal of Materials Chemistry A: Materials for Energy and Sustainability 2013, V1(8), P2913-2920 CAPLUS

实验数据与实验谱图

▾ EXPERIMENTAL SPECTRA

^{1}H NMR | ^{13}C NMR | Hetero NMR | IR | Mass | Raman | UV and Visible | X-Ray | Additional Spectra

Hetero NMR Properties	Value	Condition	Note
Metal NMR Spectrum	See full text		(8)CAS

Notes

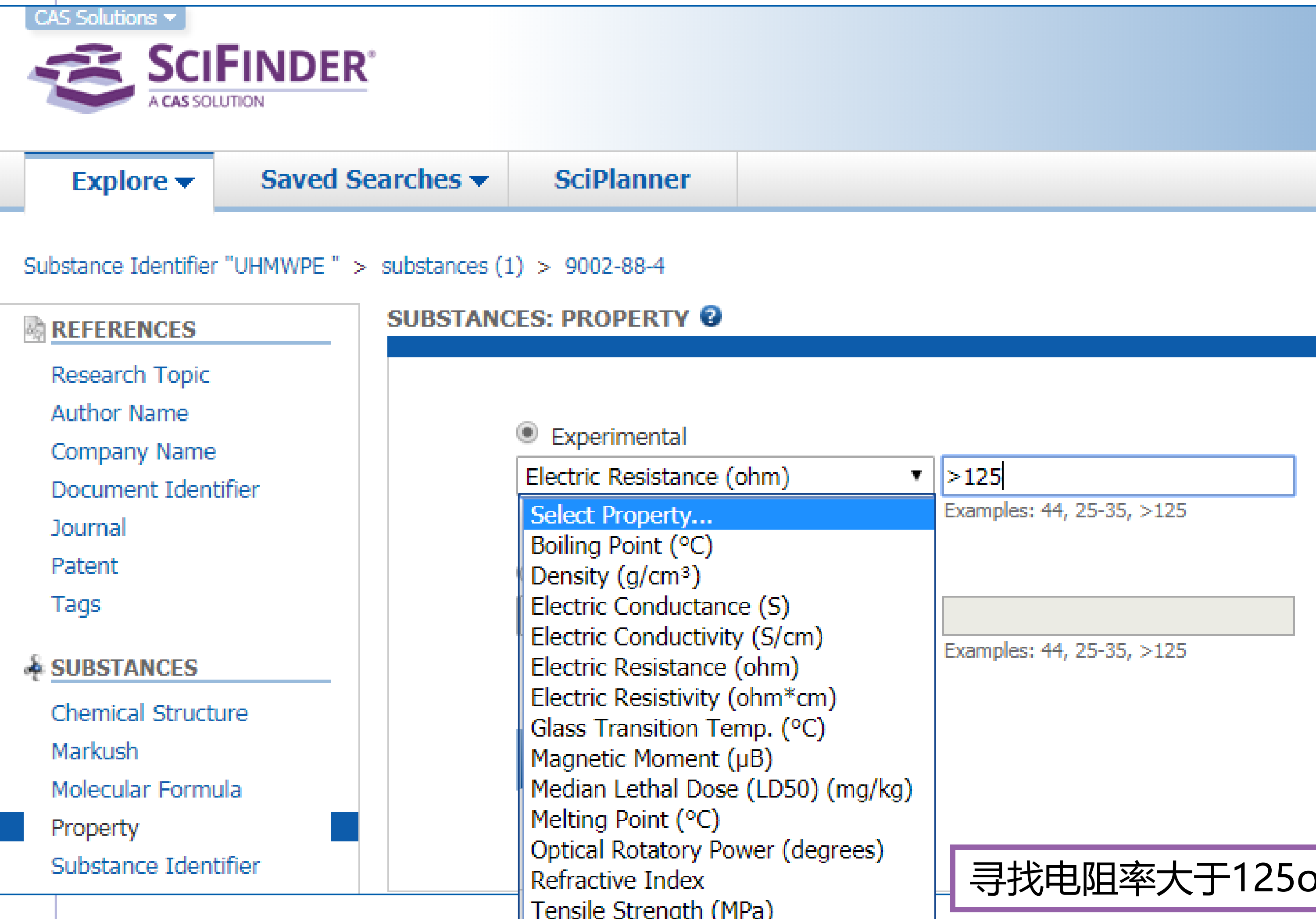
(8) Kasperovich, V. S.; Physics of the Solid State (Translation of Fizika Tverdogo Tela (Sankt-Peterburg)) 2003, V45(9), P1802-1807 CAPLUS

▸ CAS REFERENCE ROLES

▸ ADDITIONAL DETAILS

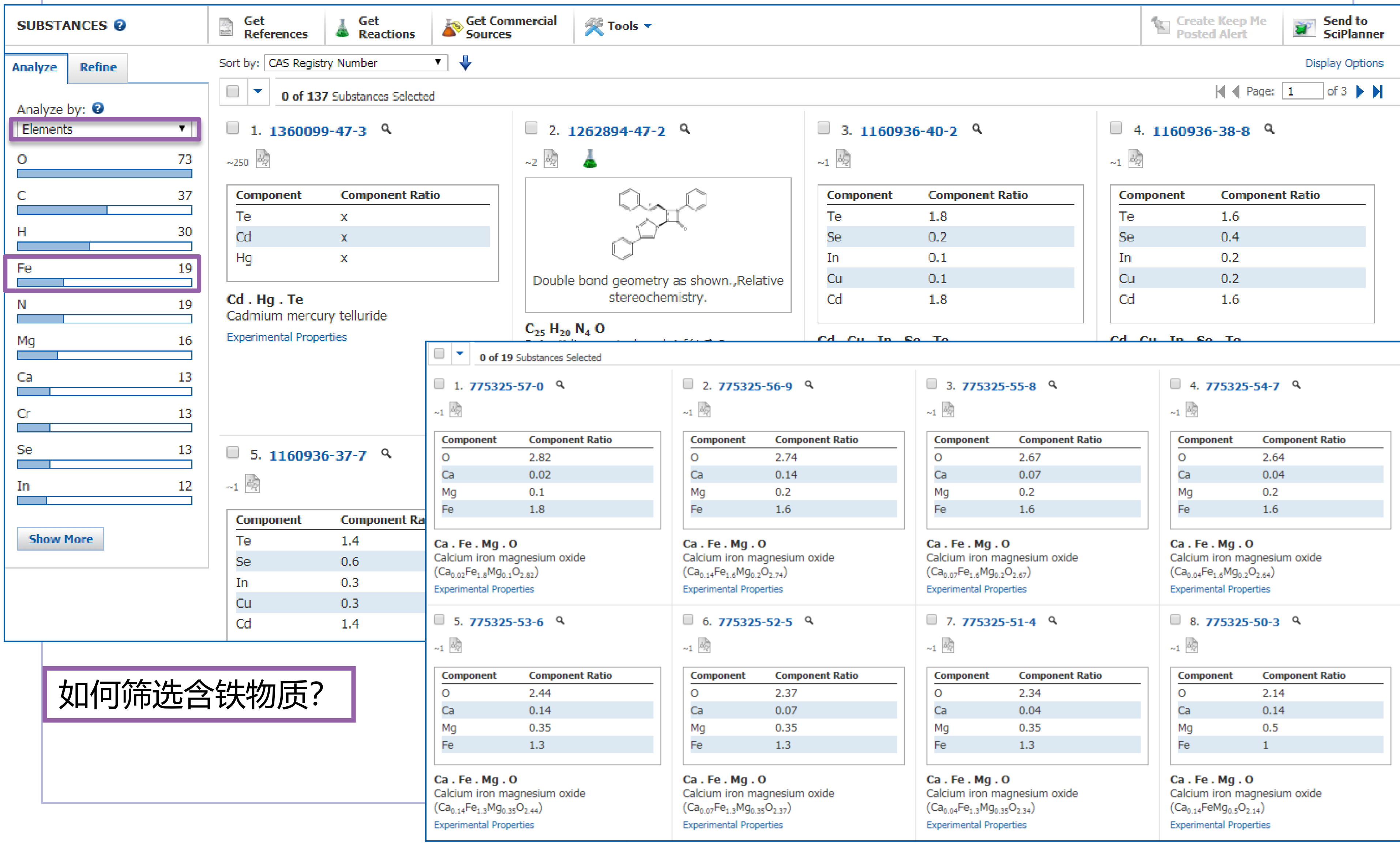
SCIFINDER®
A CAS SOLUTION

物质检索——Property explore



寻找电阻率大于125ohm的含铁物质

物质结果集的筛选——Refine



如何筛选含铁物质?

物质检索——分子式

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

C12H26O4S.Na

Examples:
H4SiO4
(C3H6O.C2H4O)x

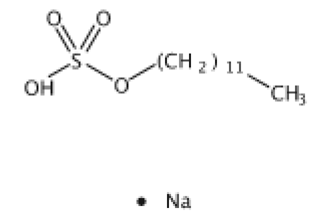
Search

金属盐：金属离子和阴离子间用点（.）分开

1. 151-21-3

(Component: 151-41-7)

~84904 ~276



$C_{12}H_{26}O_4S.Na$
Sulfuric acid monododecyl ester sodium salt (1:1)

- Key Physical Properties
- Regulatory Information
- Spectra
- Experimental Properties

分子式输入需要遵守Hill排序规则：不含碳化合物，按元素符号的字母顺序排列；分子式为含碳化合物时，则“C”在前；如有氢则紧随其后，其它元素符号按字母顺序排在氢的后面

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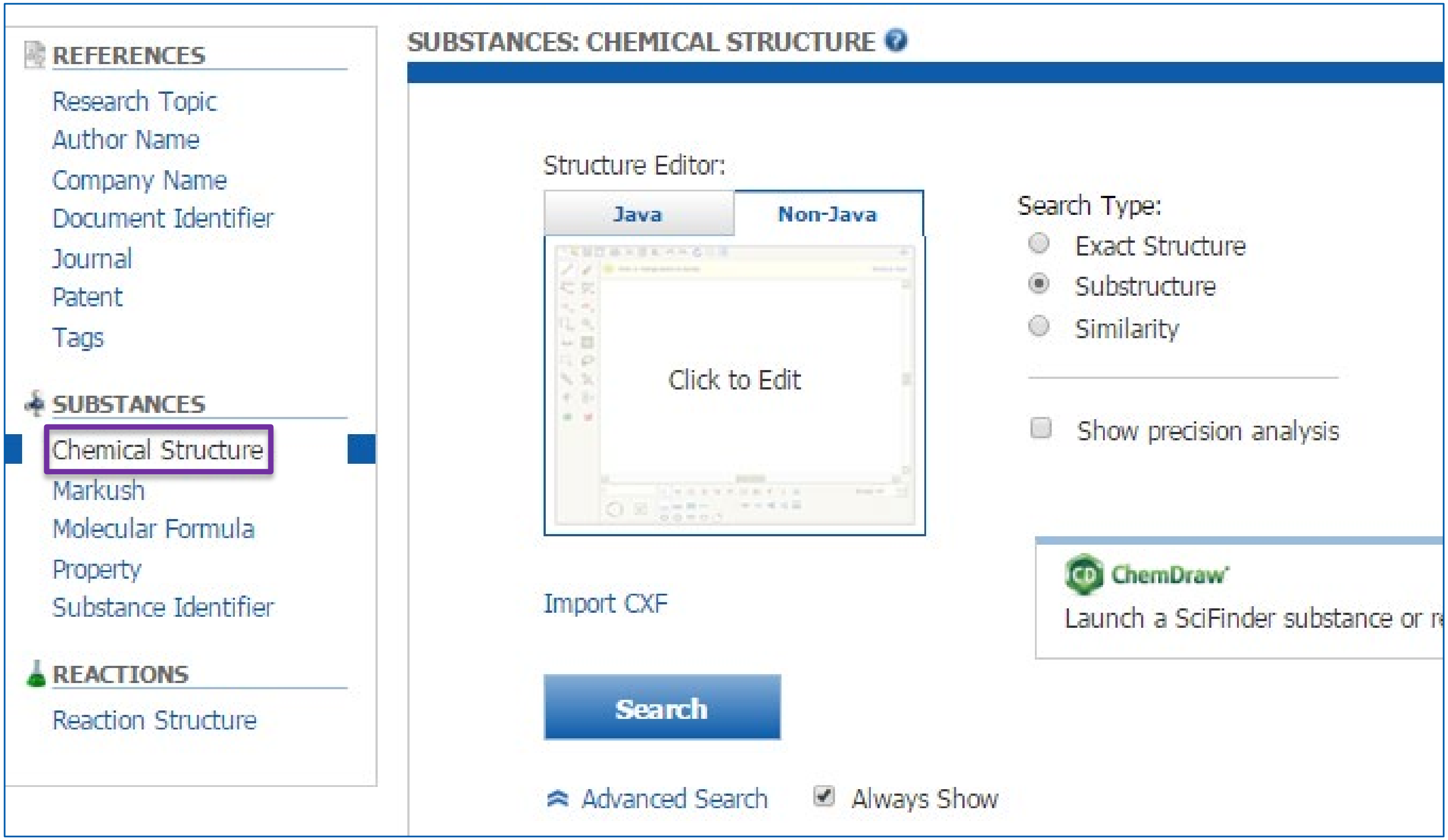
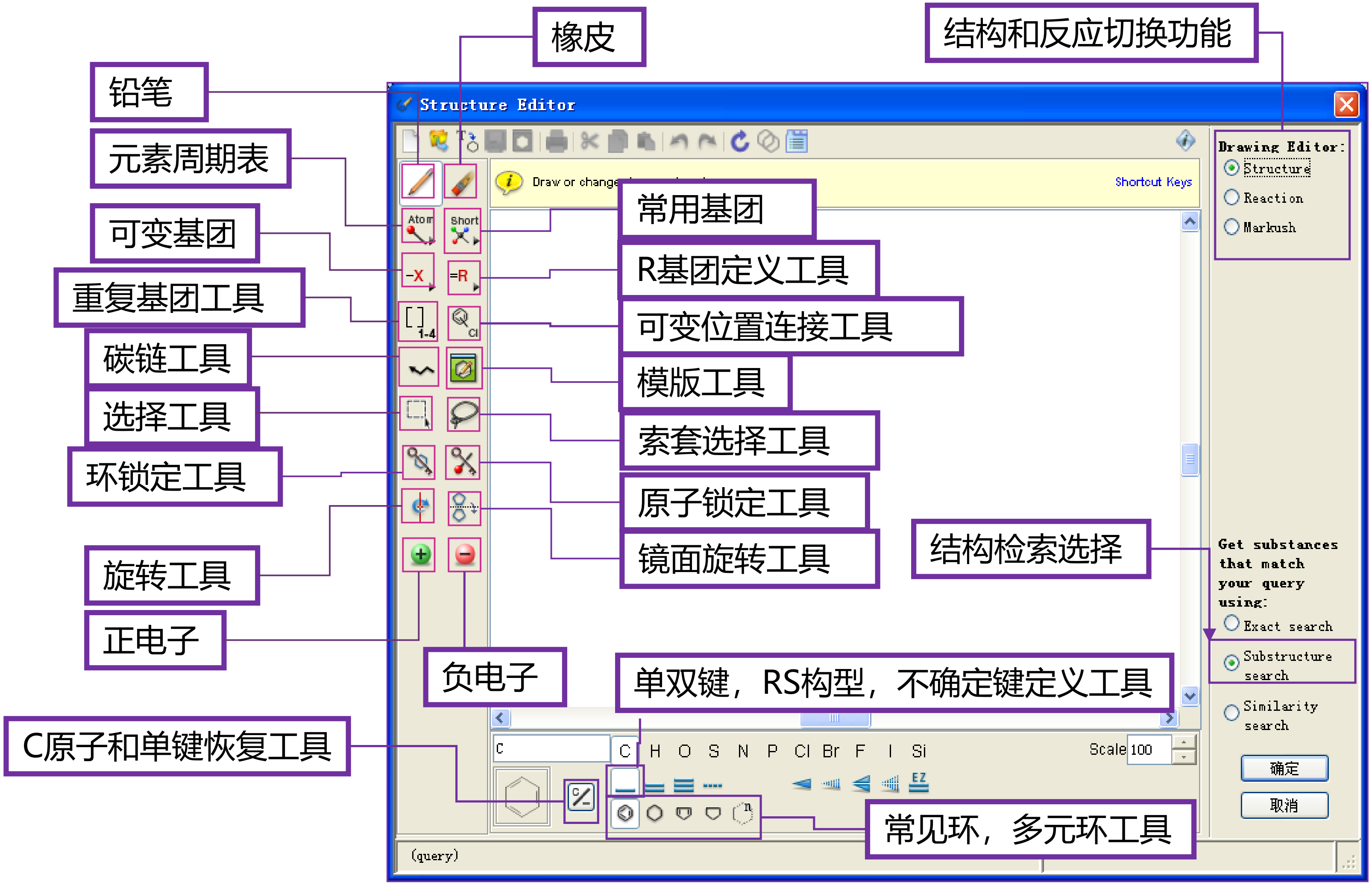
物质检索——结构

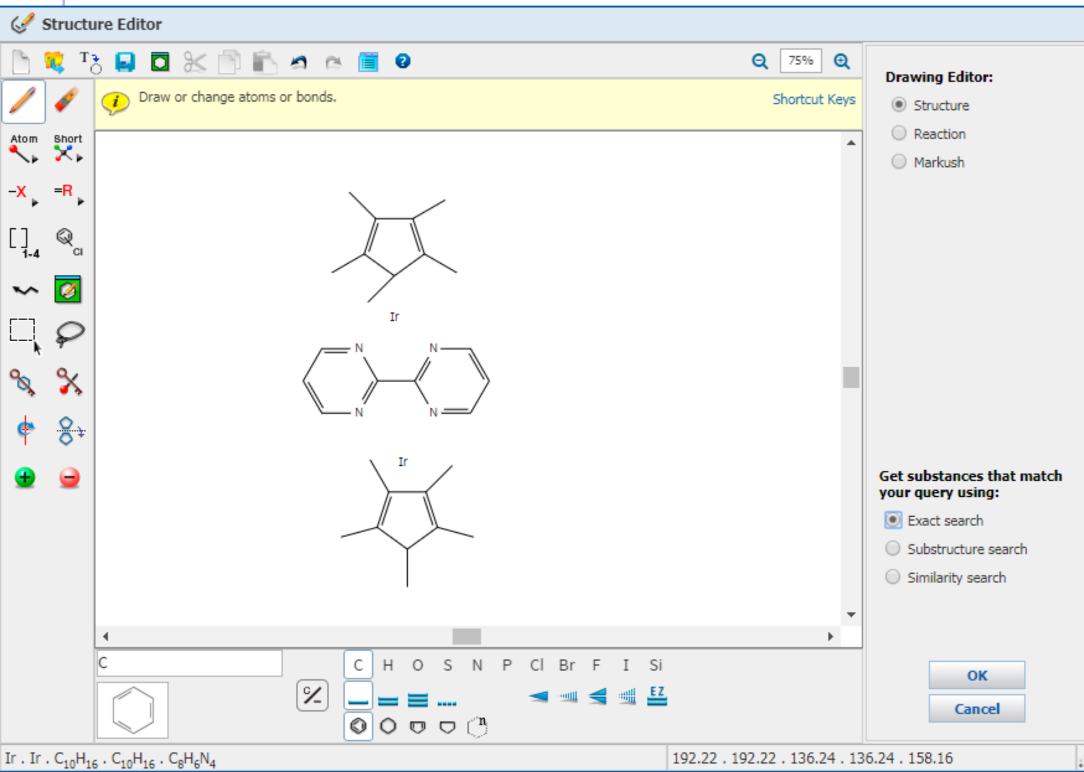

REFERENCES
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier
REACTIONS
Reaction Structure
SUBSTANCES: CHEMICAL STRUCTURE
Structure Editor:
Java
Non-Java
Click to Edit
Search Type:
Exact Structure
Substructure
Similarity
Show precision analysis
ChemDraw
Import CXF
Search
Advanced Search
Always Show

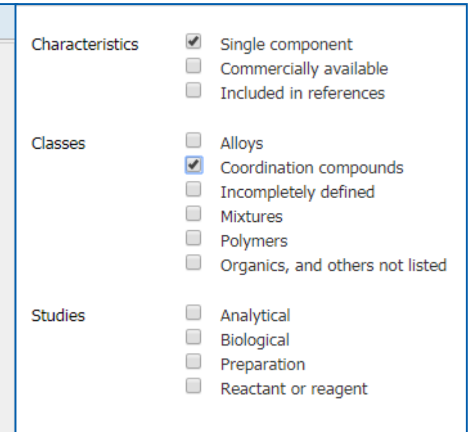
物质检索——结构



SCIFINDER® A CAS SOLUTION

物质检索——精确结构检索





限定为单一组分

精确结构检索

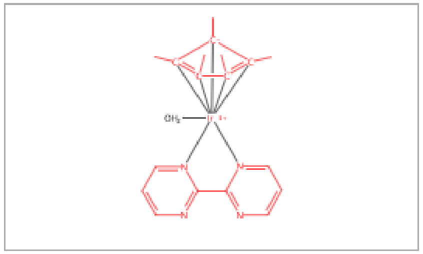
SCIFINDER®
A CAS SOLUTION

物质检索——精确结构检索

0 of 4 Substances Selected

1. 1613301-57-7

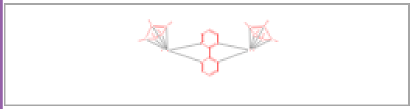
~2



$C_{18}H_{23}IrN_4O$
Iridium(2+), aqua(2,2'-bipyrimidine-κN^1,κ$N^{1'}$)[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

2. 1448751-22-1

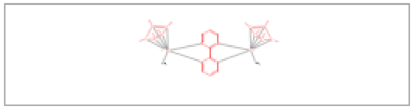
~0



$C_{28}H_{36}Ir_2N_4$
Iridium(4+), [μ-(2,2'-bipyrimidine-κN^1,κ$N^{1'}$:κN^3,κ$N^{3'}$)]bis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-

3. 1448751-19-6

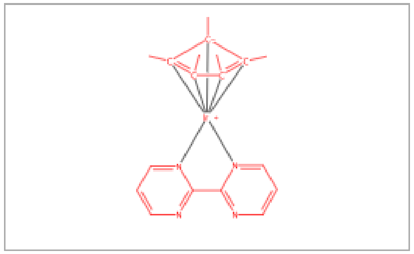
~0



$C_{28}H_{40}Ir_2N_4O_2$
Iridium(4+), diaqua[μ-(2,2'-bipyrimidine-κN^1,κ$N^{1'}$:κN^3,κ$N^{3'}$)]bis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-

4. 920966-48-9

~1



$C_{18}H_{21}IrN_4$
Iridium, (2,2'-bipyrimidine-κN^1,κ$N^{1'}$)[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-

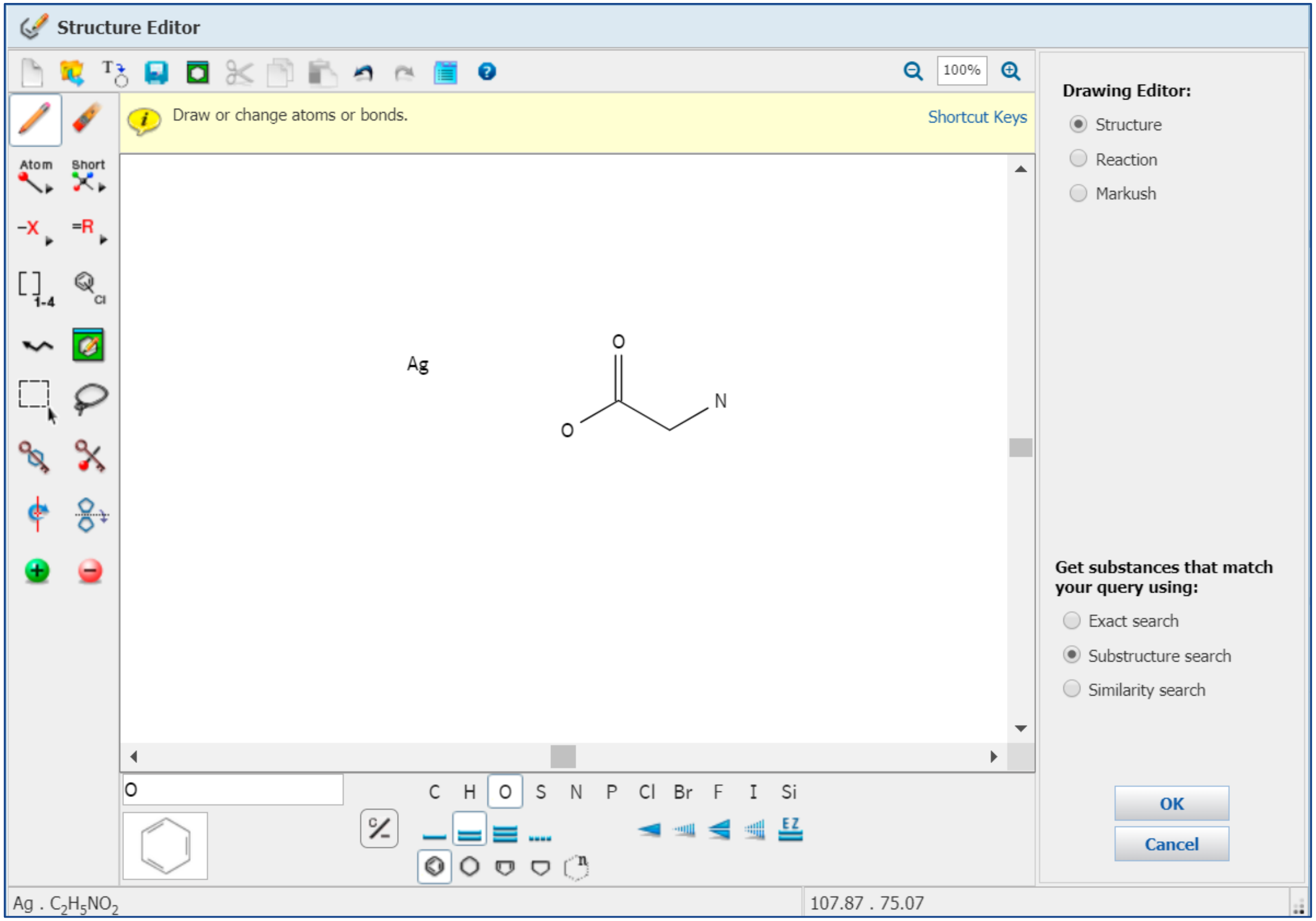
SCIFINDER® A CAS SOLUTION

物质检索——精确结构检索

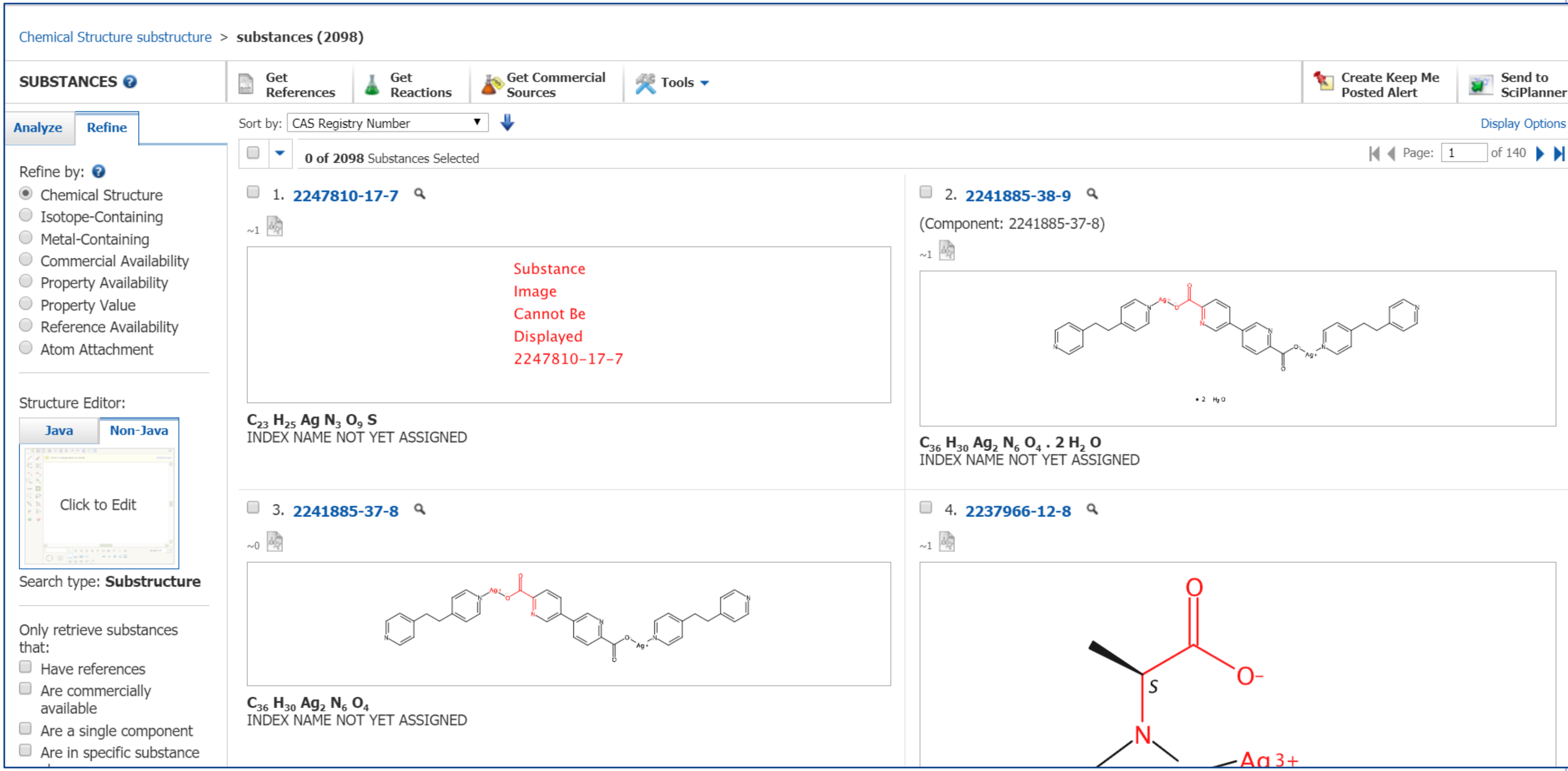
精确结构检索：

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

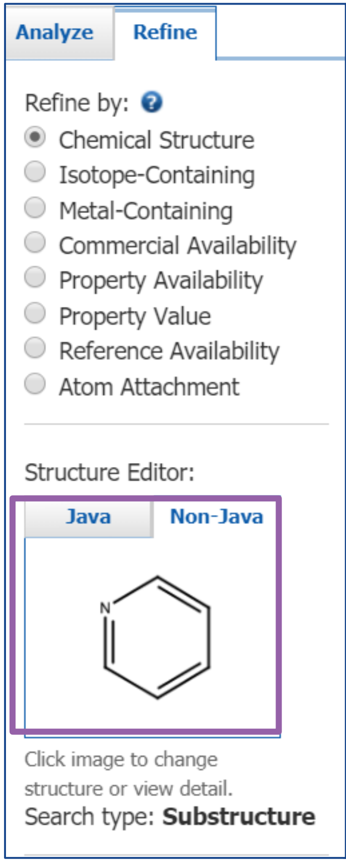

Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Atom
Short
Ag
O
O
N
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search
C H O S N P Cl Br F I Si
OK
Cancel
Ag . $C_2H_5NO_2$
107.87 . 75.07

物质检索——亚结构检索

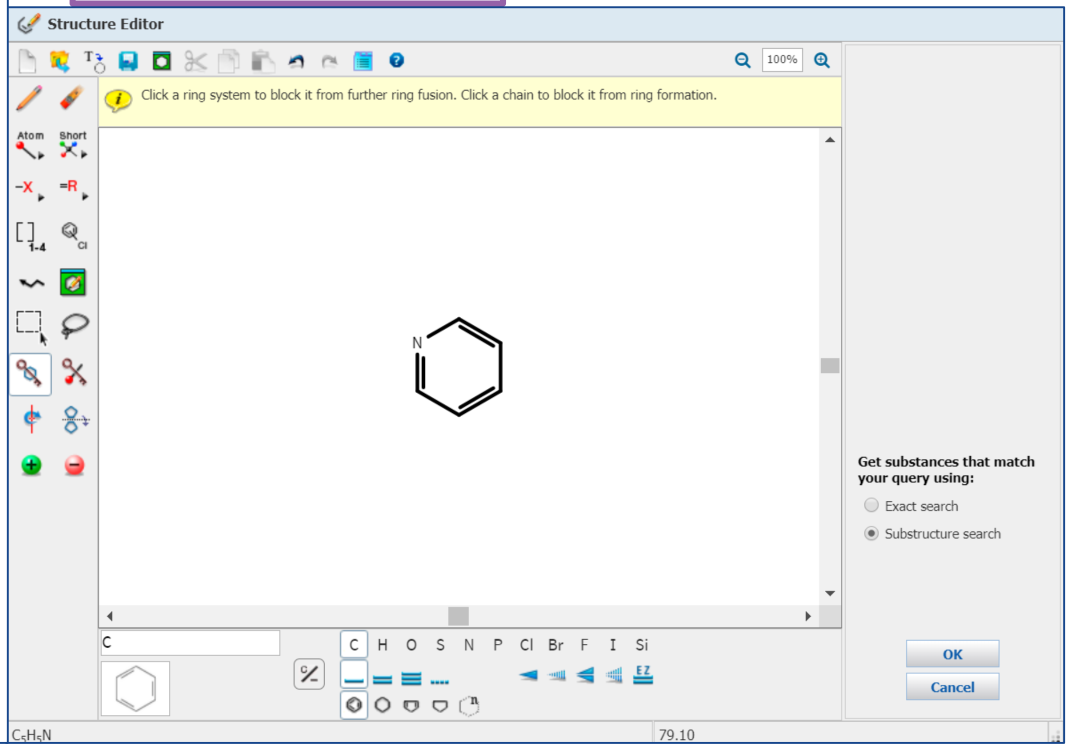


Chemical Structure substructure > substances (2098)
SUBSTANCES
Get References
Get Reactions
Get Commercial Sources
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Sort by: CAS Registry Number
Display Options
0 of 2098 Substances Selected
Page: 1 of 140
Refine by:
Chemical Structure
Isotope-Containing
Metal-Containing
Commercial Availability
Property Availability
Property Value
Reference Availability
Atom Attachment
Structure Editor:
Java
Non-Java
Click to Edit
Search type: Substructure
Only retrieve substances that:
Have references
Are commercially available
Are a single component
Are in specific substance
1. 2247810-17-7
Substance Image Cannot Be Displayed 2247810-17-7
C23 H25 Ag N3 O9 S
INDEX NAME NOT YET ASSIGNED
2. 2241885-38-9
(Component: 2241885-37-8)
C36 H30 Ag2 N6 O4 . 2 H2 O
INDEX NAME NOT YET ASSIGNED
3. 2241885-37-8
C36 H30 Ag2 N6 O4
INDEX NAME NOT YET ASSIGNED
4. 2237966-12-8
O
O-
S
N
Ag 3+

亚结构检索结果的限定



化学结构的再次限定



环锁定

亚结构检索结果的限定

SUBSTANCES

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

Analyze | Refine

Sort by: Relevance

Display Options

0 of 173 Substances Selected

Page: 1 of 12

Analyze by:

Substance Role

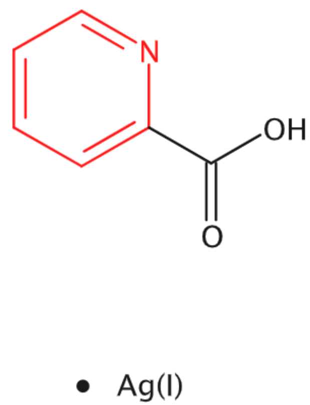
Properties	80
Preparation	66
Reactant or Reagent	30
Uses	18
Biological Study	17
Process	7
Analytical Study	1

Show More

1. 27876-60-4

(Component: 98-98-6)

~23 ~1



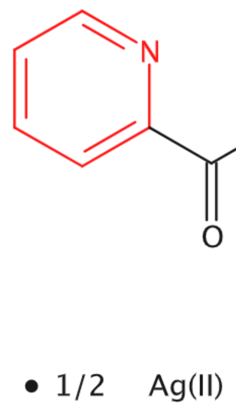
$C_6H_5NO_2 . Ag$

2-Pyridinecarboxylic acid, silver(1+) salt (1:1)

2. 22721-95-5

(Component: 98-98-6)

~4



$C_6H_5NO_2 . {}^1/_2 Ag$

2-Pyridinecarboxylic acid, silver(2+) salt (2:1)

3. 171626-32-7

(Component: 23628-31-1)

~2

4. 1622218-89-6

(Component: 499-83-2)

~1

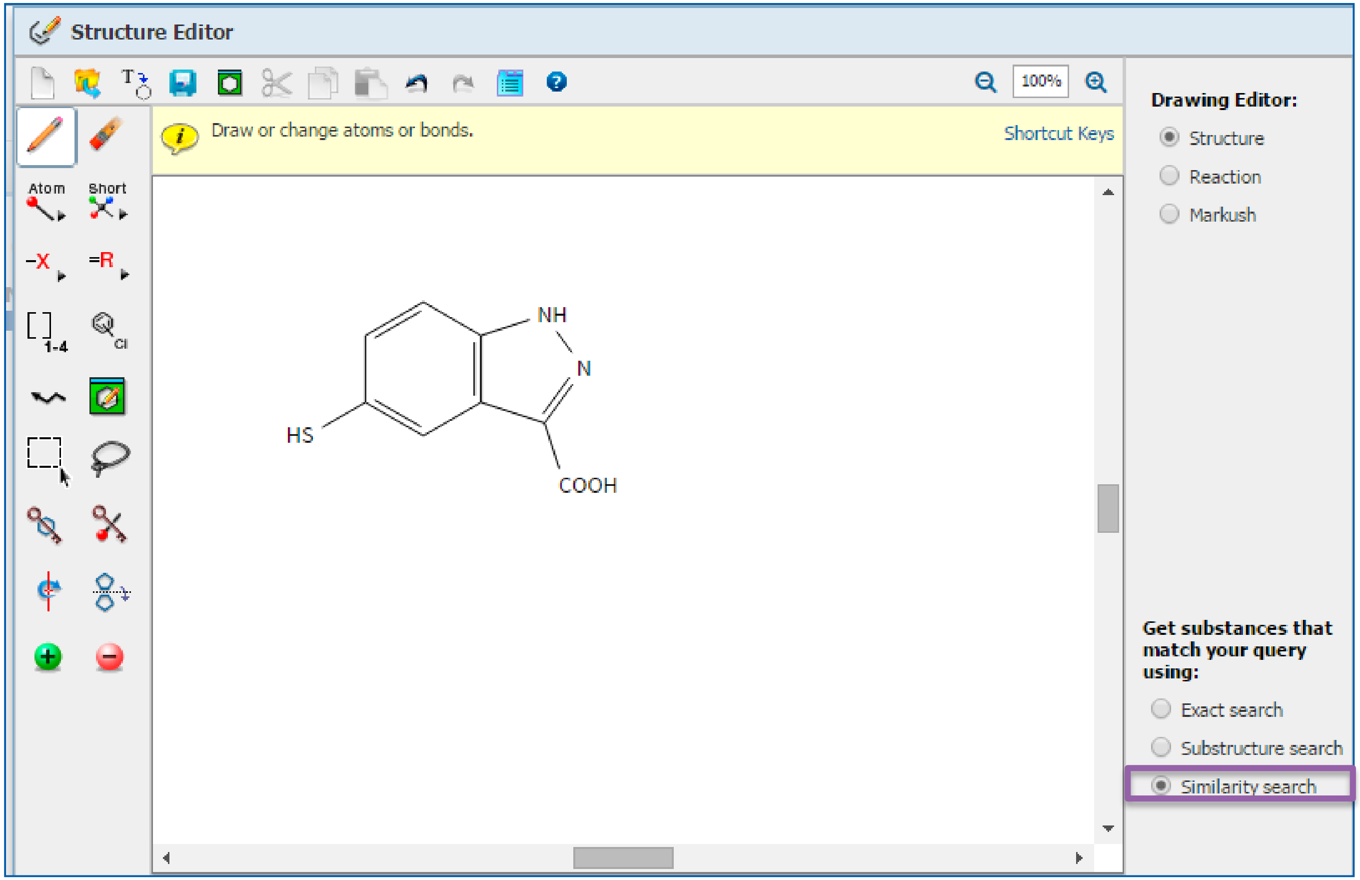
SCIFINDER® A CAS SOLUTION

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

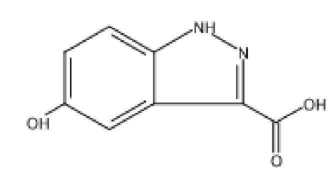
评分越高，相似度越高，结构越相似

Score: 88

1. **885518-94-5**

取代基变化

~1 ~35



$C_8 H_6 N_2 O_3$

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

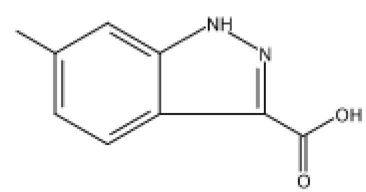
Key Physical Properties

Score: 86

5. **858227-12-0**

取代基位置变化

~7 ~41



$C_9 H_8 N_2 O_2$

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

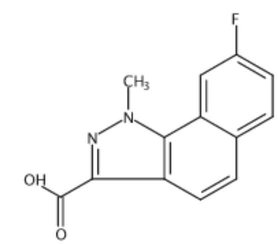
Key Physical Properties

Score: 65

541. **1100422-**

母体结构变化

~1



$C_{13} H_9 F N_2 O_2$

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

Key Physical Properties

SciFinder® A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

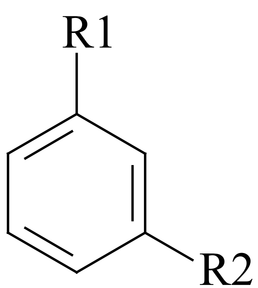
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

SCIFINDER®
A CAS SOLUTION

Markush检索

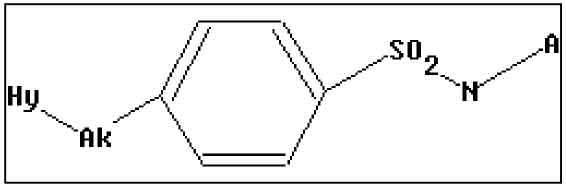
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 预测性物质[Prophetic Substance]：
  — 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
  — 专利中所陈述的预测物质，不会被分配CAS RN
  — Markush检索，能检索到通过结构检索检不到的专利

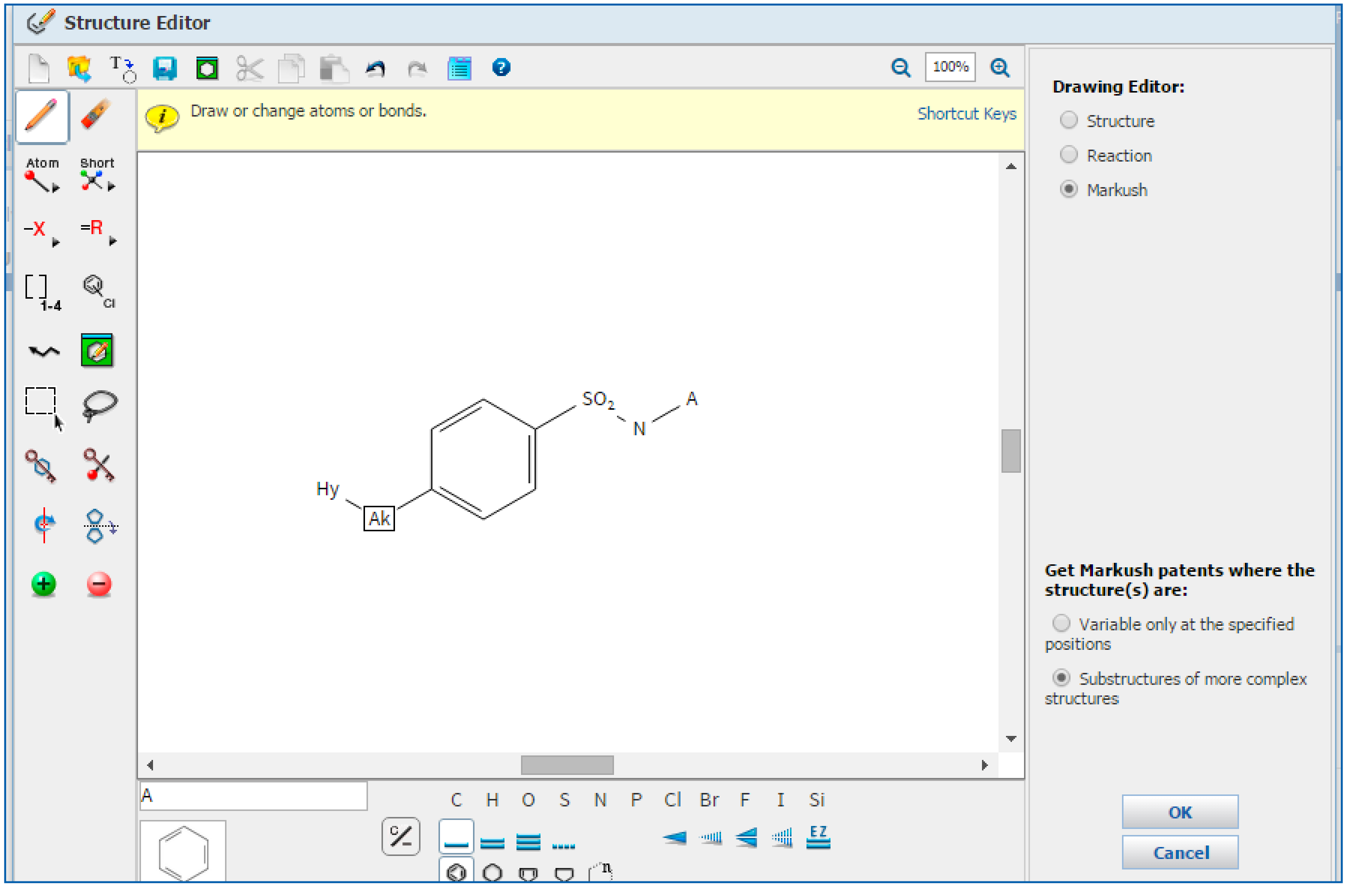


$R1 = H, Br, Cl, I$

$R2 = Br, Cl, I, -CH_2-\text{halogen}, -CH(CH_3)-\text{halogen},$



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

全部是专利

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

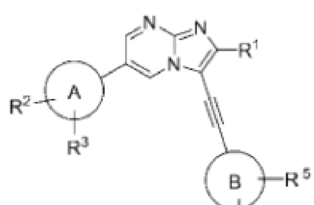
The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat 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^{a}R^b, SO_2R^b, or NR^aSO_2R^b; R^a, R^b (same...

SCIFINDER® A CAS SOLUTION

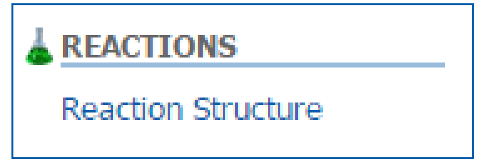
提纲

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

SciFinder检索选项——反应检索

- 反应检索方法

  结构式



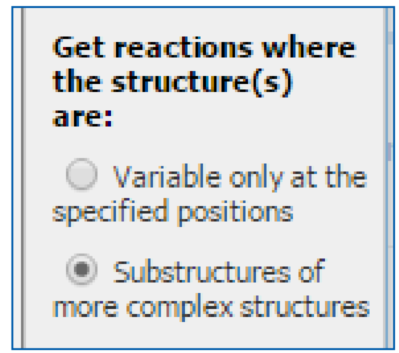
- 常用获取方法

  已知物质：由物质获取反应

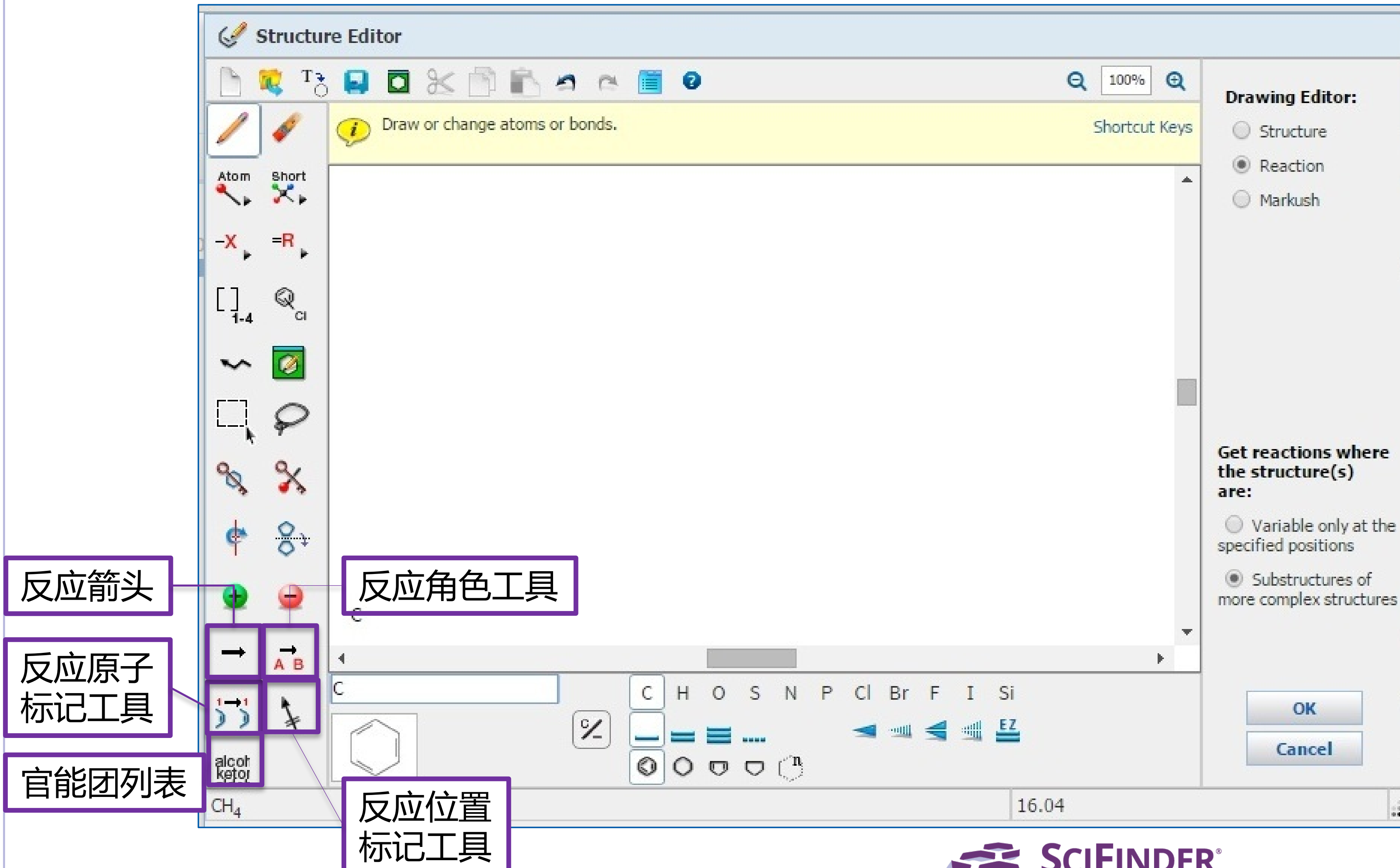
  已知文献：从文献中获取反应

  精确结构反应检索

  亚结构反应检索

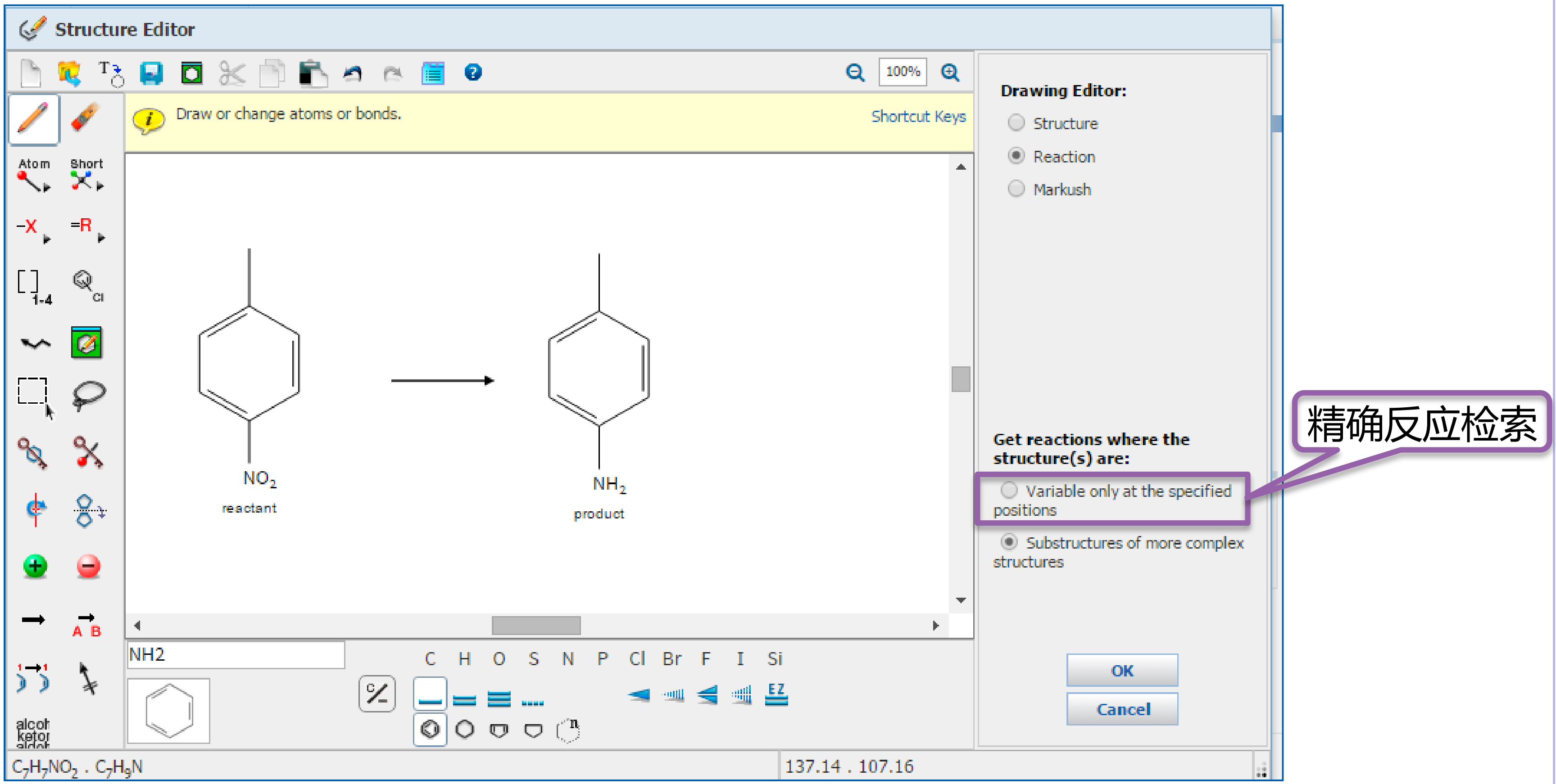


反应绘制工具



Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Atom
Short
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
C H O S N P Cl Br F I Si
OK
Cancel
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。

Get References | Tools | Send to SciPlanne

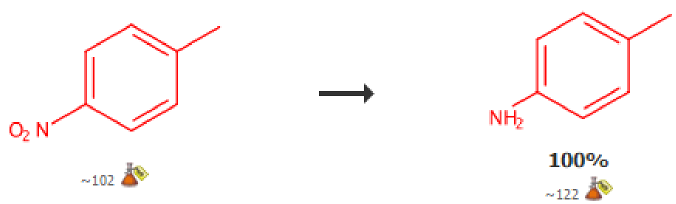
Group by: No Grouping
No Grouping
Document
Transformation

Sort by: Relevance | Display Option

Selected | Page: 1 of 11

1. **View Reaction Detail** **Link** **Similar Reactions**

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



Overview

Steps/Stages

1.1 R:$NaBH_4$, C:1832616-28-0, C:Ru, S:H_2O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

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按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼

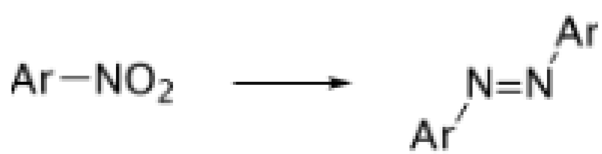
0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines

538 Reactions

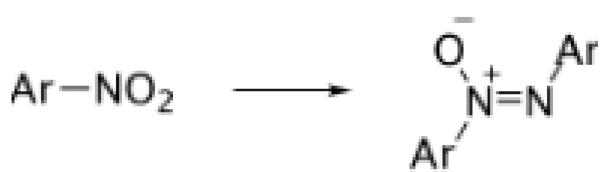
2. Reduction of Nitro to Azo Compounds

11 Reactions



3. Reduction of Nitro to Azoxy Compounds

11 Reactions

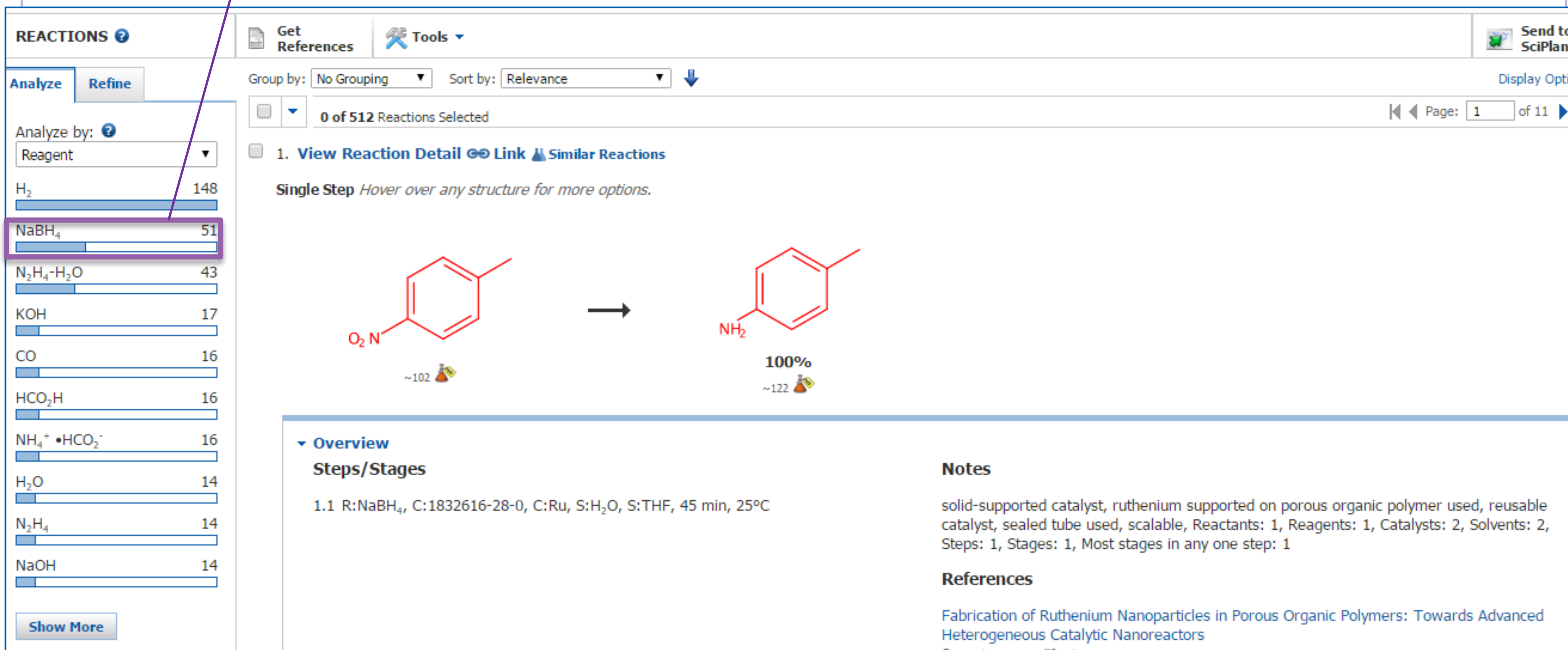


更精确的查找需要的反应

SciFinder A CAS SOLUTION

反应检索结果的筛选

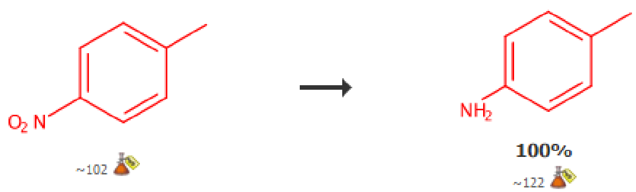
获得特定物质做还原剂的反应



SCIFINDER® A CAS SOLUTION

SciFinder囊括最大的反应实验过程合集

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



Overview

Steps/Stages

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

Notes

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

References

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

Quick View   Other Sources

By Sabater, Sara et al

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

Experimental Procedure

ACS Catalysis

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

不用阅读全文，直接获得包含实验过程的反应记录

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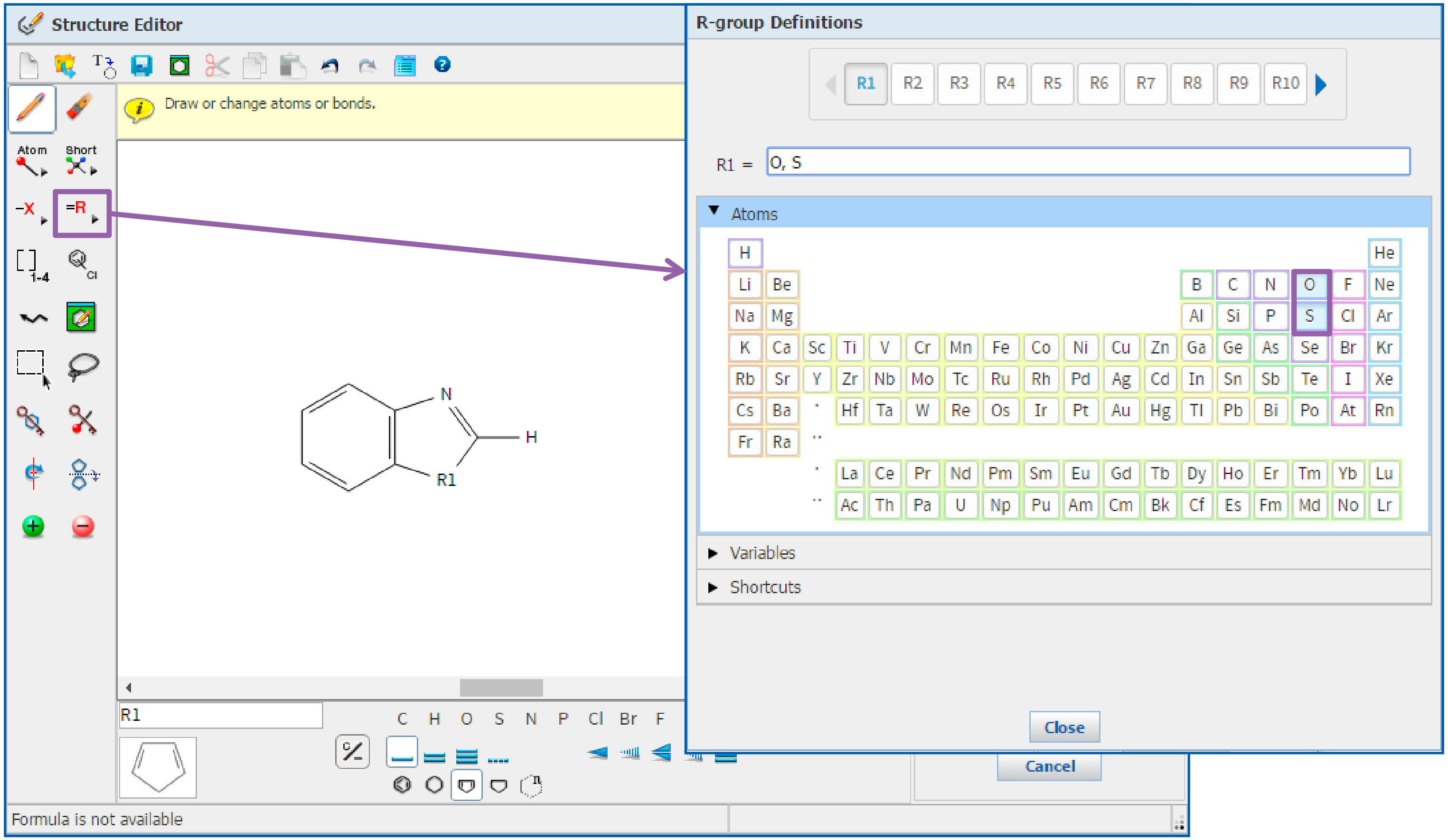
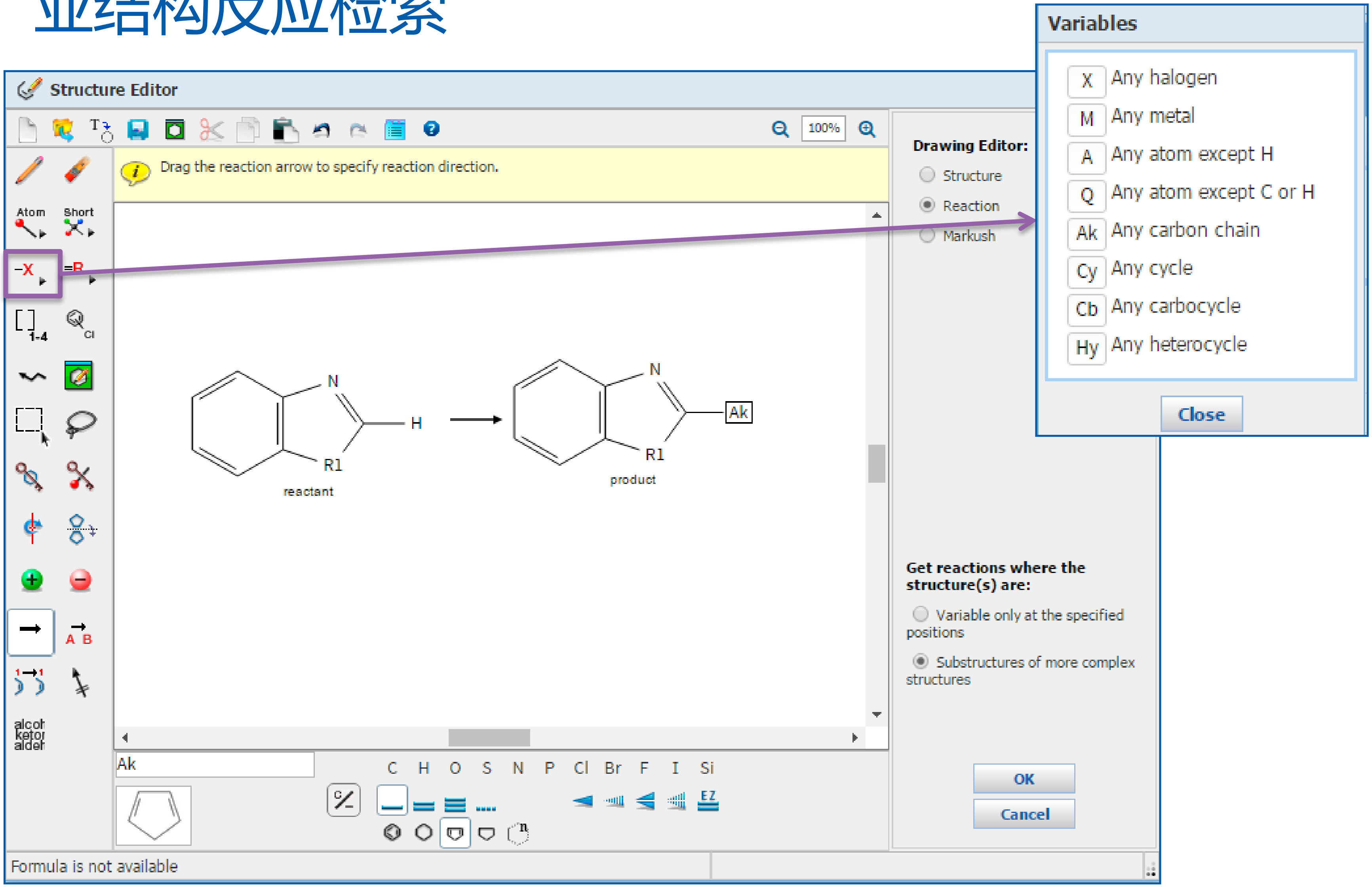
亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化

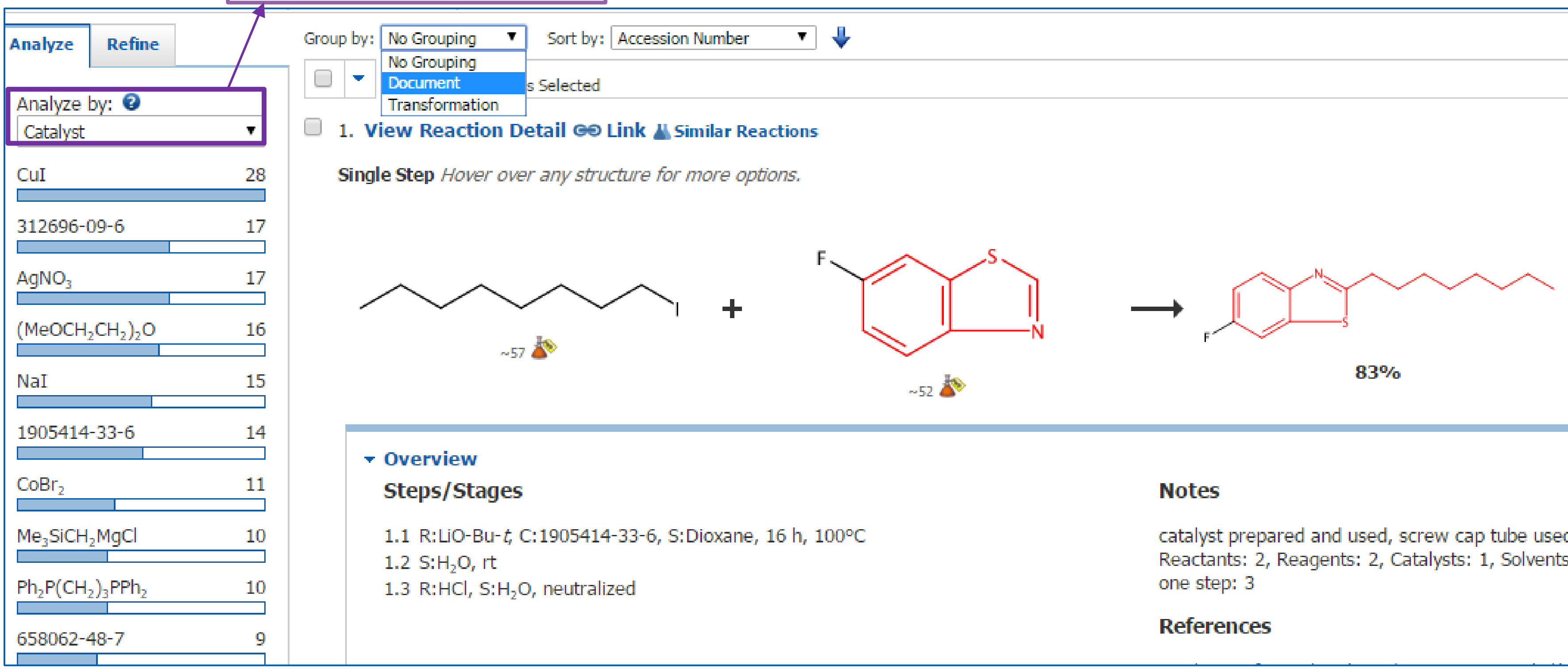


亚结构反应检索


Structure Editor
100%
Drag the reaction arrow to specify reaction direction.
Atom
Short
N
H
R1
reactant
N
Ak
R1
product
Ak
C H O S N P Cl Br F I Si
Formula is not available
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
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



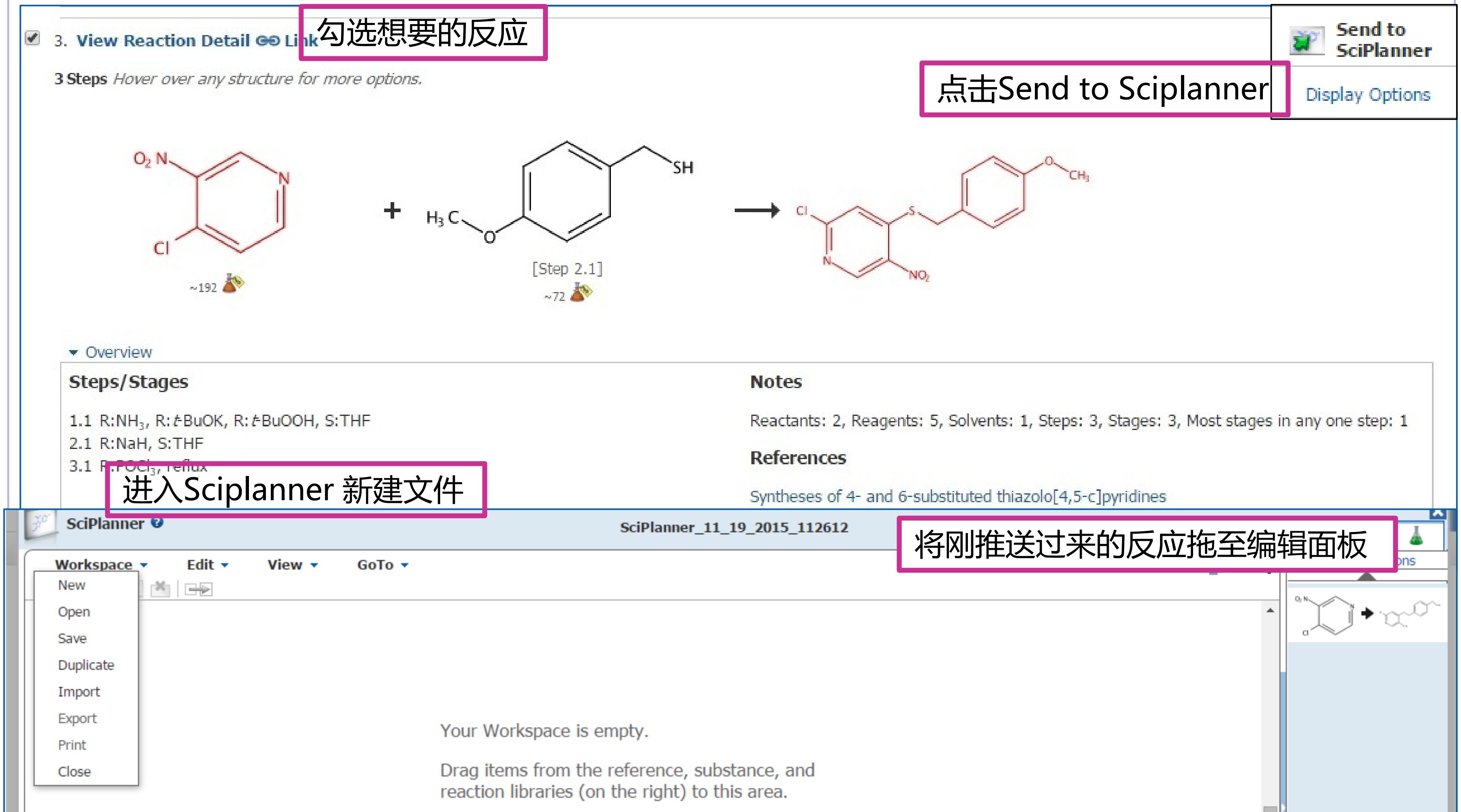
SCIFINDER® A CAS SOLUTION

提纲

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

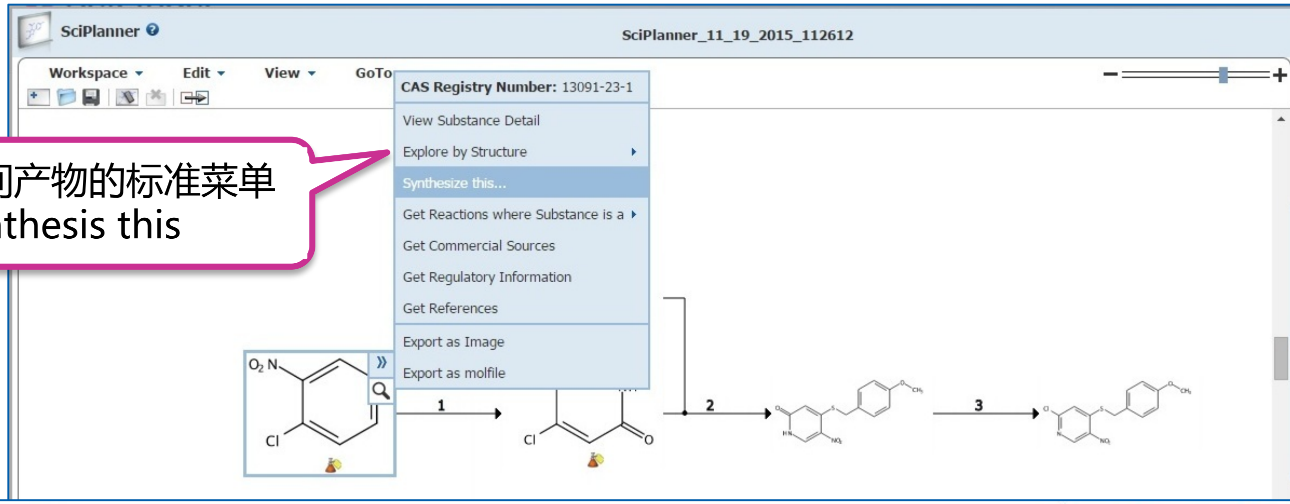
SciFinder® A CAS SOLUTION

SciPlanner使用简介

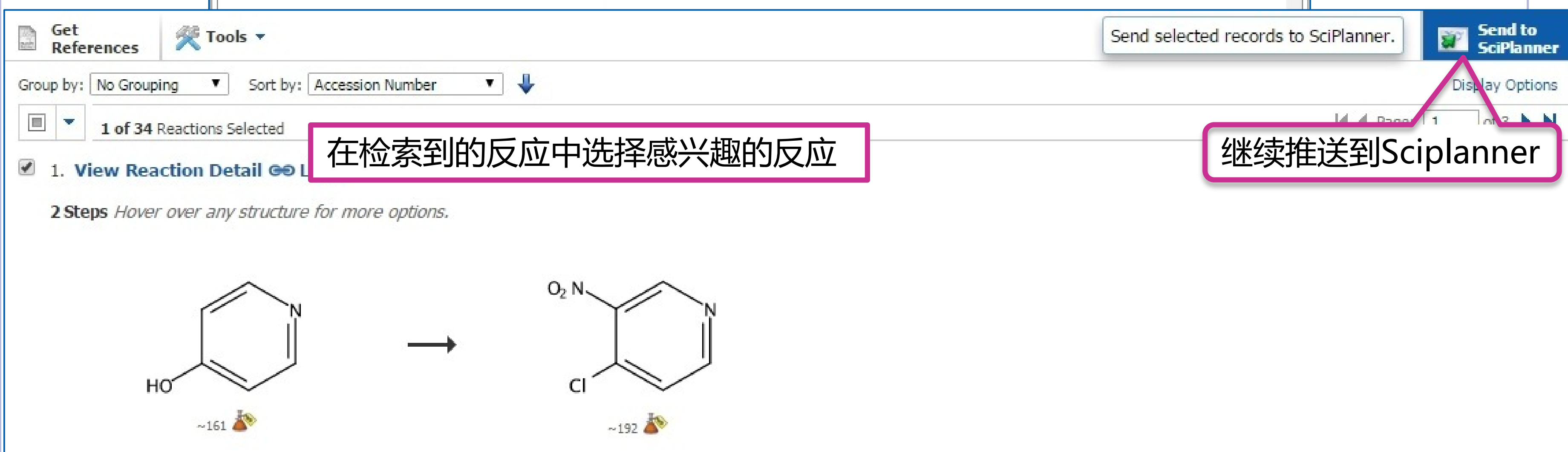


SCIFINDER® A CAS SOLUTION

SciPlanner使用简介



打开中间产物的标准菜单
选择Synthesis this

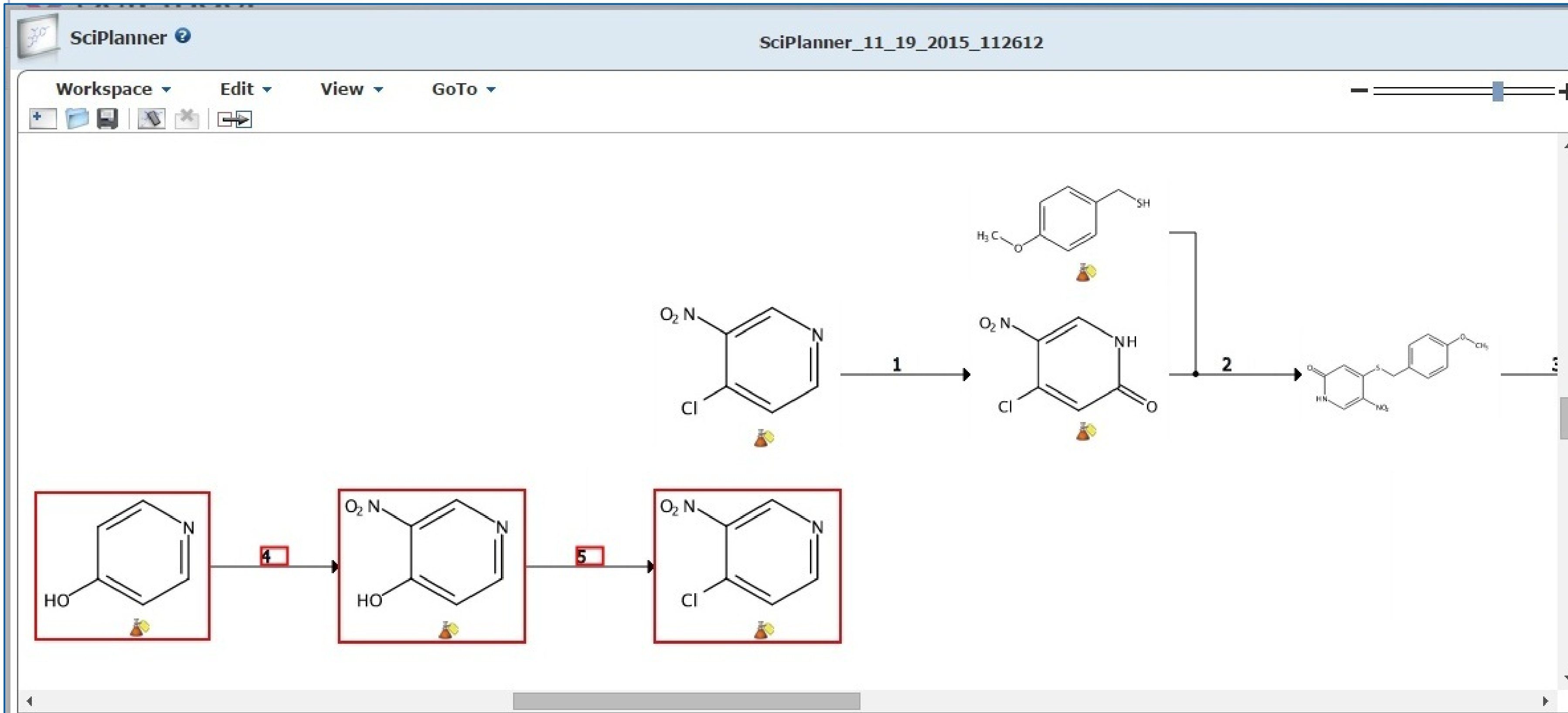


在检索到的反应中选择感兴趣的反应

继续推送到Sciplanner

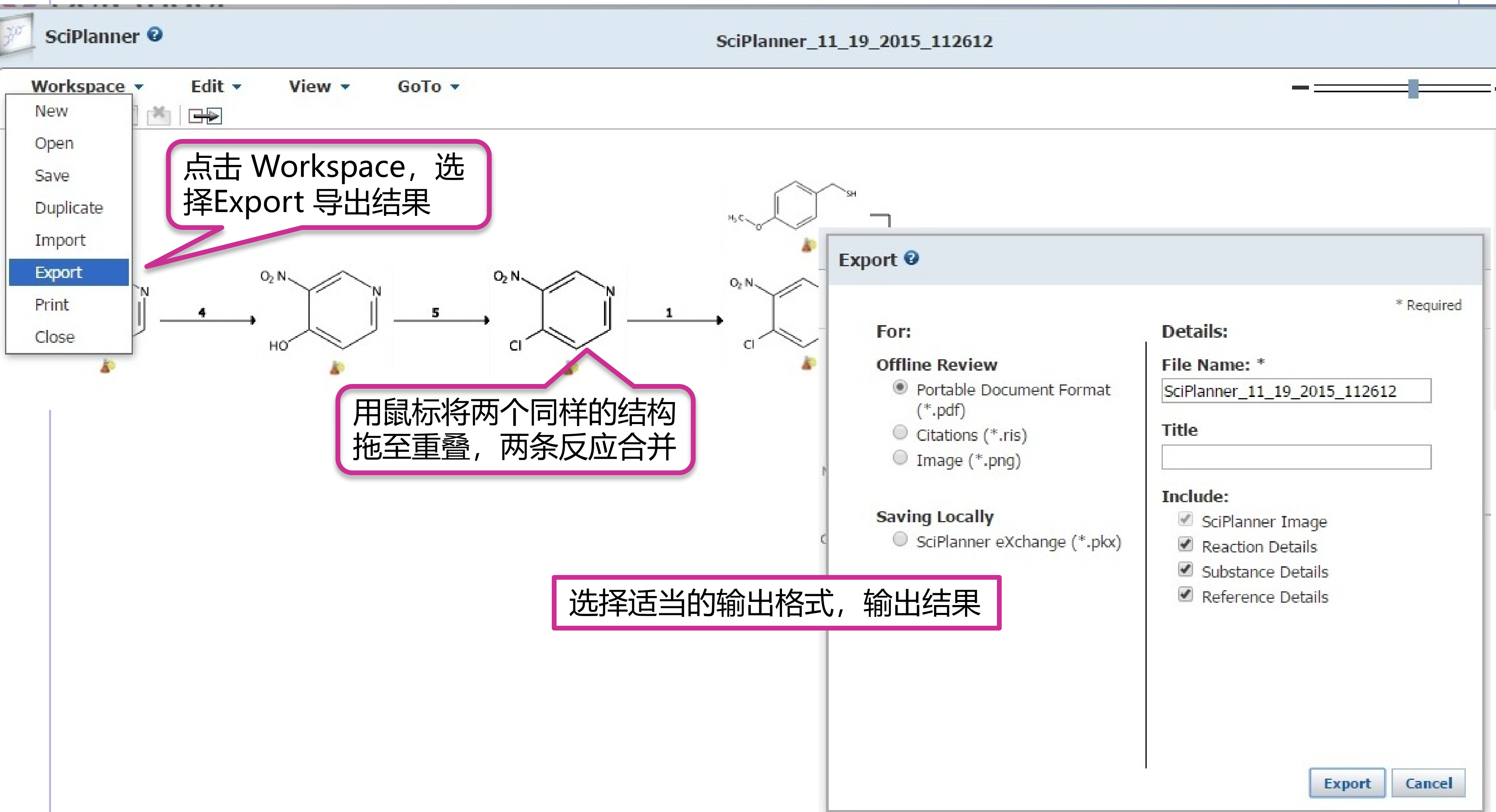
SCIFINDER®
A CAS SOLUTION

SciPlanner使用简介



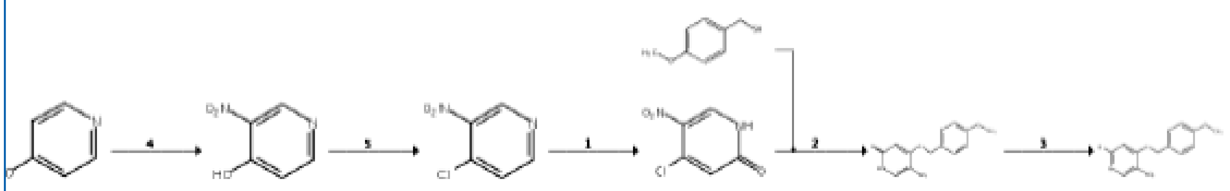
步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介



SCIFINDER®
A CAS SOLUTION

SciPlanner导出结果



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

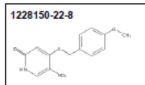
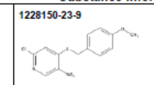
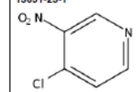
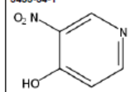
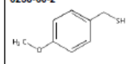
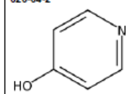
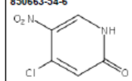
References

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		

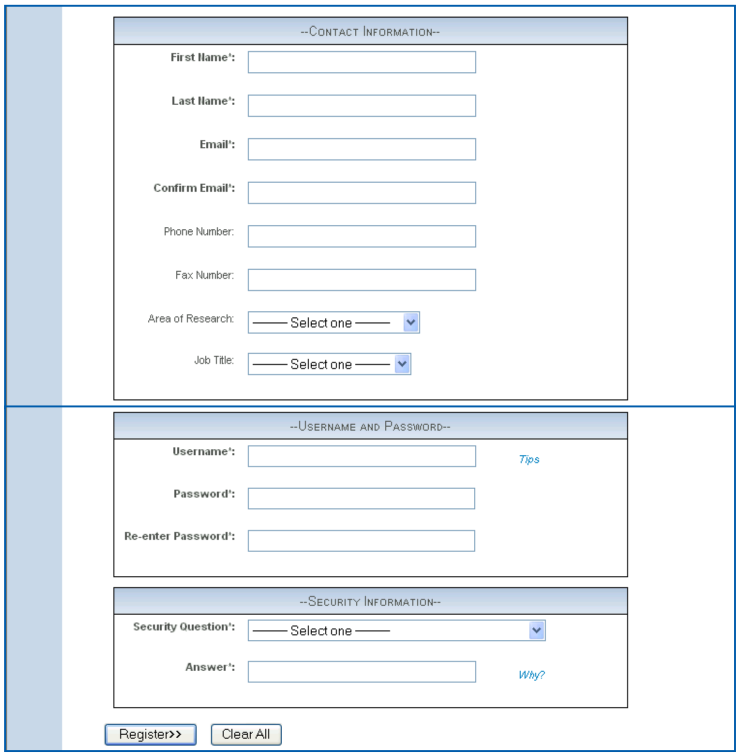
提纲

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

SciFinder浏览器选择建议

- Windows 7以上用户升级IE到10以上，不支持IE7、IE8
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

如何获取SciFinder账号



请注意：
1.必须输入真实姓名和学校邮箱。
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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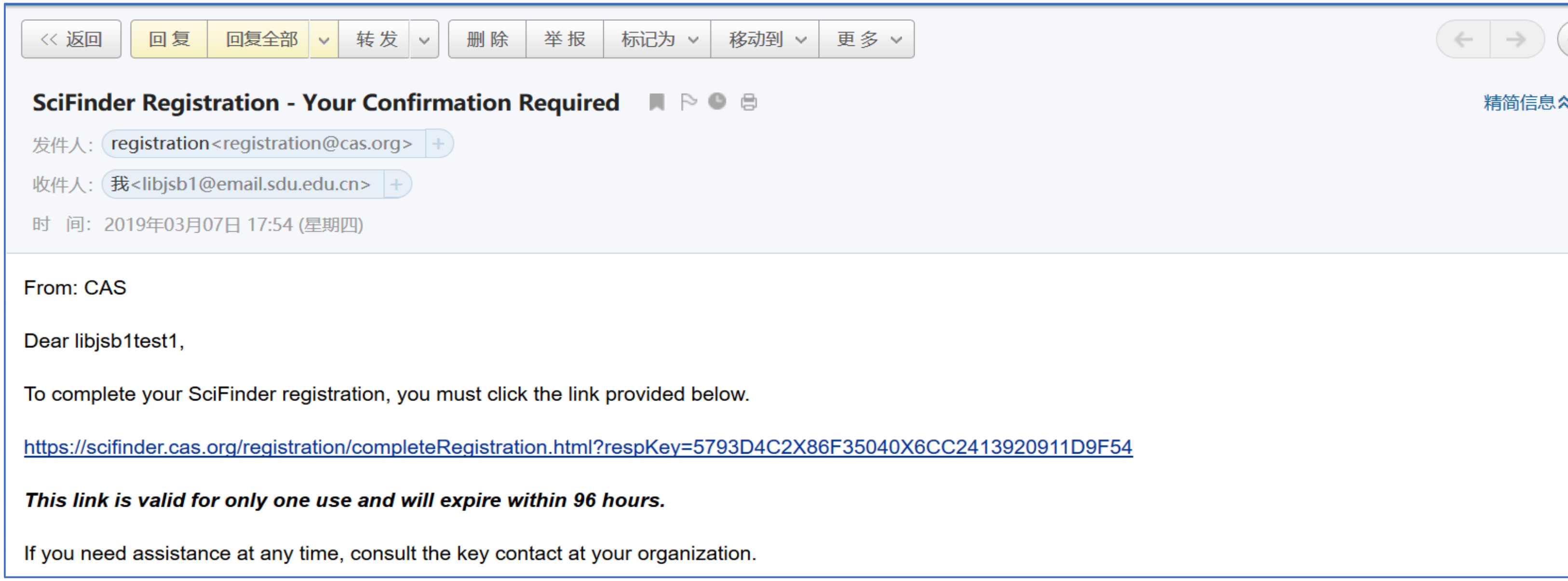
如何获取SciFinder账号


<< 返回 | 回复 | 回复全部 | 转发 | 删除 | 举报 | 标记为 | 移动到 | 更多

SciFinder Registration - Your Confirmation Required

精简信息

发件人：registration<registration@cas.org>

收件人：我<libjsb1@email.sdu.edu.cn>

时　间：2019年03月07日 17:54 (星期四)

From: CAS

Dear libjsb1test1,

To complete your SciFinder registration, you must click the link provided below.

https://scifinder.cas.org/registration/completeRegistration.html?respKey=5793D4C2X86F35040X6CC2413920911D9F54

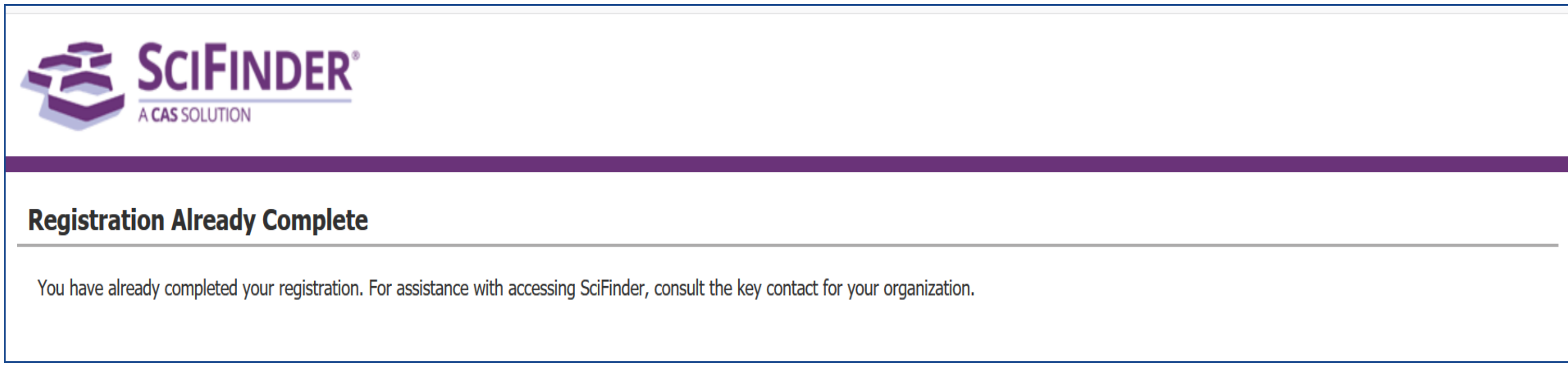
This link is valid for only one use and will expire within 96 hours.

If you need assistance at any time, consult the key contact at your organization.

打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件

如何获取SciFinder账号



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

SciFinder使用注意事项

- 在校内完成注册（教学楼、图书馆、实验室）
- 一人注册一个帐号
- 请提供真实姓名信息（中文名的汉语拼音全拼）
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

更多培训资料请访问

https://www.cas.org/support/training/scifinder

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010-62508026

china@acs-i.org