钱欣博士
Application Specialist
cqian@acs-i.org

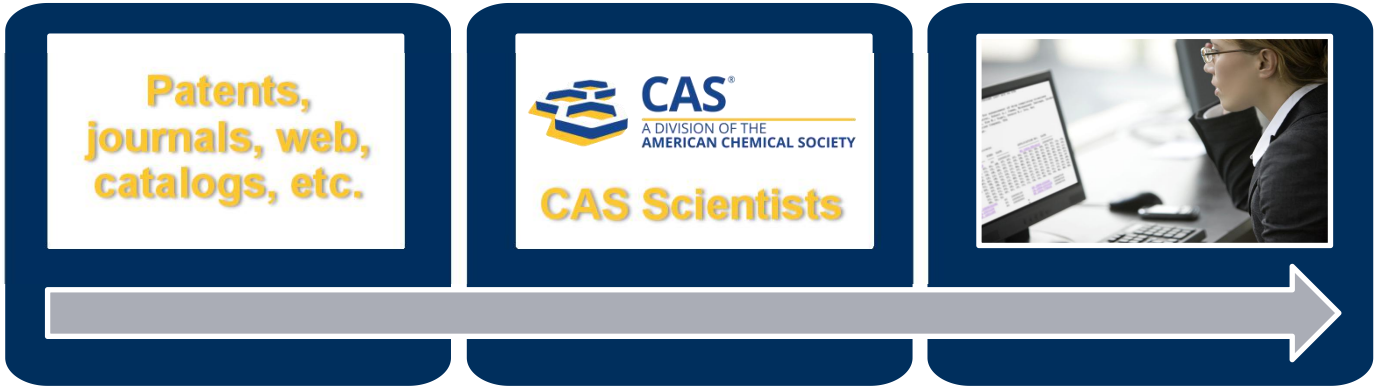
如何使用SciFinder获取科技信息

SCIFINDER®
A CAS SOLUTION

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1400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

JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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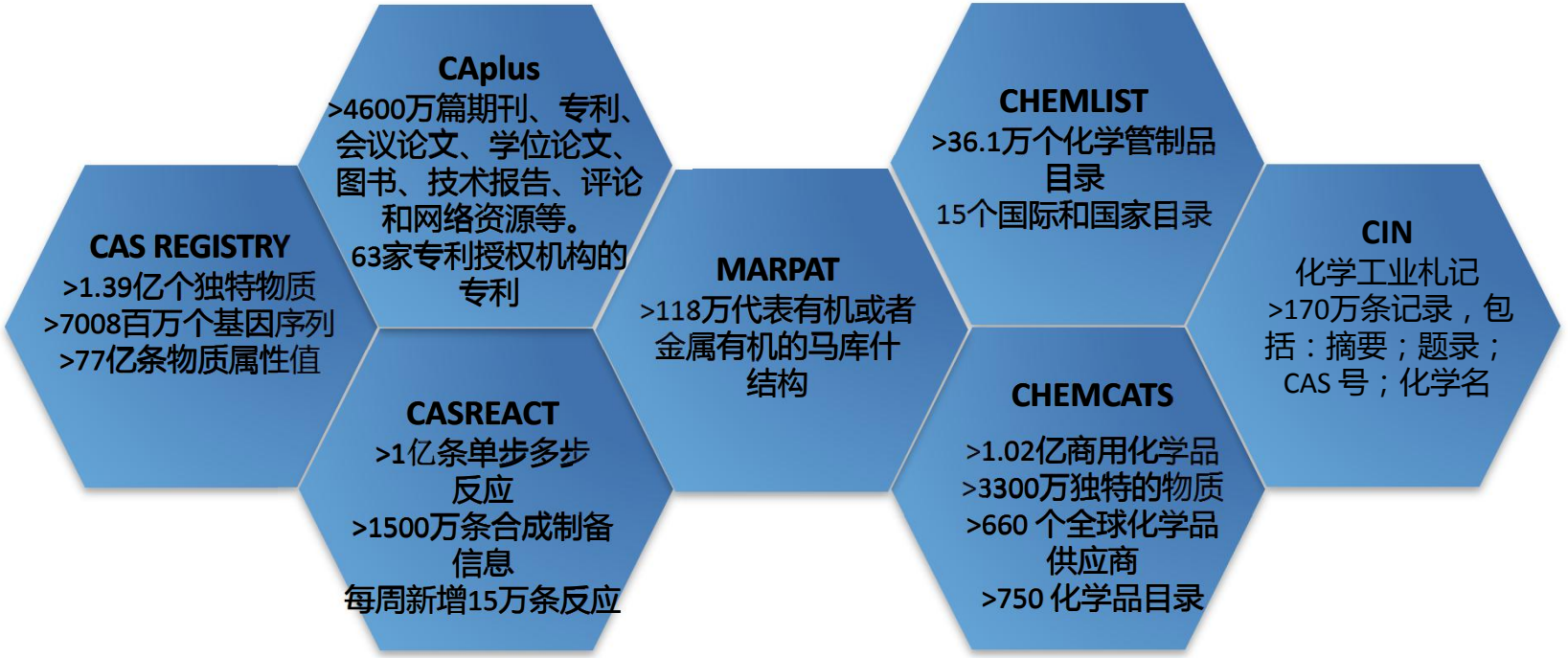

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CAS数据库——源于化学，超越化学

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

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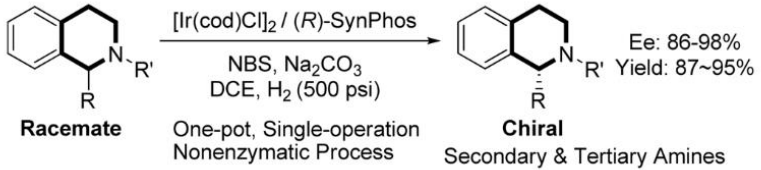
CAS数据库最具价值的内容——人工标引

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

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

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



Indexing

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

Concepts

Enantioselective synthesis
Hydrogenation catalysts
Oxidation

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

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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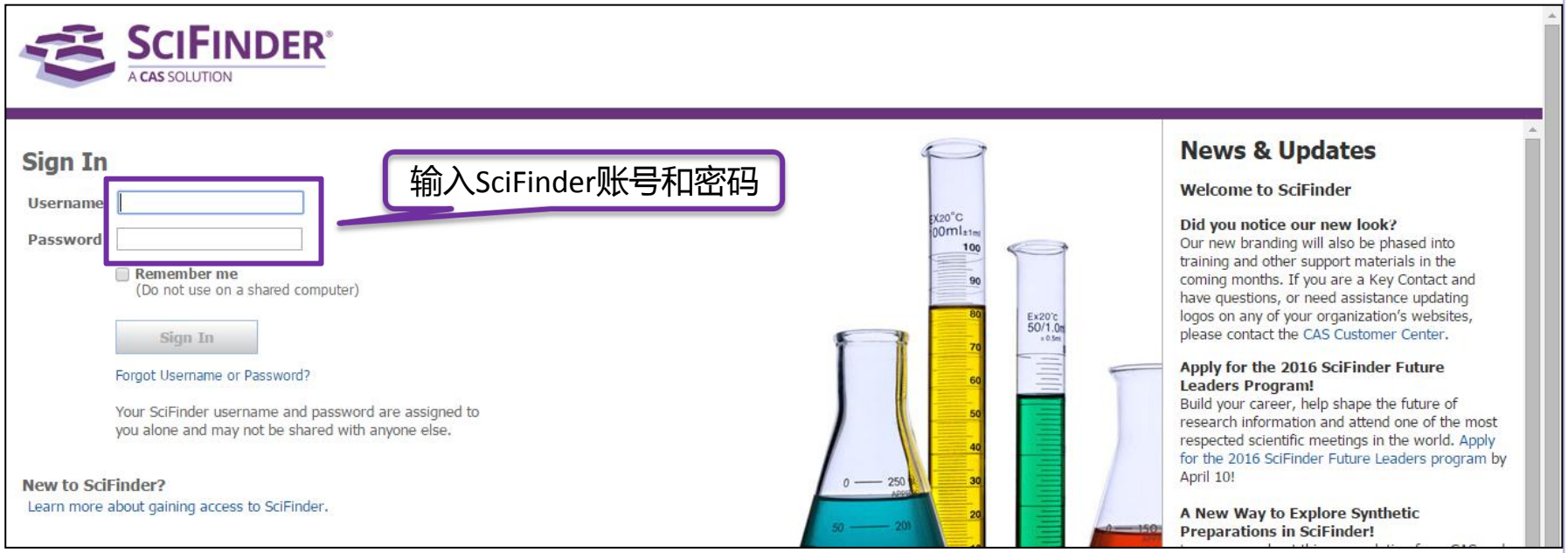
如何使用SciFinder提高科研效率

- **以“光解水”为例，如何利用SciFinder：**
  - 获取研究全景
  - 对文献结果进行分析、筛选、及精准定位所需信息
- **物质检索**
  - 如何从大量物质结果集中快速定位目标物质
  - 结构式检索；分子式检索（合金，多氧簇金属，MOF化合物）；物质属性检索
  - 如何获得物质的属性信息、谱图信息
  - 化合物分析方法检索
- **反应检索**
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何进行精确结构反应检索，并获得实验详情
  - 如何进行亚结构反应检索，以及如何处理检索结果
  - 案例分享
    - 多氧簇金属的反应信息
    - MOF化合物反应信息

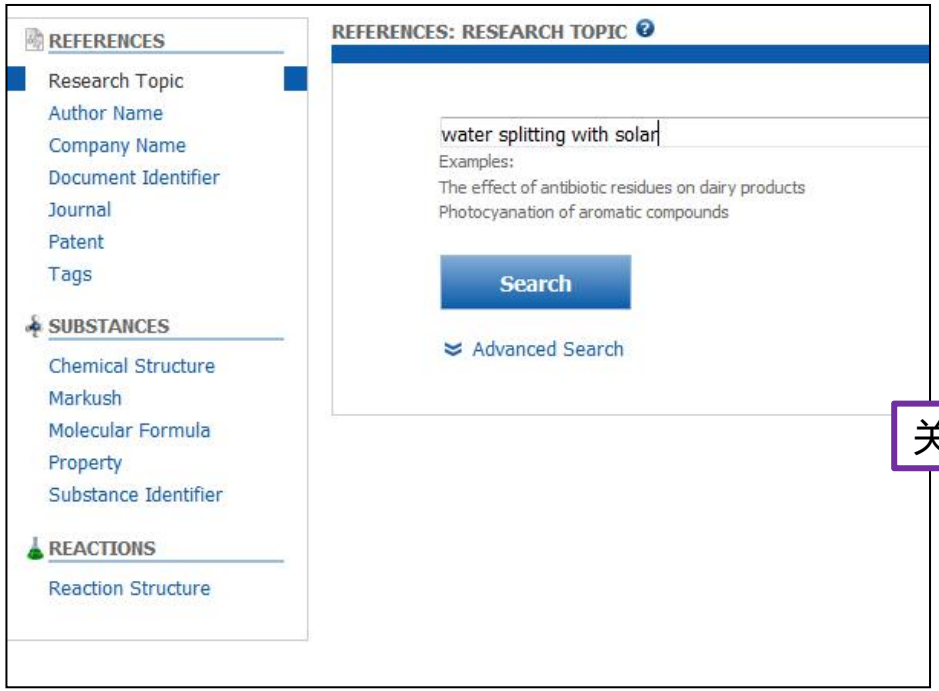
SciFinder登录网址: https://scifinder.cas.org/



SciFinder主界面

文献检索——主题: 光解水

- 检索式： water splitting with solar



关键词之间可用介词连接：in, with, of…

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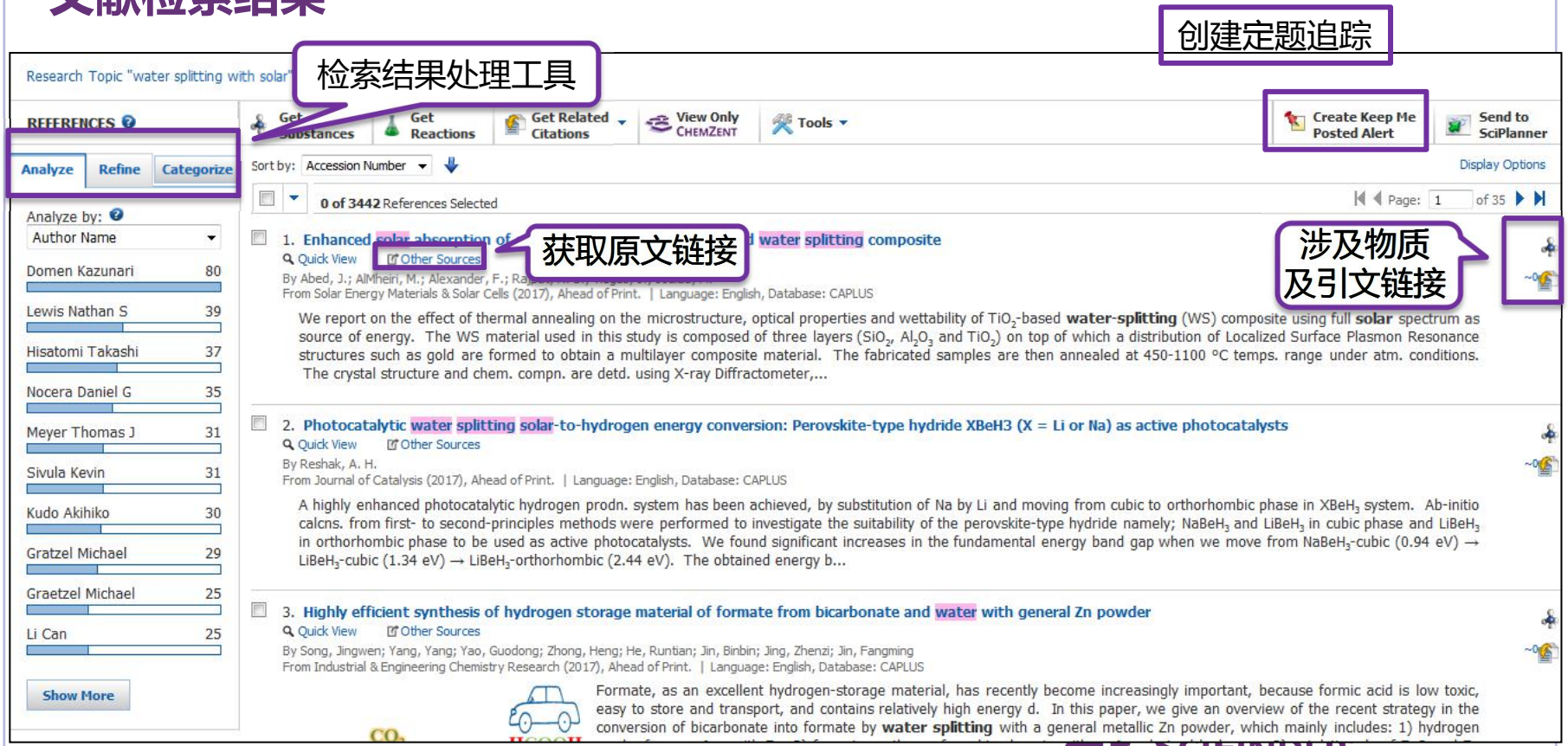
文献检索结果



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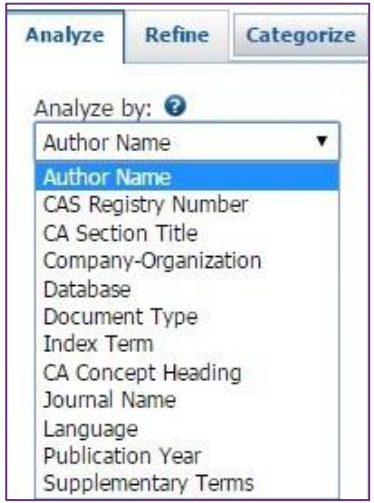
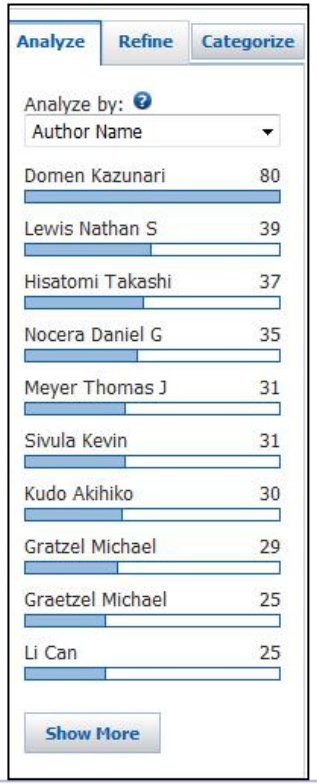
文献检索结果：Analyze

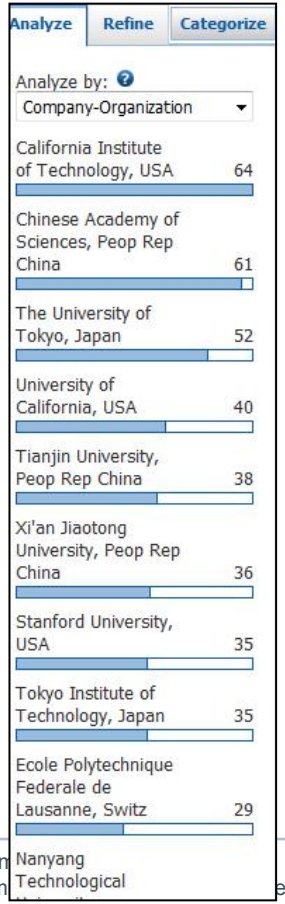
12种文献分析选项



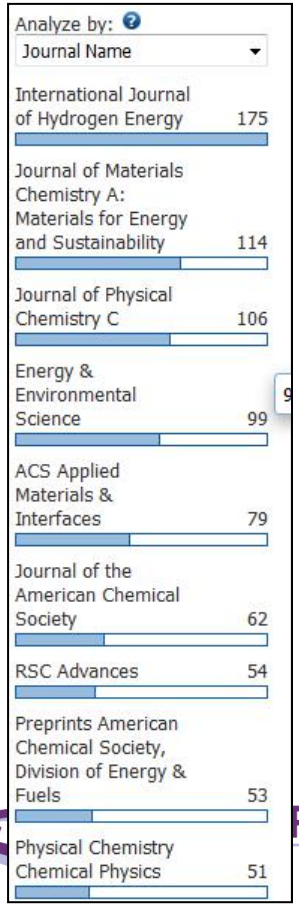
主要研究人员



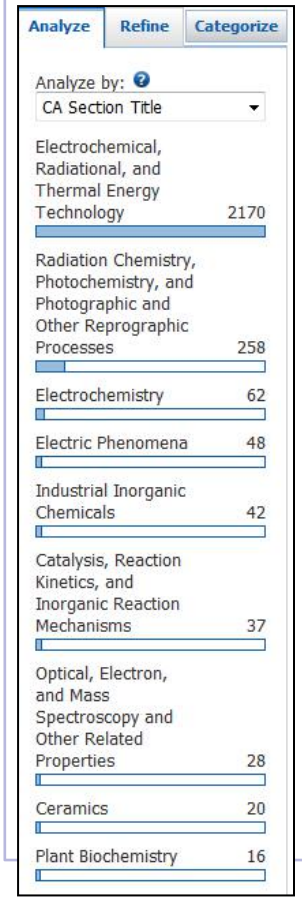
主要研究机构，
合作伙伴，竞争对手

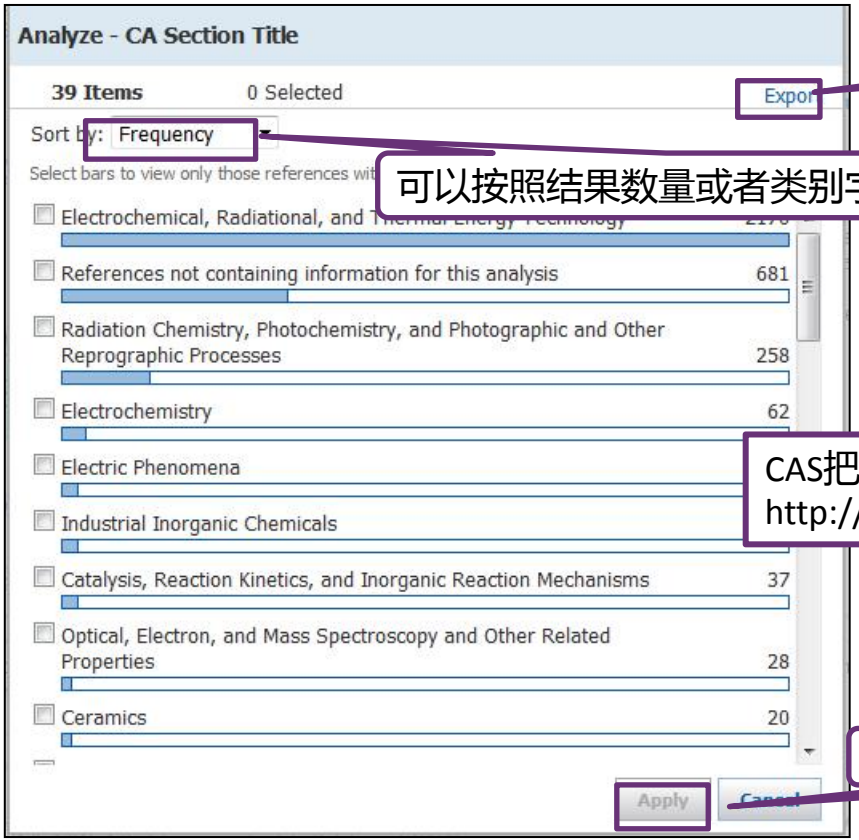


公开媒介



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:
http://www.cas.org/content/ca-sections

选择感兴趣的词语,点击Apply

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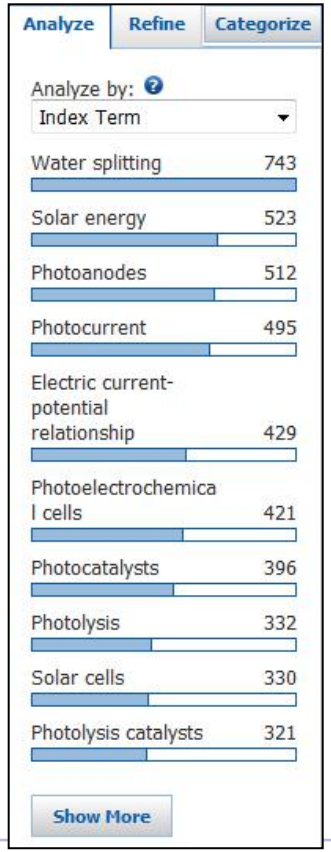
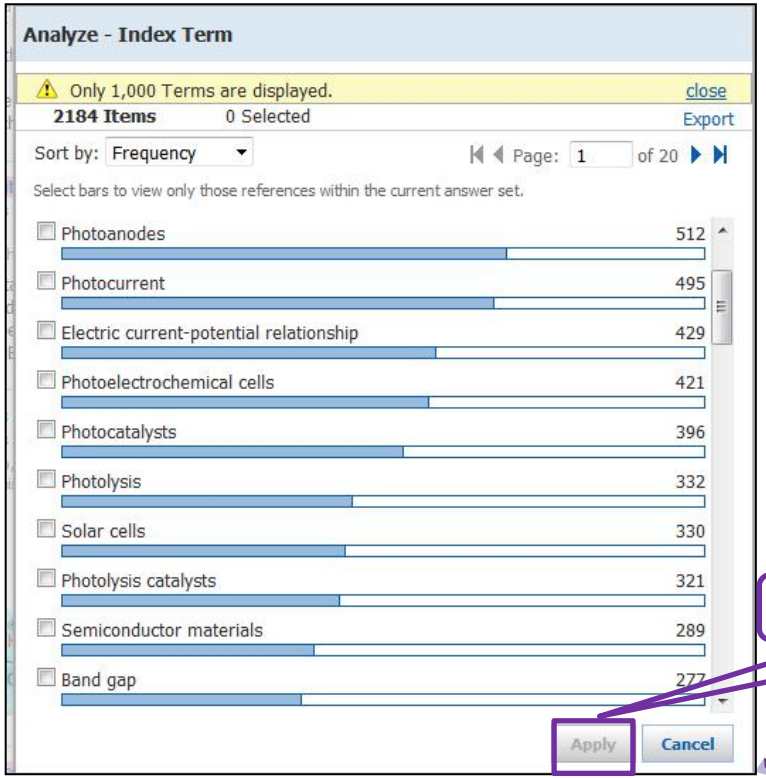
文献检索结果：Analyze



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



选择感兴趣的词语,点击Apply

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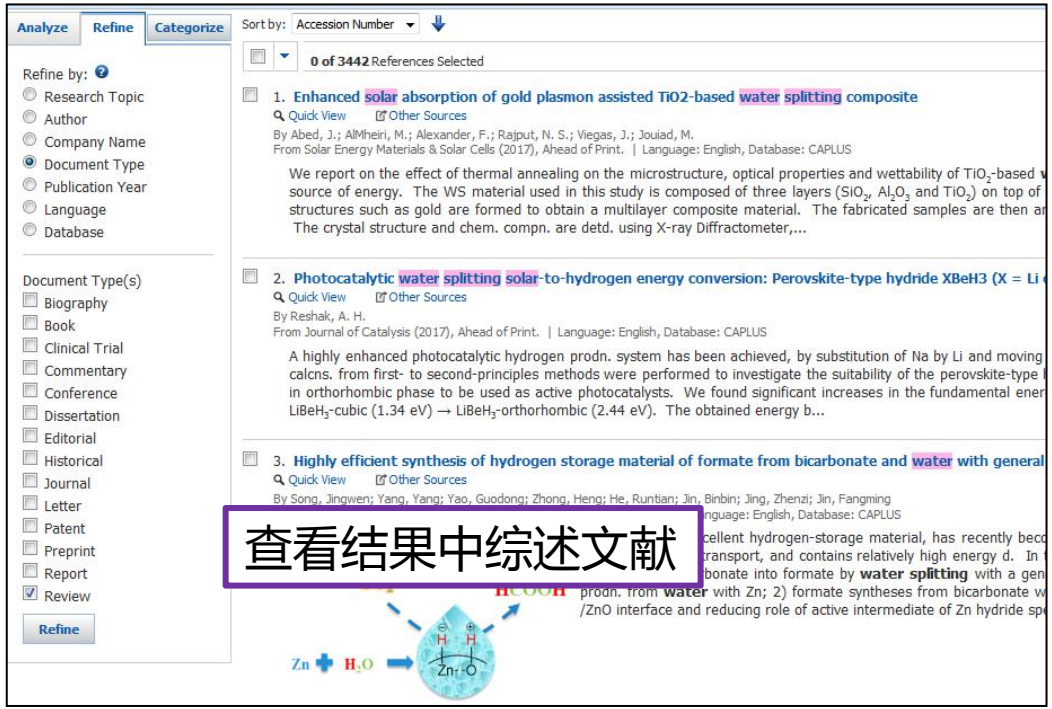
文献检索结果：Refine

- 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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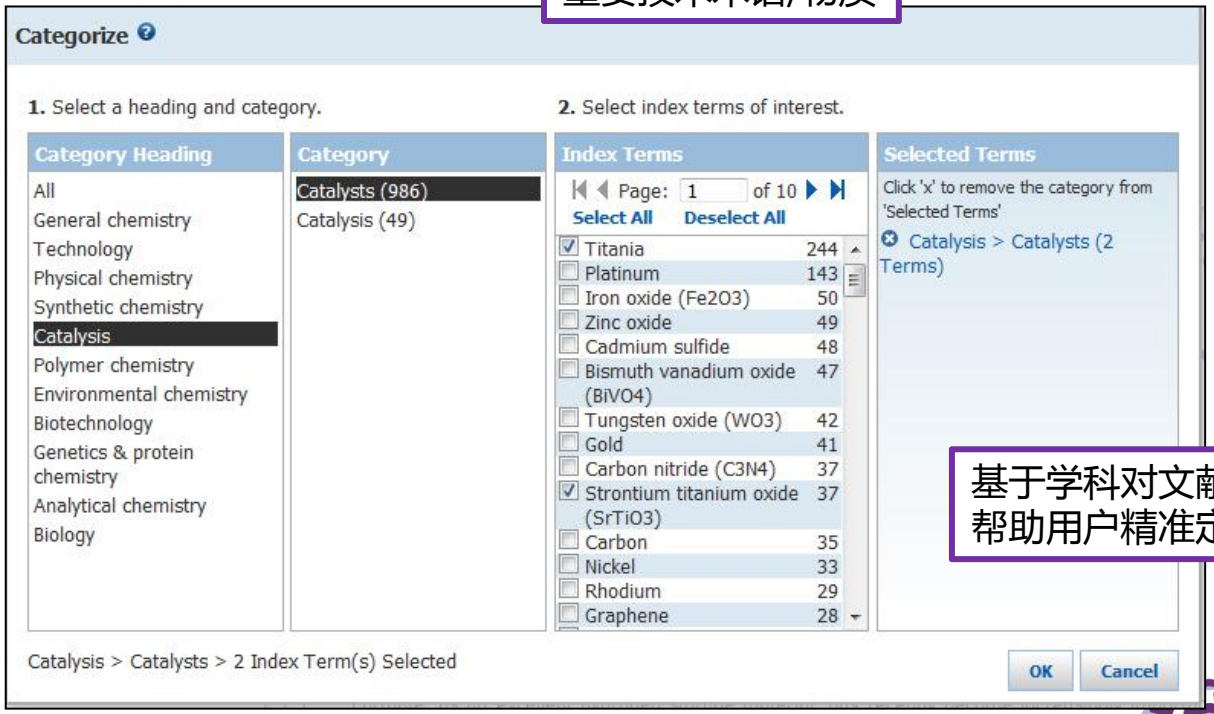
光解水中指定某催化剂的文献

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



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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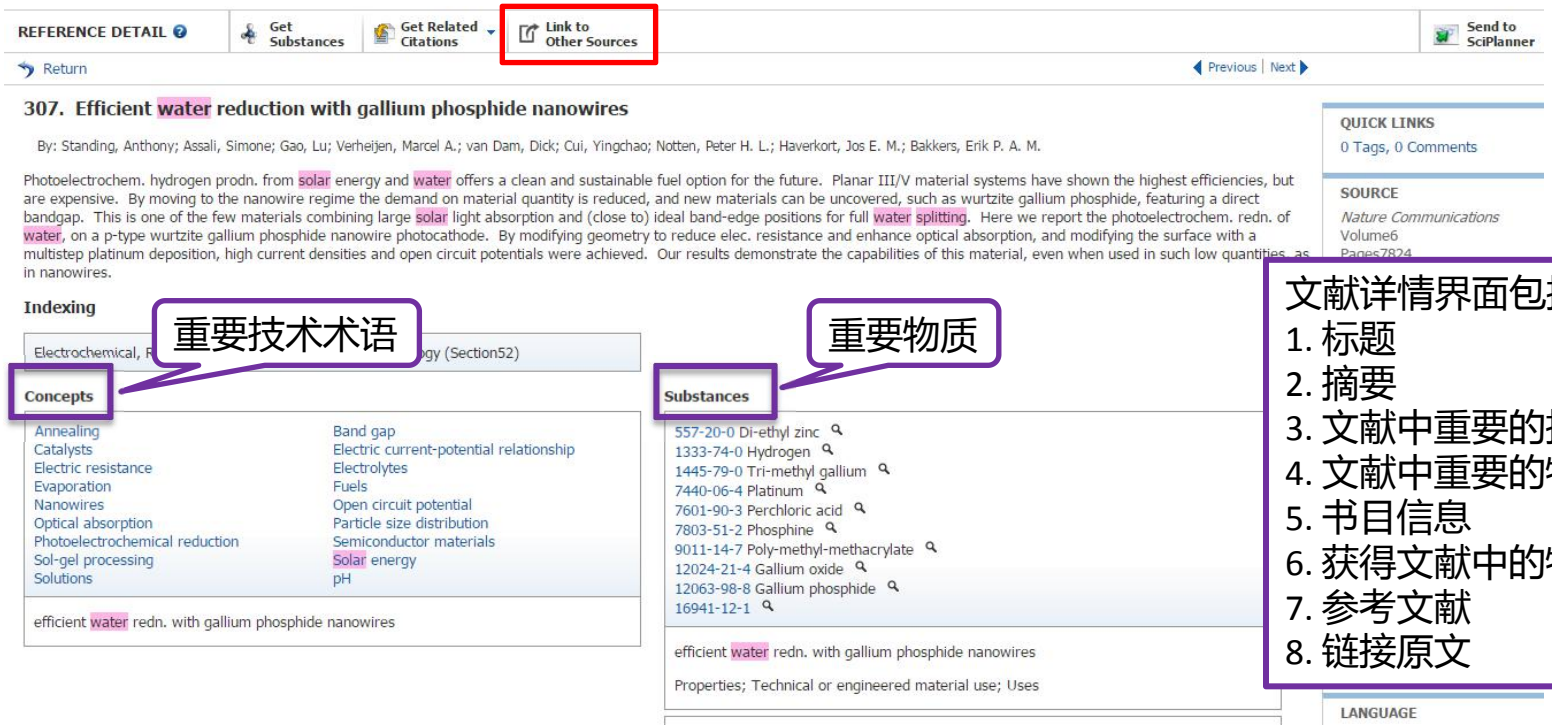
文献信息详情

文献原文链接



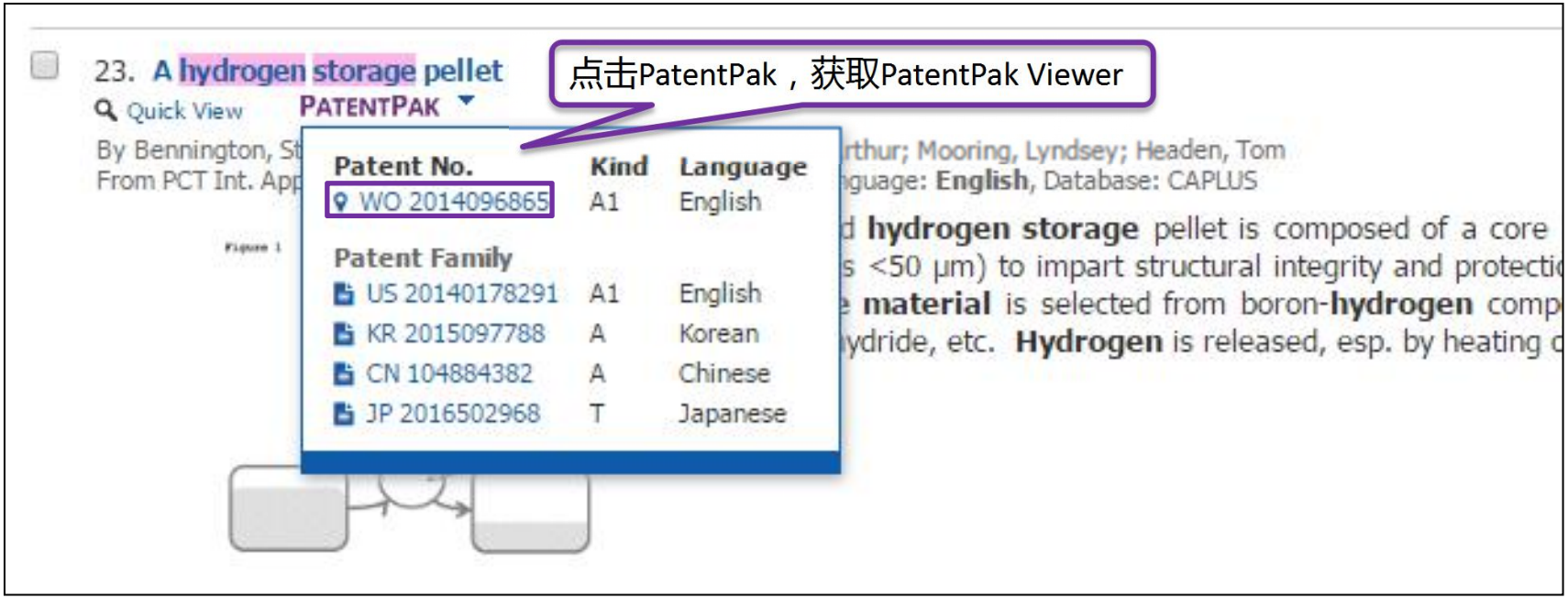
重要技术术语

重要物质

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

PatentPak——专利工作流程解决方案：检索案例：金属储氢材料

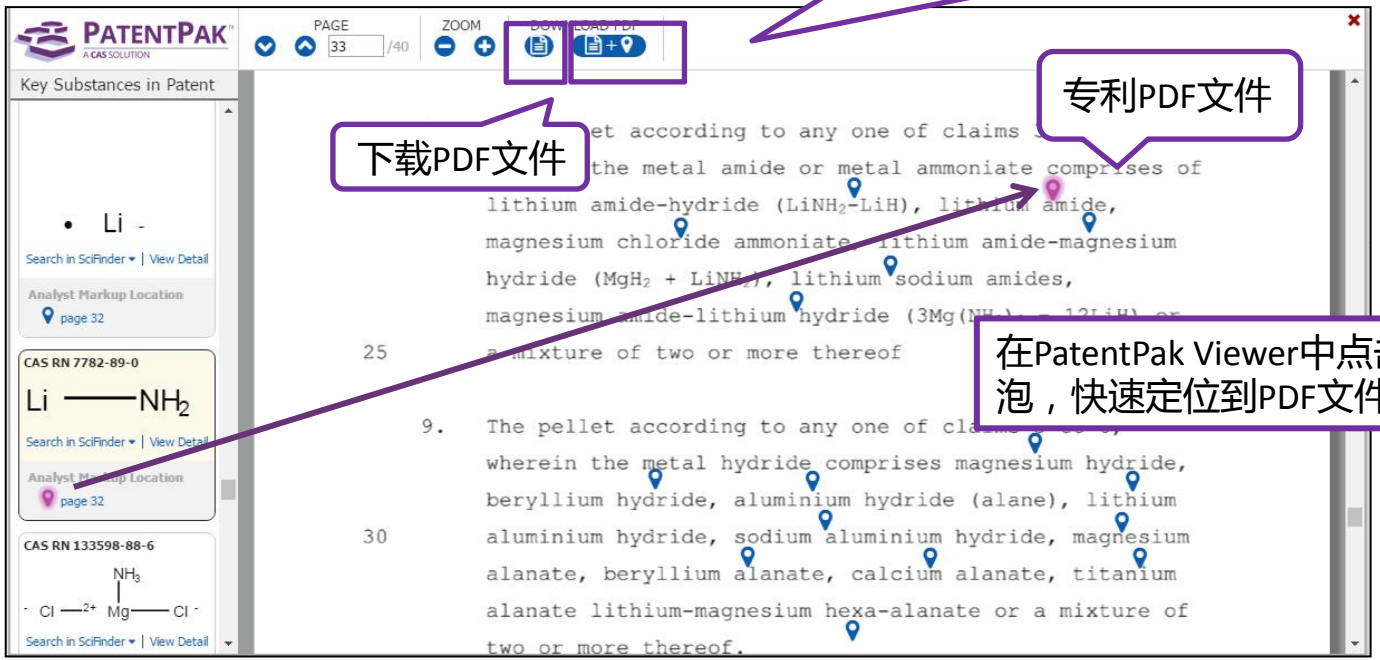
- 检索式：hydrogen storage material with metal



PatentPak——专利工作流程解决方案

PatentPak浏览器

下载包含物质位置等信息的专利PDF文件



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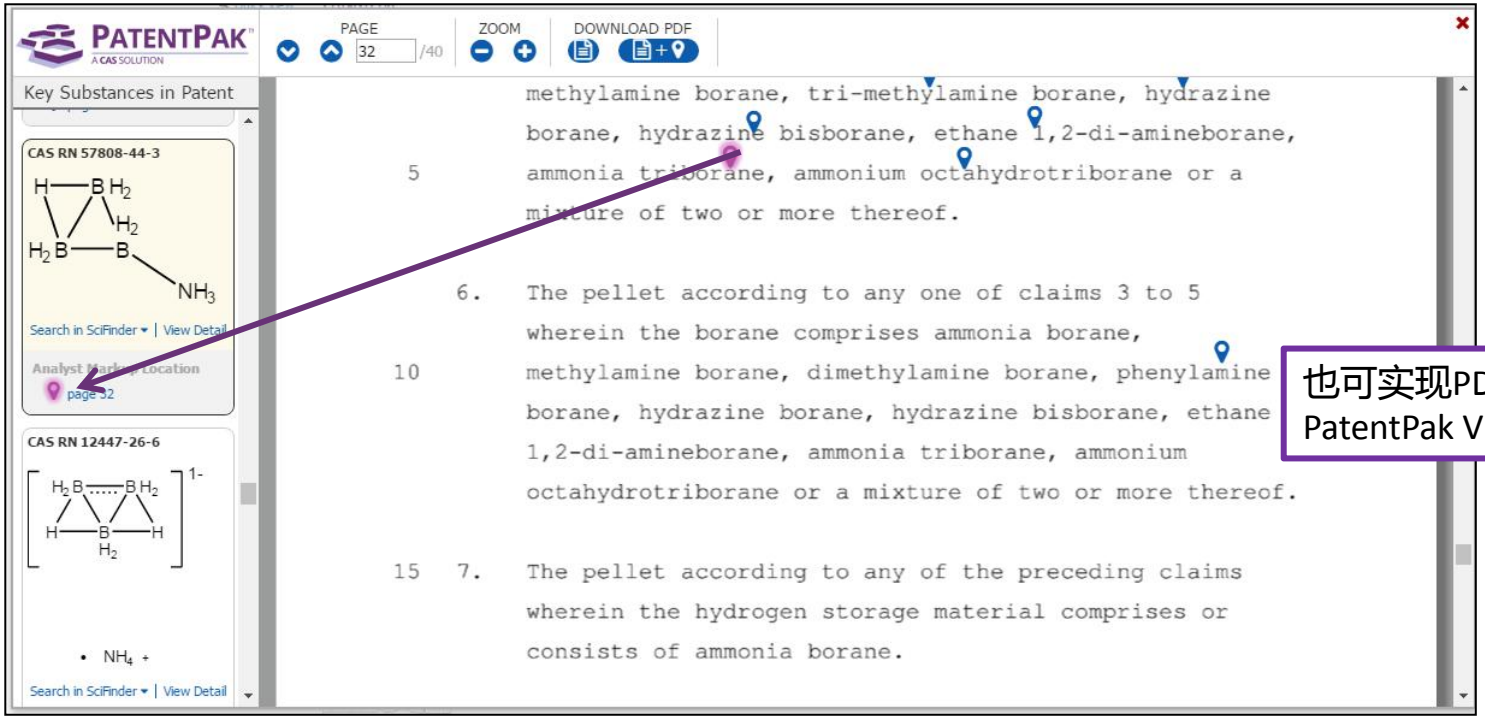

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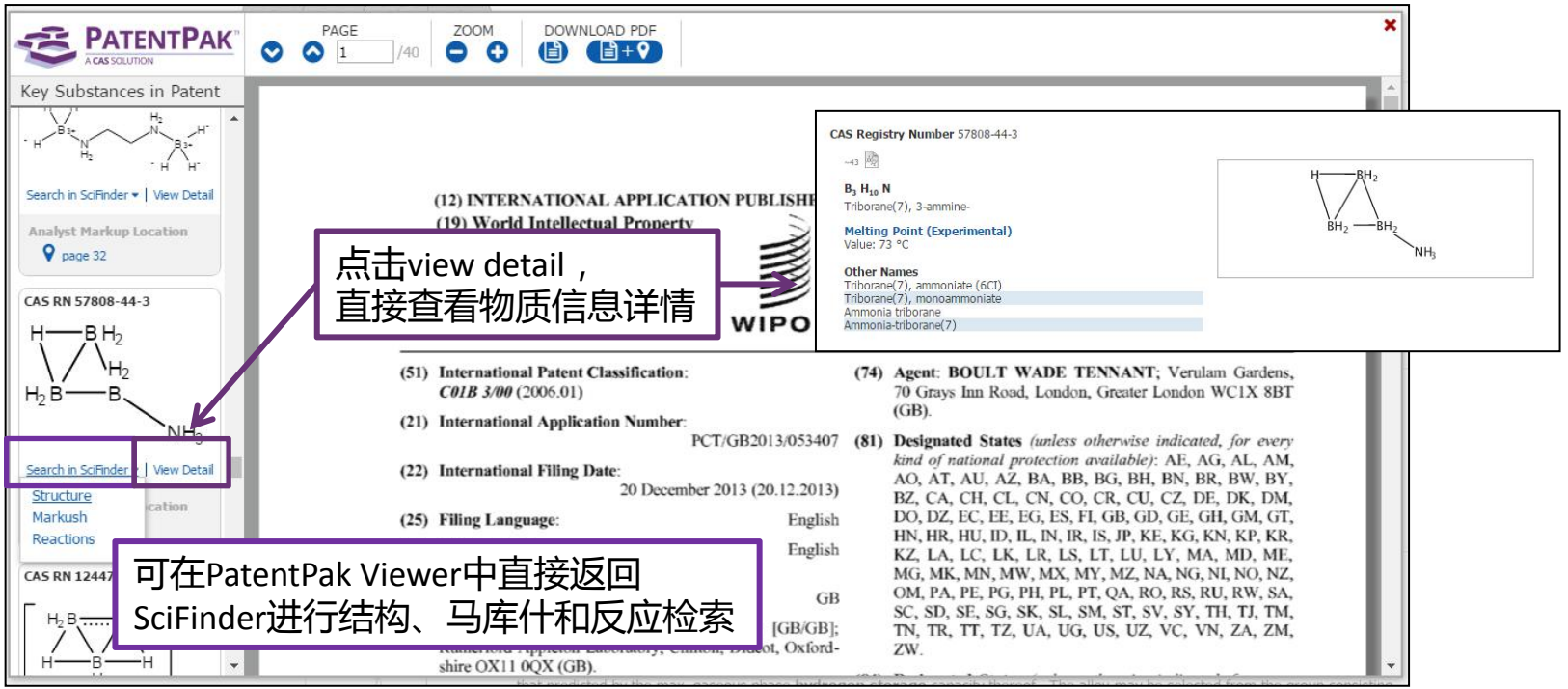
PatentPak——专利工作流程解决方案



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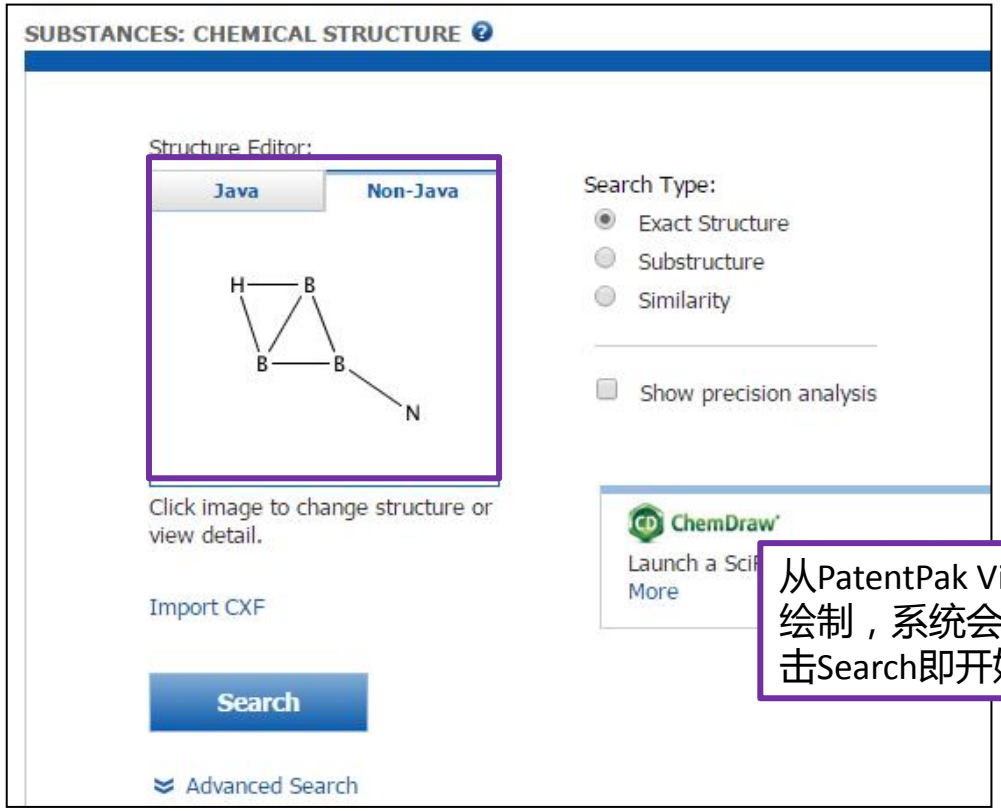
PatentPak——专利工作流程解决方案



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

如何使用SciFinder提高科研效率

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  - 如何从大量物质结果集中快速定位目标物质
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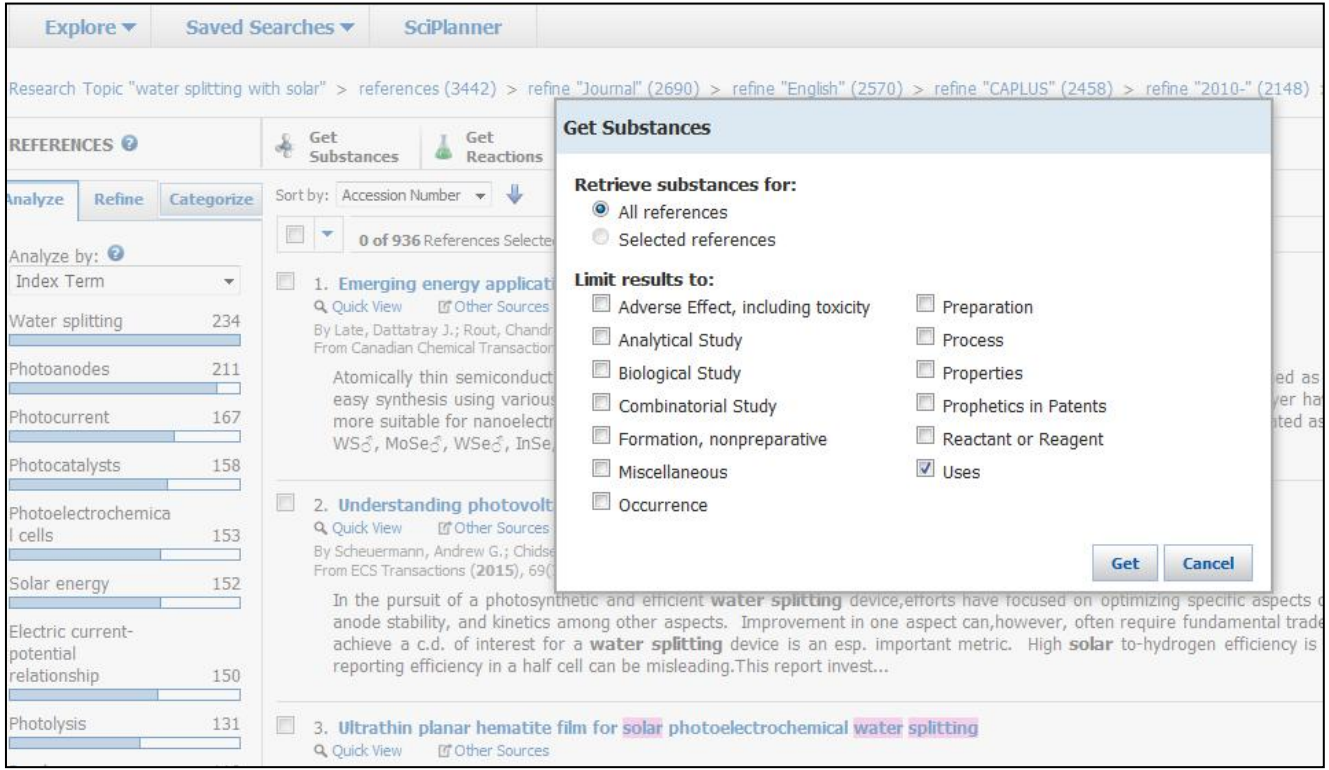
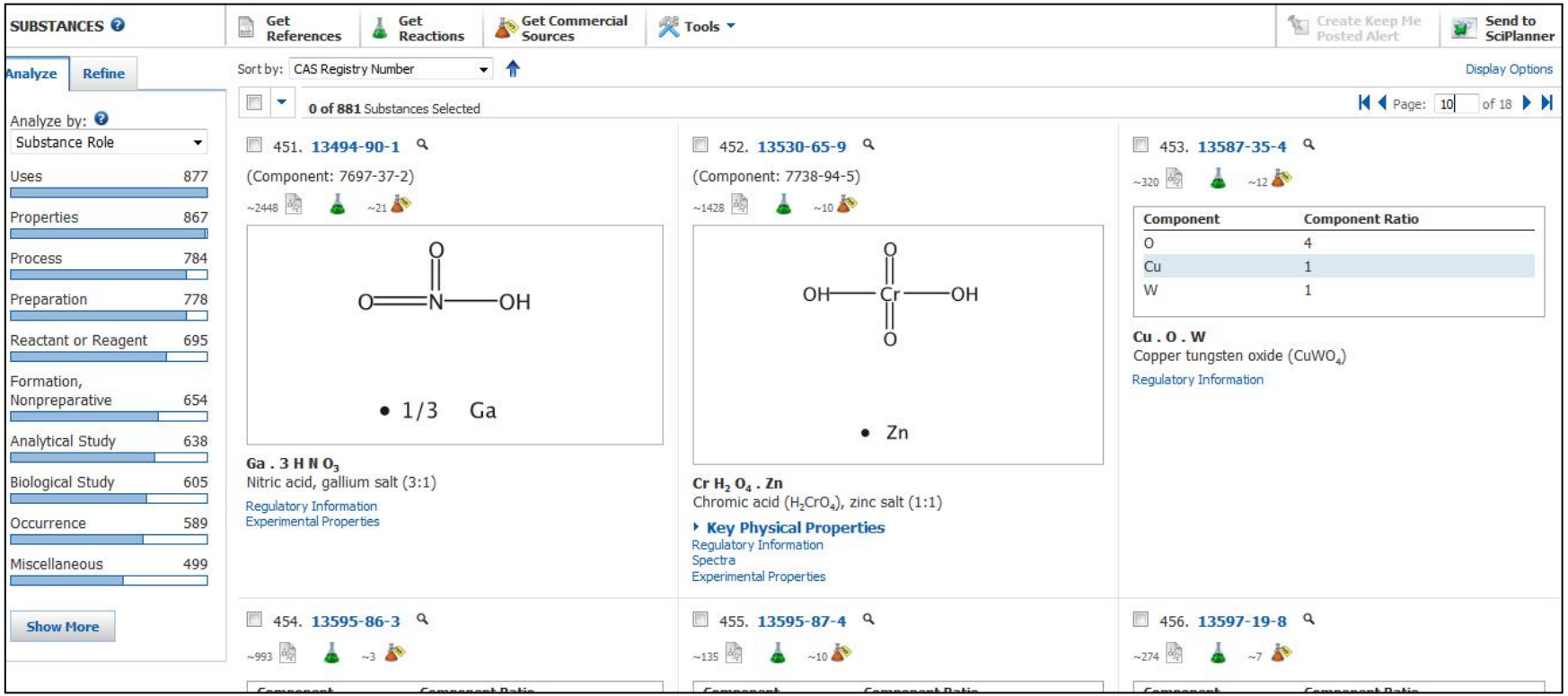
  - 如何获得物质的属性信息、谱图信息
- 反应检索：手性反应检索专题
  - 手性化合物合成方法检索
  - 手性反转反应
  - 手性拆分反应
- 聚合物检索专题
  - 聚合物物质检索
  - 聚合物反应检索

通过文献获得不同研究领域的物质

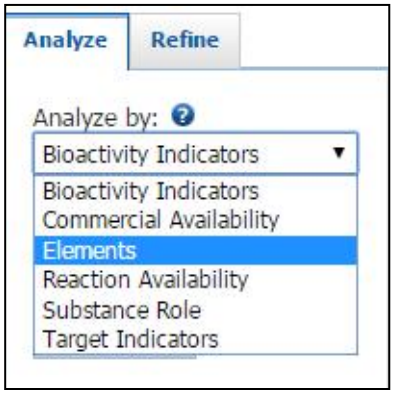


光解水中有关用途的物质



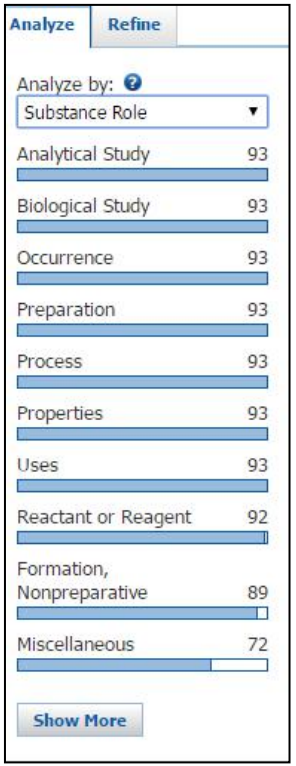
物质检索结果——Analyze

六种分析选项

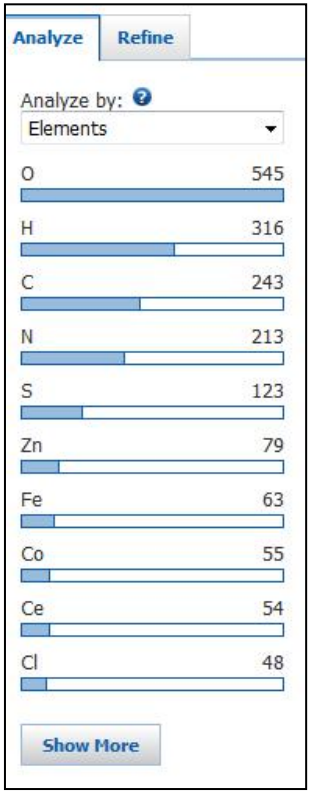


可以按照生物活性，
商业可获得性，元素，
反应可获得性，
物质角色和靶点进行分析

物质角色



元素



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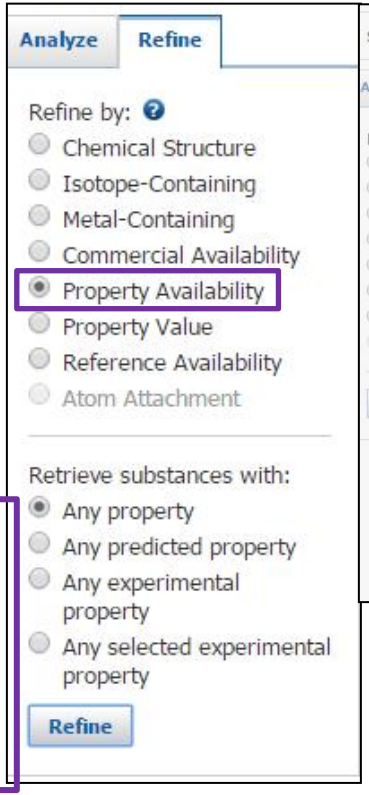
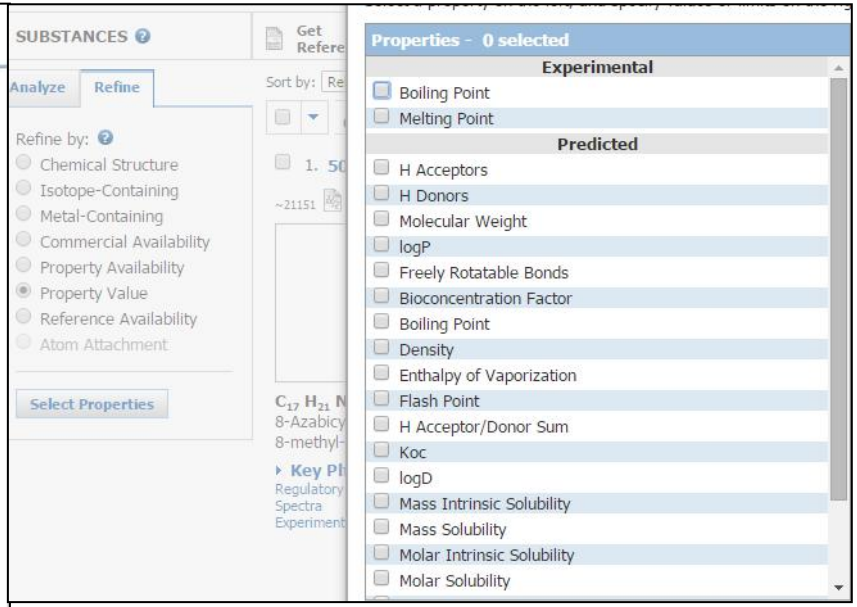
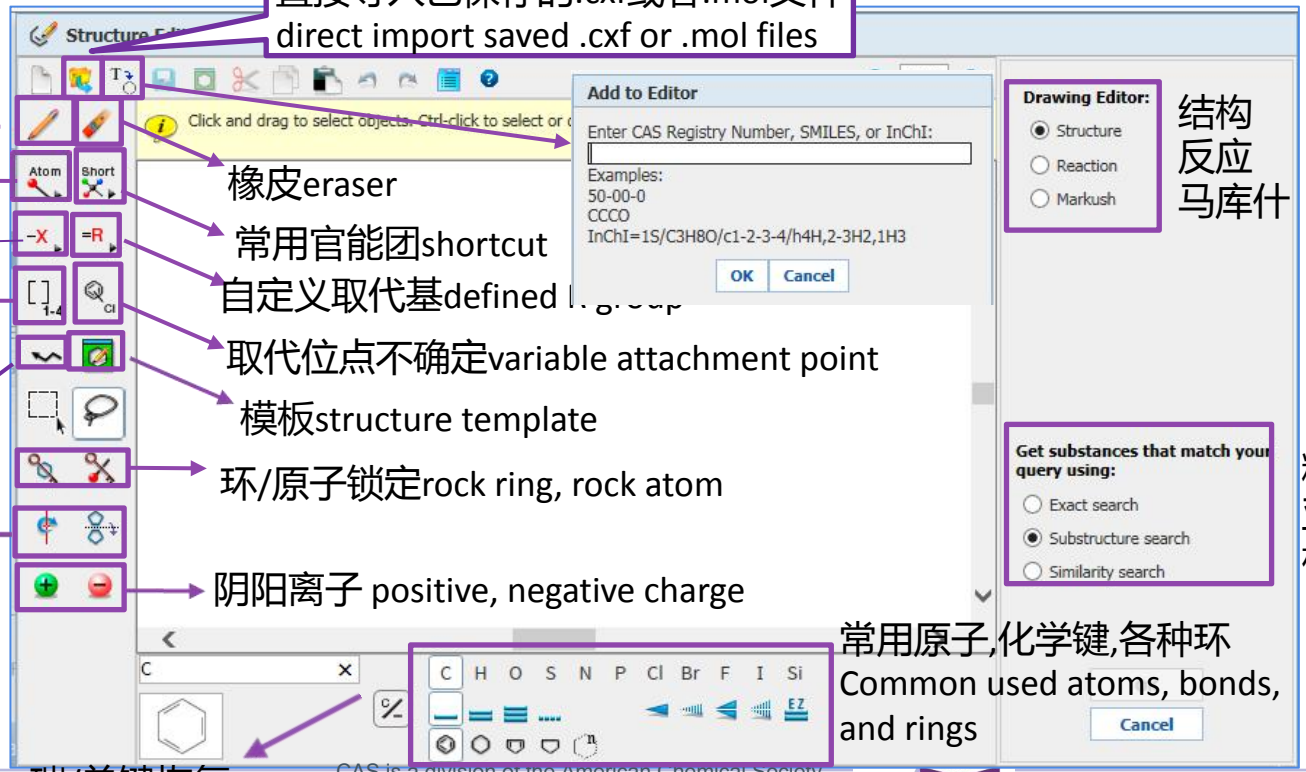
物质检索结果——Refine





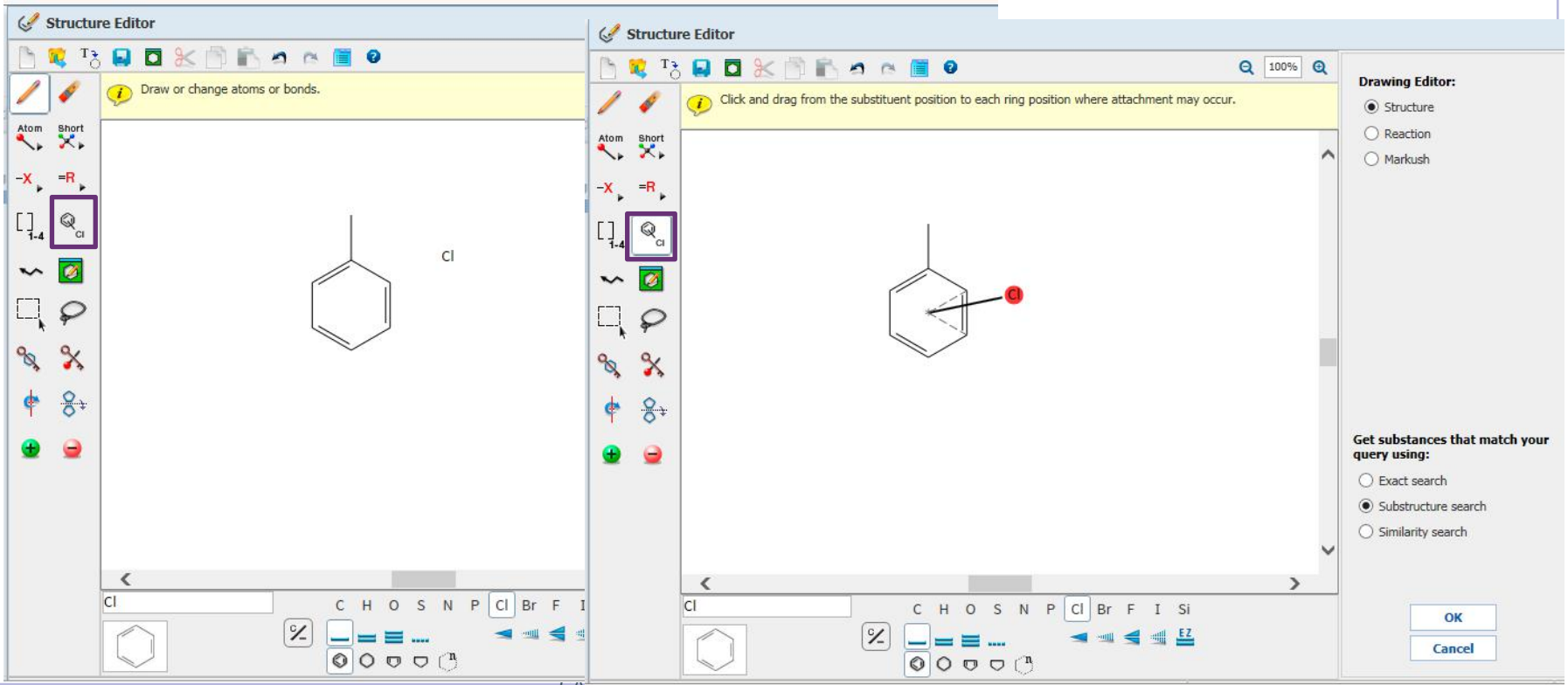
可以按照化学结构，
包含同位素化合物/金属化合物，
商业可获得性，
性质可获得性，
性质数值，文献可获得性
对结果进行限定

化学结构检索：结构编辑器



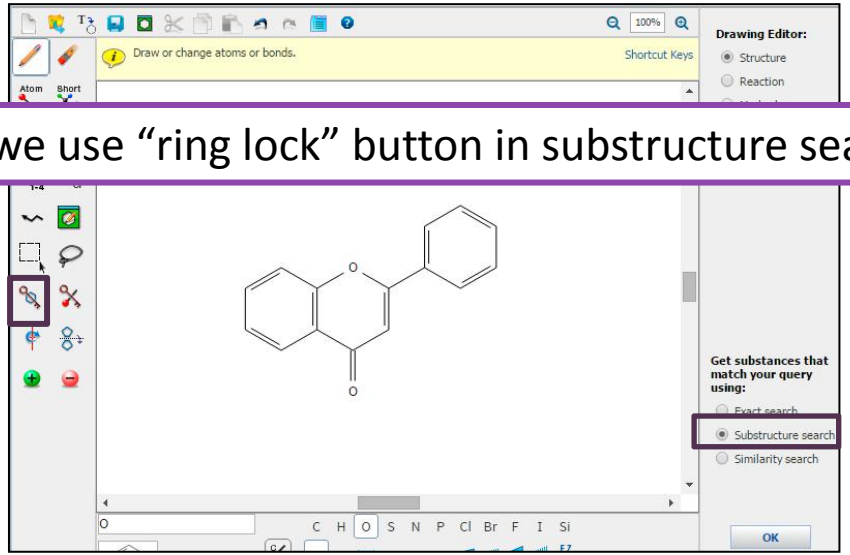
A CAS SOLUTION

举例：不固定位置取代

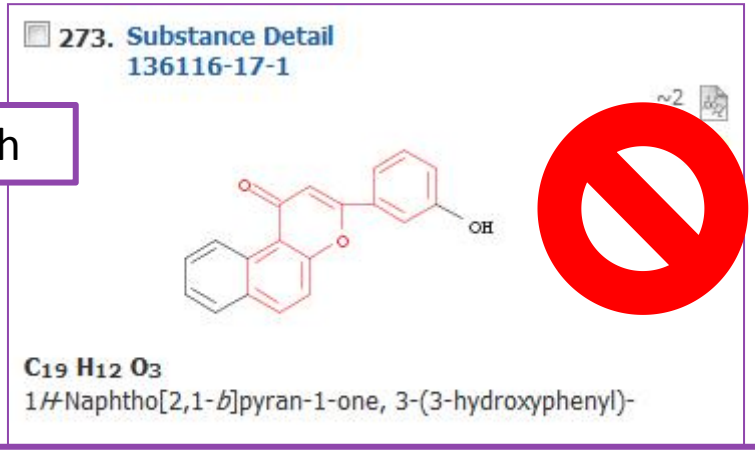


举例：环锁定

环锁定，被锁定的结构上不会出现新的环结构



If we use “ring lock” button in substructure search



These type answers will not be retrieved.

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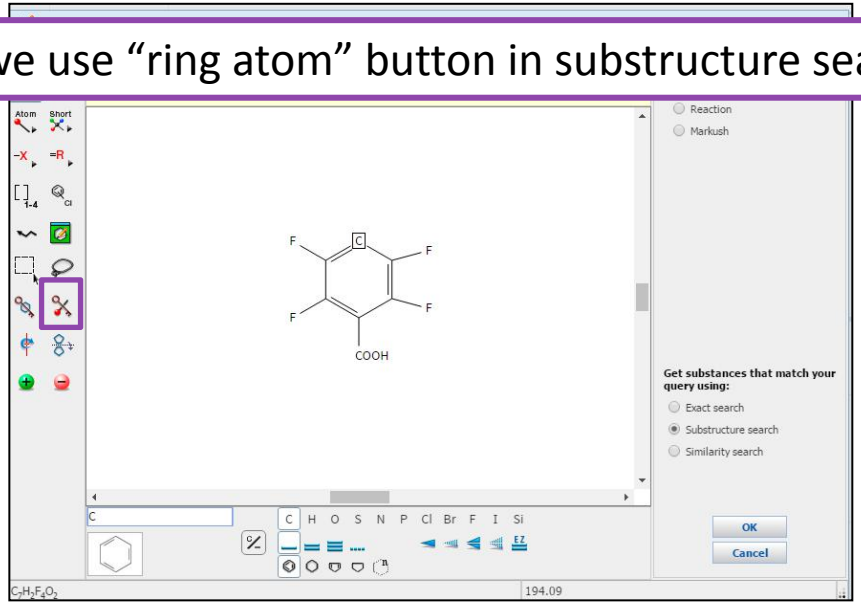
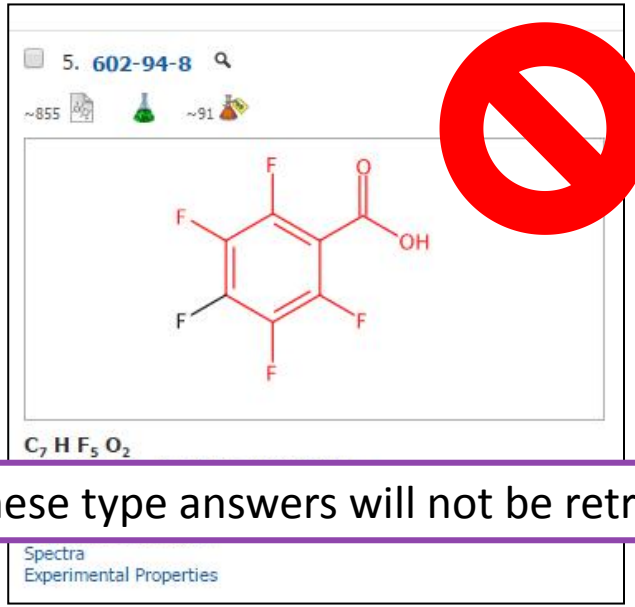
举例：原子锁定

被锁定的原子上不会出现非氢取代

If we use “ring atom” button in substructure search

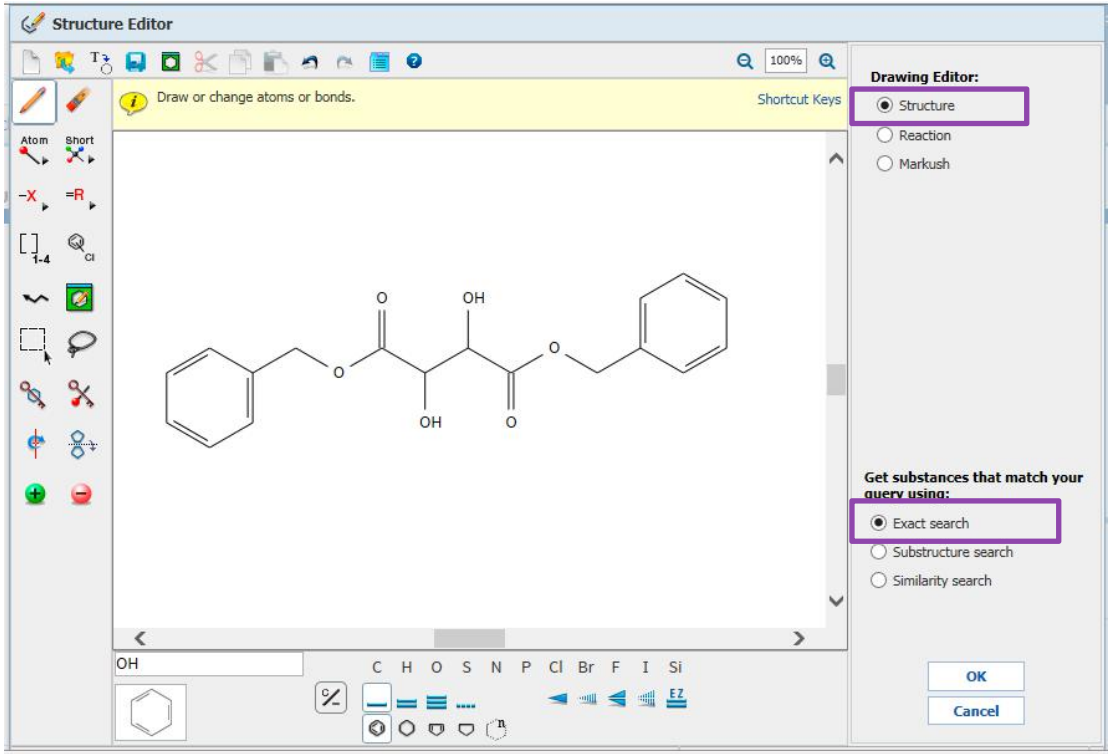




These type answers will not be retrieved.

SciFinder® A CAS SOLUTION

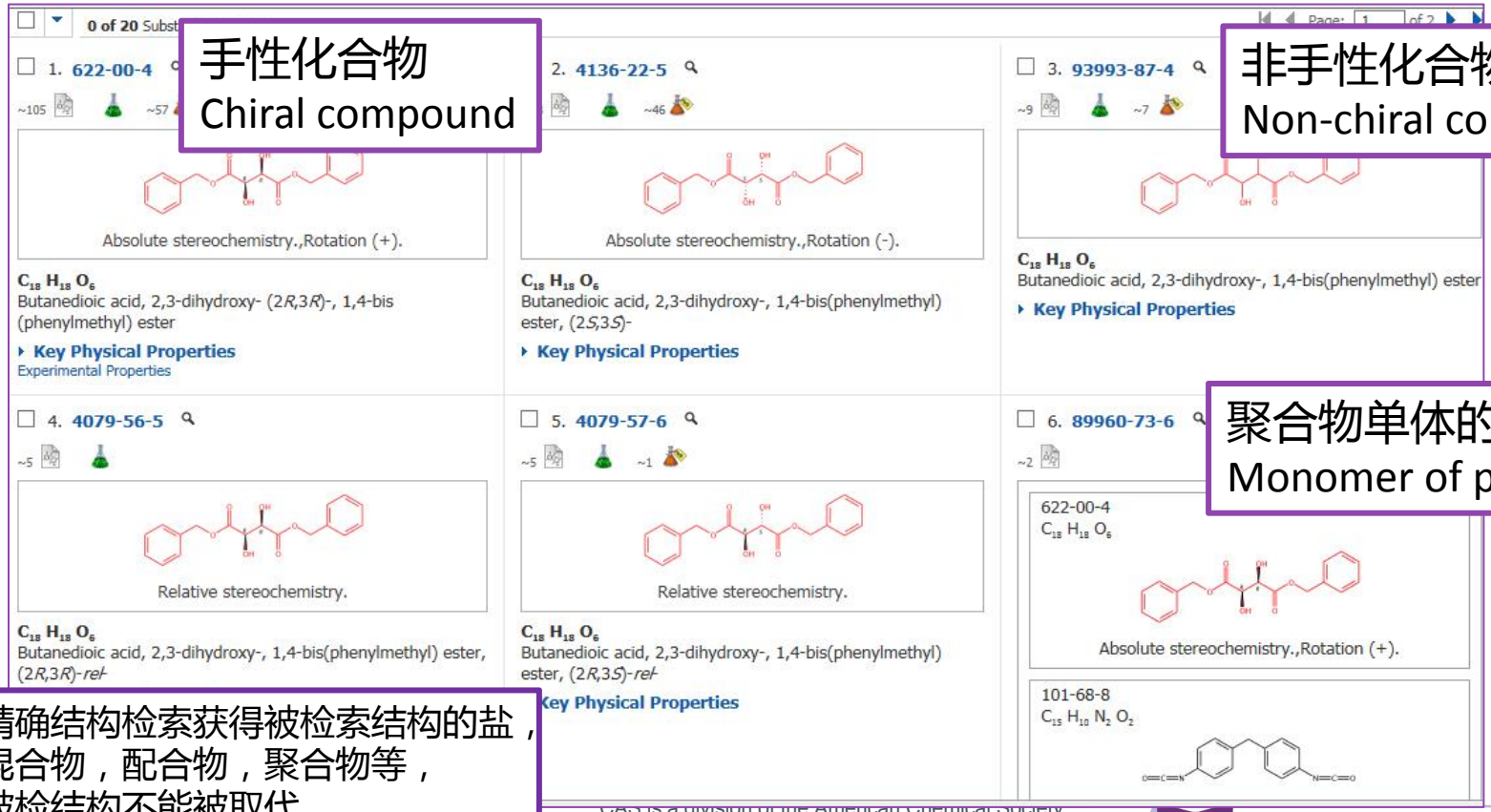
化学结构检索: 精确结构检索



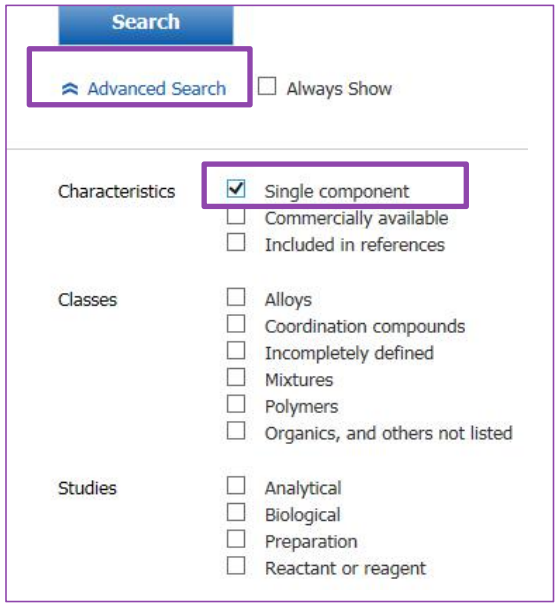
结构式中的原子和环
全部被锁定,不可被取代
All atom and ring are locked,
No substituents

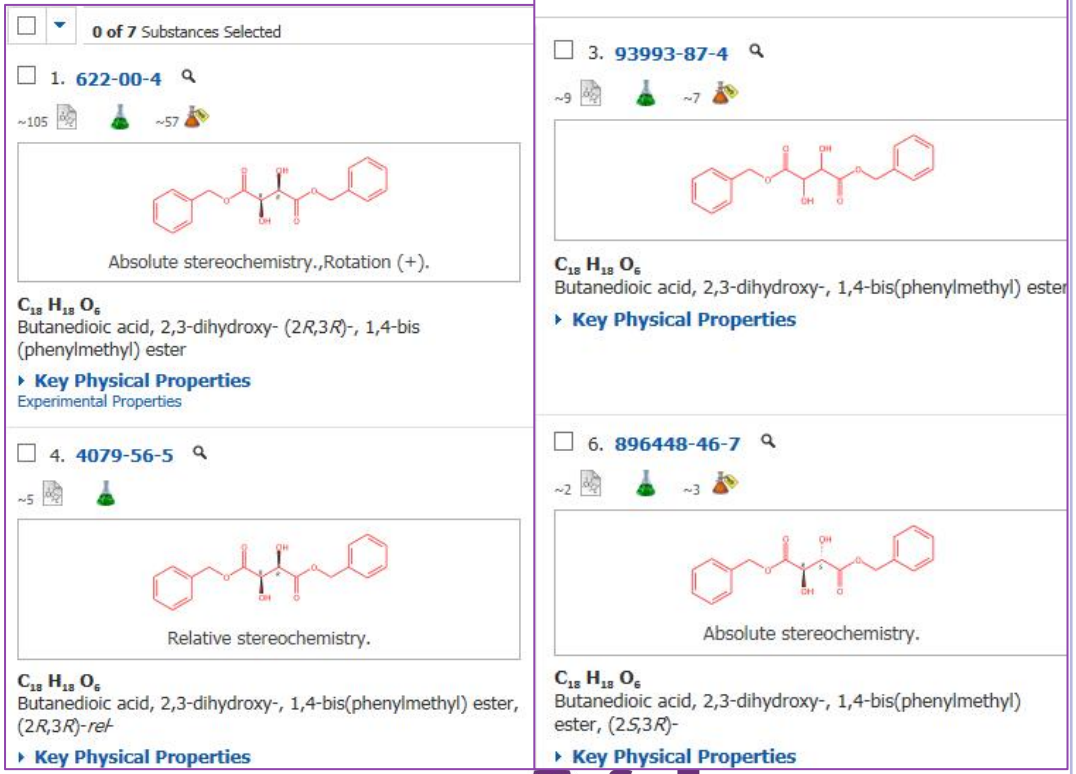
SciFinder® A CAS SOLUTION

物质结构结果集



高级检索——提前限定



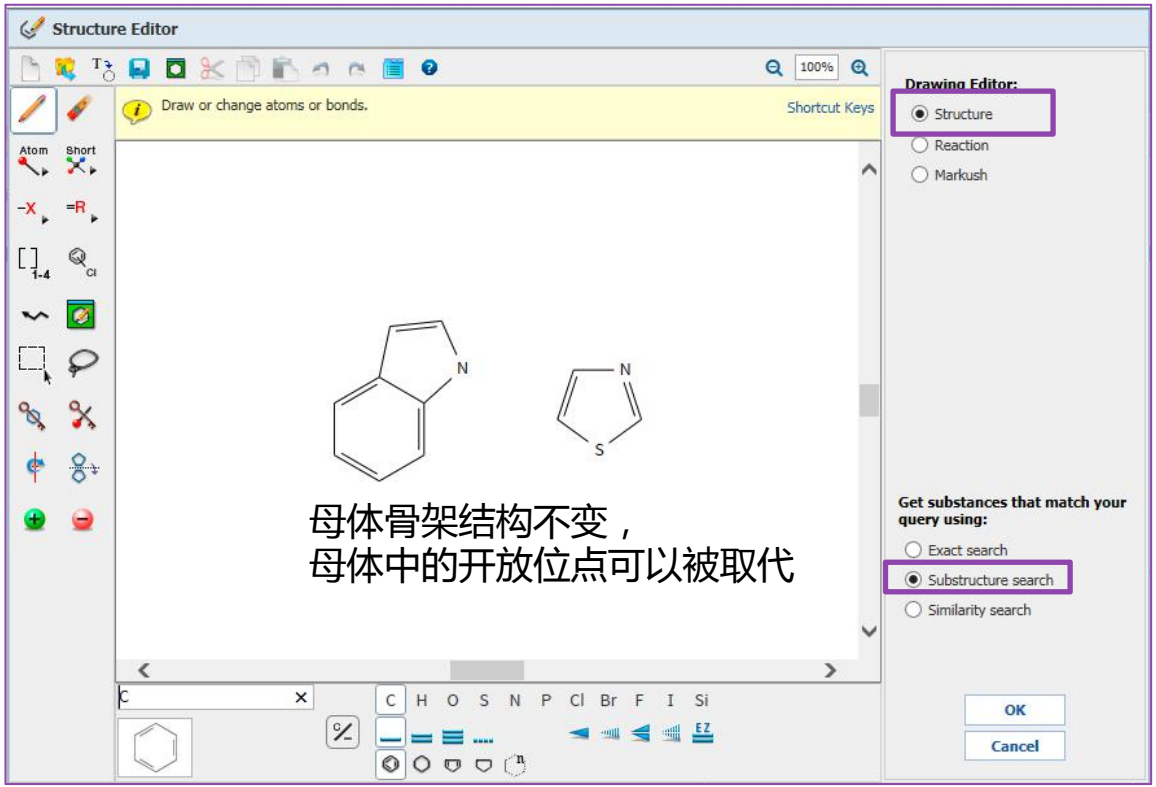


去除混合物，组合物，配合物，盐

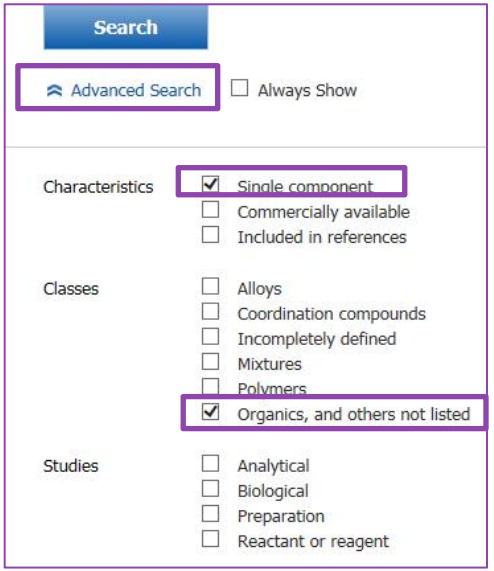
Exclude mixture, polymer, complex, salts

SCIFINDER® A CAS SOLUTION

化学结构检索：亚结构检索



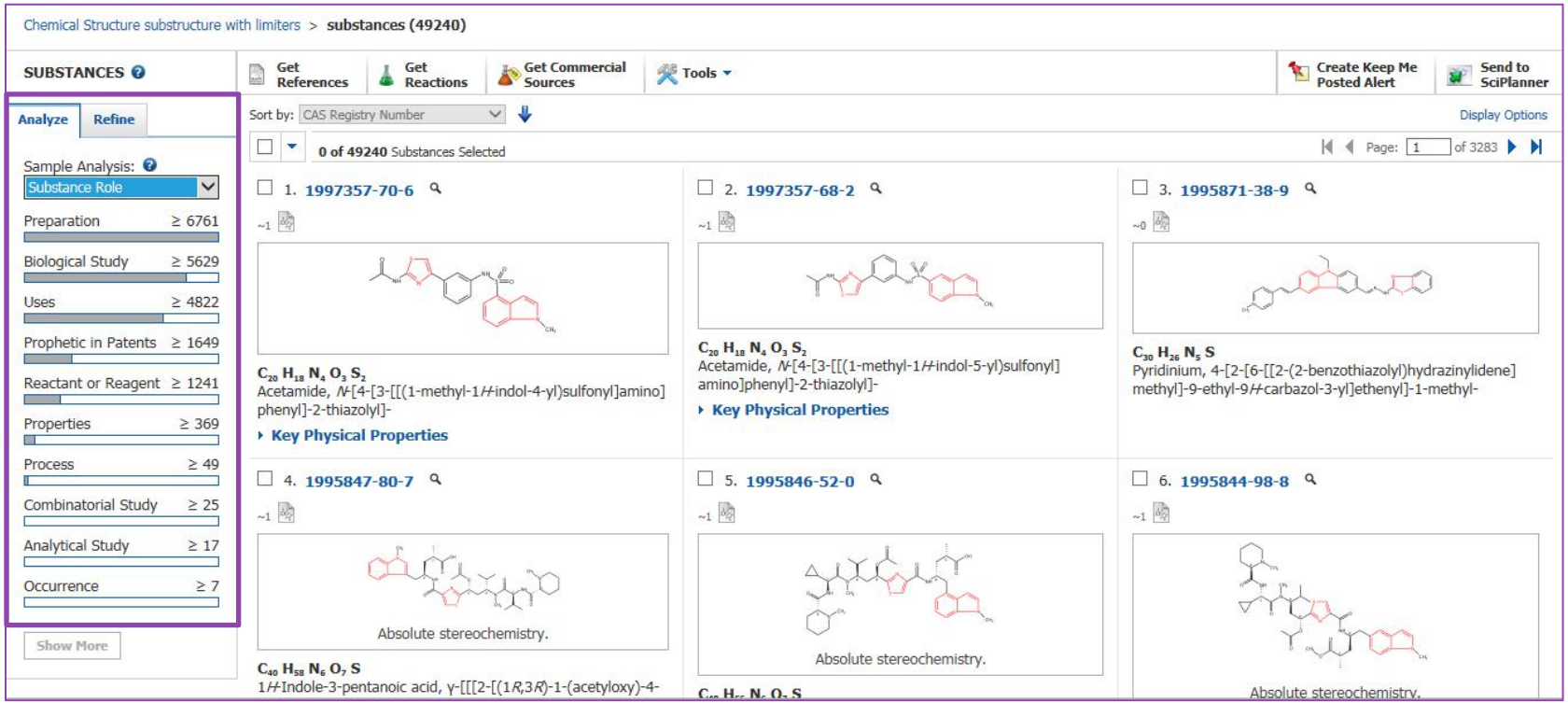
母体骨架结构不变，
母体中的开放位点可以被取代



将两个结构片段限定在同一物质中

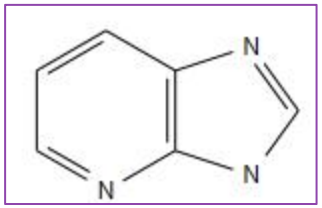
SciFinder® A CAS SOLUTION

物质结果集



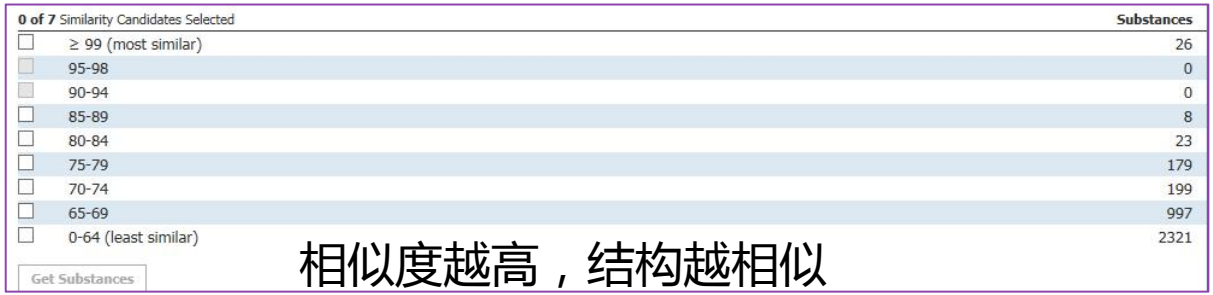
SciFinder® A CAS SOLUTION

化学结构检索: 相似结构检索

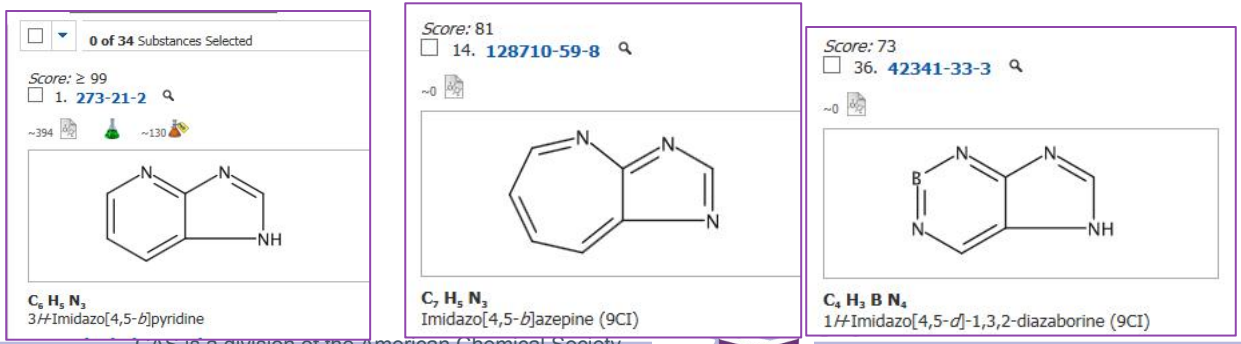


Purin

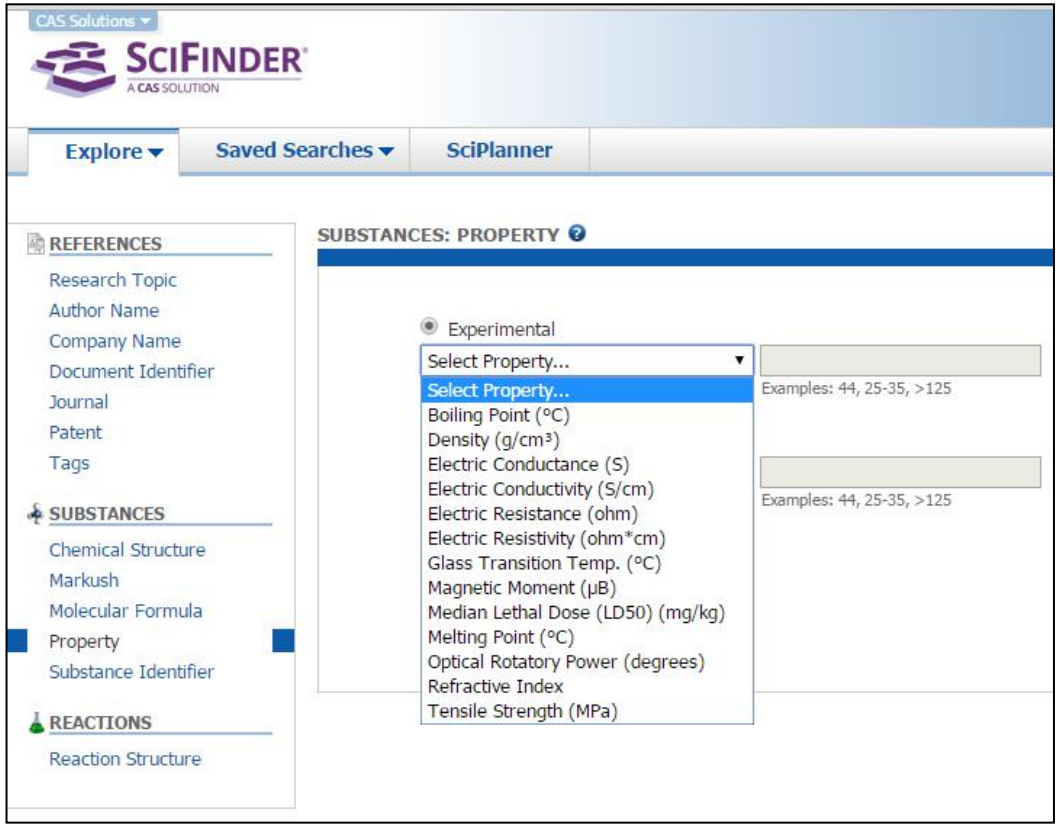
母体结构被拆分成分子片段



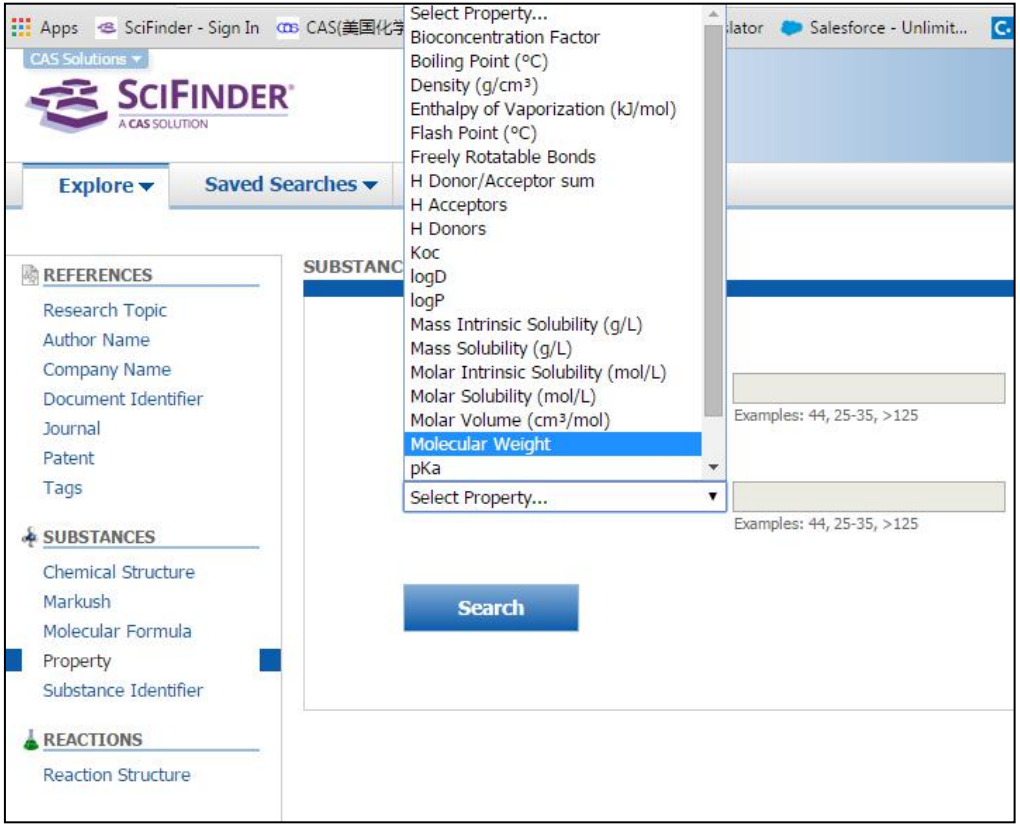
相似度越高，结构越相似



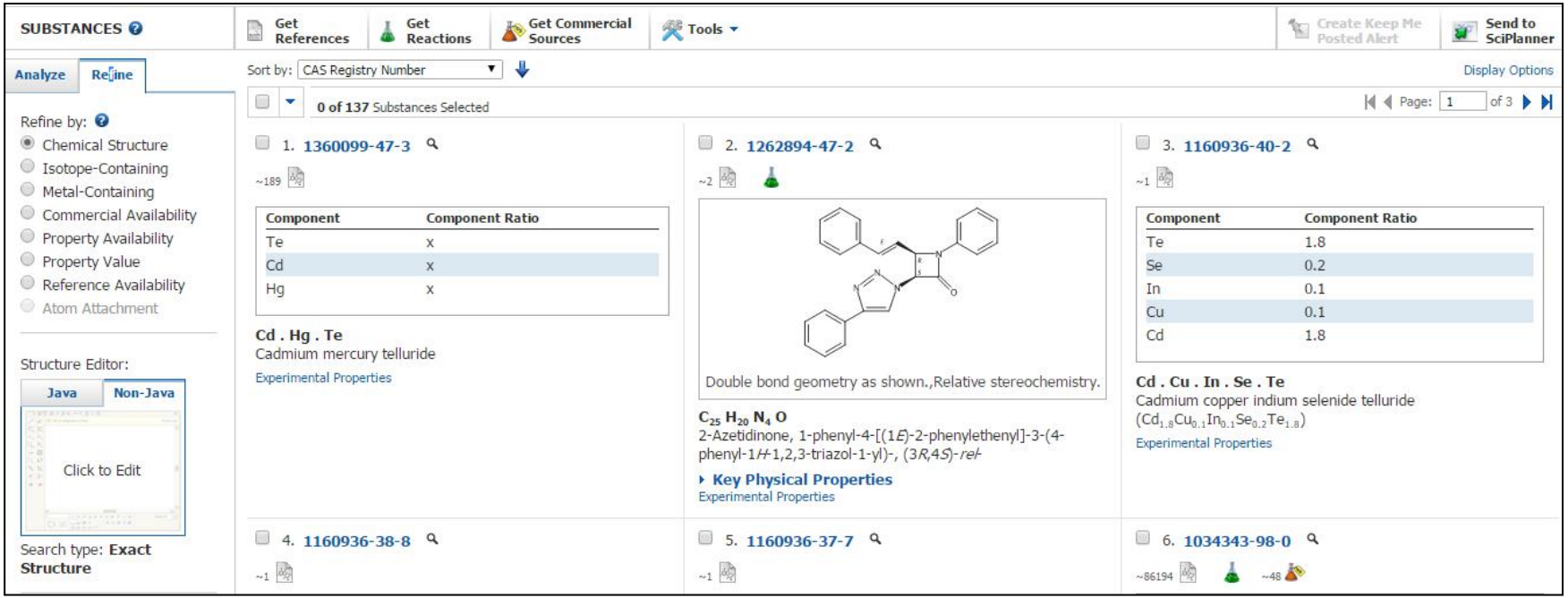
物质检索——理化性质检索：寻找电阻率大于125ohm的含铁物质



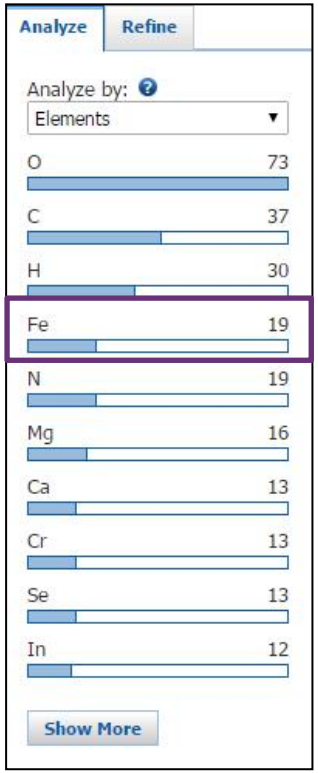
物质检索——理化性质性质检索

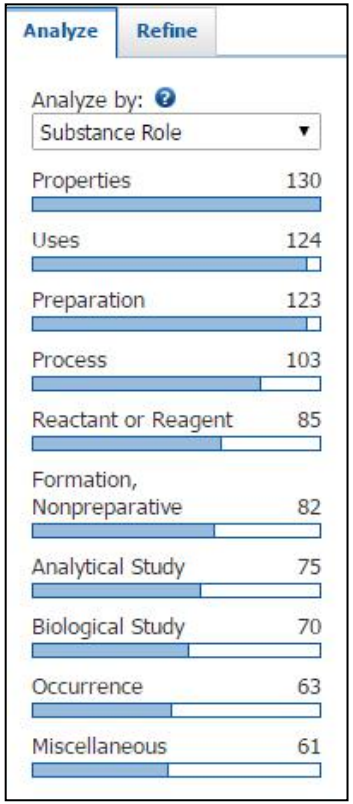


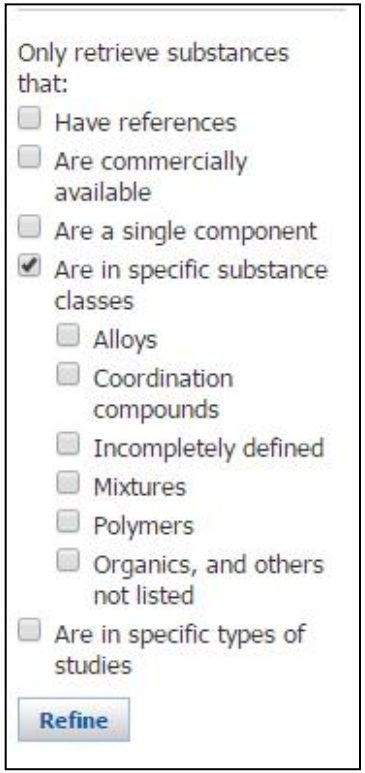
SciFinder物质检索结果



通过分析/限定工具筛选结果







提纲

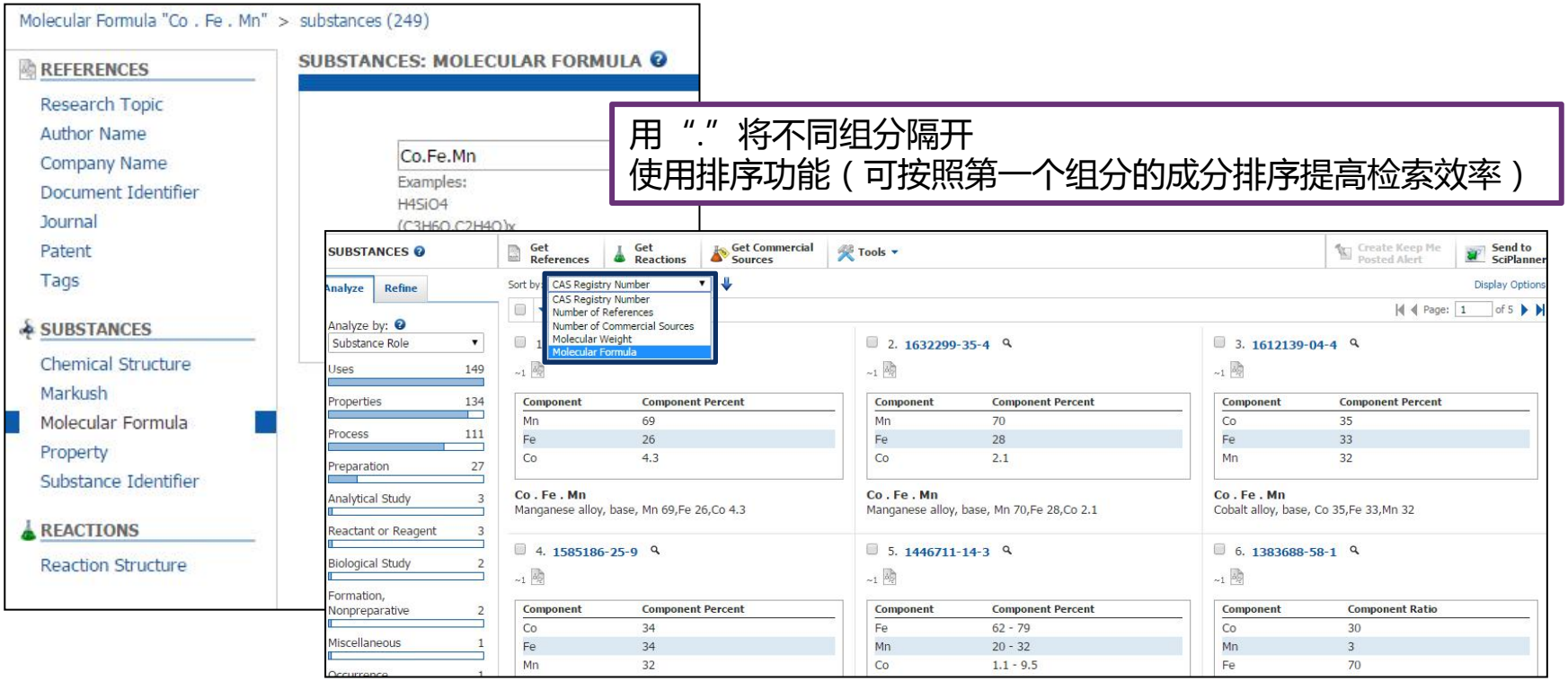
- SciFinder物质检索
  - 通过文献获得物质
    - 物质检索结果的处理：分析和限定
    - 物质信息详情
  - 理化性质检索
  - 分子式检索
  - 物质标识符检索

物质检索——分子式检索

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

合金的检索：钴铁锰合金


Molecular Formula "Co . Fe . Mn" > substances (249)
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
Co.Fe.Mn
Examples:
H4SiO4
用 "." 将不同组分隔开
使用排序功能（可按照第一个组分的成分排序提高检索效率）
SUBSTANCES
Get References
Get Reactions
Get Commercial Sources
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Analyze
Refine
Sort by
CAS Registry Number
Number of References
Number of Commercial Sources
Molecular Weight
Molecular Formula
Display Options
Page: 1 of 5
Analyze by:
Substance Role
Uses 149
Properties 134
Process 111
Preparation 27
Analytical Study 3
Reactant or Reagent 3
Biological Study 2
Formation, Nonpreparative 2
Miscellaneous 1
2. 1632299-35-4
3. 1612139-04-4
Component
Component Percent
Mn 69
Fe 26
Co 4.3
Co . Fe . Mn
Manganese alloy, base, Mn 69,Fe 26,Co 4.3
Mn 70
Fe 28
Co 2.1
Co . Fe . Mn
Manganese alloy, base, Mn 70,Fe 28,Co 2.1
Co 35
Fe 33
Mn 32
Co . Fe . Mn
Cobalt alloy, base, Co 35,Fe 33,Mn 32
4. 1585186-25-9
5. 1446711-14-3
6. 1383688-58-1
Co 34
Fe 34
Mn 32
Fe 62 - 79
Mn 20 - 32
Co 1.1 - 9.5
Component Ratio
Co 30
Mn 3
Fe 70

多氧簇金属：七钼酸铵

CAS Registry Number 12027-67-7

(Component: 12274-10-1)

~7,729 ~40

$H_4\,N\,.\,{}^1/_6\,Mo_7\,O_{24}$

Molybdate ($Mo_7O_{24}^{6-}$), ammonium (1:6)

Coordination Compound

Other Names

Ammonium molybdate(VI) ($(NH_4)_6Mo_7O_{24}$) (6CI)

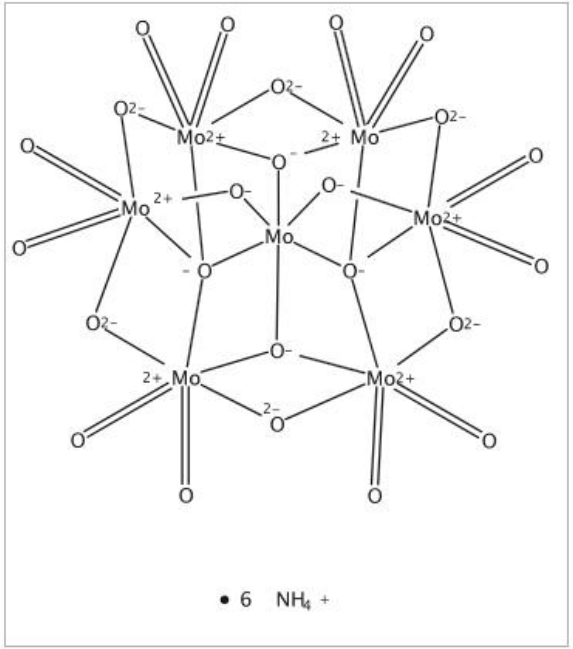
Molybdate ($Mo_7O_{24}^{6-}$), hexaammonium (9CI)

Molybdic acid ($H_6Mo_7O_{24}$), hexaammonium salt (8CI)

Ammonium heptamolybdate

Ammonium heptamolybdate ($(NH_4)_6Mo_7O_{24}$)

View more...



$H_4\,N\,.\,{}^1/_6\,Mo_7\,O_{24}$

如何查找MOF化合物，以Cu-BTC为例

Substance Identifier "222404-02-6 " > substances (1) > **222404-02-6**

SUBSTANCE DETAIL | Get References | Get Reactions

Return

CAS Registry Number 222404-02-6

~1,274

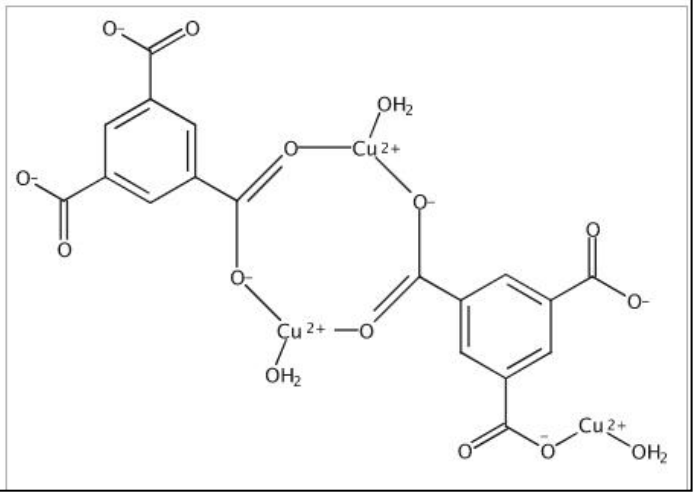
$C_{18}H_{12}Cu_3O_{15}$

Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO^1:κO^1]][$μ_3$-[1,3,5-benzenetricarboxylato(3-)-κO^1:κO^3:κO^1]]tri-

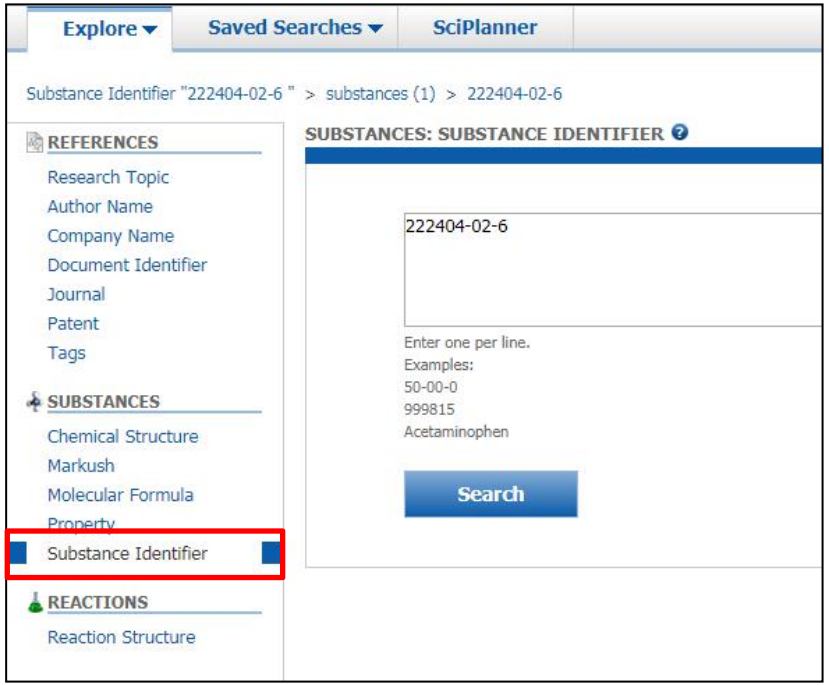
Coordination Compound

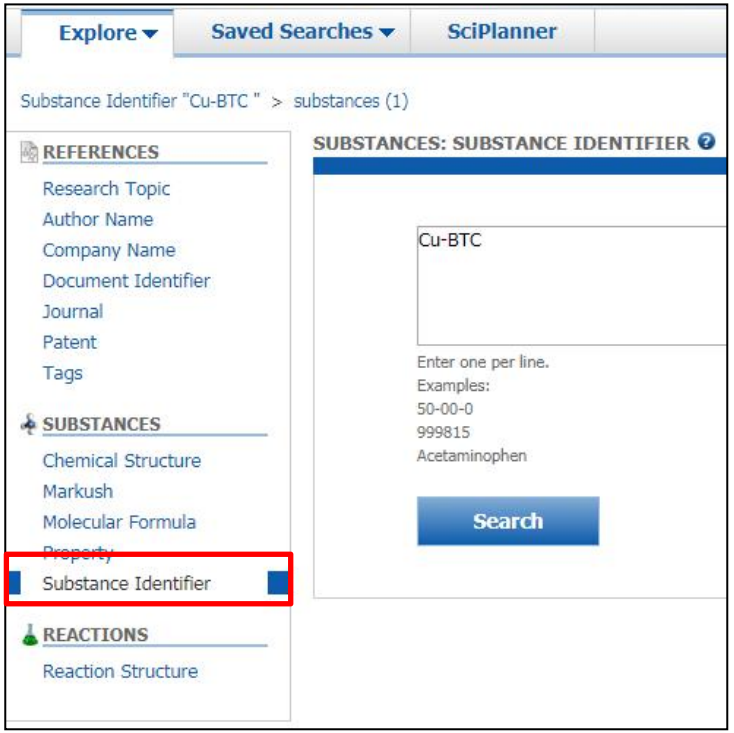
Density (Experimental)
Value: 0.879 g/cm3

Other Names
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO^1:κO^1]][$μ_3$-[1,3,5-benzenetricarboxylato(3-)-κO^1:κO^1:κO^3]]tri- (9CI)
Triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO^1:κO^1]][$μ_3$-[1,3,5-benzenetricarboxylato(3-)-κO^1:κO^3:κO^1]]tricopper
Basolite C 300
Cu-BTC
Cu_3BTC_2
View more...

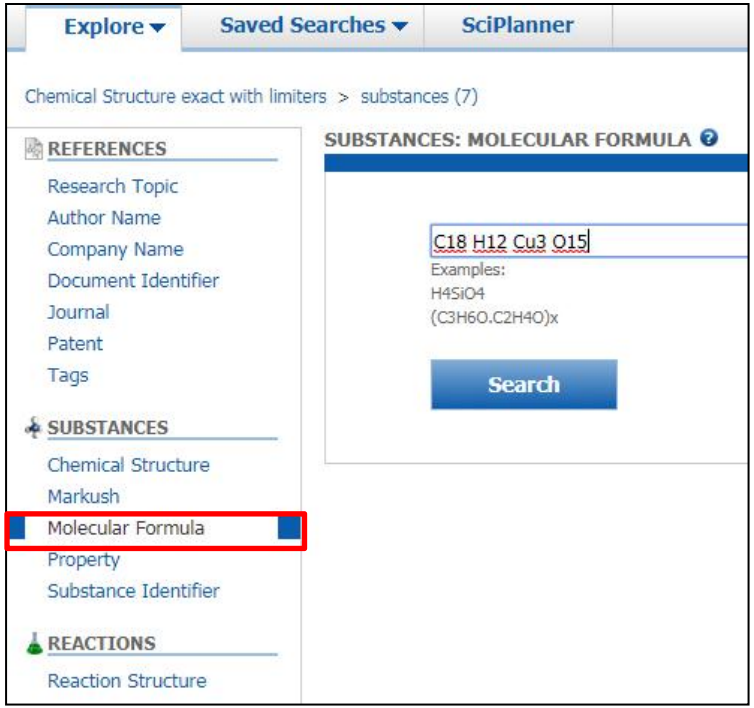


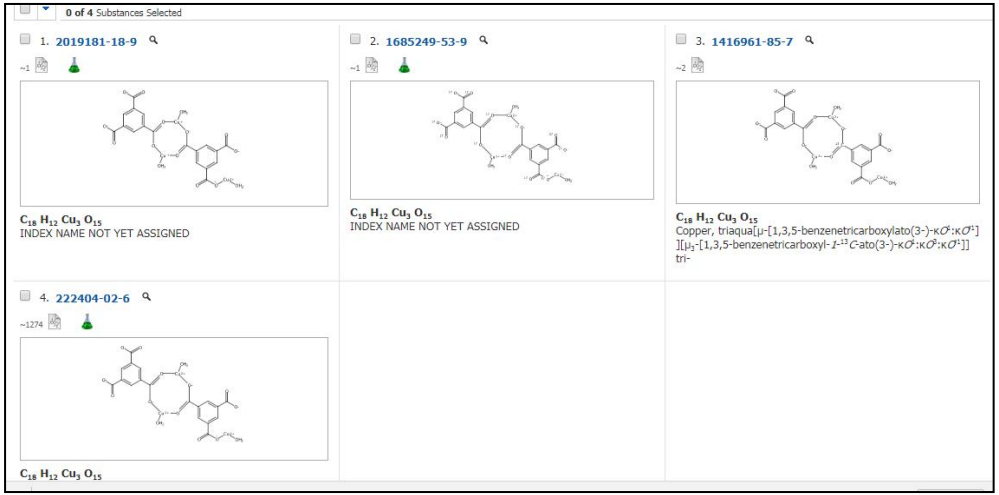
方法1：若已知物质的CAS号码，物质名称，使用Substance Identifier



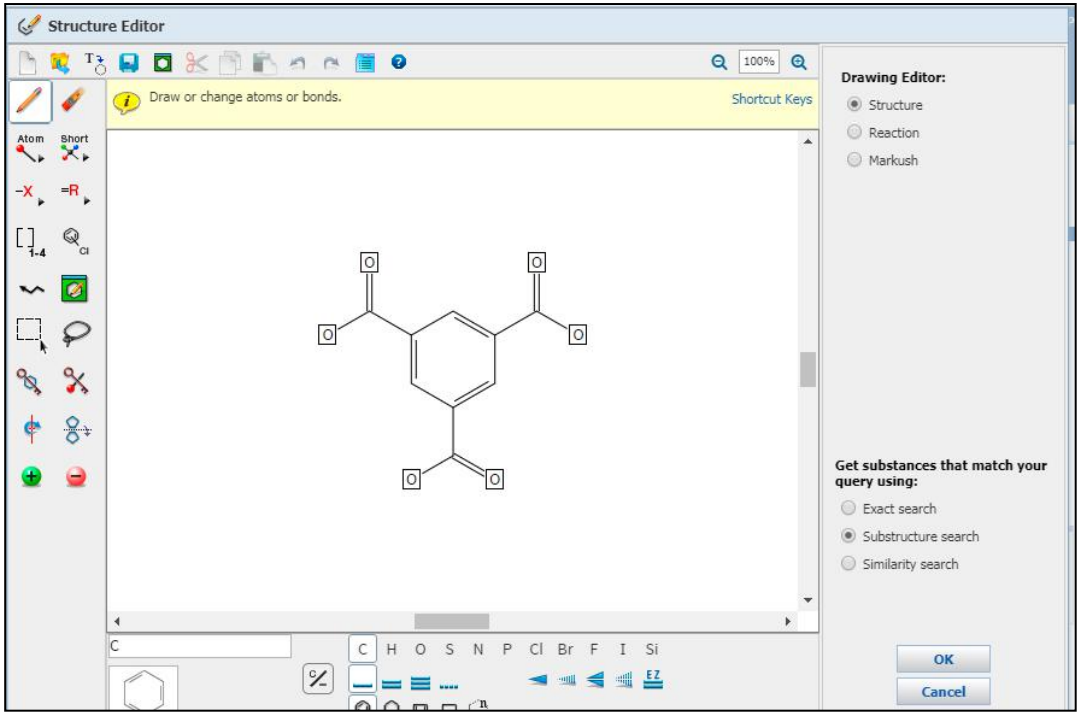


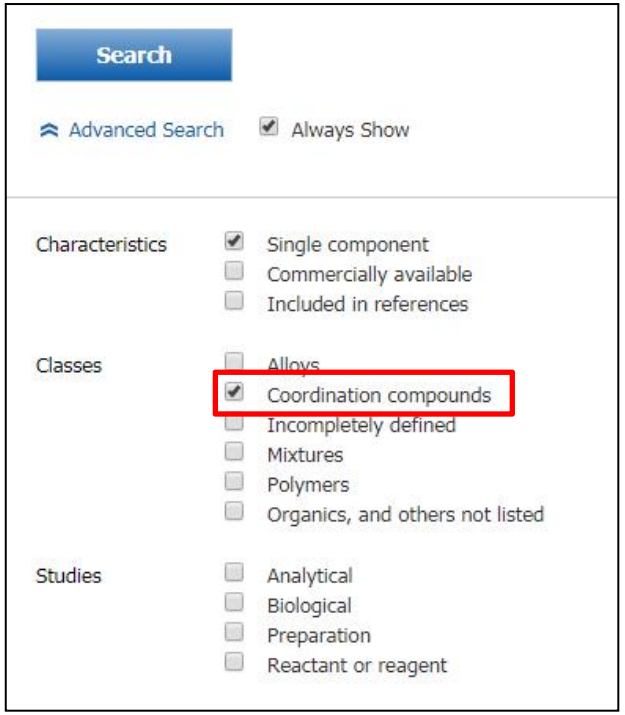
方法2：已知MOF化合物单元分子式，可以使用分子式检索





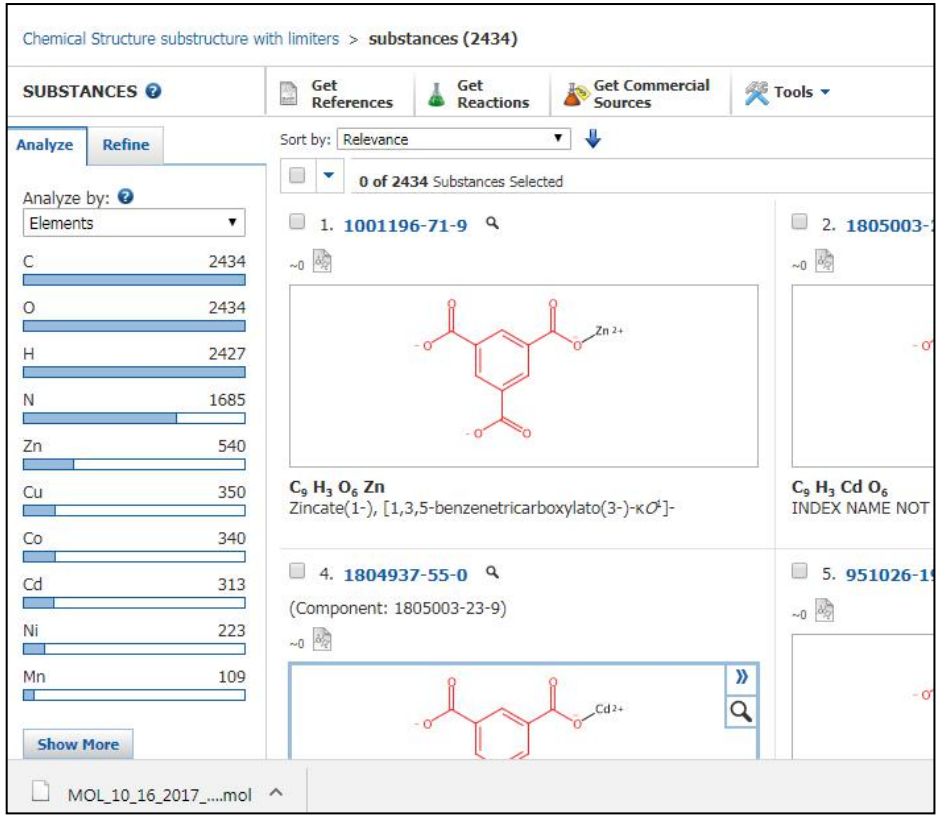
方法3：已知配合物配体，可以先结构检索配体，然后获得相关配合物



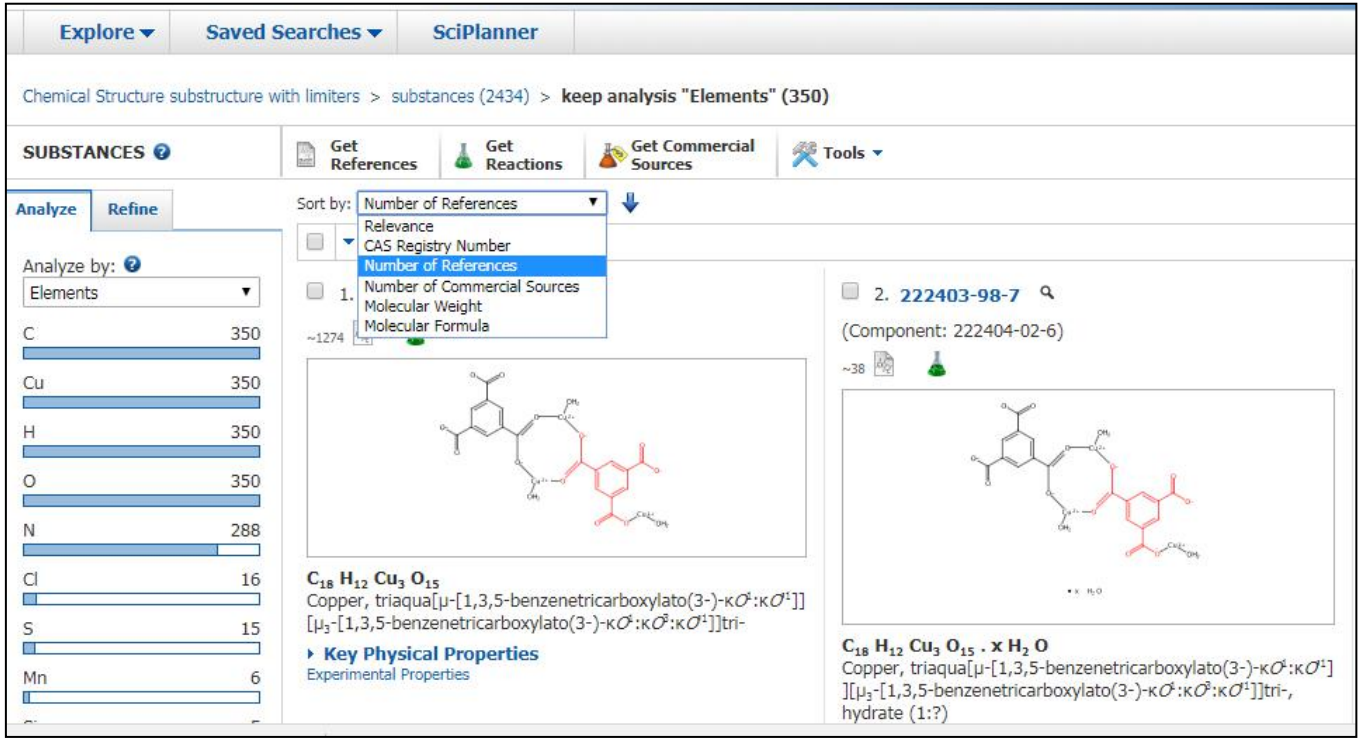


注：此种方法可能结果噪音较多

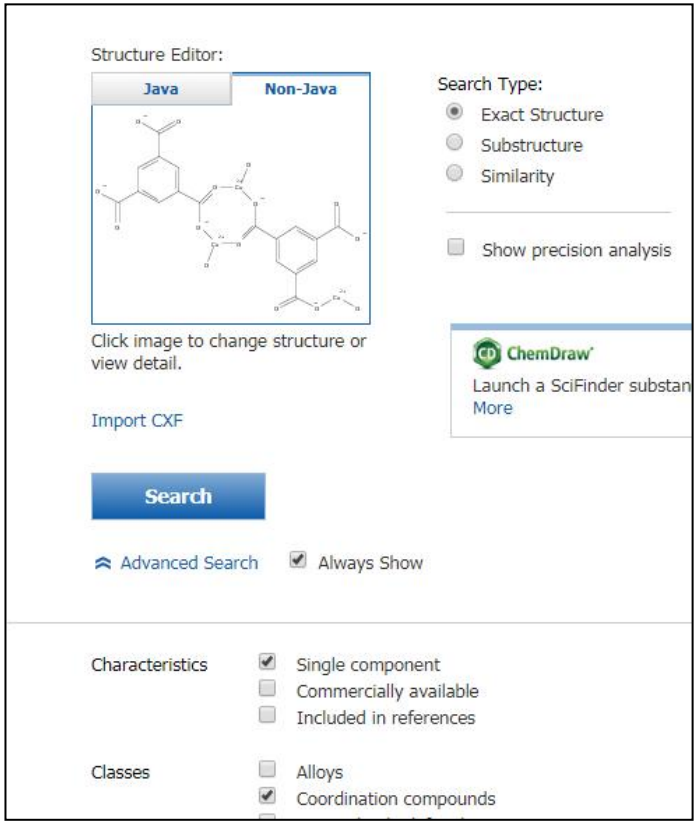
在结果集中通过Analyze by Elements，选择Cu

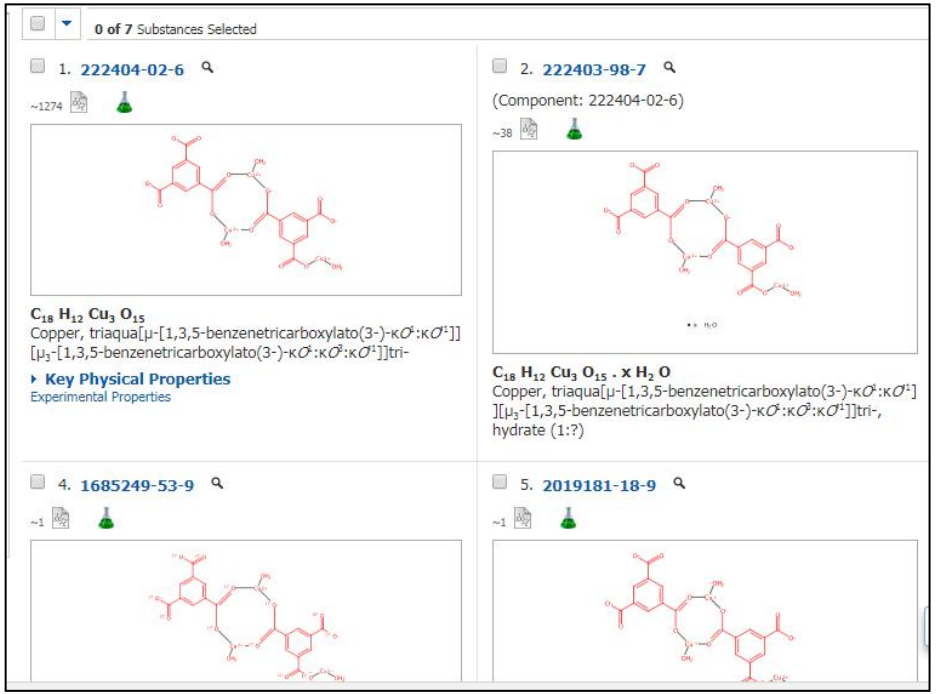


结果会有噪音，可以通过结构等进一步进行筛选

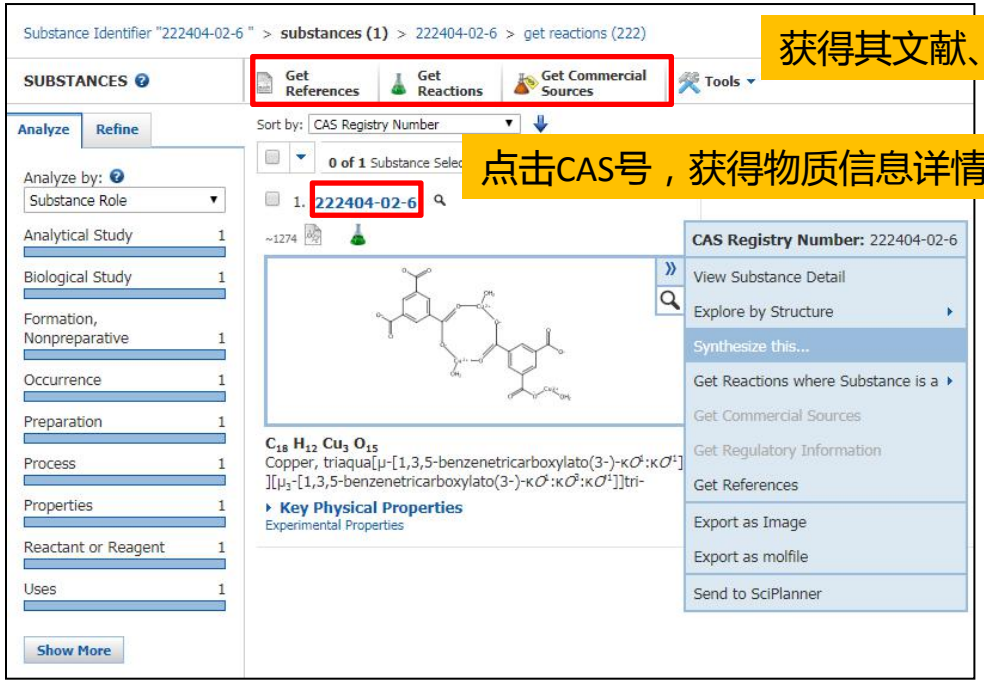


方法4：已知MOF化合物单元结构式，可以绘制完整结构进行检索





SciFinder中的物质记录



获得其文献、反应和供应商信息

点击CAS号，获得物质信息详情

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 Identifier "222404-02-6 " > substances (1) > **222404-02-6**

SUBSTANCE DETAIL | Get References | Get Reactions

Return

CAS Registry Number 222404-02-6

~1,274

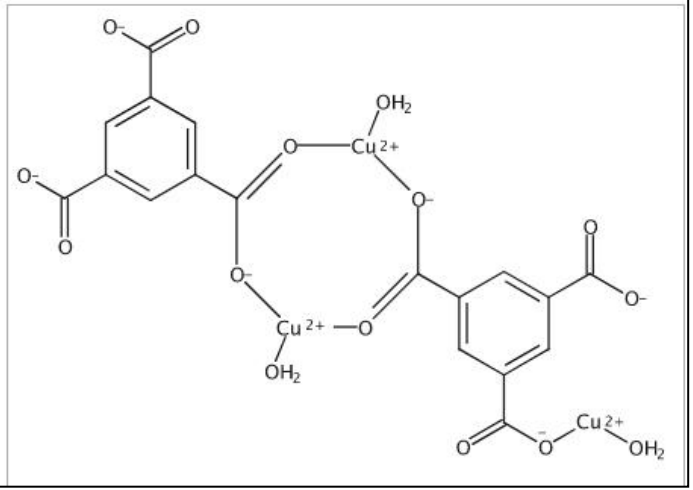
$C_{18}H_{12}Cu_3O_{15}$

Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO^1:κ$O^{1'}$]][$μ_3$-[1,3,5-benzenetricarboxylato(3-)-κO^1:κO^3:κ$O^{1'}$]]tri-

Coordination Compound

Density (Experimental)
Value: 0.879 g/cm3

Other Names
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO^1:κ$O^{1'}$]][$μ_3$-[1,3,5-benzenetricarboxylato(3-)-κO^1:κ$O^{1'}$:κO^3]]tri- (9CI)
Triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO^1:κ$O^{1'}$]][$μ_3$-[1,3,5-benzenetricarboxylato(3-)-κO^1:κO^3:κ$O^{1'}$]]tricopper
Basolite C 300
Cu-BTC
Cu_3BTC_2
View more...



实验数据与实验谱图

EXPERIMENTAL PROPERTIES

Density | Electrical | Mechanical | Nuclear | Optical and Scattering | Structure Related | Thermal

Density Properties	Value	Condition	Note
Density	0.879 g/cm3		(5)CAS
Density	See full text	1 of 3	(6)CAS

Notes

(5) Chen, Banglin; US 20110269984 A1 2011 CAPLUS

(6) Liu, Ying Dan; Chemical Communications (Cambridge, United Kingdom) 2012, V48(45), P5635-5637 CAPLUS

EXPERIMENTAL SPECTRA

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

^{1}H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See full text		(15)CAS

Notes

(15) Chen, Joseph J.; Angewandte Chemie, International Edition 2013, V52(46), P12043-12046 CAPLUS

SciFinder® A CAS SOLUTION

SciFinder中的物质记录

CAS REFERENCE ROLES

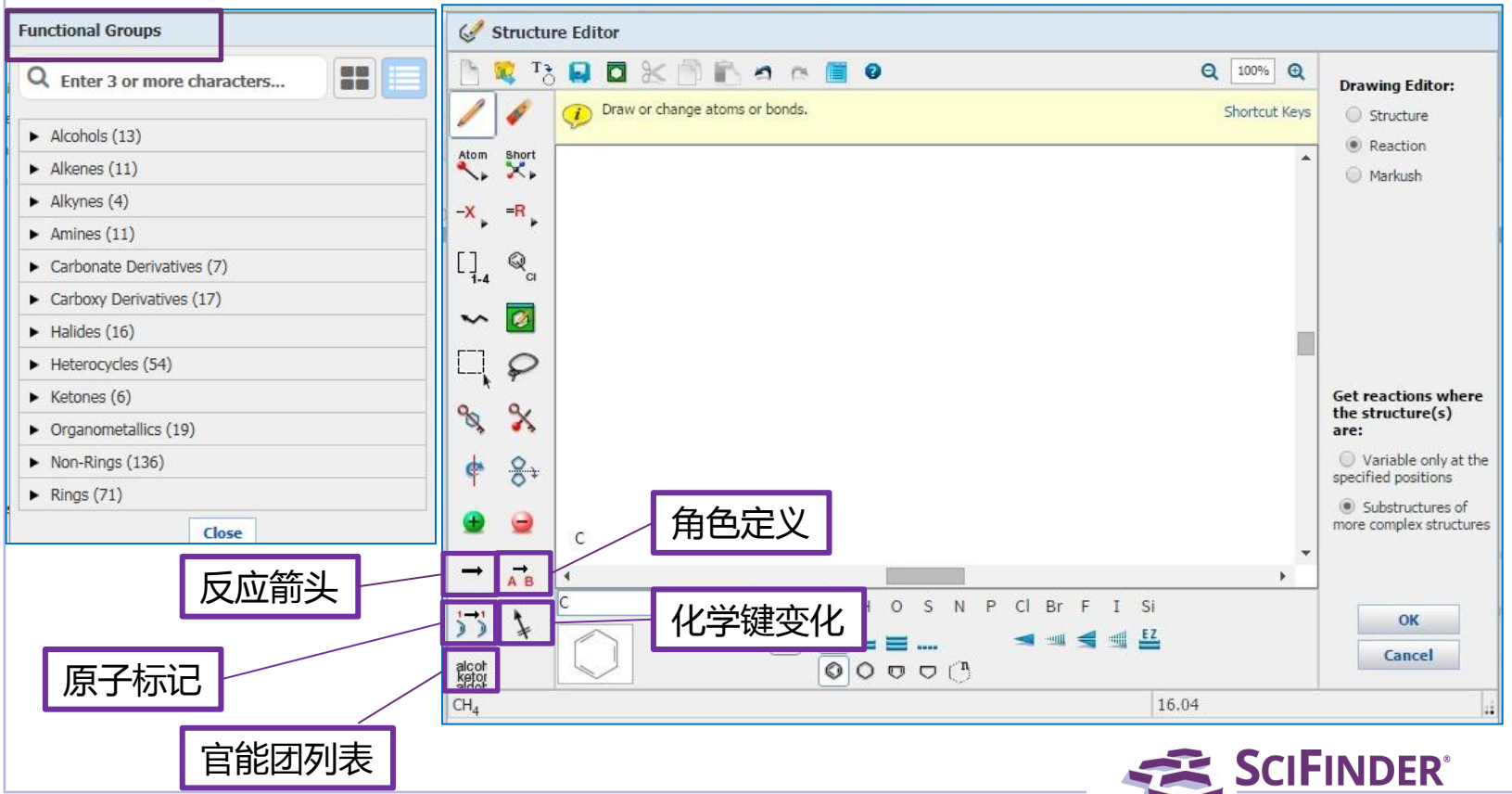
Roles	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Combinatorial Study	✓	✓	✓	
Formation, Nonpreparative	✓	✓	✓	✓
Miscellaneous	✓	✓	✓	✓
Occurrence	✓	✓	✓	✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties		✓	✓	
Prophetic in Patents			✓	
Reactant or Reagent			✓	✓
Uses	✓	✓	✓	✓

选中任何一项即可获得相关文献

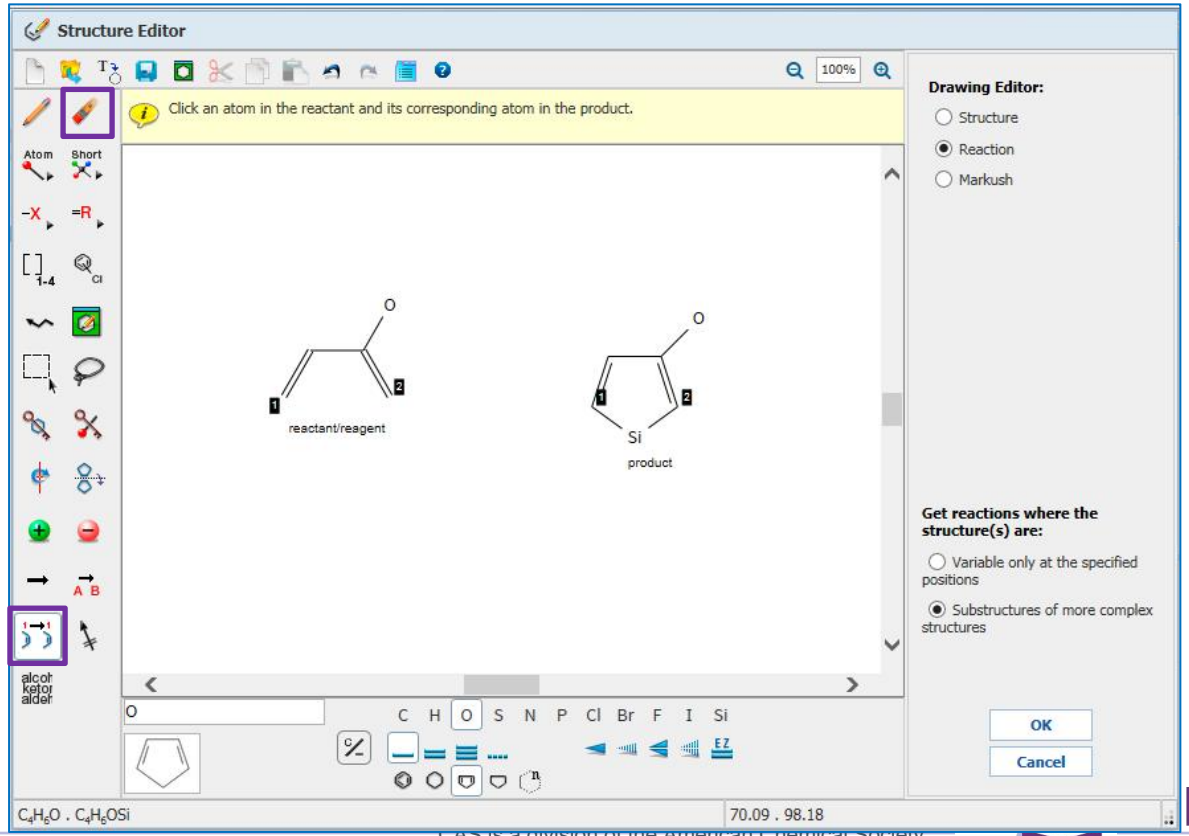
如何使用SciFinder提高科研效率

- 以“光解水”为例，如何利用SciFinder：
  - 获取研究全景
  - 对文献结果进行分析、筛选、及精准定位所需信息
- 物质检索
  - 如何从大量物质结果集中快速定位目标物质
  - 结构式检索；分子式检索（合金，多氧簇金属，MOF化合物）；物质属性检索
  - 如何获得物质的属性信息、谱图信息
  - 化合物分析方法检索
- **反应检索**
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何进行精确结构反应检索，并获得实验详情
  - 如何进行亚结构反应检索，以及如何处理检索结果
  - 案例分享
    - 多氧簇金属的反应信息
    - MOF化合物反应信息

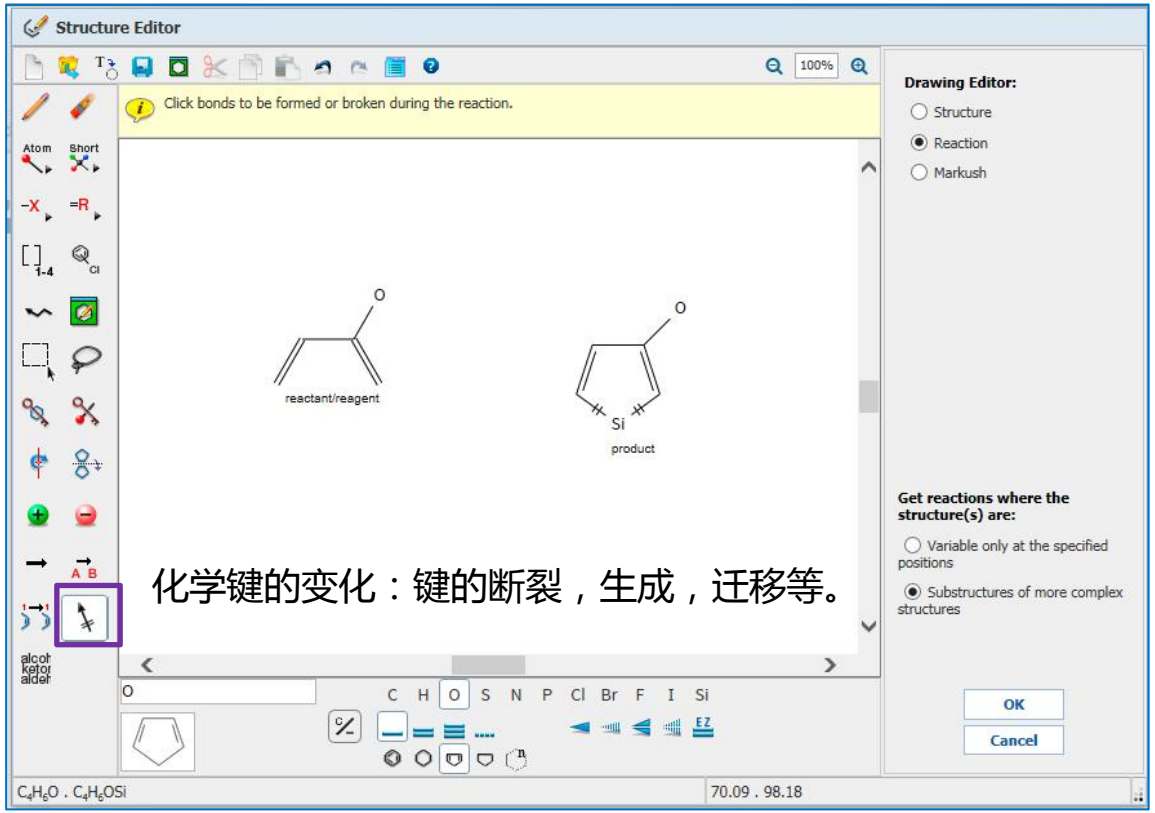
结构编辑器：绘制反应工具



例1：反应前后物质中的原子标记



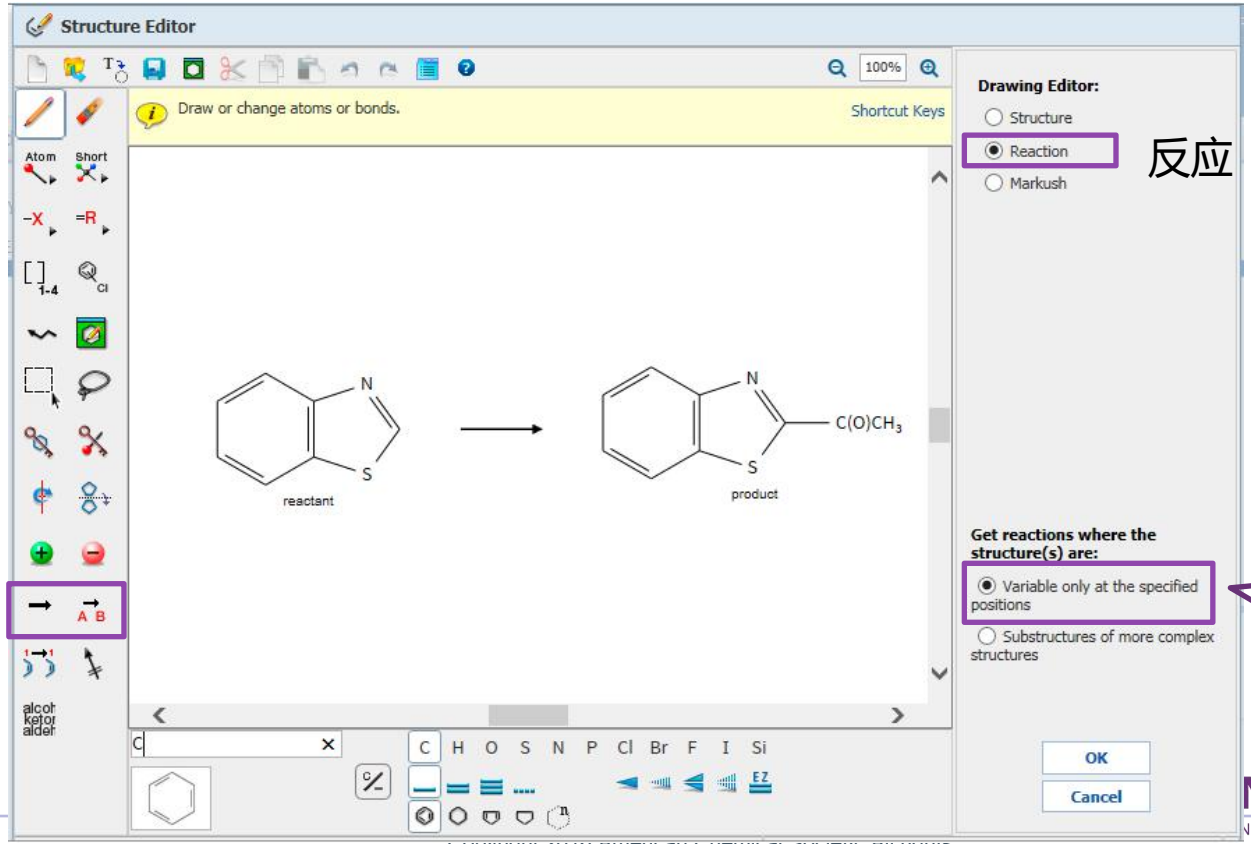
例2：发生变化的化学键标记



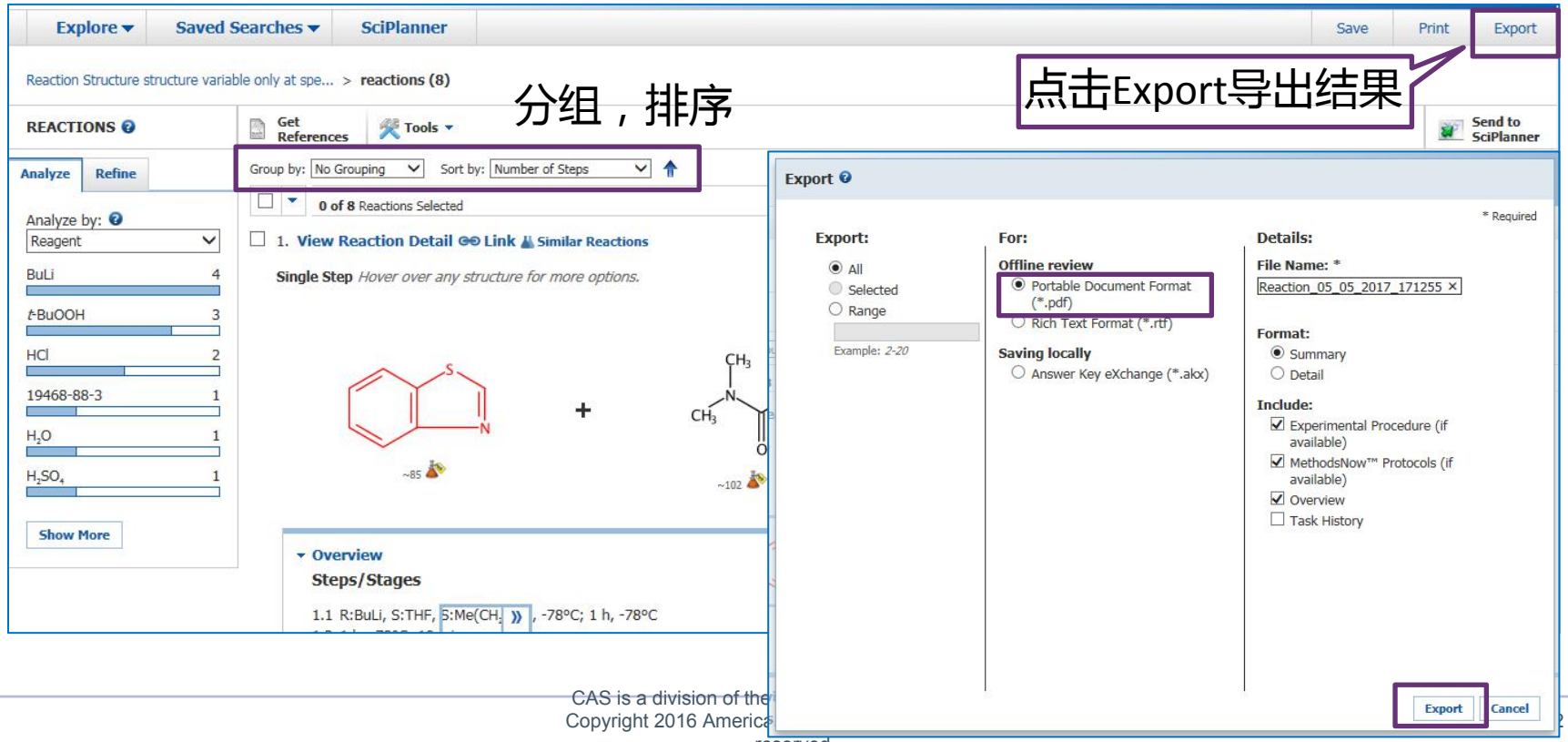
化学键的变化：键的断裂，生成，迁移等。

SciFinder® A CAS SOLUTION

精确结构反应检索：绘制反应式

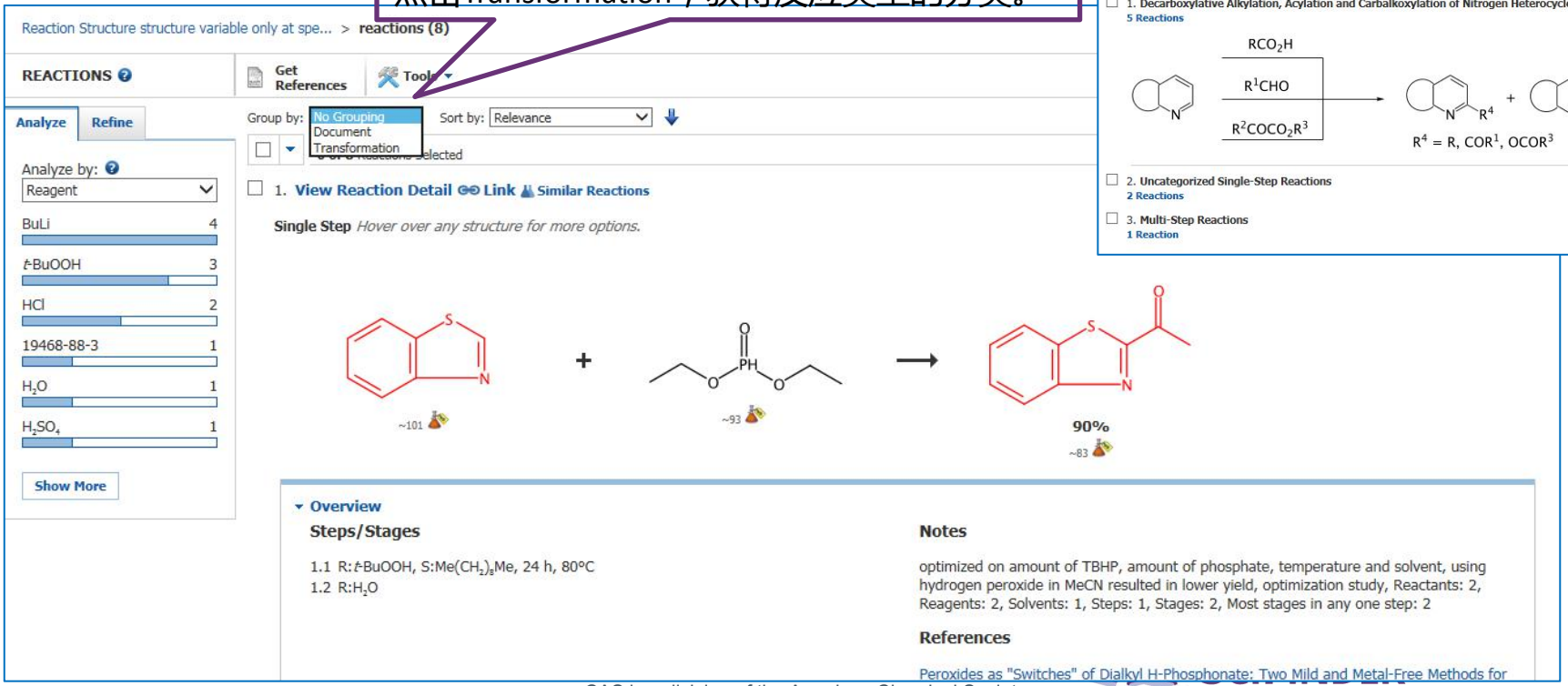


精确结构反应检索：查看反应结果集

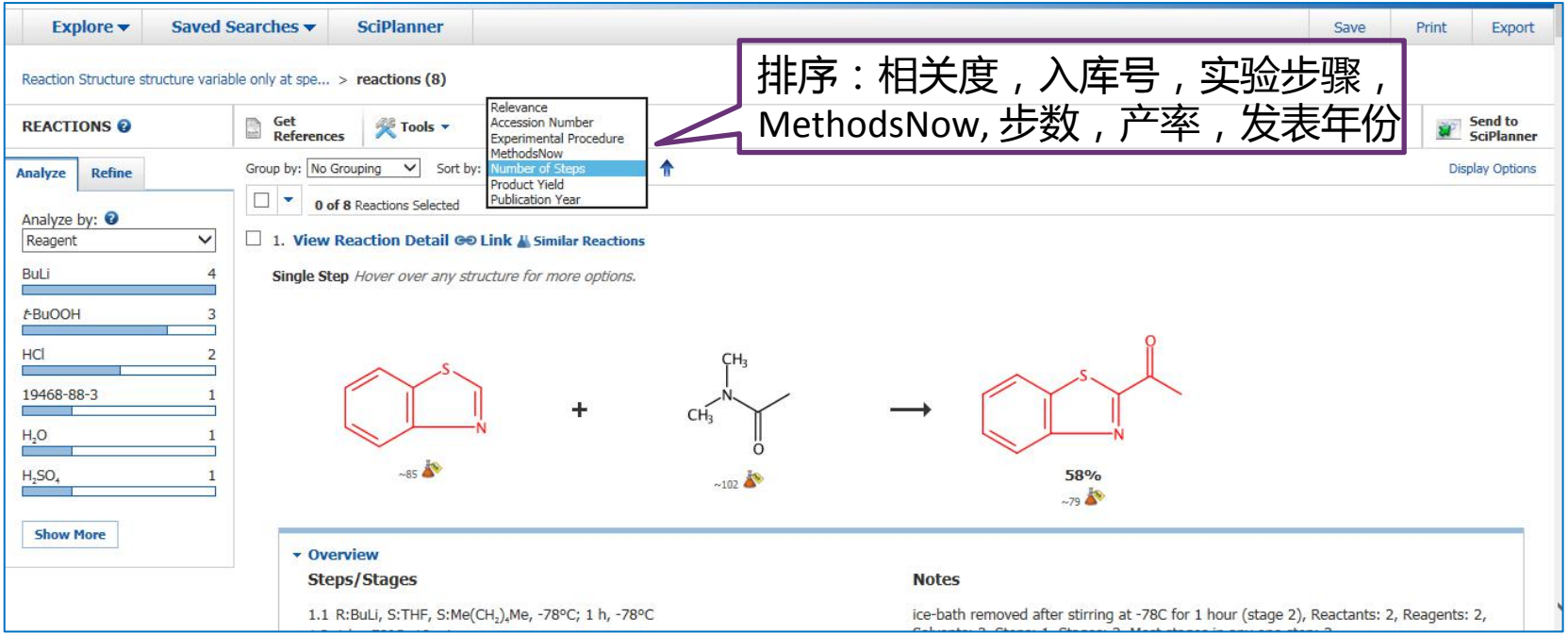


精确结构反应检索：查看反应结果集

点击Document，合并来自同一篇文献的反应；
点击Transformation，获得反应类型的分类。



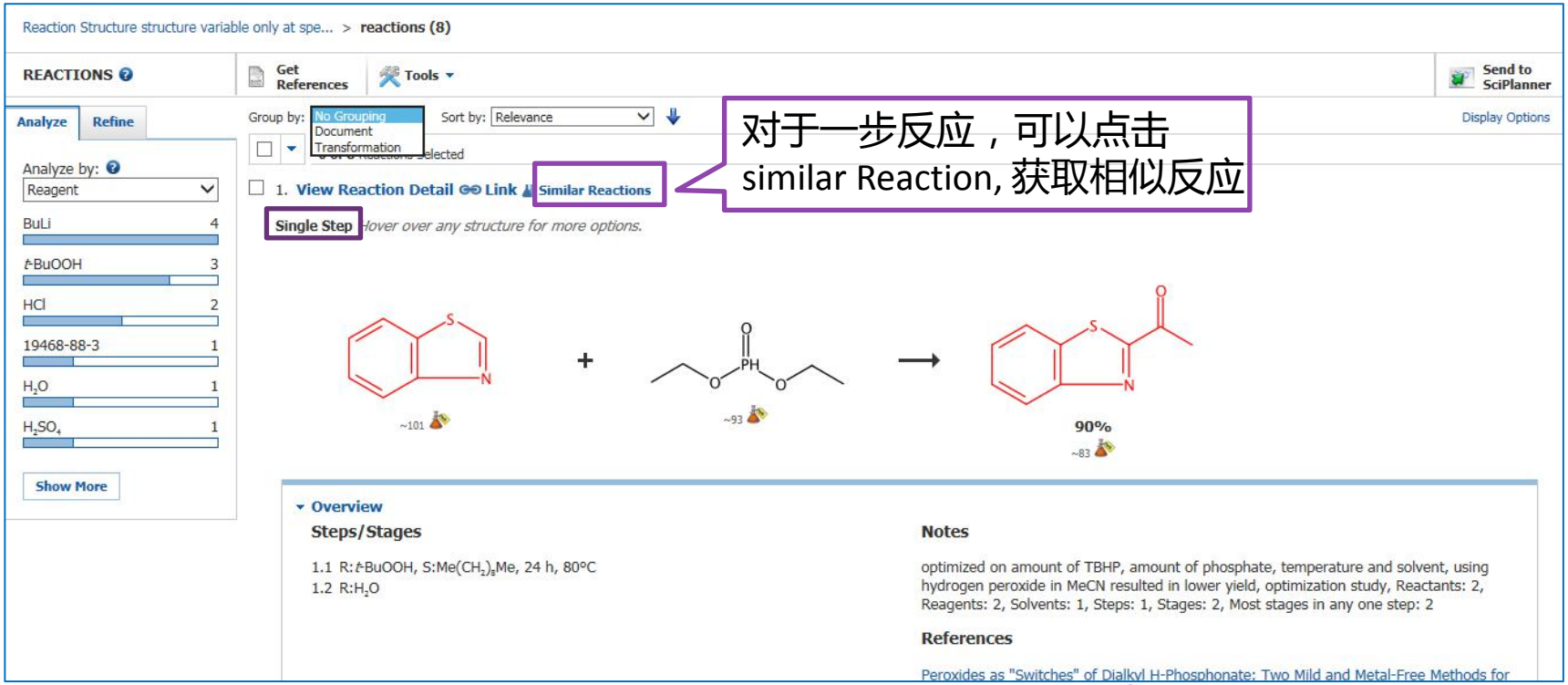
精确结构反应检索：查看反应结果集



排序：相关度，入库号，实验步骤，MethodsNow, 步数，产率，发表年份

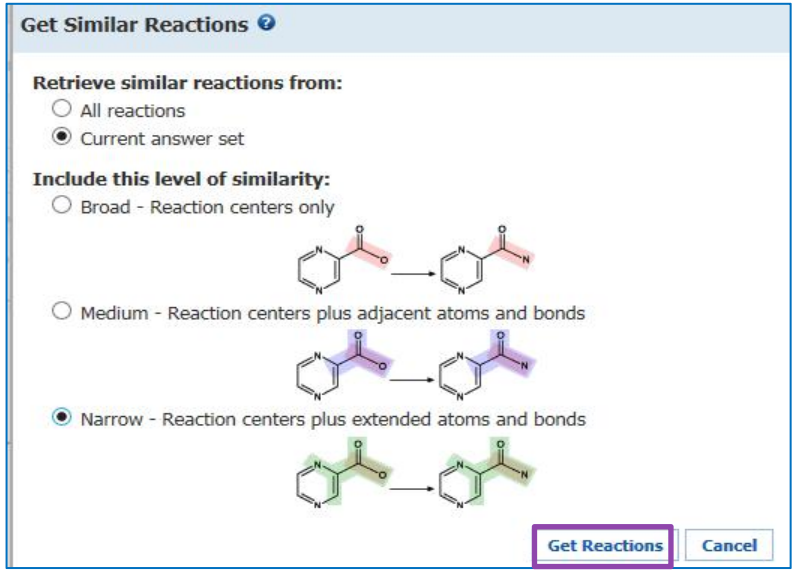
SciFinder® A CAS SOLUTION

精确结构反应检索：查看反应结果集



SCIFINDER® A CAS SOLUTION

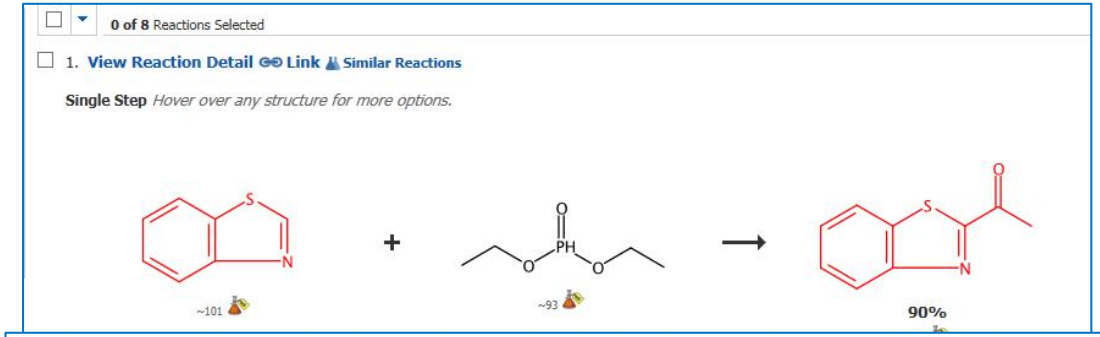
精确结构反应检索：获取相似反应



相似度限制：
Broad：仅反应中心相似
Medium：反应中心及附属原子和键
Narrow：反应中心及扩展的原子和键

SciFinder® A CAS SOLUTION

精确结构反应检索：查看感兴趣的反应信息



实验步骤

Overview

Steps/Stages

1.1 R:*t*-BuOOH, S:$Me(CH_2)_8Me$, 24 h, 80°C
1.2 R:H_2O

Notes

optimized on amount of TBHP, amount of phosphate, temperature and solvent, using hydrogen peroxide in MeCN resulted in lower yield, optimization study, Reactants: 2, Reagents: 2, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Peroxides as "Switches" of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for Preparation of 2-Acylbenzothiazoles and Dialkyl Benzothiazol-2-ylphosphonates
Quick View Other Sources
By Chen, Xiao-Lan et al
From Journal of Organic Chemistry, 79(17), 8407-8416; 2014

Experimental Procedure

JOC The Journal of Organic Chemistry

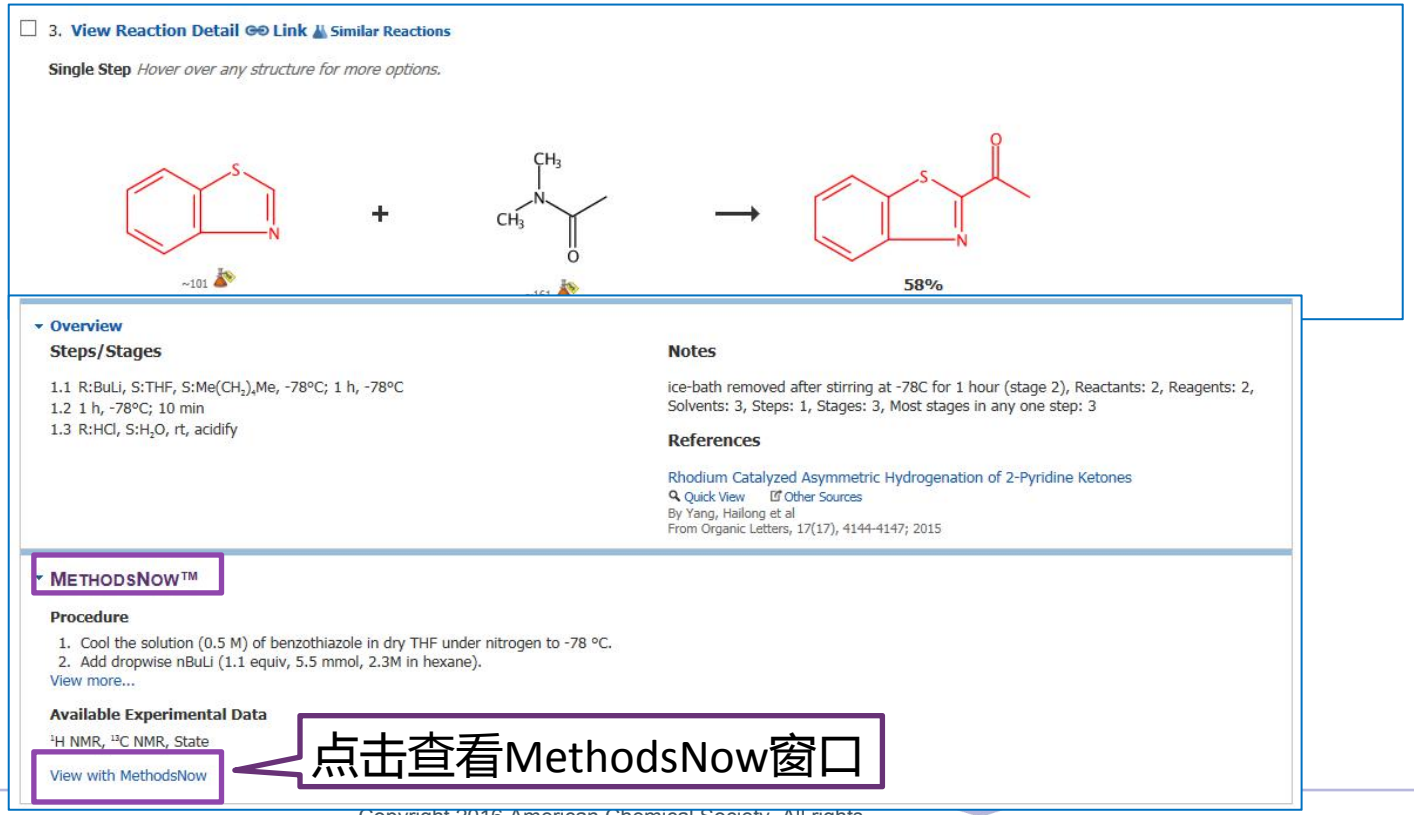
Experimental Procedures for the Synthesis of 2-Acylbenzothiazoles (3a 3ab). A mixture of benzothiazole (135.0 mg, 1.0 mmol), phosphonate (5.0 mmol), and TBHP (10.0 mmol) in CH_3CN (2.0 mL) was stirred at 80 °C for 24 h. The reaction mixture was quenched with water (5.0 mL) and extracted with ethyl acetate (3 x 5.0 mL). The combined organic layers were washed with brine (15.0 mL) and dried over anhydrous $MgSO_4$. After filtration, the solvent was evaporated in vacuo. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate 20/1) to give the desired product *1-(Benzo[d]thiazol2-yl) ethanone (3a):* Yield 90%. mp 107 110 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 2.83 (s, 3H), 7.53 (td, *J* = 7.6, 1.3 Hz, 1H), 7.58 (td, *J* = 8.0, 1.3 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 8.18 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.2, 122.5, 125.5, 127.0, 127.7, 137.5, 153.6, 166.5, 193.2; HRMS (ESI) calcd for C_9H_7NOS [M + H]$^+$, 178.0321, found 178.0320.

MethodsNow Synthesis——人工标引的反应信息，节省您宝贵的时间

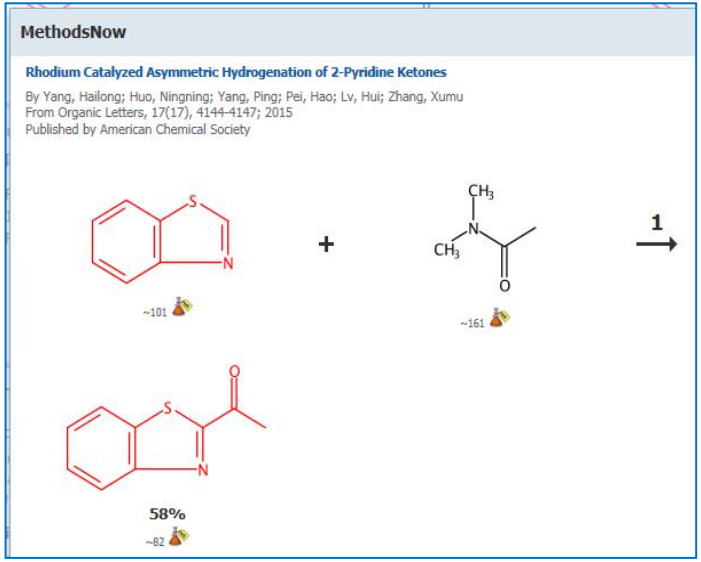
- 详细、明确的物质信息
- 全面、有条理的实验过程信息
- 更好的阅读体验——表格形式
- 无需查看原文直接获取实验详情——反应物，反应条件，步骤，产物性质，谱图等

SciFinder®
A CAS SOLUTION

MethodsNow Synthesis: 通过Analyze，选择有MethodsNow标引的反应，点击MethodsNow查看实验详情



MethodsNow Synthesis: 实验详情展示窗口



Products	Ethanone, 1-(2-benzothiazolyl)-, 58%, CAS RN: 1629-78-3
Reactants	Benzothiazole, CAS RN: 95-16-9 Dimethylacetamide, CAS RN: 127-19-5
Reagents	Butyllithium, CAS RN: 109-72-8 Hydrochloric acid, CAS RN: 7647-01-0
Solvents	Tetrahydrofuran, CAS RN: 109-99-9 Hexane, CAS RN: 110-54-3 Water, CAS RN: 7732-18-5
Procedure	1. Cool the solution (0.5 M) of benzothiazole in dry THF under nitrogen to -78 °C. 2. Add dropwise nBuLi (1.1 equiv, 5.5 mmol, 2.3M in hexane). 3. Keep the resulted mixture for 1 h under -78 °C. 4. Add N,N-dimethylacetamide (1 equiv, 5 mmol) to the stirred solution at -78 °C. 5. Stir the mixture was continuously for 1 h. 6. Remove the cold bath and stir the mixture for additional 10 min. 7. Hydrolyze with concd hydrochloric acid (1 mL). 8. Stir the acidic solution continuously until the temperature reach to room temperature. 9. Pour the mixture into same amount of water. 10. Extract the aqueous mixture with ethyl acetrate 3 times. 11. Dry the combined organic solution with Na_2SO_4. 12. Purify by flash column chromatography to afford product.
Transformation	Decarboxylative Alkylation, Acylation and Carbalkoxylation of Nitrogen Heterocycle
^{1}H NMR	(400 MHz, $CDCl_3$)δ8.22 (d,J = 8.0Hz,1H), 8.01 (d, J = 7.6Hz, H), 7.55-7.63 (m, 2H), 2.87 (s, 3H);
^{13}C NMR	(101MHz, $CDCl_3$)δ193.2, 166.5, 153.6, 137.4, 127.7, 127.0, 125.5, 122.5, 26.2.
State	white solid
CAS Method Number	3-219-CAS-1662290

点击CAS RN，
即时查看物质

产物，反应物，试剂，溶剂，步骤，
反应类型，规模，核磁氢谱，核磁碳谱，
产物状态，CAS方法号

PDF or XLS格式

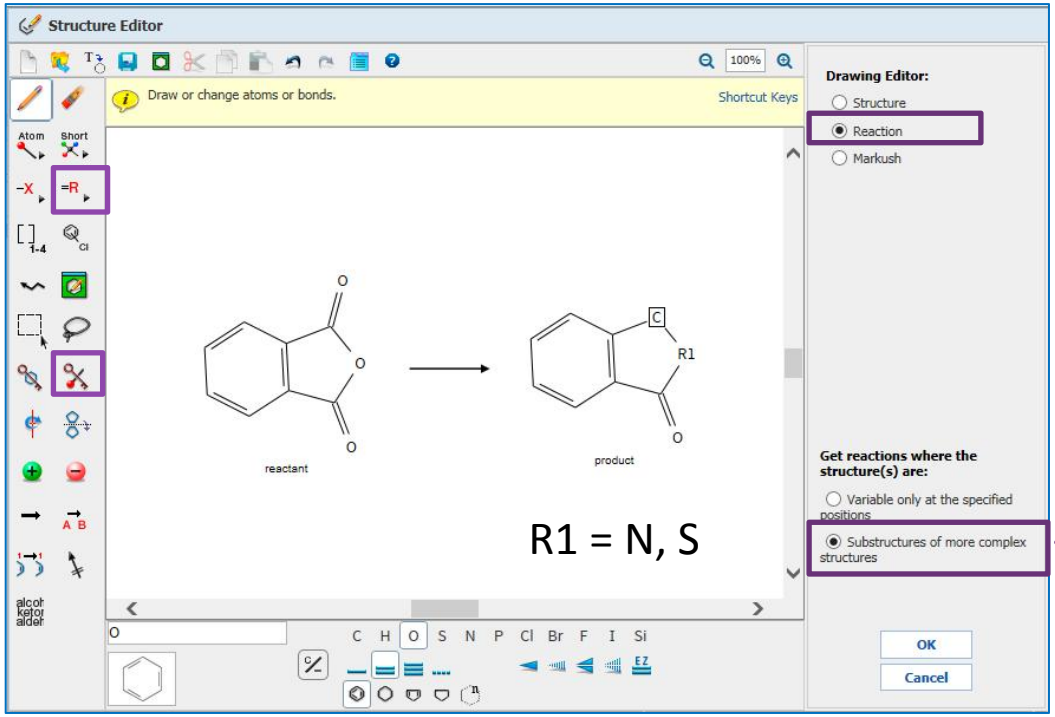
Print/Export Close

SciFinder® A CAS SOLUTION

提纲

- SciFinder中获取化合物制备信息的方法
- 物质相关信息获取方法
  - 结构编辑器的使用（绘图工具，定义和限定化合物等）
  - 如何进行物质检索（结构，属性，识别号检索等）
  - 如何查看物质详情
- 反应相关信息获取方法
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何进行精确结构反应检索，并获得实验详情
  - 如何进行亚结构反应检索，以及如何处理检索结果
  - 反应检索案例分享

亚结构反应检索: 绘制反应式



输入的反应物和产物结构可以被修饰，但母体结构不变

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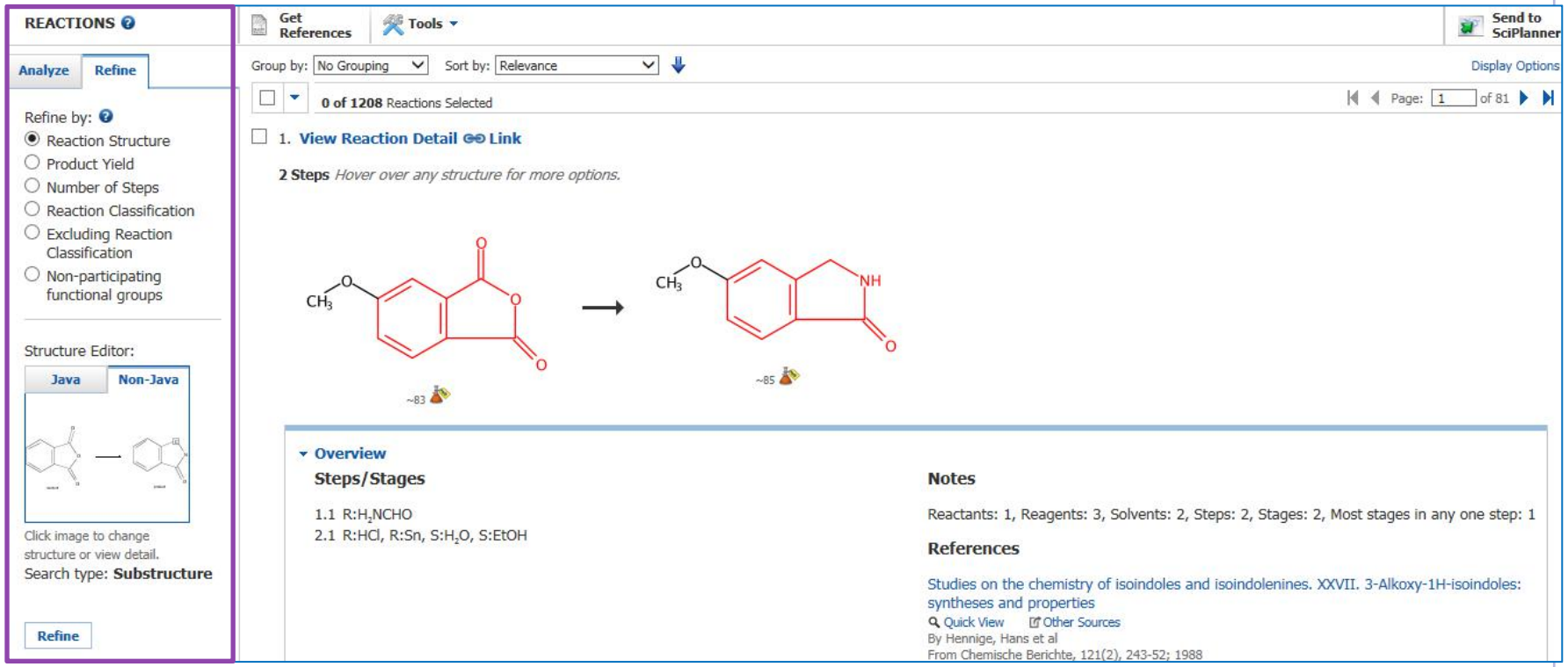
亚结构反应检索：获得反应结果集



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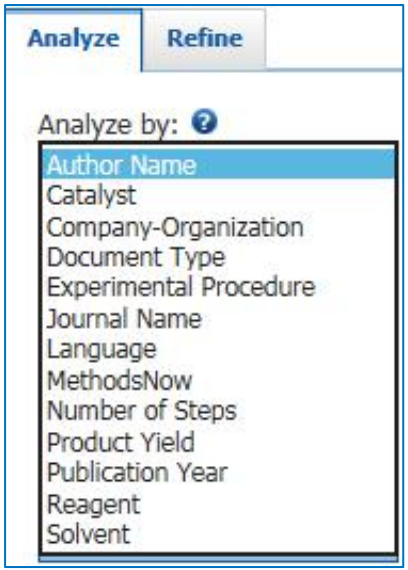
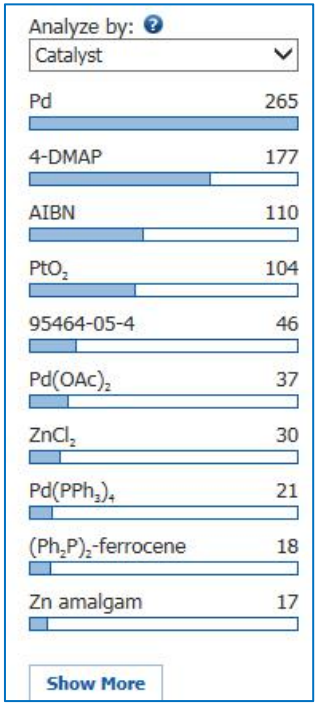
亚结构反应检索：分析处理

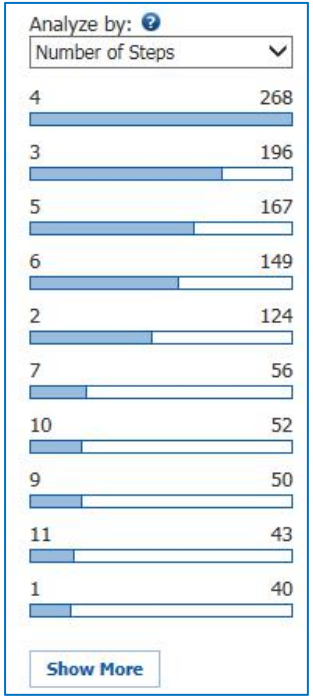
13种分析选项



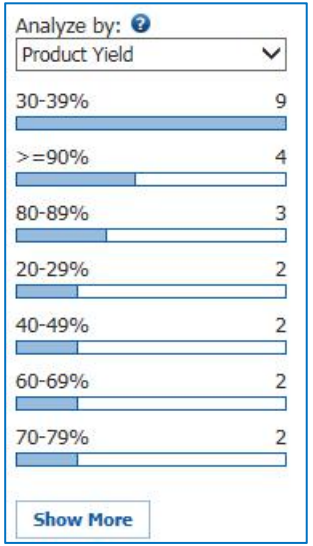
催化剂



反应步数



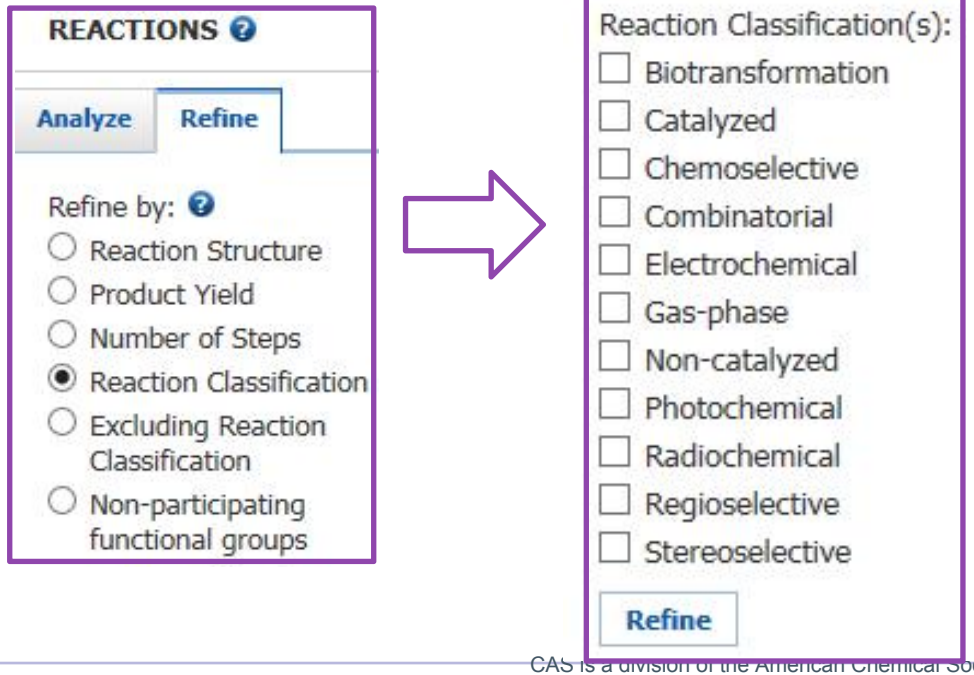
产率



SciFinder® A CAS SOLUTION

亚结构反应检索：筛选处理

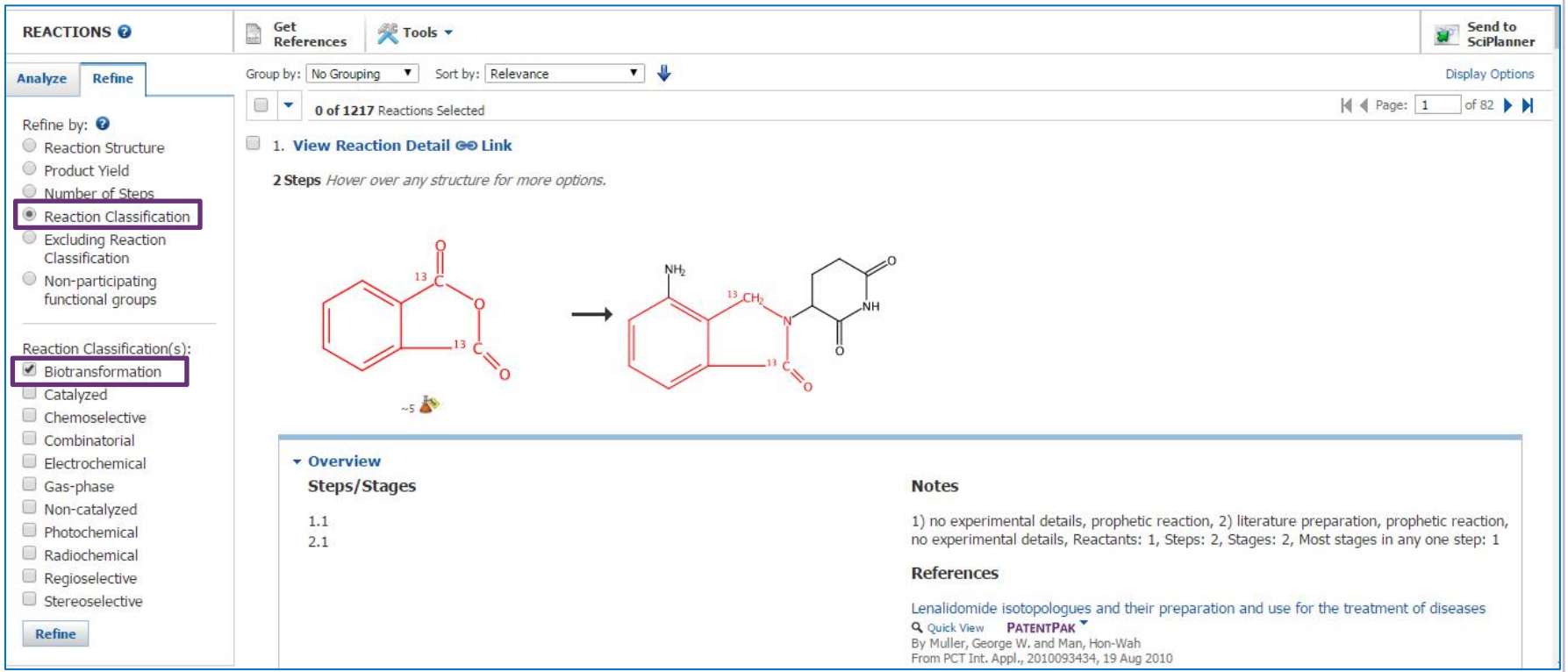
6种筛选选项：反应结构、产率、反应步数、包含/排除的反应类型(11种)、反应官能团(217种)



- ❑ 生物转化
- ❑ 催化反应
- ❑ 化学选择性
- ❑ 组合化学
- ❑ 电子化学
- ❑ 气相反应
- ❑ 非催化反应
- ❑ 光化学
- ❑ 放射化学
- ❑ 区域选择反应
- ❑ 立体选择反应

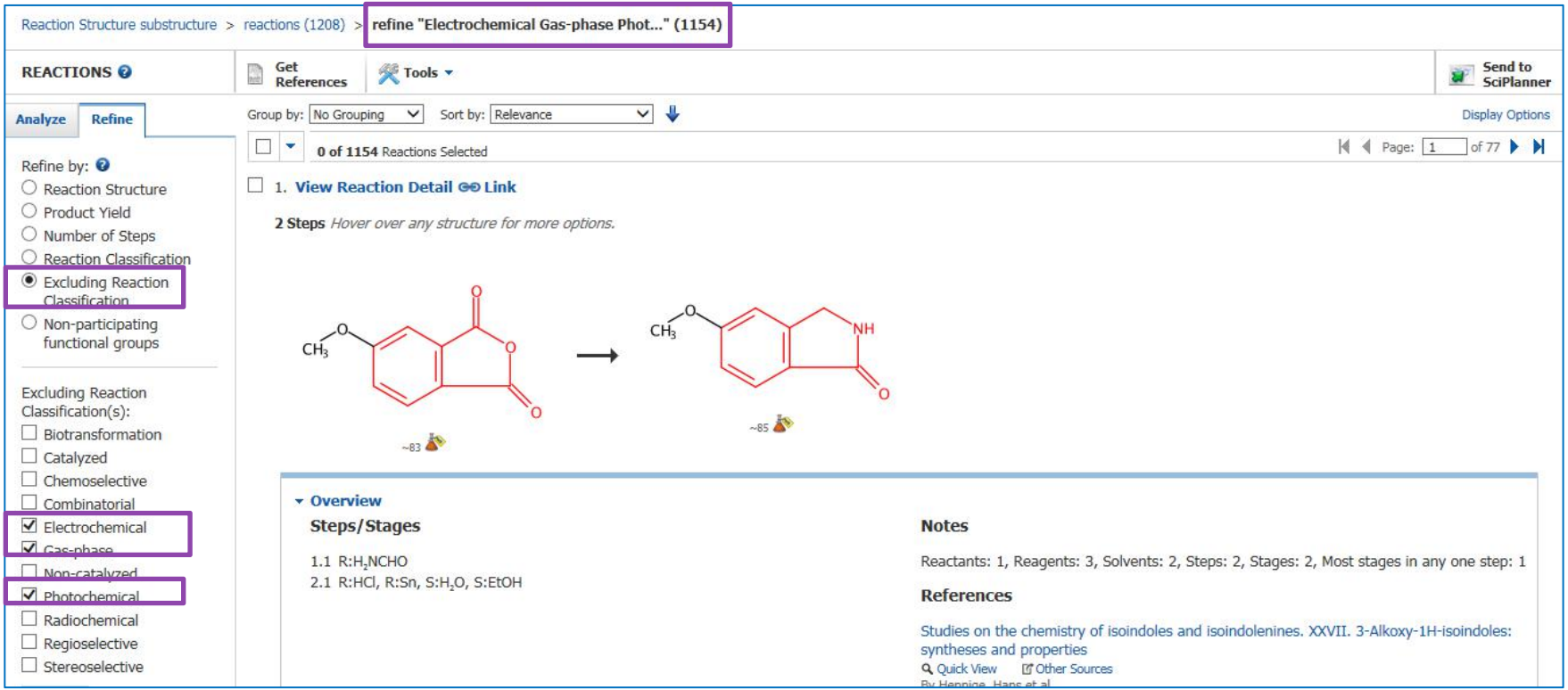
SciFinder® A CAS SOLUTION

亚结构反应检索：勾选反应类型



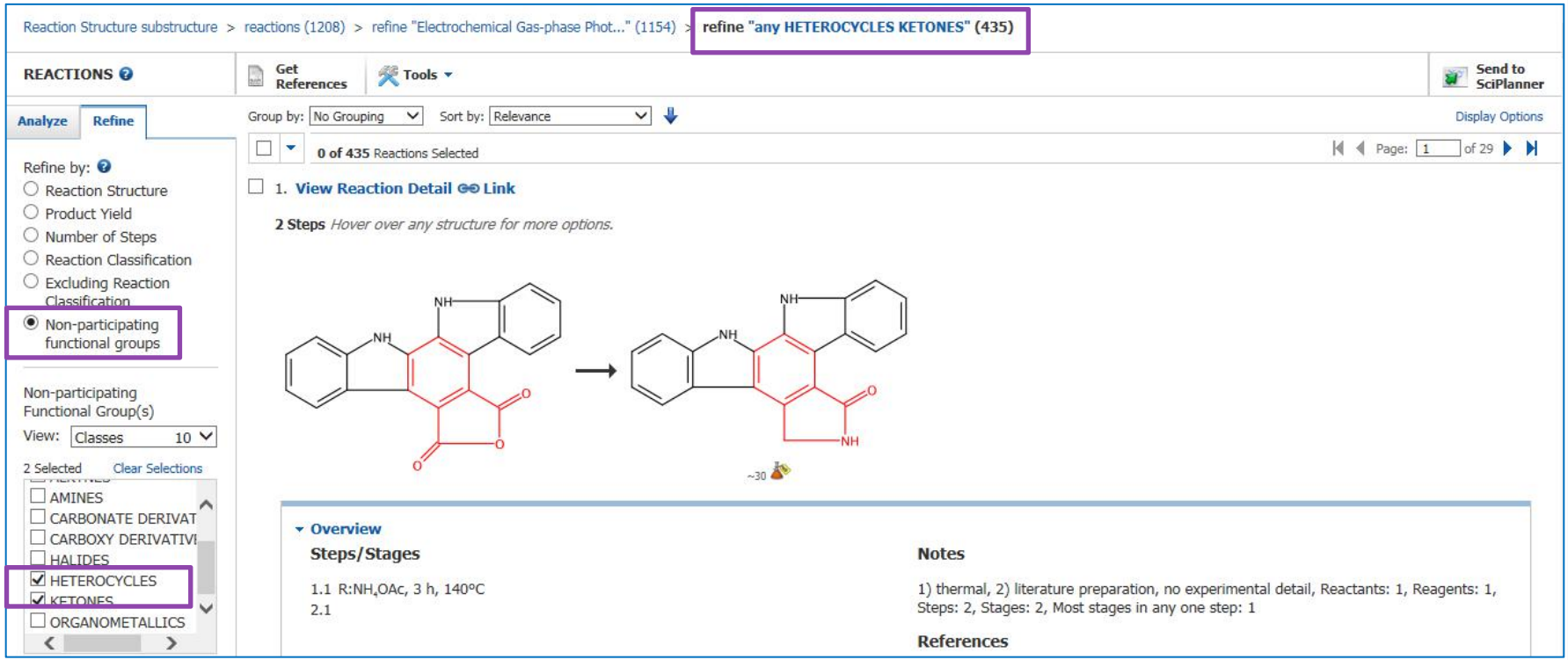
SciFinder® A CAS SOLUTION

亚结构反应检索：排除反应类型



SciFinder® A CAS SOLUTION

亚结构反应检索：筛选官能团



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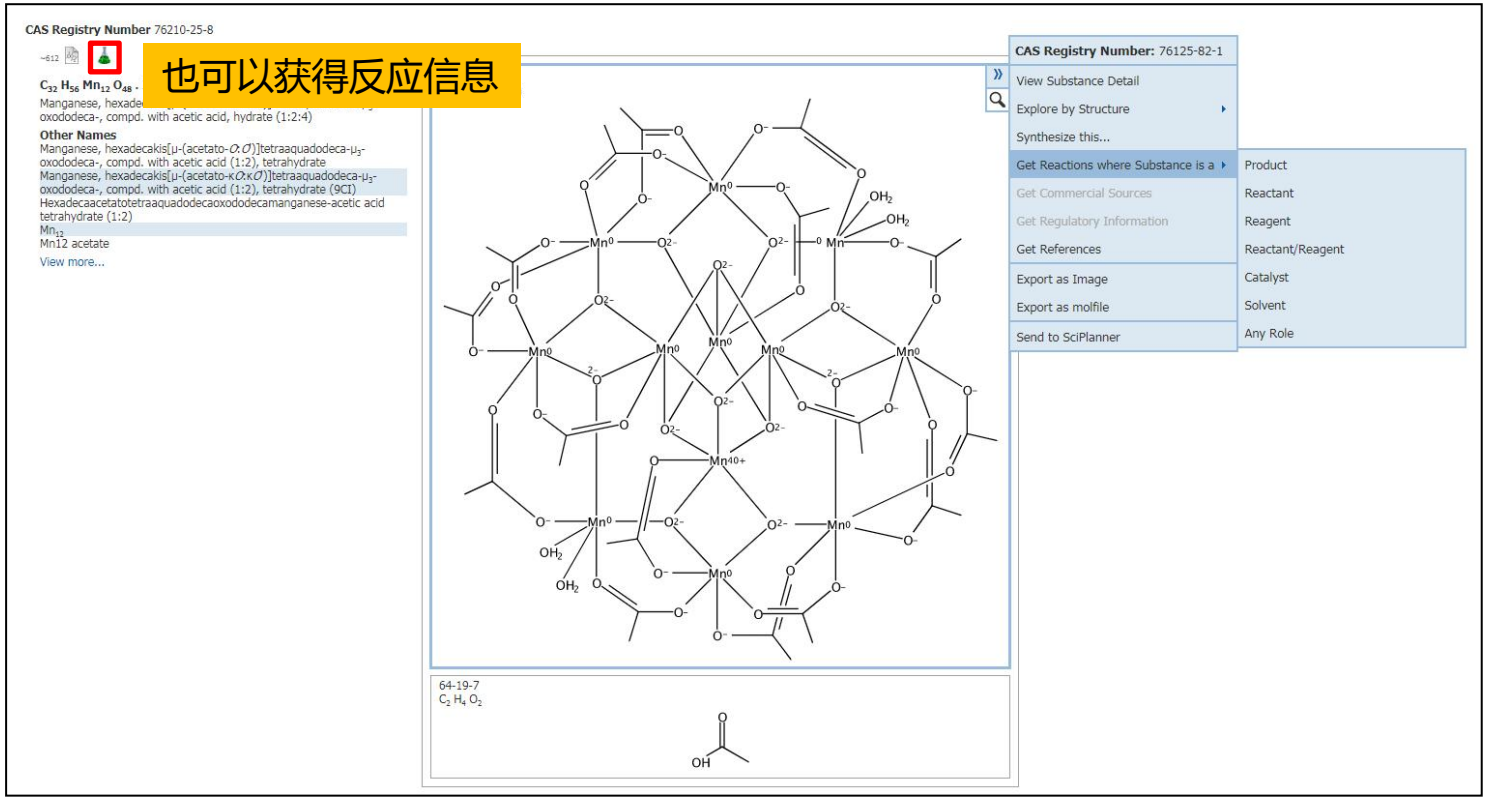
查找多氧簇金属的反应信息：



SciFinder® A CAS SOLUTION

查看反应信息详情

Analyze | Refine

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

Analyze by: Reagent

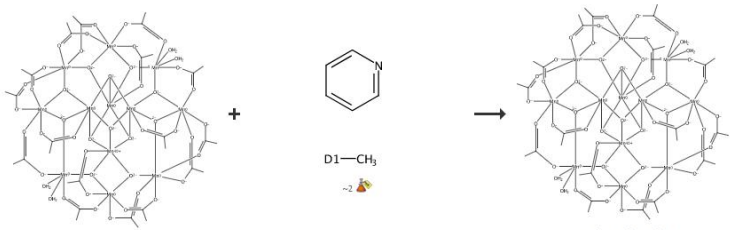
- $KMnO_4$ 6
- TEA chloride 2
- 110743-42-5 1
- $Ce(NH_4)_2(NO_3)_6$ 1
- H_2O 1
- $Mn(OAc)_2$ 1

Show More

0 of 12 Reactions Selected

1. View Reaction Detail Link

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



complex with picoline

Overview

Steps/Stages

1.1 R:$Ce(NH_4)_2(NO_3)_6$, S:MeCN, rt; 15 min, rt

Notes

crystals formed after 3 days at room temperature, Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Manganese/Cerium Clusters Spanning a Range of Oxidation Levels and CeMn8, Ce2Mn4, and Ce6Mn4 Nuclearities: Structural, Magnetic, and EPR Properties

Quick View | Other Sources

By Lampropoulos, Christos et al

From Inorganic Chemistry, 53(13), 6805-6816; 2014

Experimental Procedure

Inorganic Chemistry

General/Typical Procedure: ***Method B.*** To a stirred solution of $[Mn_{12}O_{12}(O_2CMe)_{16}(H_2O)_4]$ (0.50 g, 0.25 mmol) in a solvent mixture comprising MeCN (15 mL) and pyridine (10 mL) was slowly added solid $(NH_4)_2[Ce(NO_3)_6]$ (0.28 g, 0.50 mmol). The resulting solution was stirred for 15 min, during which time the color changed slightly from dark brown to redbrown. The solution was filtered and left undisturbed for a period of 3 d, during which time black needles of **1**·2py·6MeCN grew. They were isolated as for Method A; the yield was based on Ce. The identity of the product was confirmed by elemental analysis, IR spectral comparison, and unit cell determination to be identical to material from Method A. The picoline version $[Ce_6Mn_4O_{12}(O_2CMe)_{10}(NO_3)_4(pic)_4]$ (**1'**) can be obtained in comparable yield by the same method using picoline instead of pyridine. Anal. Calcd (Found) for **1**·$2H_2O$: C, 21.14 (21.25); H, 2.50 (2.75); N, 4.48 (4.26)%.

METHODSNOW™

Procedure

1. Slowly add solid $(NH_4)_2[Ce(NO_3)_6]$ (0.28 g, 0.50 mmol) to a stirred solution of $[Mn_{12}O_{12}(O_2CMe)_{16}(H_2O)_4]$ (0.50 g, 0.25 mmol) in a solvent mixture comprising MeCN (15 mL) and picoline (10 mL).
2. Stir the resulting solution for 15 min.

View more...

Available Experimental Data

Elemental Analysis

View with MethodsNow

查找MOF的反应信息：

Substance Identifier "222404-02-6 " > substances (1) > **222404-02-6**

SUBSTANCE DETAIL | Get References | Get Reactions

Return

CAS Registry Number 222404-02-6

~1.274

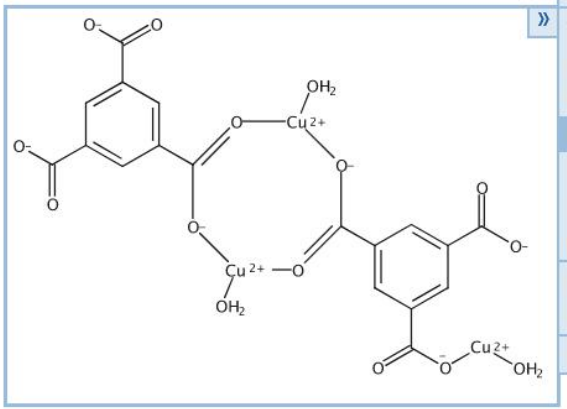
$C_{18}H_{12}Cu_3O_{15}$

Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO¹]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO³:κO¹]]tri-

Coordination Compound

Density (Experimental)
Value: 0.879 g/cm3

Other Names
Copper, triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO³]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO³:κO³]]tri- (9CI)
Triaqua[μ-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO¹]][μ₃-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO³:κO¹]]tricopper
Basolite C 300
Cu-BTC
Cu_3BTC_2
View more...



CAS Registry Number: 222404-02-6

- View Substance Detail
- Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
  - Product
  - Reactant
  - Reagent
  - Reactant/Reagent
  - Catalyst
  - Solvent
  - Any Role
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile
- Send to SciPlanner

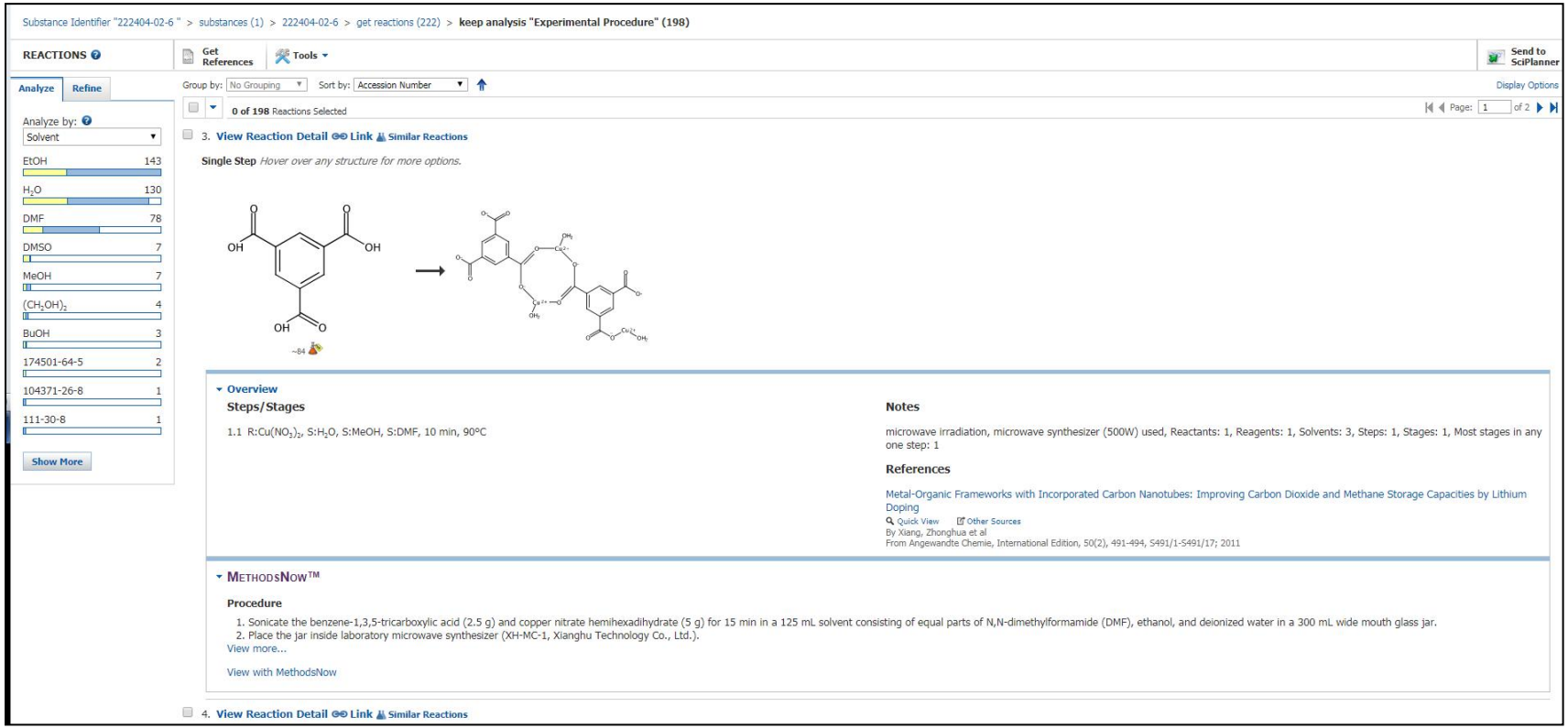
▸ EXPERIMENTAL PROPERTIES

▸ EXPERIMENTAL SPECTRA

▸ CAS REFERENCE ROLES

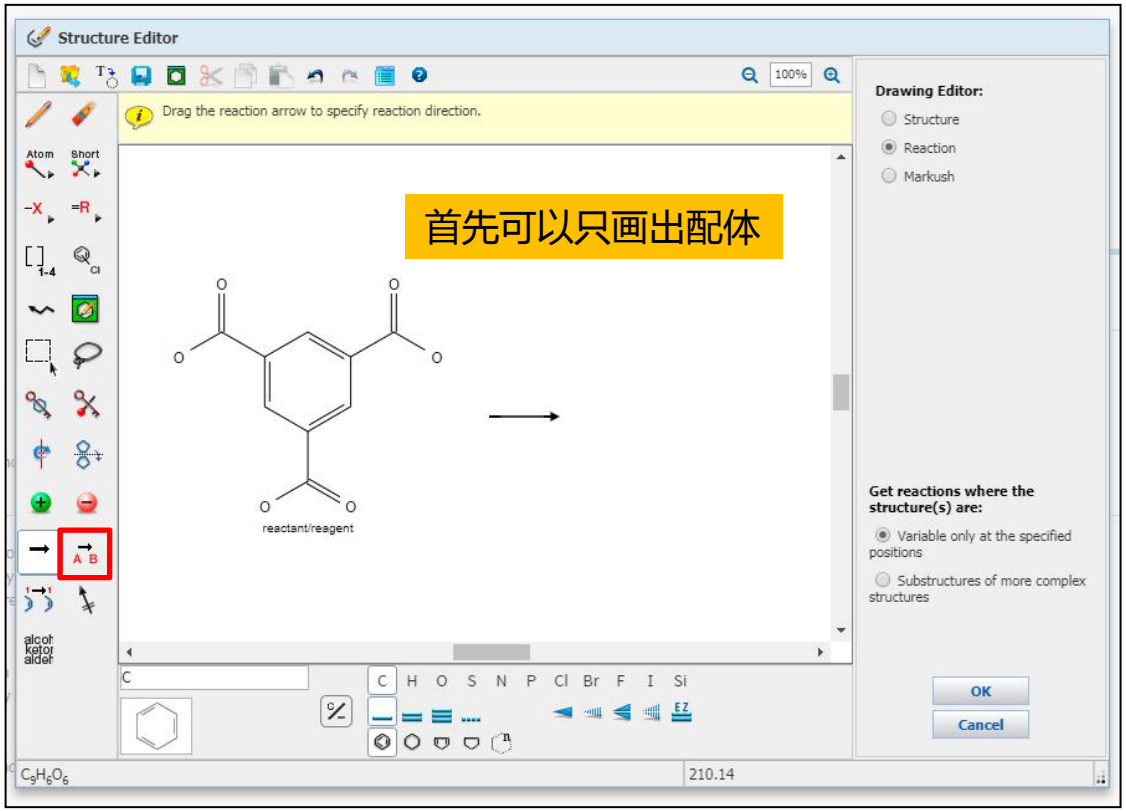
▸ ADDITIONAL DETAILS

查看反应信息详情



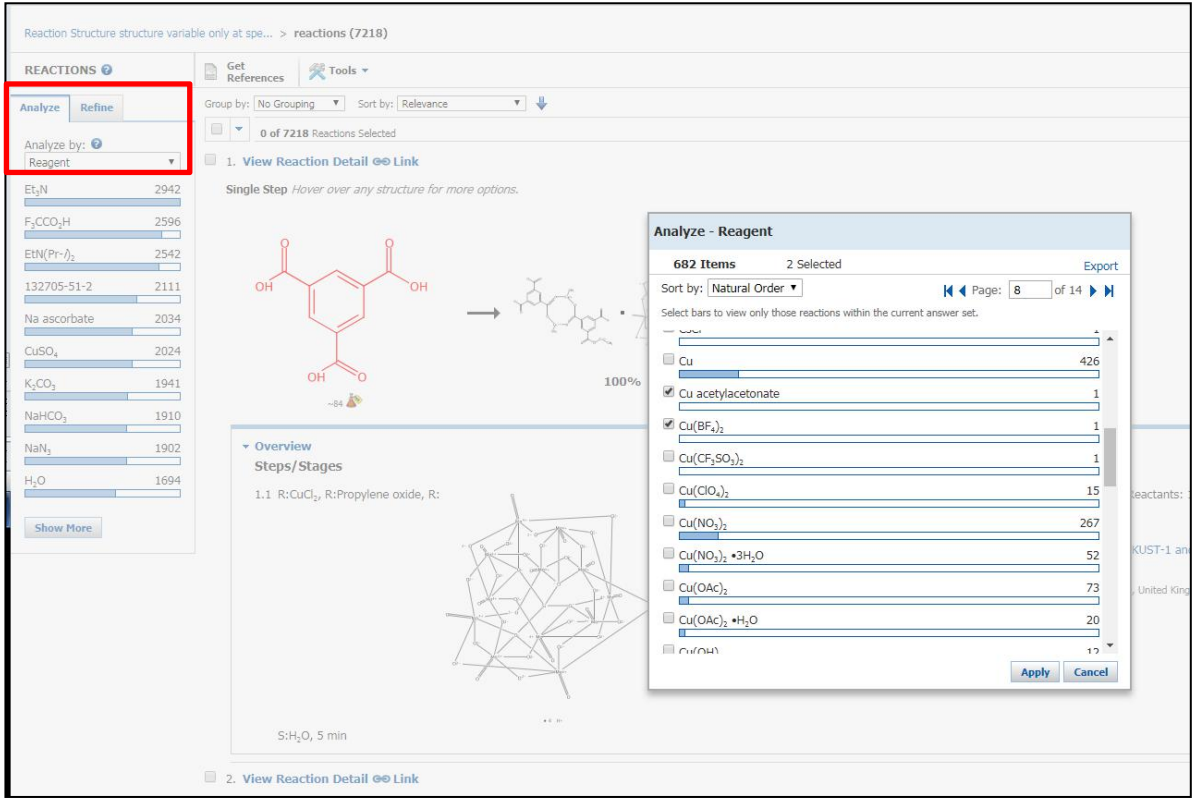
SCIFINDER® A CAS SOLUTION

已知配体查找MOF的合成信息



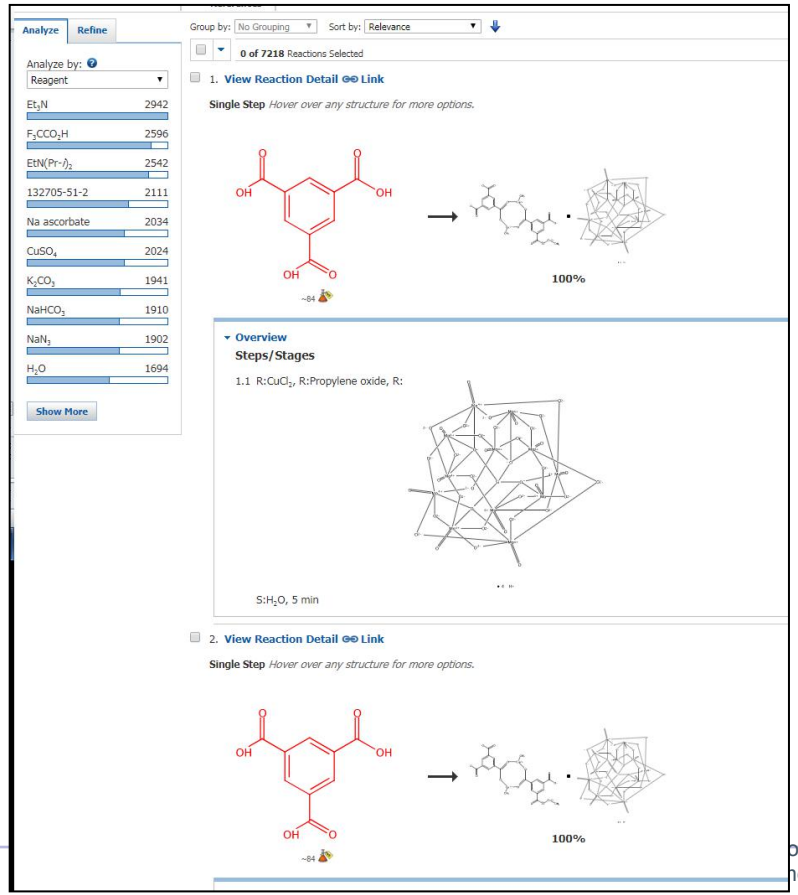
SciFinder® A CAS SOLUTION

在反应结果集中选择Analyze by Reagent, 找到相应金属盐



SciFinder® A CAS SOLUTION

获得相应反应信息



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谢谢关注！

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英文网站：http://www.cas.org/

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