钱欣博士
Application Specialist
cqian@acsi.info

如何使用SciFinder获取科技信息

2016年10月27日

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
  - 反应检索
  - 聚合物检索
- SciFinder常见问题及解决

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美国化学文摘社—Chemical Abstracts Service

- ACS的分支机构，愿景：运用化学的力量改善人们的生活
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 全面收集、文摘、标引全球化学相关文献
- 总部位于美国俄亥俄州哥伦布市
- 超过1,400名员工
- 精通50多种语言的科学家

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

J|A|C|S JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical Neuroscience

Cornell University Library

THE JOURNAL OF PHYSICAL CHEMISTRY Letters

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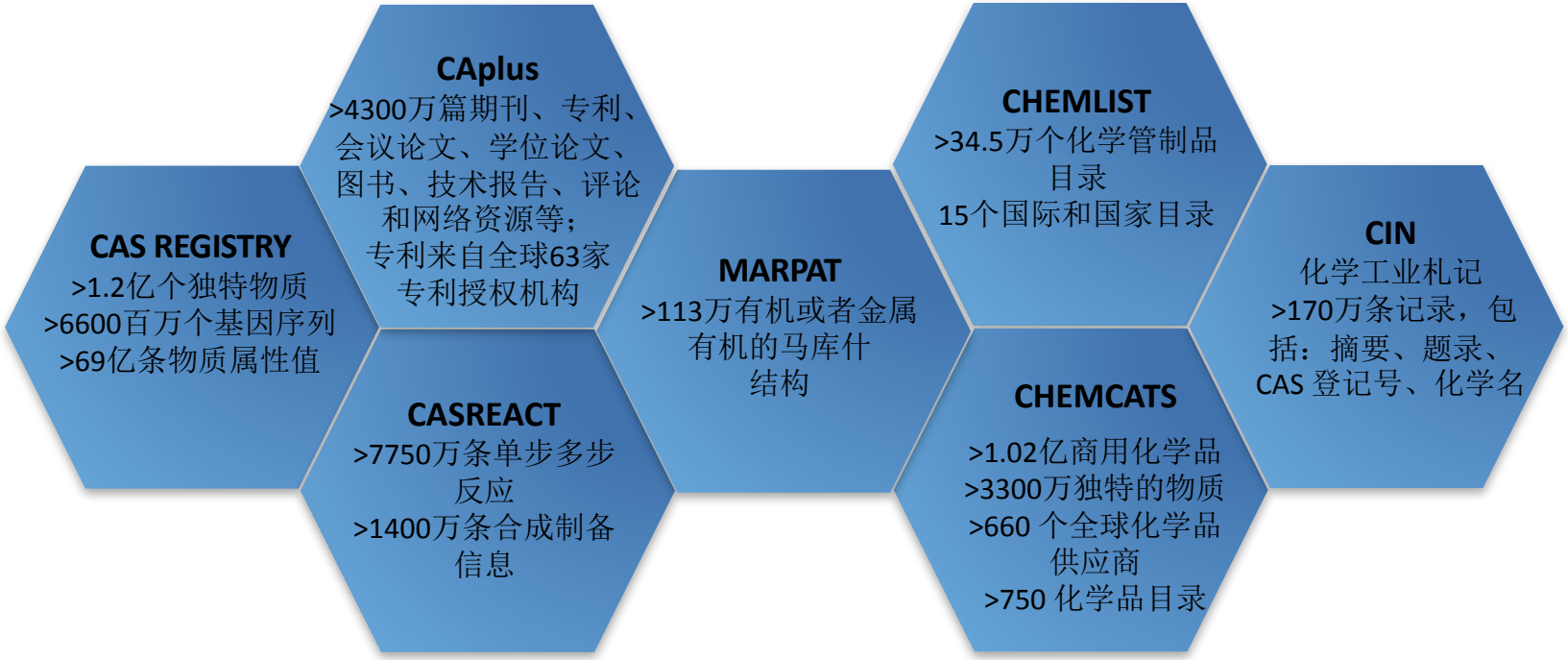
CAS——构建最高质量的化学数据库



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CAS解决方案——加速科学探索的步伐

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CAS数据库——源于化学，超越化学

- **生物化学：**
  - 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学
- **有机化学各领域：**
  - 氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇
- **大分子化学各领域：**
  - 纤维素、木质素、造纸、涂料、墨水
  - 染料、有机颜料、合成橡胶、纺织品、纤维
- **应用化学各领域 ：**
  - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- **物理、无机、分析化学各领域：**
  - 表面化学、催化剂、相平衡、核现象、电化学

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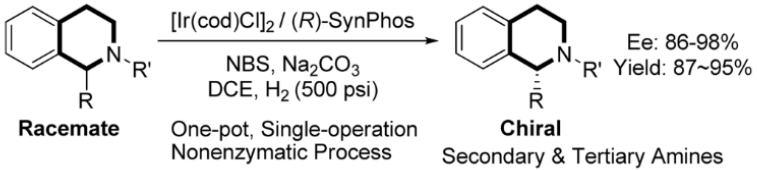
CAS数据库最具价值的内容——人工标引

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

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

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



Indexing

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

Concepts

Enantioselective synthesis
Hydrogenation catalysts
Oxidation

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

Chiral ligands

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

Catalyst use; Uses

Substances

12112-67-3 Dichlorobis(cyclooctadiene)diiridium
76189-55-4
133545-16-1
445467-61-8
503538-68-9 (S)-SynPhos
503538-69-0

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

Journal of the American Chemical Society
Volume137
Issue33
Pages10496-10499
Journal; Online Computer File
2015
CODEN:JACSAT
ISSN:0002-7863
DOI:10.1021/jacs.5b06659

COMPANY/ORGANIZATION

State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics
Chinese Academy of Sciences
Dalian, Peop. Rep. China
116023

ACCESSION NUMBER

2015:1340032

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

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CAS人工标引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好地解决了该问题，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

- 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
  - 设计合成路线——SciPlanner使用简介
- SciFinder常见问题及解决

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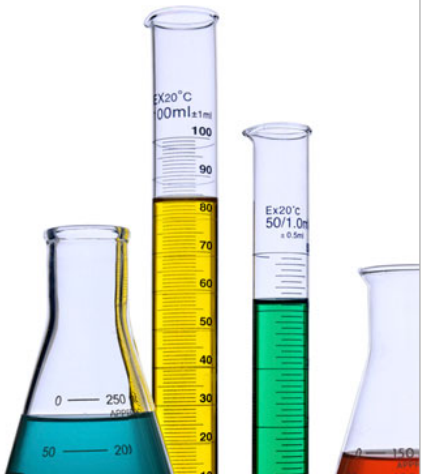

News & Updates

Welcome to SciFinder

Did you notice our new look?
Our new branding will also be phased into training and other support materials in the coming months. If you are a Key Contact and have questions, or need assistance updating logos on any of your organization's websites, please contact the CAS Customer Center.

Apply for the 2016 SciFinder Future Leaders Program!
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A New Way to Explore Synthetic Preparations in SciFinder!

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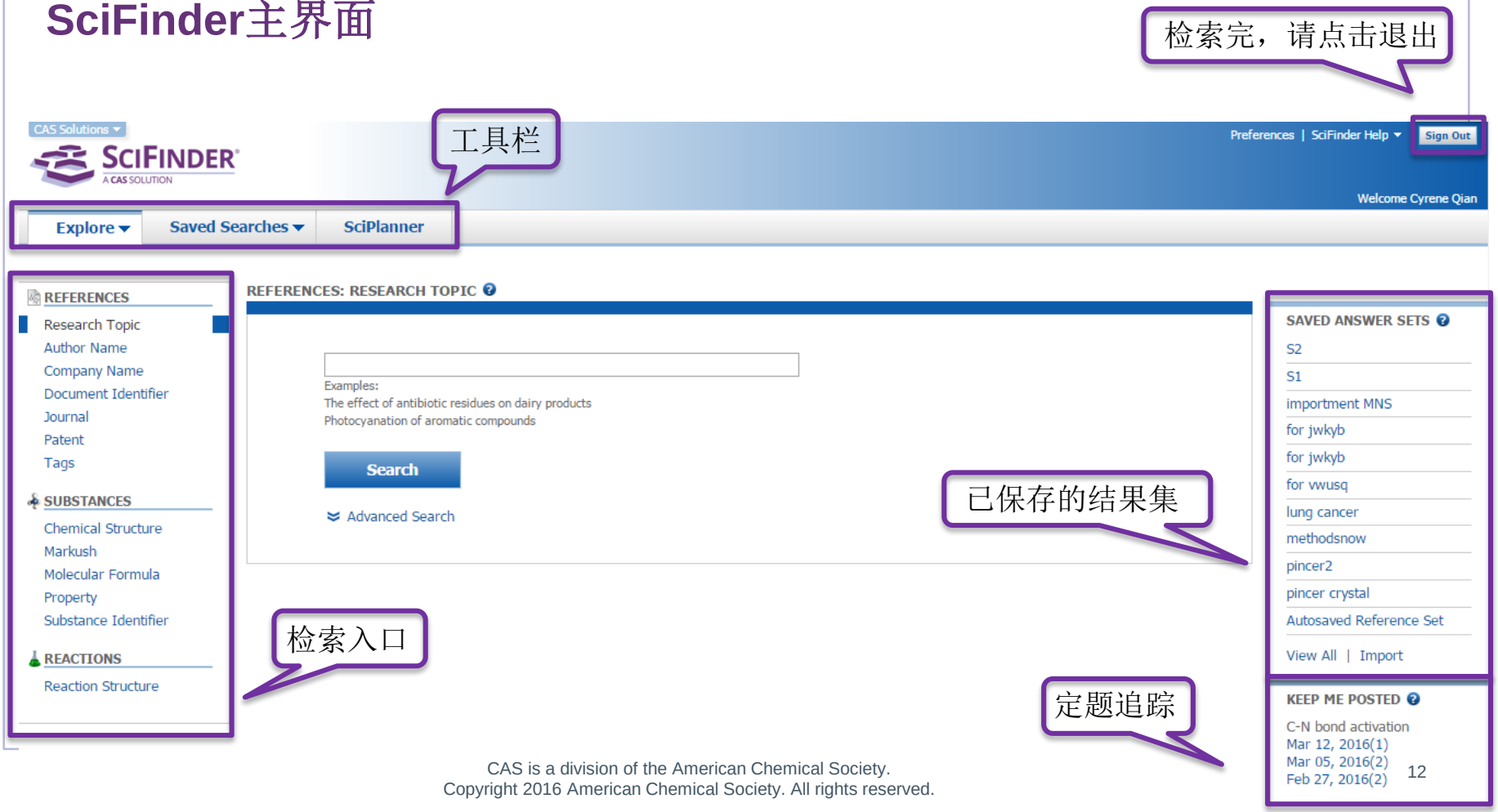
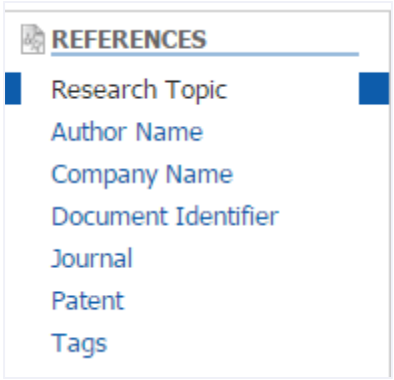
SciFinder主界面



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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以“OLED发光材料”为例：

- 如何快速了解到领域研究动态
- 如何查找到分析化学的相关文献
- 如何获得光谱学/电子传输的相关文献
- 如何通过PatentPak快速获得发光材料的专利信息

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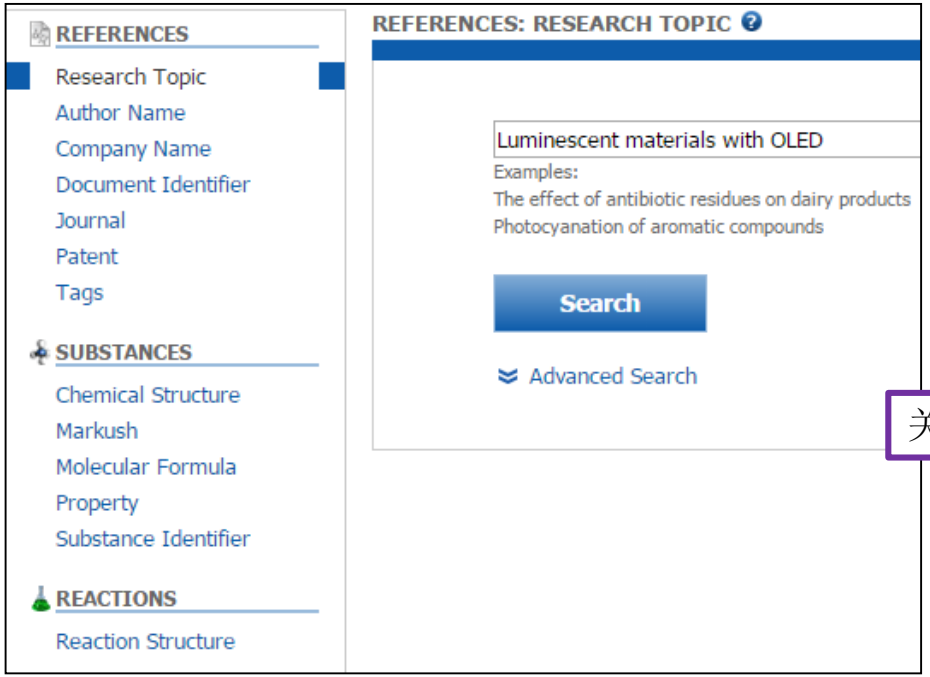
文献检索——主题: OLED发光材料

- 检索式： Luminescent materials with OLED



关键词之间可用介词连接：in, with, of…

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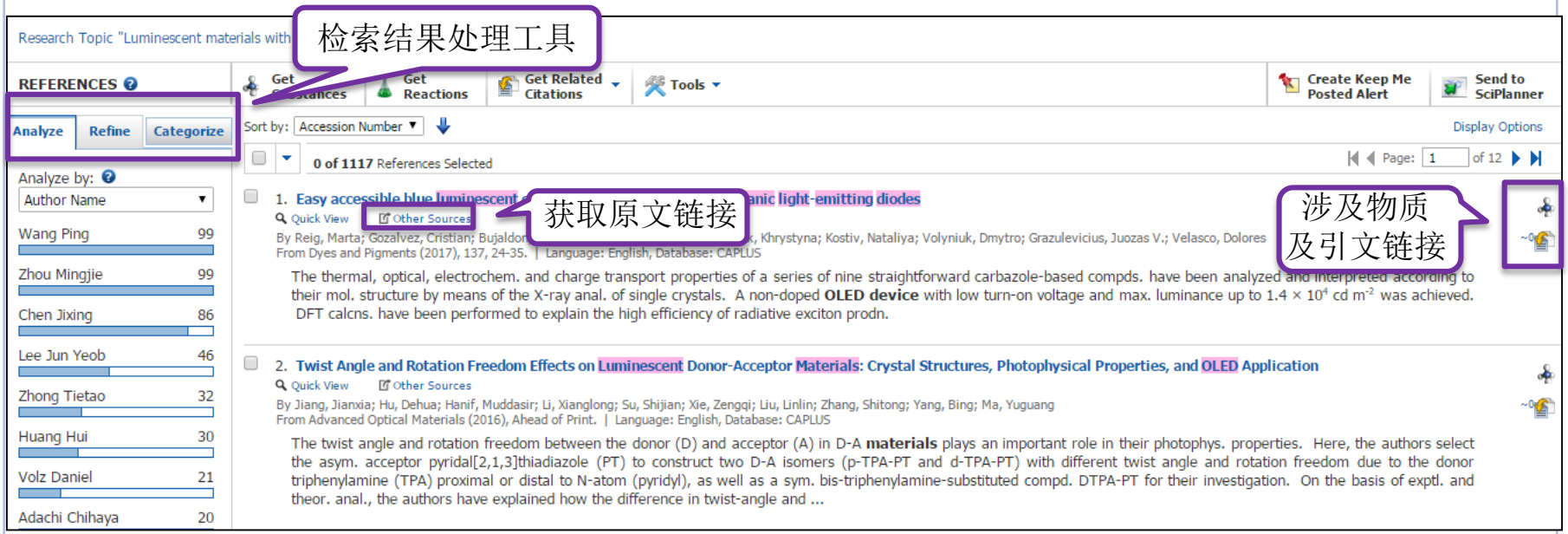
文献检索结果



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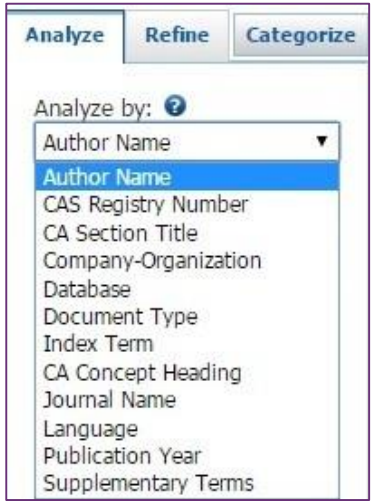
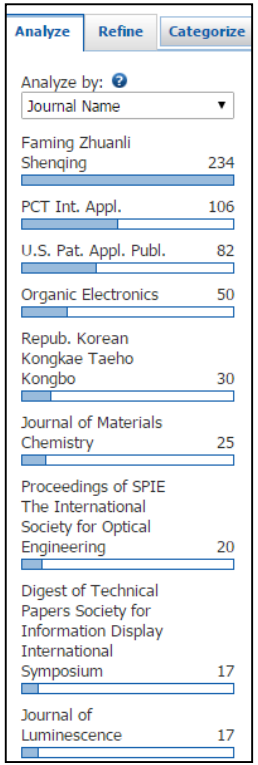
文献检索结果：Analyze

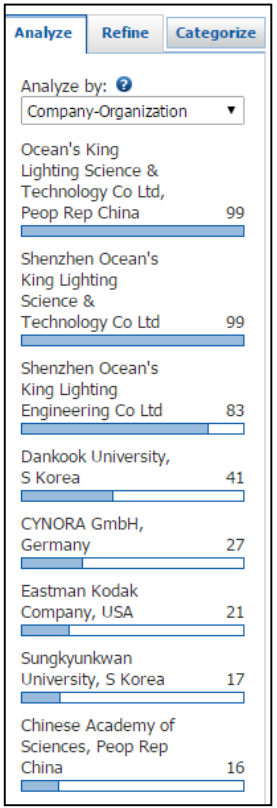
12种文献分析选项



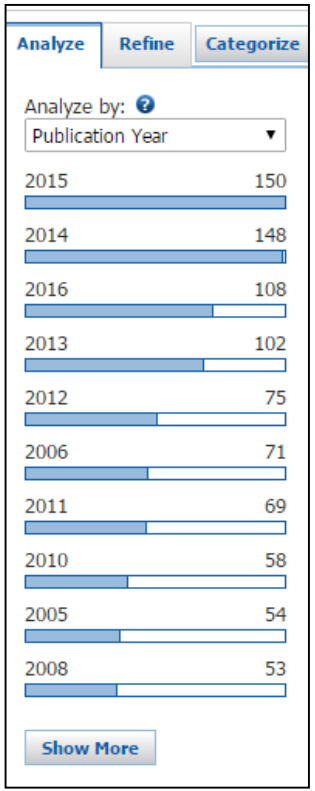
成果披露媒介



主要研究机构，
合作伙伴，竞争对手



年度发表数量



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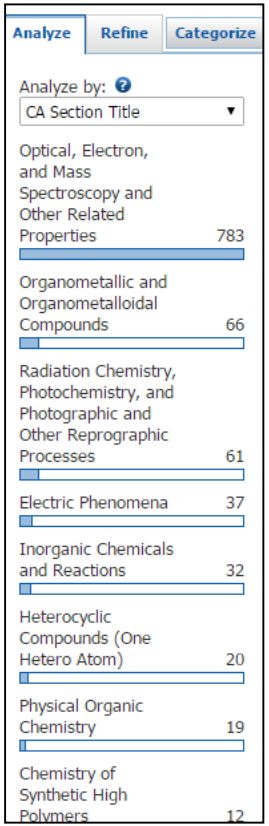
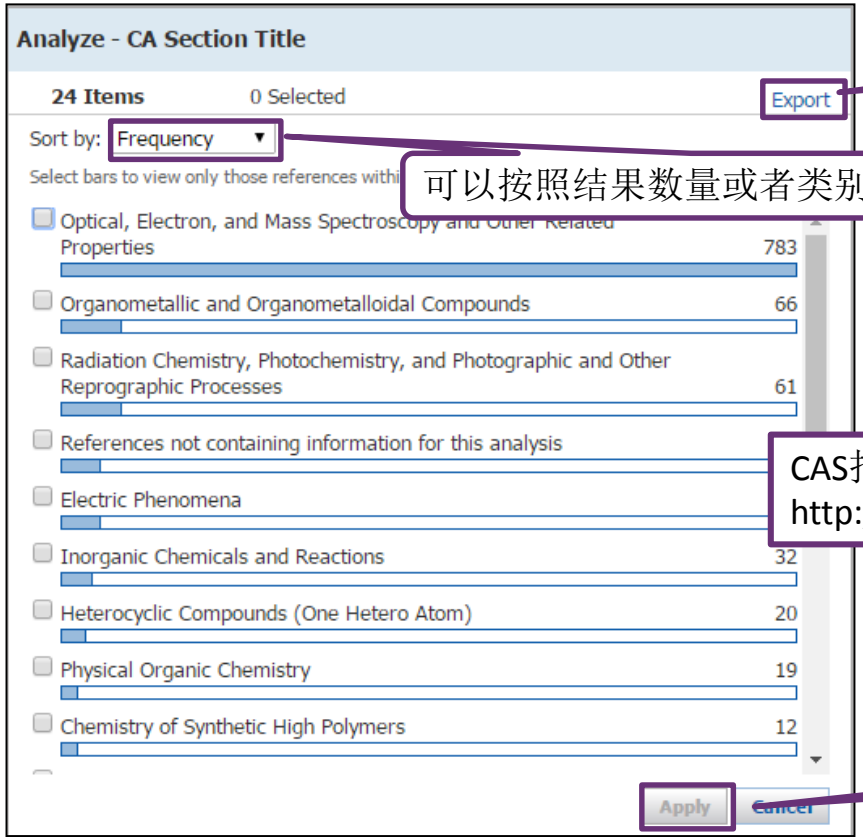
文献检索结果：Analyze





可以将分析结果导出xls文件

可以按照结果数量或者类别字母顺序排序

CAS把收录的信息分为5个大类80个小类:
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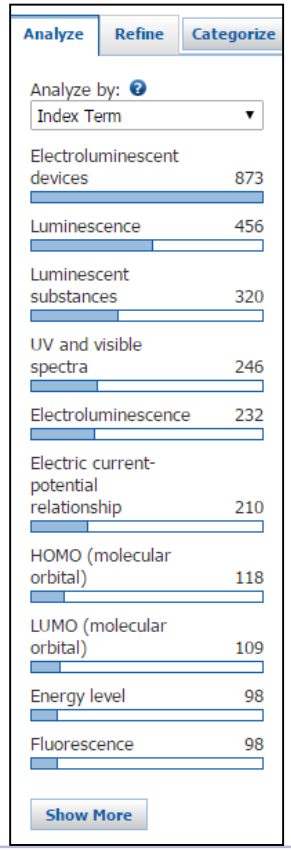
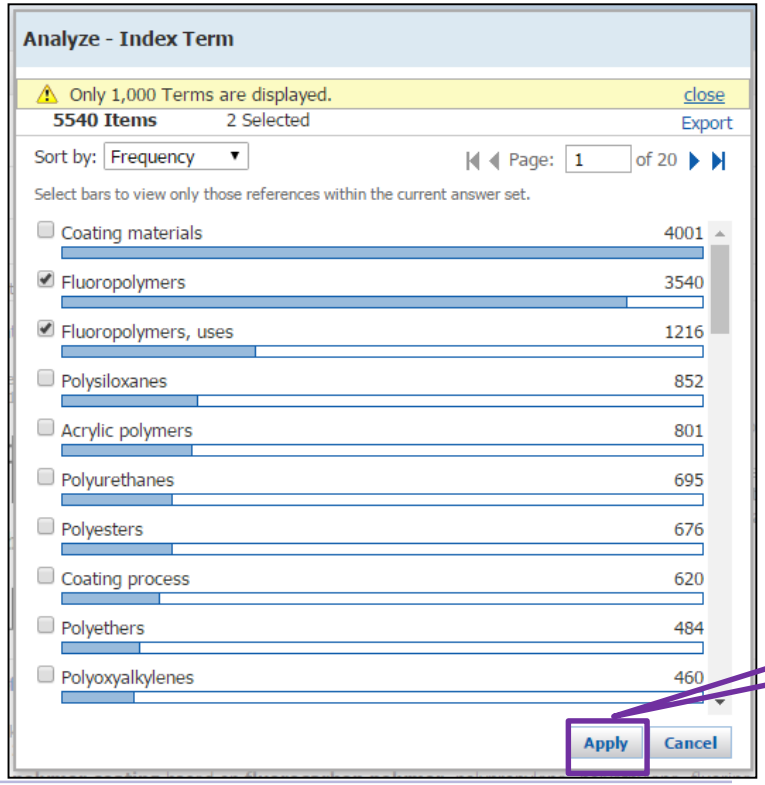
文献检索结果：Analyze



Index Term:帮助用户全景了解本领域涉及的重要技术术语，精选文献



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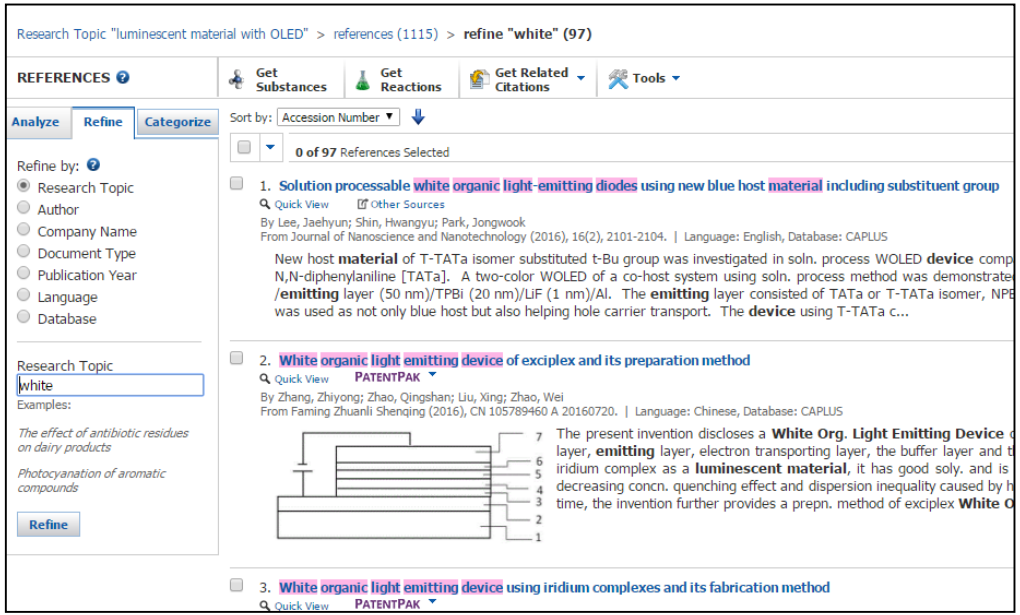
文献检索结果：Refine

- 七种限定选项，包括主题词、作者姓名、机构名称、出版年代、语言、所属数据库



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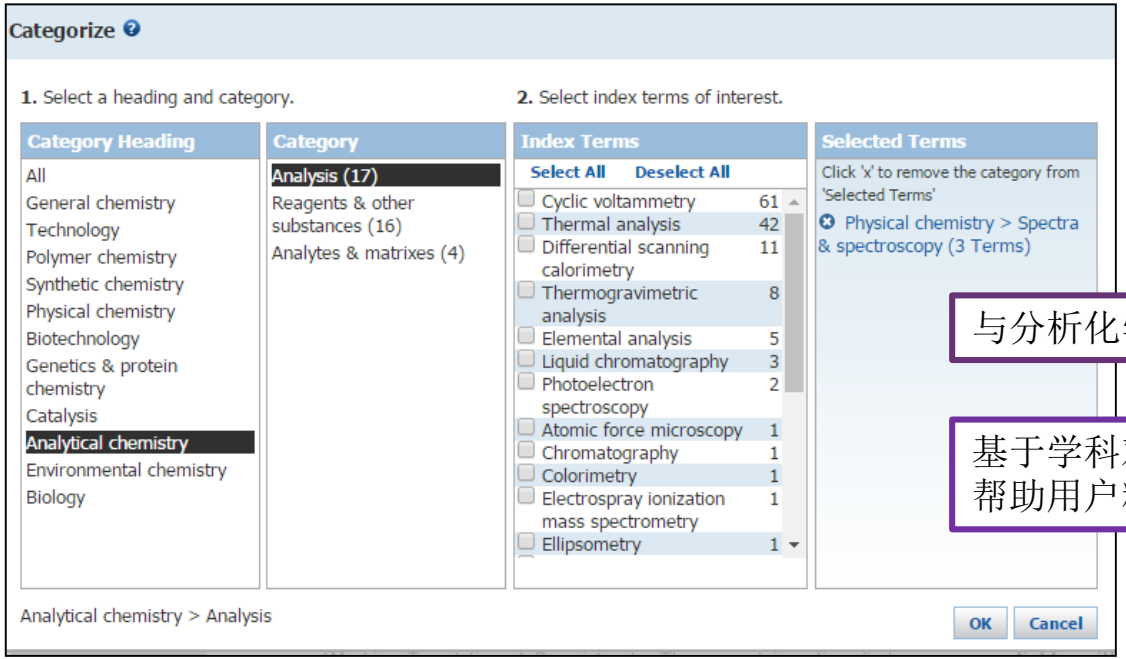
文献检索结果：Categorize

学科主分类

学科副分类

学科副分类涉及的
重要技术术语/物质



与分析化学相关的文献

基于学科对文献进行自动分类，
帮助用户精准定位所关注的学科和技术术语

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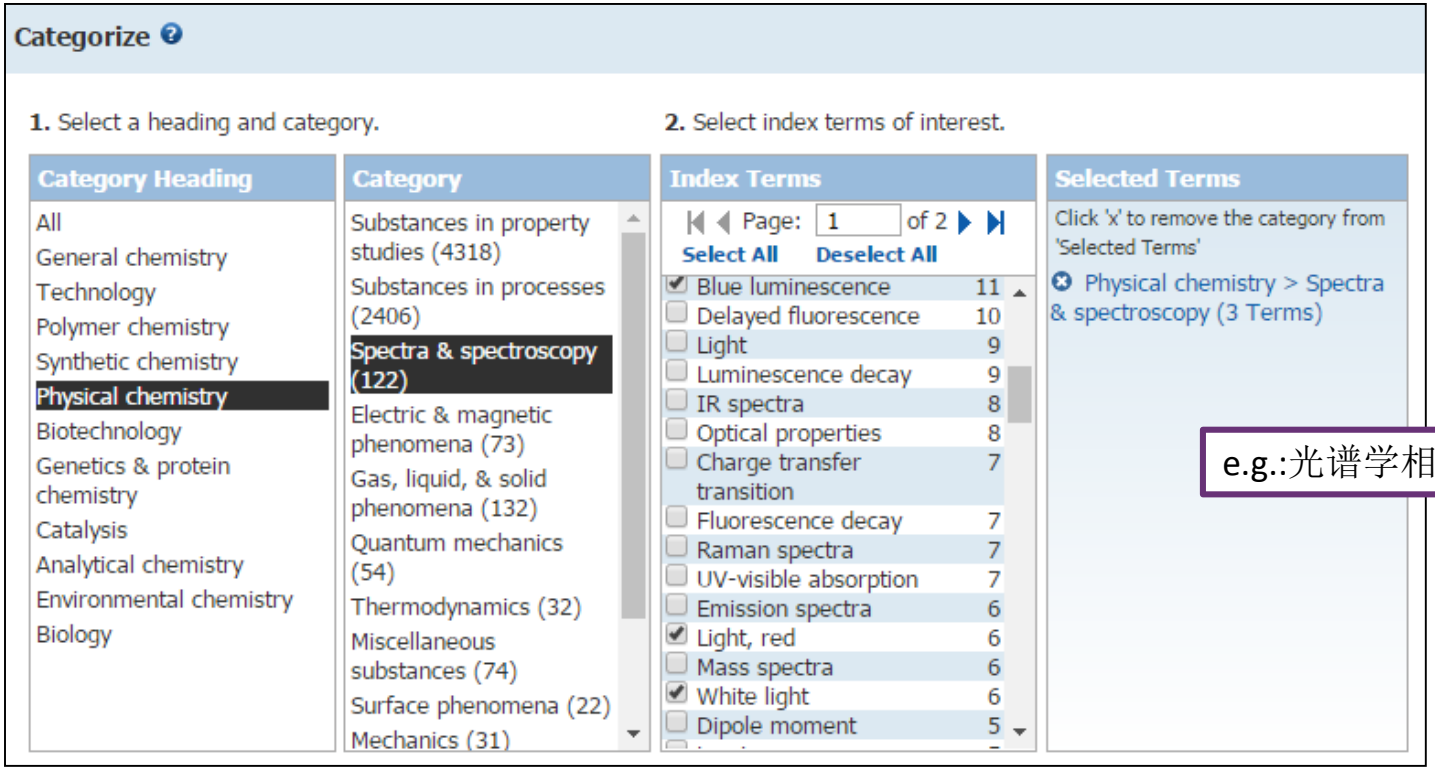
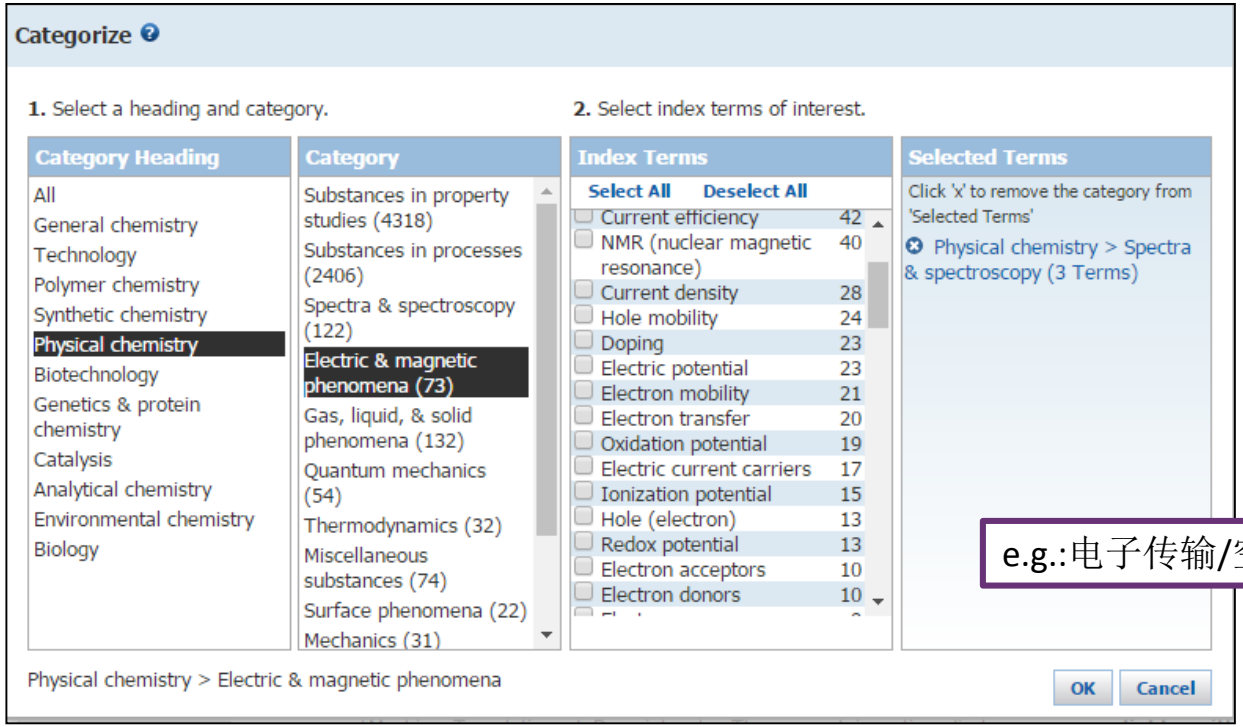
文献检索结果：Categorize



e.g.:光谱学相关的文献

文献检索结果：Categorize



e.g.:电子传输/空穴传输相关的文献

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在各种专利检索工具中，PatentPak™是唯一提供快速定位物质相关化学信息的工具

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  - 新的专利文件每日上传更新
- **通过PatentPak 浏览器，快速定位专利PDF文件中的重要物质页码信息，迅速找到难以查找的化学信息**
- **在CAS专利族文献中找到你所熟悉语言的专利**

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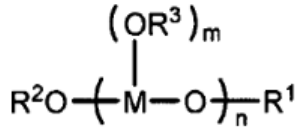
17. **Compound, desiccant, sealing structure and organic electroluminescent element**

Quick View PATENTPAK

By Hoshina, Yusuke; Takakura, Yoshie
From Ger. Offen. (**2015**), DE 102015209342 A1 20151126. | Language: German, Database: CAPLUS



(1)

A compd. represented by the formula $R^2O(M(OR^3)_mO)_nR^1$ (wherein M represents an aluminum atom, a titanium atom, a silicon atom or a boron atom; m represents 1 or 2; n is a pos. integer; R^1, R^2 and R^3 each independently represent a C_{1-16} alkyl group which is optionally substituted with one or more fluorine atoms, or a C_{2-17} acyl group which is optionally substituted with one or more fluorine atoms, represent, and when a plurality of R^3 are present, the plurality of R^3 may be the same or different from each other) is described for uses as a desiccant in top-emission type org. electroluminescent el...

18. **Organic compounds and composition, and organic optoele… …ristics employing the organic compounds as electroluminescent hosts**

Quick View PATENTPAK

By Lee, Han-Ill; Si… …lin, Soo-Hyun; Yu, Eun-Sun; Jung, Ho-Kuk
From Eur. Pat. Ap… …ge: English, Database: CAPLUS

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Patent No.	Kind	Language
EP 2947071	A1	English
Patent Family		
KR 2015133566	A	Korean
US 20150340626	A1	English
JP 2015218165	A	Japanese
CN 105085412	A	Chinese

…d are org. compd. represented by Formula (I), where X, L^{1-6}, R^{1-22}, and n1-4 are described in the detailed description; a … for an org. optoelec. device including the org. compd., an org. optoelec. device including the org. compd. or the compn., and … y device including the org. optoelec. device. Thus, org. electroluminescent devices with remarkably improves luminous … y and life-span characteristics were fabricated using the org. compds. as electroluminescent hosts.

19. **Condensed cyclic compounds with excellent elec. characteristics and thermal stability, and organic light-emitting devices including the compounds in emitting or electron-transporting layer**

Quick View PATENTPAK

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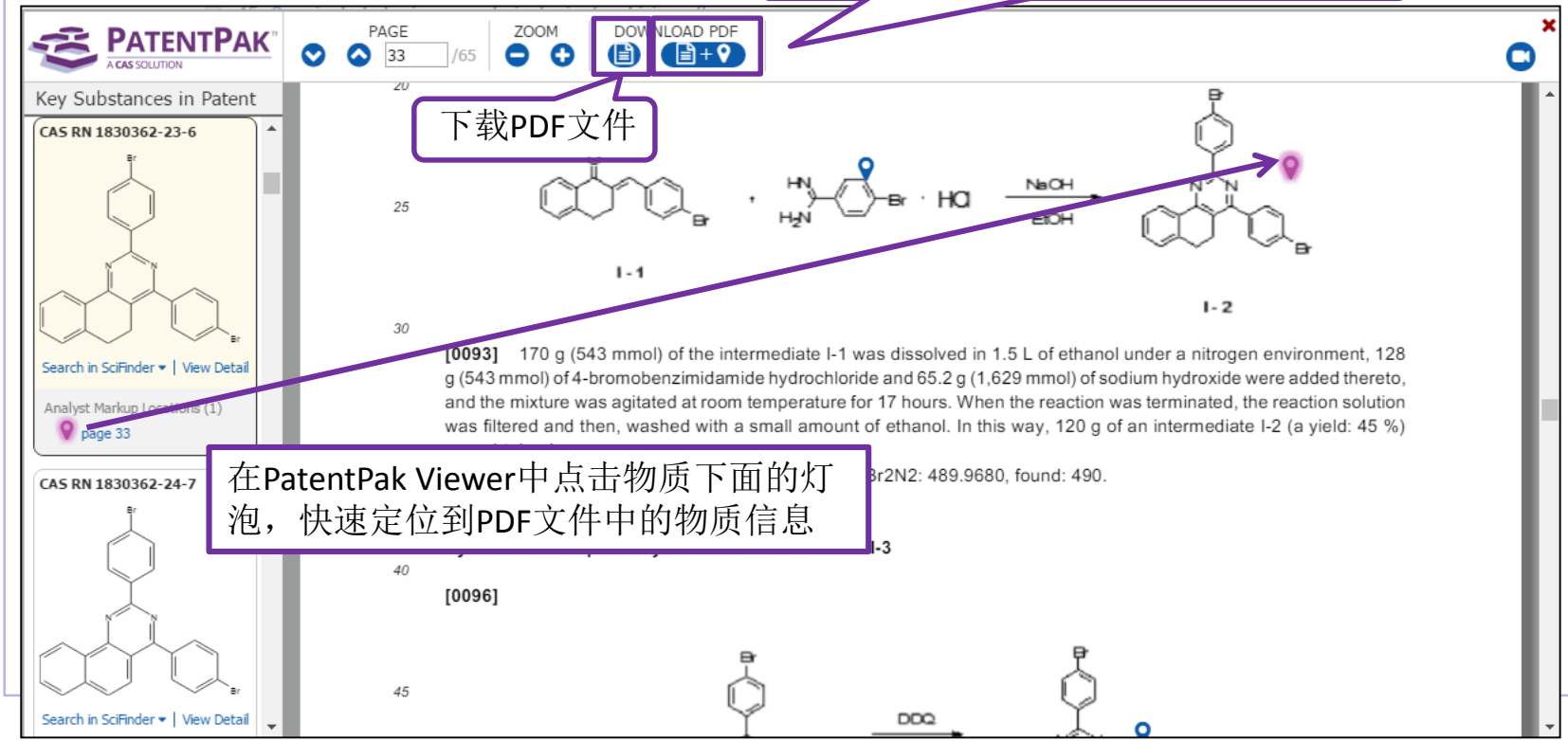
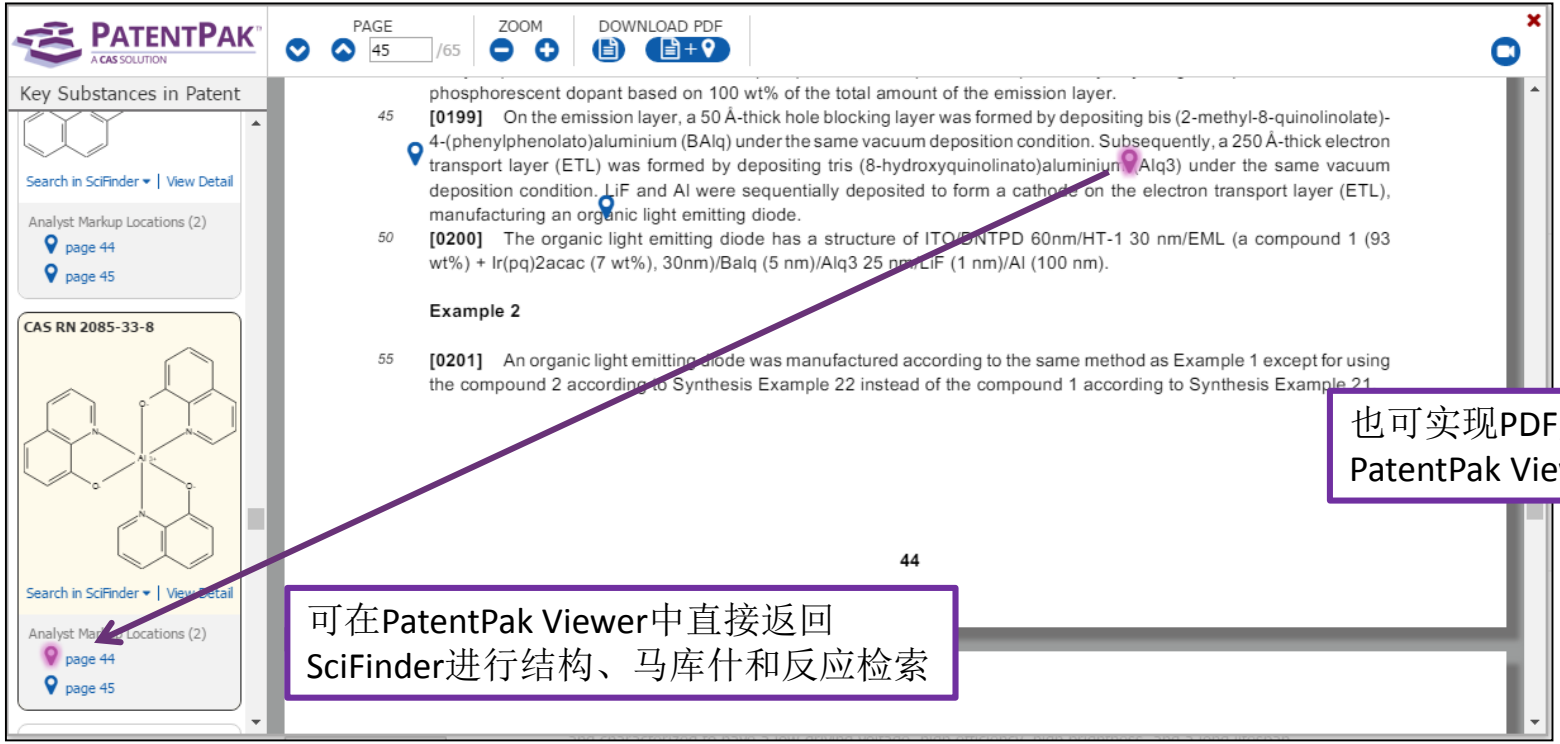


PatentPak——专利工作流程解决方案



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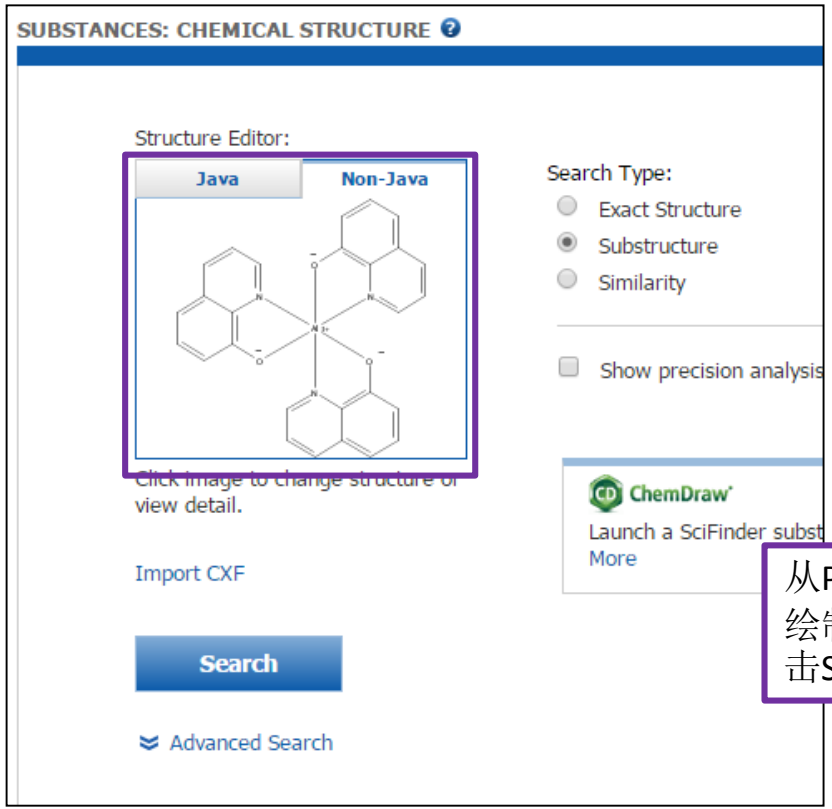
PatentPak——专利工作流程解决方案



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

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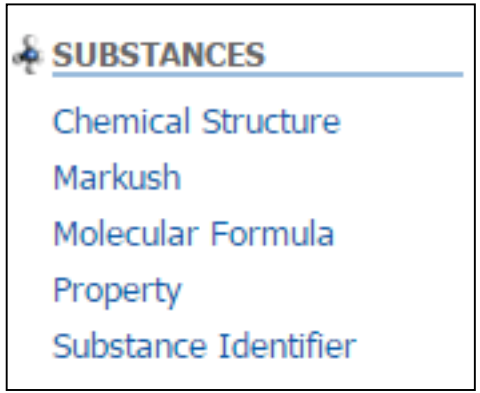
SciFinder检索选项——物质检索

- 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
  - 有机物化合物、天然产物：结构检索
  - 无机化合物、合金：分子式检索
  - 高分子化合物：分子式检索和结构检索



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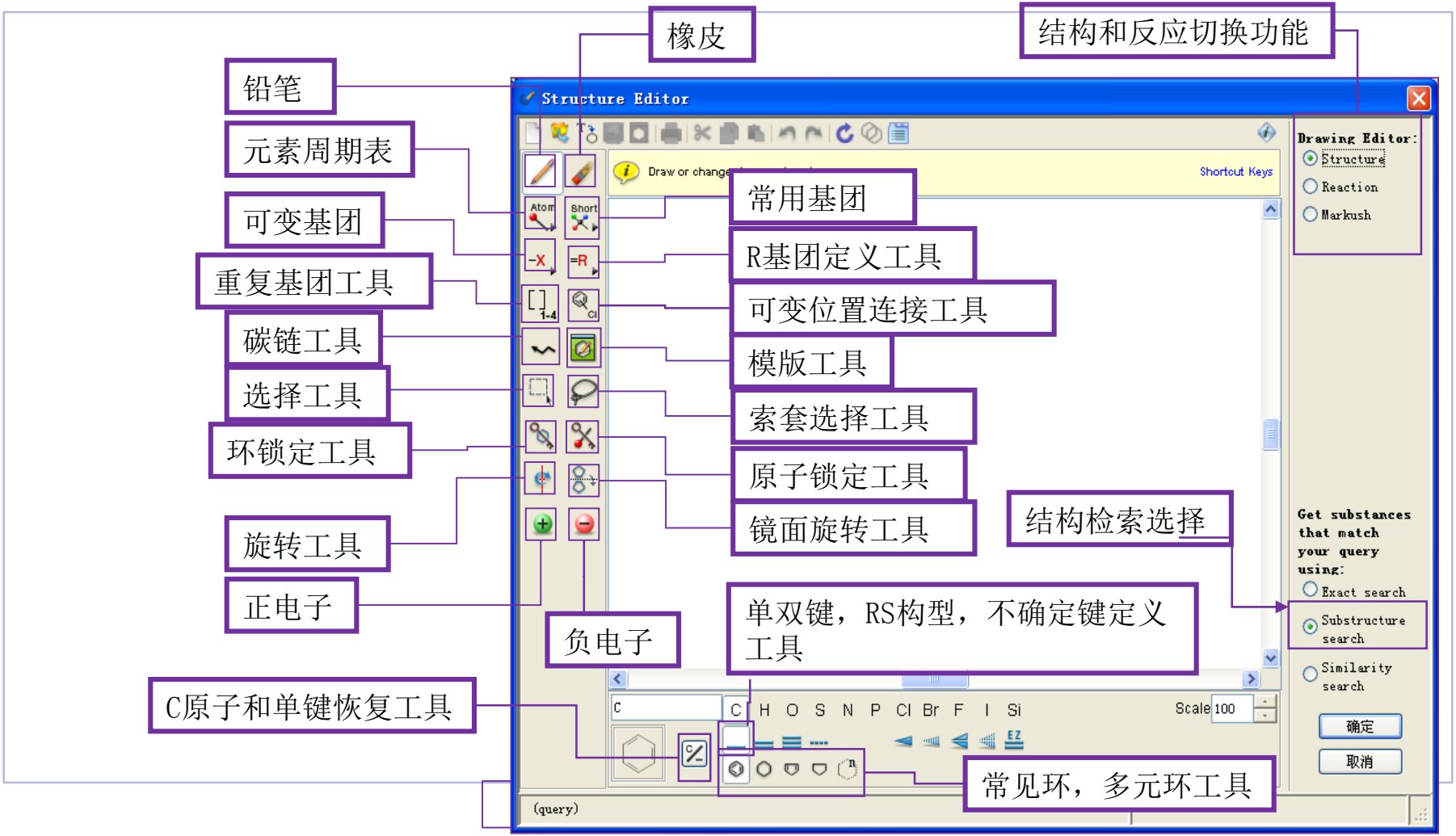
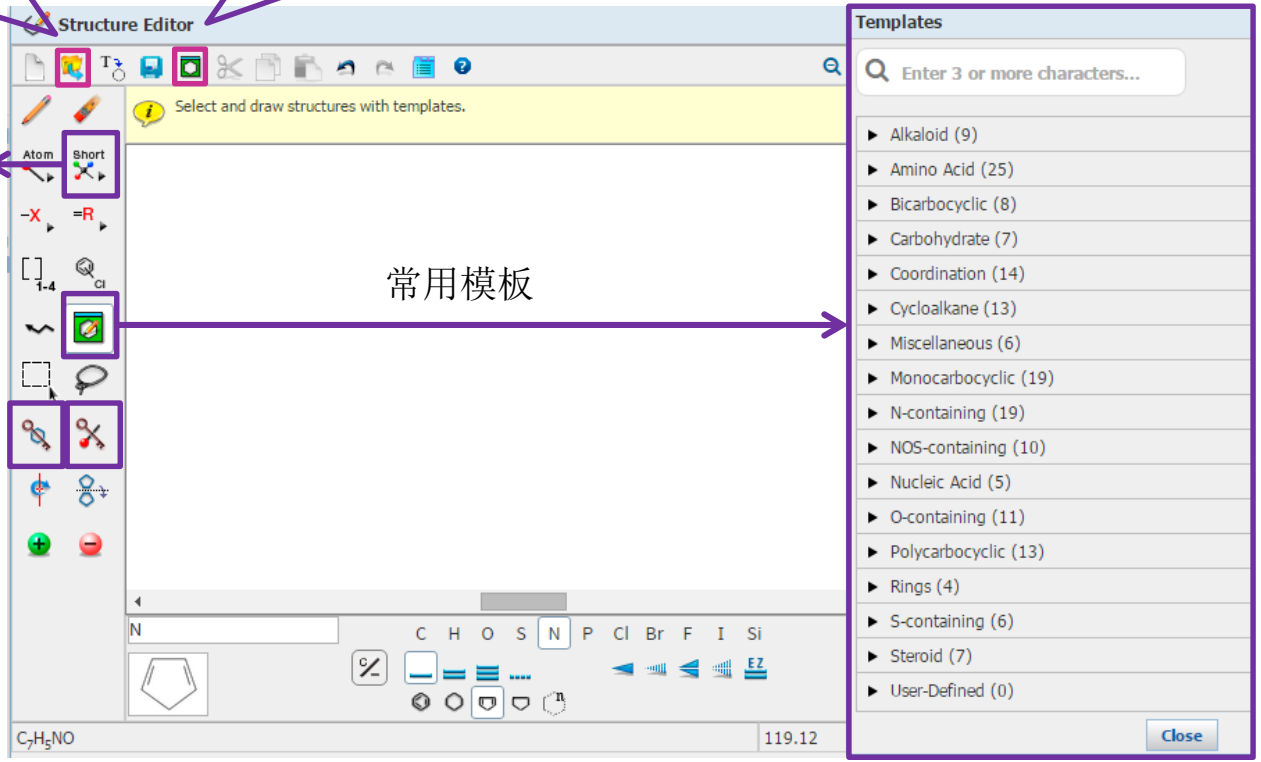
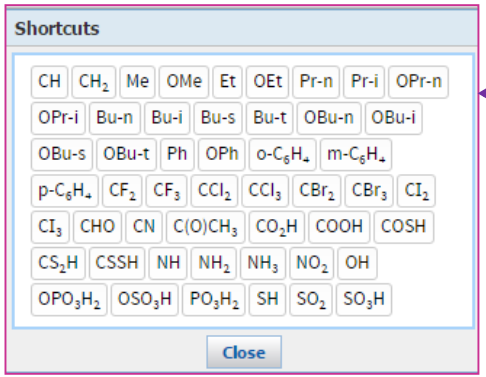

橡皮
结构和反应切换功能
铅笔
元素周期表
可变基团
重复基团工具
碳链工具
选择工具
环锁定工具
旋转工具
正电子
C原子和单键恢复工具
常用基团
R基团定义工具
可变位置连接工具
模版工具
索套选择工具
原子锁定工具
镜面旋转工具
结构检索选择
负电子
单双键，RS构型，不确定键定义工具
常见环，多元环工具
Structure Editor
Drawing Editor:
Structure
Reaction
Markush
Shortcut Keys
Get substances that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
Scale 100
(query)

直接导入已保存的.cxf或者.mol文件

将绘制结构存为模板



常用模板



常用基团

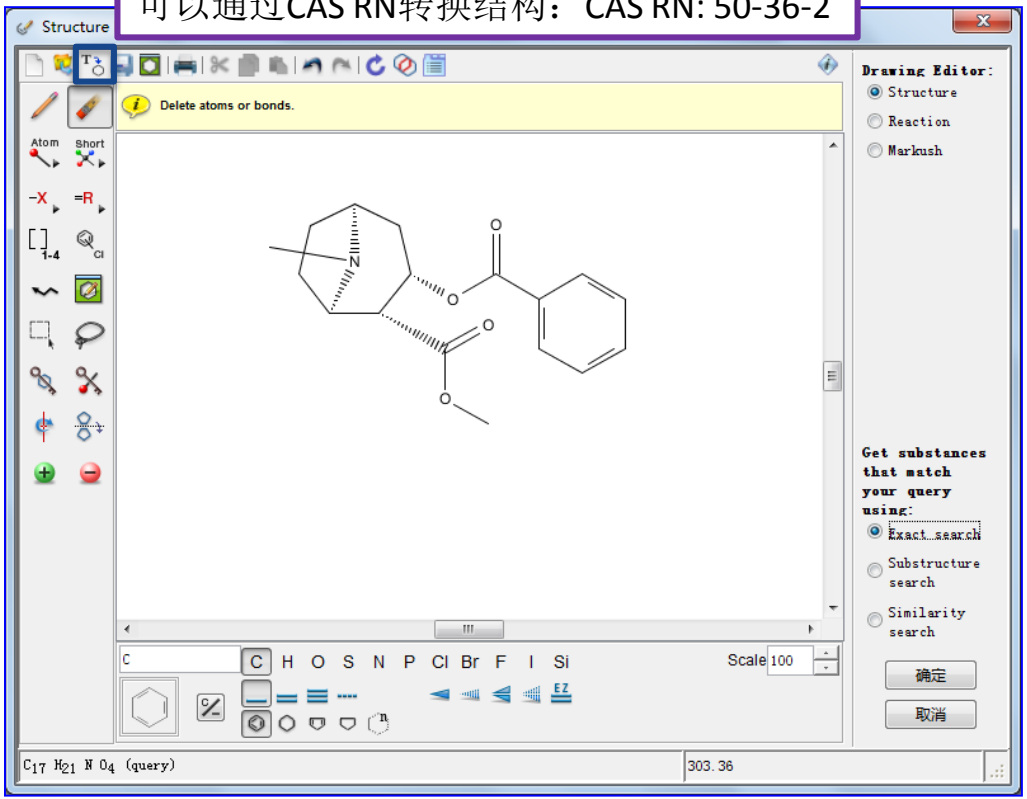
环锁定工具

原子锁定工具

SciFinder® A CAS SOLUTION

物质检索——精确结构检索

可以通过CAS RN转换结构：CAS RN: 50-36-2

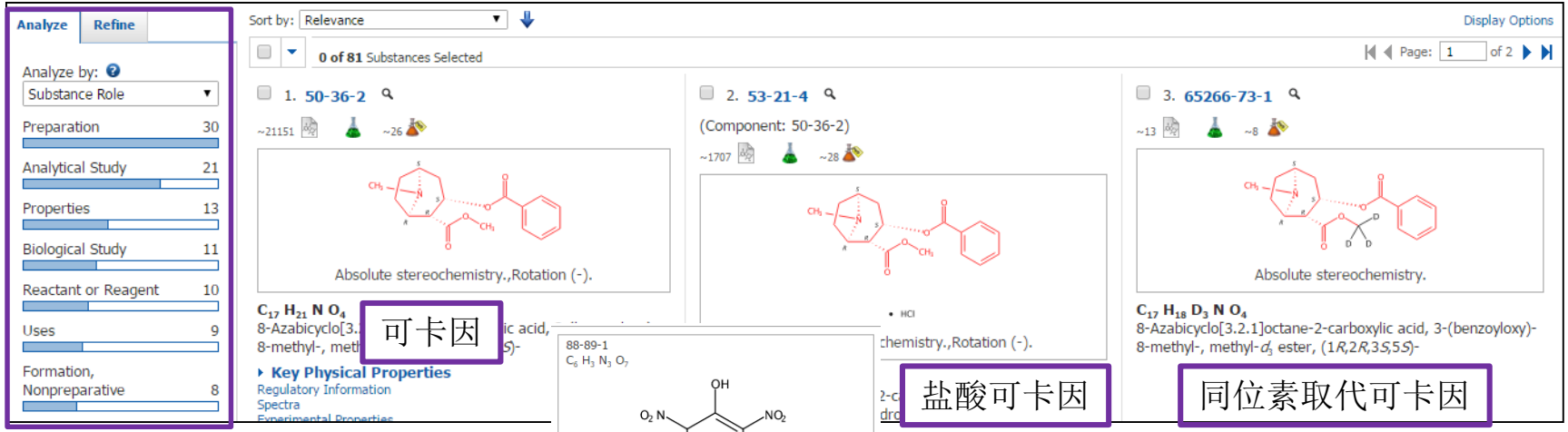


精确结构检索

SciFinder® A CAS SOLUTION

浏览精确结构检索结果

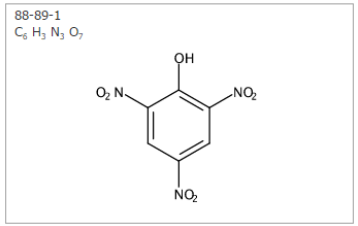
可以通过分析/限定筛选结果集

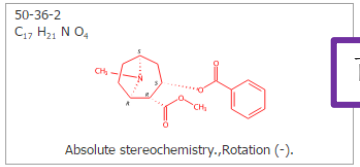


可卡因

盐酸可卡因

同位素取代可卡因





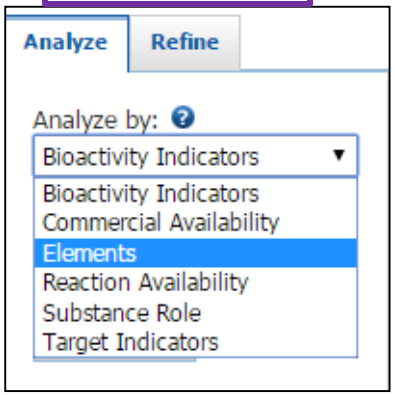
可卡因组合物

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

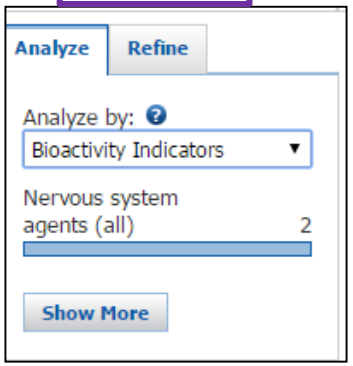
SciFinder® A CAS SOLUTION

物质检索结果——Analyze

六种分析选项

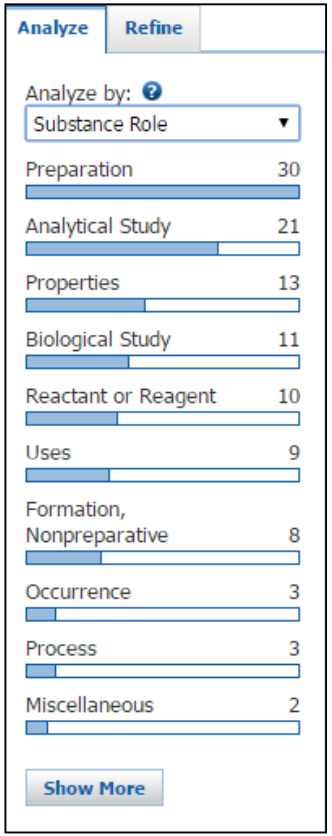


生物活性

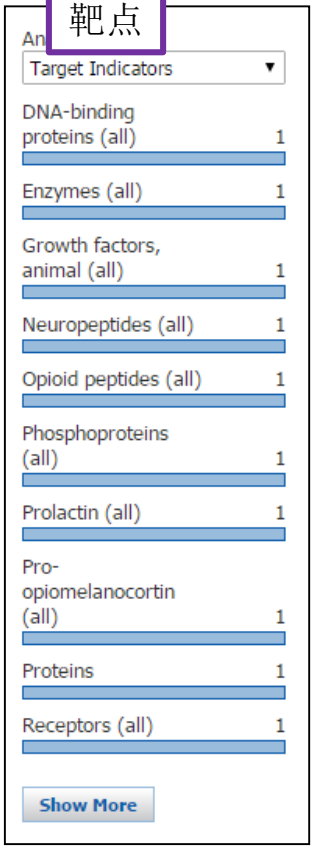


可以按照生物活性，商业可获得性，元素，反应可获得性，物质角色和靶点进行分析

物质角色

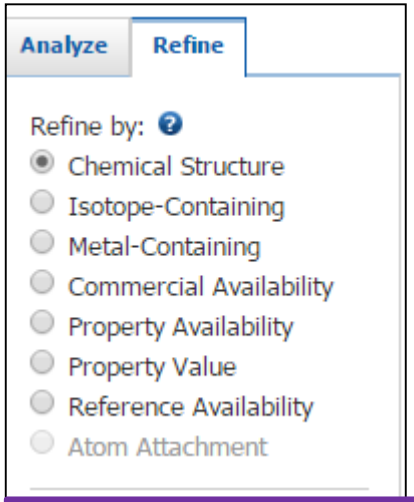


靶点

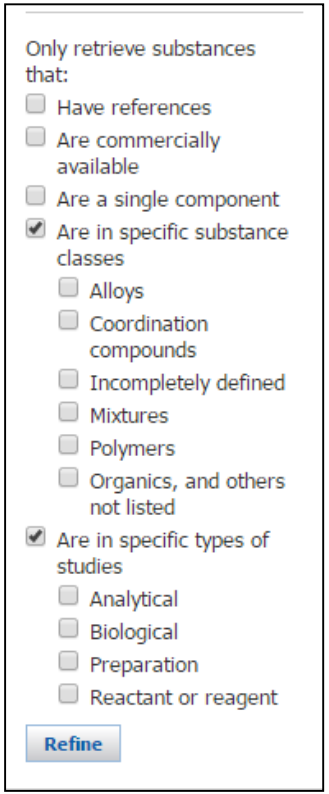


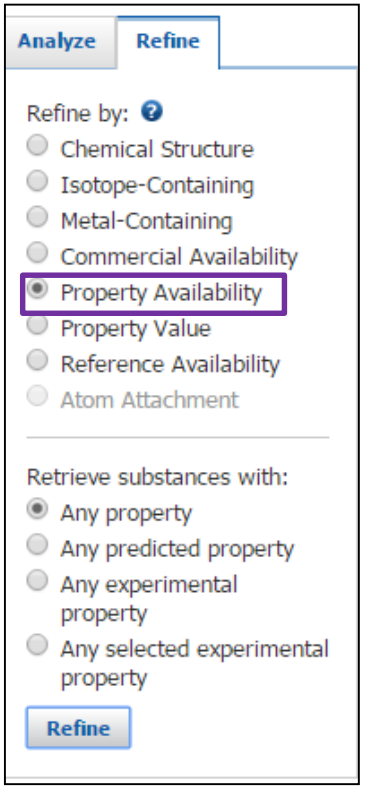
SciFinder® A CAS SOLUTION

物质检索结果——Refine



可以按照化学结构，
包含同位素化合物/金属化合物，
商业可获得性，
性质可获得性，
性质数值，文献可获得性
对结果进行限定

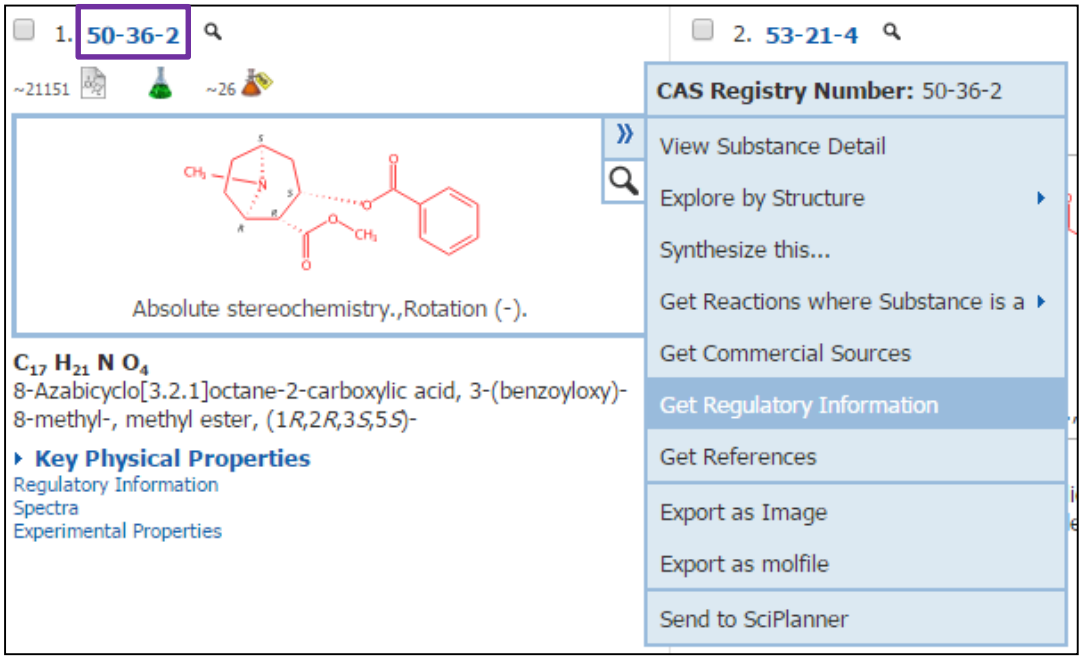




SciFinder® A CAS SOLUTION

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

获得文献，反应，供应商信息

Return

1. CAS Registry Number 50-36-2

~21,151 ~26

$C_{17}H_{21}NO_4$

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

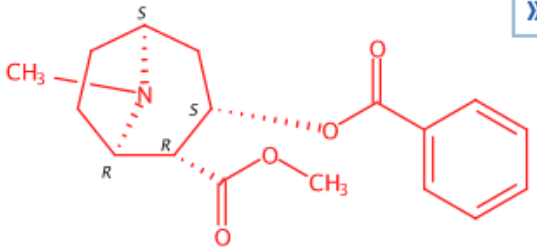
Molecular Weight
303.35

Melting Point (Experimental)
Value: 98 °C

Boiling Point (Experimental)
Value: 187 °C | Condition: Press: 0.1 Torr

Density (Predicted)
Value: 1.22±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

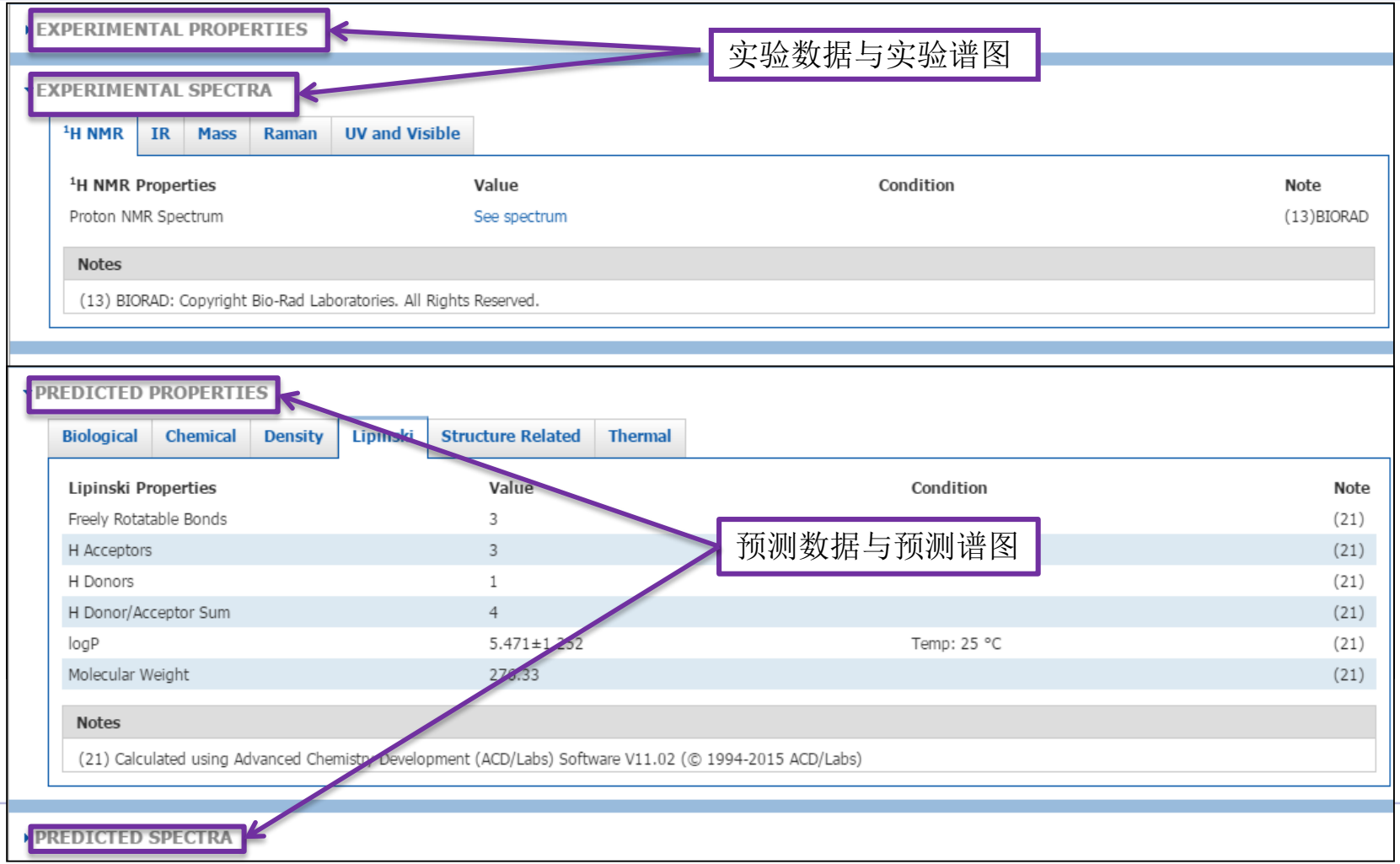
pKa (Predicted)
Value: 8.97±0.60 | Condition: Most Basic Temp: 25 °C



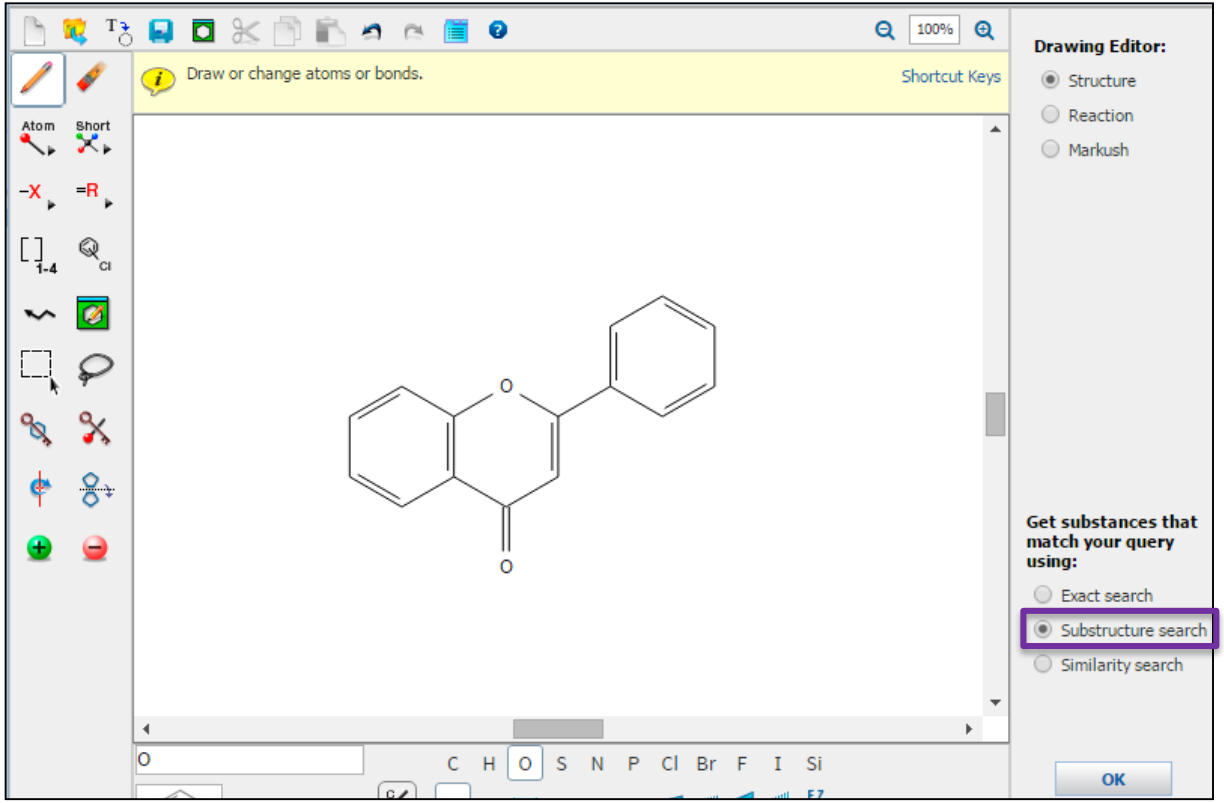
Absolute stereochemistry.,Rotation (-).

物质信息详情

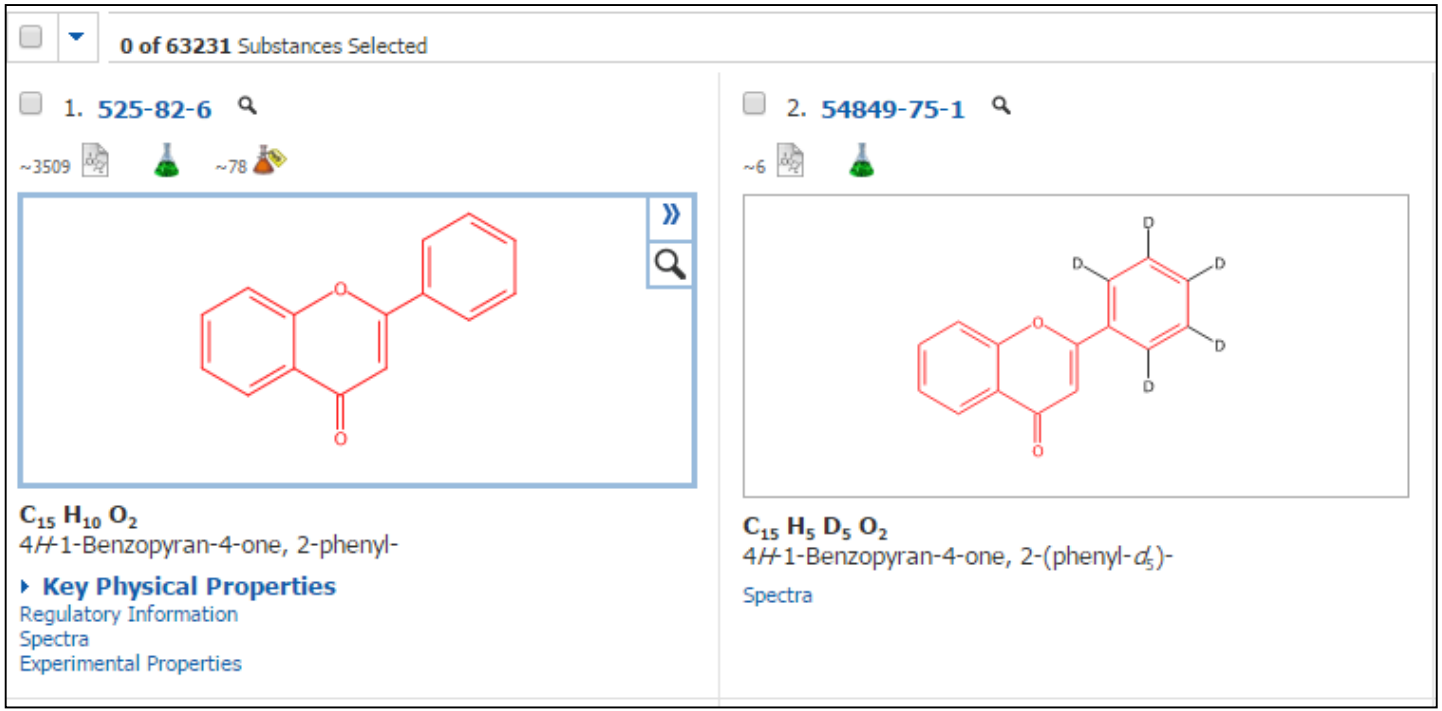
SciFinder® A CAS SOLUTION


EXPERIMENTAL PROPERTIES
EXPERIMENTAL SPECTRA
实验数据与实验谱图
¹H NMR
IR
Mass
Raman
UV and Visible
¹H NMR Properties
Value
Condition
Note
Proton NMR Spectrum
See spectrum
(13)BIORAD
Notes
(13) BIORAD: Copyright Bio-Rad Laboratories. All Rights Reserved.
PREDICTED PROPERTIES
Biological
Chemical
Density
Lipinski
Structure Related
Thermal
Lipinski Properties
Value
Condition
Note
Freely Rotatable Bonds
3
(21)
H Acceptors
3
(21)
H Donors
1
(21)
H Donor/Acceptor Sum
4
(21)
logP
5.471±1.252
Temp: 25 °C
(21)
Molecular Weight
276.33
(21)
预测数据与预测谱图
Notes
(21) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2015 ACD/Labs)
PREDICTED SPECTRA

物质检索——亚结构检索



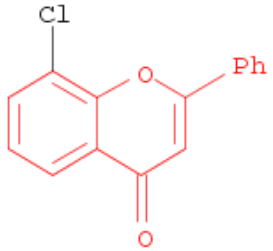
浏览亚结构检索结果



浏览亚结构检索结果

251. Substance Detail
1148-20-5

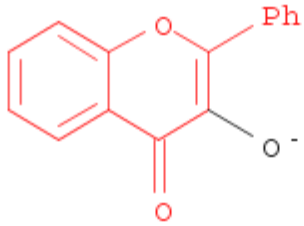
取代物



C15 H9 Cl O2
4*H*-1-Benzopyran-4-one, 8-chloro-2-phenyl-

261. Substance Detail
85481-91-0

离子

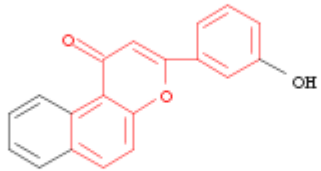


C15 H9 O3
4*H*-1-Benzopyran-4-one, 3-hydroxy-2-phenyl-, ion

273. Substance Detail
136116-17-1

稠环物质

~2



C19 H12 O3
1*H*-Naphtho[2,1-*b*]pyran-1-one, 3-(3-hydroxyphenyl)-

Experimental Properties

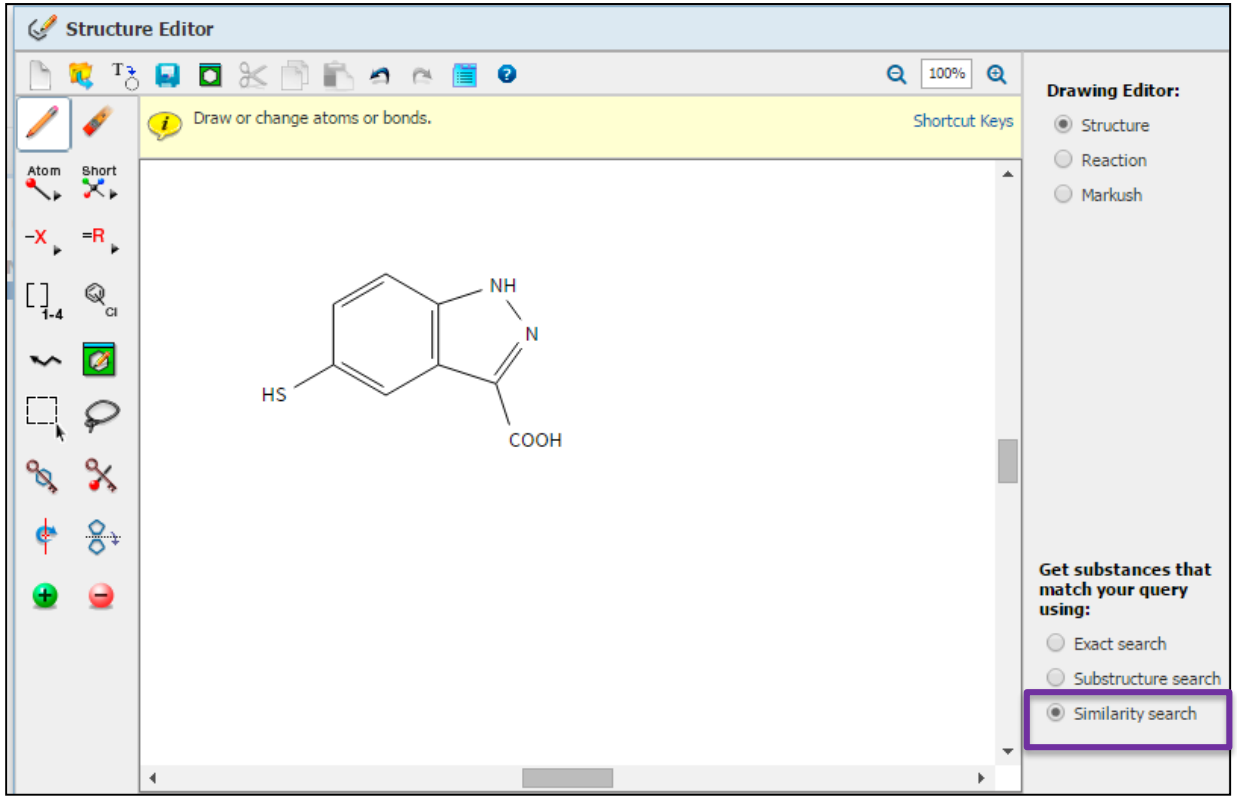
SciFinder® A CAS SOLUTION

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



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Select All Deselect All

相似结构检索候选项

1 of 6 Similarity Candidates Selected

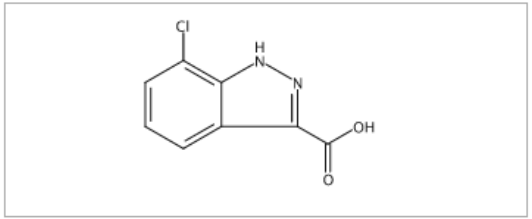
	Substances
≥ 99 (most similar)	0
95-98	0
90-94	0
85-89	11
80-84	34
75-79	82
70-74	254
65-69	633
0-64 (least similar)	1636

相似度越高，结构越相似

相似结构检索结果

1. 129295-32-5

~3 ~96



$C_8 H_5 Cl N_2 O_2$

1*H*-Indazole-3-

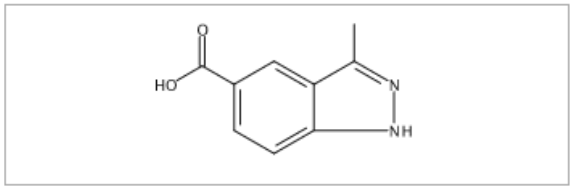
Key Physica

取代基变化

Score: 79

3. 885223-58-5

~11 ~34



$C_9 H_8 N_2 O_2$

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

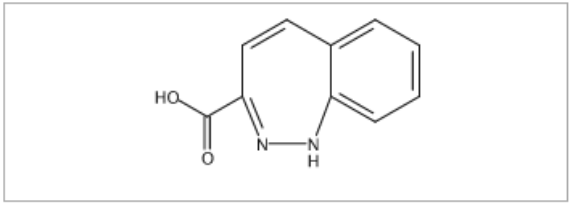
Key Physical Properties

取代基位置变化

Score: 71

117. 72119-92-7

~1



$C_{10} H_8 N_2 O_2$

1*H*-1,2-Benzodiazepine-3-carboxylic acid

Key Physical Properties

Experimental Properties

母体结构变化

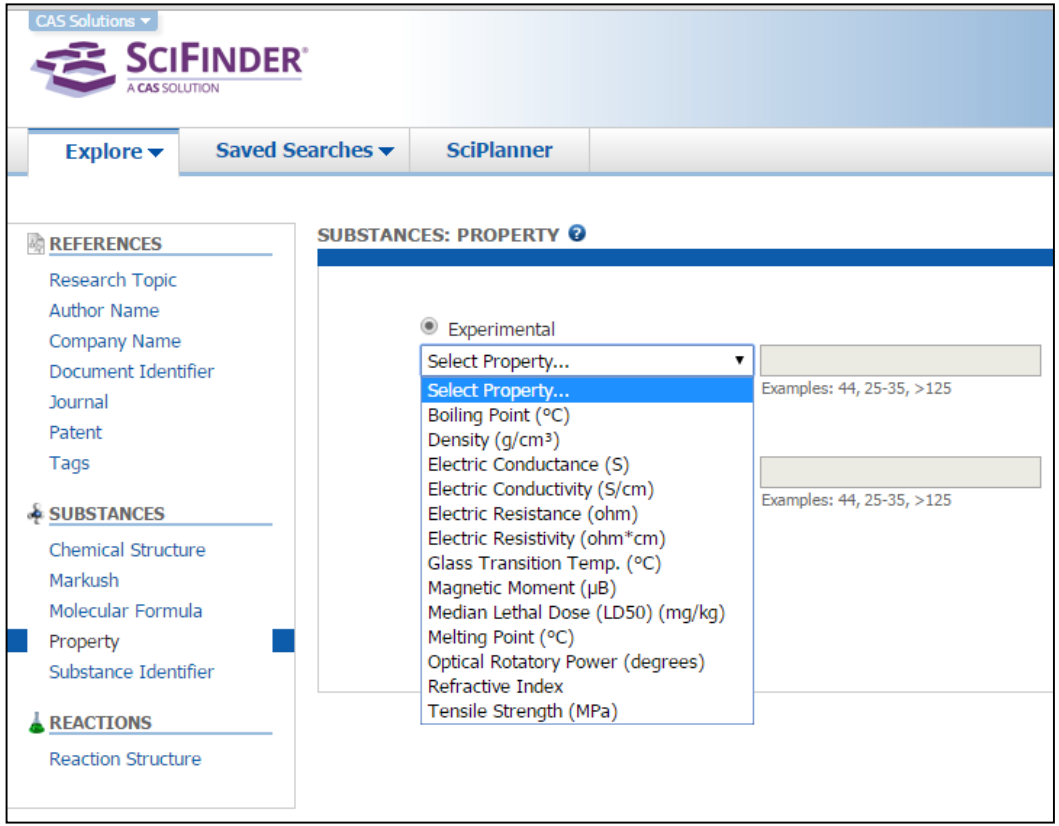
SciFinder® A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

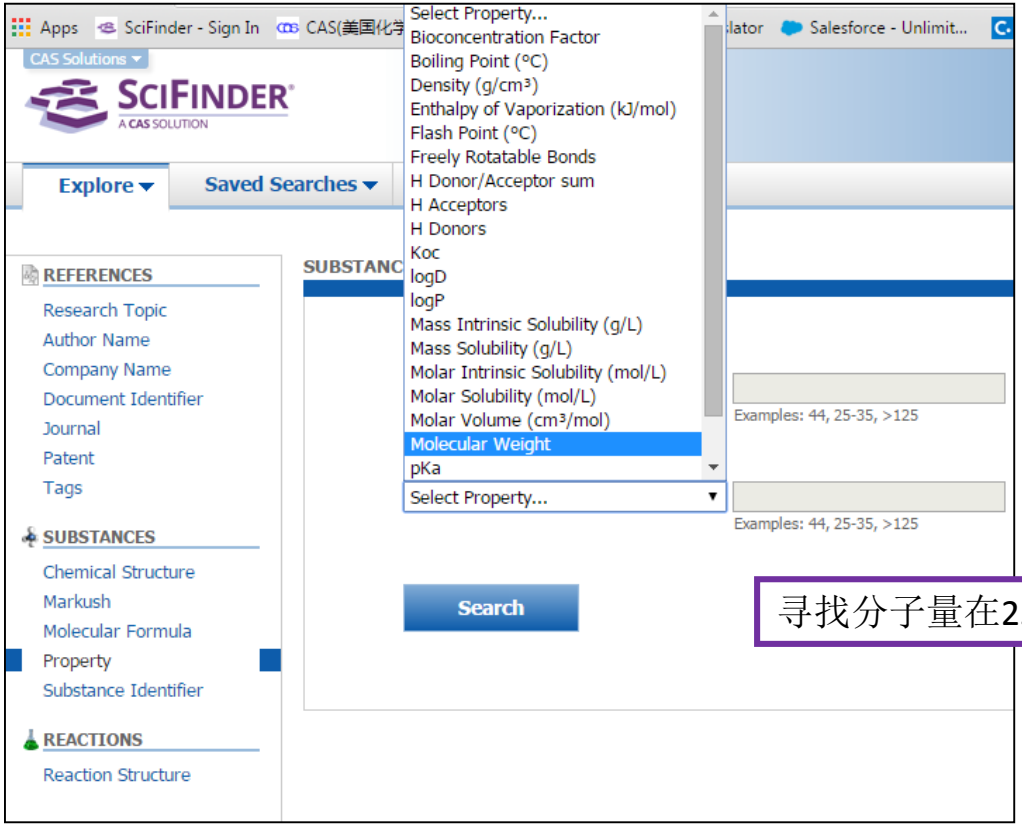
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

物质检索——性质检索



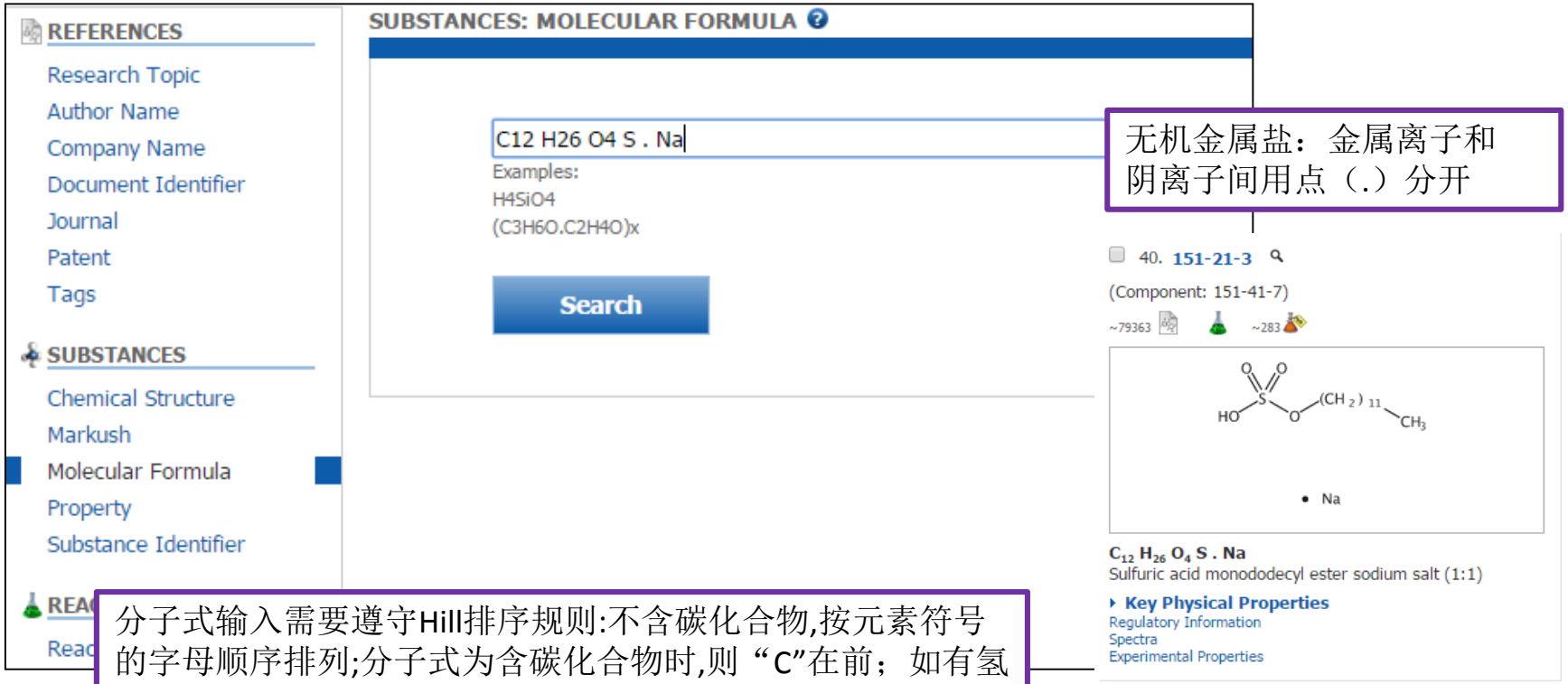
SciFinder® A CAS SOLUTION

物质检索——性质检索



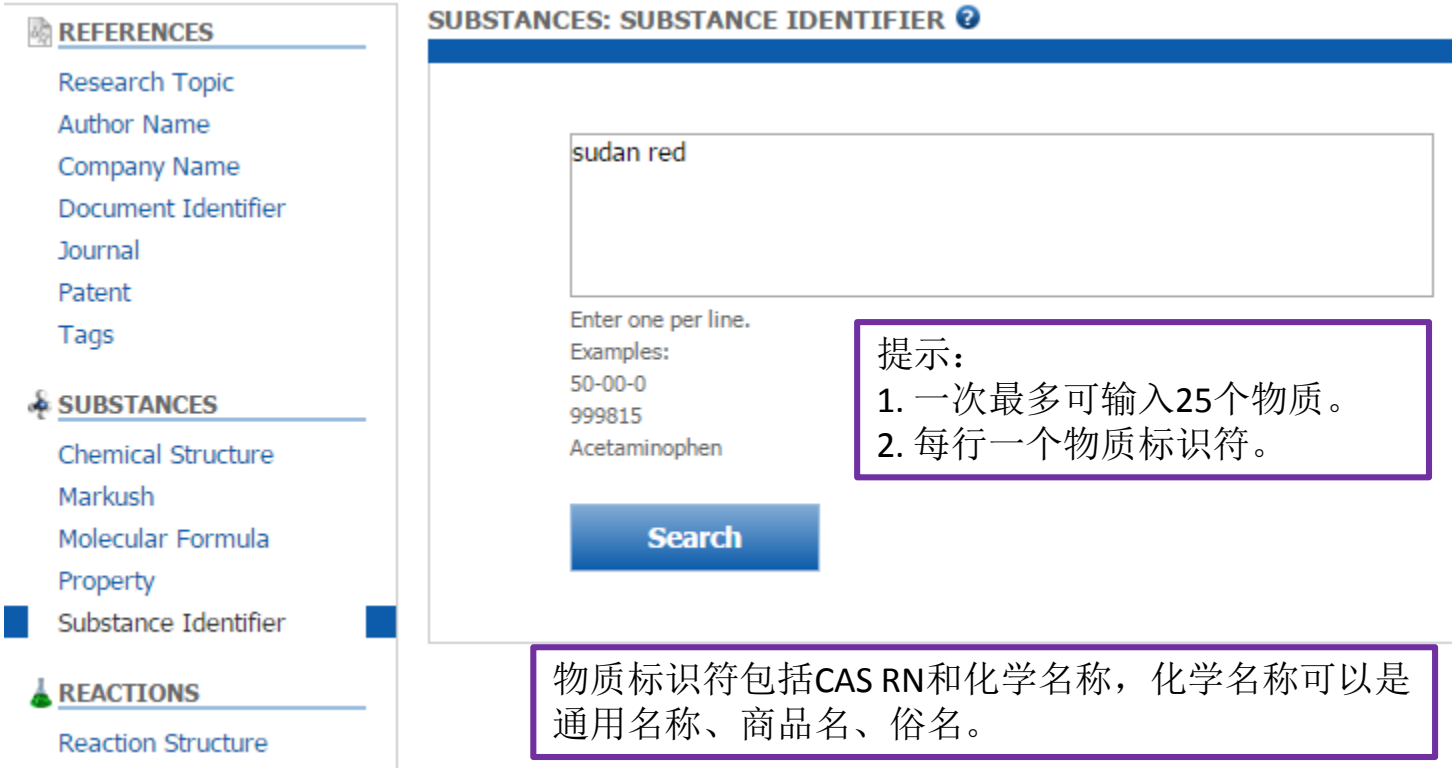
寻找分子量在250-400之间的物质

物质检索——分子式检索



SciFinder® A CAS SOLUTION

物质检索——标识符检索

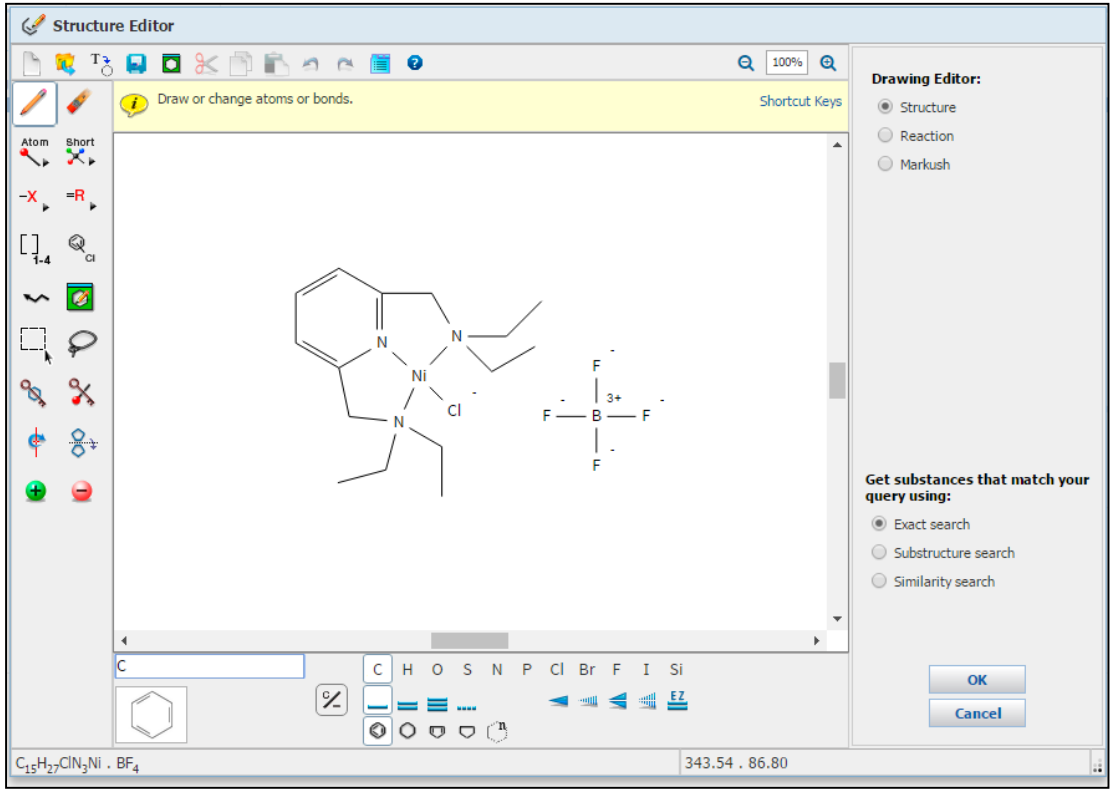


提示：
1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

SciFinder® A CAS SOLUTION

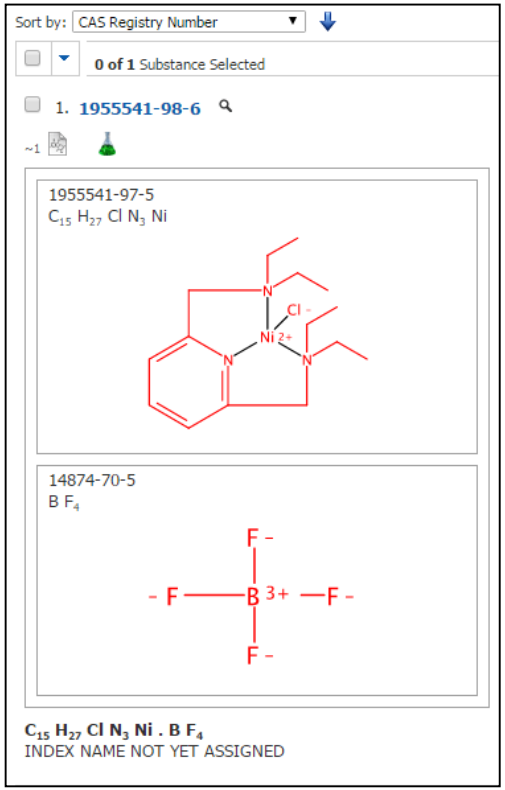
精确结构检索配合物



SciFinder® A CAS SOLUTION

获得精确结构检索结果

Characteristics	☑ Single component
	☐ Commercially available
	☐ Included in references
Classes	☐ Alloys
	☑ Coordination compounds
	☐ Incompletely defined
	☐ Mixtures
	☐ Polymers
	☐ Organics, and others not listed
Studies	☐ Analytical
	☐ Biological
	☐ Preparation
	☐ Reactant or reagent



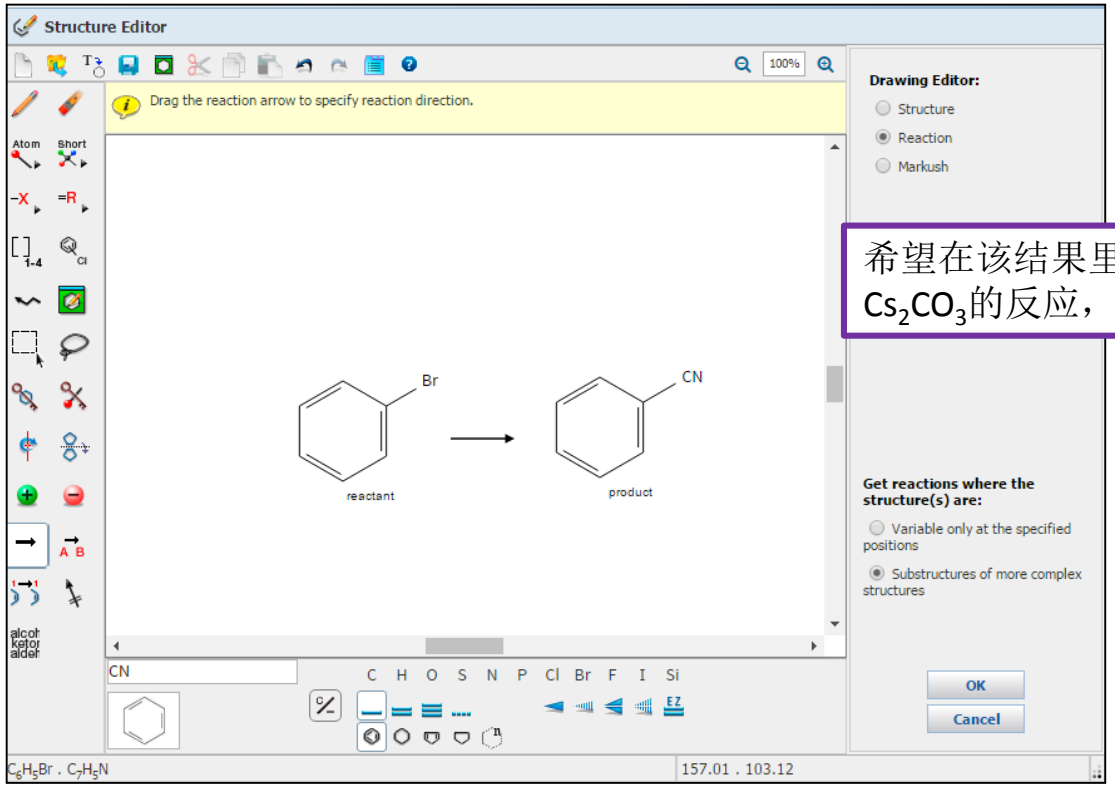
SciFinder® A CAS SOLUTION

提纲

- 反应检索
  - 如何使用反应结构编辑器功能键提高反应检索精度
  - 如何使用Analyze/Refine处理反应结果集
  - 如何通过MethodsNow Synthesis快速获得权威可靠的合成方法

SciFinder® A CAS SOLUTION

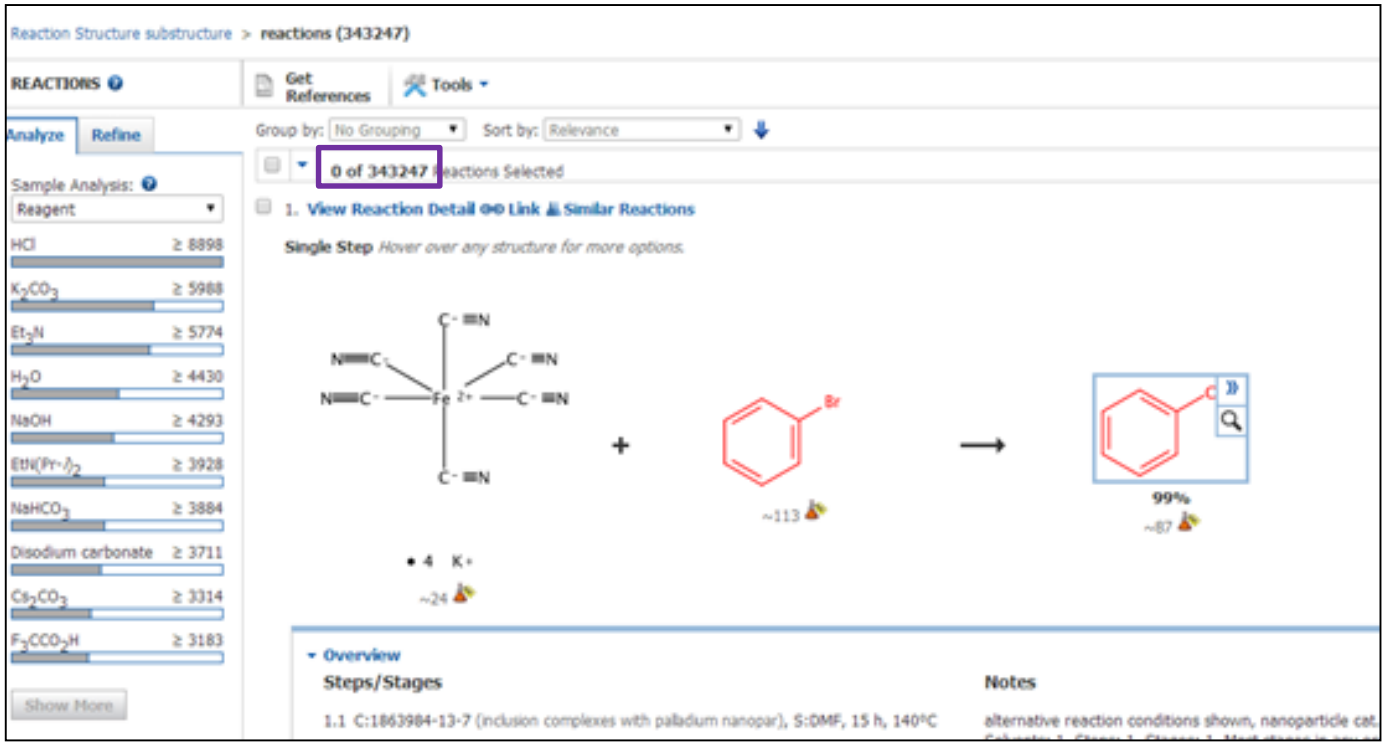
案例一：检索由溴苯转化为苯腈的反应



希望在该结果里进一步限定:溶剂为DMF，试剂为Cs_2CO_3的反应，应如何操作？

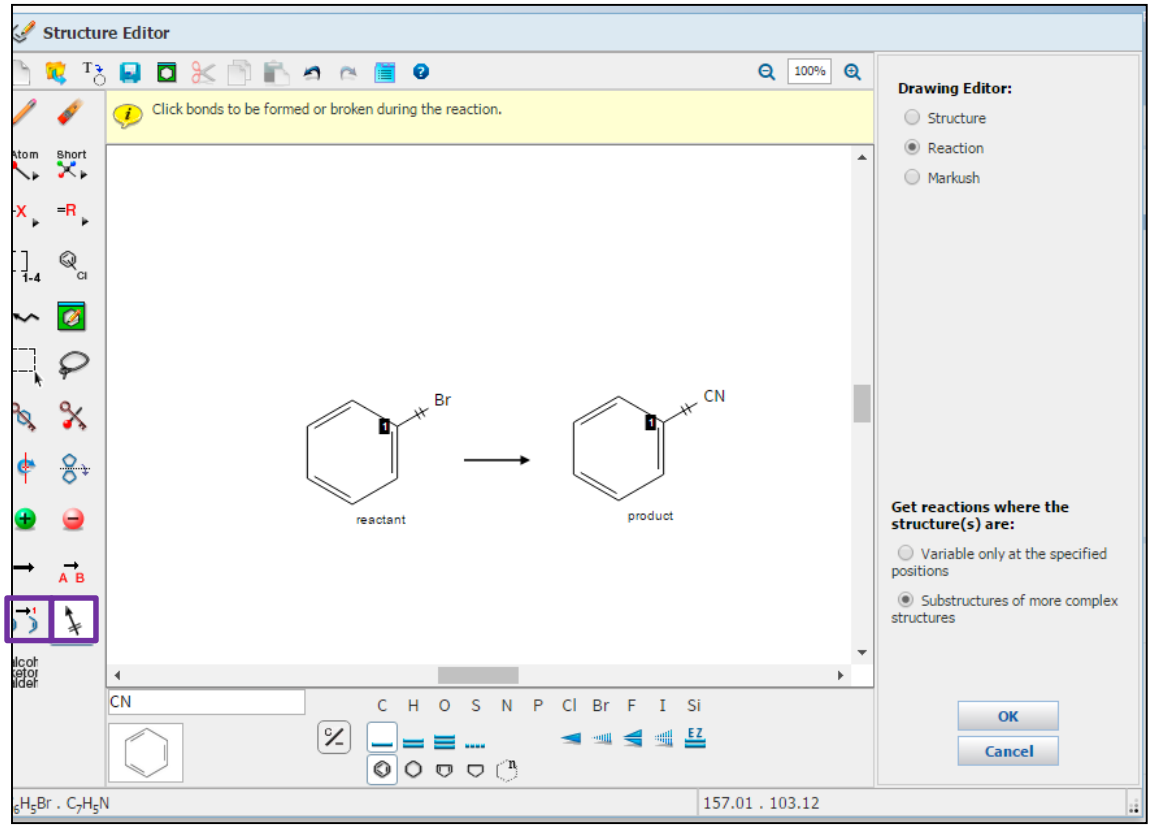
SciFinder® A CAS SOLUTION

获得34万多条反应，噪音较大



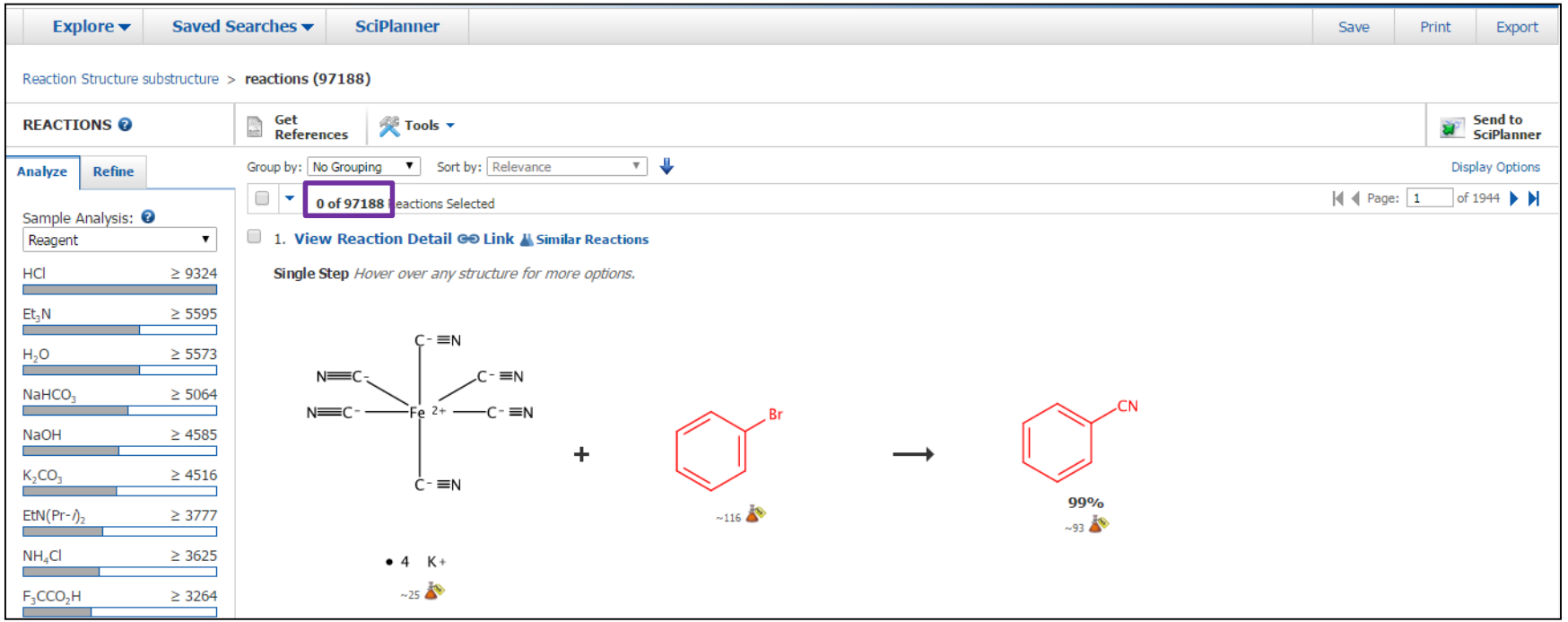
SciFinder® A CAS SOLUTION

可以通过反应原子标记工具和反应位置标记工具提高反应检索精度



SciFinder® A CAS SOLUTION

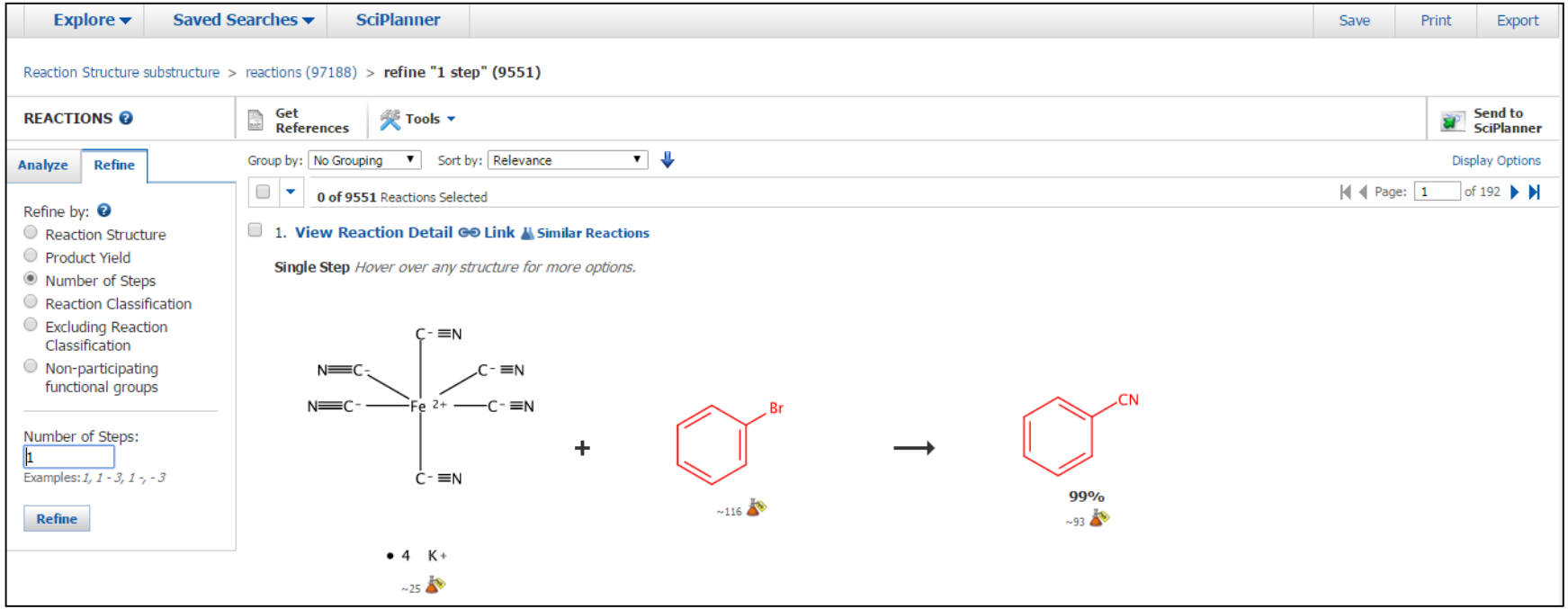
获得反应97188条



使用反应结果集中的Analyze功能，需要将结果集压缩到20000以下

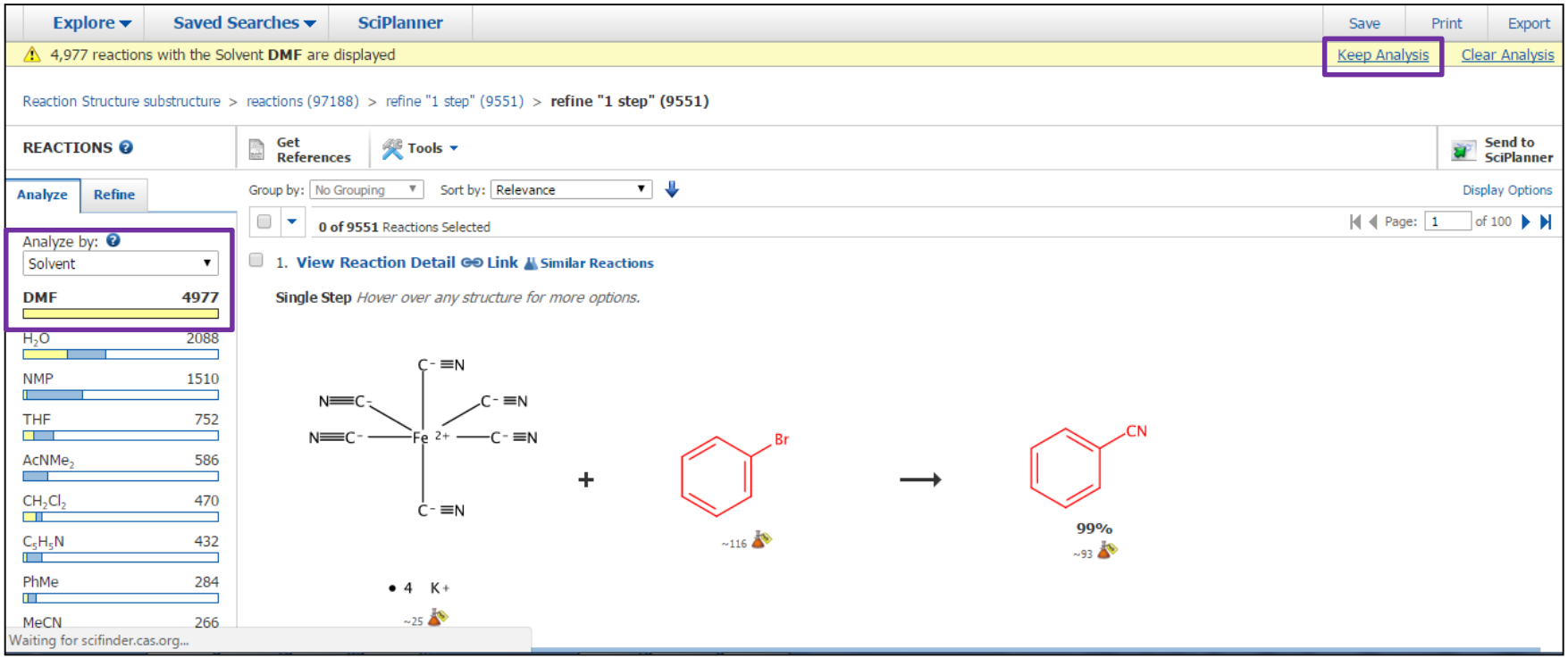
SciFinder® A CAS SOLUTION

将反应限定为1步反应



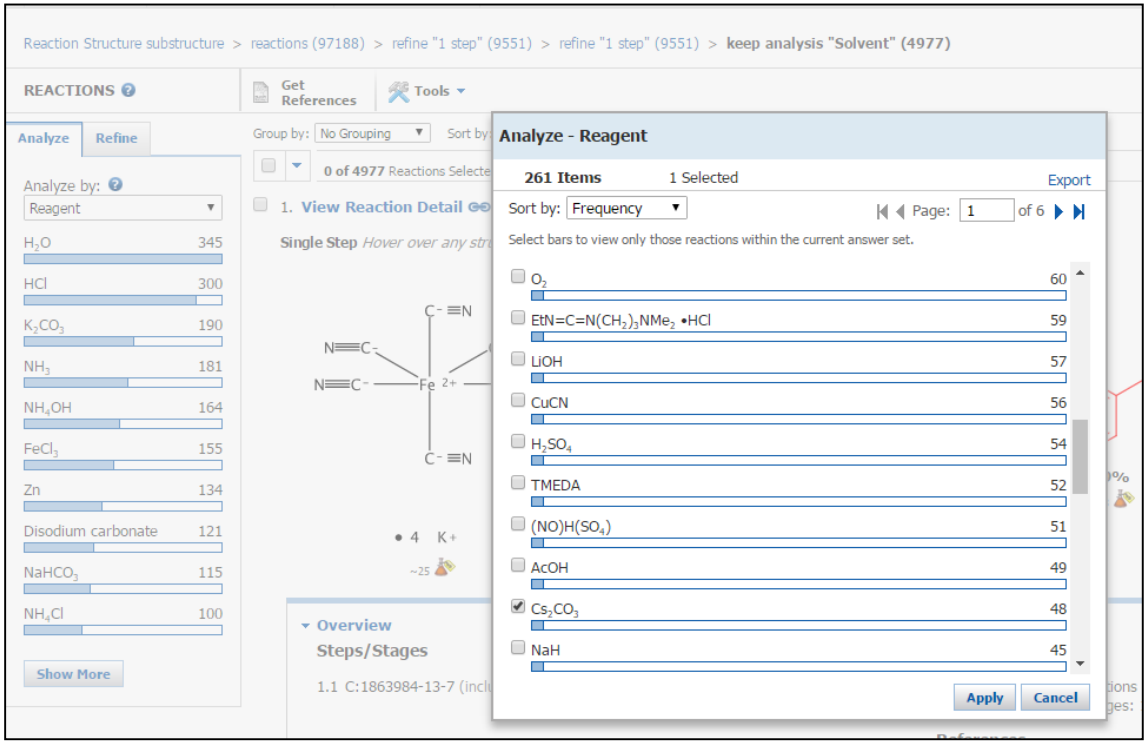
SciFinder® A CAS SOLUTION

通过Analyze by Solvent选择在DMF溶剂中进行的反应



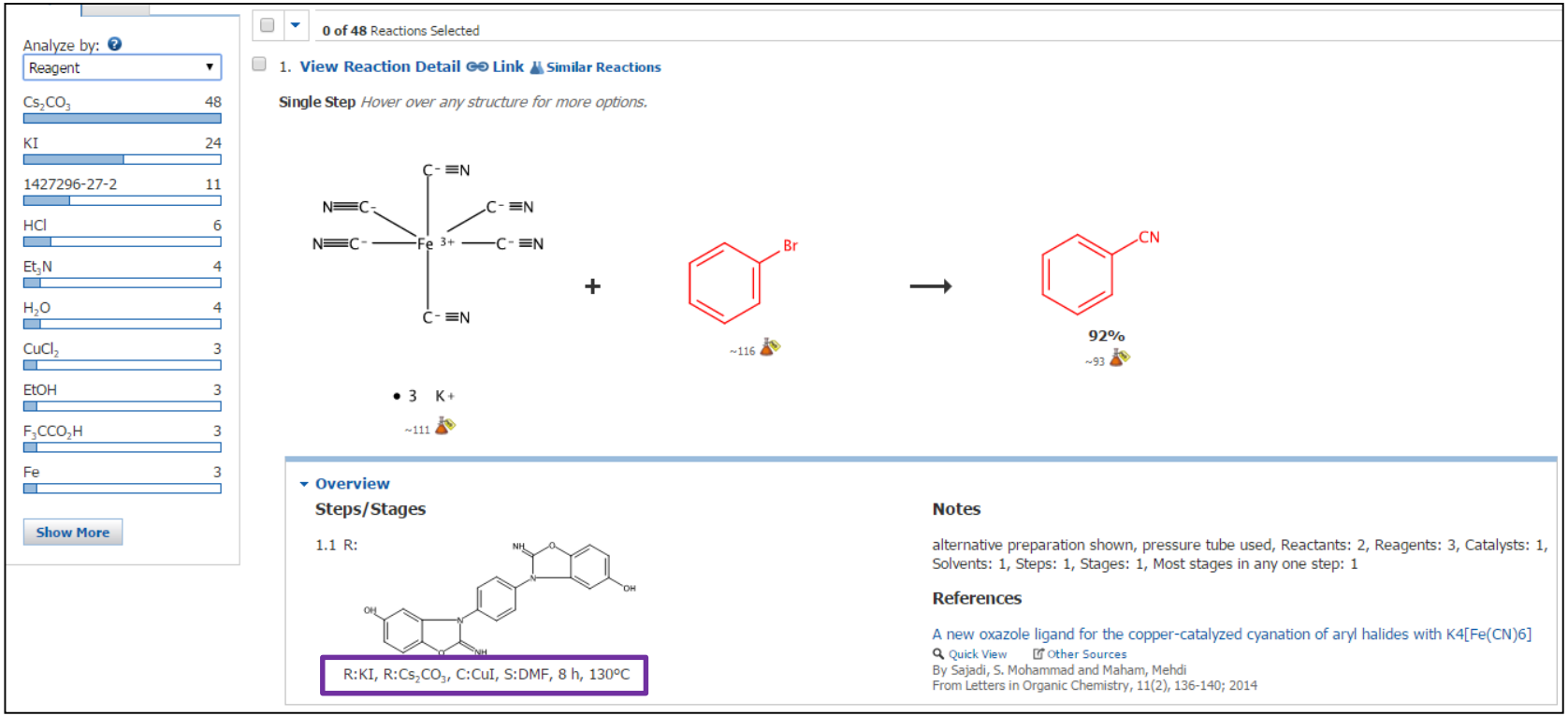
SciFinder® A CAS SOLUTION

在反应结果集中继续通过Analyze by Reagent选择Cs_2CO_3作为试剂的反应



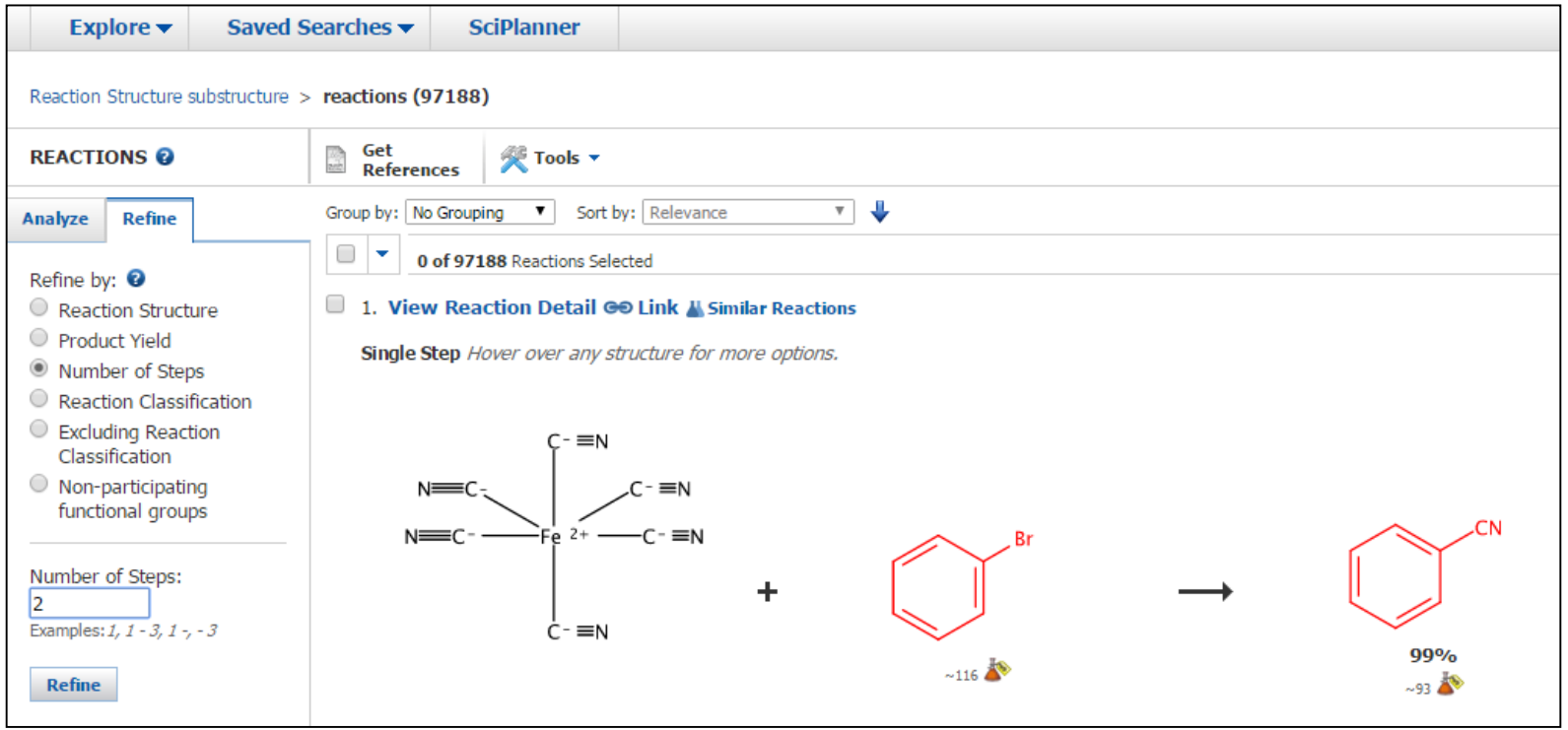
SciFinder® A CAS SOLUTION

获得以 DMF为溶剂， Cs_2CO_3为试剂的一步反应，保存结果集

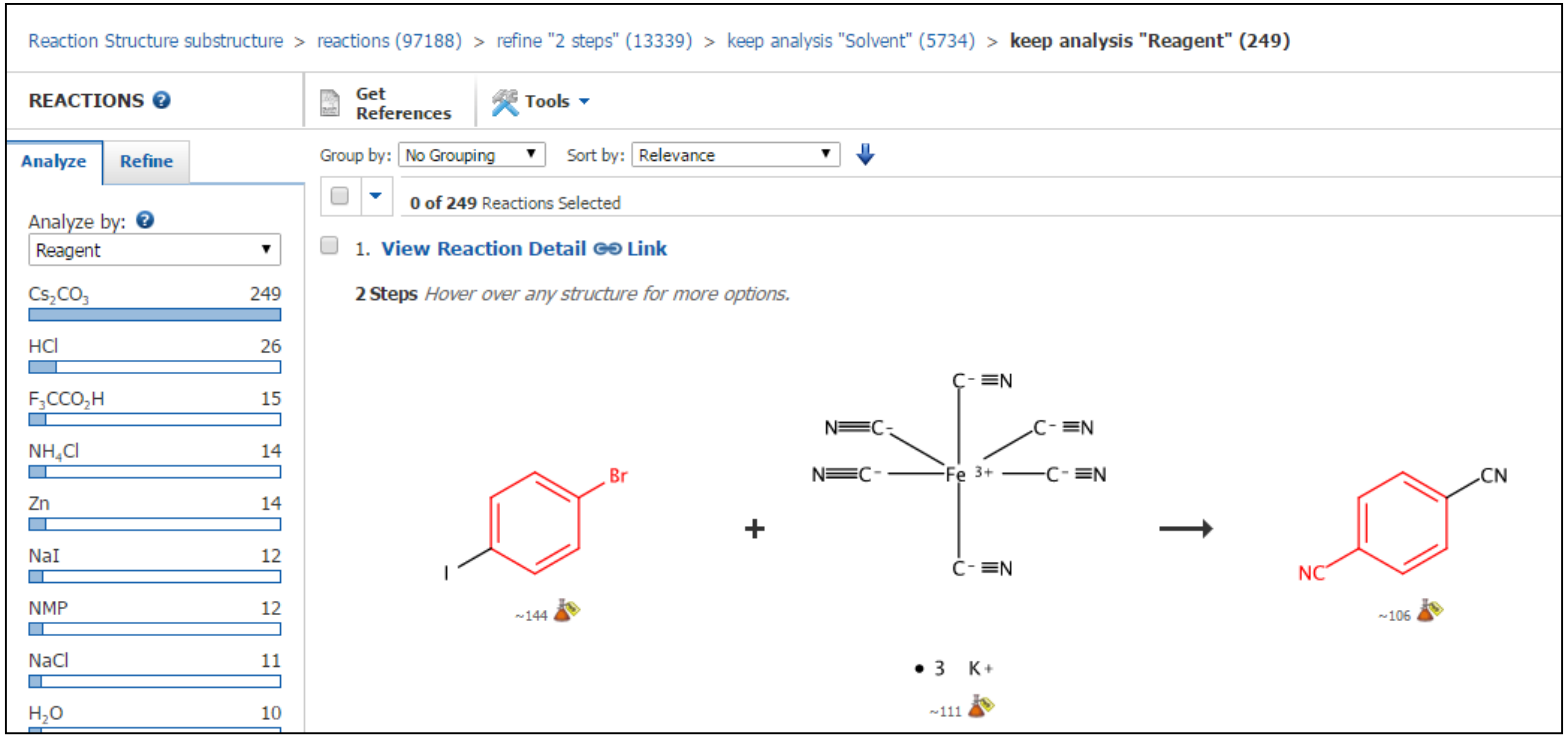


SciFinder® A CAS SOLUTION

在初始反应结果集中限定2步反应，重复刚才的步骤

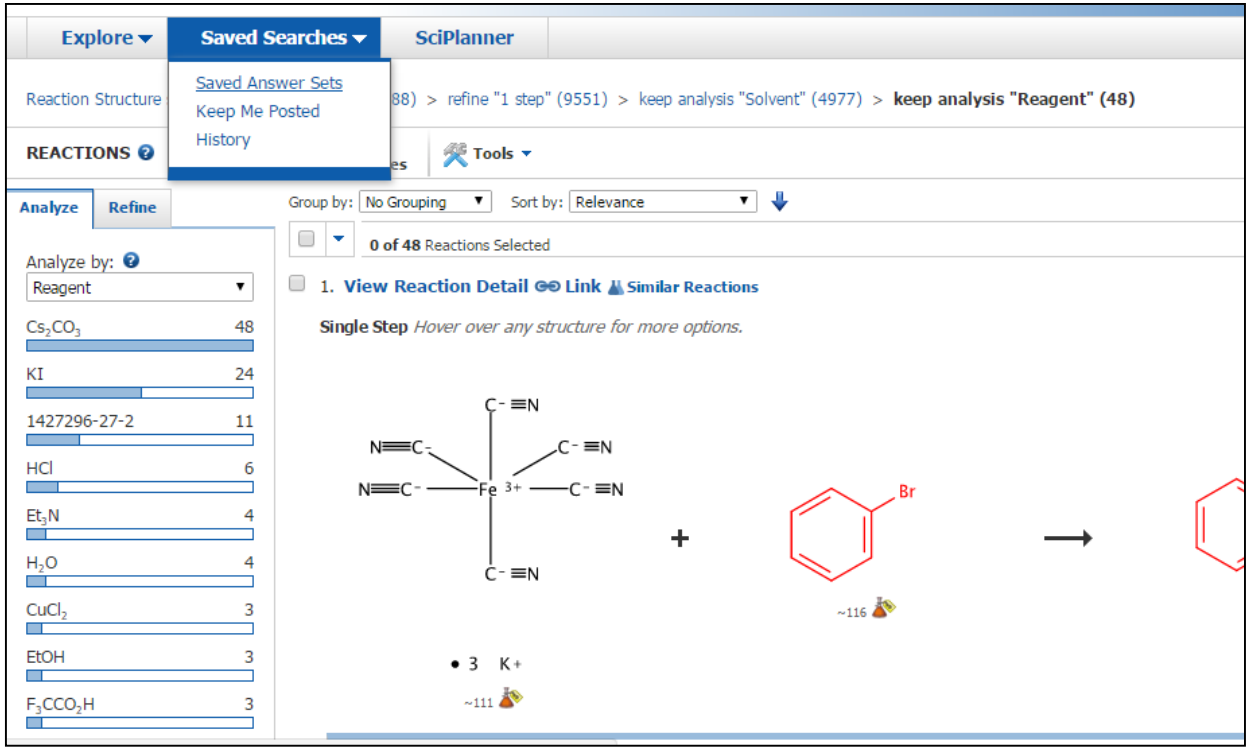


获得以 DMF为溶剂， Cs_2CO_3为试剂的2步反应，保存结果集

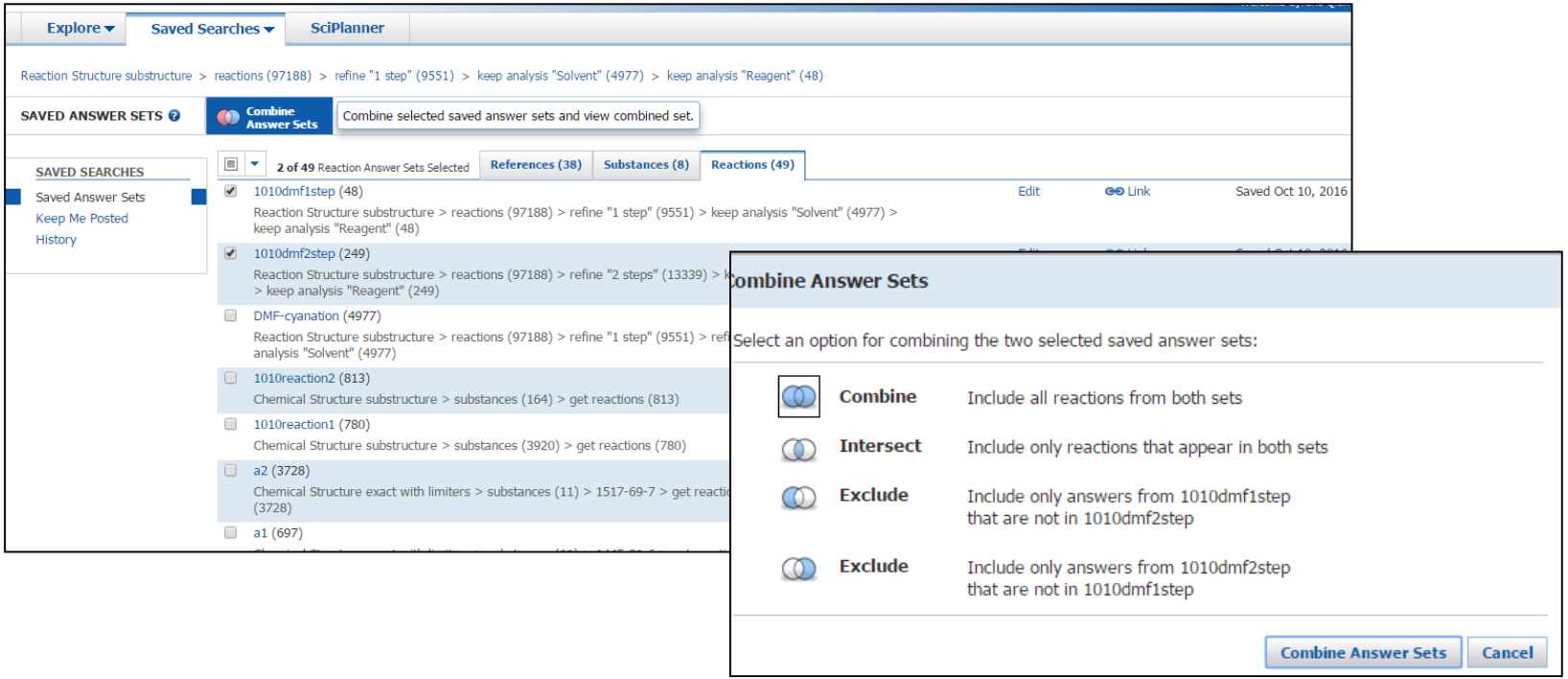


SciFinder® A CAS SOLUTION

在Saved Searches中的反应结果集中找到刚保存过的结果集

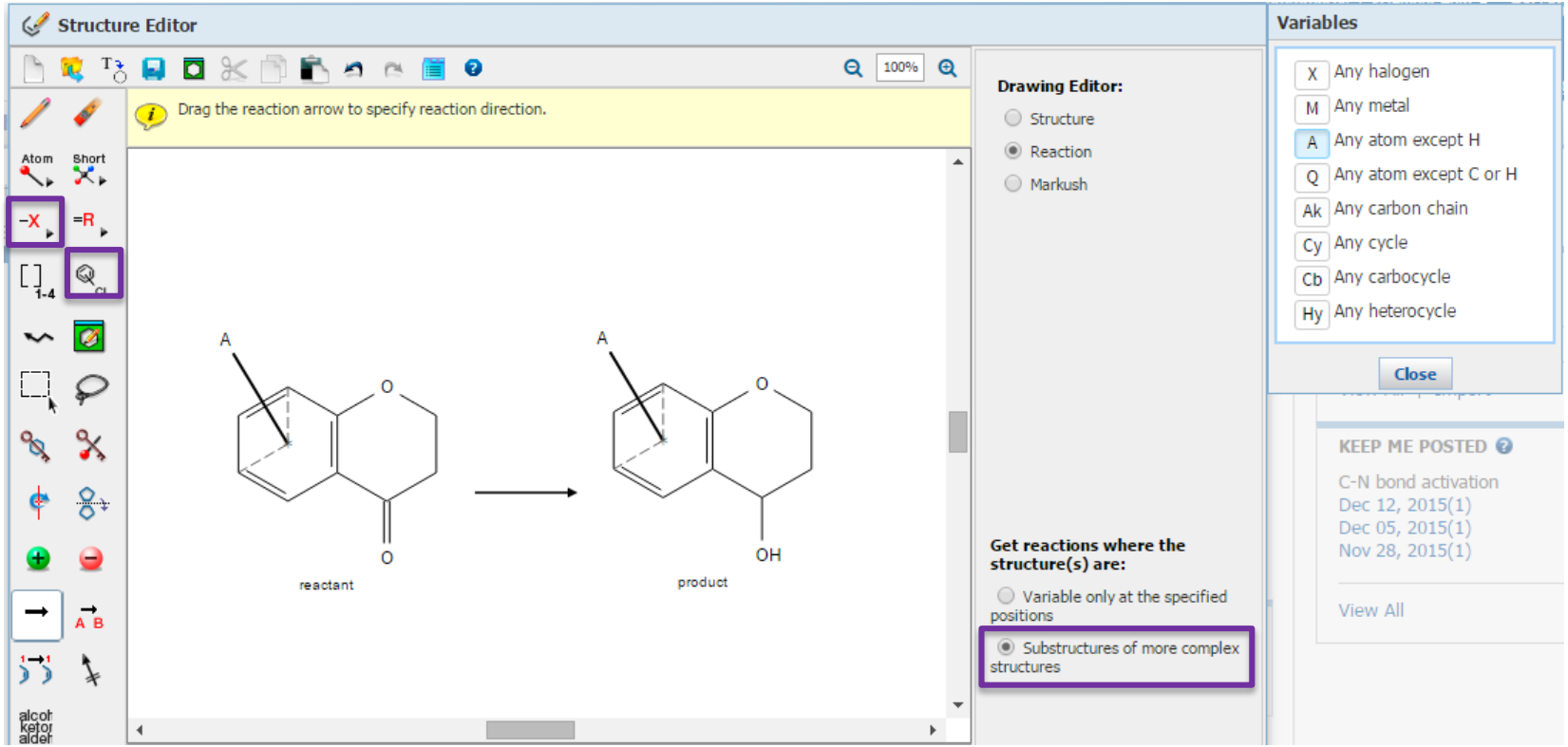


合并结果集

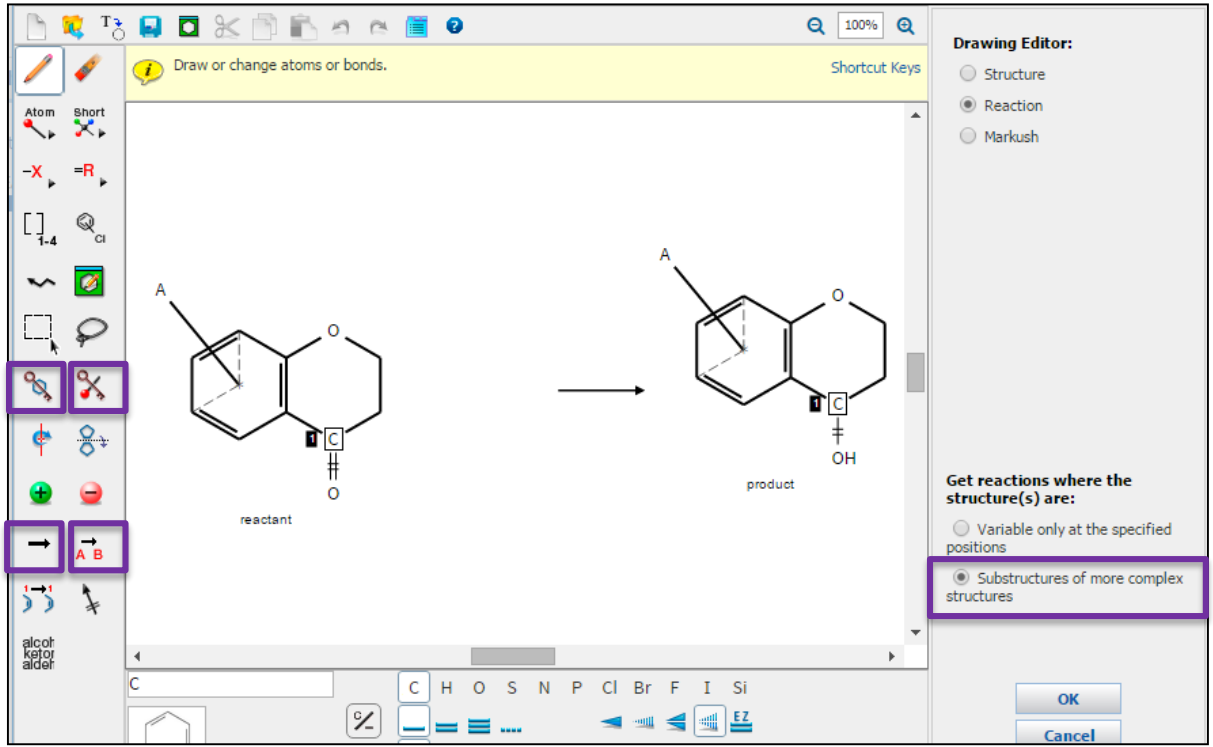


SciFinder® A CAS SOLUTION

亚结构检索2：酮基的还原反应



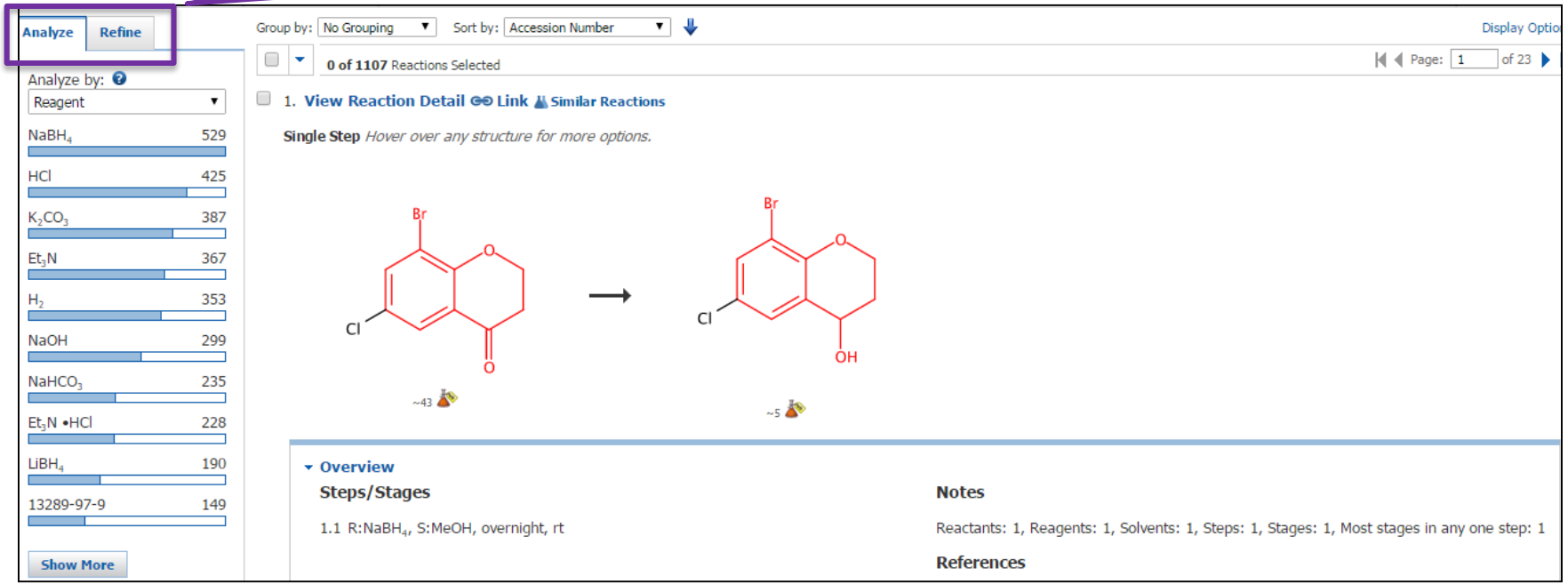
亚结构检索2：酮基的还原反应



检索酮基的还原反应，需将碳原子锁定

亚结构反应检索结果

通过Analyze或者Refine处理检索结果



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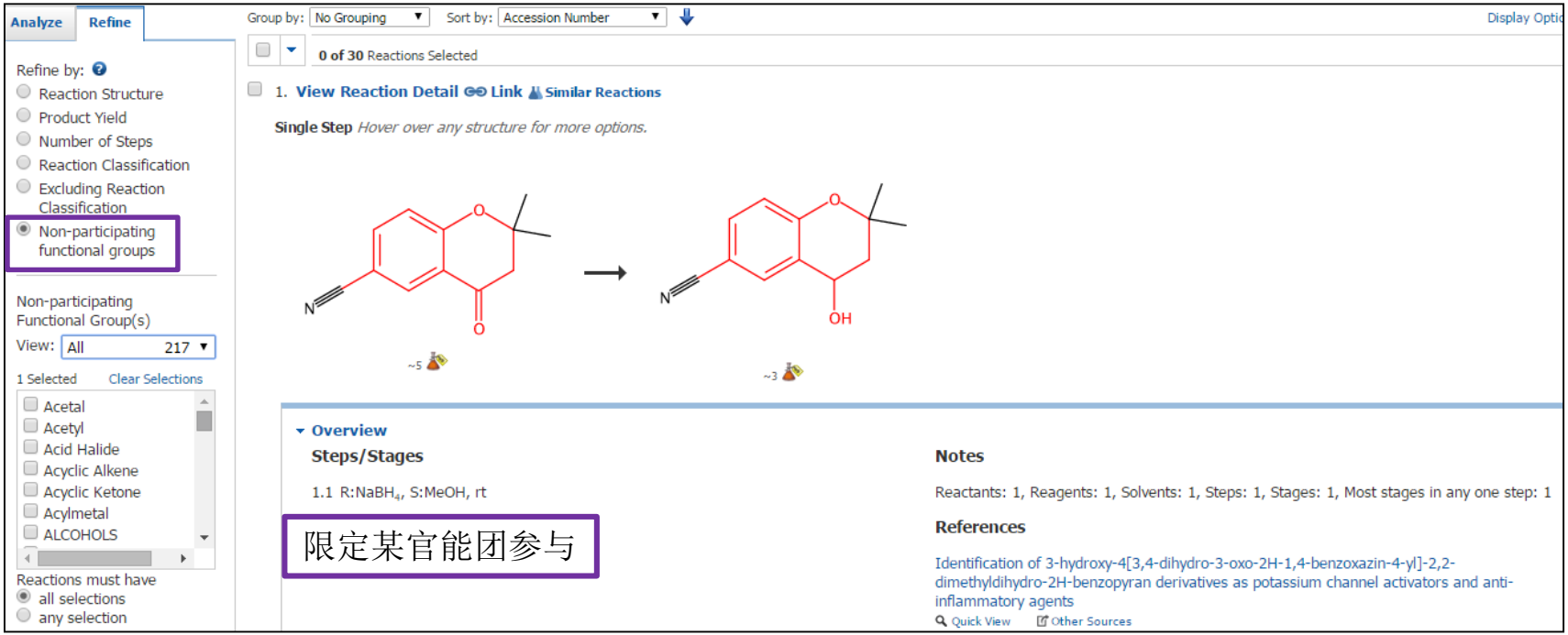
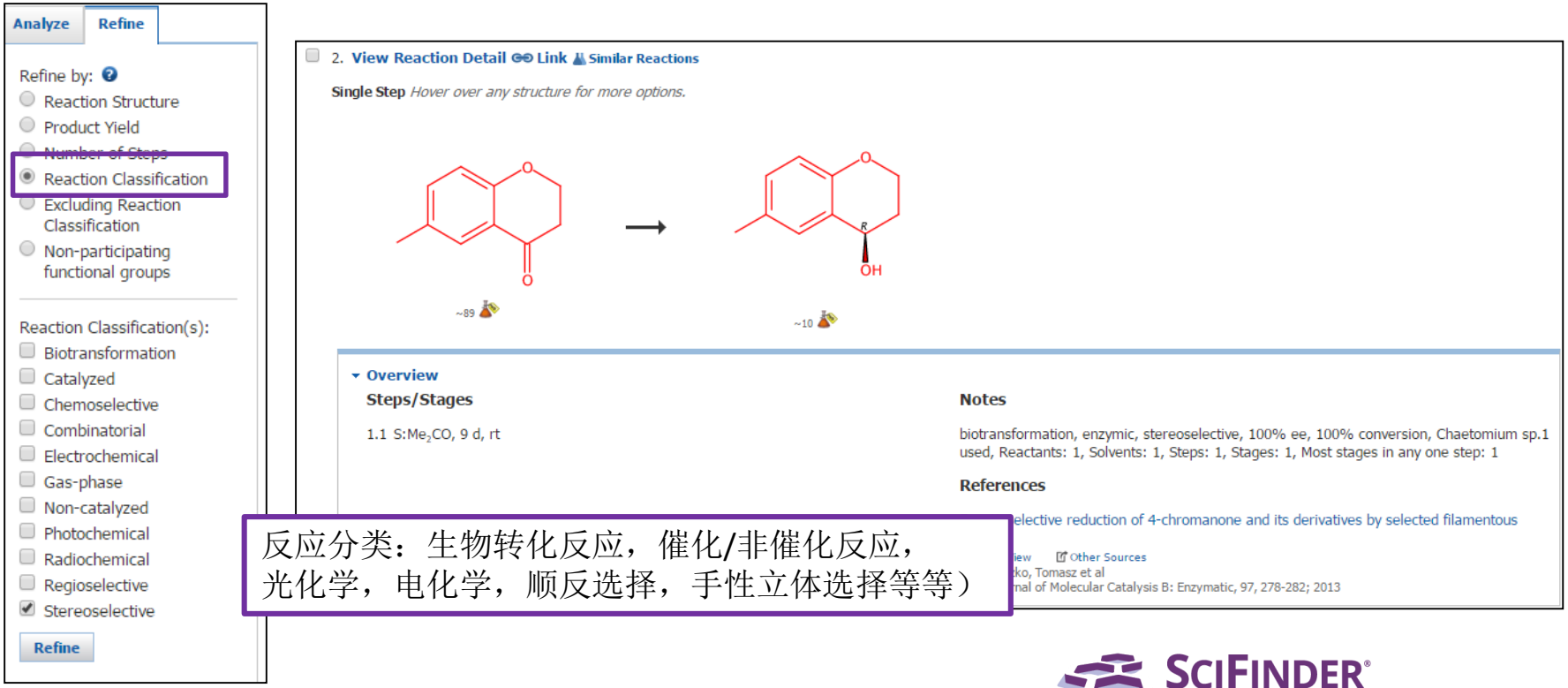
亚结构反应检索结果



SciFinder® A CAS SOLUTION

亚结构反应检索结果



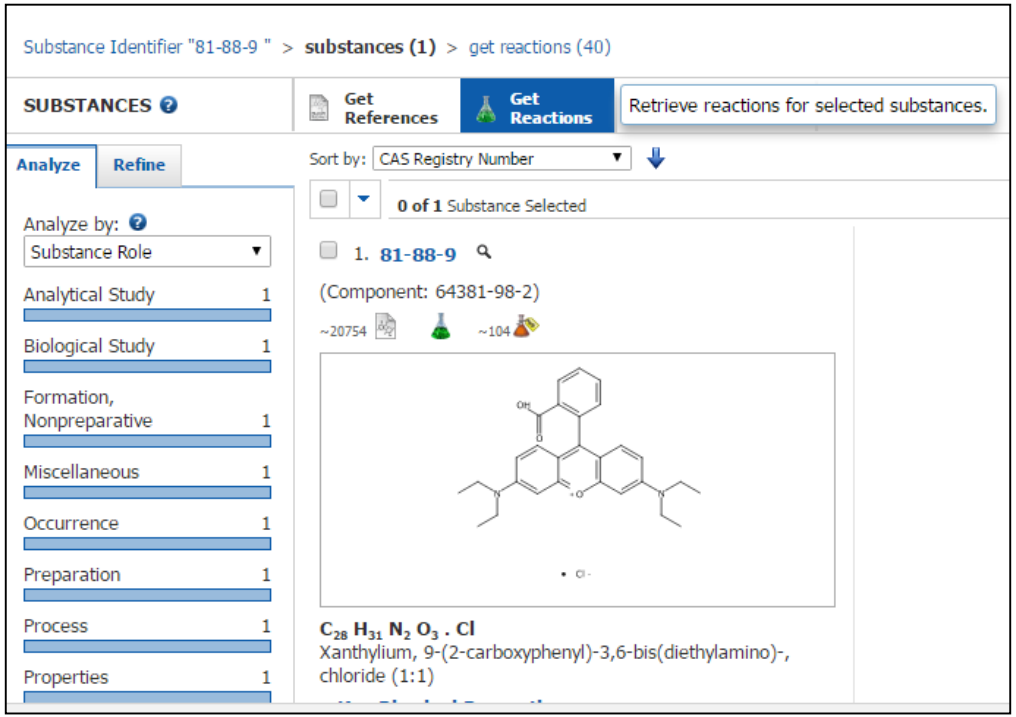
反应分类：生物转化反应，催化/非催化反应，
光化学，电化学，顺反选择，手性立体选择等等）

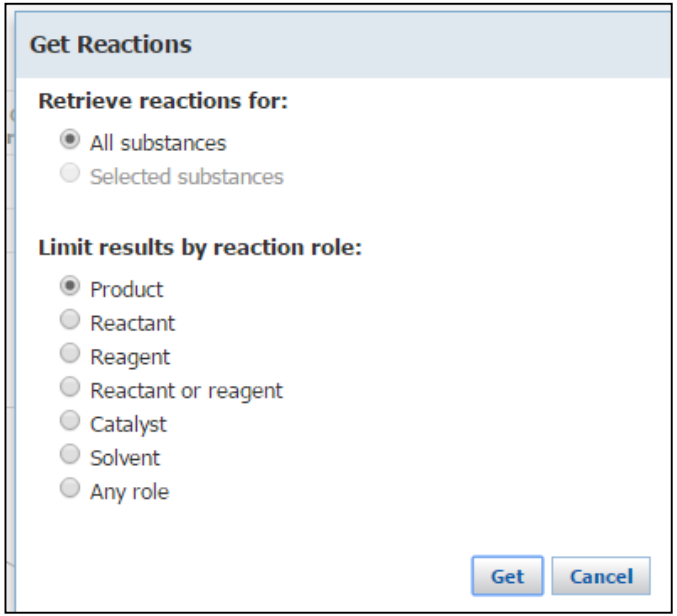
提纲

- 反应检索
  - 如何使用反应结构编辑器功能键提高反应检索精度
  - 如何使用Analyze/Refine处理反应结果集
  - 如何通过MethodsNow Synthesis快速获得权威可靠的合成方法

SciFinder® A CAS SOLUTION

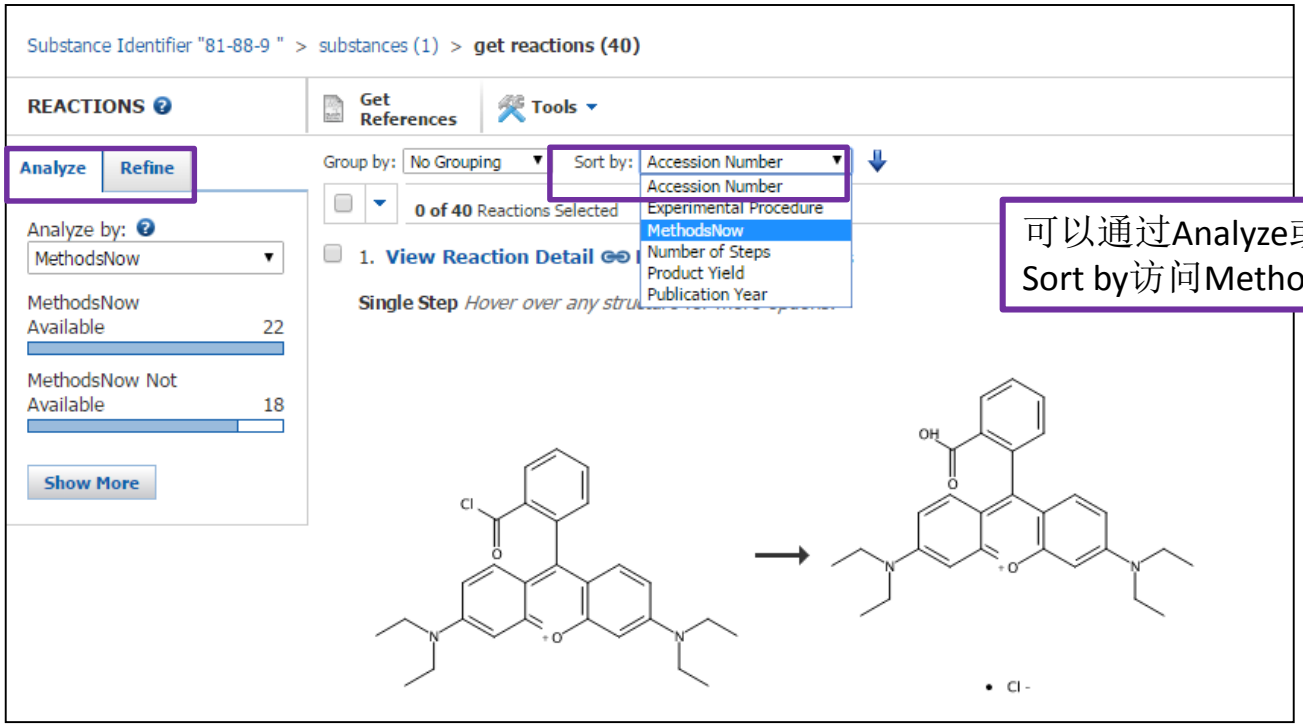
通过罗丹明物质获得反应





SciFinder® A CAS SOLUTION

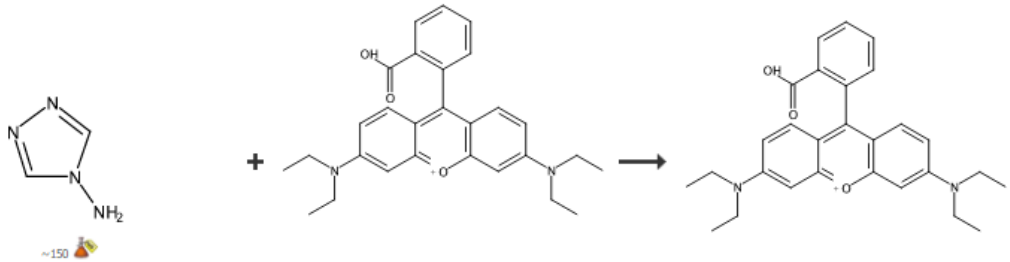
由罗丹明的制备信息获得相关反应



可以通过Analyze或者
Sort by访问MethodsNow Synthesis

SciFinder® A CAS SOLUTION

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



~150 [Step 2.1] ~104

graft compd. with iron triazole

▸ **Overview**

▾ **METHODSNOW™**

Procedure

1. Add a 50 mL methanol solution containing 3 mmol 4-NH_2-1,2,4-triazole at room temperature into a 50 mL methanol solution containing 1 mmol $Fe(ClO_4)_2 \cdot 6H_2O$ and 5 mg ascorbic acid.
2. Stir the resulting limpid mixture for half an hour.

View more...

Available Experimental Data

Elemental Analysis, State

View with MethodsNow

SciFinder® A CAS SOLUTION

MethodsNow

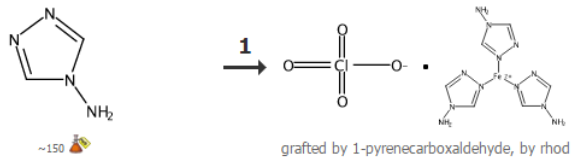
Synergetic Spin Crossover and Fluorescence in One-Dimensional Hybrid Complexes

By Wang, Chun-Feng; Li, Ren-Fu; Chen, Xue-Yuan; Wei, Rong-Jia; Zheng, Lan-Sun; Tao, Jun
From Angewandte Chemie, International Edition, 54(5), 1574-1577; 2015
Published by Wiley-VCH Verlag GmbH & Co. KGaA

书目信息

Reaction Steps 1 2

点击步数，获得相应步骤反应



grafted by 1-pyrenecarboxaldehyde, by rhod

Products	Iron(2+), tris(4*H*-1,2,4-triazol-4-amine-*N*^{1})-, diperchlorate, hydrate, grafted by 1-pyrenecarboxaldehyde, by rhod, CAS RN: 151592-05-1
Reactants	4*H*-1,2,4-Triazol-4-amine, CAS RN: 584-13-4
Reagents	Perchloric acid, iron(2+) salt (2:1), CAS RN: 13933-23-8 L-Ascorbic acid, CAS RN: 50-81-7
Solvents	Methanol, CAS RN: 67-56-1
Procedure	1. Add a 50 mL methanol solution containing 3 mmol 4-NH_2-1,2,4-triazole at room temperature into a 50 mL methanol solution containing 1 mmol $Fe(ClO_4)_2 \cdot 6H_2O$ and 5 mg ascorbic acid. 2. Stir the resulting limpid mixture for half an hour. 3. Evaporate the mixture to dryness by a rotary evaporator at about 333 K. 4. Precipitate the product as powder that turnspurple on cooling.
Scale	milligram
Elemental Analysis	Calcd (%) for $C_8H_{12}N_{12}O_8Cl_2Fe$: C 14.21, H 2.38, N 33.15. Found: C 14.32, H 2.32, N 32.56.
State	purple powder.
CAS Method Number	3-562-CAS-1814872

Print/Export Close

更清楚的物质展示
更清楚的实验过程展示

经过CAS科学家重写的实验步骤

物质表征信息

打印或者导出分析方法

SciFINDER® A CAS SOLUTION

SciFinder® Page 1

Synergetic Spin Crossover and Fluorescence in One-Dimensional Hybrid Complexes
By Wang, Chun-Feng; Li, Ren-Fu; Chen, Xue-Yuan; Wei, Rong-Jia; Zheng, Lan-Sun; Tao, Jun
From Angewandte Chemie, International Edition, 54(5), 1574-1577; 2015
Published by Wiley-VCH Verlag GmbH & Co. KGaA

Step 2

grafted by 1-pyrenecarboxaldehyde, by rhod | [Reactant] | graft compd. with iron triazole

Products	Rhodamine B, graft compd. with iron triazole, CAS RN: 81-88-9
Reactants	Iron(2+), tris(4*H*-1,2,4-triazol-4-amine-*N*^{1})-, diperchlorate, hydrate, grafted by 1-pyrenecarboxaldehyde, by rhod, CAS RN: 151592-05-1 Rhodamine B, CAS RN: 81-88-9
Solvents	Toluene, CAS RN: 108-88-3
Procedure	1. Disperse 100 mg FeL in 30 mL toluene. 2. Add 0.21 mmol rhodamine B. 3. Reflux the mixture under N_2 for 24 hours. 4. Collect the resulting materials by filtration. 5. Wash the resulting materials properly with ethanol to remove any unreacted reagent. 6. Dry the solids under vacuum.
Scale	milligram
Elemental Analysis	Calcd (%) for$[Fe(C_2H_4N_4)_{2.71}(C_{30}H_{33}N_6O_2Cl)_{0.29}]\cdot(ClO_4)_2$: C 28.14, H 3.41, N 22.94. Found: C 28.13, H 2.97, N 26.92.
State	red solid.
CAS Method Number	3-614-CAS-1824301

更好的阅读体验

SciFinder® A CAS SOLUTION

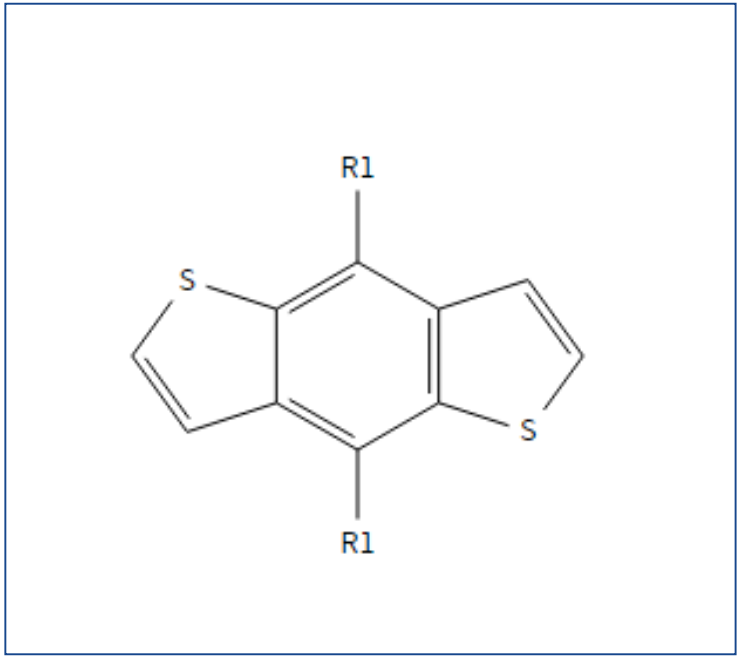
提纲

- 聚合物结构检索
- 聚合物分子式检索
- 聚合物反应检索
  - 检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）
  - 尼龙1212（单体：十二胺、十二酸）的聚合方法

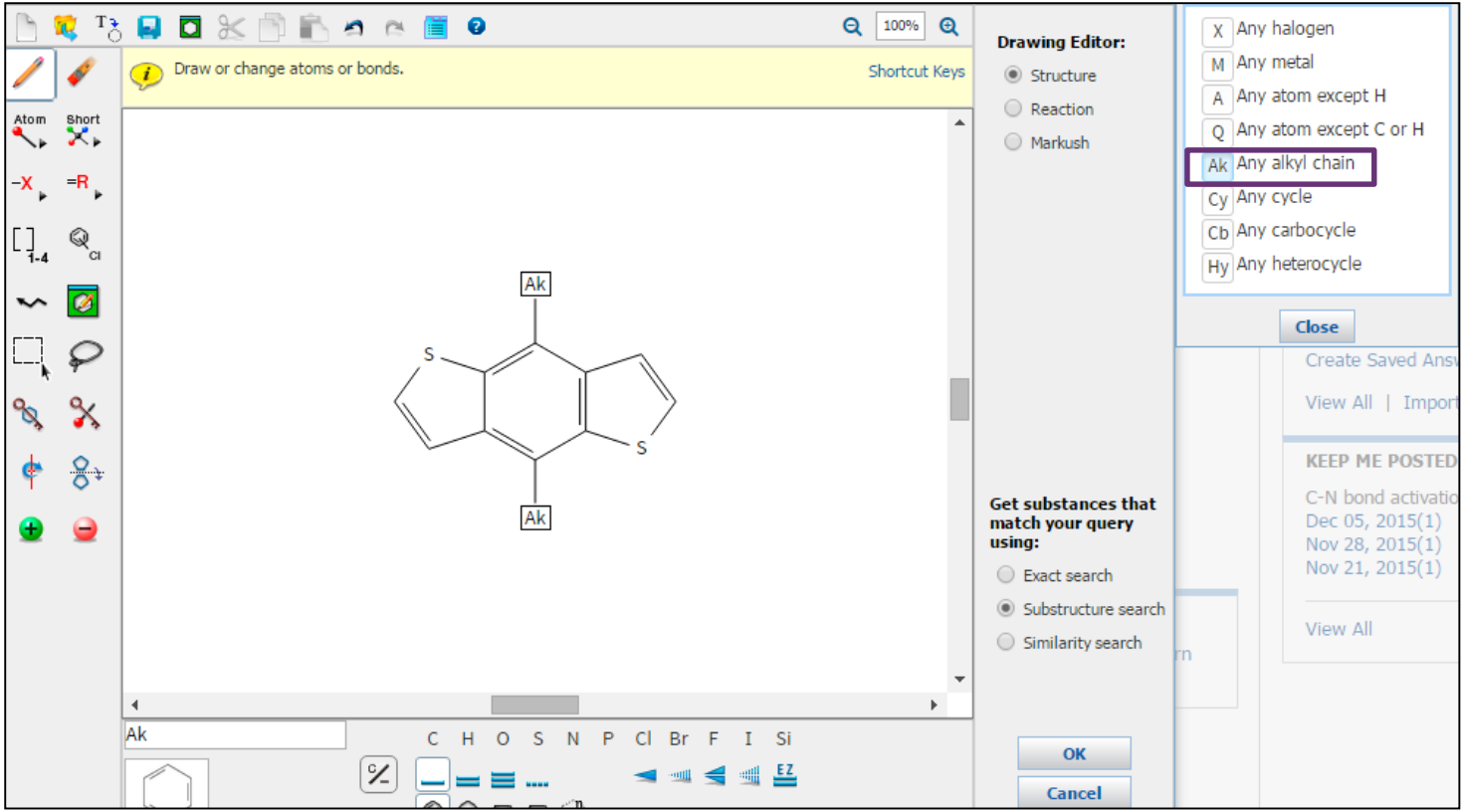
SciFinder® A CAS SOLUTION

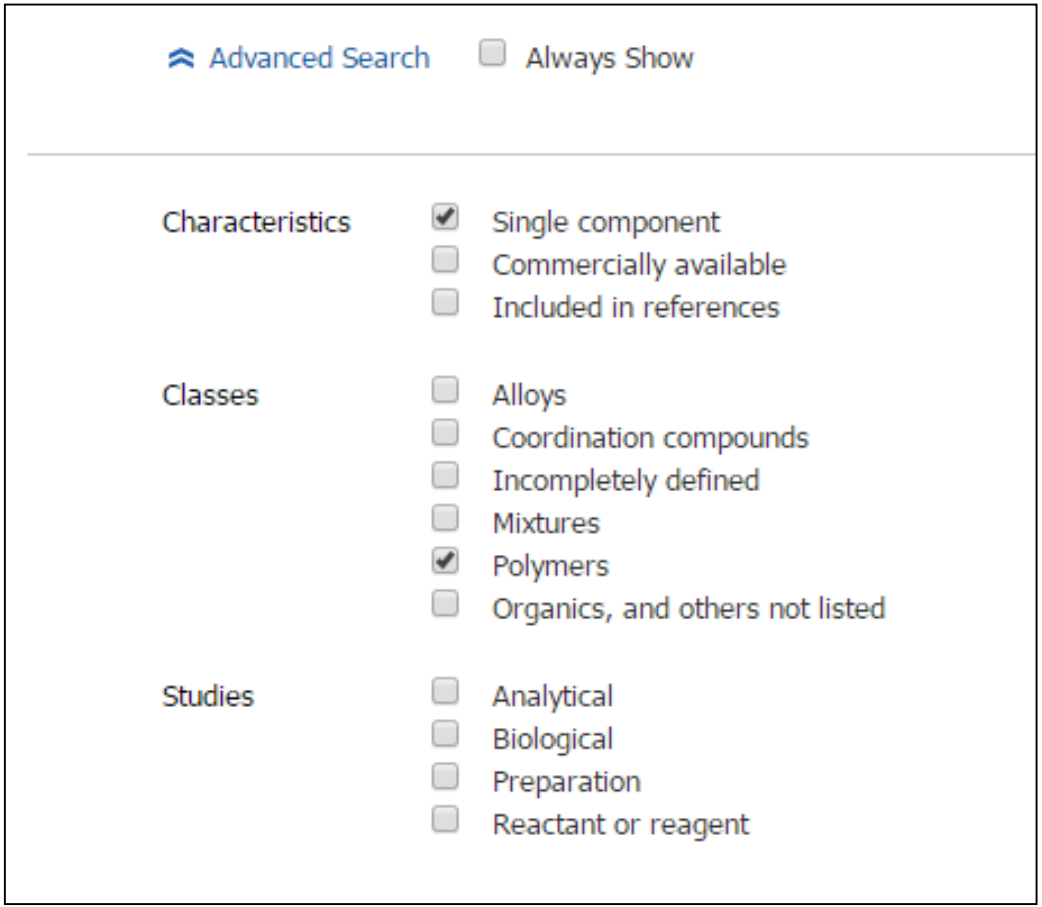
聚合物检索——结构式检索

- 案例：检索以下结构作为聚合单体的均聚物信息并对检索结果进行筛选



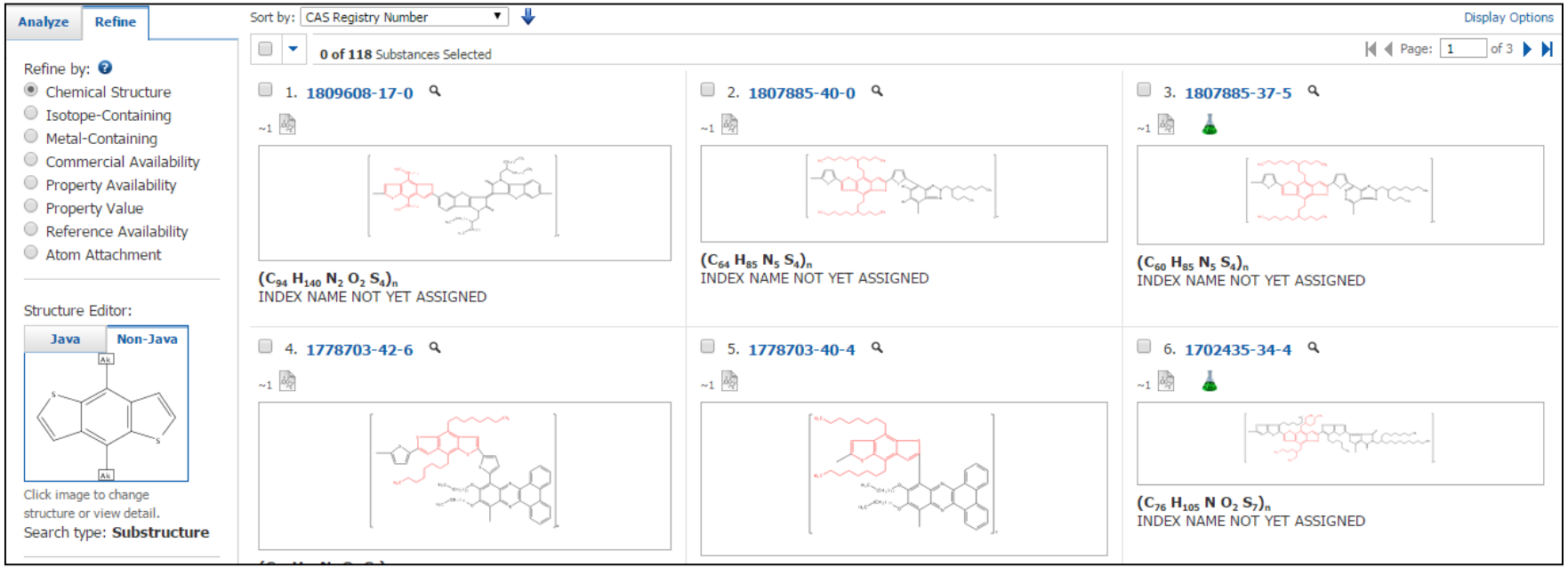
R1 = alkyl chains



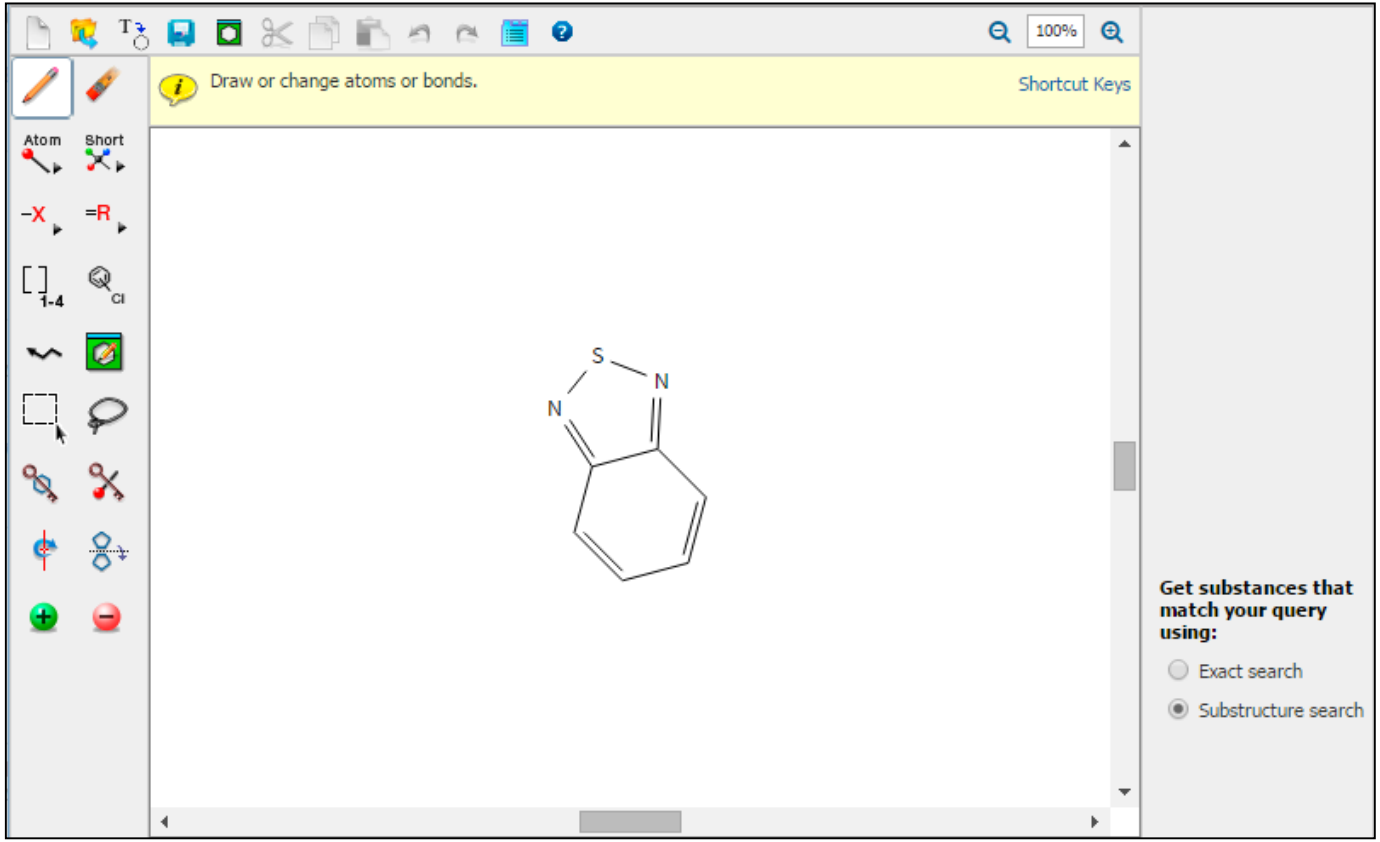


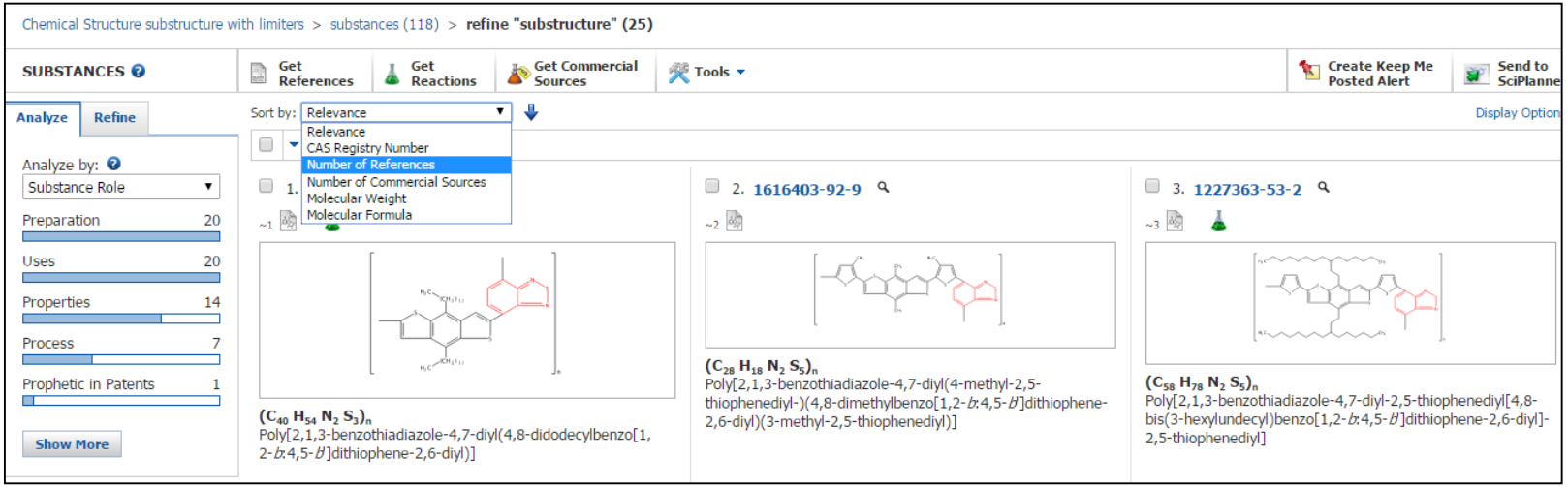
SciFinder® A CAS SOLUTION

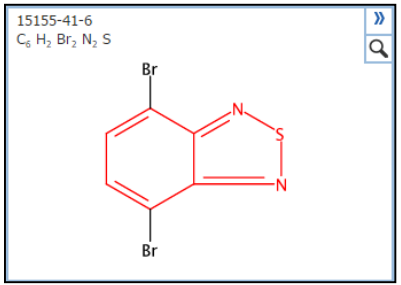
通过化学结构限定检索结果

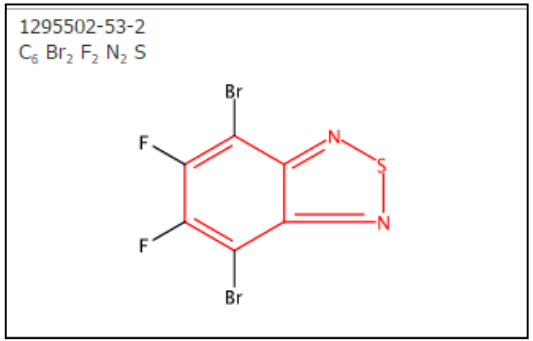


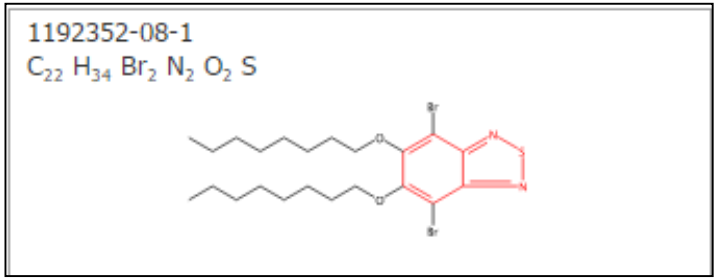
SciFinder® A CAS SOLUTION











SciFinder® A CAS SOLUTION

提纲

- 聚合物结构检索
- 聚合物分子式检索
- 聚合物反应检索
  - 检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）
  - 尼龙1212（单体：十二胺、十二酸）的聚合方法

SciFinder® A CAS SOLUTION

聚合物检索——分子式检索

- 聚合物的分子式表现形式

  分子式中带有括号

  括号外为n，嵌段聚合物（有首尾端或无首尾段都可）

  有端基嵌段聚合物分子式：(C6H10O2)n C3H4O2

  无端基嵌段聚合物分子式：（C12 H12 O4)n

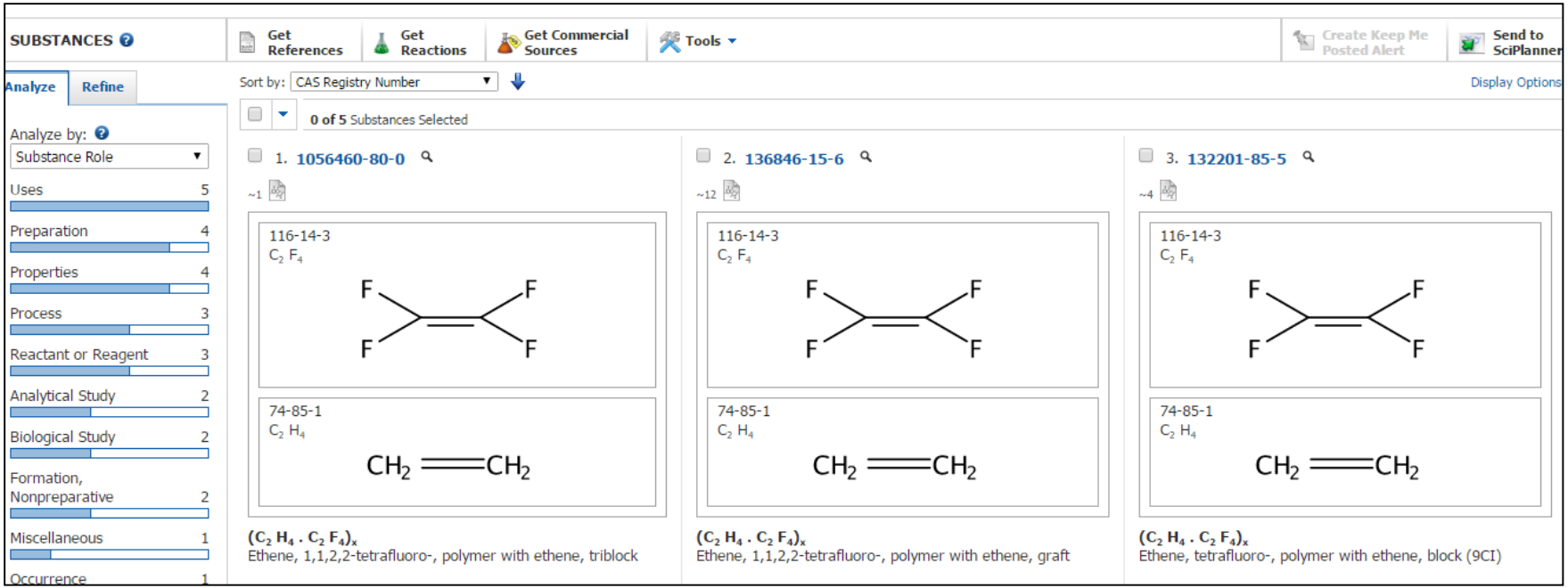
  括号外为x，对于均聚物和共聚物，将以单体进行标引，聚合度不影响标引

  共聚物：(C2 H4 . C2 F4)x

  均聚物：(C2H4)x

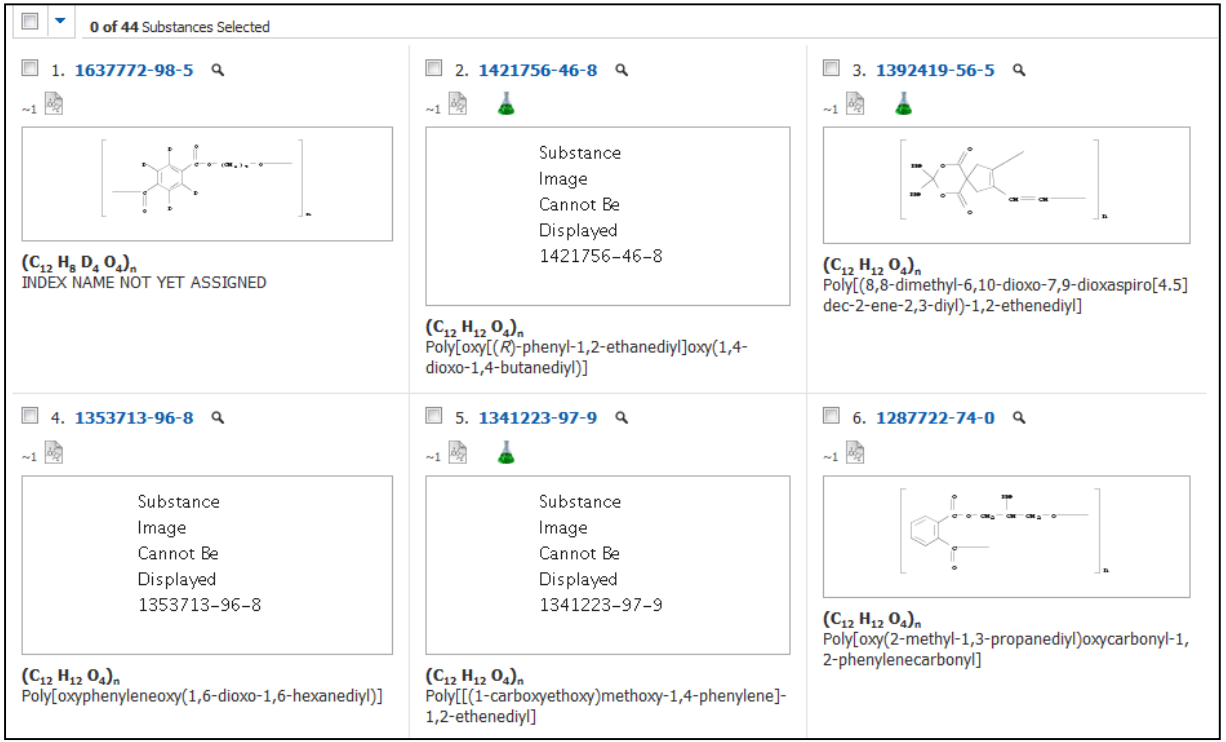
SciFinder® A CAS SOLUTION

(C2 H4 . C2 F4)x——SciFinder检索结果



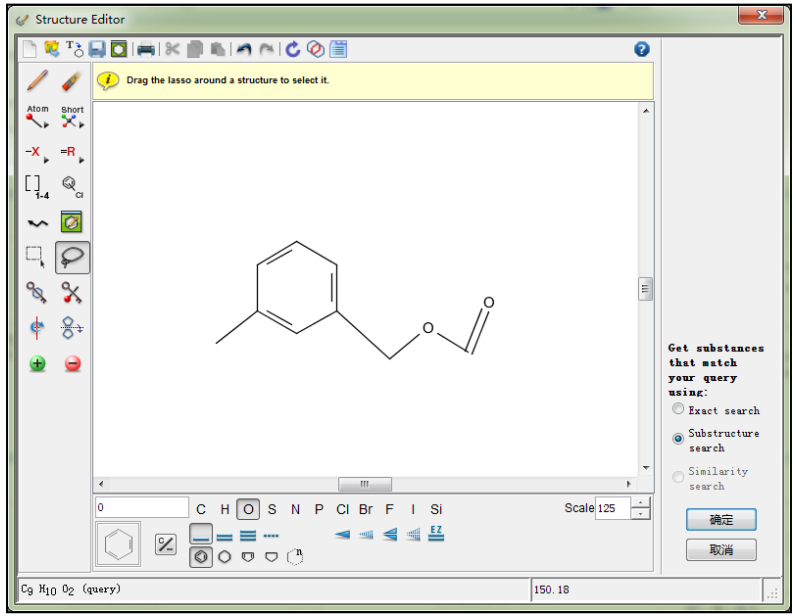
SCIFINDER® A CAS SOLUTION

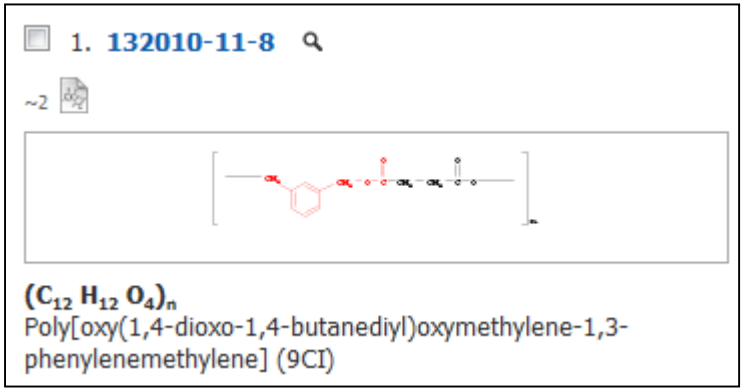
(C12 H12 O4)n——SciFinder检索结果



SciFinder® A CAS SOLUTION

用结构限定





SciFinder® A CAS SOLUTION

提纲

- 聚合物结构检索
- 聚合物分子式检索
- 聚合物反应检索
  - 检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）
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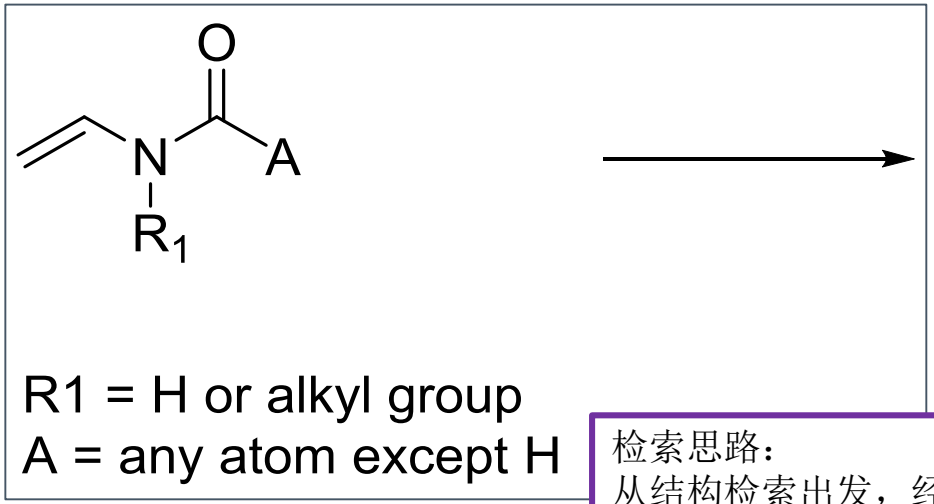
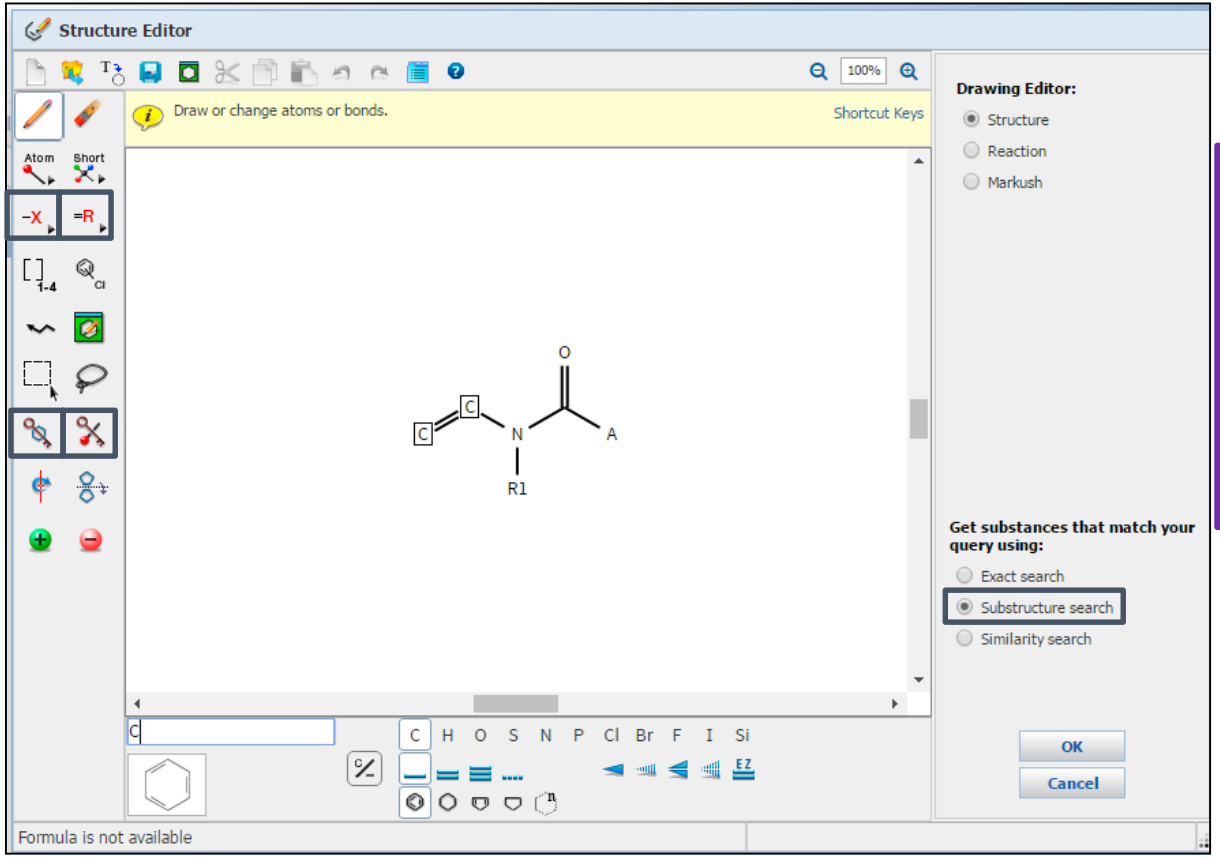
检索案例：检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）



检索思路：
从结构检索出发，经过限定后，得到聚合物物质结果集
方案一：由物质获得反应，再获得相关合成制备文献；
方案二：由物质获得文献，再通过文献检索结果处理工具精选文献



打开物质检索结构编辑器，
绘制起始物结构，
使用可变基团工具，
R基团定义工具，
环锁定工具
原子锁定工具对结构进行限定。

选择亚结构检索

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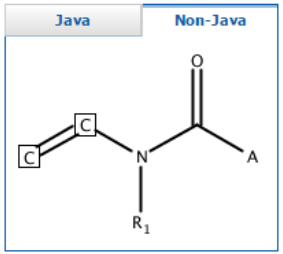
Structure Editor:

Java | Non-Java



Click image to change structure or view detail.

Import CXF

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. Learn More

Search

Advanced Search | Always Show

Characteristics

- Single component
- Commercially available
- Included in references

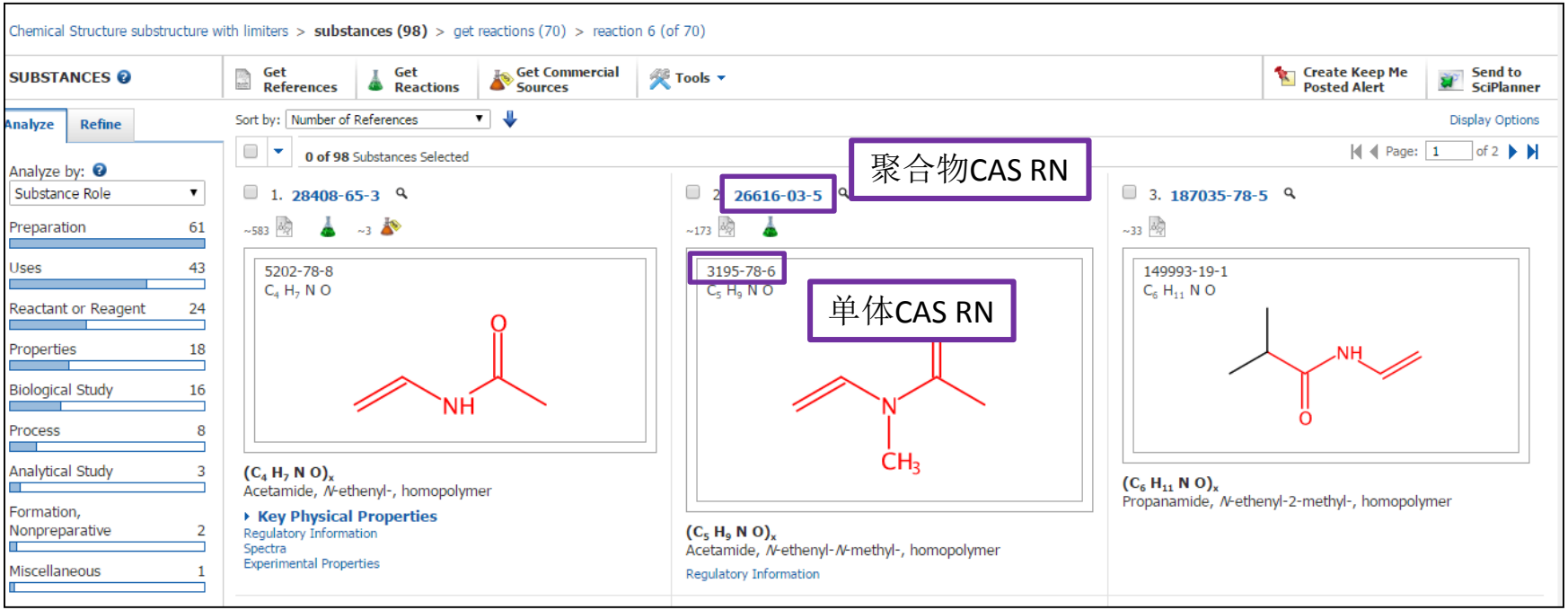
Classes

- Alloys
- Coordination compounds
- Incompletely defined
- Mixtures
- Polymers
- Organics, and others not listed

在Advanced Search中，选中Single component和Polymers

SciFinder® A CAS SOLUTION

获得98个均聚物物质结果

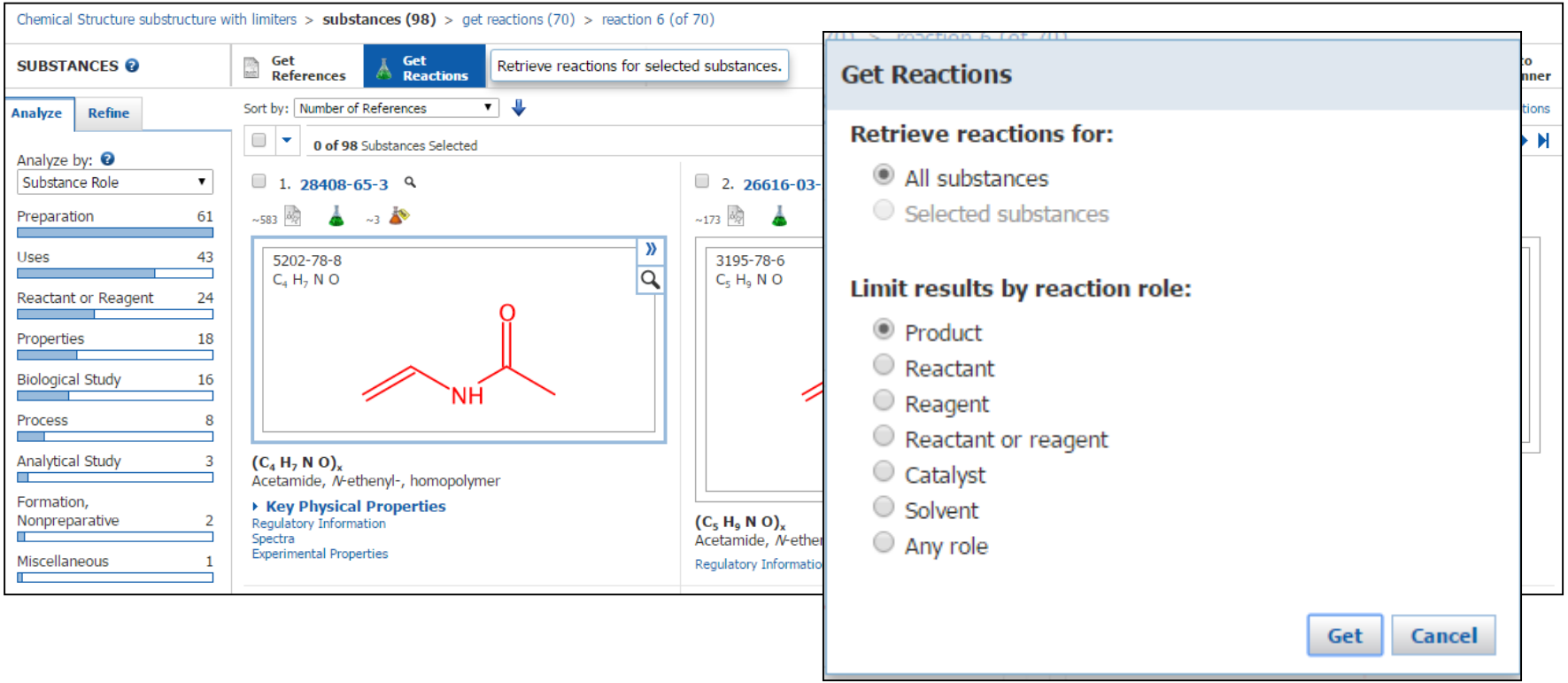


SCIFINDER® A CAS SOLUTION

方案一：
由物质获得反应，再获得相关合成制备文献

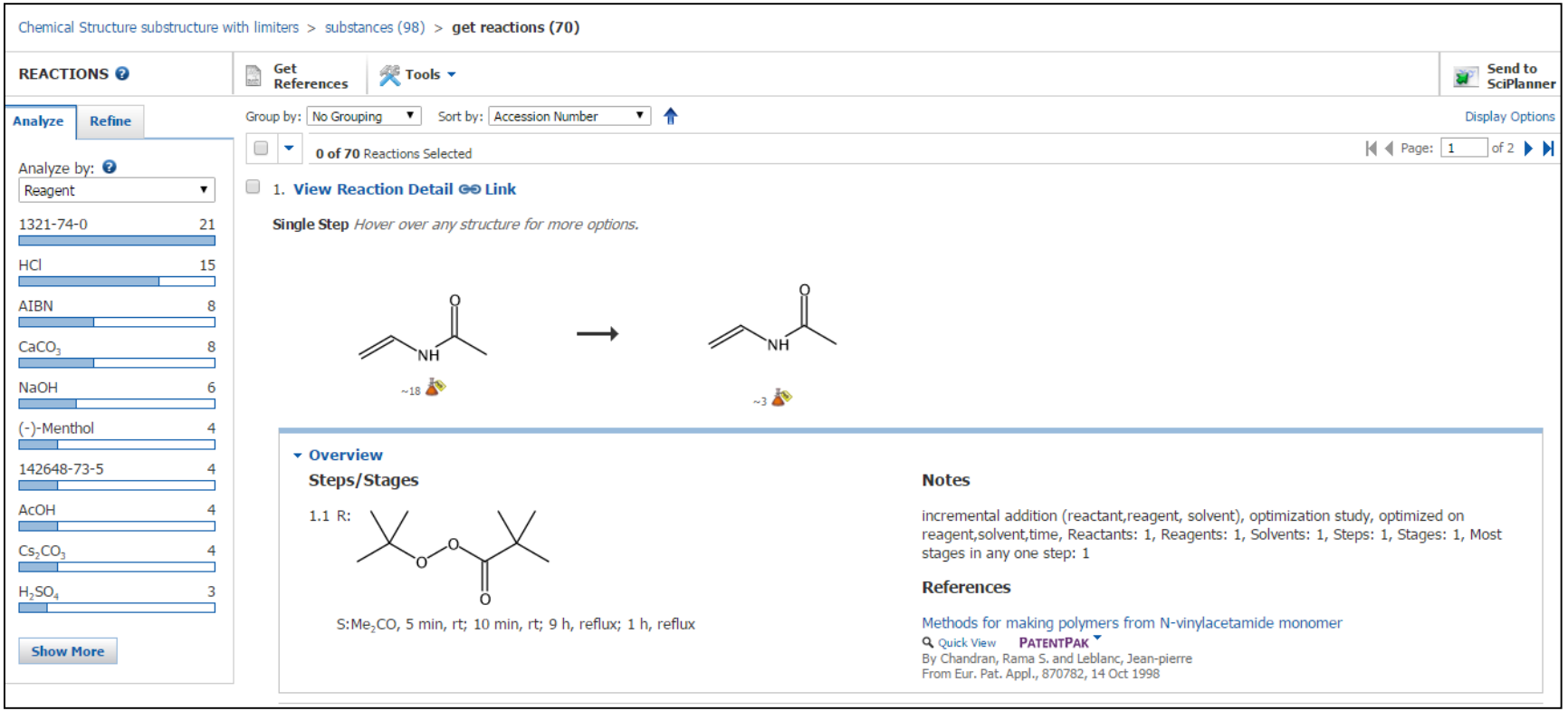
SciFinder® A CAS SOLUTION

方案一：通过物质（限定为产物）获得反应



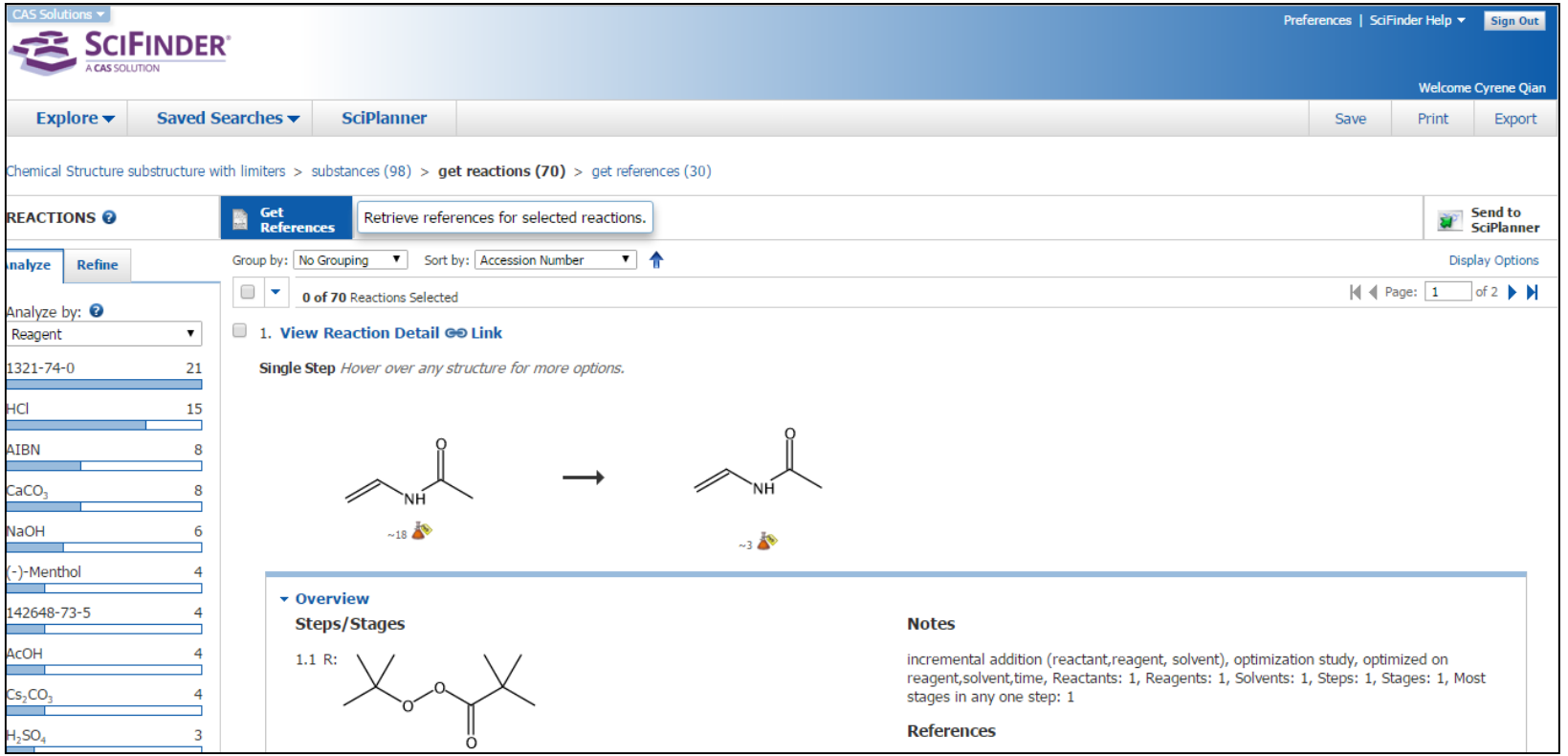
SciFinder® A CAS SOLUTION

获得70条满足检索需要的反应



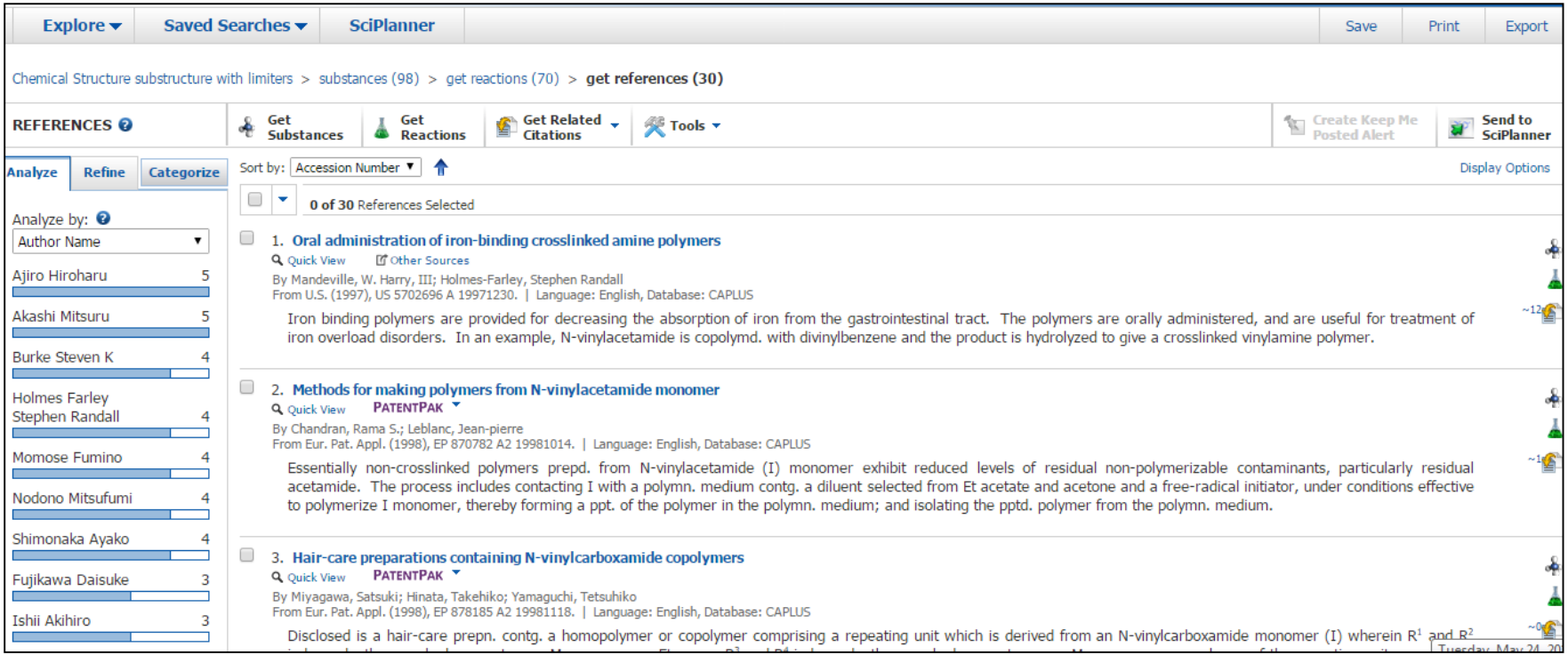
SciFinder® A CAS SOLUTION

通过反应获得文献



SciFinder® A CAS SOLUTION

获得30篇和聚合物制备相关的文献

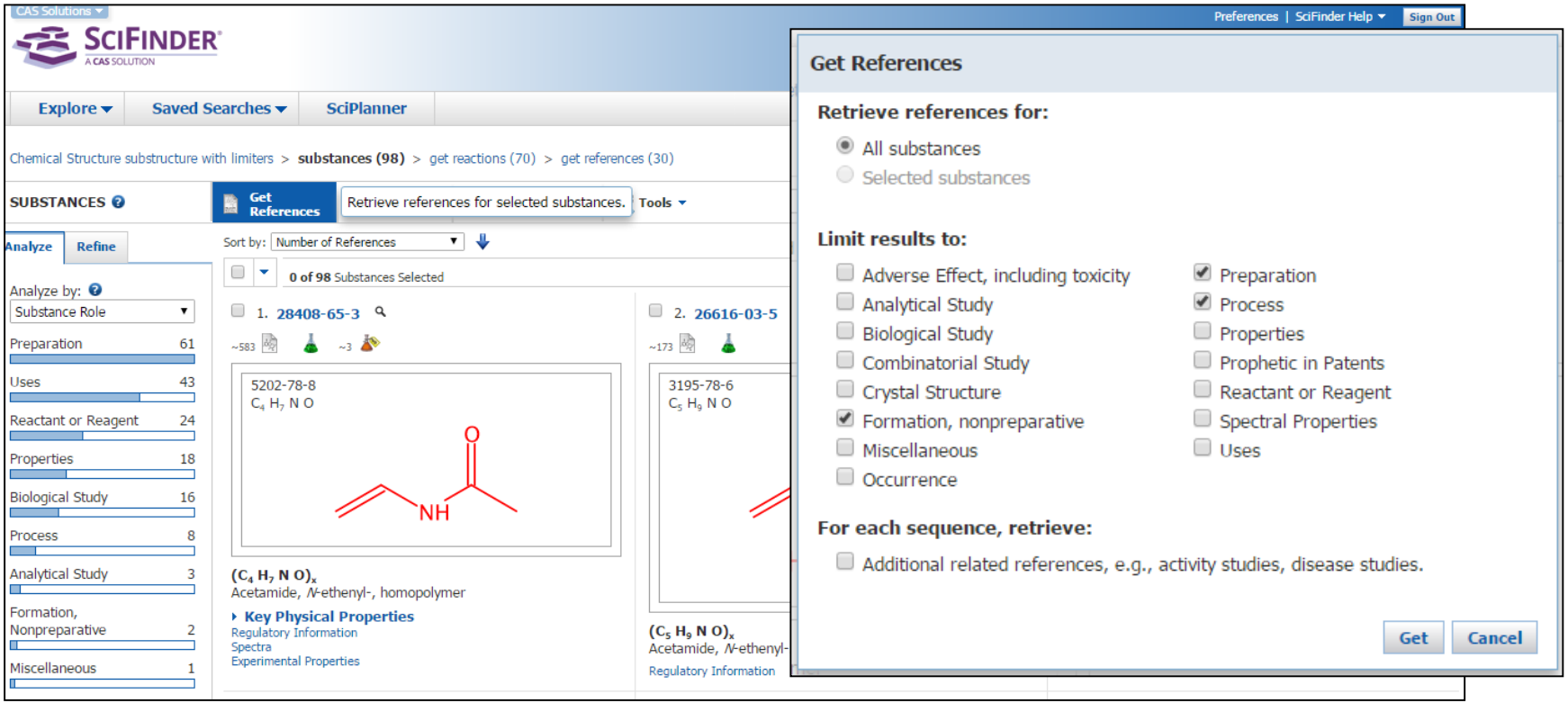


SciFinder® A CAS SOLUTION

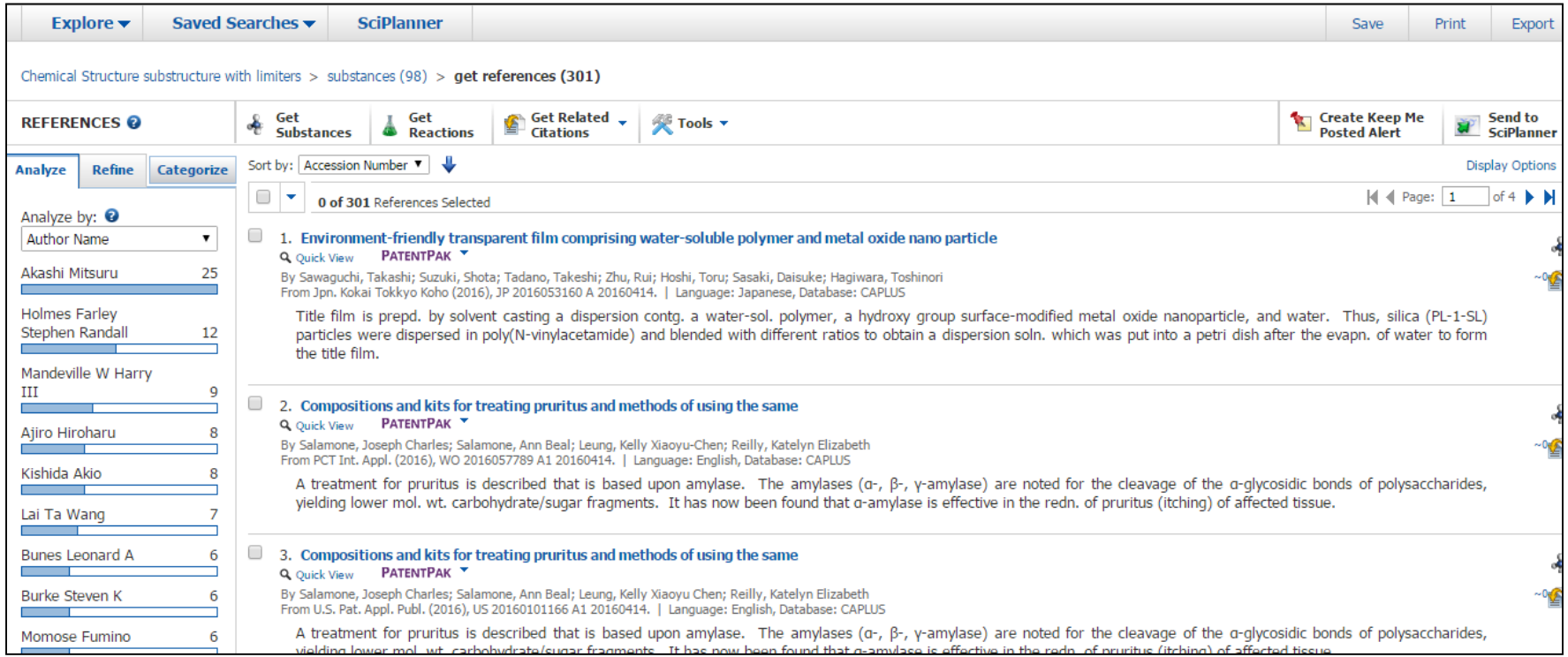
方案二：
由物质获得文献，再通过文献检索结果处理工具精选文献

SciFinder® A CAS SOLUTION

方案二：通过物质获得文献（限定为合成/制备/工艺）



获得301篇文献



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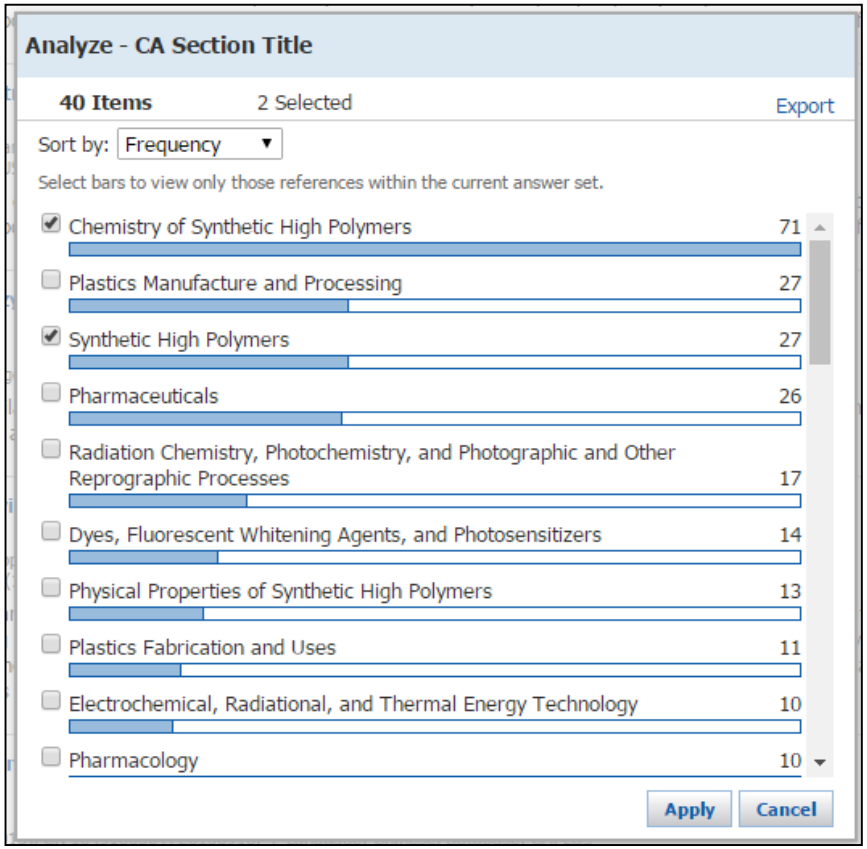
可以通过CA Section Title等选项进行分析，甄选文献



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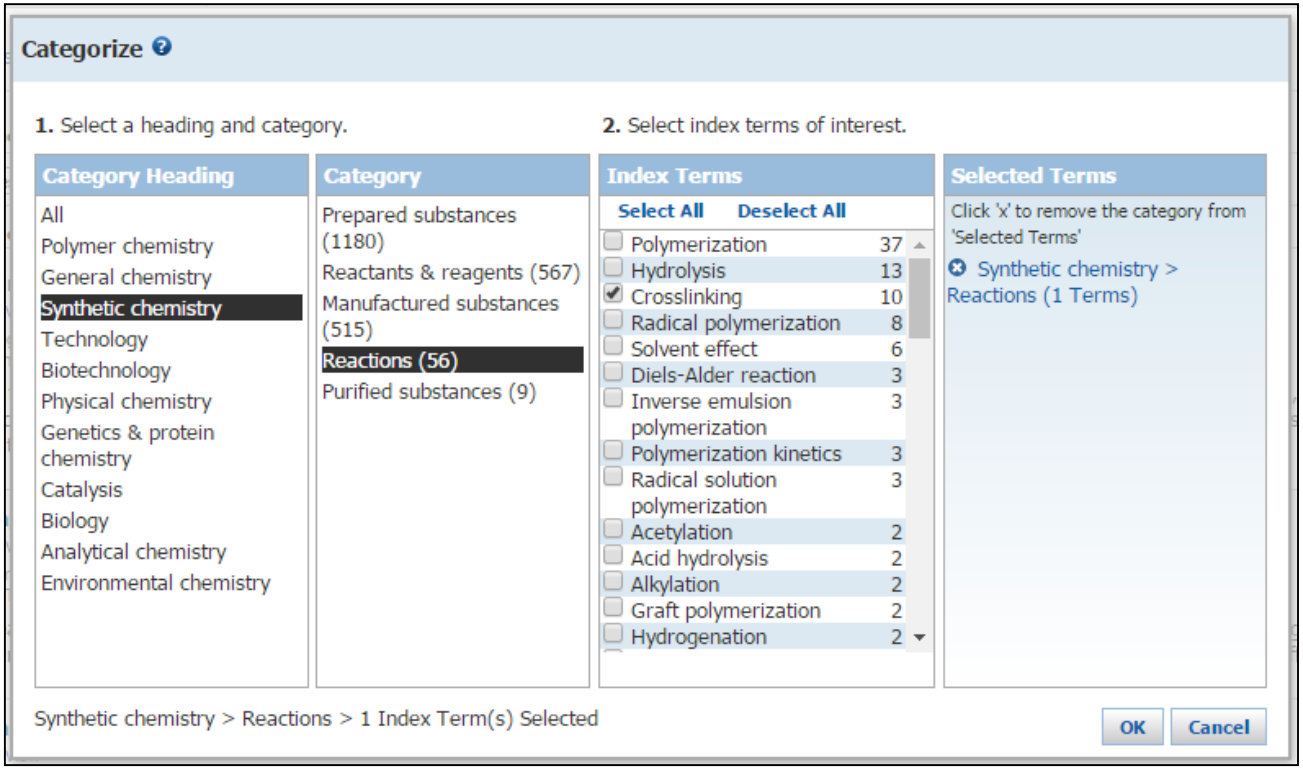
通过分类工具，可以对反应类型/关键词等进行限定，筛选文献



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均聚物合成/制备检索技巧总结

- 如果需要用结构式检索均聚物合成、制备信息，则可用以下操作步骤：
  1. 直接绘制单体的结构式，并在执行检索之前，将条件设置为单组分、聚合物
  2. 获取到物质结果集后：
     - A) 如果希望获取到精准的化学反应，则可通过物质获取化学反应，并限定物质在反应过程中的角色（产物）
     - B) 如果希望获取最完整、全面的文献信息，则可通过物质获取文献信息，并将结果限定为工艺，制备等

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提纲

- 聚合物结构检索
- 聚合物分子式检索
- 聚合物反应检索
  - 检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）
  - 尼龙1212（单体：十二胺、十二酸）的聚合方法

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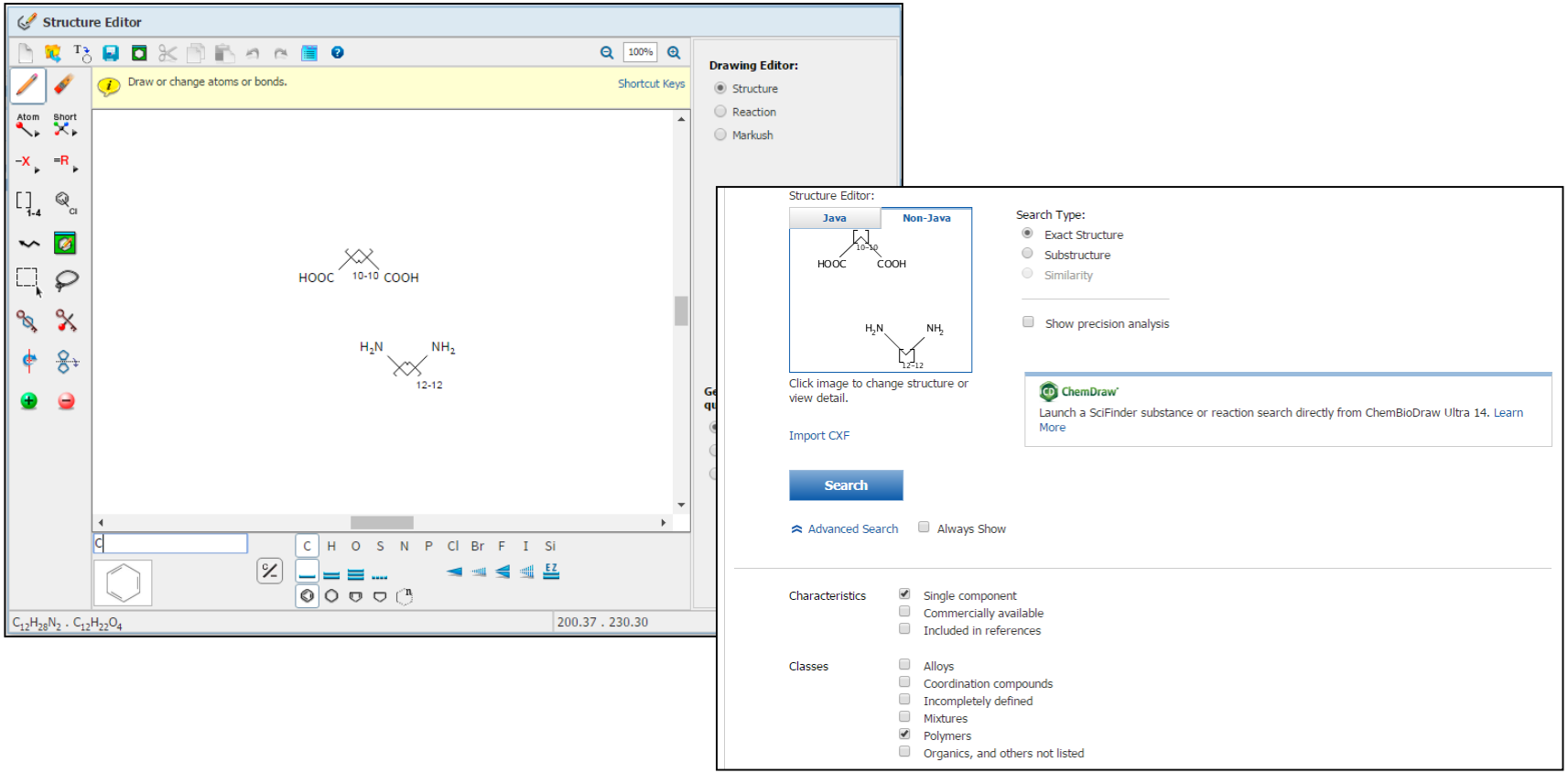

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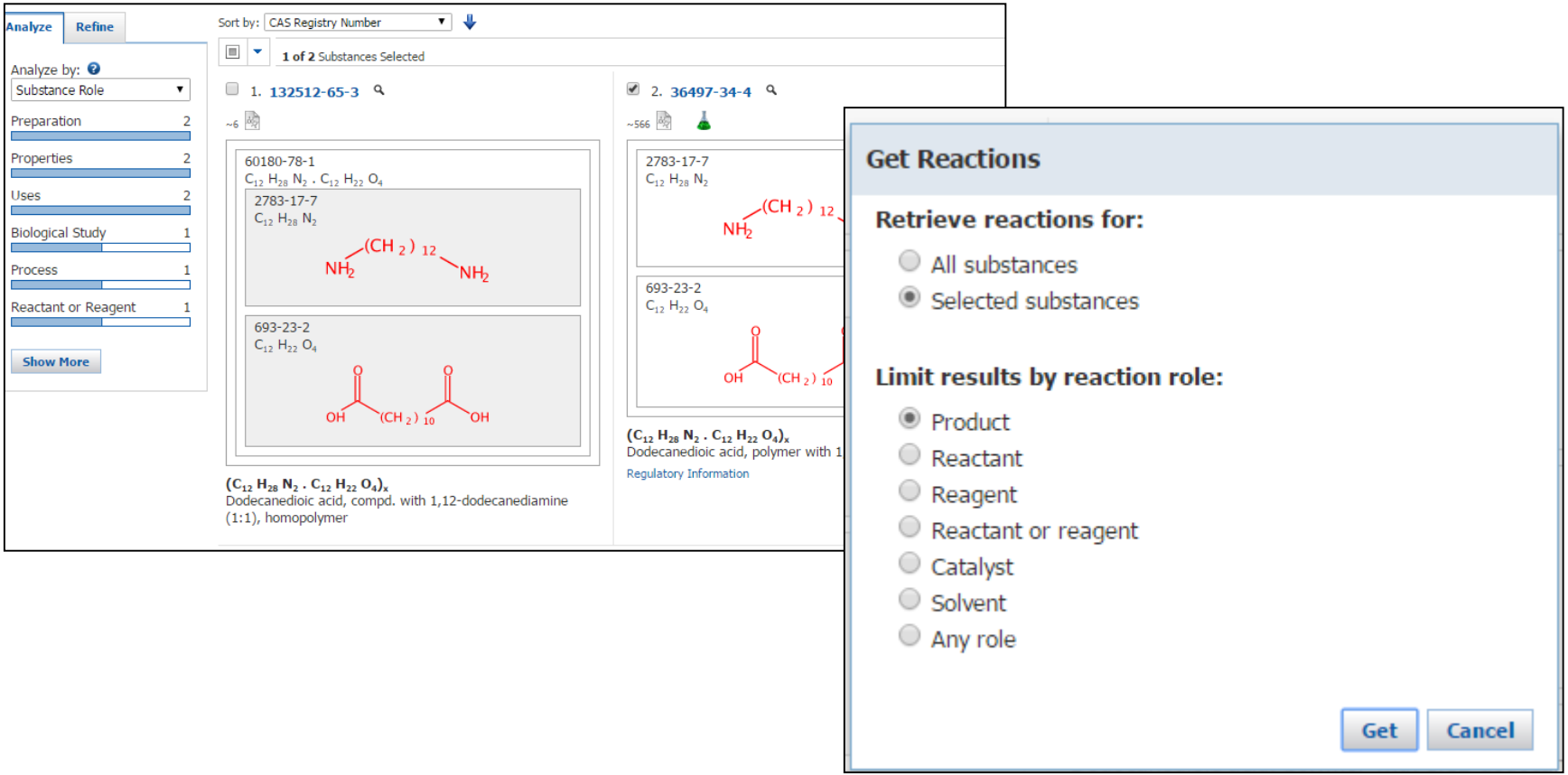

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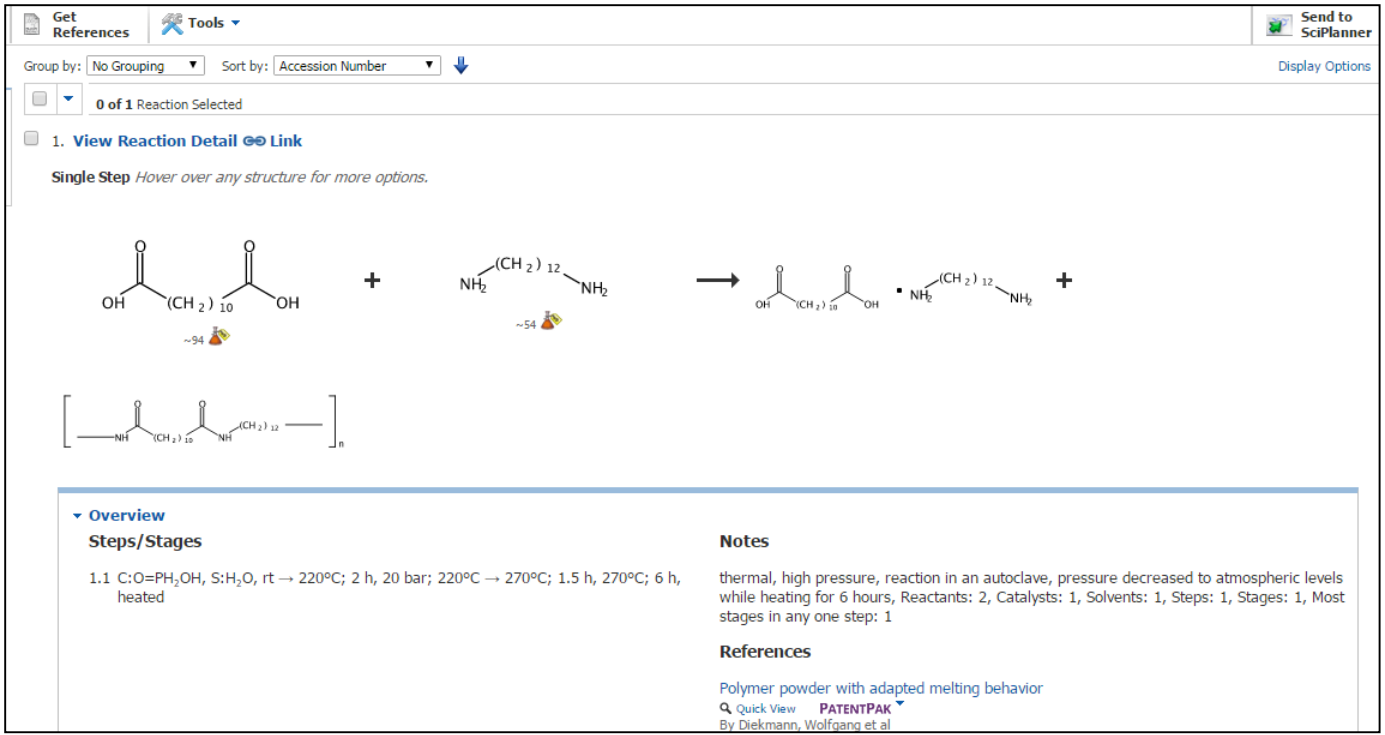
尼龙1212（单体：十二胺、十二酸）的聚合方法



注意事项

- 一人注册一个帐号
- 严禁过量下载
- 严禁将帐号用于非学术研究
- 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
- Mac电脑，如使用Safari浏览器请注意及时升级版本，不要拦截SciFinder插件，或者安装火狐或者谷歌浏览器使用SciFinder

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谢谢关注！

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