朱传娴
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hzhu@acs-i.org

如何使用SciFinder获取科技信息

中南民族大学

2018.5.21

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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

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

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CAS——构建最高质量的化学数据库

arXiv.org

Aldrichimica ACTA

ACS chemical biology

BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

division of polymer chemistry, inc American Chemical Society

JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical Neuroscience

Cornell University Library

THE JOURNAL OF PHYSICAL CHEMISTRY Letters

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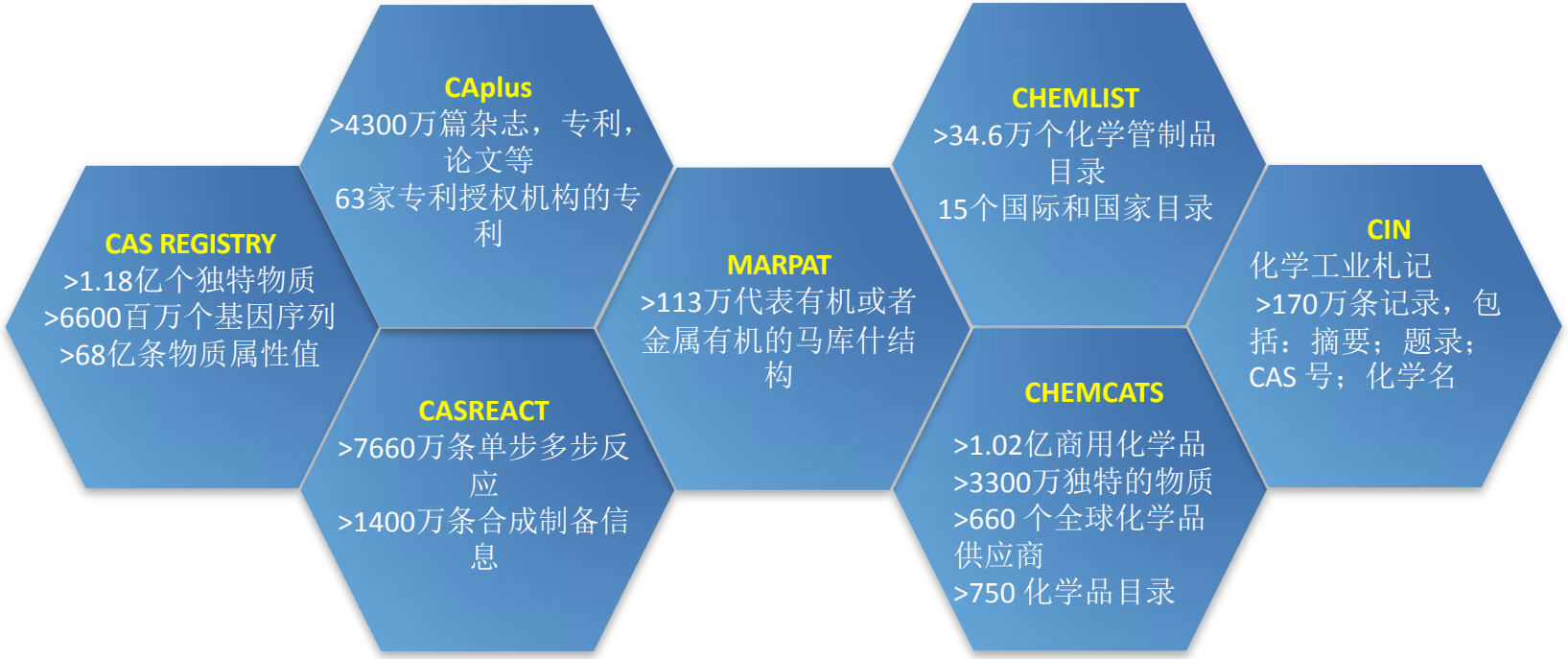

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CAS数据库——源于化学，超越化学

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——人工索引

4. Process for preparation of novel sofosbuvir crystal

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

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

Patent Information

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

Priority Application

CN 2014-10742897	Dec 9, 2014

Indexing

Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

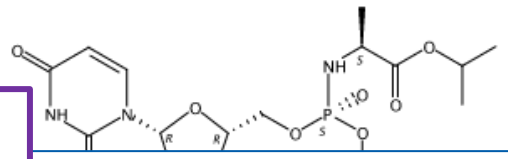
Concepts

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

Substances

1190307-88-0P Sofosbuvir
Absolute stereochemistry.

Page 2 in PATENTPAK



Tips:

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

SCIFINDER® A CAS SOLUTION

CAS人工标引解决的问题

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

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CAS最新动向—解决方案

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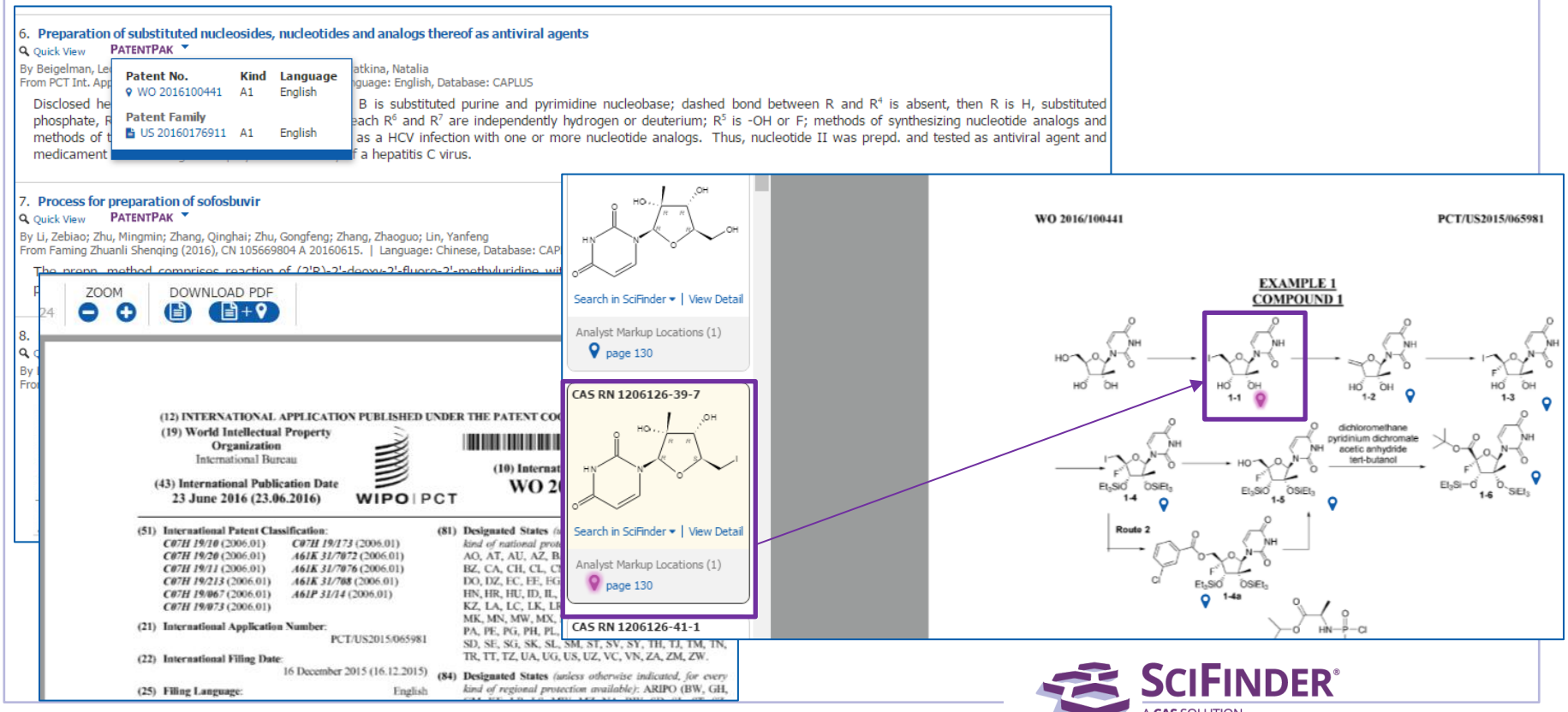
CAS最新动向—解决方案

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



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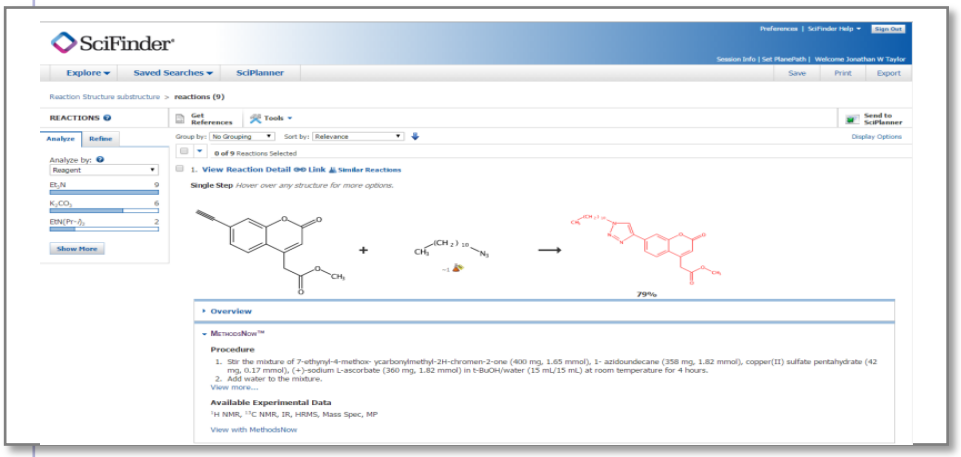
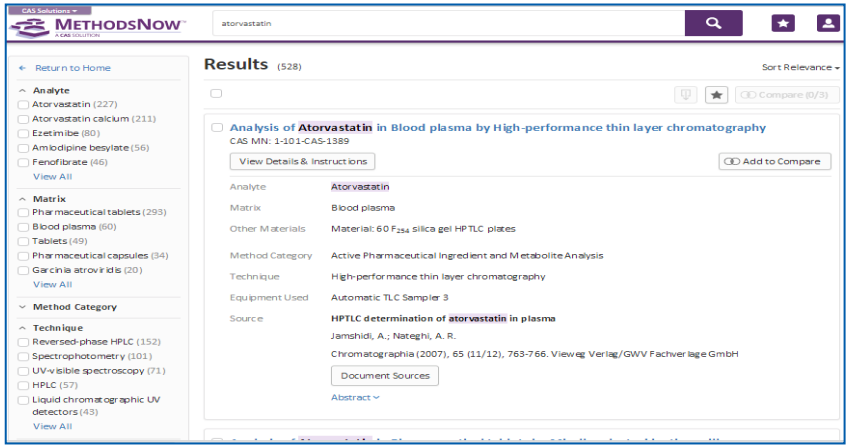
CAS最新动向—解决方案

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



嵌在SciFinder中的合成模块



单独的分析界面

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提纲

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

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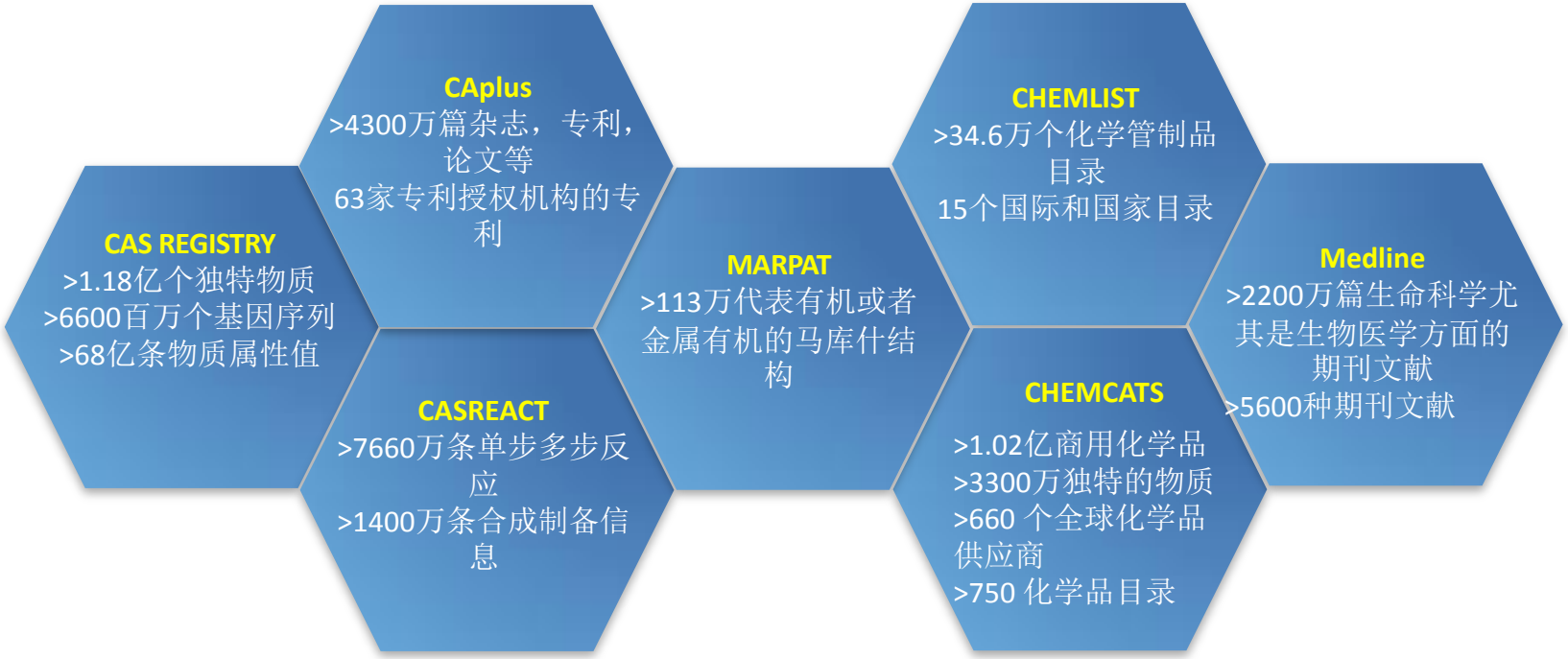
SciFinder覆盖的数据库



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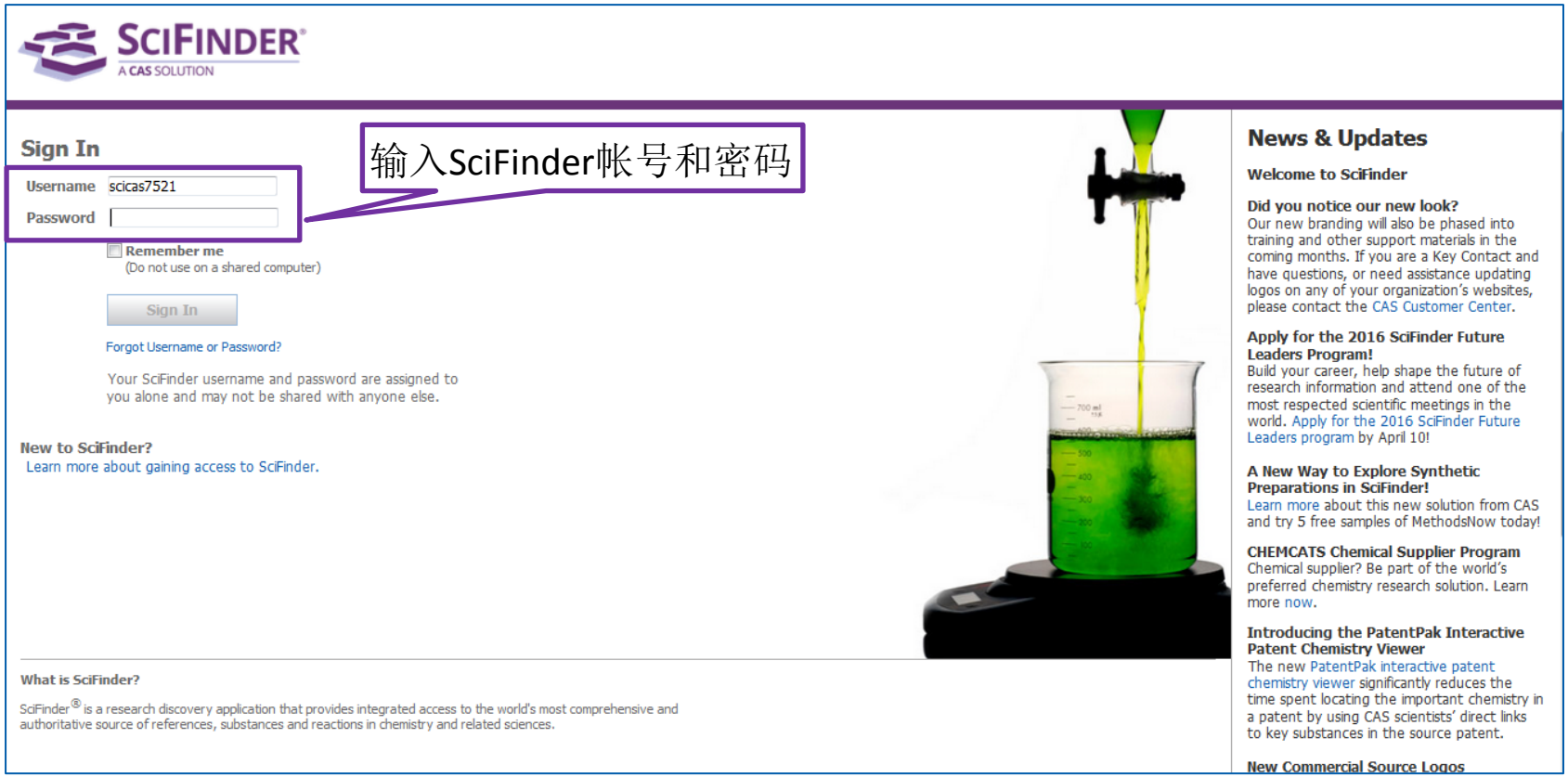
SciFinder登录网址: https://scifinder.cas.org/



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SciFinder主界面

SciFinder检索——文献检索

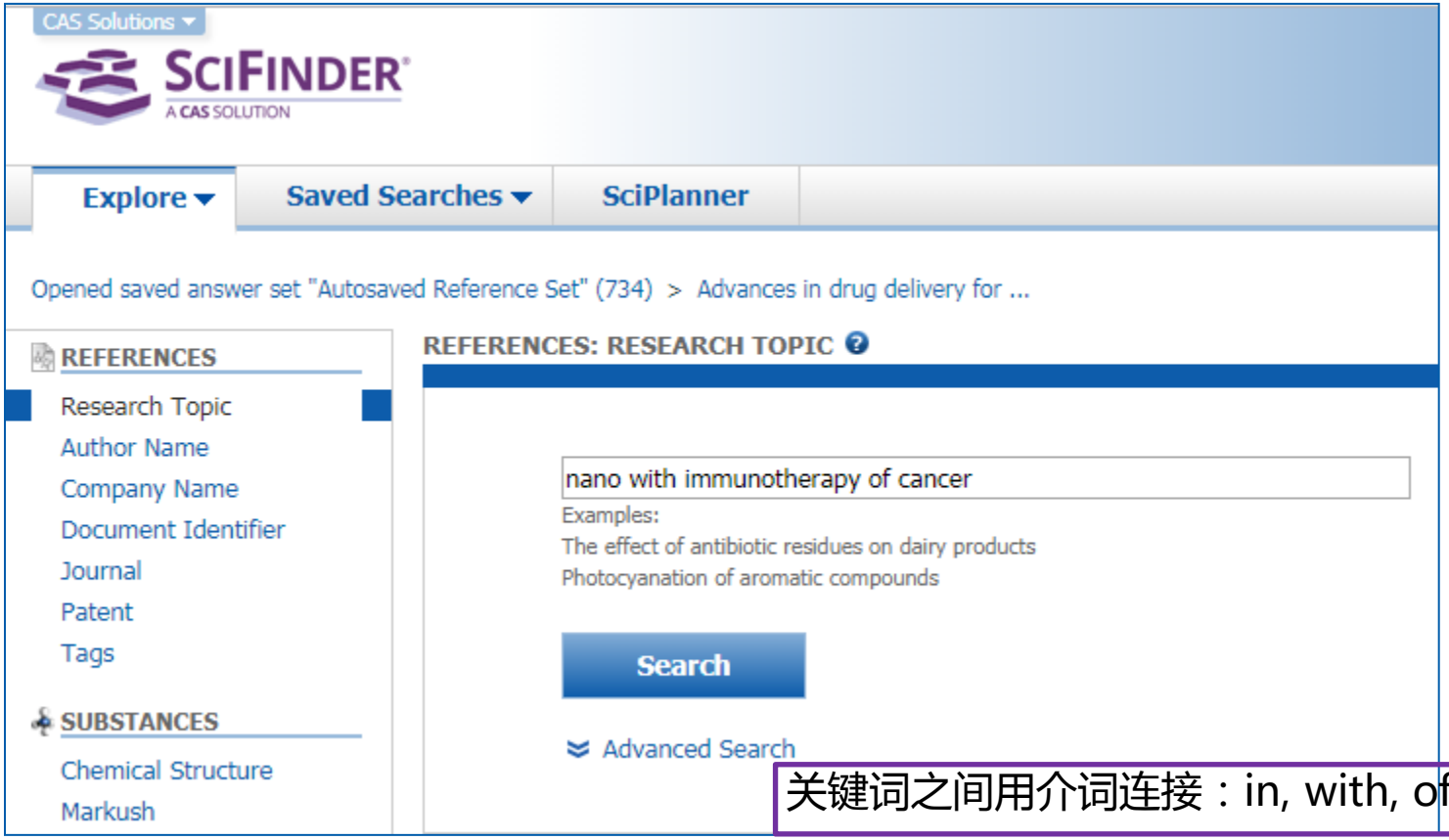
- 文献检索方法
  - 主题检索
  - 作者名检索
  - 机构名检索
  - 文献标识符检索
  - 期刊名称和专利信息（公开号，申请号等）
  - 从物质，反应获得文献

- 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

文献检索——主题

主题检索： 纳米技术在癌症免疫疗法中的应用

检索式：nano with Immunotherapy of cancer



关键词之间用介词连接：in, with, of...

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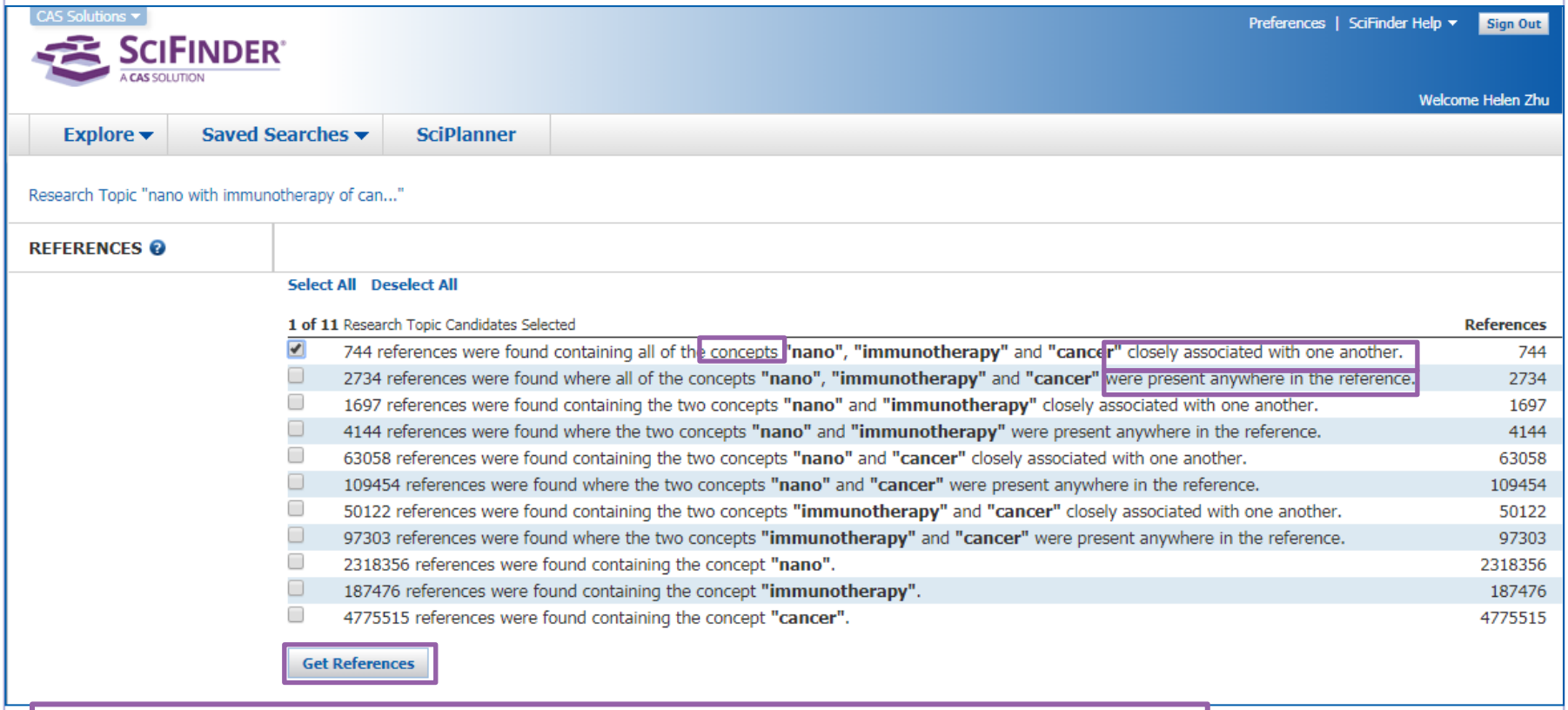
主题检索的候选项



“Concepts”表示对主题词做了同义词的扩展；

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

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

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按被引次数排序— Citing References

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Research Topic "nano with immunotherapy of can..." > **references (580)**

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Analyze | Refine | Categorize

Analyze by: Author Name

Lu Xiaoling	18
Zhao Yongxiang	17
Liu Zhuang	9
Lim Yong Taik	8
Santos Helder A	7
Xu Ligeng	7
Ito Atsuo	6
Shahbazi Mohammad Ali	6
Wang Chao	6
Wang Xiupeng	6

Sort by: Citing References ▼ (Accession Number / Author Name / **Citing References** / Publication Year / Title)

Display Options

s Selected

Page: 1 of 29

1. Photothermal Cancer Therapy: Impending Clinical Impact

Quick View | Other Sources

~720

By Lal, Surbhi; Clare, Susan E.; Halas, Naomi J.
From Accounts of Chemical Research (2008), 41(12), 1842-1851. | Language: English, Database: CAPLUS

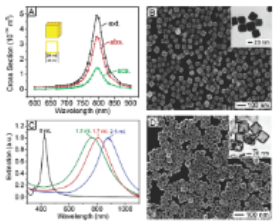
A review. Much of the current excitement surrounding **nanoscience** is directly connected to the promise of new **nanoscale** applications in **cancer** diagnostics and therapy. Because of their strongly resonant light-absorbing and light-scattering properties that depend on shape, noble metal **nanoparticles** provide a new and powerful tool for innovative light-based approaches. **Nanoshells**-spherical, dielec. core, gold shell **nanoparticles**-have been central to the development of photothermal **cancer** therapy and diagnostics for the past several years. By manipulating **nanoparticle** shape, researchers can tu...

2. Immuno Gold Nanocages with Tailored Optical Properties for Targeted Photothermal Destruction of Cancer Cells

Quick View | Other Sources

~632

By Chen, Jingyi; Wang, Danling; Xi, Jiefeng; Au, Leslie; Siekkinen, Andy; Warsen, Addie; Li, Zhi-Yuan; Zhang, Hui; Xia, Younan; Li, Xingde
From Nano Letters (2007), 7(5), 1318-1322. | Language: English, Database: CAPLUS



Gold **nanocages** with a relatively small size (e.g., ~45 nm in edge length) have been developed, and the structure of these **nanocages** was tailored to achieve strong absorption in the near-IR (NIR) region for photothermal **cancer** treatment. Numerical calcns. show that the **nanocage** has a large absorption cross section of 3.48×10^{-14} m^2, facilitating conversion of NIR irradn. into heat. The gold **nanocages** were conjugated with monoclonal antibodies (anti-HER2) to target epidermal growth factor receptors (EGFR) that are overexpressed on the surface of breast **cancer** cells (SK-BR-3). Our preliminary p...

Citing Reference: 帮助找到最重要的文献

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文献检索结果

SciFinder提供强大的文献处理工具，帮助处理文献

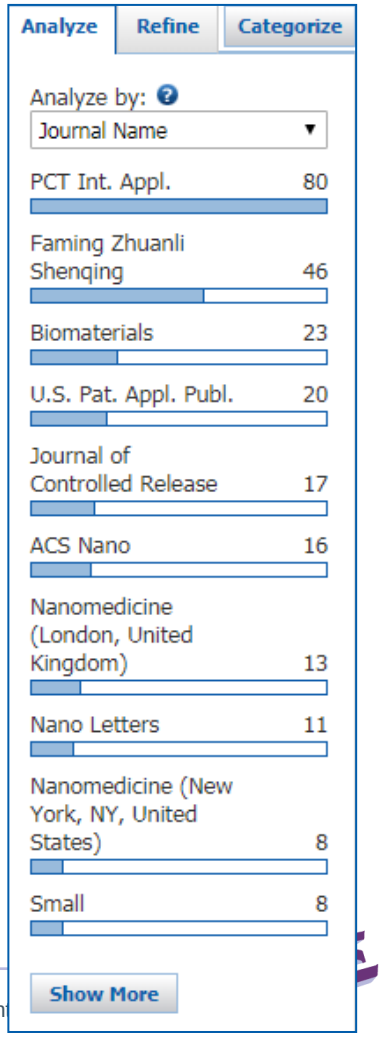
SciFinder A CAS SOLUTION

文献检索结果的Analyze

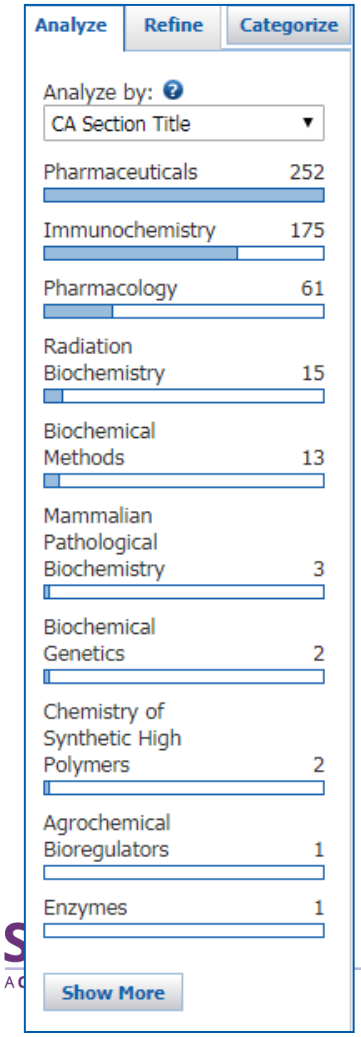
本领域研究人员

本领域研究机构、合作伙伴、竞争对手

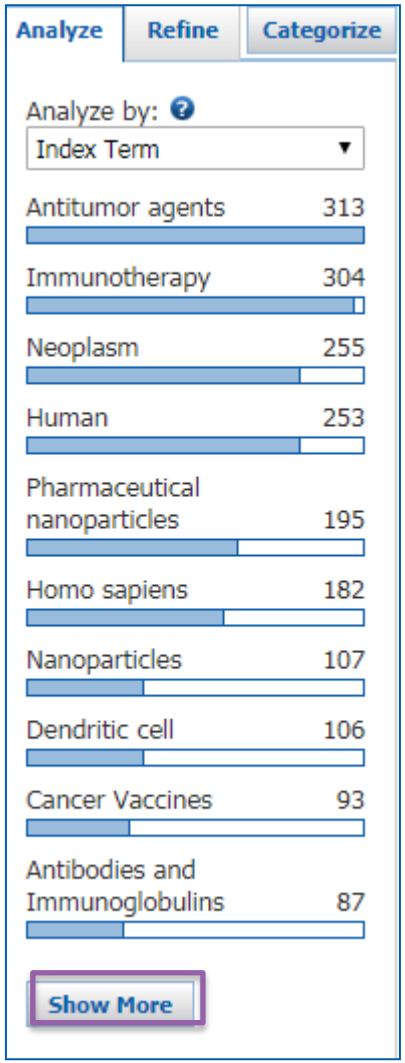
期刊



涉及学科领域

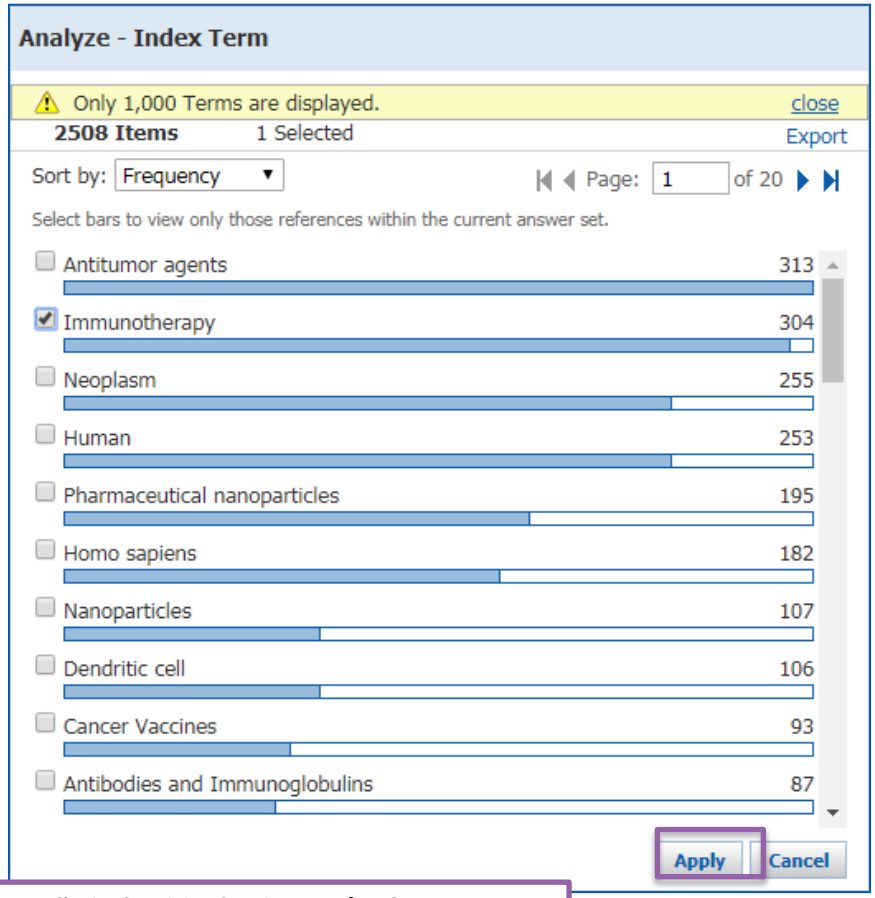


文献检索结果的Analyze



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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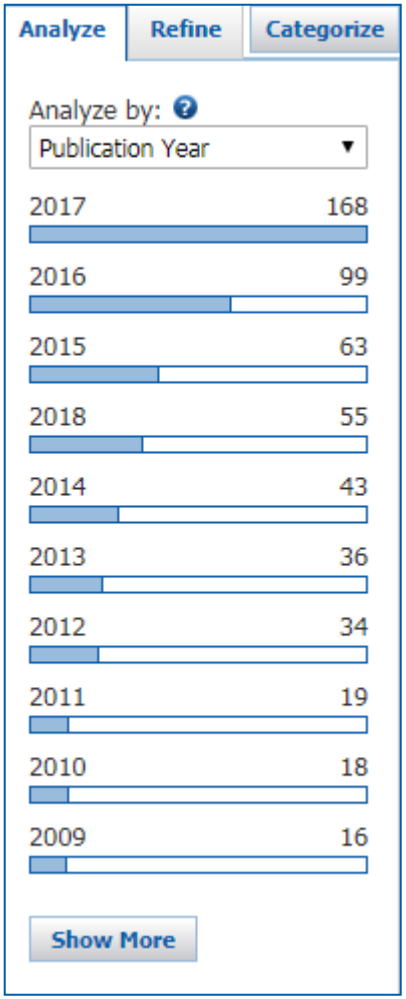

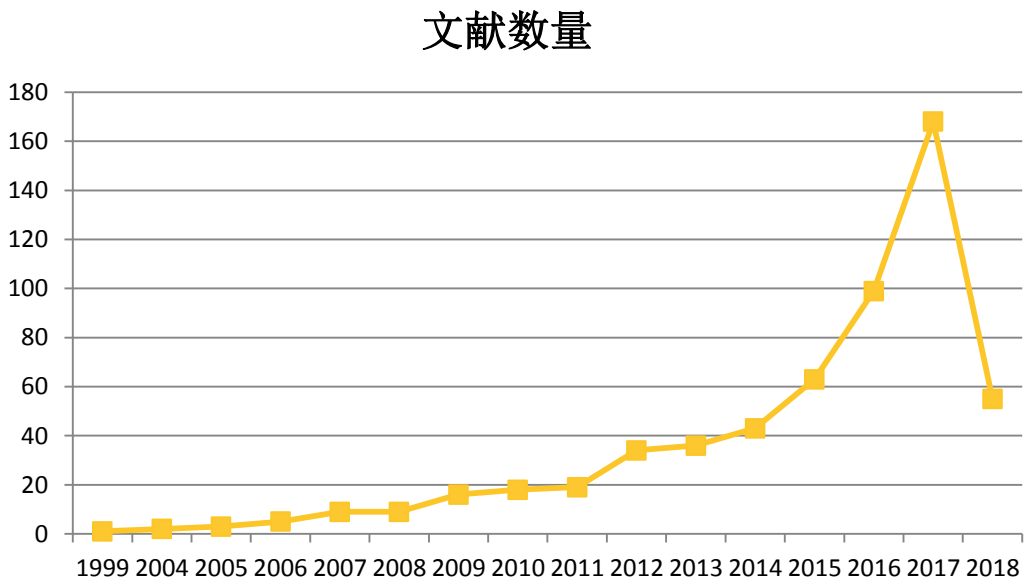

Publication Year: 分析领域发展趋势

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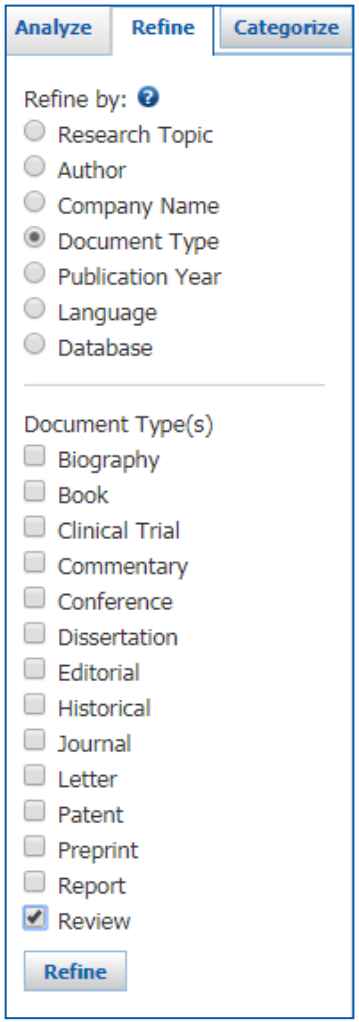
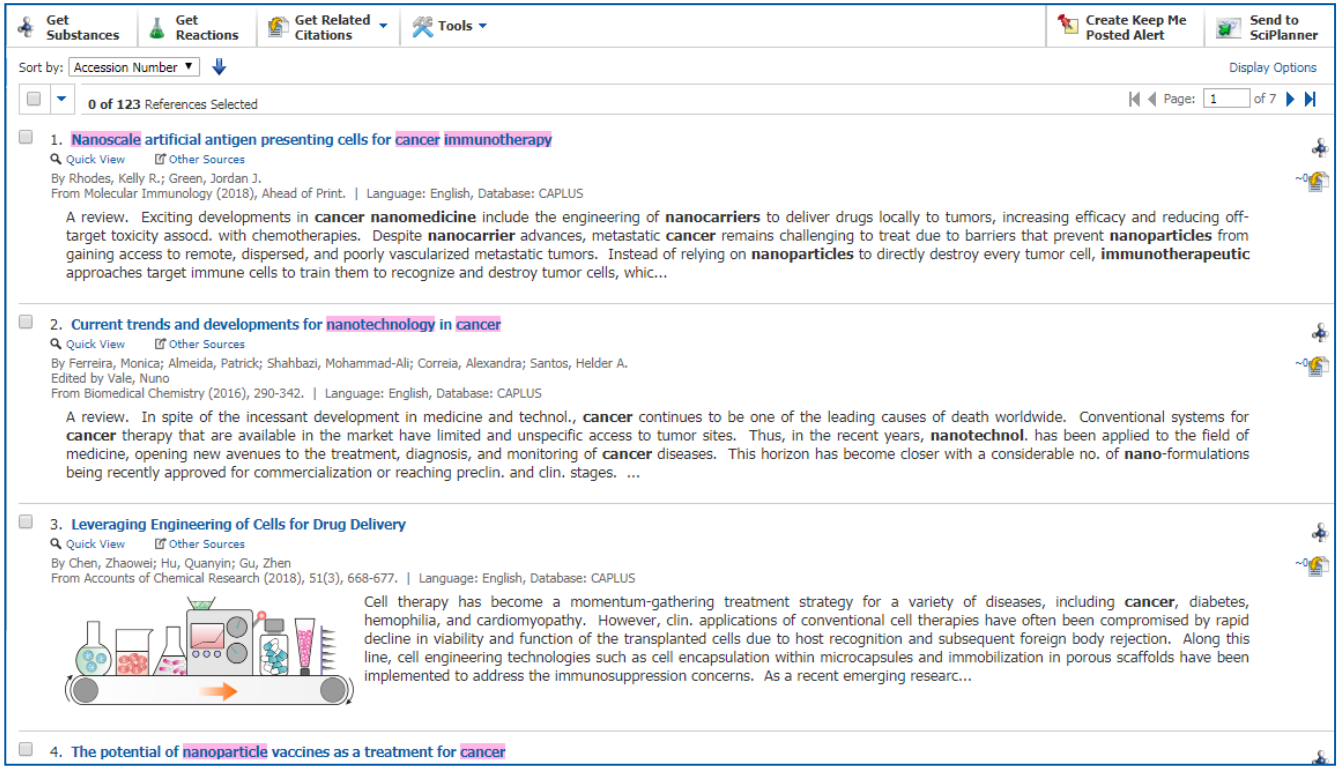
文献检索结果的Refine





Refine：帮助用户迅速获得需要的文献

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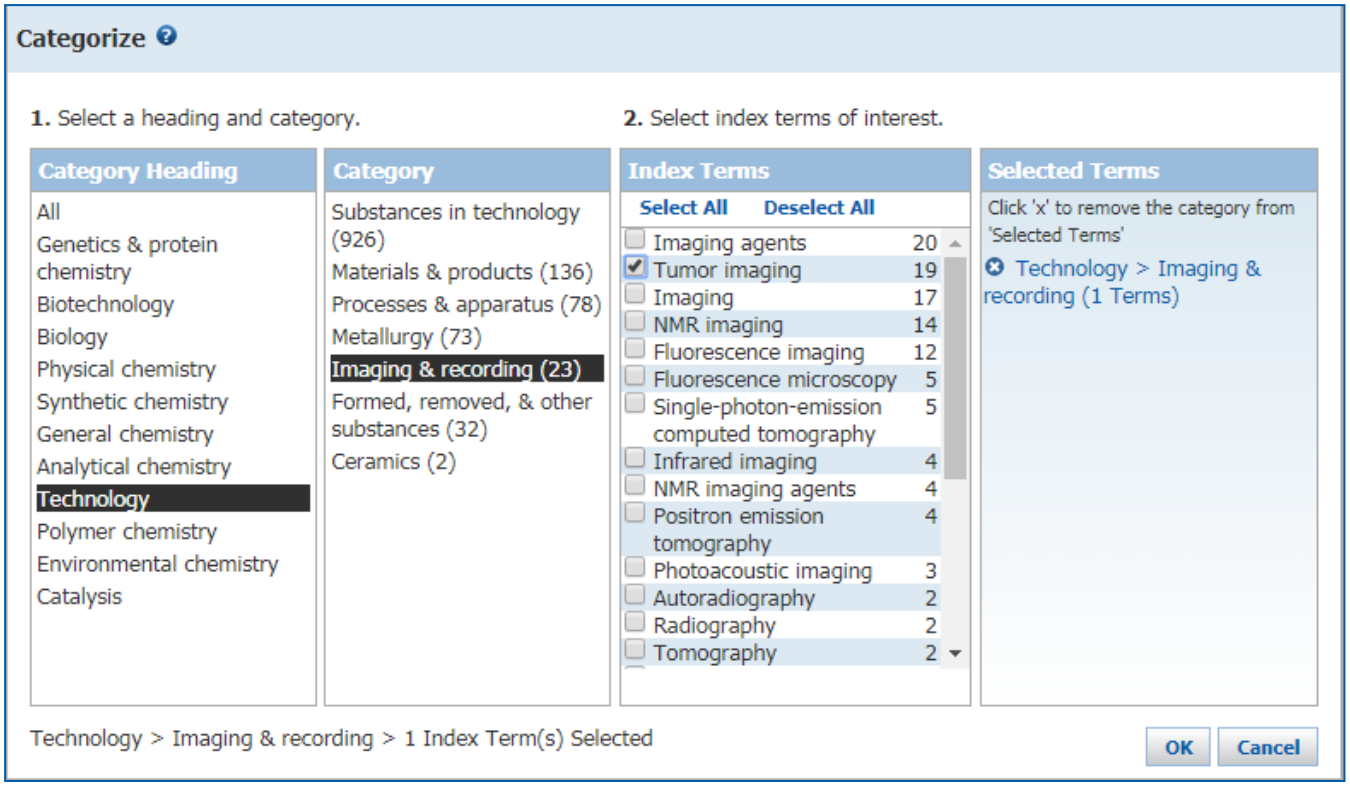
文献检索结果的Categorize

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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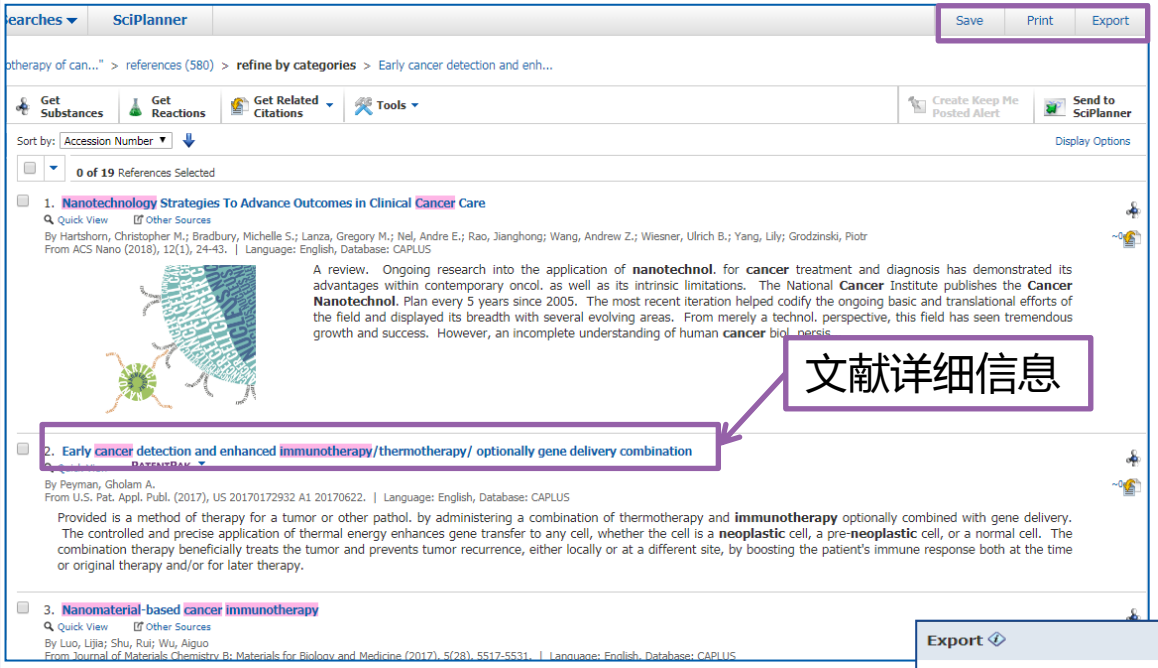
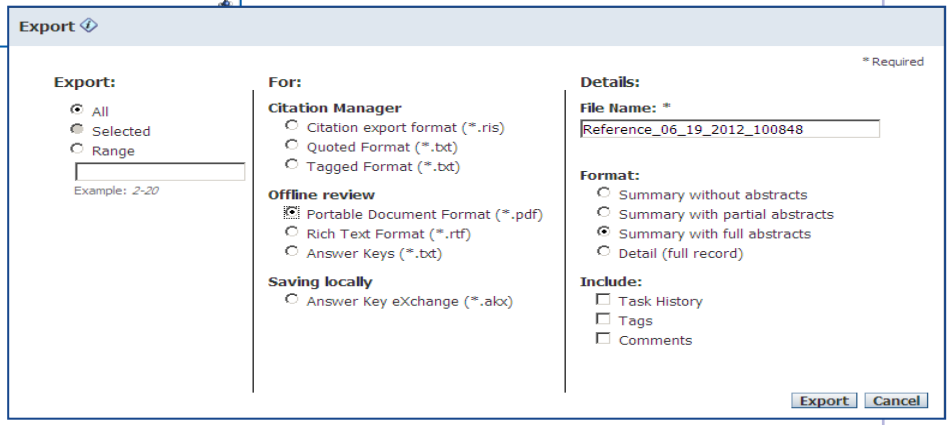
结果集的保存— Save, Print, Export



Save：保存在服务器上，方便以后登陆查看，每次可存2万条记录。

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

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文献信息—题录、摘要、索引

2. Early cancer detection and enhanced immunotherapy/thermotherapy/ optionally gene delivery combination

By: Peyman, Gholam A.
Assignee: USA

Provided is a method of therapy for a tumor or other pathol. by administering a combination of thermotherapy and immunotherapy optionally combined with gene delivery. The controlled and precise application of thermal energy enhances gene transfer to any cell, whether the cell is a neoplastic cell, a pre-neoplastic cell, or a normal cell. The combination therapy beneficially treats the tumor and prevents tumor recurrence, either locally or at a different site, by boosting the patient's immune response both at the time or original therapy and/or for later therapy.

Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
US 20170172932	PDF | PDF+ | Viewer	A1		Jun 22, 2017	US 2016-15143981	May 2, 2016
US 9849092	PDF	B2	English	Dec 26, 2017		
US 20170173191	PDF | PDF+ | Viewer	A1	English	Jun 22, 2017	US 2015-14976321	Dec 21, 2015

Priority Application

US 2015-14976321	A2	Dec 21, 2015

Indexing

Immunochemistry (Section15-3)

Section cros

重要概念

Concepts

Clustered regularly interspaced short palindromic repeat

ermotherapy/ optionally

重要物质

Substances

1425049-49-5 Cas9 nuclease Page 21 in PATENTPAK

CRISPR/cas9 complex; early cancer detection and enhanced immunotherapy/thermotherapy/ optionally gene delivery combination

Therapeutic use; Biological study; Uses

QUICK LINKS
0 Tags, 0 Comments

PATENT INFORMATION
Jun 22, 2017
US 20170172932
A1

APPLICATION
May 2, 2016
US 2016-15143981

PRIORITY
Dec 21, 2015
US 2015-14976321

SOURCE
U.S. Pat. Appl. Publ.
22pp., Cont.-in-part of U.S. Ser. No. 976,321.
Patent
2017
CODEN:USXXCO

ACCESSION NUMBER
2017:1034814
CAN167:99362
CAPLUS

LANGUAGE
English

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

文献检索小结

- 主题检索时，使用介词 in, with, of 等作为连接词
- 跟据检索要求选择合适的候选项
- 通过SciFinder 的Analyze/Refine功能来缩小检索的范围
- 尝试将不同的Analyze/Refine功能组合起来用，会有更多的收益
- 使用Categorize可以让系统来实现自动分类

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

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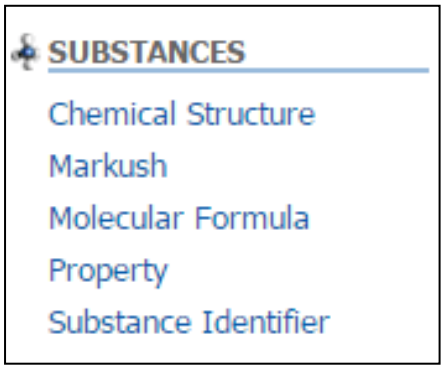
SciFinder检索选项——物质检索

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



- 物质检索策略推荐
  - —有机化合物，天然产物：结构检索
  - —无机物，合金：分子式检索
  - —高分子化合物：分子式检索和结构检索

物质检索——标识符检索

提示：
1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

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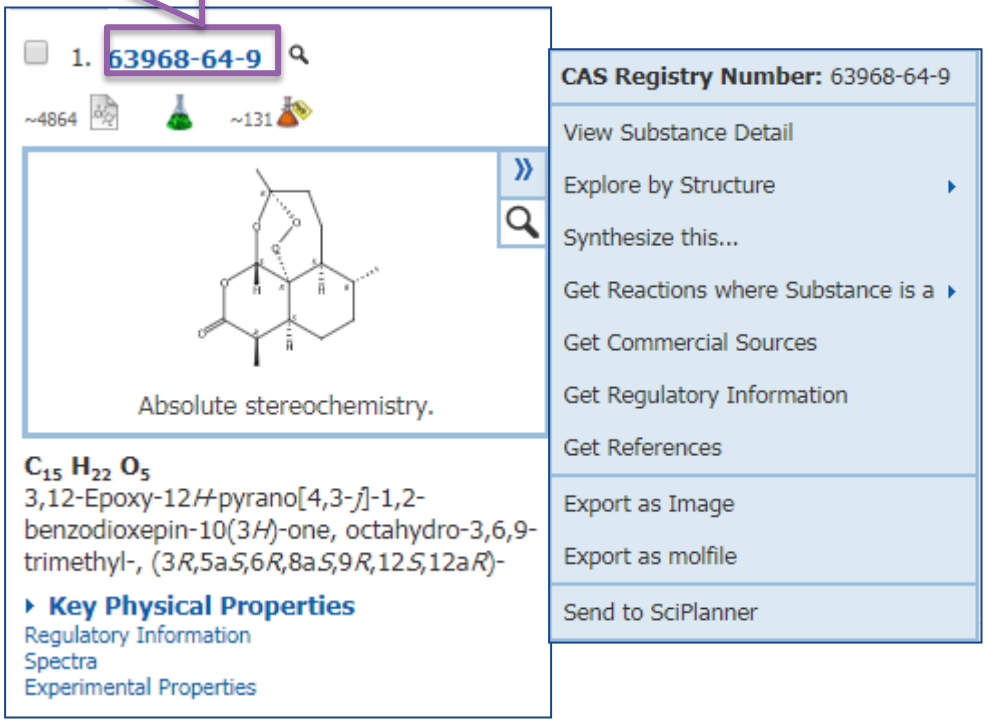
SciFinder中的物质记录

点击CAS RN 获得物质详细信息



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

SciFinder中的物质记录

SUBSTANCE DETAIL

Get References | Get Reactions | Get Commercial Sources

Return

由物质获得文献，反应，供应商等信息

CAS Registry Number 63968-64

~4,864 ~131

$C_{15}H_{22}O_5$

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

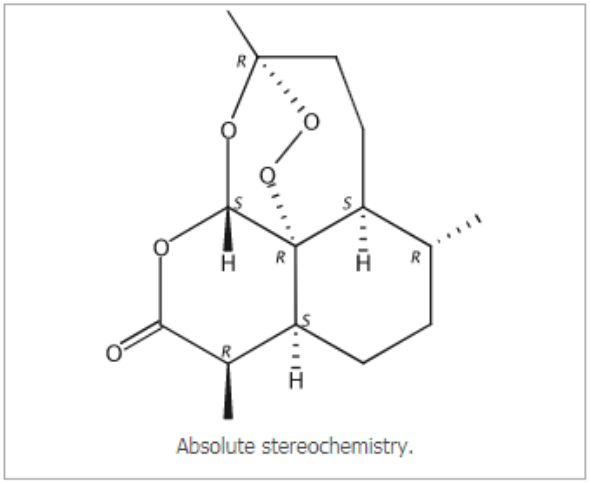
Molecular Weight
282.33

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

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

Density (Experimental)
Value: 1.300 g/cm3

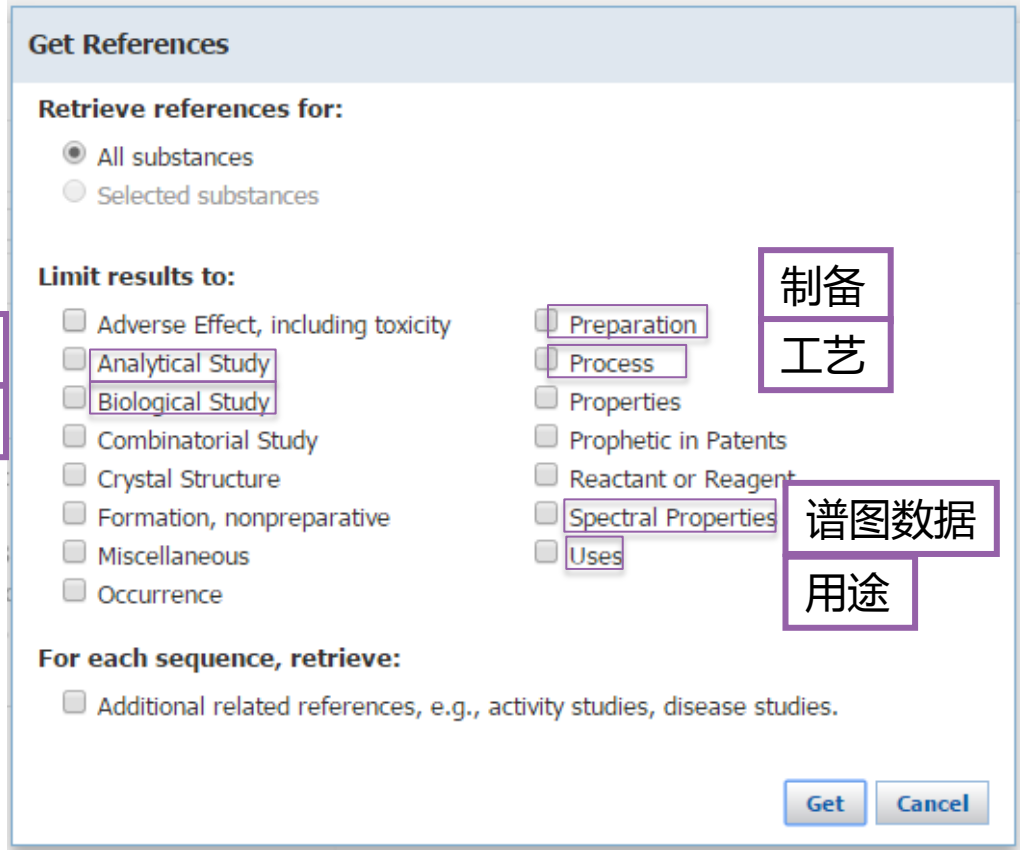
Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3α,5aβ,6β,8aβ,9α,12β,12a*R**)]-
(3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Arteannuin
(+)-Artemisinin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



Absolute stereochemistry.

物质详情

通过物质获得文献



分析化学

生物研究

制备

工艺

谱图数据

用途

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

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

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

Notes

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

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

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

预测数据与预测谱图

PREDICTED PROPERTIES

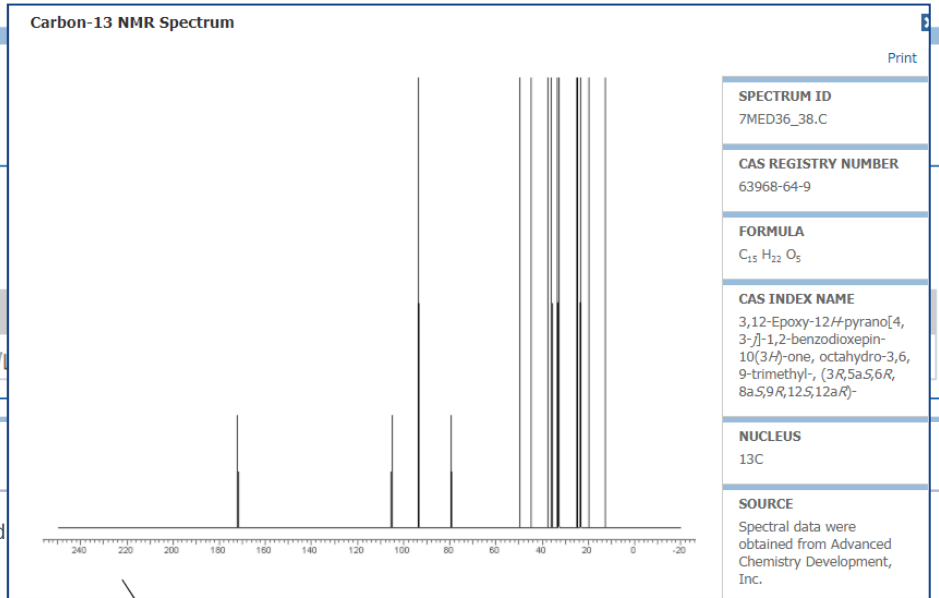
PREDICTED SPECTRA

¹H NMR | ¹³C NMR

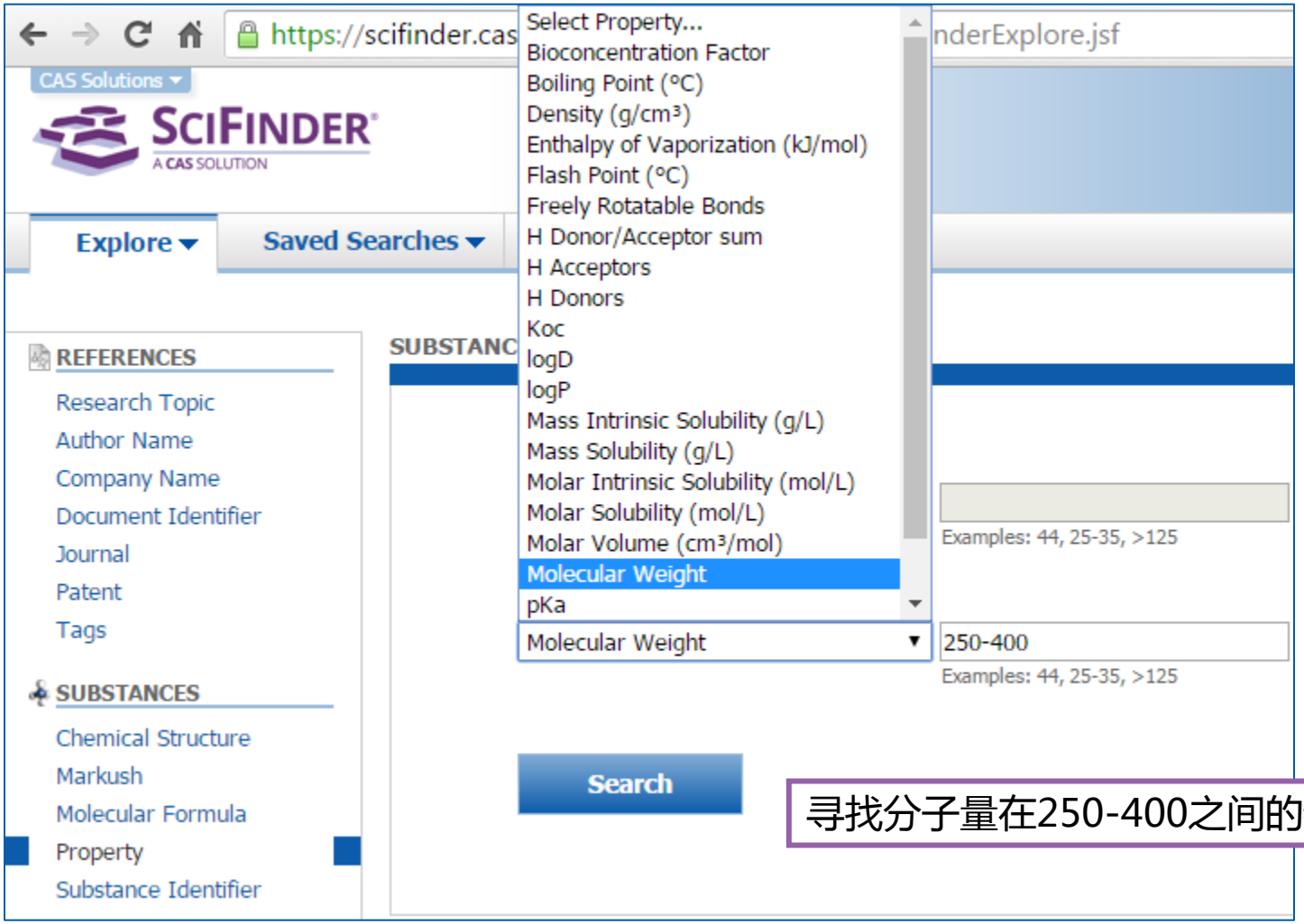
¹H NMR Properties	Value
Proton NMR Spectrum	See spectrum

Notes

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

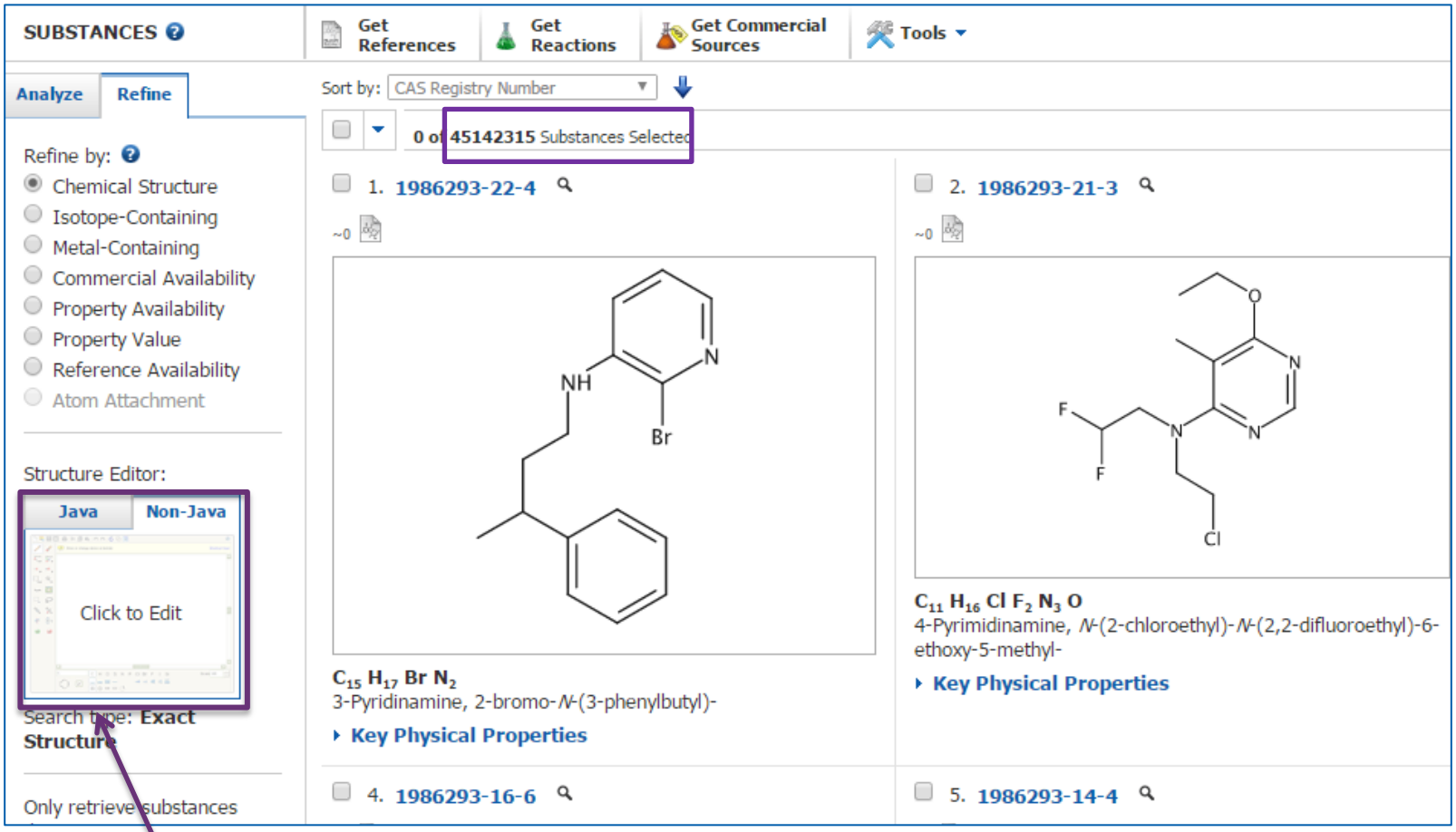


物质检索——Property explore



寻找分子量在250-400之间的物质

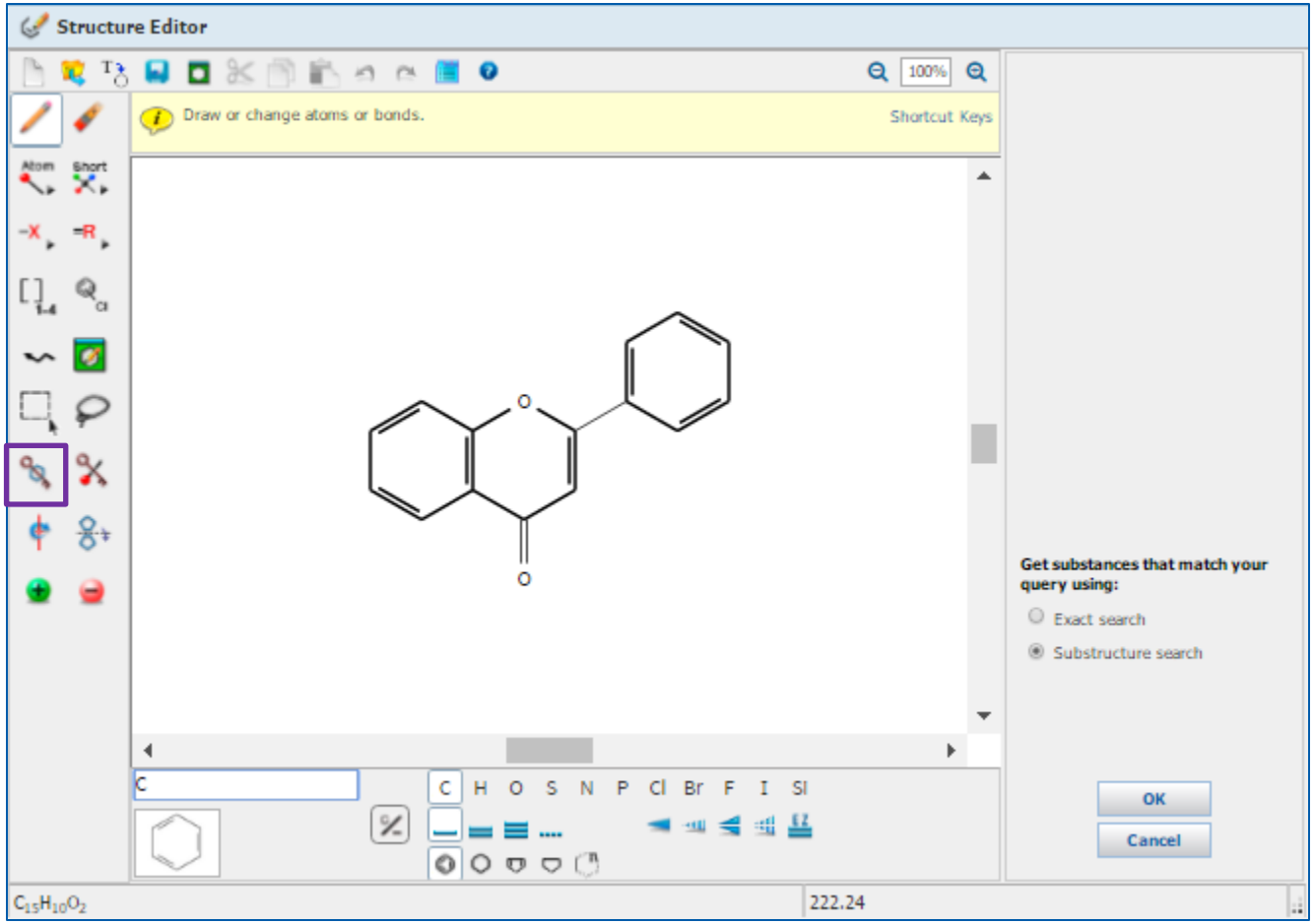
物质结果集的筛选——Refine

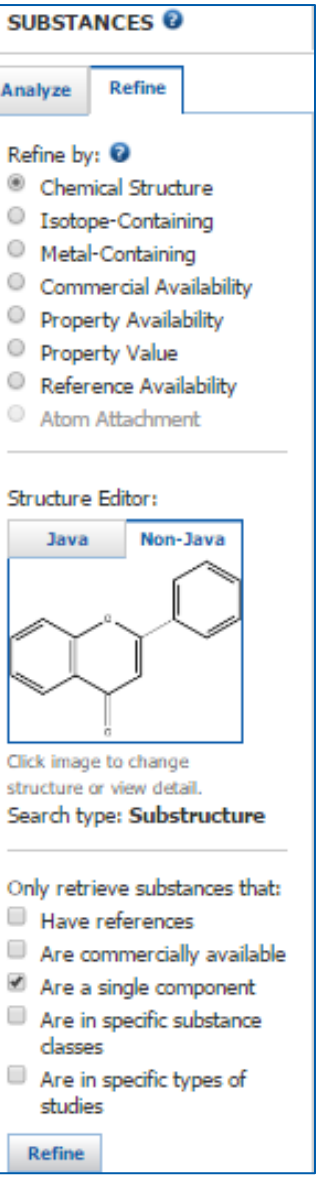


4500多万个结构，

如何筛选黄酮类物质？

物质结果集的筛选——Refine

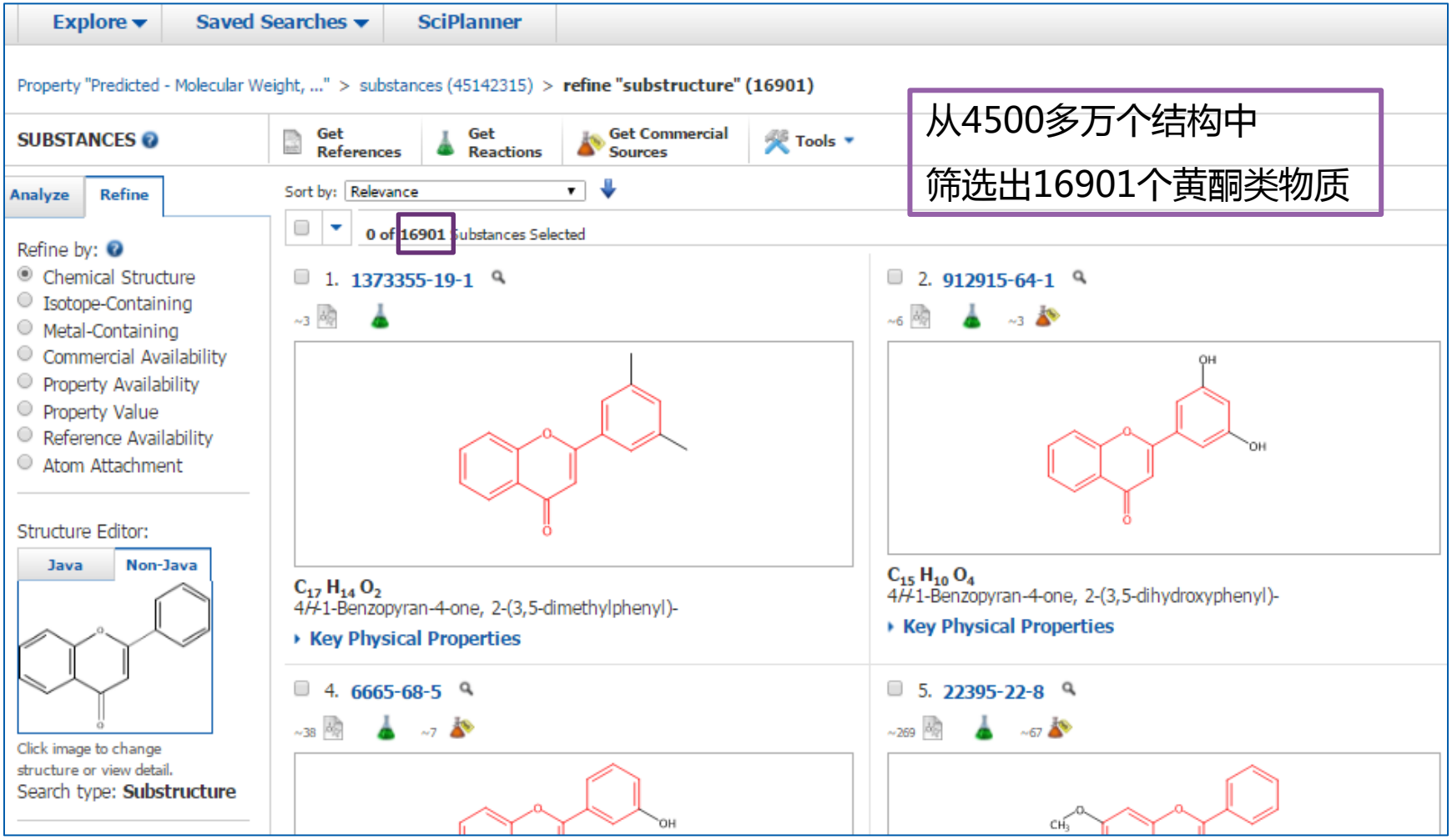




锁环工具：避免在被锁定的环结构上出现新的环结构

SciFinder® A CAS SOLUTION

物质检索结果集

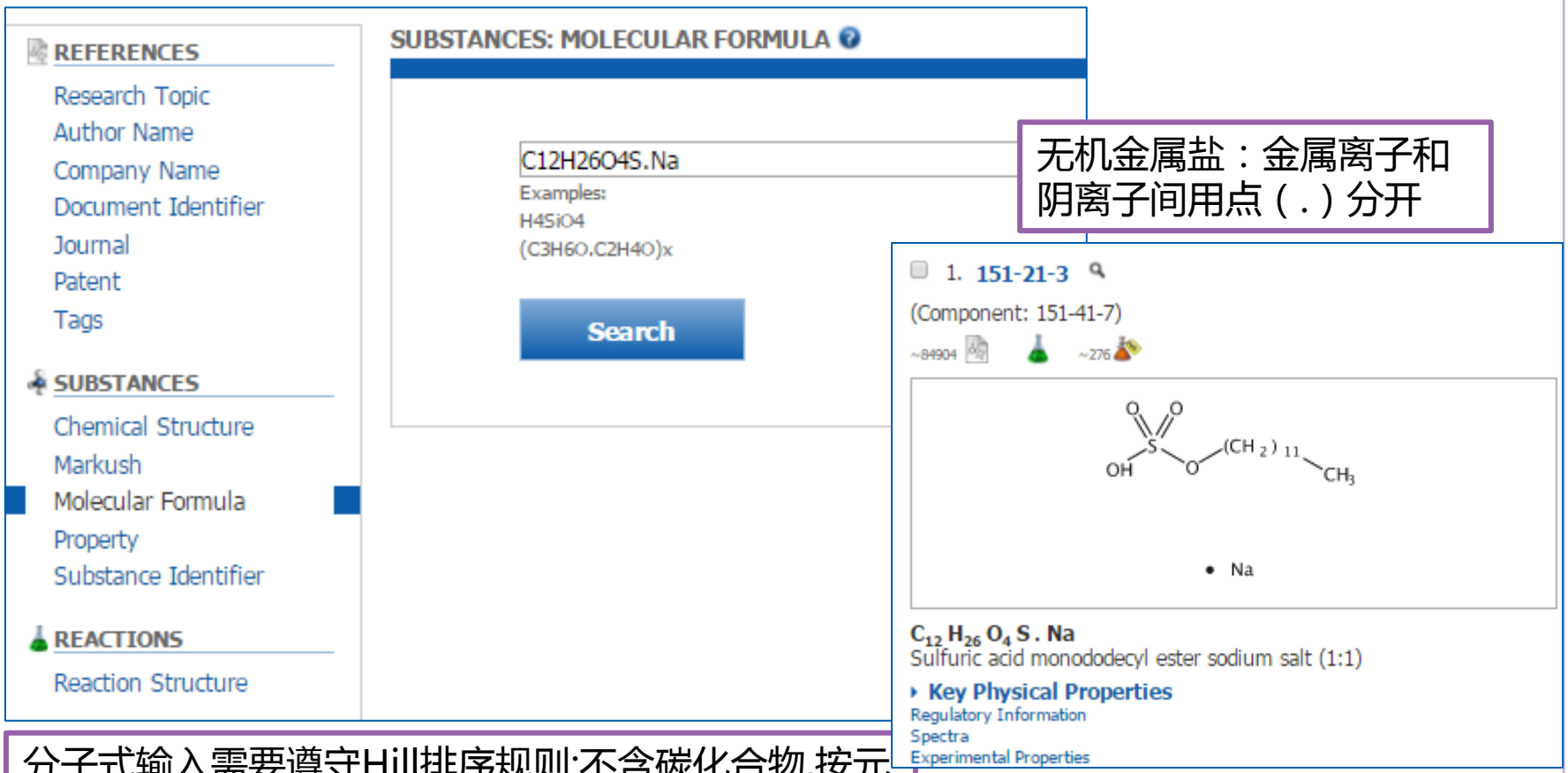


从4500多万个结构中

筛选出16901个黄酮类物质

SciFinder® A CAS SOLUTION

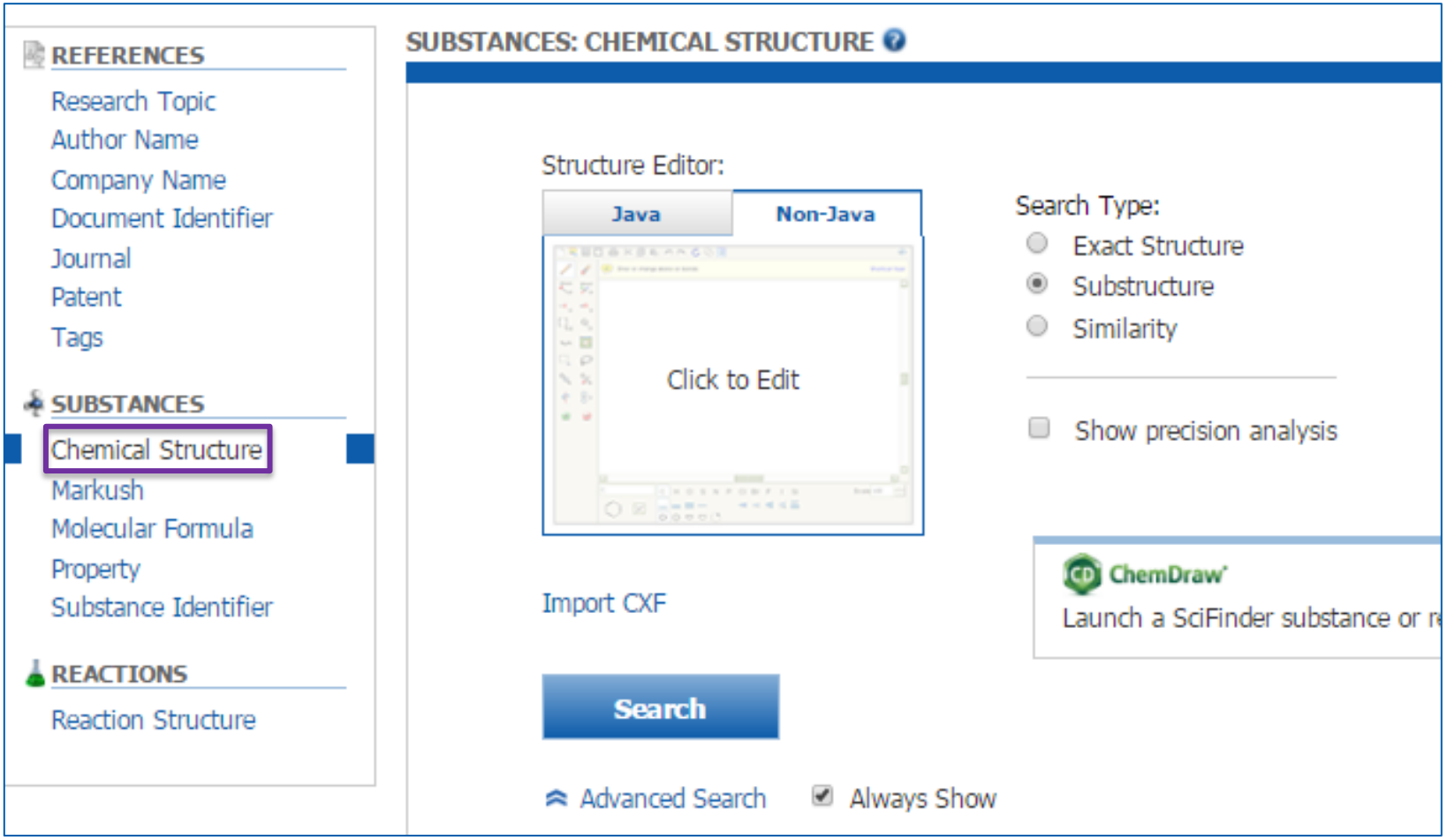
物质检索——分子式



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

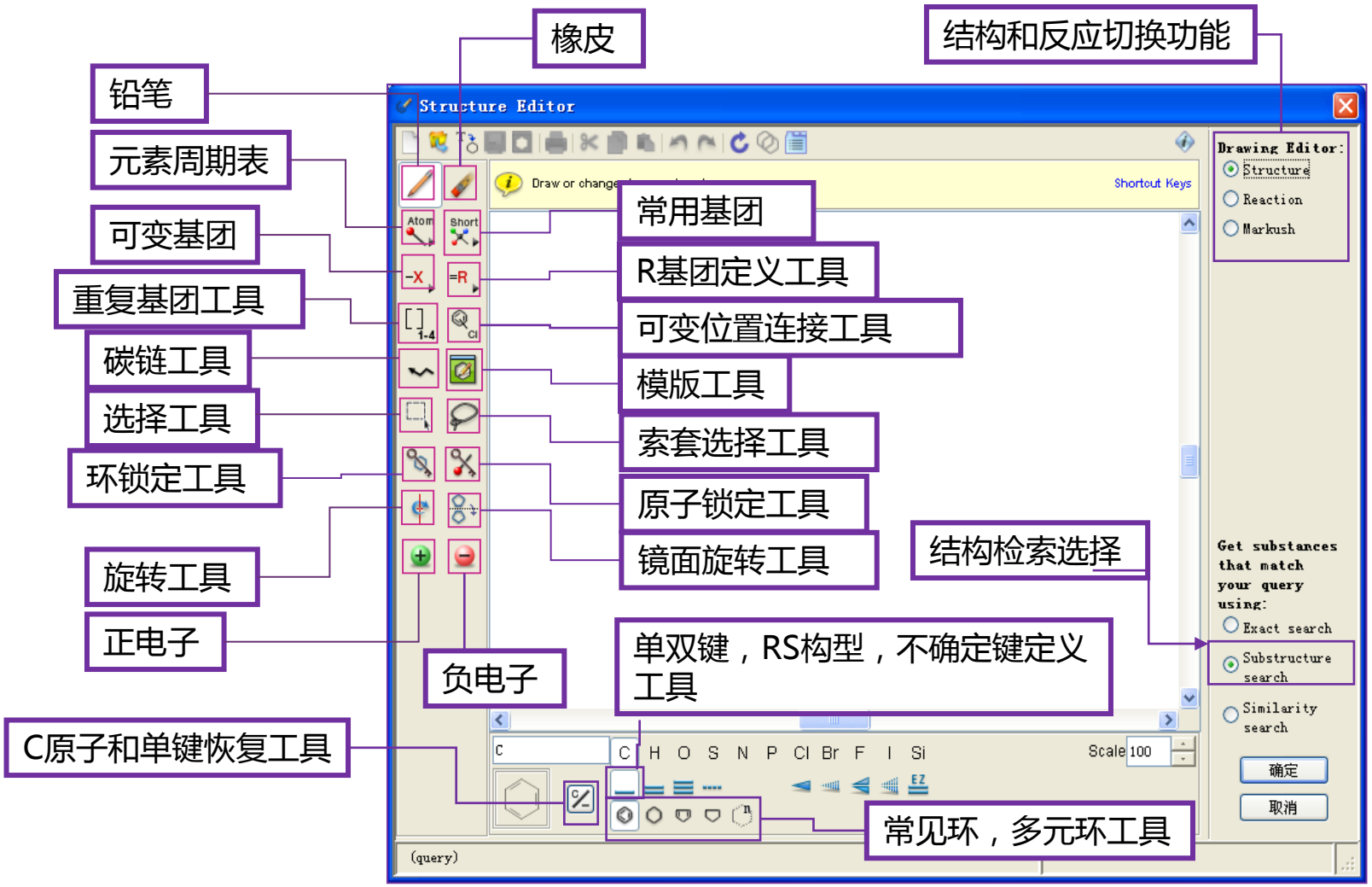
SciFinder® A CAS SOLUTION

物质检索——结构

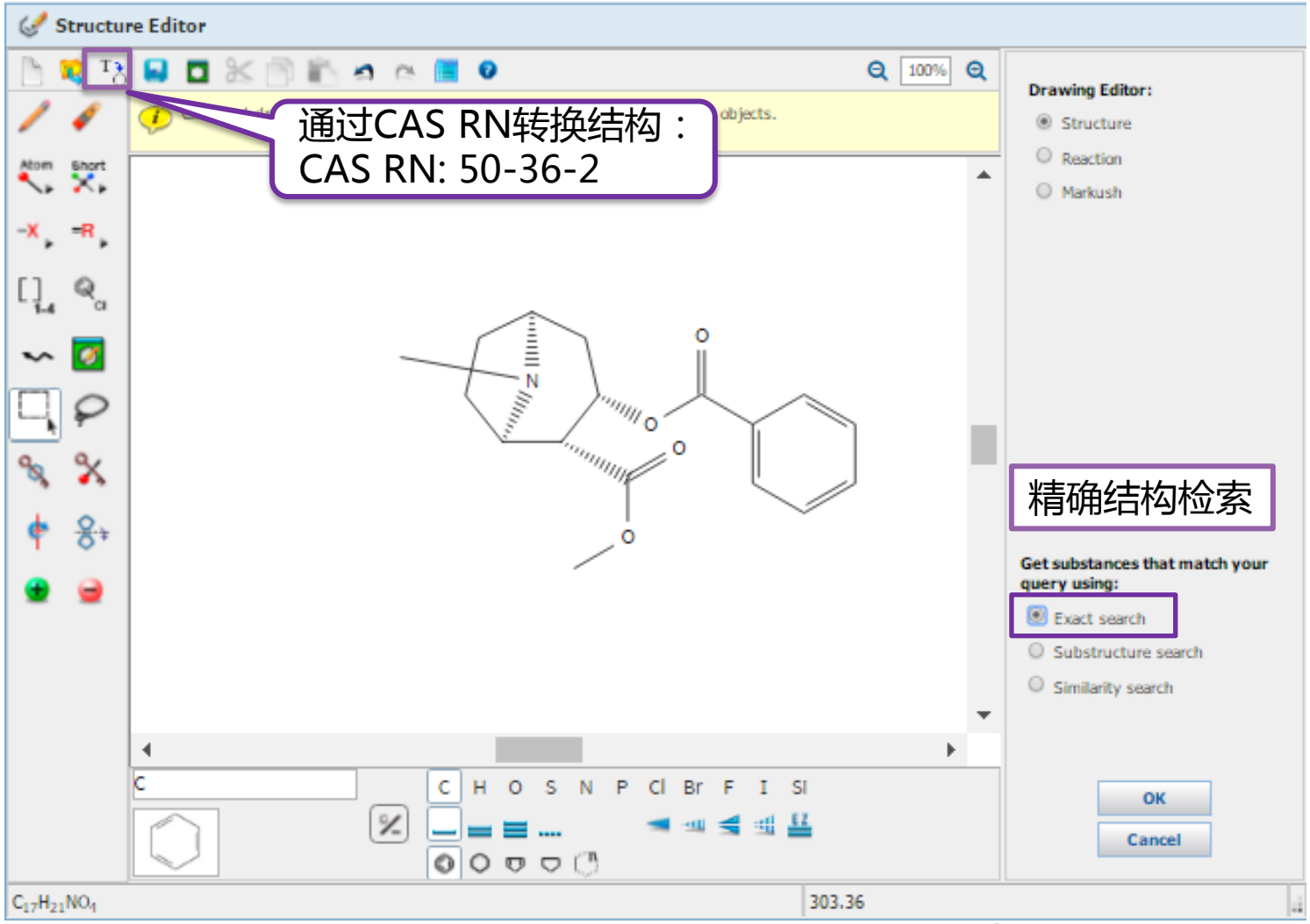


SciFinder® A CAS SOLUTION

物质检索——结构


橡皮
结构和反应切换功能
铅笔
元素周期表
可变基团
重复基团工具
碳链工具
选择工具
环锁定工具
旋转工具
正电子
C原子和单键恢复工具
负电子
常用基团
R基团定义工具
可变位置连接工具
模版工具
索套选择工具
原子锁定工具
镜面旋转工具
结构检索选择
单双键，RS构型，不确定键定义工具
常见环，多元环工具
Structure Editor
Drawing Editor:
Structure
Reaction
Markush
Shortcut Keys
Get substances that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
(query)

物质检索——精确结构检索



SciFinder® A CAS SOLUTION

精确结构检索结果

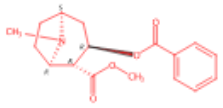
Get References | Get Reactions | Get Commercial Sources | Tools | Create Posted

Sort by: Relevance

0 of 6 Substances Selected

1. 668-19-9

~18 ~1



Absolute stereochemistry.

$C_{17}H_{21}NO_4$

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

▸ Key Physical Properties

Spectra

可卡因

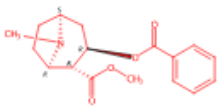
2. 114599-38-1

~5

可卡因组合物

668-19-9

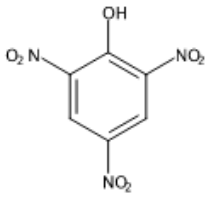
$C_{17}H_{21}NO_4$



Absolute stereochemistry.

88-89-1

$C_6H_3N_3O_7$



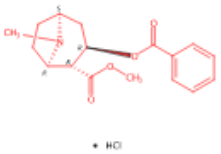
$C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$

Allococaine, picrate (6CI)

3. 109496-04-0

(Component: 668-19-9)

~1



Absolute stereochemistry.

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

Allococaine, hydrochloride (6CI)

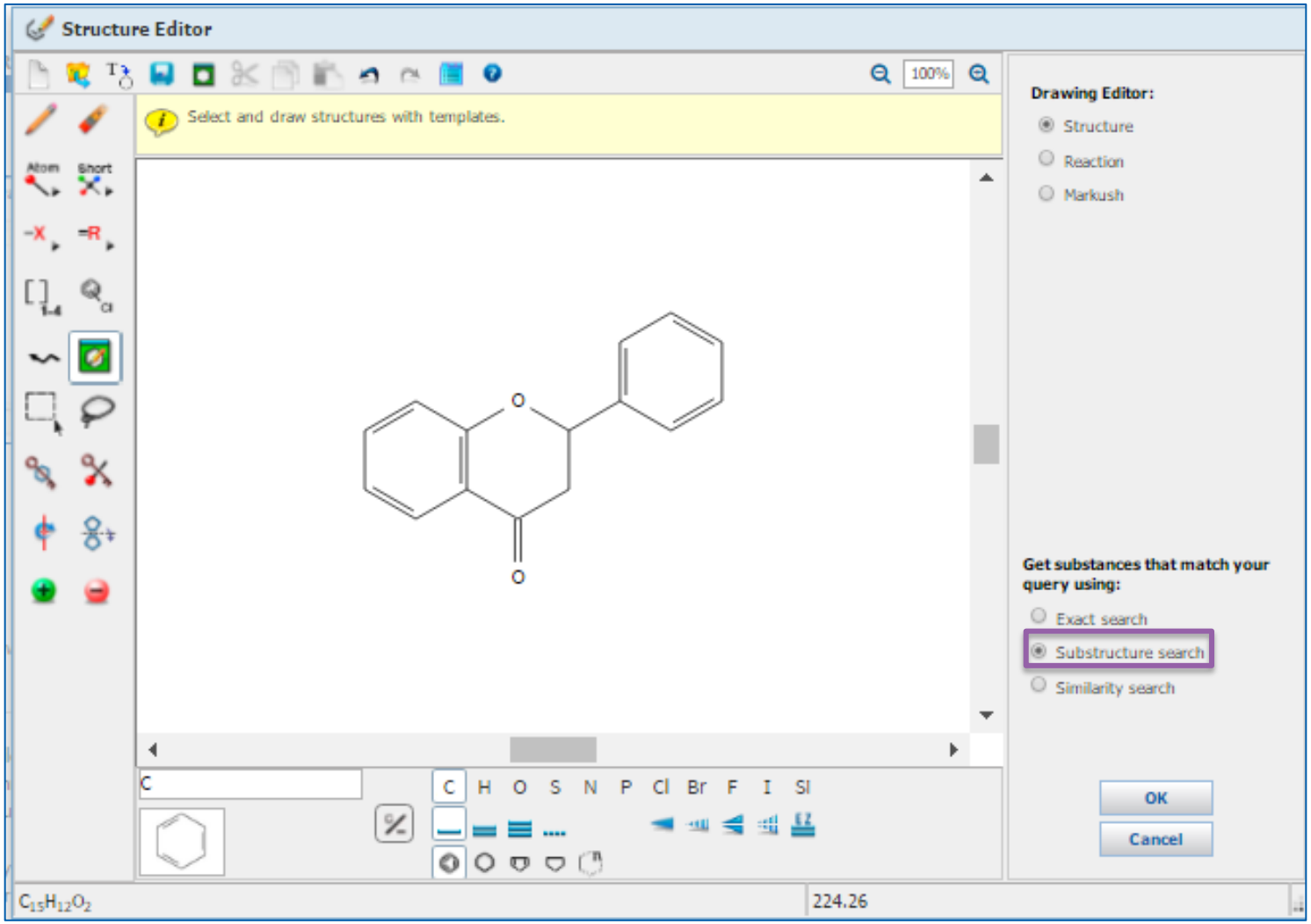
盐酸可卡因

物质检索——精确结构检索

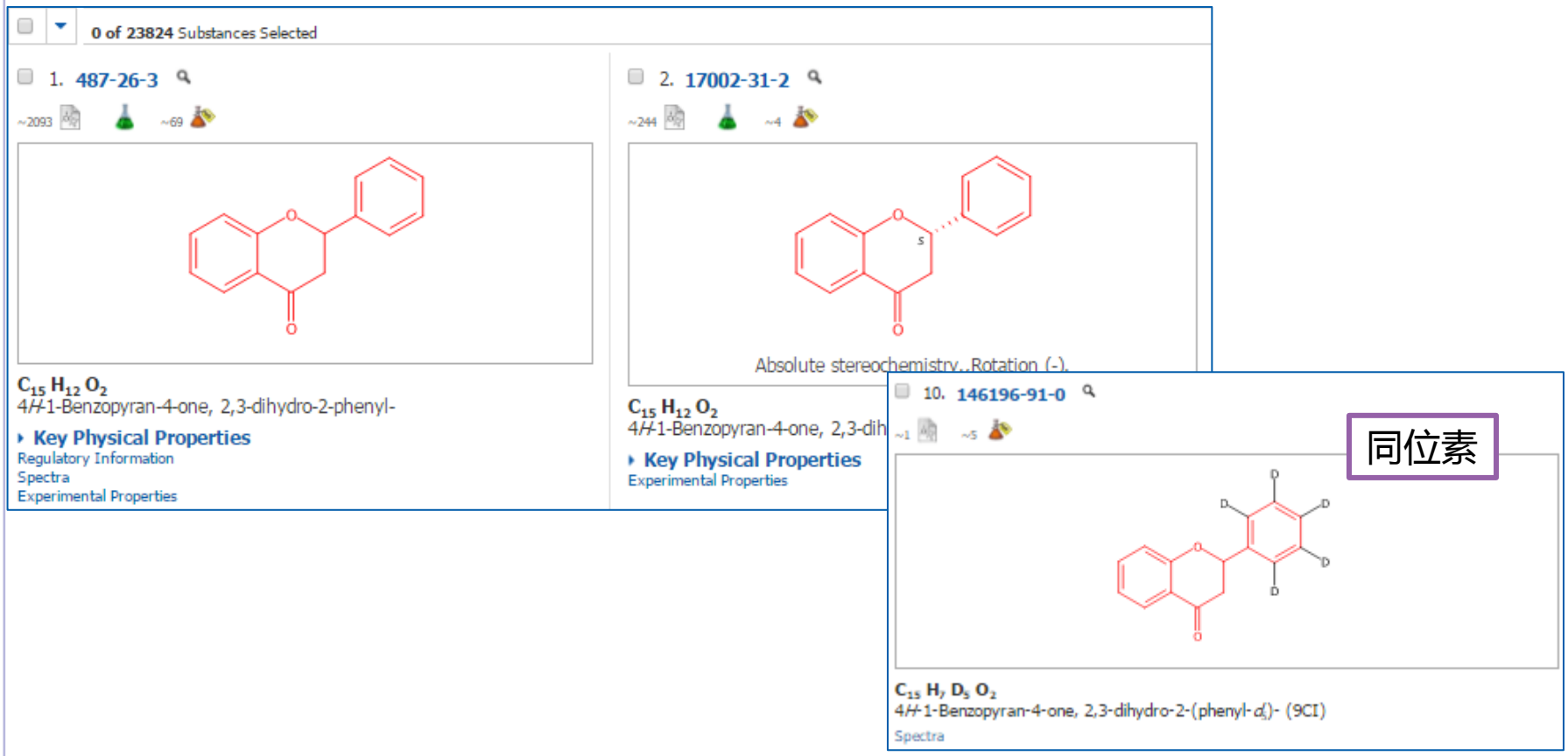
精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索


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

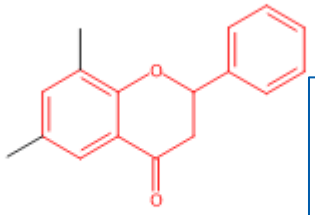
物质检索——亚结构检索


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

亚结构检索结果

281. 123251-10-5

取代物



$C_{17}H_{16}O_2$

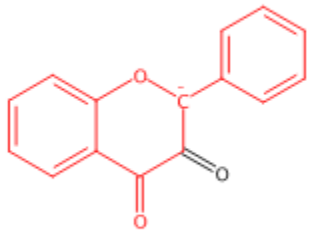
4*H*-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl

Key Physical Properties

Experimental Properties

295. 780723-19-5

离子

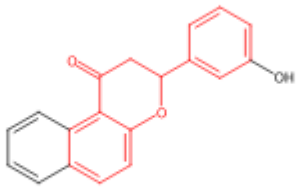


$C_{15}H_9O_3$

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

284. 136116-23-9

稠环物质



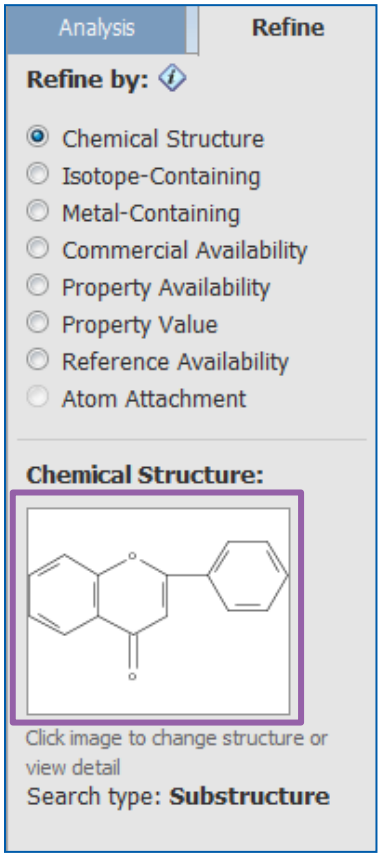
$C_{19}H_{14}O_3$

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

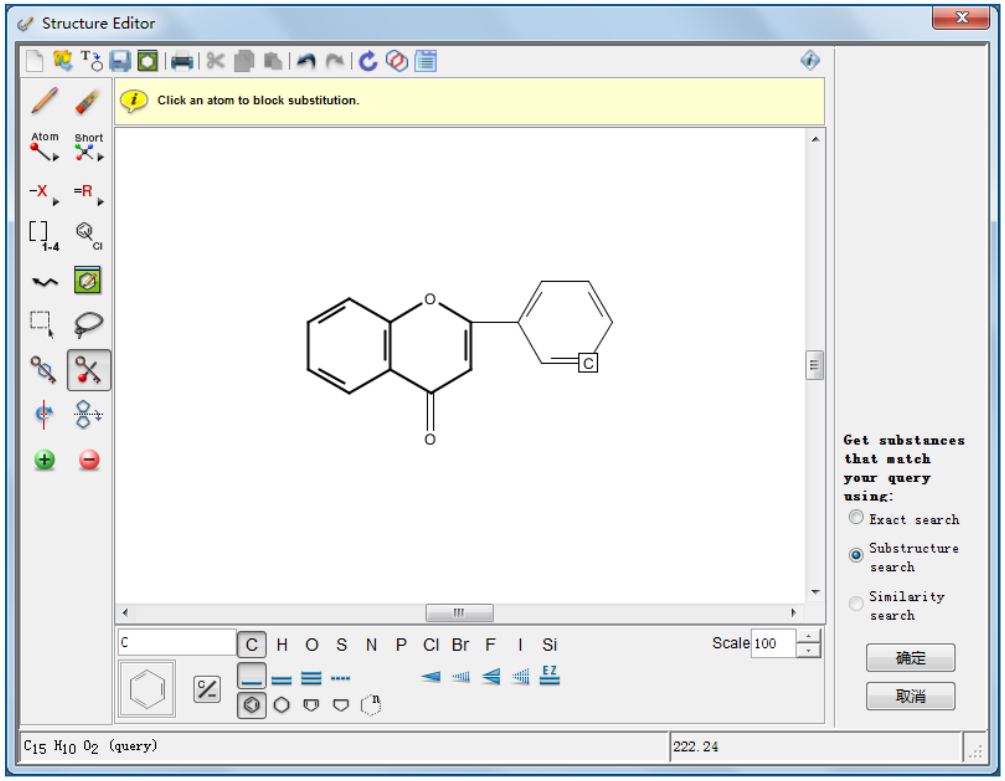
Key Physical Properties

SciFinder® A CAS SOLUTION

亚结构检索结果的限定



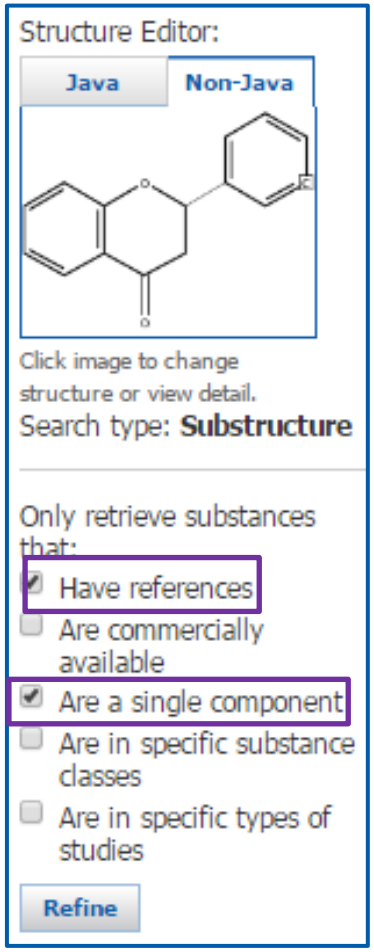
化学结构的再次限定

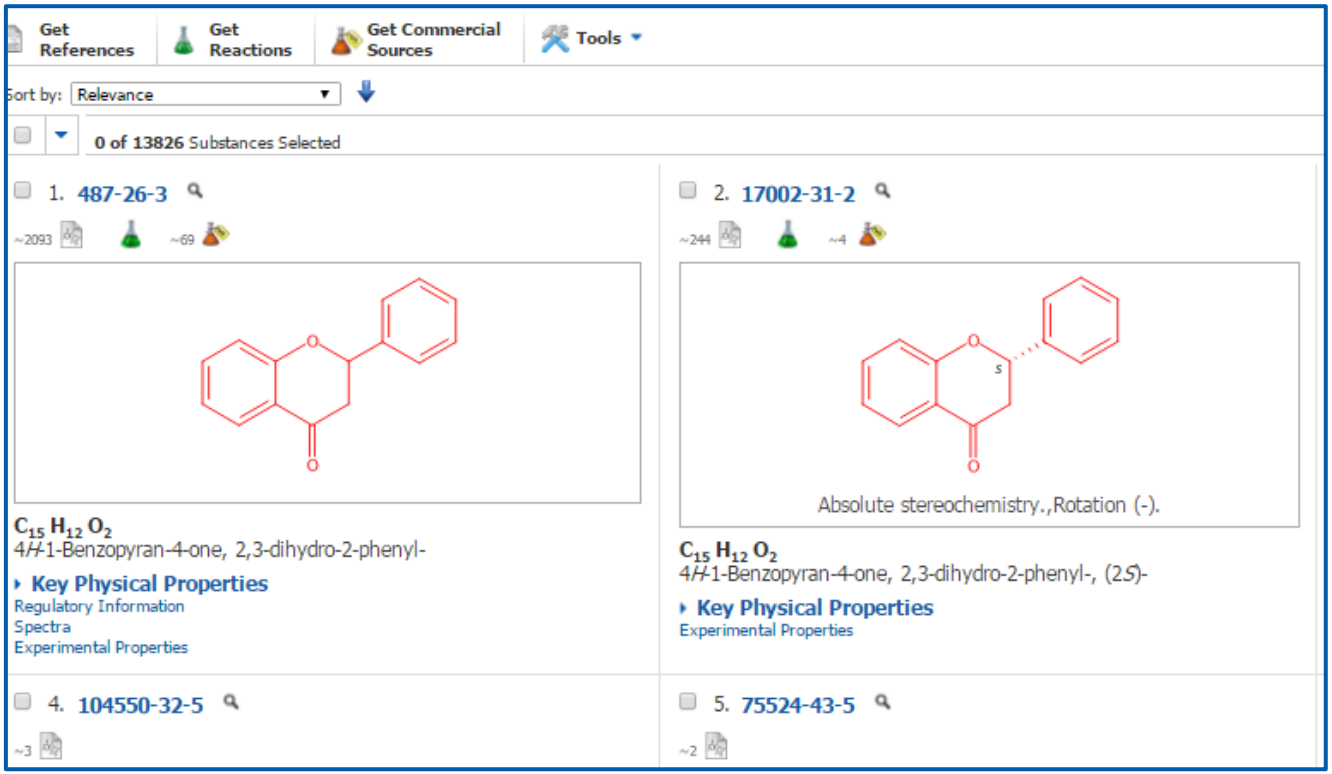


环锁定

原子锁定

亚结构检索结果的限定


Structure Editor:
Java
Non-Java
Click image to change structure or view detail.
Search type: Substructure
Only retrieve substances that:
Have references
Are commercially available
Are a single component
Are in specific substance classes
Are in specific types of studies
Refine

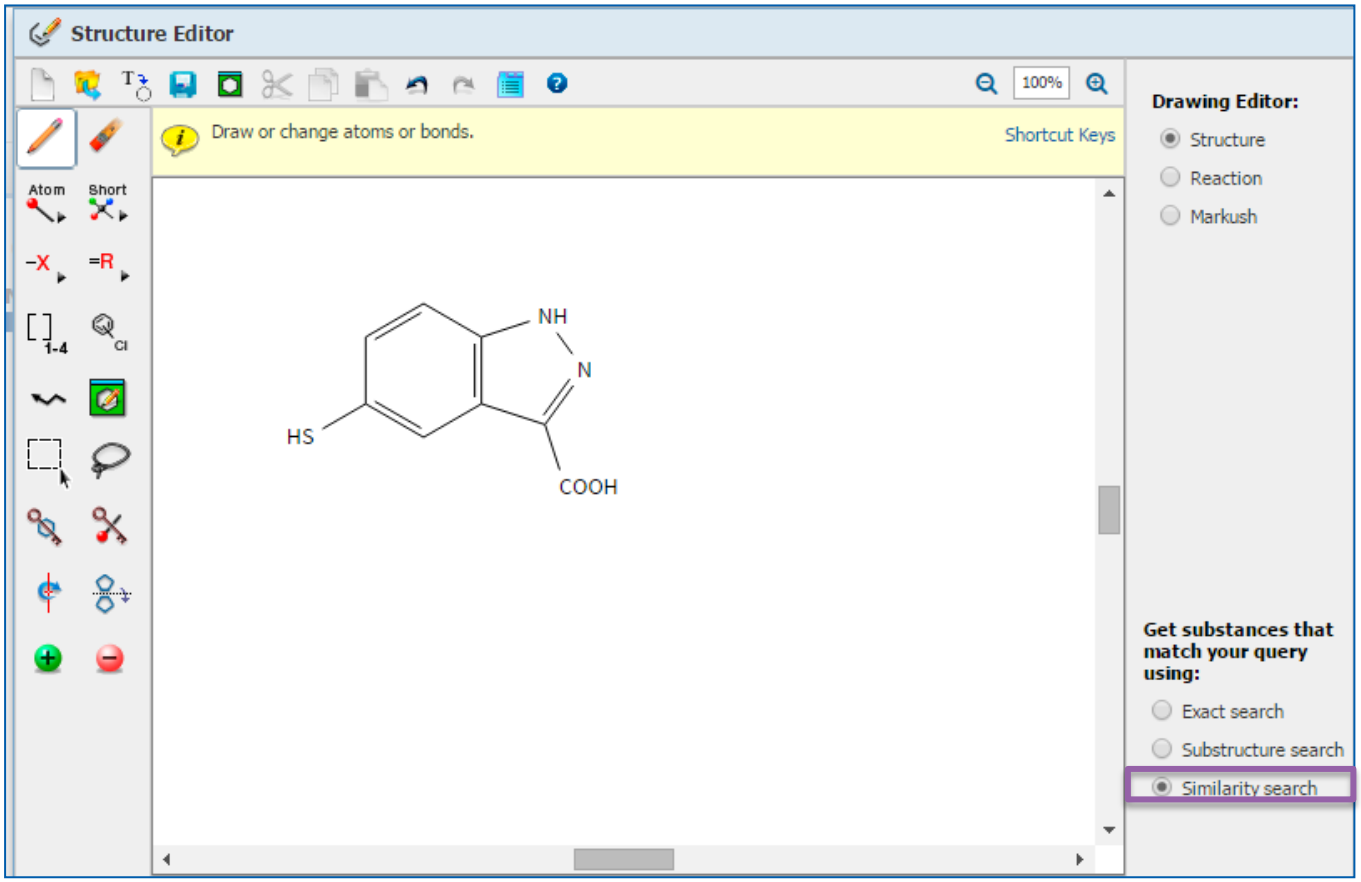

Get References
Get Reactions
Get Commercial Sources
Tools
Sort by: Relevance
0 of 13826 Substances Selected
1. 487-26-3
2. 17002-31-2
Absolute stereochemistry.,Rotation (-).
C15 H12 O2
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-
Key Physical Properties
Regulatory Information
Spectra
Experimental Properties
C15 H12 O2
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-
Key Physical Properties
Experimental Properties
4. 104550-32-5
5. 75524-43-5

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

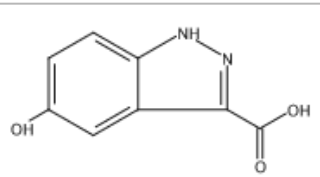
0 of 6 Similarity Candidates Selected	Substances
≥ 99 (most similar)	0
95-98	0
90-94	0
85-89	11
80-84	34
75-79	84
70-74	267
65-69	696
0-64 (least similar)	1818

Get Substances

相似度越高，结构越相似

Score: 88
1. **885518-94-5**

~1 ~35



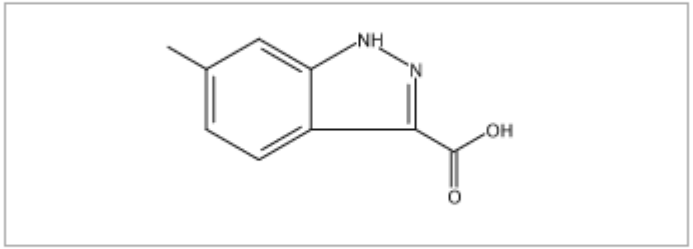
$C_8H_6N_2O_3$
1*H*-Indazole-3-carboxylic acid, 5-hydroxy-

Key Physical Properties

取代基变化

Score: 86
5. **858227-12-0**

~7 ~41



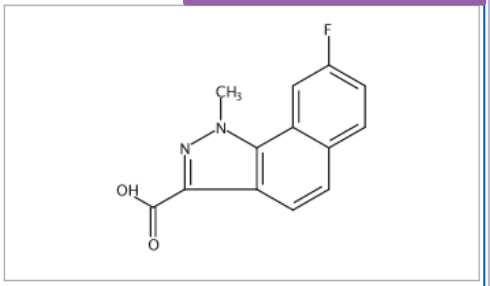
$C_9H_8N_2O_2$
1*H*-Indazole-3-carboxylic acid, 6-methyl-

Key Physical Properties

取代基位置变化

Score: 65
541. **1100422-**

~1



$C_{13}H_9FN_2O_2$
1*H*-Benz[*g*]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

Key Physical Properties

母体结构变化

SciFinder® A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

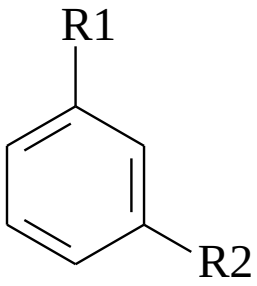
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

Markush检索

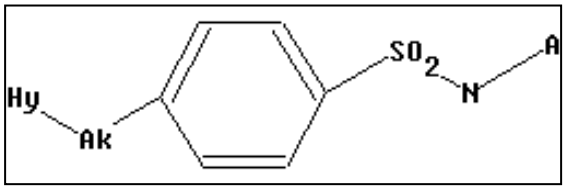
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

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

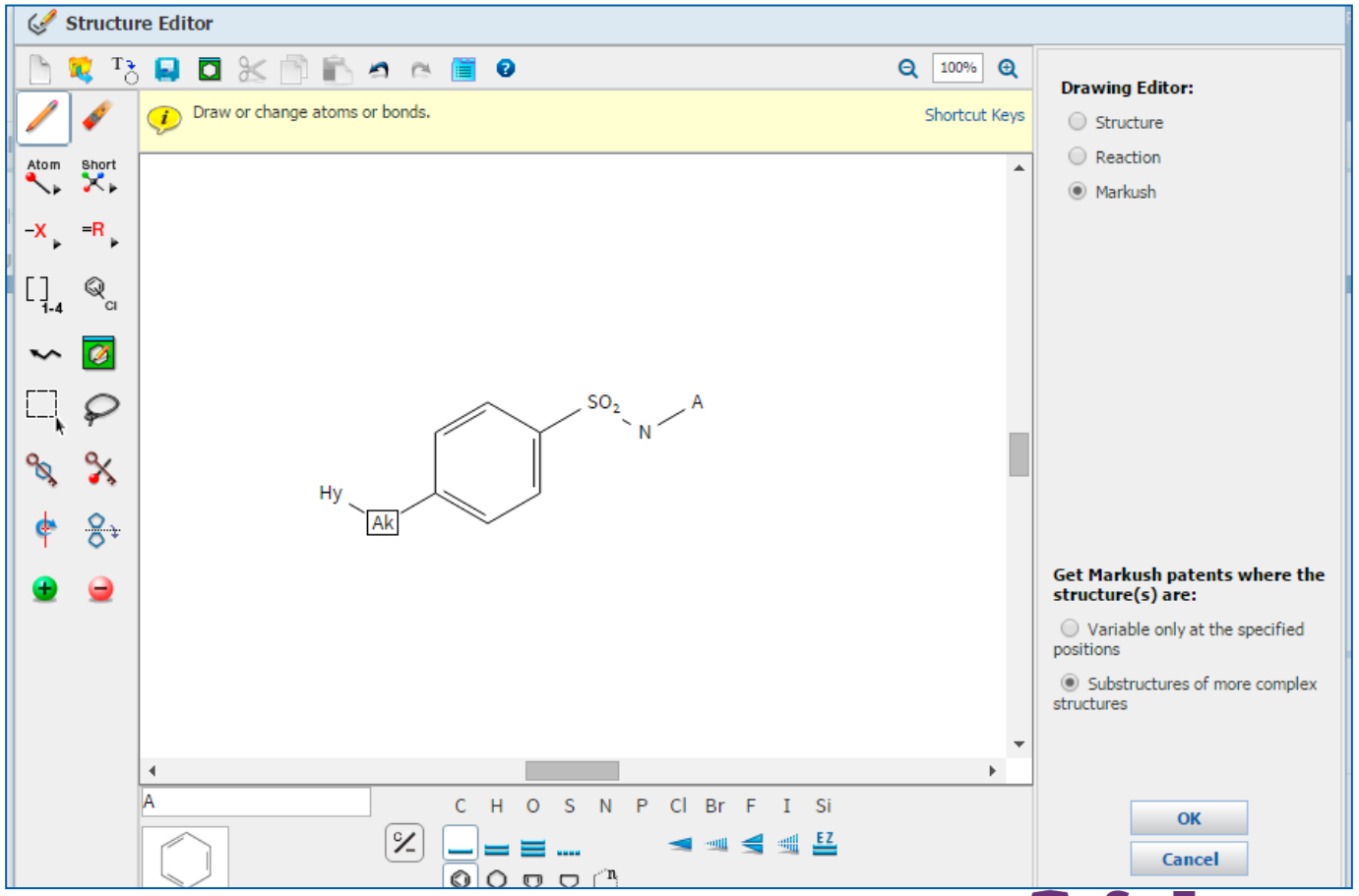


R1 = H, Br, Cl, I

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



可用SciFinder中的Markush检索查看专利中化合物结构保护范围。



Markush检索

SciFinder A CAS SOLUTION

Welcome Helen Zhu

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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

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Analyze by: Document Type ▾

Patent 1969

Journal 1

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0 of 1969 References Selected Page: 1 of 99

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

Quick View PATENTPAK ▾

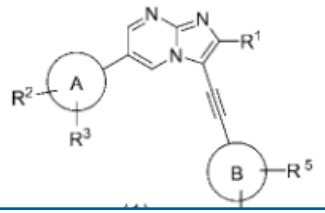
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

2. **Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)**

Quick View PATENTPAK ▾

By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji
From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS



The title imidazo[1,2-a]pyrimidine derivs. I [R^1 = H or halogen; ring A Ph or pyridyl; R^2, R^3 (same or different) = hydrogen, halogen, C_{1-4} alkyl or C_{1-4} alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R^2 and R^3 are at the adjacent substitution position, R^2 and R^3 together with ring A form C_{5-8} carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R^4, R^5 (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^{a}R^b, SO_3H, $SO_2NR^aR^b$, SO_2R^b, or $NR^aSO_2R^b$; R^a, R^b (same...

全部是专利

SciFinder A CAS SOLUTION

提纲

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

SCIFINDER® A CAS SOLUTION

SciFinder检索选项——反应检索

- 反应检索方法

  结构式

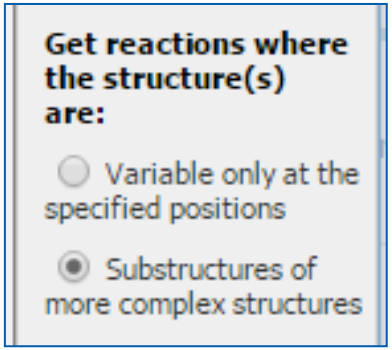
- 常用获取方法

  已知物质：由物质获取反应

  已知文献：从文献中获取反应

  精确结构反应检索

  亚结构反应检索



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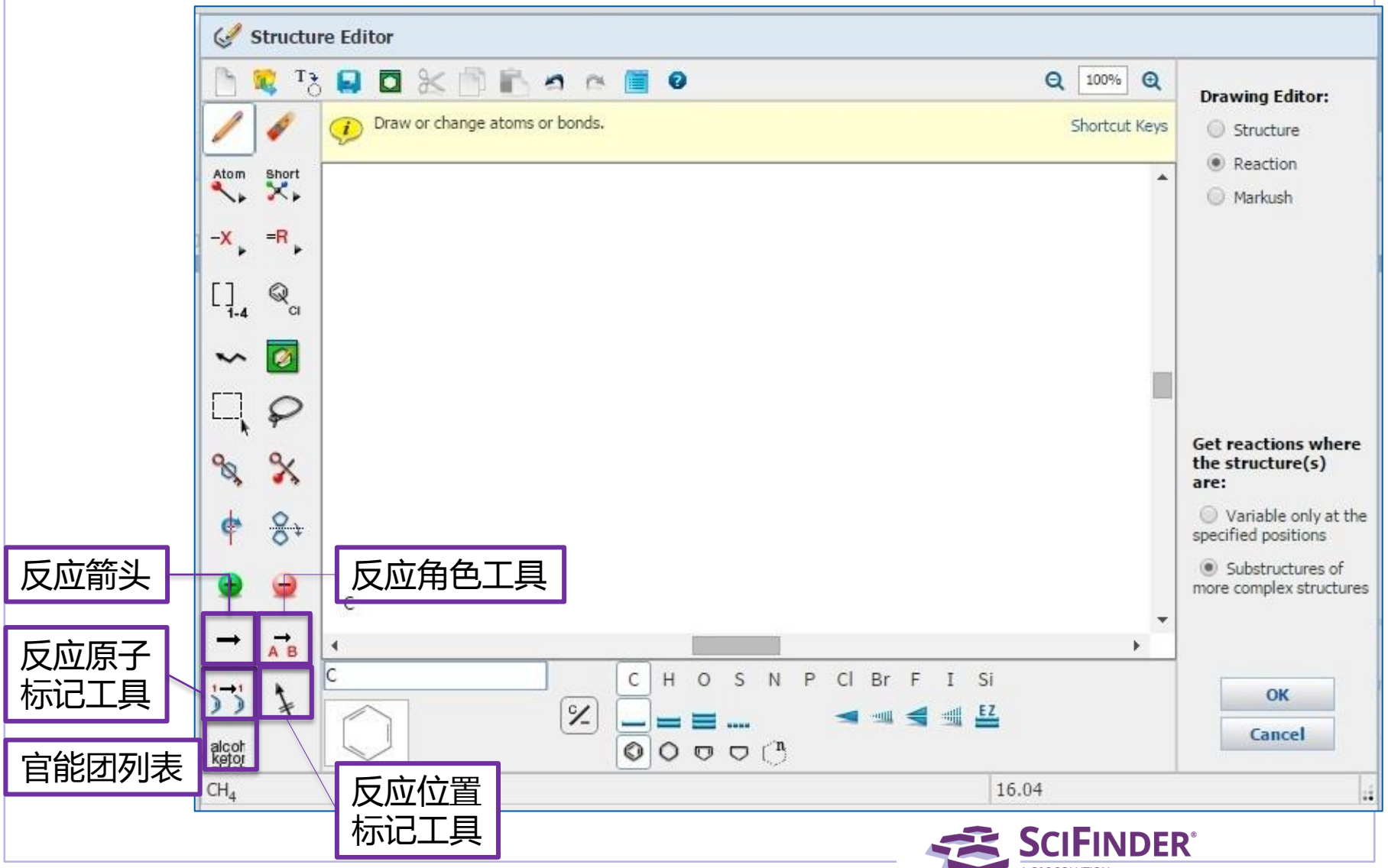
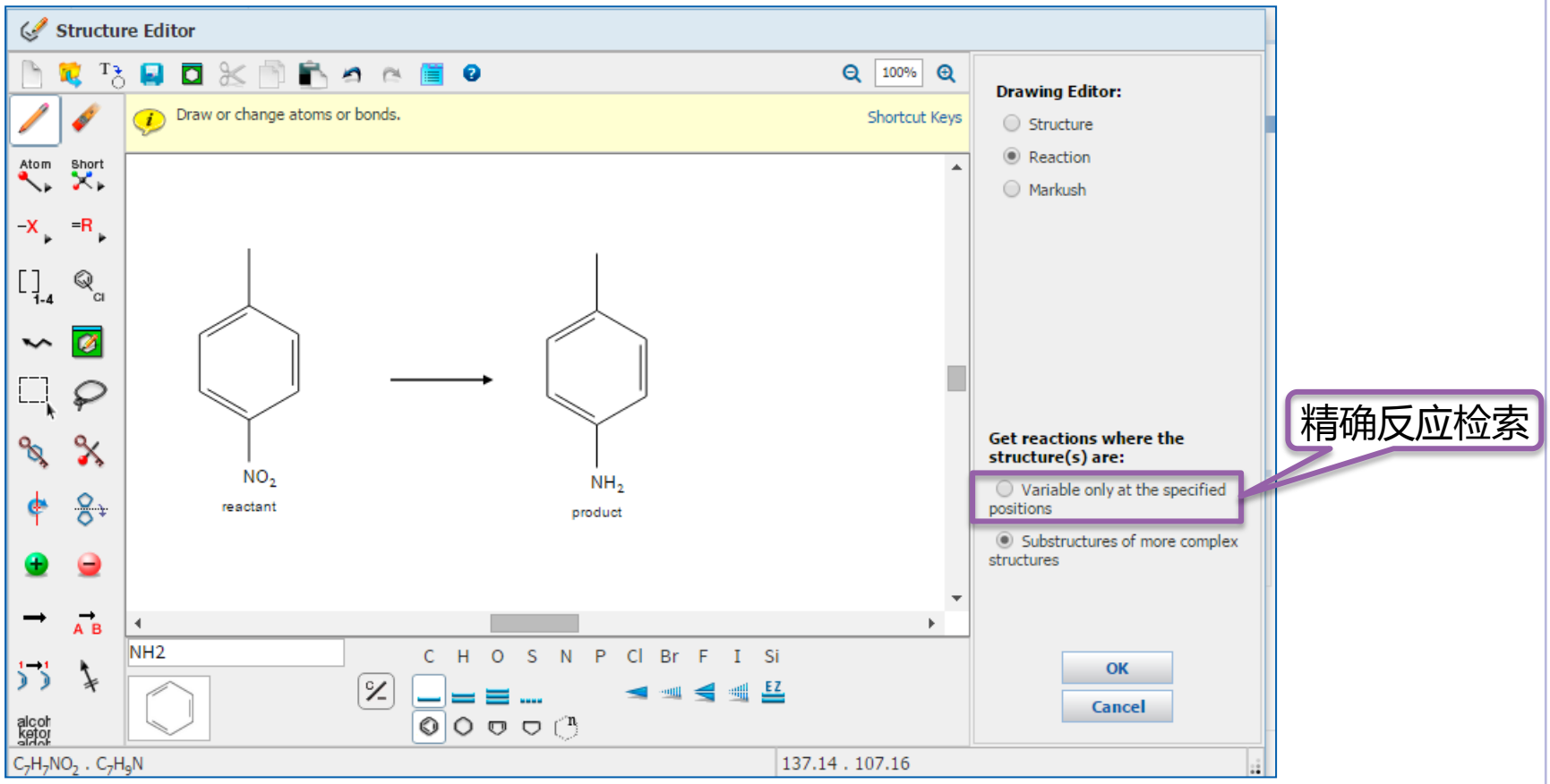
反应绘制工具

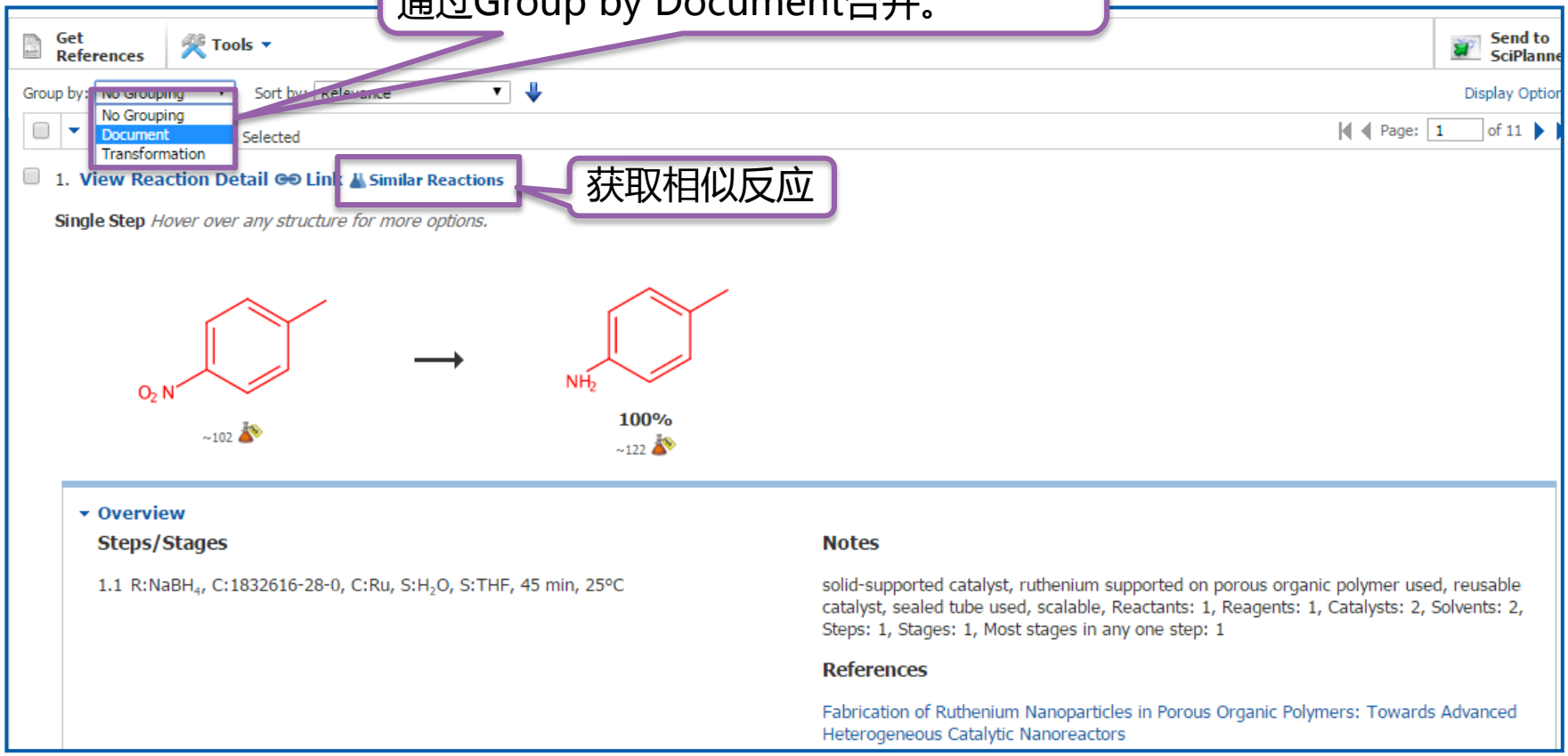

Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
C H O S N P Cl Br F I Si
CH4
16.04
反应箭头
反应角色工具
反应原子标记工具
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

SciFinder反应检索——精确反应检索



反应检索结果

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



SciFinder® A CAS SOLUTION

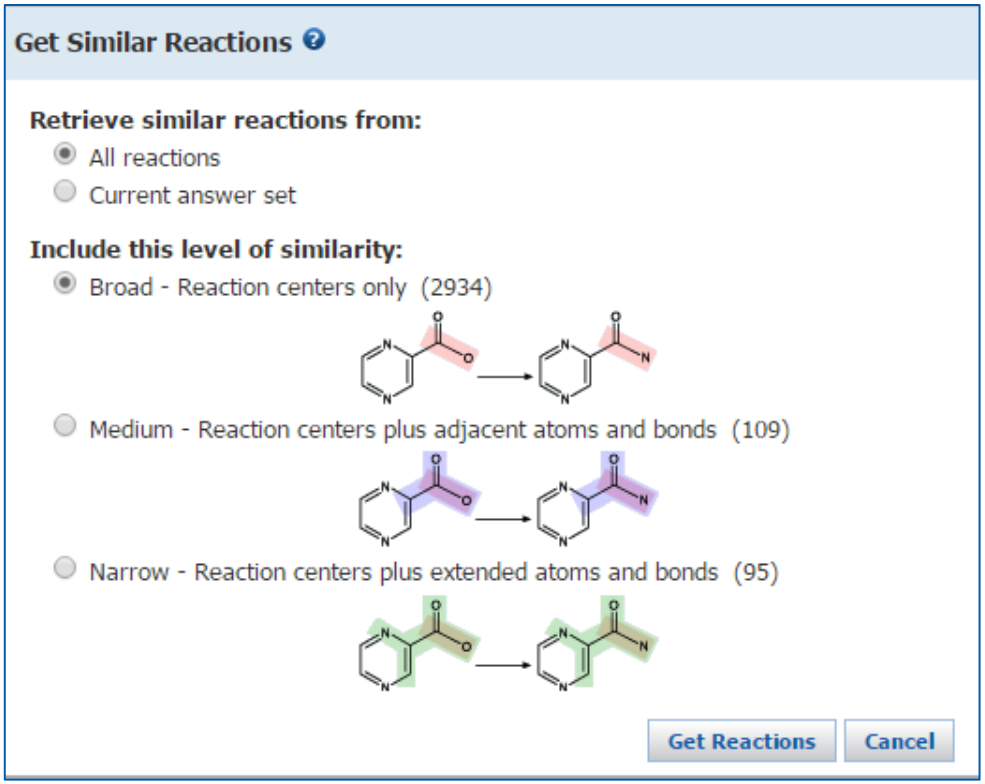
获取相似反应

选择相似反应的相似限制：

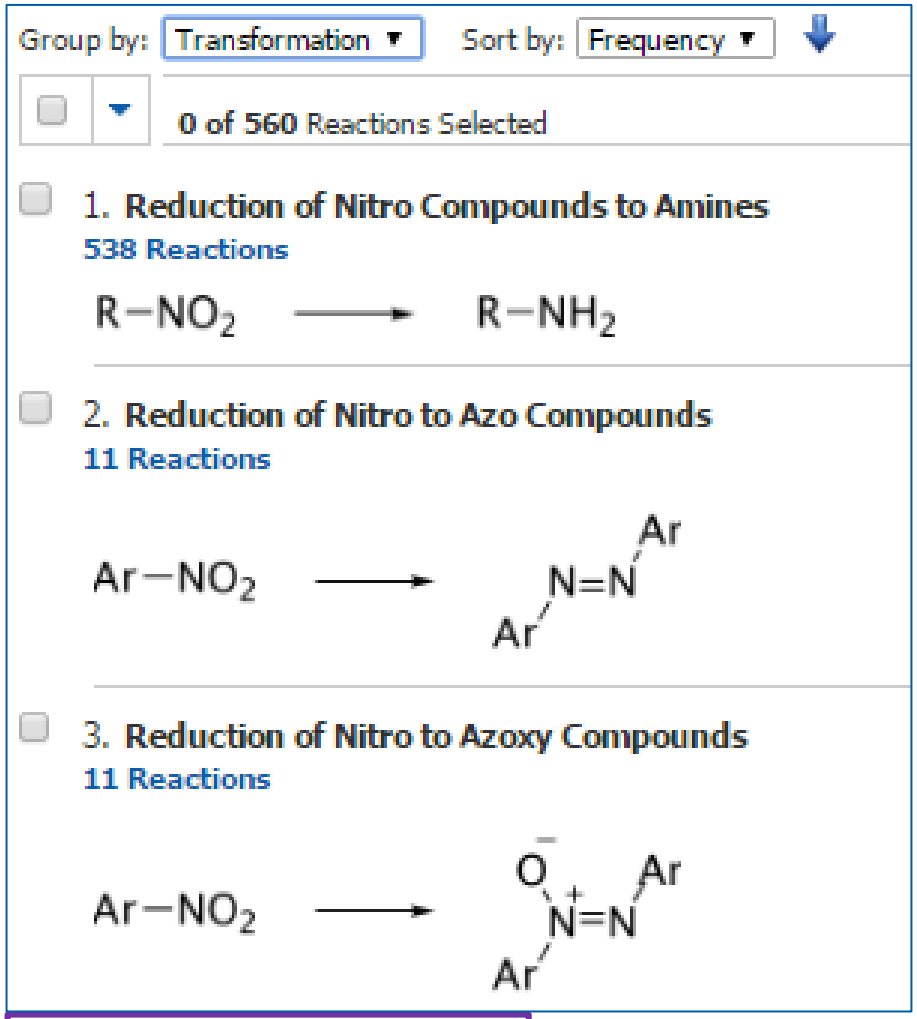
Broad：仅反应中心相似

Miedum：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键



按照反应类型排序



更精确的查找需要的反应

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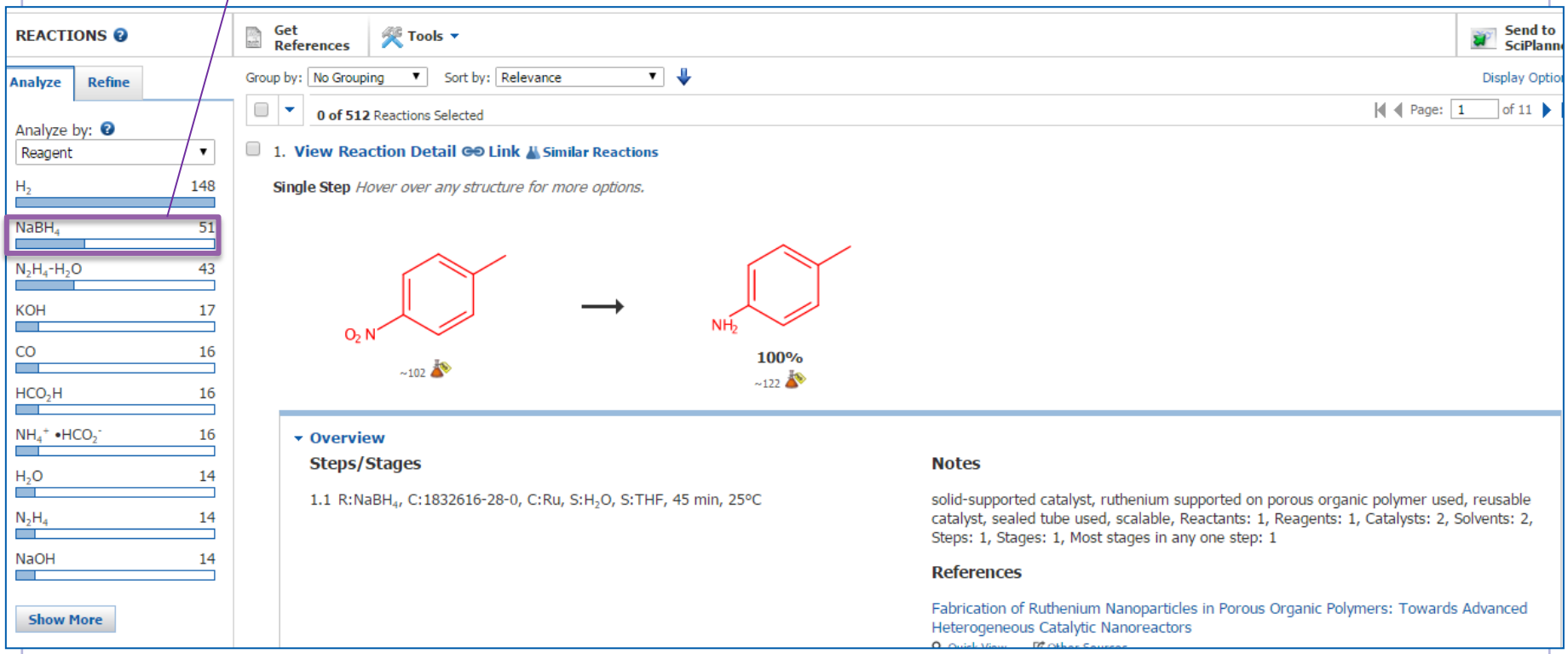
反应检索结果的筛选

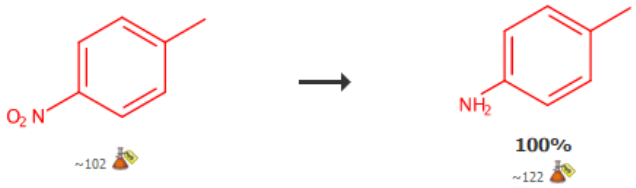
获得特定物质做还原剂的反应



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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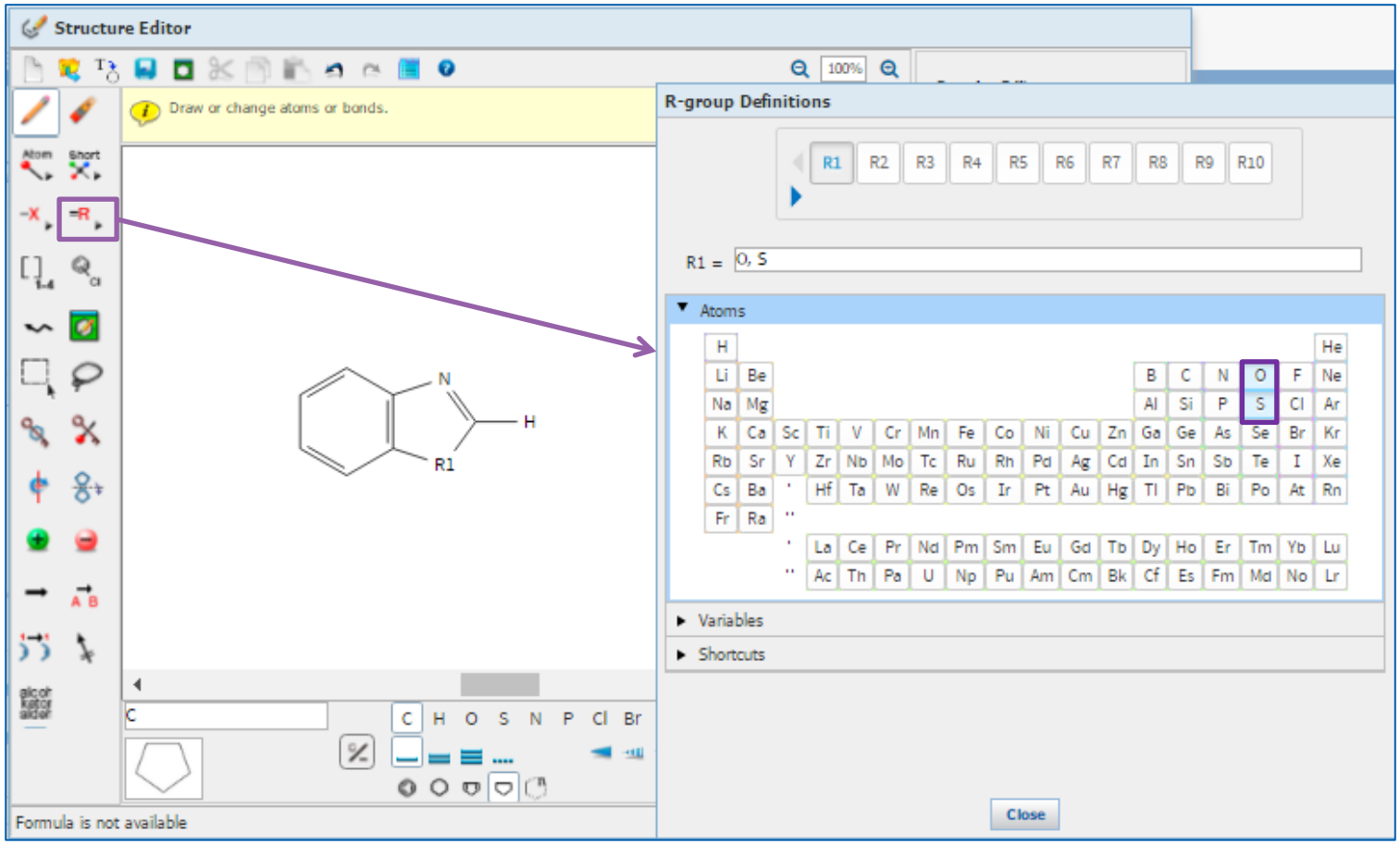
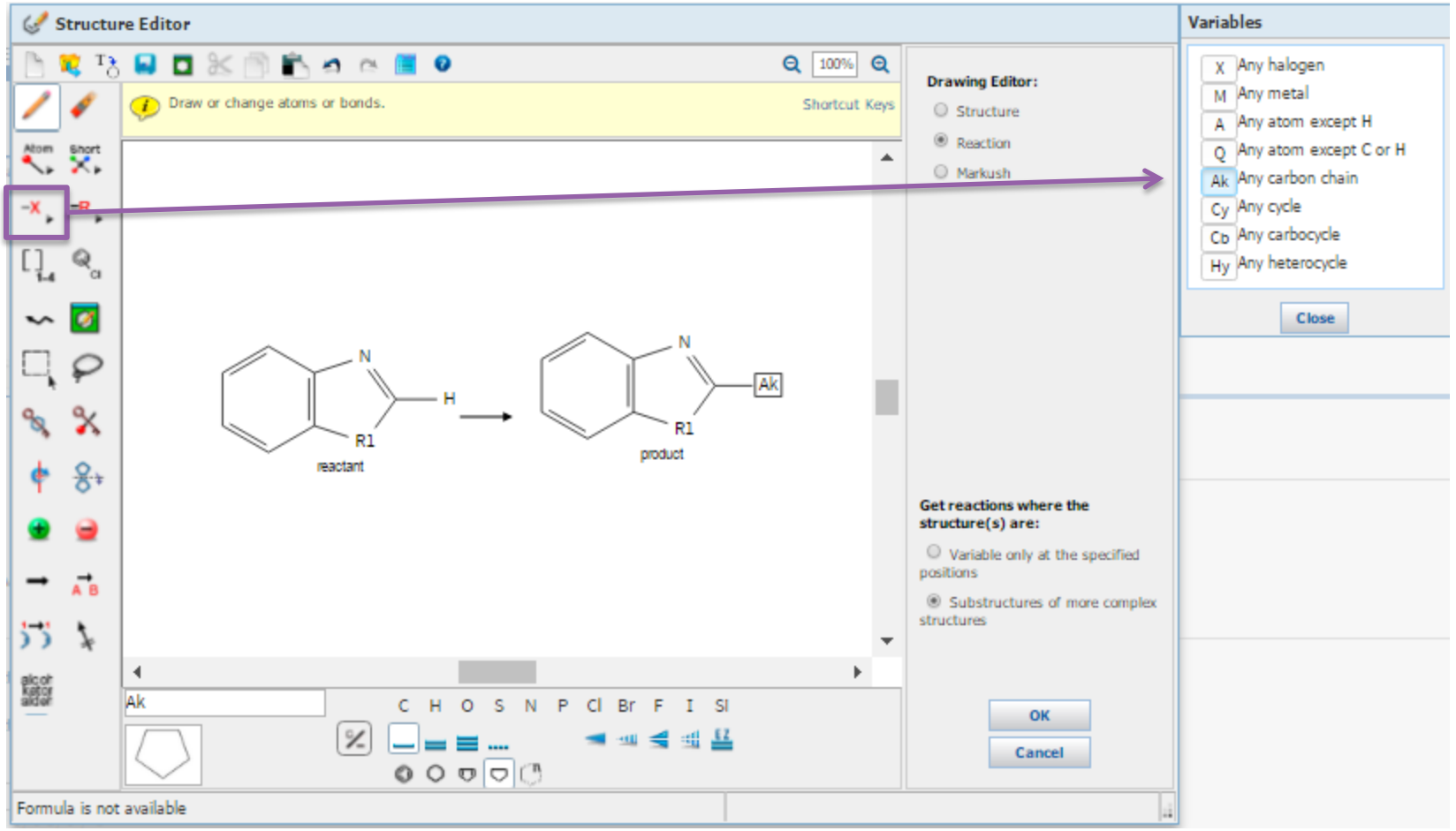
亚结构反应检索

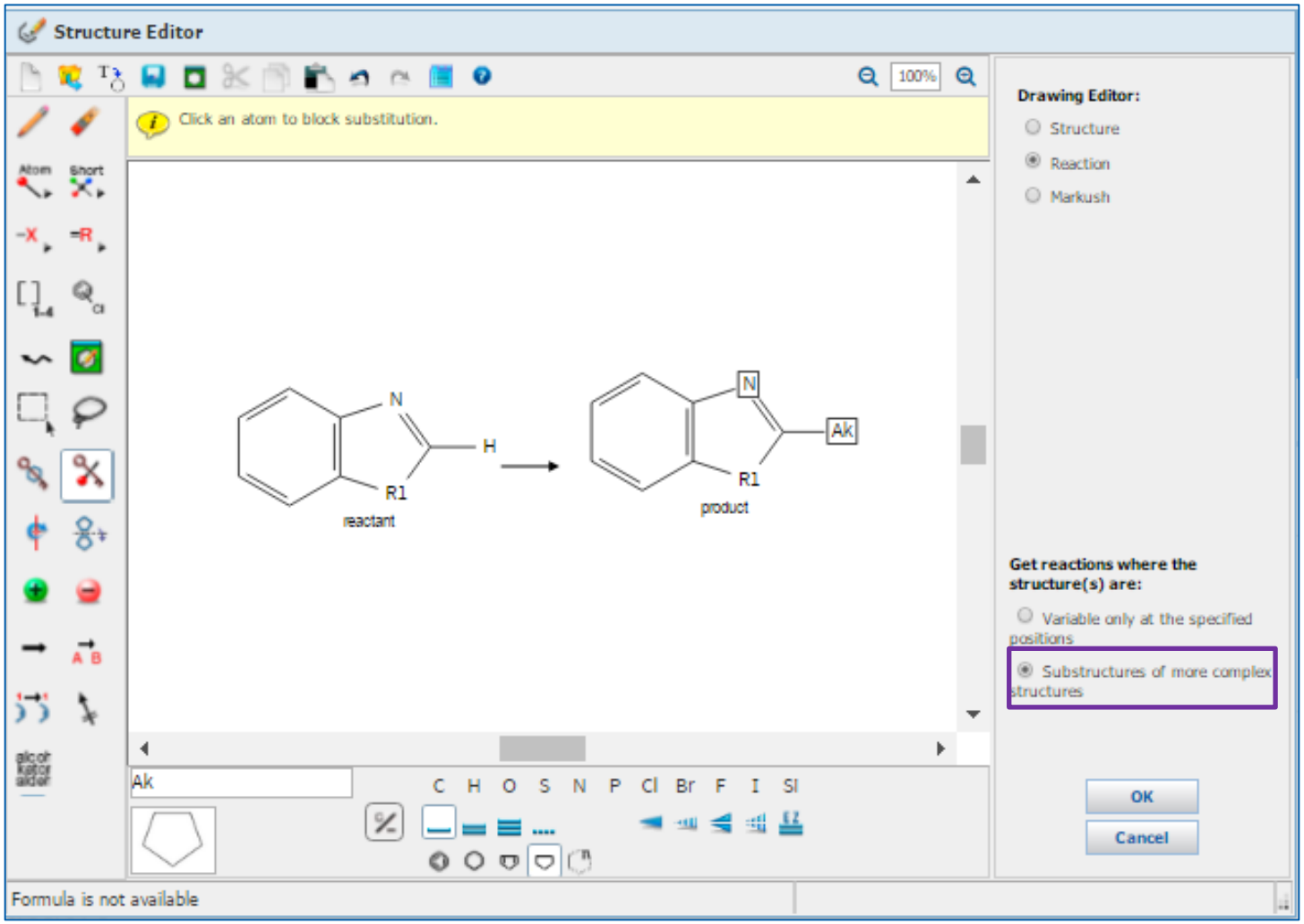
通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索

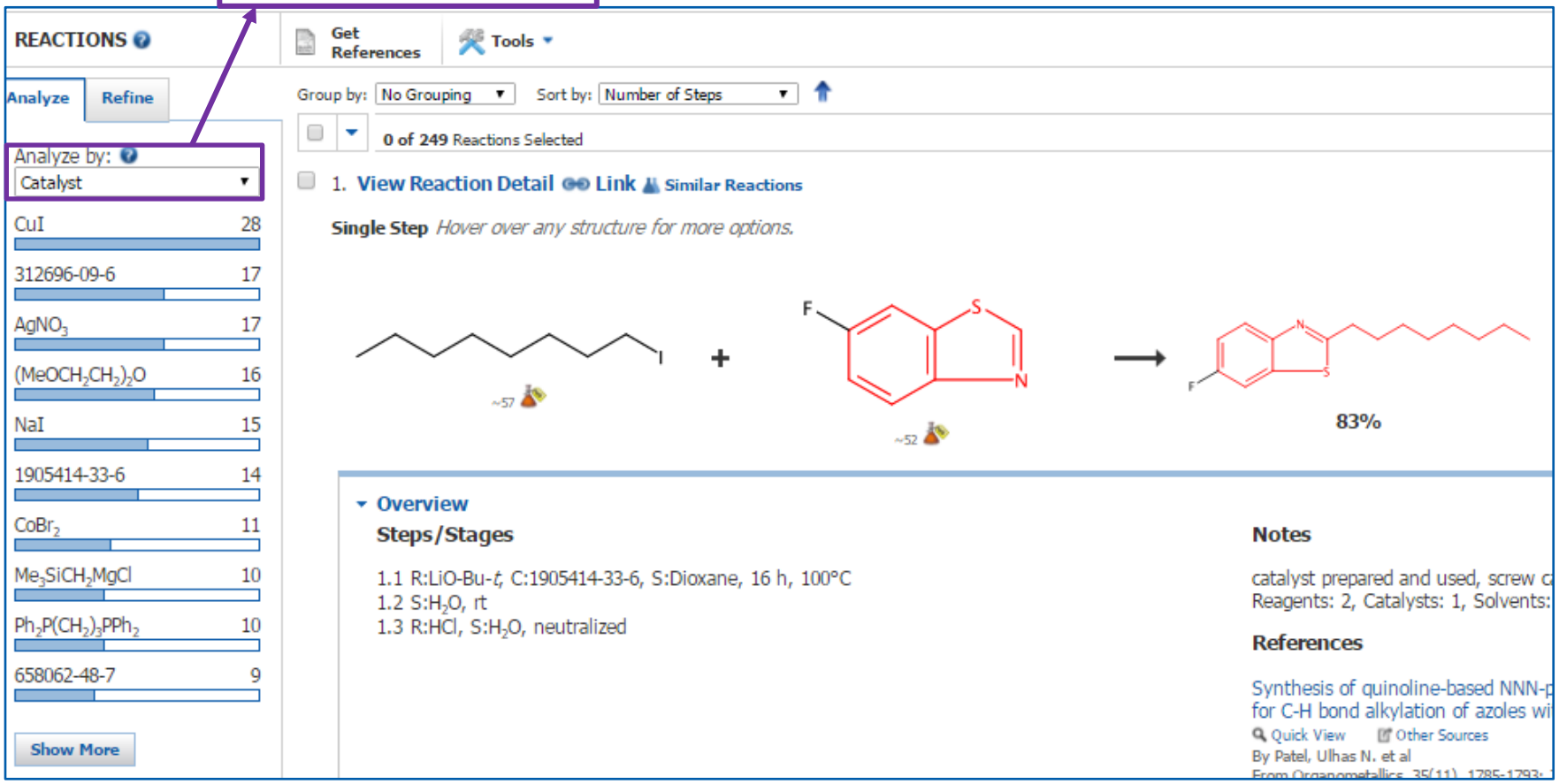

Structure Editor
Draw or change atoms or bonds.
Shortcut Keys
100%
Drawing Editor:
Structure
Reaction
Markush
N
H
R1
reactant
N
Ak
R1
product
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
Ak
C H O S N P Cl Br F I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

亚结构反应检索


Structure Editor
100%
Click an atom to block substitution.
Drawing Editor:
Structure
Reaction
Markush
N
H
R1
reactant
N
Ak
R1
product
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
Ak
C H O S N P Cl Br F I Si
OK
Cancel
Formula is not available

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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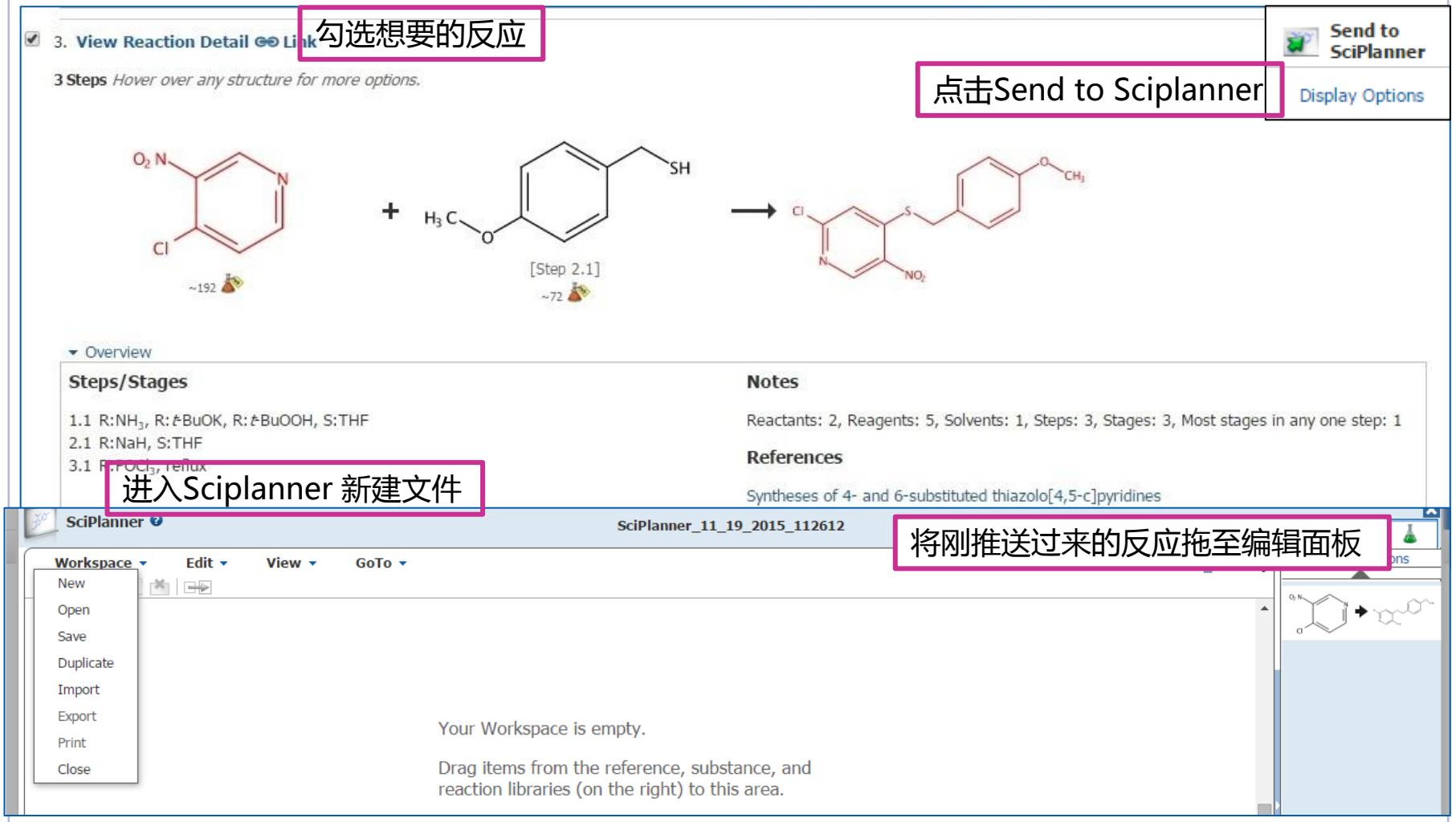
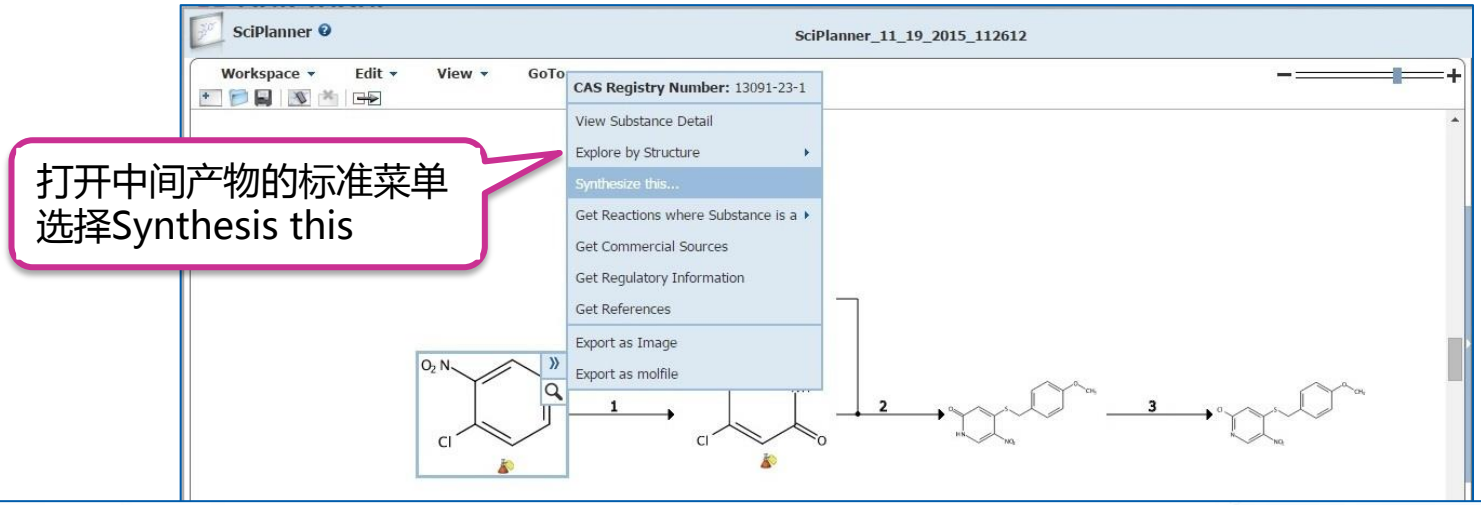
提纲

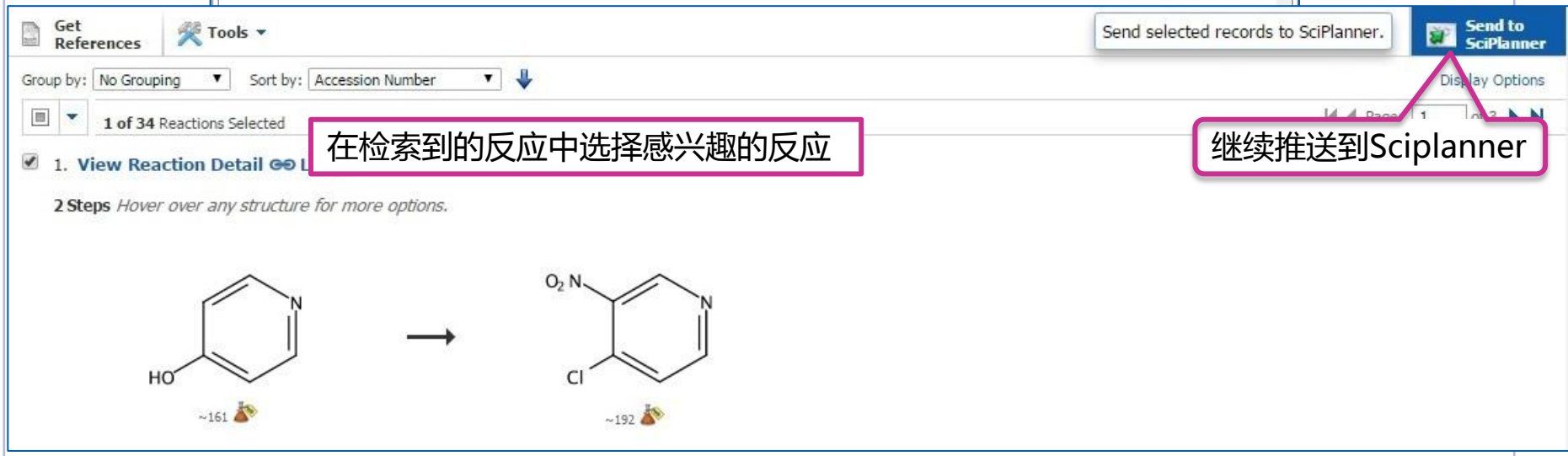
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索
  - SciPlanner
- SciFinder常见问题及解决

SciPlanner使用简介

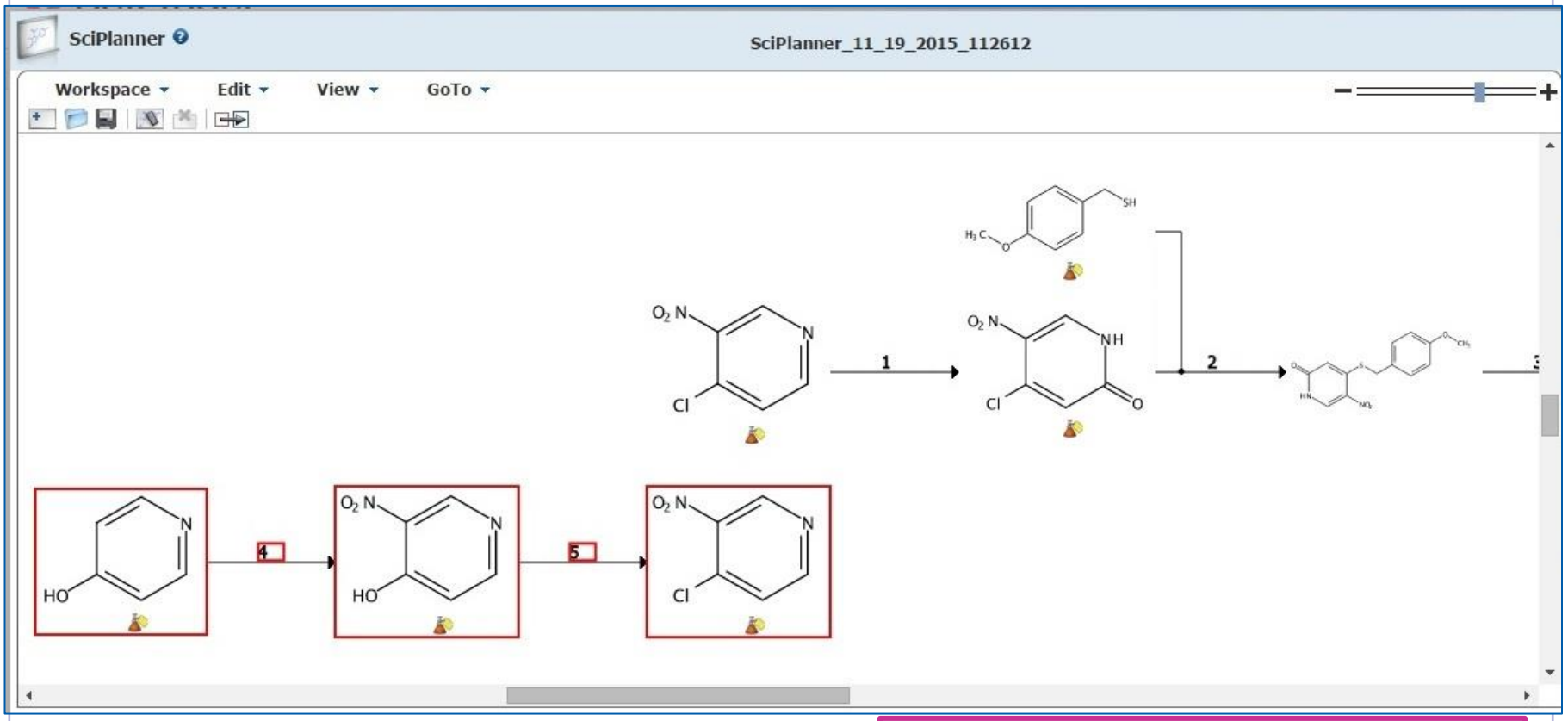


SciPlanner使用简介



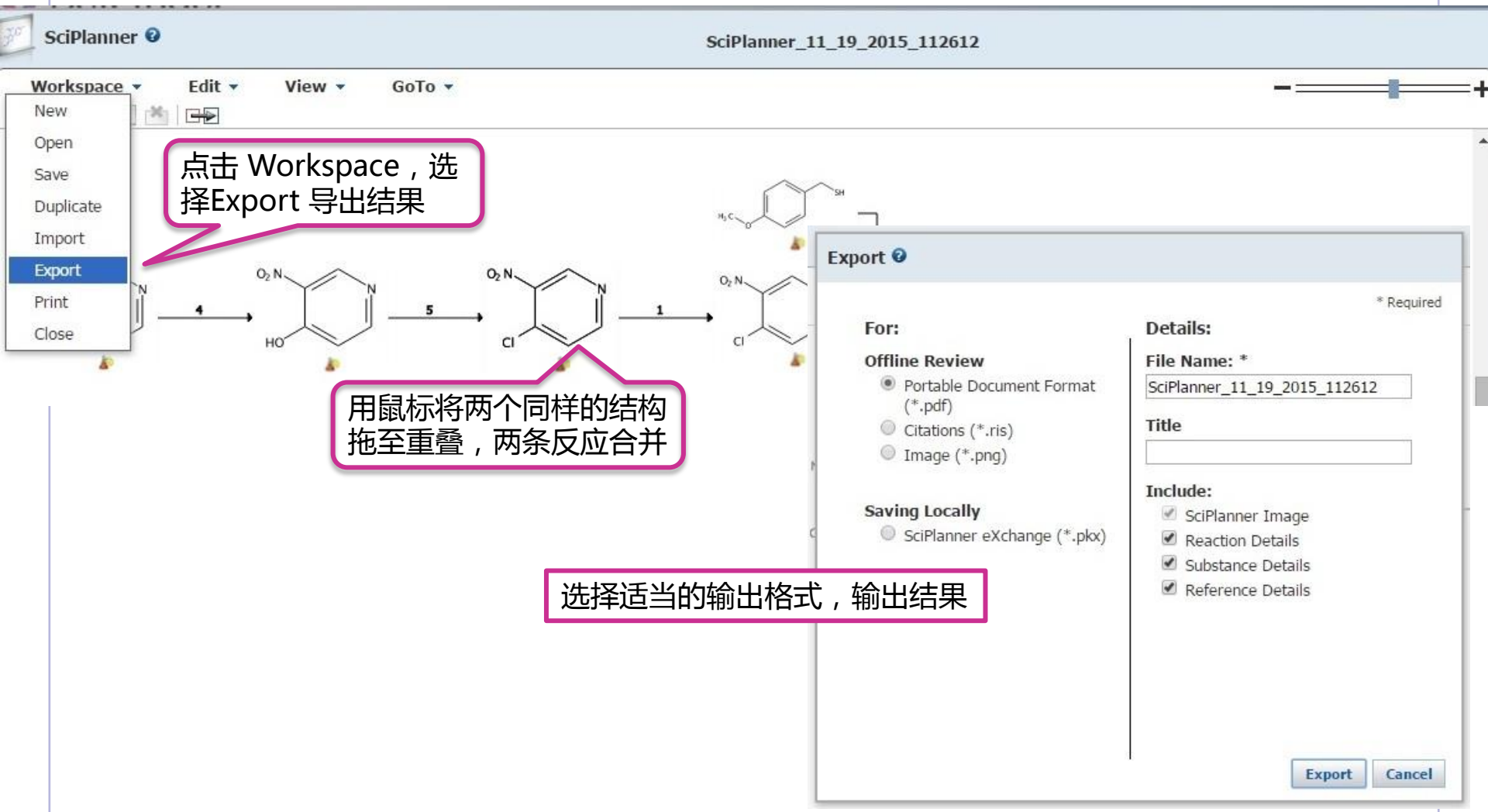


SciPlanner使用简介



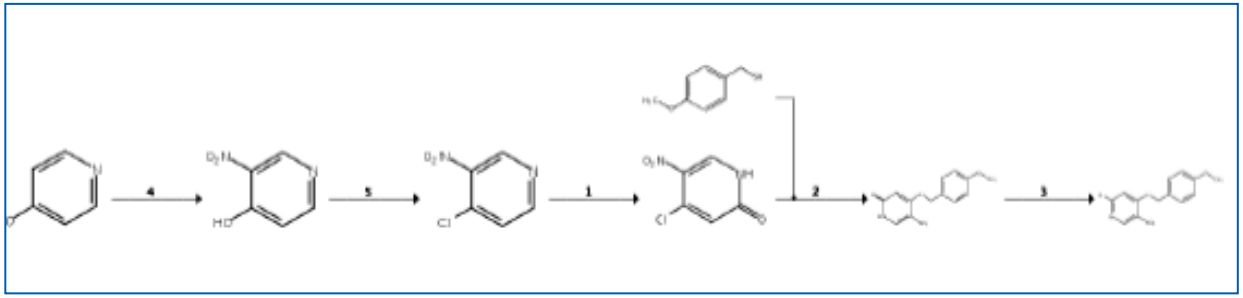
步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介



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	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	

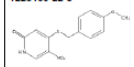
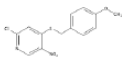
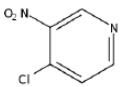
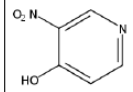
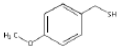
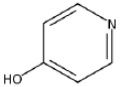
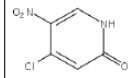
References

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
  - SciPlanner
- SciFinder常见问题及解决

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

如何获取SciFinder账号

点击注册链接，按照要求提交信息

https://scifinder.cas.org/registration/index.html?corpKey=50B8E71AX86F3503FX3002D4D11EB02026EA

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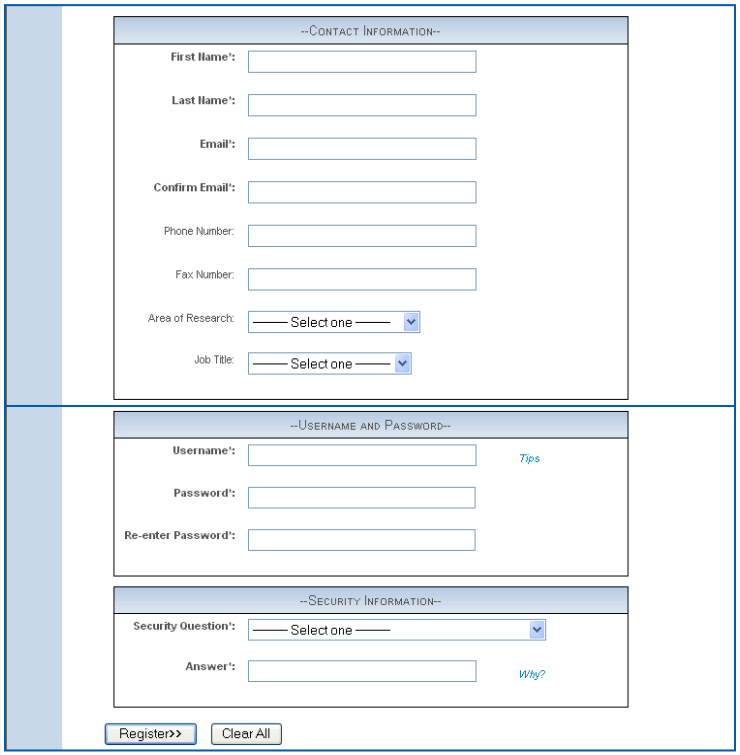
如何获取SciFinder账号



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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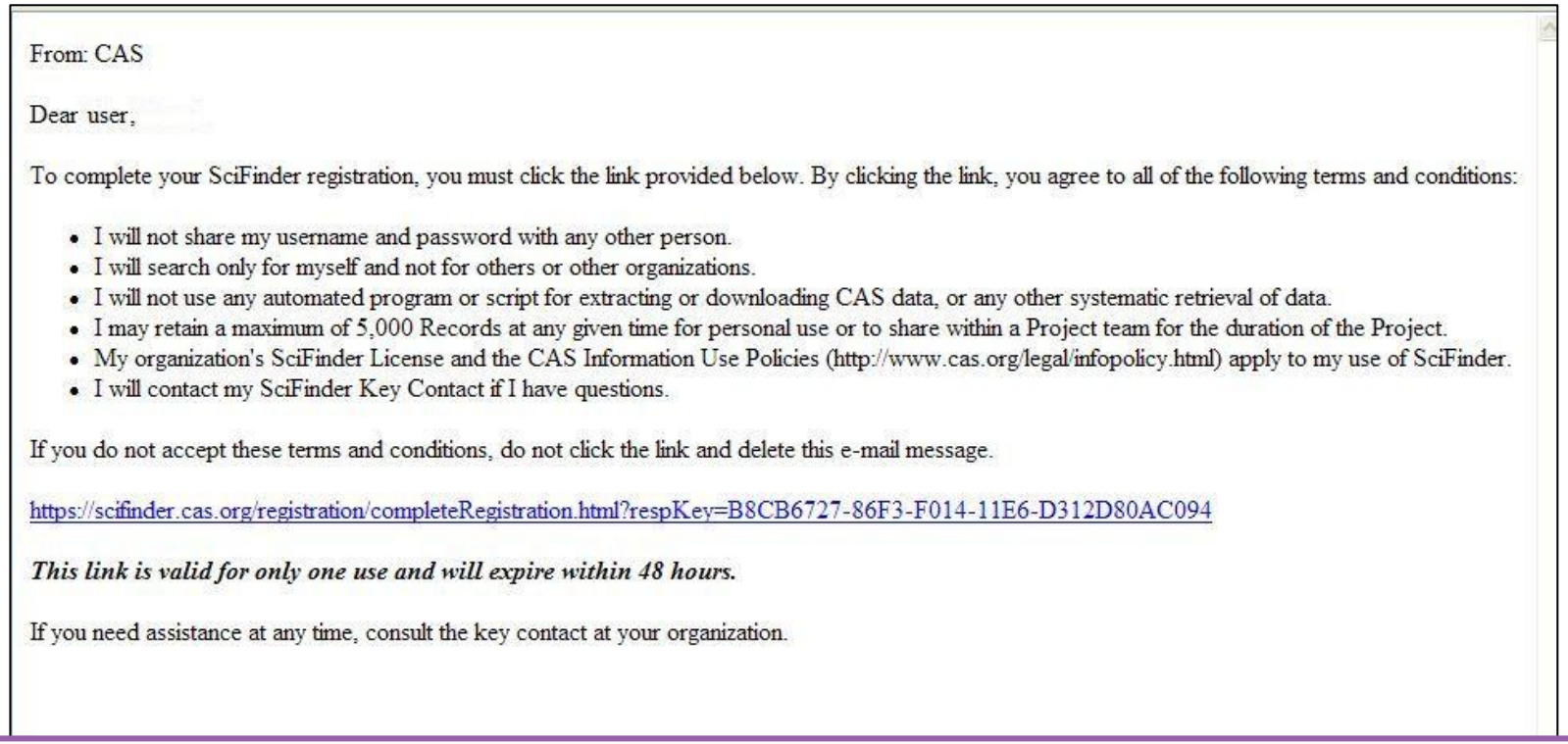

From: CAS

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