钱欣博士
Application Specialist
cqian@acsi.info

如何通过SciFinder获得科技信息

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索 （增值的专利信息：PatentPak)
  - 物质检索
  - 反应检索 (MethodsNow Synthesis)
  - 分析方法查询 (MethodsNow Analysis)
- SciFinder常见问题及解决

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

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

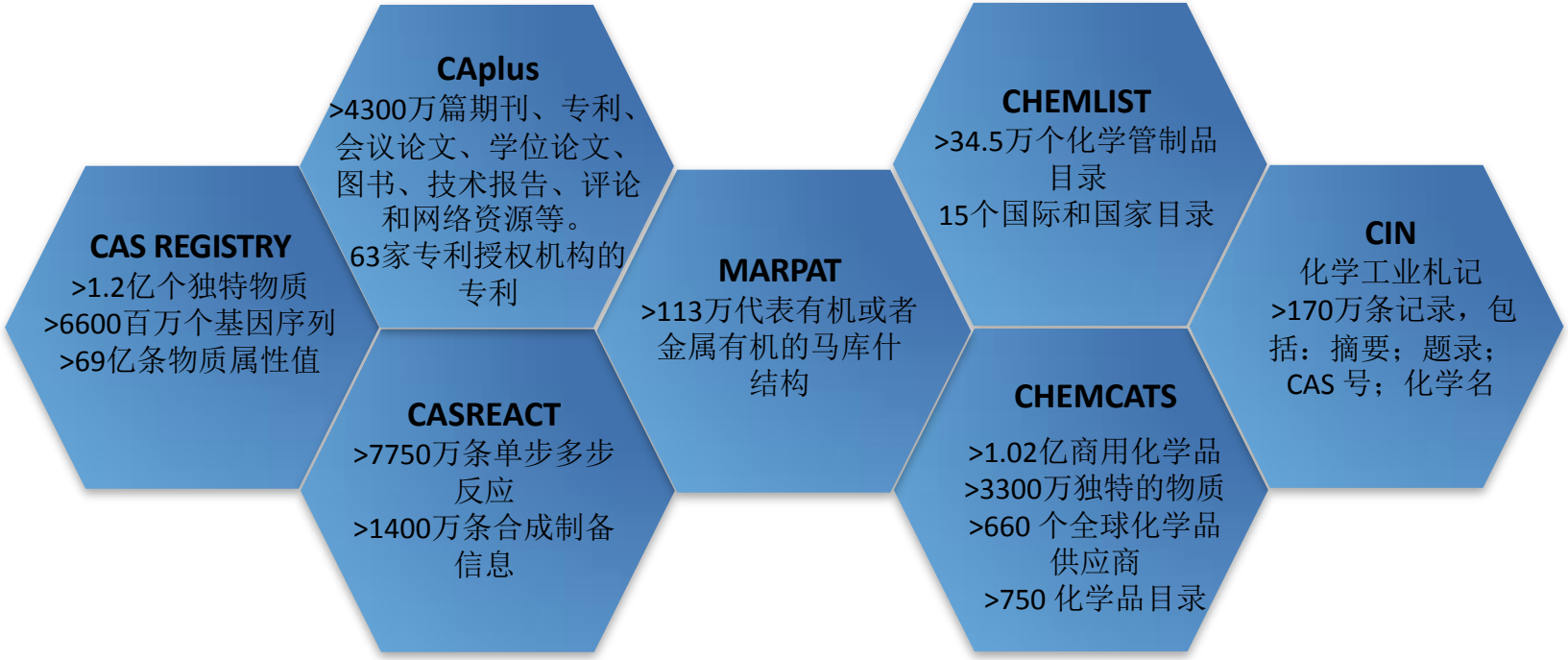
ACS Chemical Neuroscience

Cornell University Library

THE JOURNAL OF PHYSICAL CHEMISTRY Letters

CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

CAS——构建最高质量的化学数据库



CAS数据库——加速科学探索的步伐

CAS
A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

CAS数据库——源于化学，超越化学

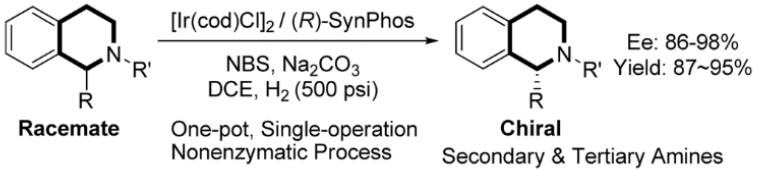
- **生物化学：**
  - 农化产品管控信息,生化遗传学,发酵,免疫化学,药理学
- **有机化学各领域：**
  - 氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇
- **大分子化学各领域：**
  - 纤维素、木质素、造纸;涂料、墨水
  - 染料、有机颜料 ;合成橡胶 ;纺织品、纤维
- **应用化学各领域 ：**
  - 大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金
- **物理、无机、分析化学各领域：**
  - 表面化学,催化剂,相平衡,核现象,电化学

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-catal
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

CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

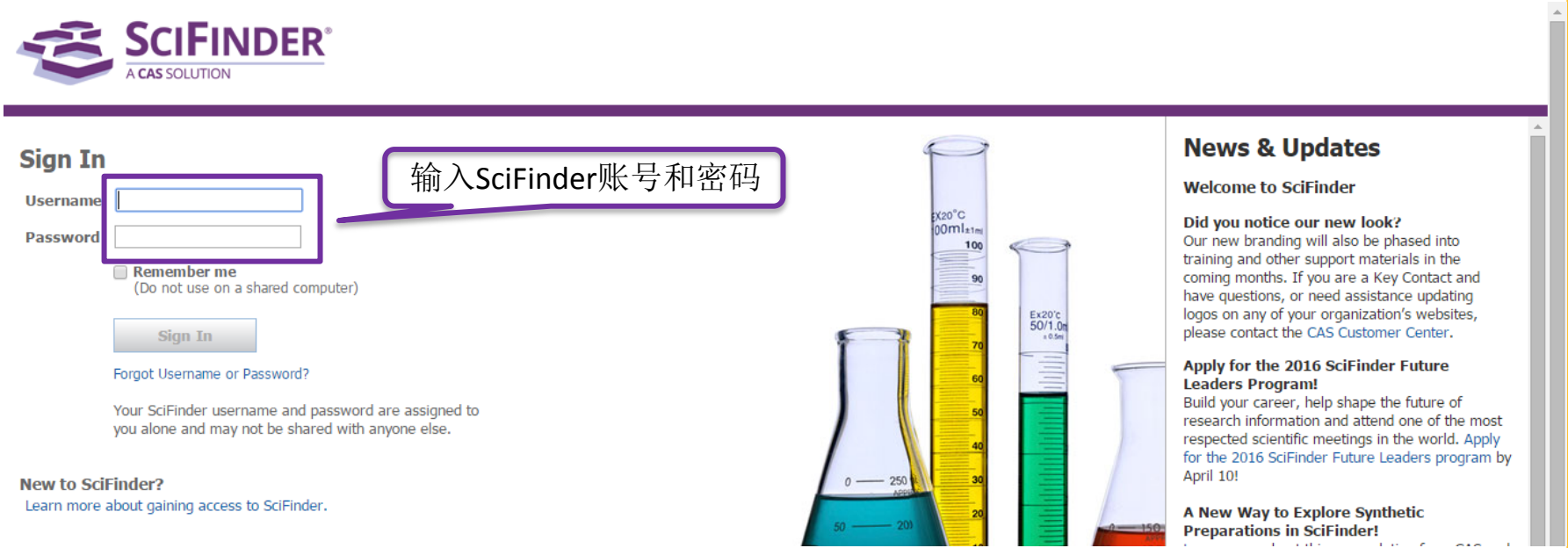
CAS人工标引解决的问题

- 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。

提纲

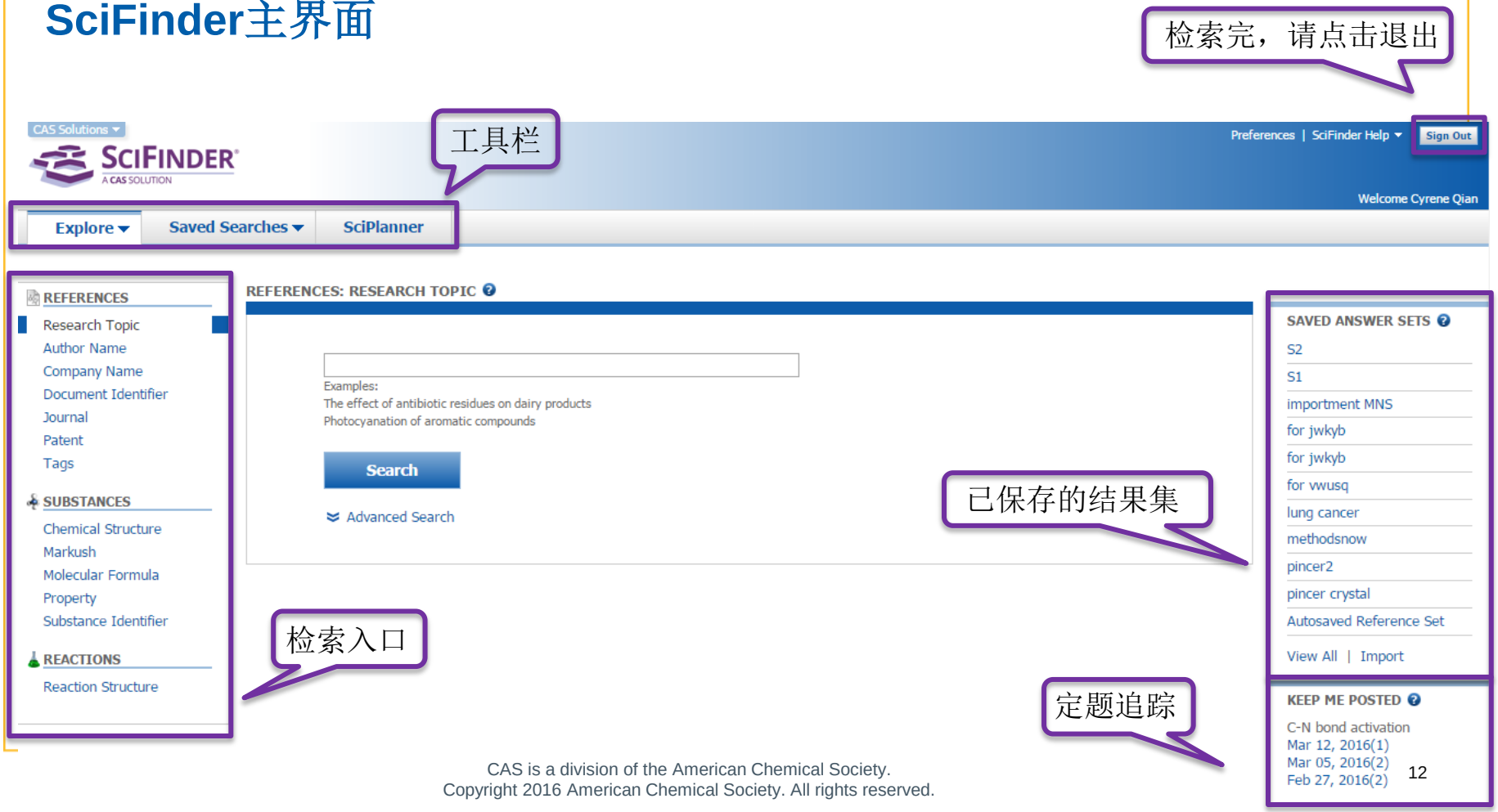
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - 反应检索
  - 分析方法查询
- SciFinder常见问题及解决

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



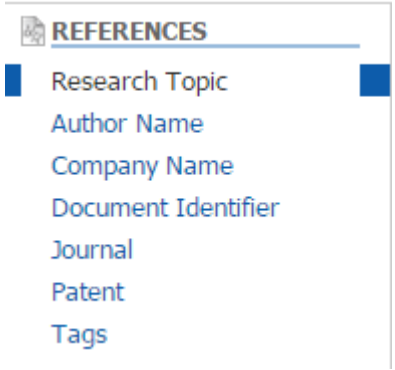
CAS
A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

SciFinder主界面



SciFinder检索——文献检索

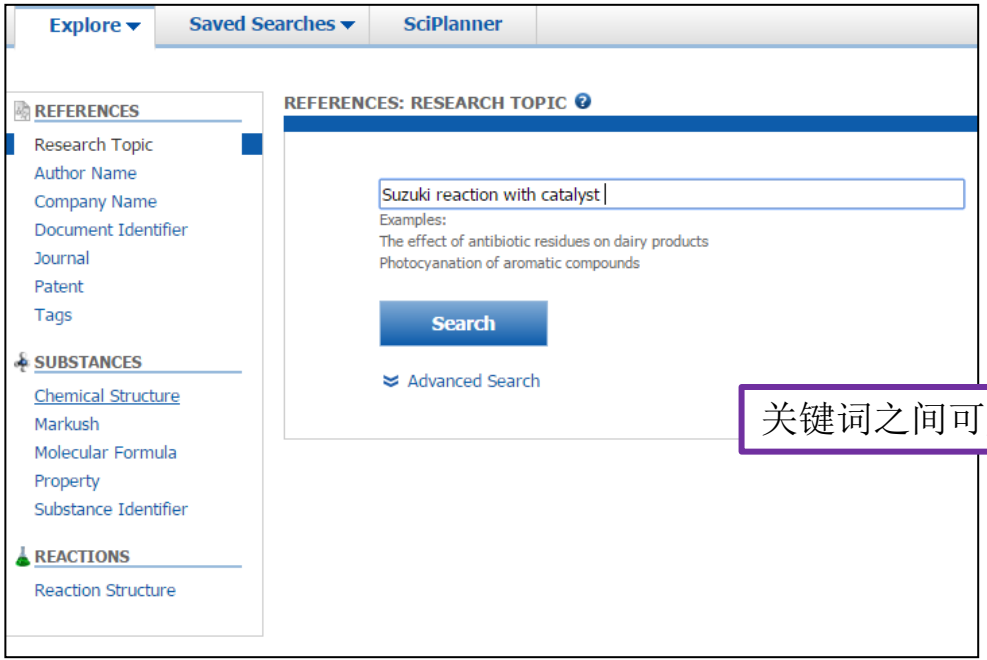
- 文献检索方法
  - 主题检索
  - 作者名检索
  - 机构名检索
  - 文献标识符检索
  - 期刊名称和专利信息（公开号，申请号等）
  - 从物质，反应获得文献
- 检索策略推荐
  - 关注某特定领域的文献：主题检索
  - 关注物质有关的文献：先获得物质，再获得文献
  - 关注某科研人员的文献：作者名检索
  - 关注某机构科研进展：机构名检索



CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

文献检索——主题: Suzuki催化反应

- 检索式： Suzuki reaction with catalyst

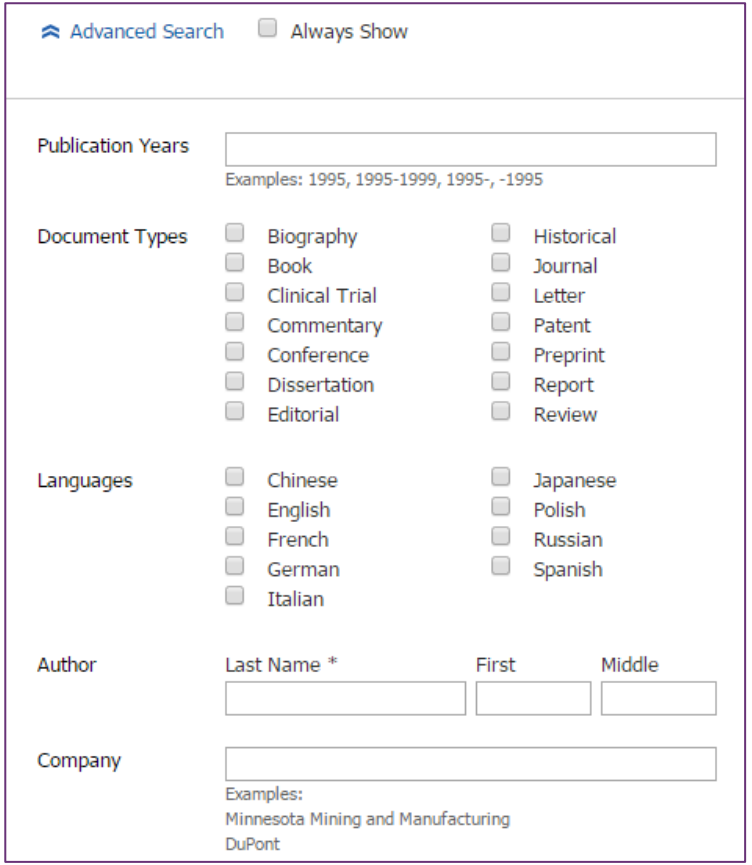


关键词之间可用介词连接：in, with, of…

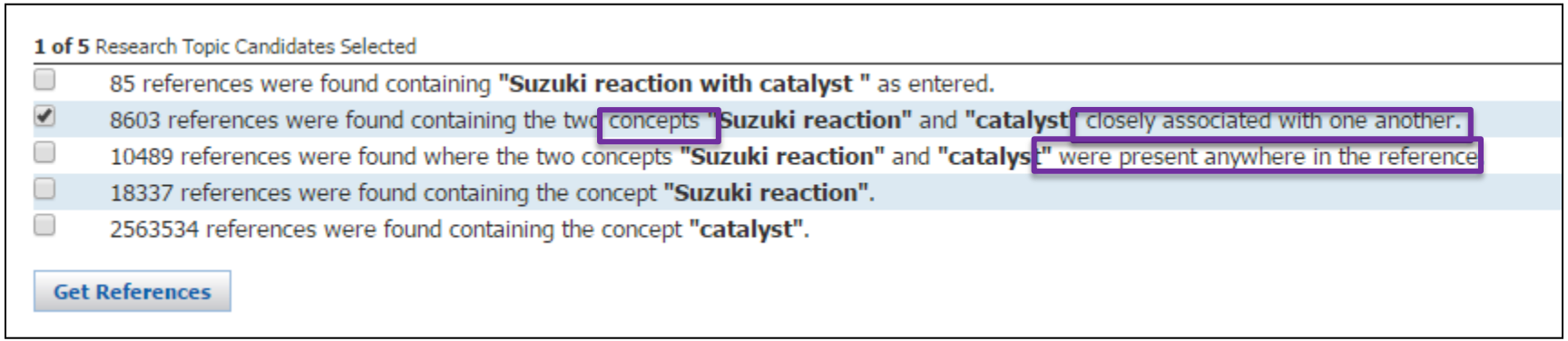
文献检索——主题: Suzuki催化反应

- 检索式： Suzuki reaction with catalyst

提前限制出版年限，语言，文献类型等

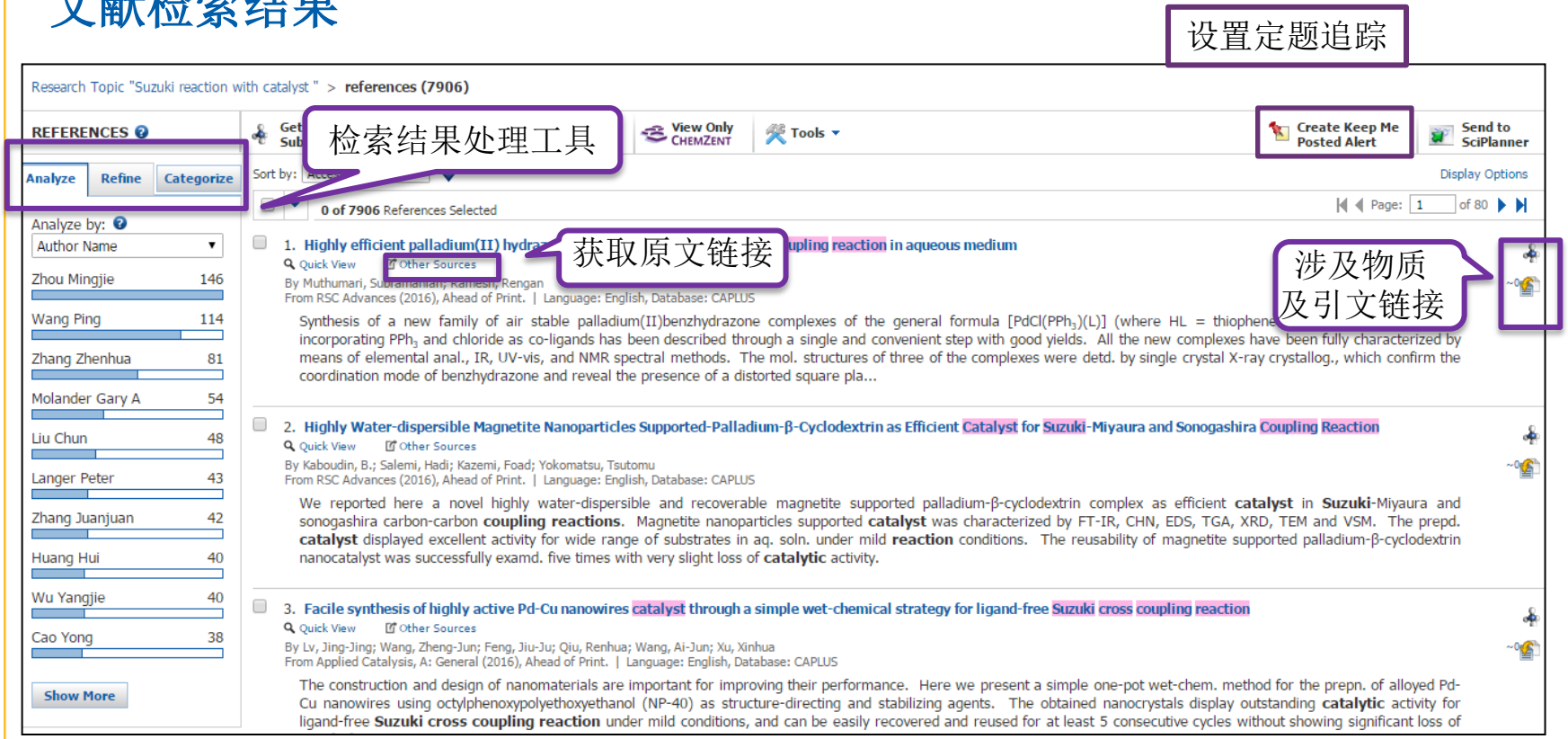


主题检索的候选项

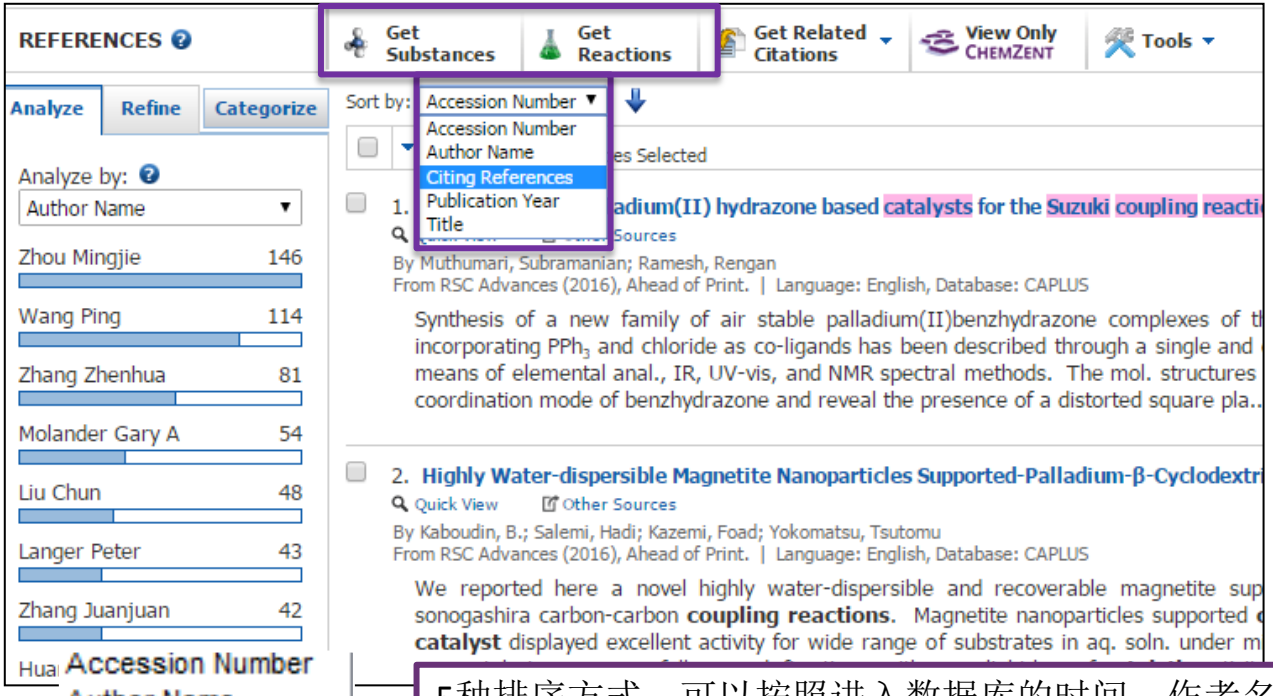


“Concepts”表示对主题词做了同义词的扩展；
“Closely associated with one another”表示同时出现在一个句子中;
“were present anywhere in the reference”表示同时出现在一篇文献中；

文献检索结果


设置定题追踪
Research Topic "Suzuki reaction with catalyst " > references (7906)
检索结果处理工具
REFERENCES
Analyze
Refine
Categorize
Analyze by:
Author Name
Zhou Mingjie 146
Wang Ping 114
Zhang Zhenhua 81
Molander Gary A 54
Liu Chun 48
Langer Peter 43
Zhang Juanjuan 42
Huang Hui 40
Wu Yangjie 40
Cao Yong 38
Show More
View Only ChemZent
Tools
Create Keep Me Posted Alert
Send to SciPlanner
Sort by:
Display Options
0 of 7906 References Selected
Page: 1 of 80
获取原文链接
涉及物质及引文链接
1. Highly efficient palladium(II) hydra... upling reaction in aqueous medium
Quick View
Other Sources
By Muthumari, Subramanian; Ramesh, Rengan
From RSC Advances (2016), Ahead of Print. | Language: English, Database: CAPLUS
Synthesis of a new family of air stable palladium(II)benzhydrazone complexes of the general formula [PdCl(PPh3)(L)] (where HL = thiophene incorporating PPh3 and chloride as co-ligands has been described through a single and convenient step with good yields. All the new complexes have been fully characterized by means of elemental anal., IR, UV-vis, and NMR spectral methods. The mol. structures of three of the complexes were detd. by single crystal X-ray crystallog., which confirm the coordination mode of benzhydrazone and reveal the presence of a distorted square pla...
2. Highly Water-dispersible Magnetite Nanoparticles Supported-Palladium-β-Cyclodextrin as Efficient Catalyst for Suzuki-Miyaura and Sonogashira Coupling Reaction
Quick View
Other Sources
By Kaboudin, B.; Salemi, Hadi; Kazemi, Foad; Yokomatsu, Tsutomu
From RSC Advances (2016), Ahead of Print. | Language: English, Database: CAPLUS
We reported here a novel highly water-dispersible and recoverable magnetite supported palladium-β-cyclodextrin complex as efficient catalyst in Suzuki-Miyaura and sonogashira carbon-carbon coupling reactions. Magnetite nanoparticles supported catalyst was characterized by FT-IR, CHN, EDS, TGA, XRD, TEM and VSM. The prepd. catalyst displayed excellent activity for wide range of substrates in aq. soln. under mild reaction conditions. The reusability of magnetite supported palladium-β-cyclodextrin nanocatalyst was successfully examd. five times with very slight loss of catalytic activity.
3. Facile synthesis of highly active Pd-Cu nanowires catalyst through a simple wet-chemical strategy for ligand-free Suzuki cross coupling reaction
Quick View
Other Sources
By Lv, Jing-Jing; Wang, Zheng-Jun; Feng, Jiu-Ju; Qiu, Renhua; Wang, Ai-Jun; Xu, Xinhua
From Applied Catalysis, A: General (2016), Ahead of Print. | Language: English, Database: CAPLUS
The construction and design of nanomaterials are important for improving their performance. Here we present a simple one-pot wet-chem. method for the prepn. of alloyed Pd-Cu nanowires using octylphenoxypolyethoxyethanol (NP-40) as structure-directing and stabilizing agents. The obtained nanocrystals display outstanding catalytic activity for ligand-free Suzuki cross coupling reaction under mild conditions, and can be easily recovered and reused for at least 5 consecutive cycles without showing significant loss of

文献检索结果

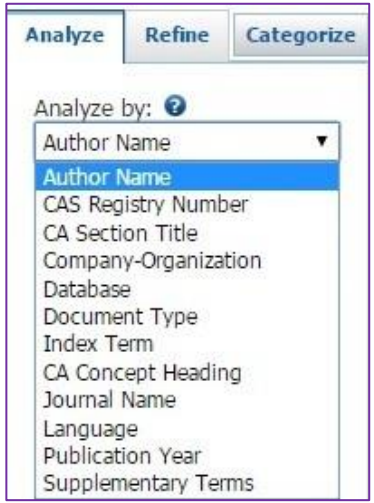


5种排序方式，可以按照进入数据库的时间、作者名、引文、公开年限、标题对文献检索结果进行重新排序

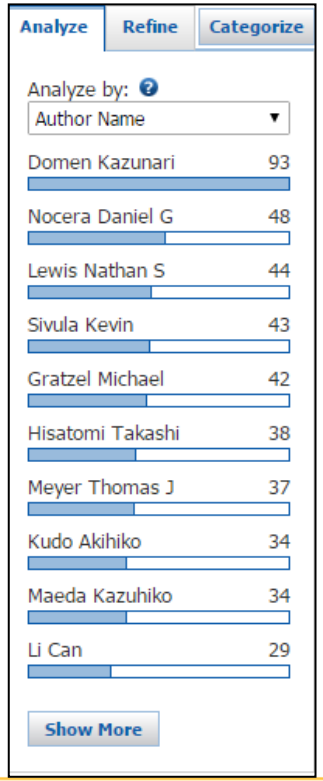
Citing Reference: 可能帮助找到最重要的文献

文献检索结果：Analyze

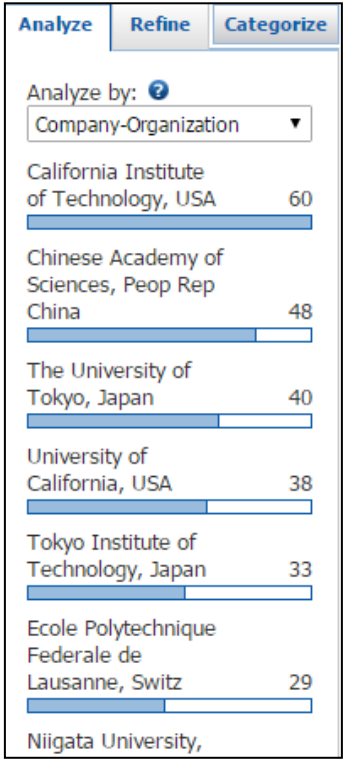
12种文献分析选项



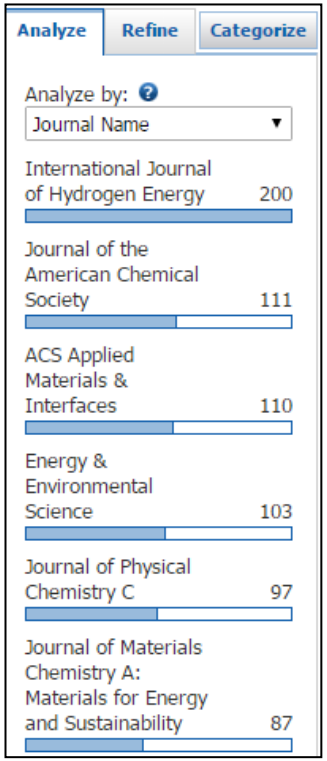
主要研究人员



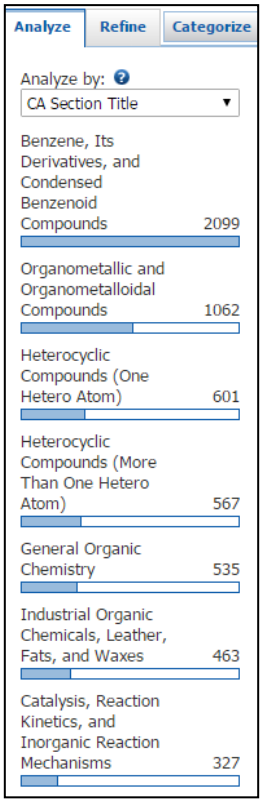
主要研究机构，
合作伙伴，竞争对手

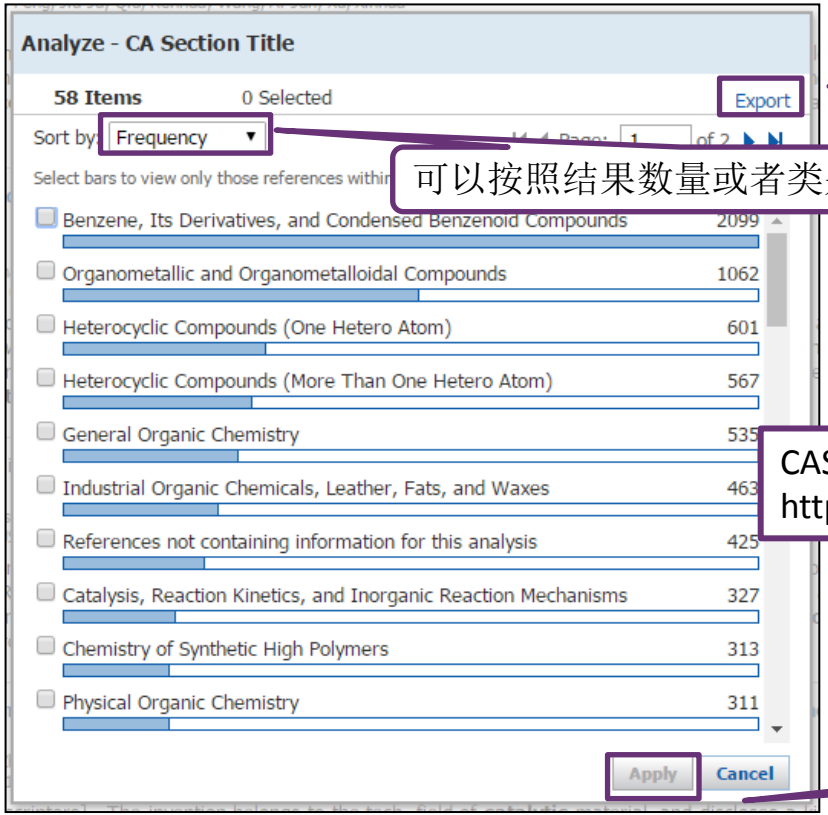


主要发表期刊



文献检索结果：Analyze





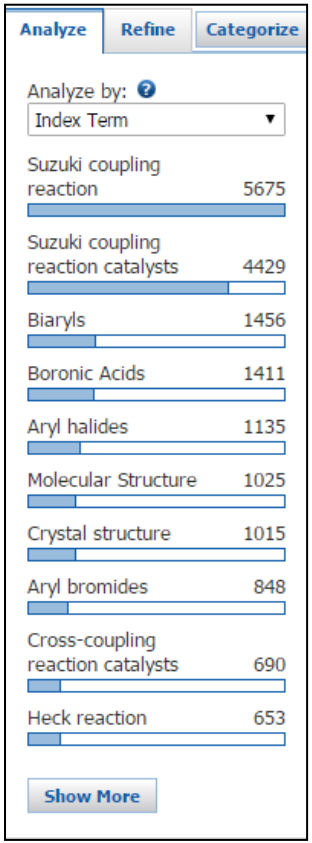
可以将分析结果导出xls文件

可以按照结果数量或者类别字母顺序排序

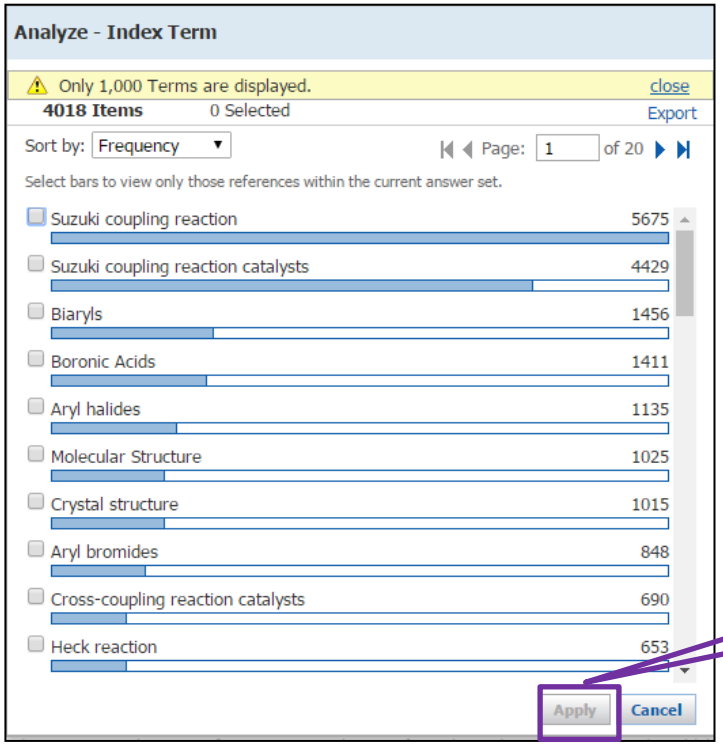
CAS把收录的信息分为5个大类80个小类:
http://www.cas.org/content/ca-sections

选择感兴趣的词语,点击Apply

文献检索结果：Analyze



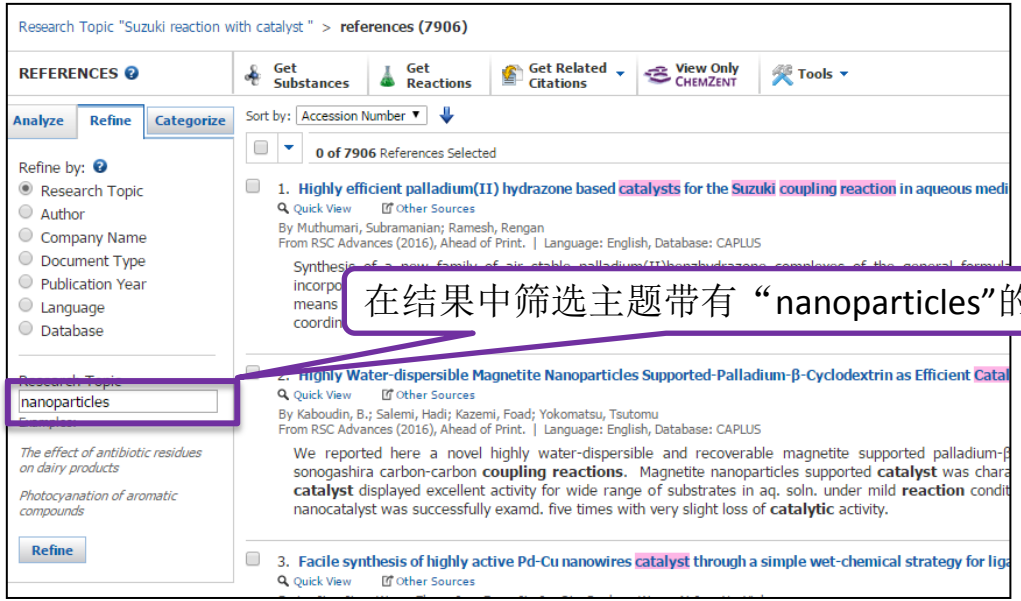
Index Term:帮助用户全景了解本领域涉及的重要技术术语，精选文献



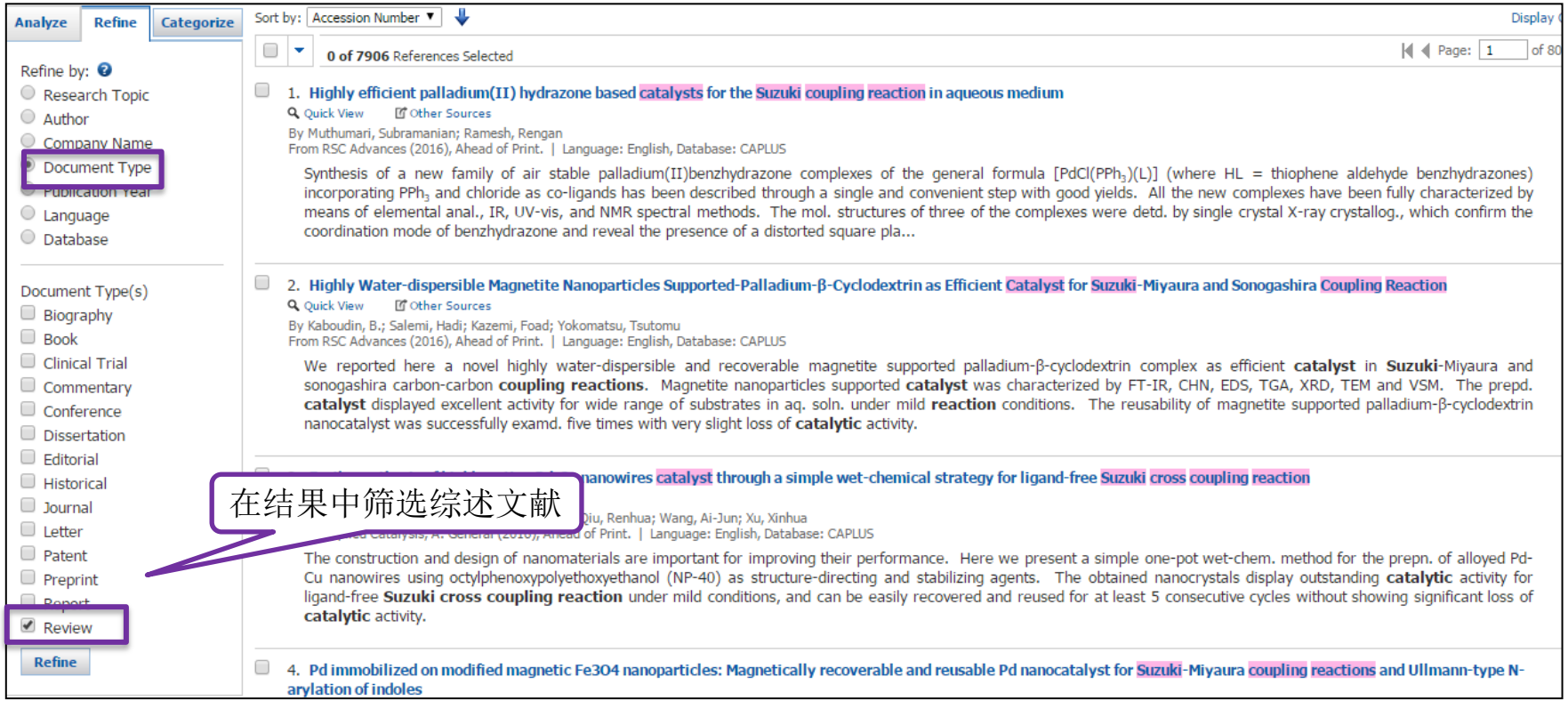
选择感兴趣的词语,点击Apply

文献检索结果：Refine

- 六种限定选项，包括主题词、作者姓名、机构名称、出版年代、语言、所属数据库



文献检索结果：Refine

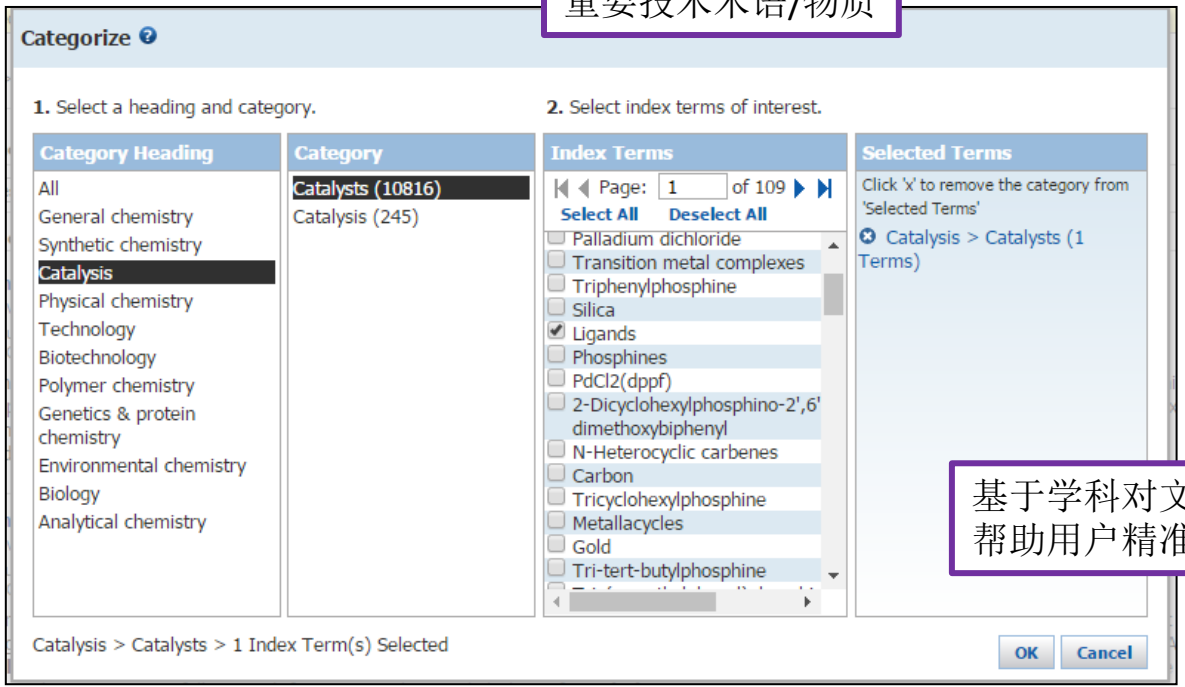


文献检索结果：Categorize

学科主分类

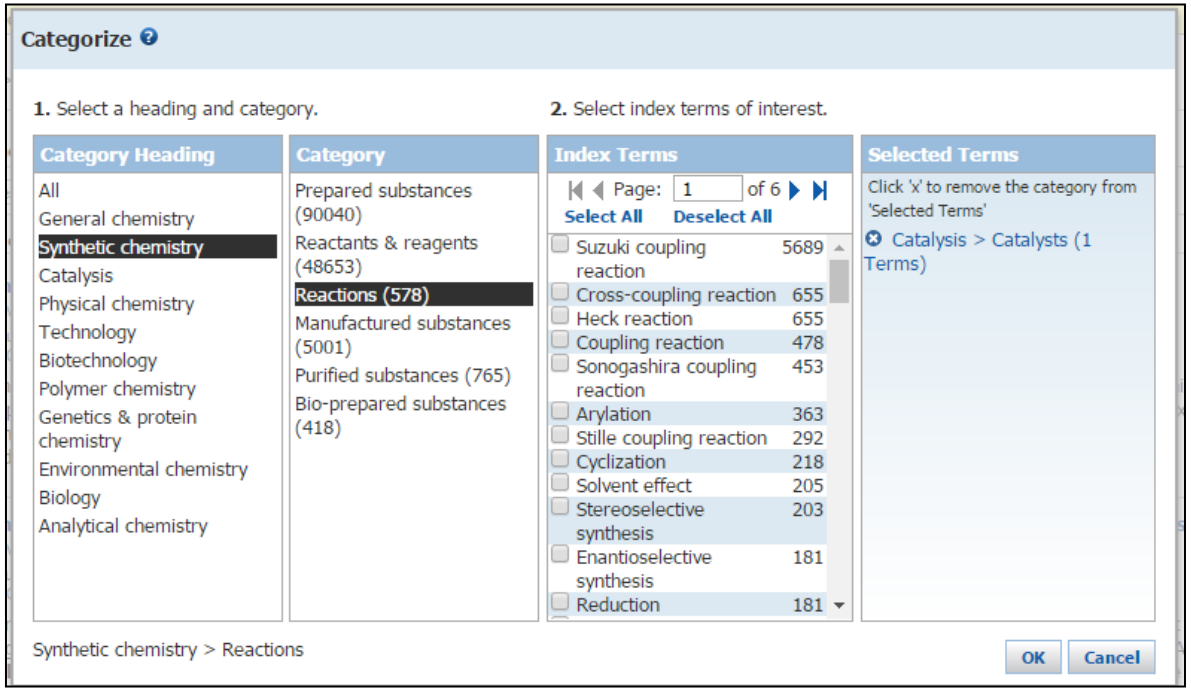
学科副分类

学科副分类涉及的
重要技术术语/物质



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

文献检索结果：Categorize



提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索（增值的专利信息）
  - 物质检索
  - 反应检索
  - 分析方法查询
- SciFinder常见问题及解决

CAS收录了全世界范围的专利

CAS依照特定筛选标准，收录了来自世界上63个国家和地区的专利文献。
其中9个主要专利授权机构的专利，在其公布48小时内即可被CAplus[SM]收录，CAS科学家在27天内能够完成完全标引。

SciFinder提供多种语言的专利文献，并就关键信息提供高质量的英文翻译

WO 2010/092287 PCT/FR2010/050204

DERIVES DE N-[(6-AZA-BICYCLO[3.2.1]OCT-1-YL)-ARYL-METHYL]-BENZAMIDE, LEUR PREPARATION ET LEUR APPLICATION EN THERAPEUTIQUE

La présente invention se rapporte à des dérivés de *N*-[(6-aza-bicyclo[3.2.1]oct-1-yl)-

Quick View

Preparation of N-[(6-azabicyclo[3.2.1]oct-1-yl)(aryl)methyl]benzamide derivatives as inhibitors of glycine transporters glyt1

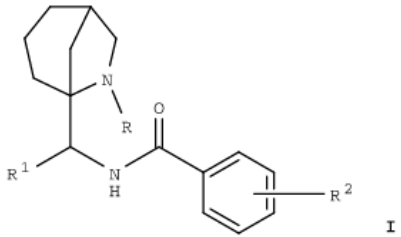
PatentPak

By Dargazanli, Ghad; Estenne-Bouhtou, Genevieve; Medaisko, Florence

From PCT Int. Appl. (2010), WO 2010092287 A1 Aug 19, 2010. | Language: French, Database: CAPLUS

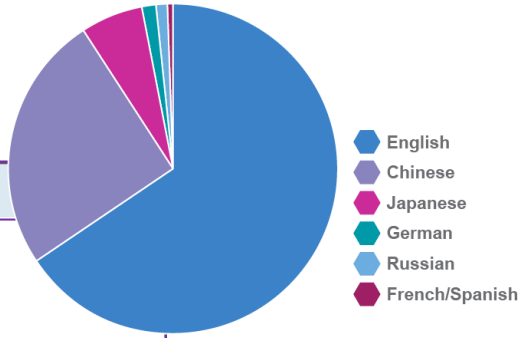
The invention also relates to the therapeutic use thereof and to a method for synthesizing same. Title compds. I [R = H, (un)substituted alkyl, cycloalkyl; R1 = (un)substituted Ph, naphthyl; R2 = H, halo, CN, heteroaryl, etc.; and their acid addn. salts] were prepd. as inhibitors of glycine transporters glyt1. Thus, reaction of 6-((R)-1-phenylethyl)-6-azabicyclo[3.2.1]octane-5-carbonitrile with phenyllithium, cleavage of the 1-phenylethyl group, amidation of 2,6-dichloro-3-trifluoromethylbenzoic acid with the resulting amine and acidulation with HCl gave II. I inhibited glycine transport via glyt1 and displayed an IC50 in the range of 0.001 to 10 μM in vitro.

Reference Images | Substance Images



I

Original publication languages not in English **35%**



CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

CAS的科学家对专利进行必要改写，使其更容易被理解和获取

WO 2006/016684 PCT/JP2005/014867

1

DESCRIPTION

PDF原文中的标题和摘要

METHOD FOR SYNTHESIS OF AROMATIC AMINE

(57) Abstract: One embodiment of the present invention provides a method for synthesis of substituted secondary amine by the reaction of aniline with aryl halide by using a Pd catalyst including $(t\text{-}Bu)_3P$ as a ligand.

Process for synthesis of substituted secondary amines via condensation of aniline with aryl halides with a palladium catalyst and (t-Bu)3P as a ligand as an electroluminescence source for display devices

By: Nakashima, Harue; Kawakami, Sachiko
Assignee: Semiconductor Energy Laboratory Co., Ltd., Japan

A process for the synthesis of secondary amines is presented via condensation of aniline with an aryl halide using palladium as a catalyst and $(t\text{-}Bu)_3P$ as a ligand in the key step. Thus, N-(4-diphenylamino)phenylaniline is synthesized in 42% yield by condensation of N,N-diphenyl-N-(4-bromophenyl)amine with aniline. The process avoids protecting groups though the use of a palladium catalyst and $(t\text{-}Bu)_3P$ as a ligand. N-(4-diphenylamino)phenylaniline can be used as an electroluminescence source for display devices including a light-emitting diodes, flat panel displays, liq. crystal display devices (no data).

CAS科学家重写的标题和摘要

节省你最宝贵的资源——时间

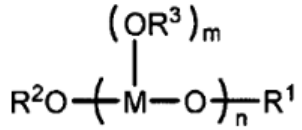
- 即时获得来自世界上主要专利授权机构的专利PDF文件
- 专利族涵盖了多种语言
- 定位标引的重要化学物质所在专利页码
- 专利研究安全保密
- 每日更新
- SciFinder检索功能中内置交互式浏览器

点击PatentPak，一键获得专利pdf文件，快速定位到关键物质

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

点击PatentPak，获取PatentPak Viewer

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

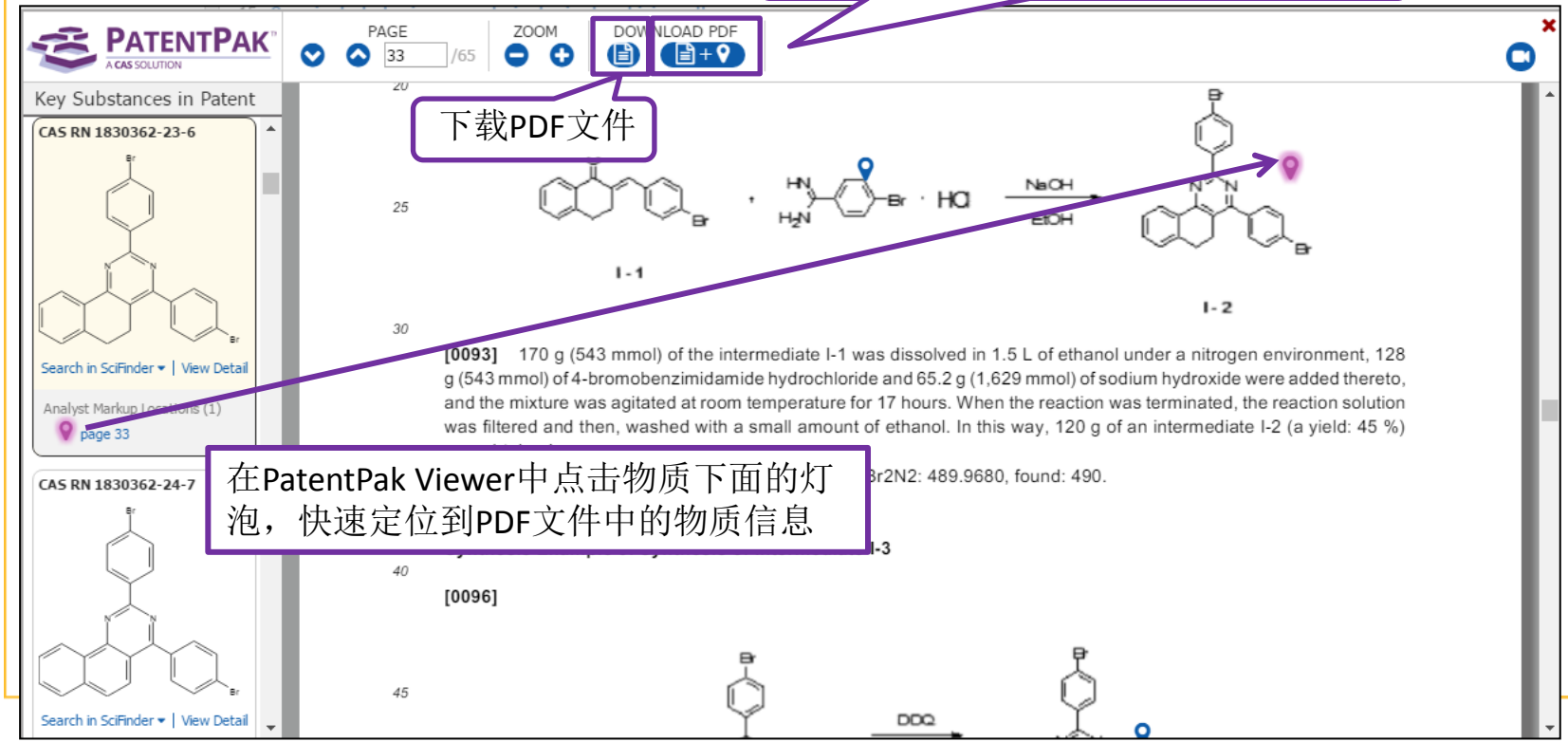
点击PatentPak，一键获得专利pdf文件，快速定位到关键物质

PatentPak浏览器

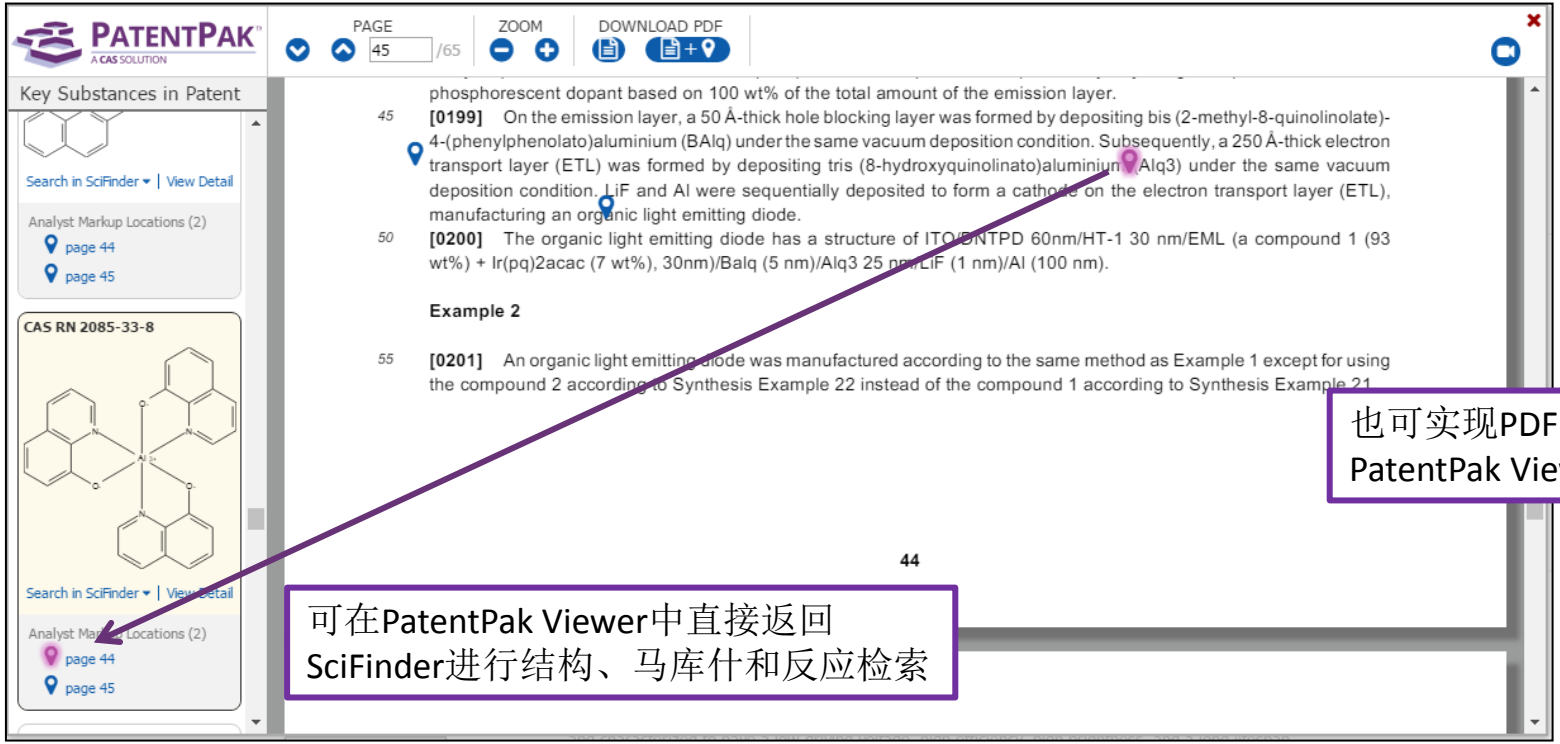
下载包含物质位置等信息的专利PDF文件

下载PDF文件

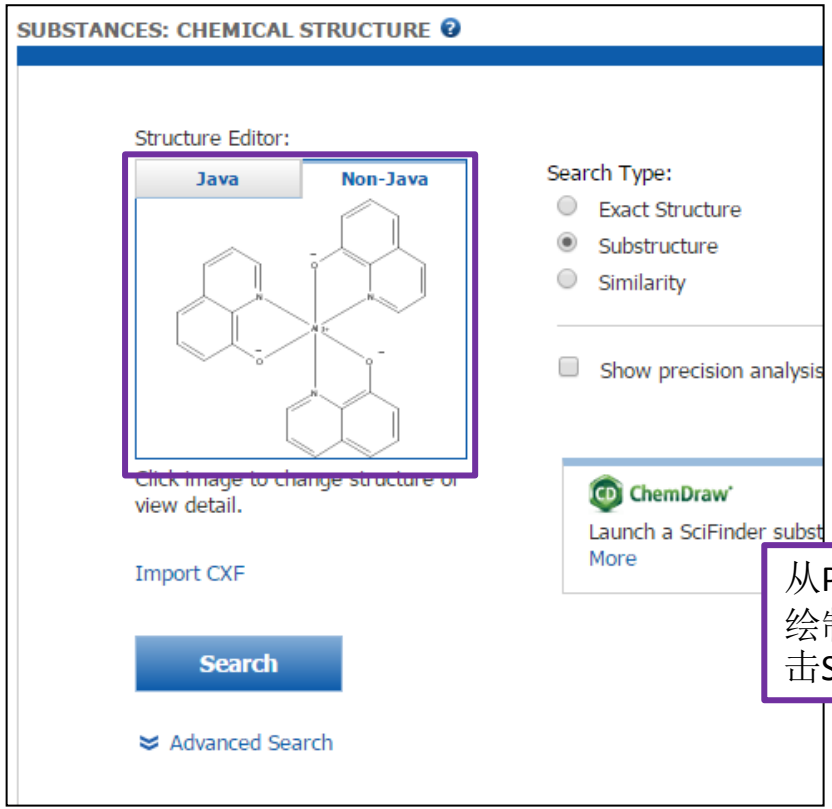
在PatentPak Viewer中点击物质下面的灯泡，快速定位到PDF文件中的物质信息



PatentPak——专利工作流程解决方案



PatentPak——专利工作流程解决方案



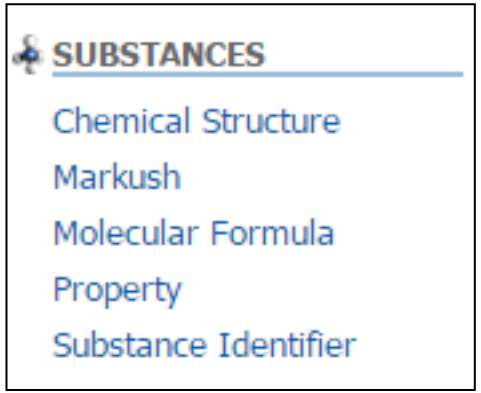
从PatentPak Viewer直接跳转到结构检索界面，同时无需绘制，系统会自动将相应的结构直接导入到绘图面板，点击Search即开始SciFinder检索，拓展新的研究方向

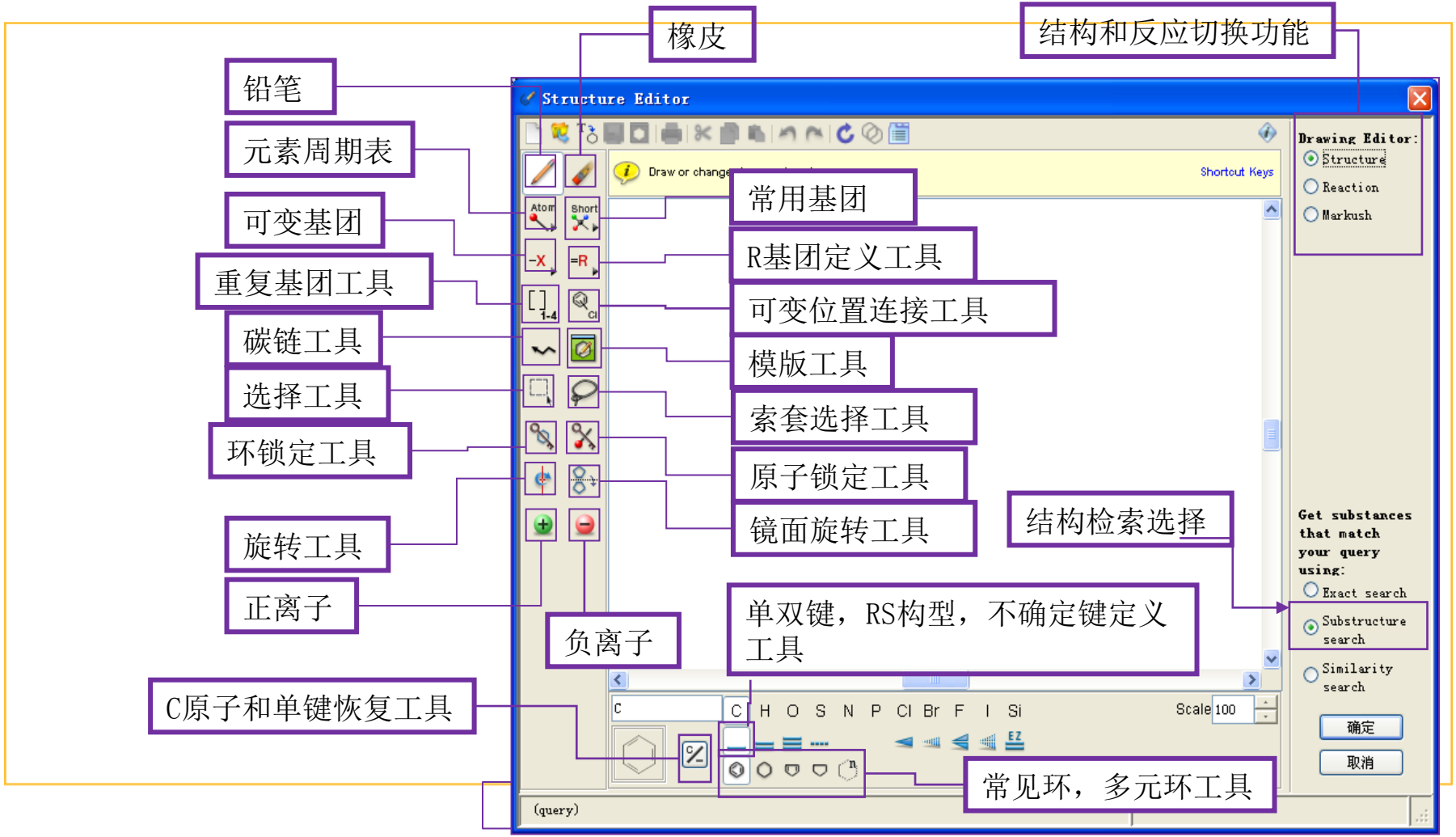
提纲

- 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
  - 分析方法查询
- SciFinder常见问题及解决

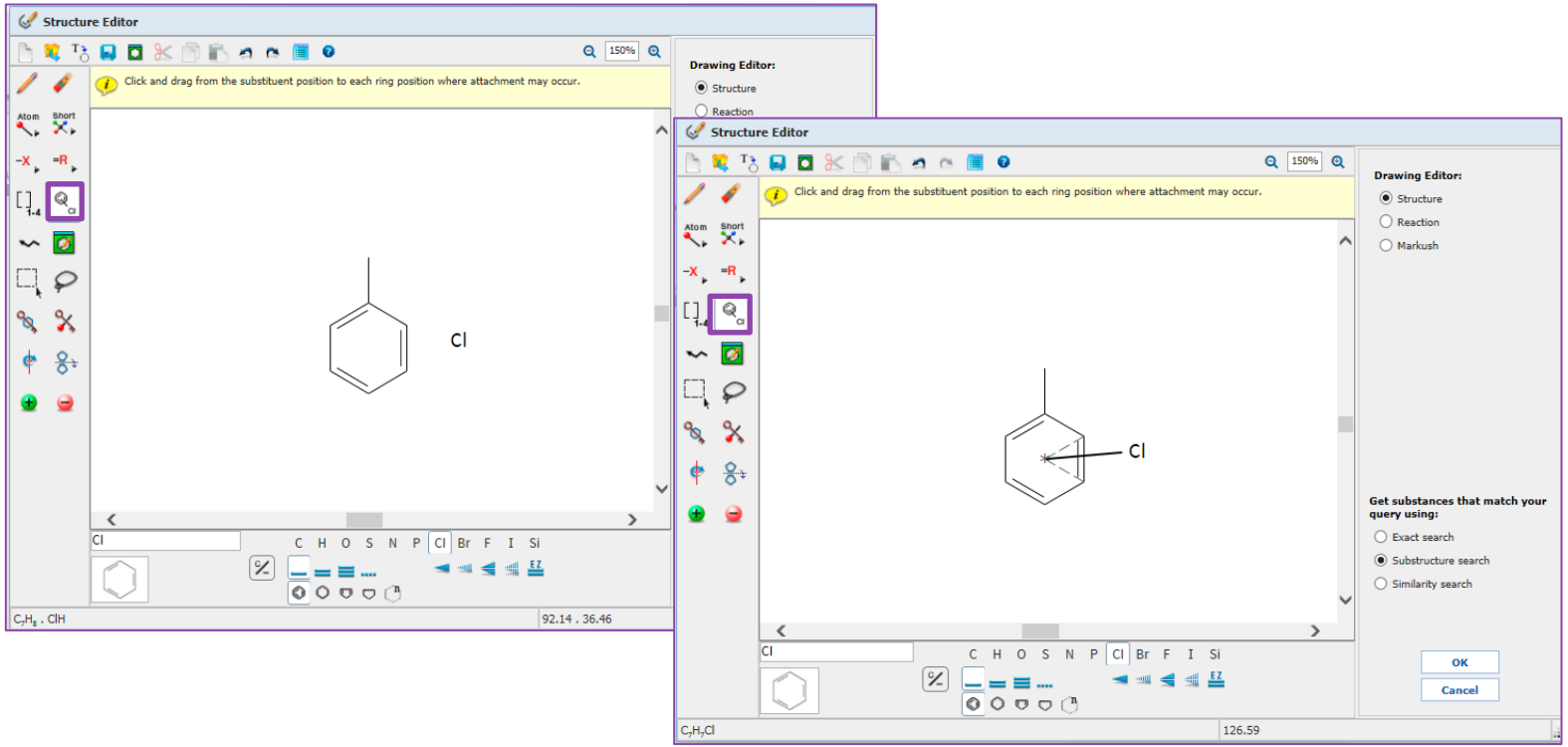
SciFinder检索选项——物质检索

- 物质检索方法
  - 结构式检索
  - 分子式检索
  - 理化性质检索
  - 物质标识符检索：化学名称，CAS RN
- 物质检索策略推荐
  - 有机物化合物、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




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
正离子
负离子
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
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)

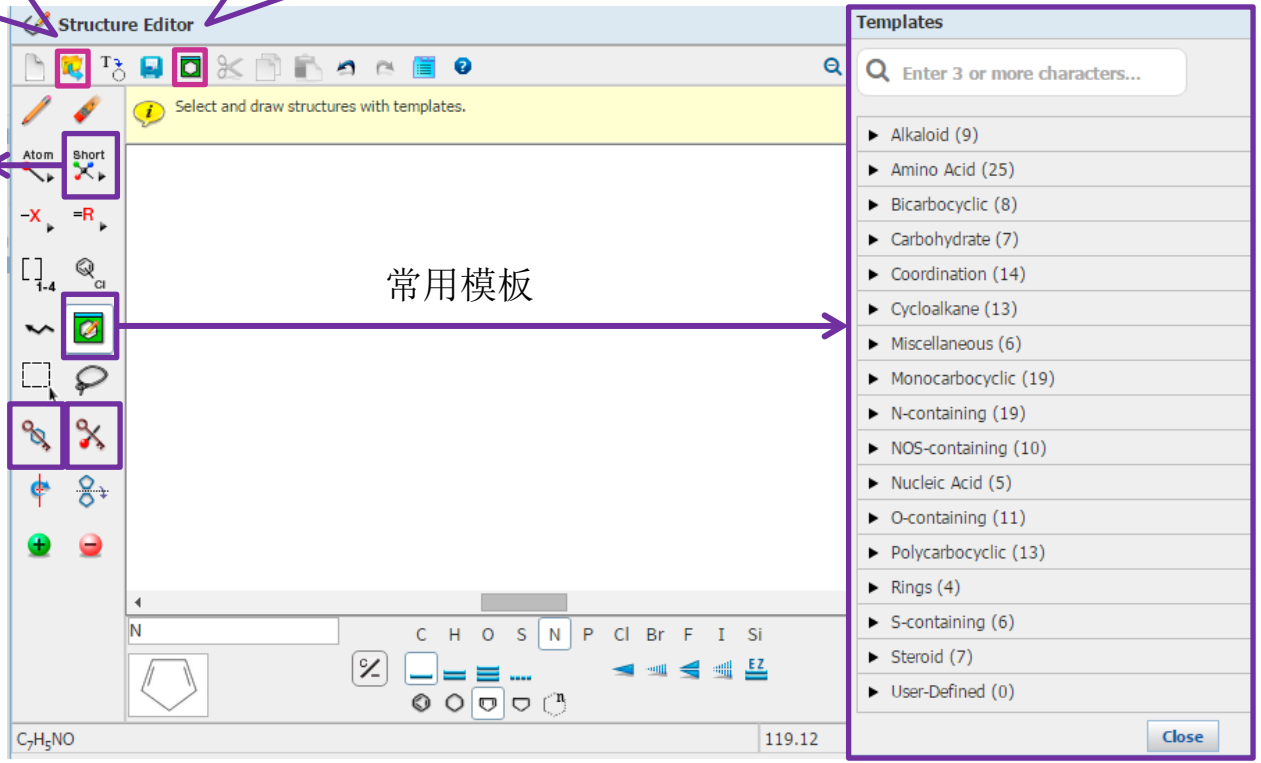
举例：不固定位置取代

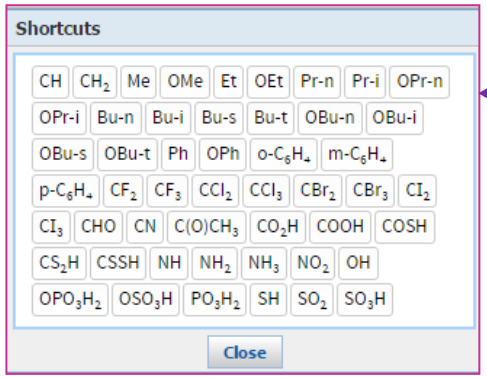


CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

直接导入已保存的.cxf或者.mol文件

将绘制结构存为模板



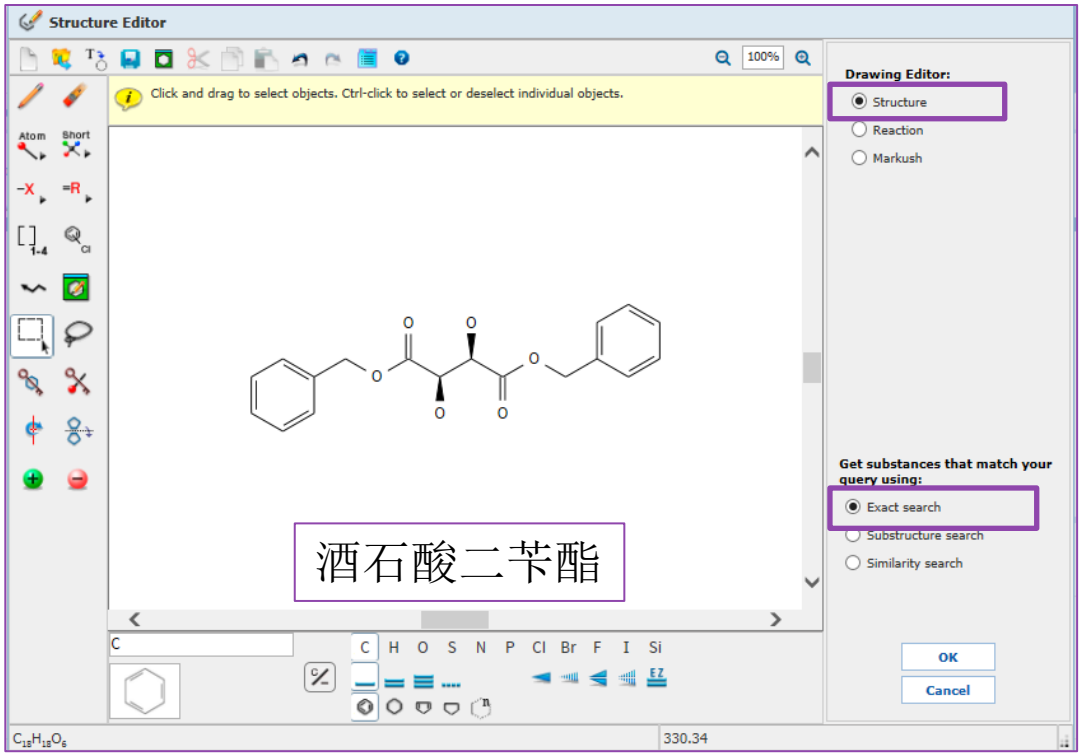


常用基团

环锁定工具

原子锁定工具

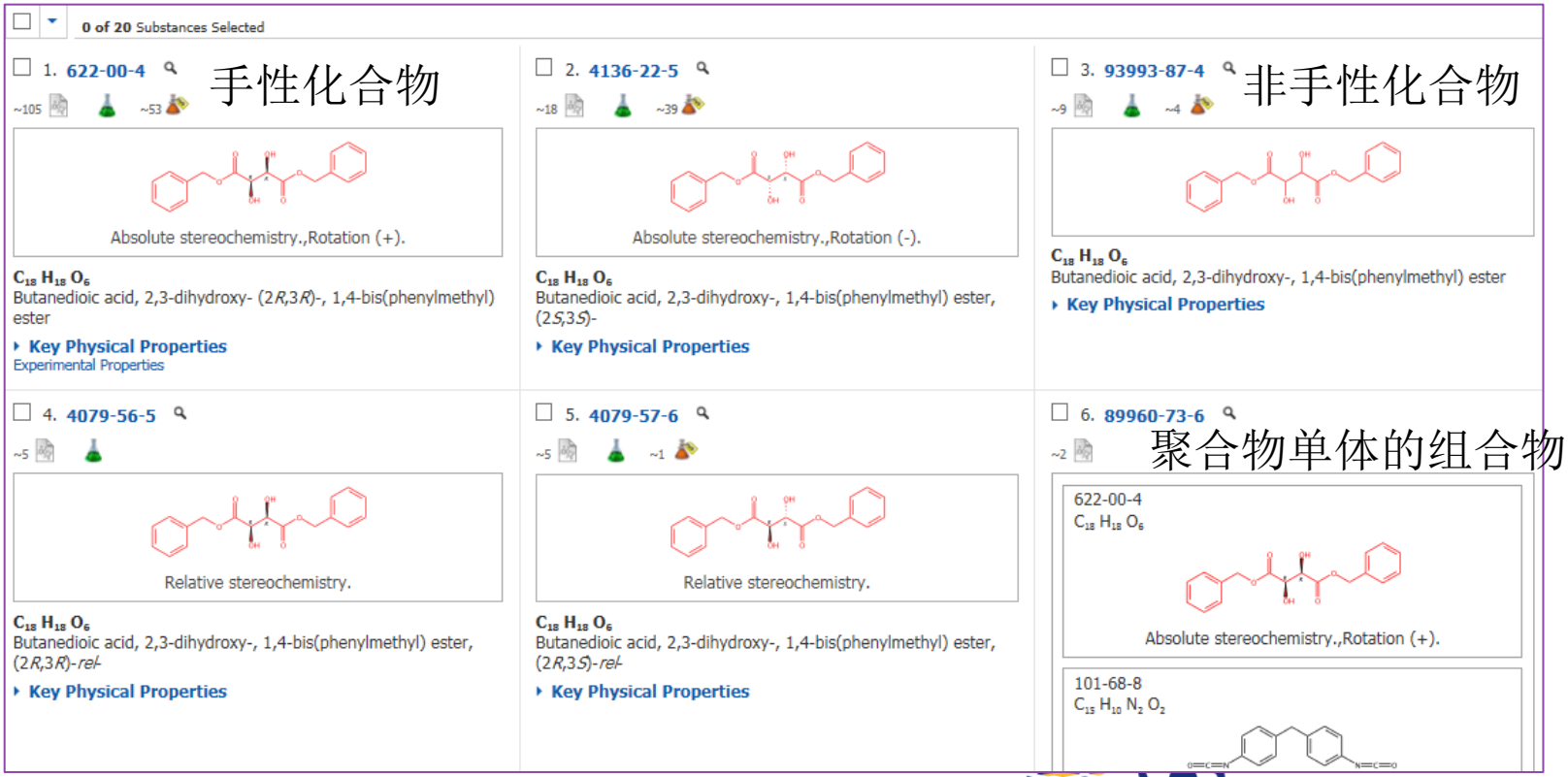
化学结构检索: 精确结构检索



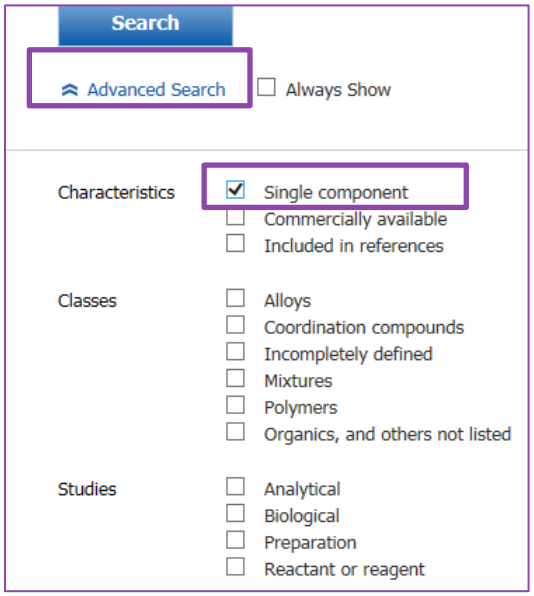
结构式中的原子和环
全部被锁定,不可被取代

CAS
A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

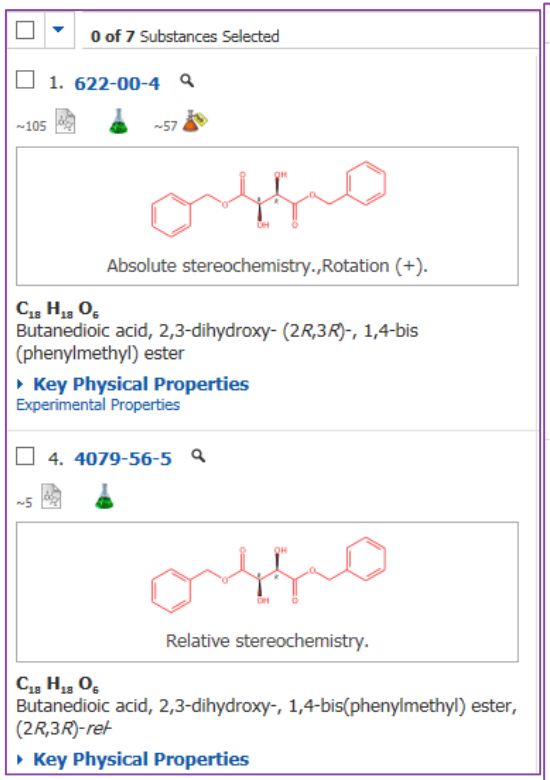
物质结构结果集

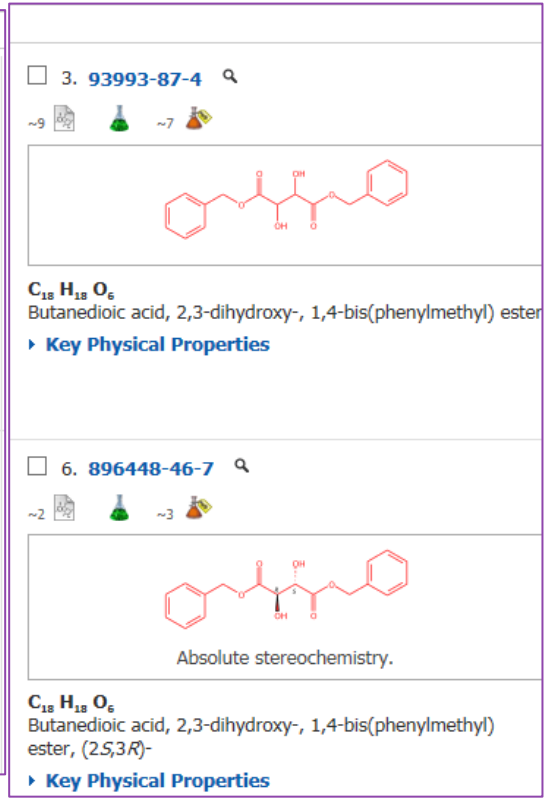


高级检索——提前限定



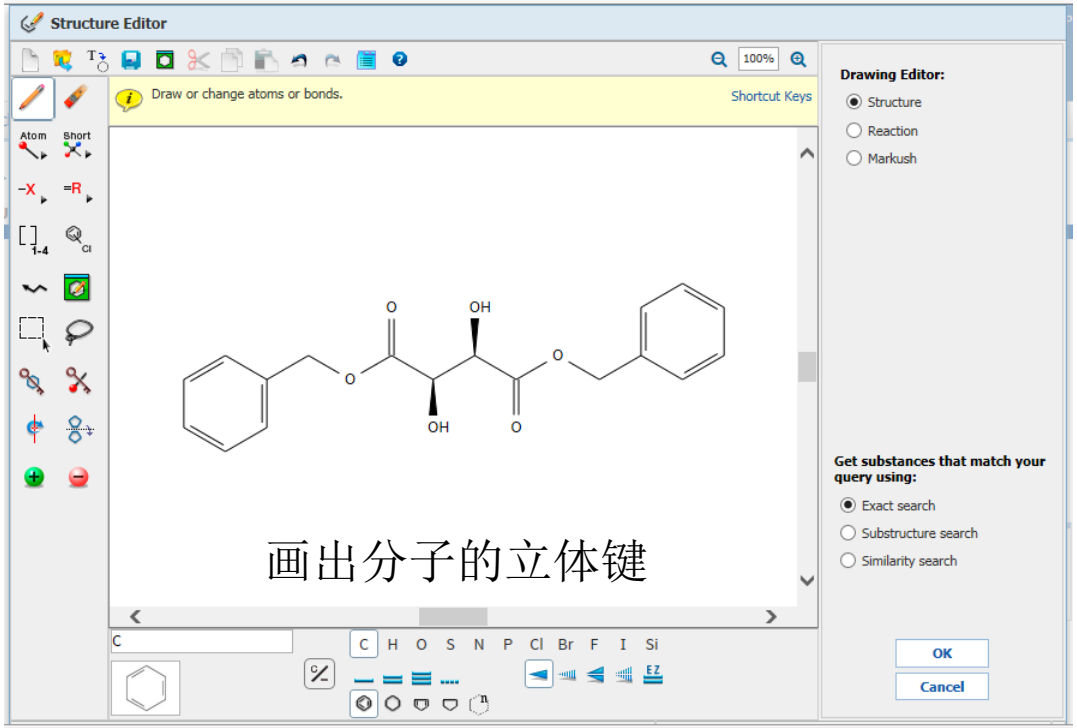
去除混合物，组合物，配合物，盐等



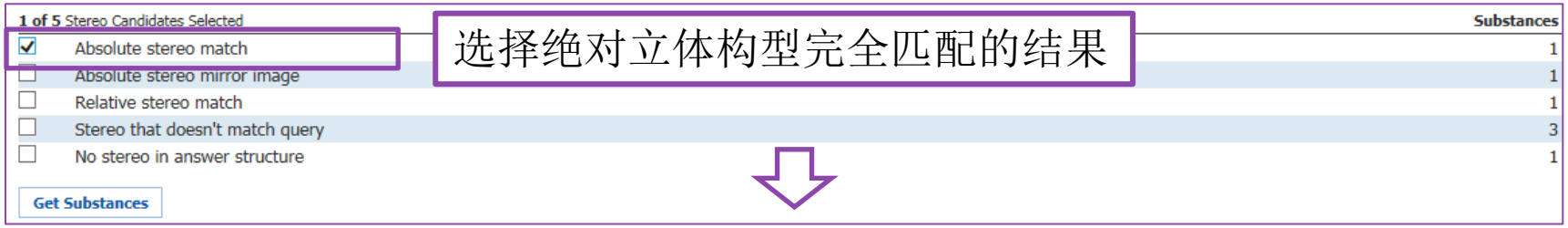


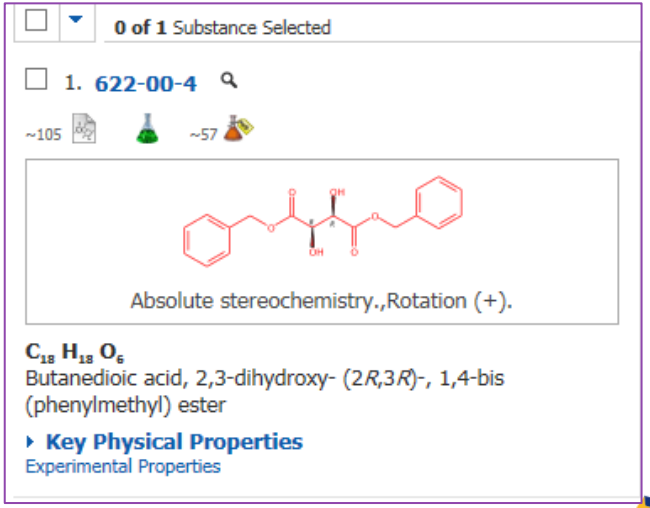
CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

举例：检索特定立体构型的分子

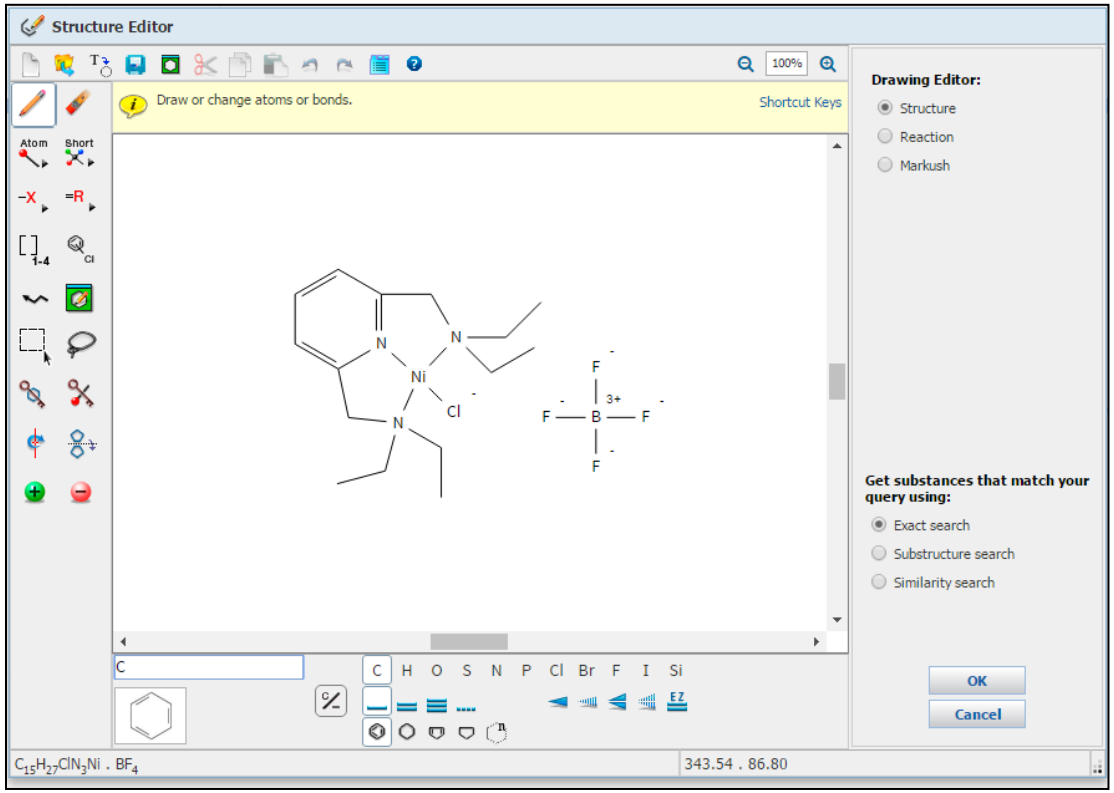


获得绝对立体构型的物质结果集



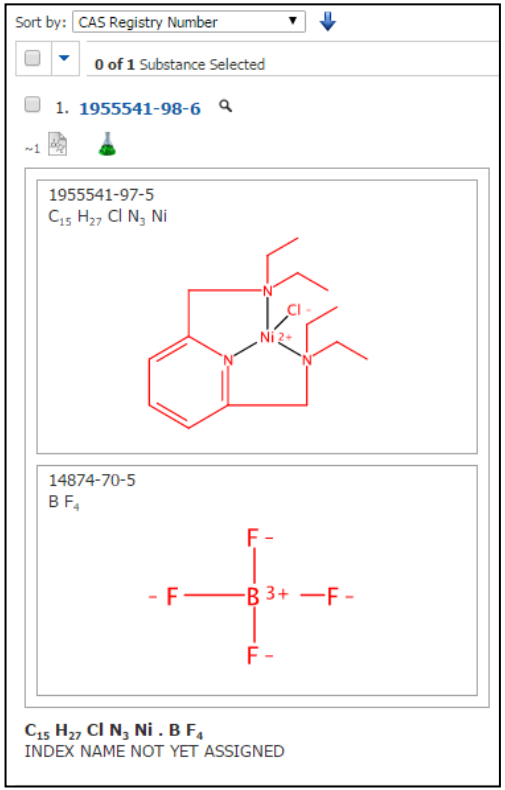


精确结构检索配合物



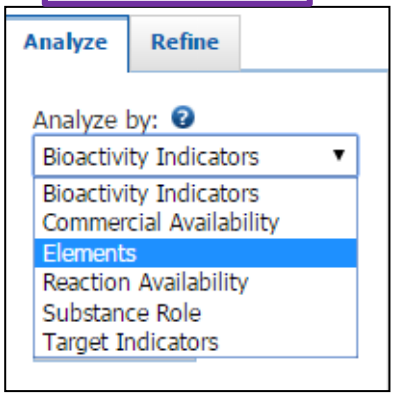
获得精确结构检索结果

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

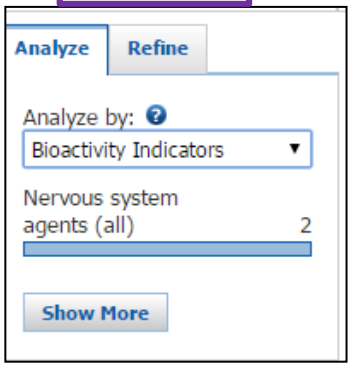


物质检索结果——Analyze

六种分析选项

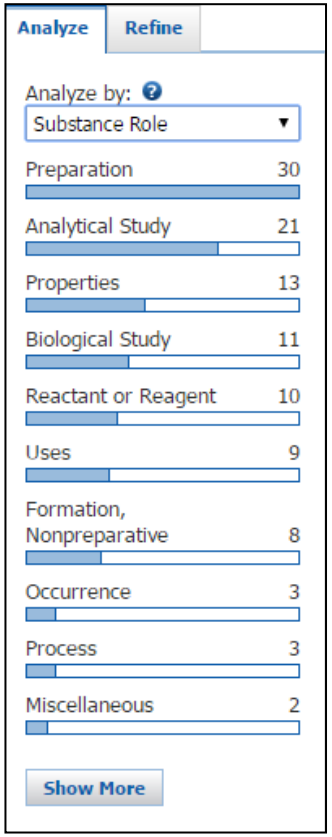


生物活性

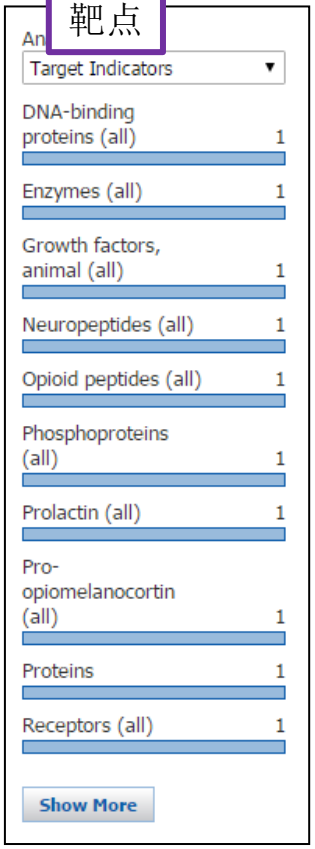


可以按照生物活性，商业可获得性，元素，反应可获得性，物质角色和靶点进行分析

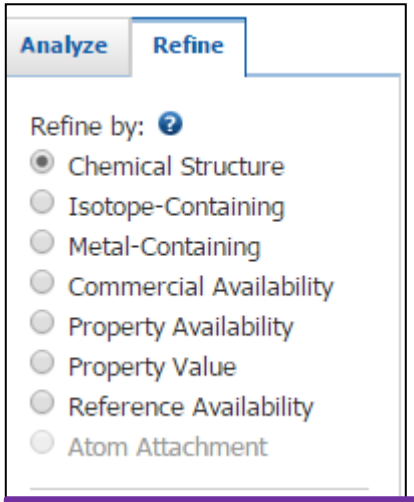
物质角色



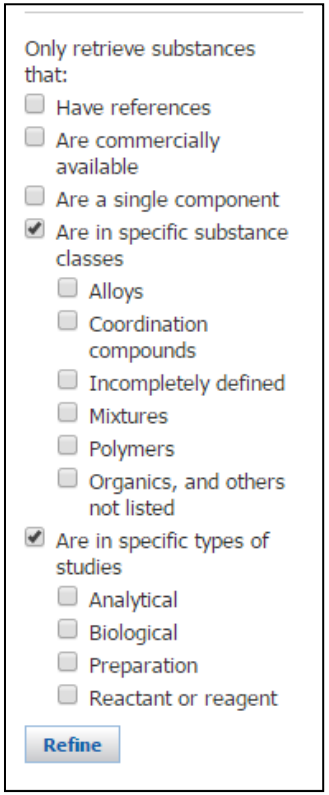
靶点

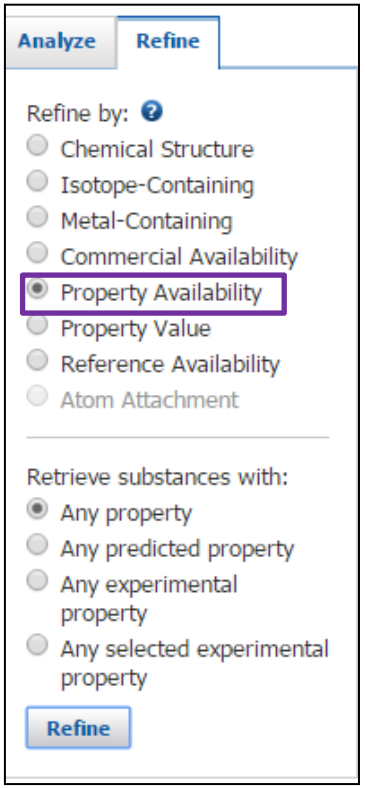


物质检索结果——Refine



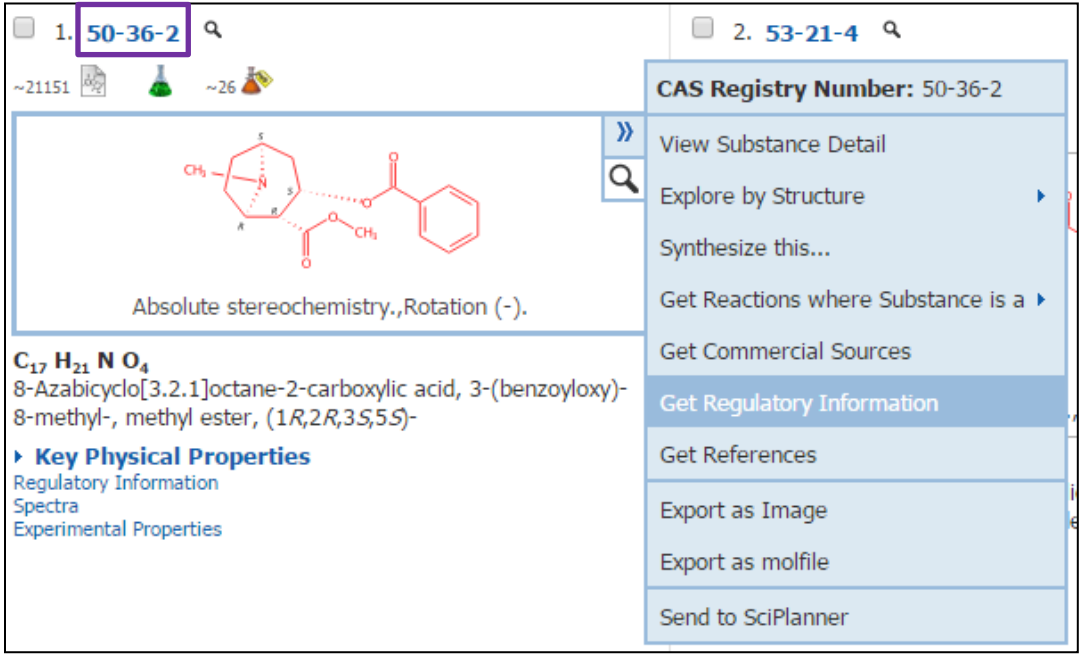
可以按照化学结构，
包含同位素化合物/金属化合物，
商业可获得性，
性质可获得性，
性质数值，文献可获得性
对结果进行限定





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

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*)-

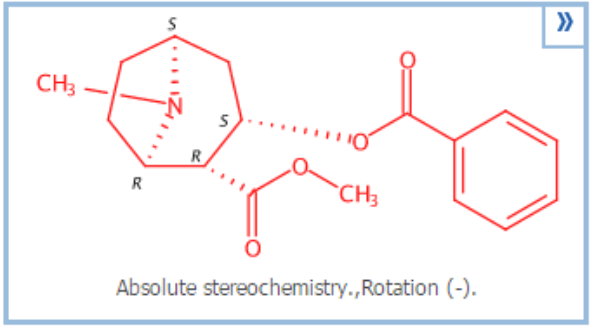
Molecular Weight
303.35

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

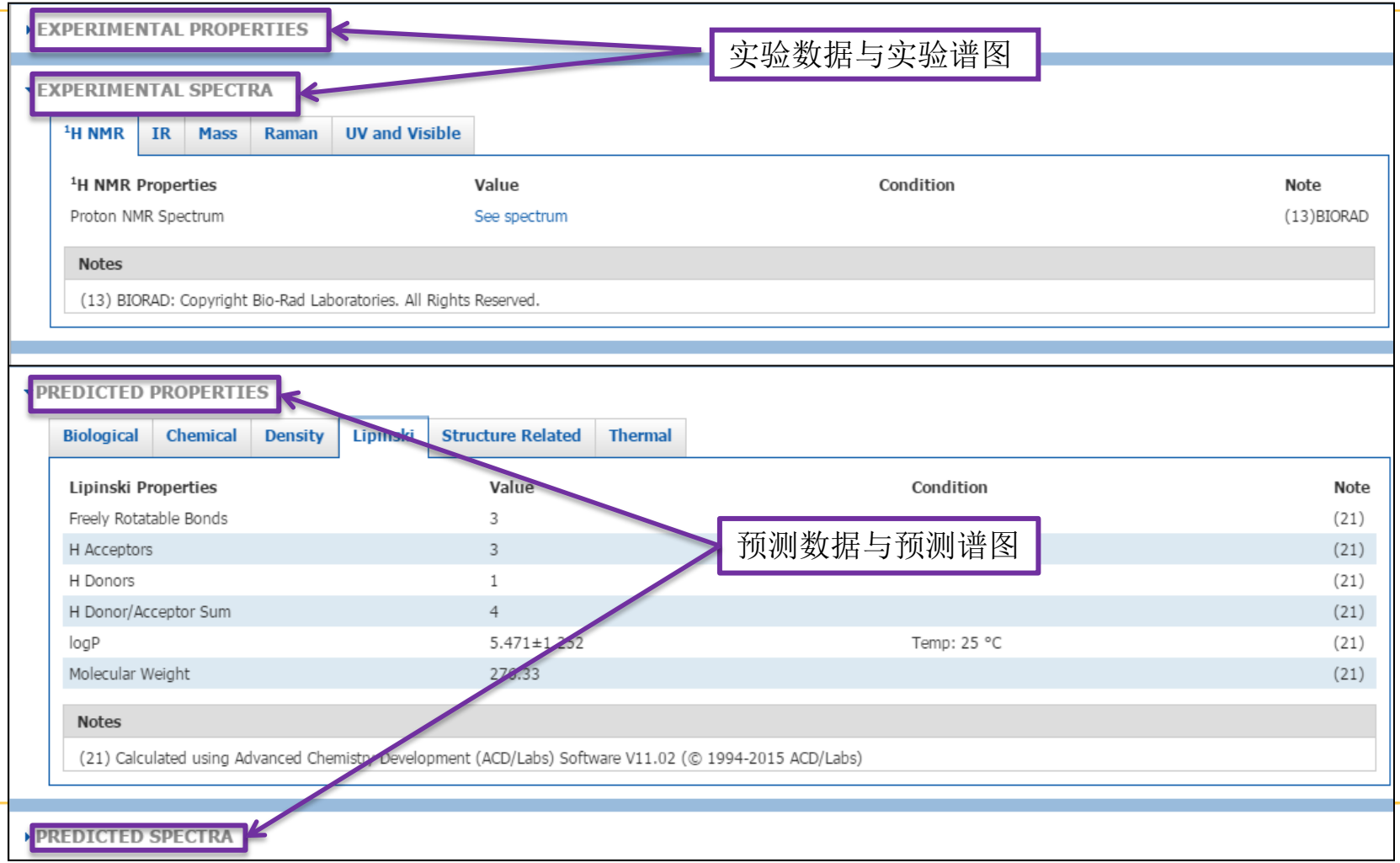
pKa (Predicted)
Value: 8.97±0.60 | Condition: Most Basic Temp: 25 °C



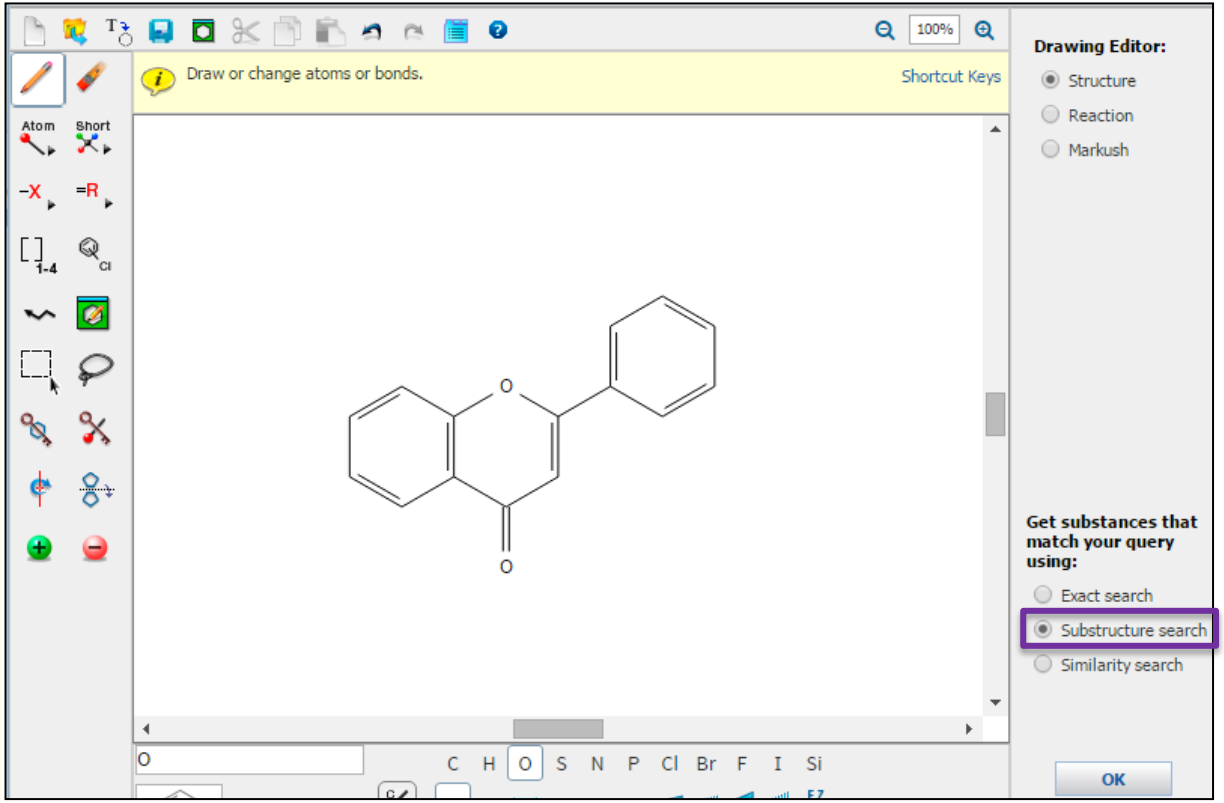
Absolute stereochemistry.,Rotation (-).

物质信息详情

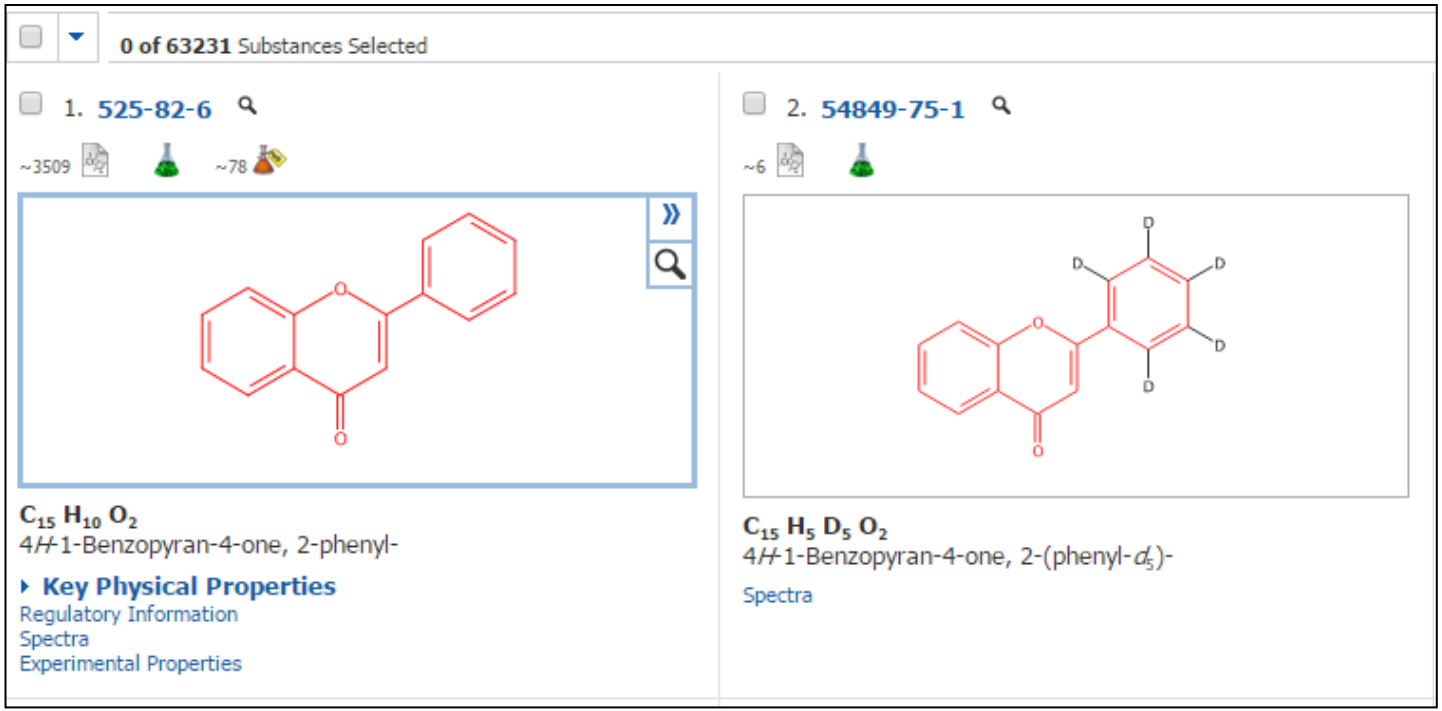
CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY


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



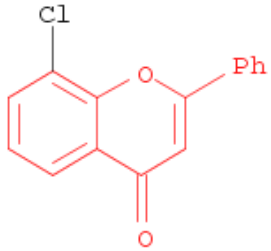
浏览亚结构检索结果



浏览亚结构检索结果

251. Substance Detail
1148-20-5

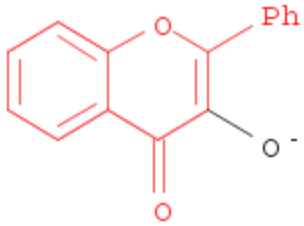
取代物



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

261. Substance Detail
85481-91-0

离子

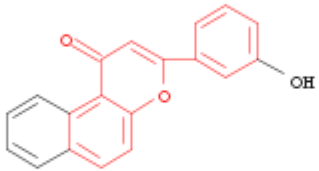


C15 H9 O3
4*H*-1-Benzopyran-4-one, 3-hydroxy-2-phenyl-, ion

273. Substance Detail
136116-17-1

稠环物质

~2

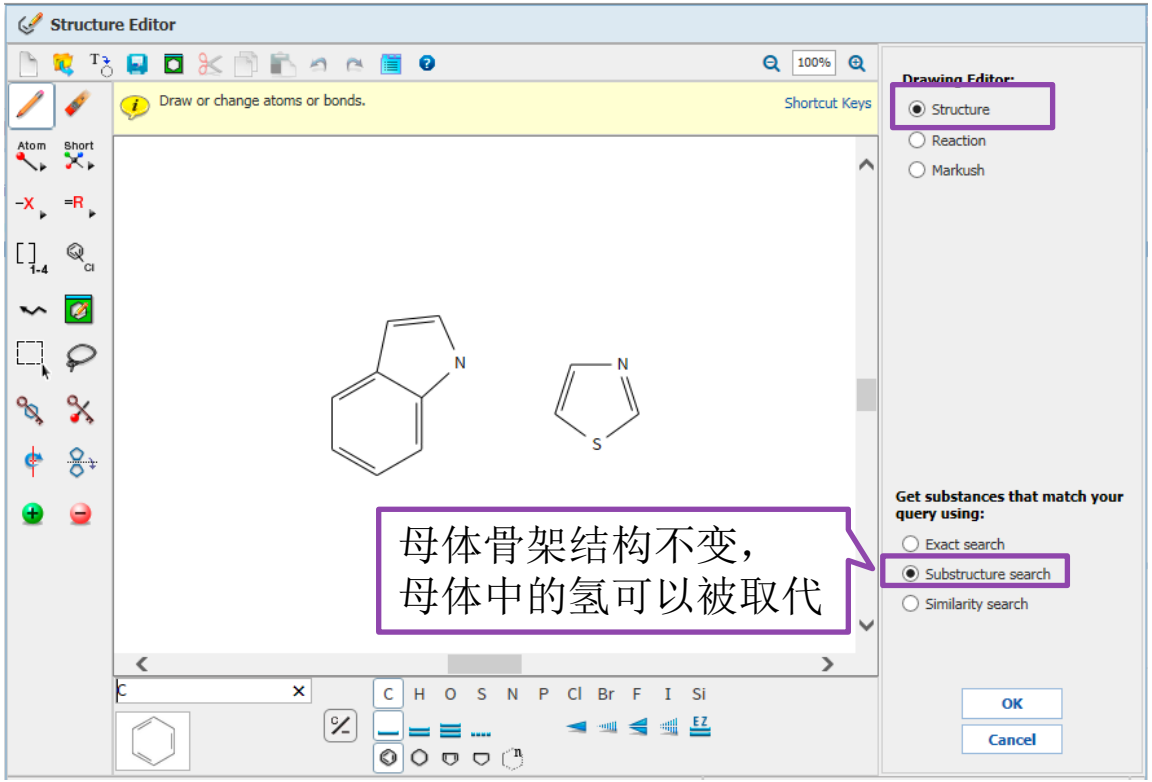


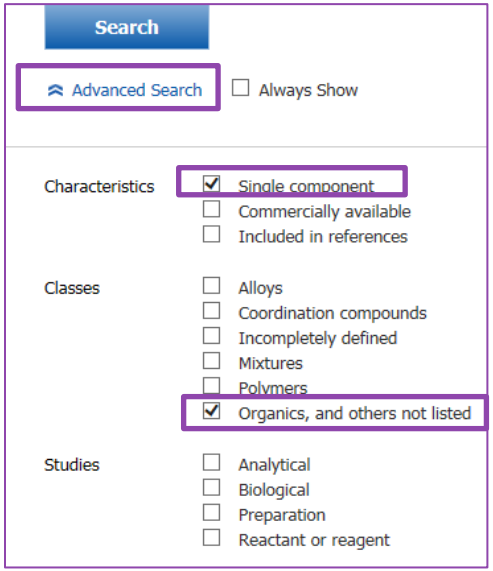
C19 H12 O3
1*H*-Naphtho[2,1-*b*]pyran-1-one, 3-(3-hydroxyphenyl)-

Experimental Properties

包括精确结构检索结果，及被检索结构的修饰结构

化学结构检索：亚结构检索

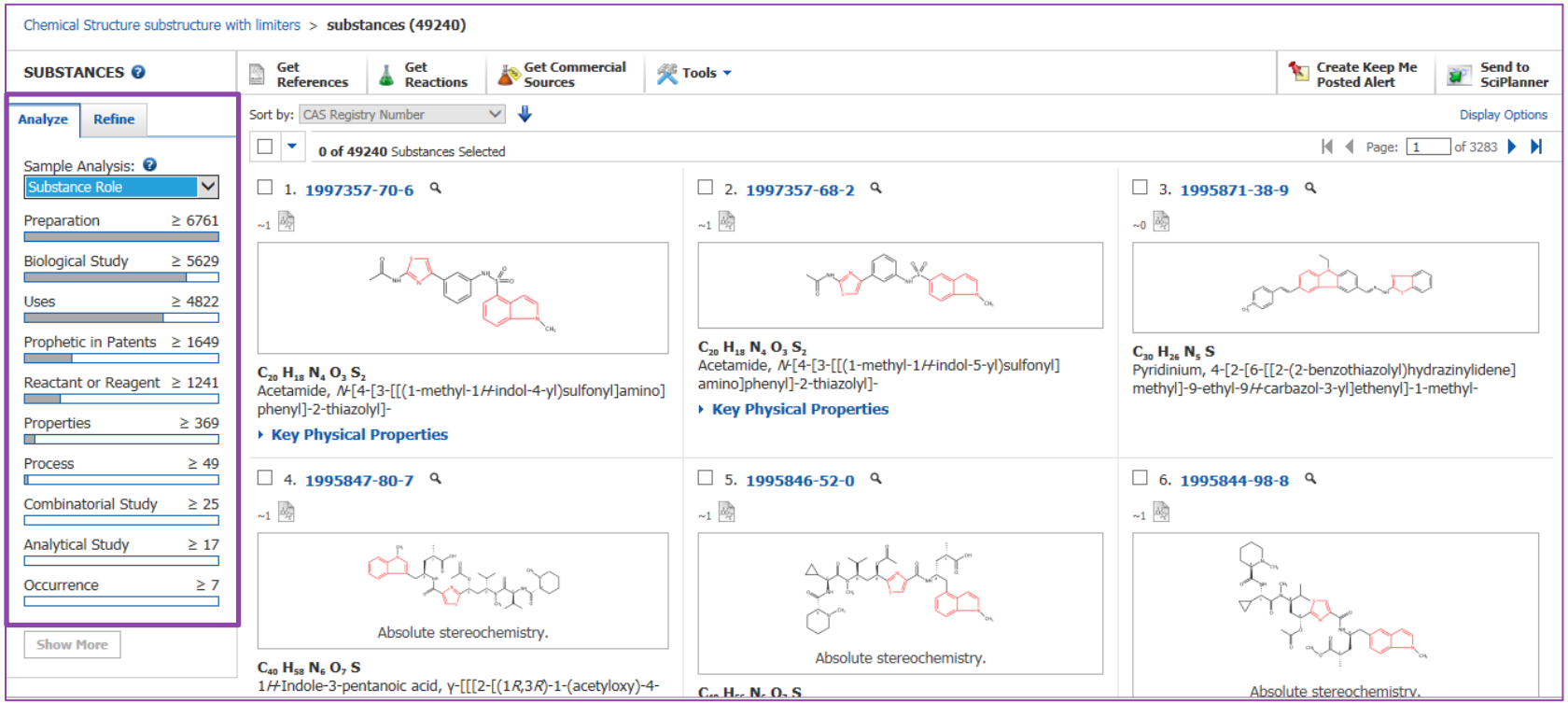




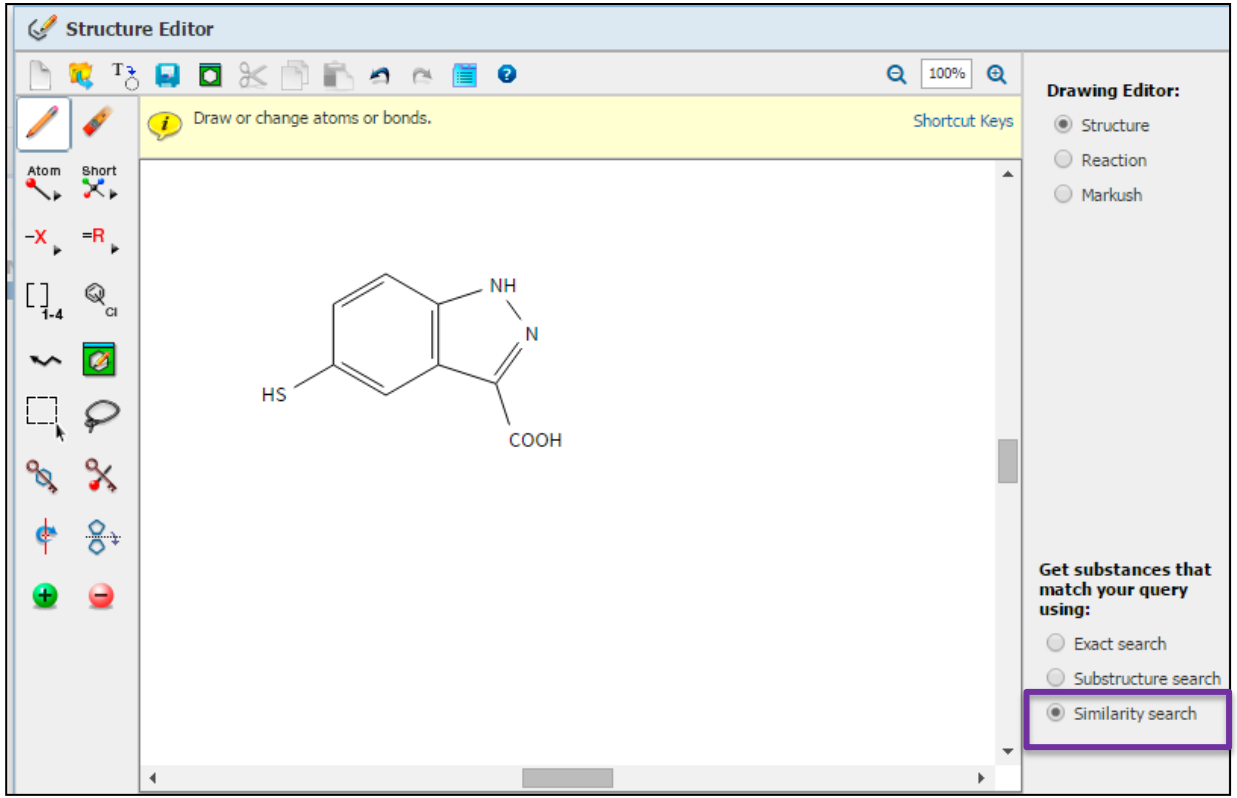
将两个活性分子片段
限定在同一物质中

CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

两个分子片段出现在同一物质中



物质检索——相似结构检索



Select All Deselect All

相似结构检索候选项

1 of 6 Similarity Candidates Selected

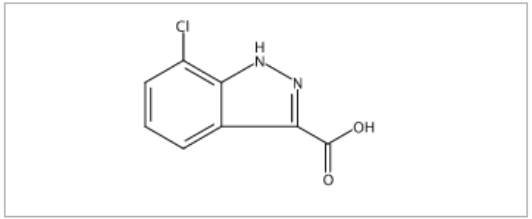
	Substances
≥ 99 (most similar)	0
95-98	0
90-94	0
85-89	11
80-84	34
75-79	82
70-74	254
65-69	633
0-64 (least similar)	1636

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-

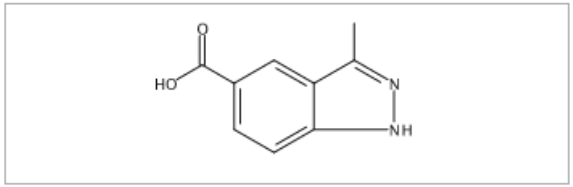
Key Physica

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-

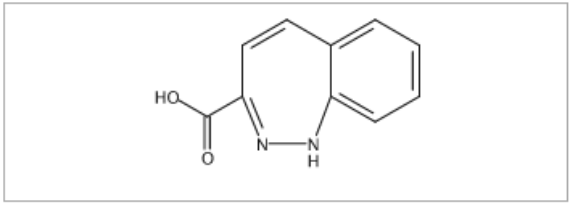
Key Physical Properties

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

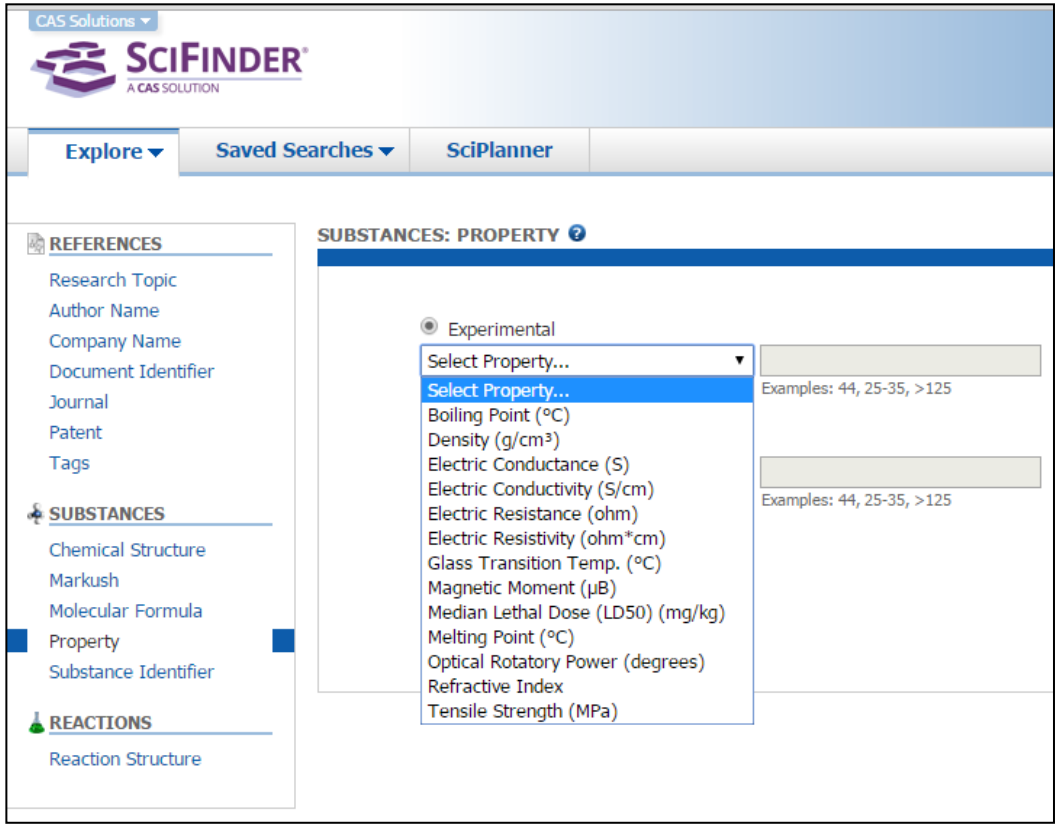
CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

物质检索——相似结构检索

- 相似结构检索：

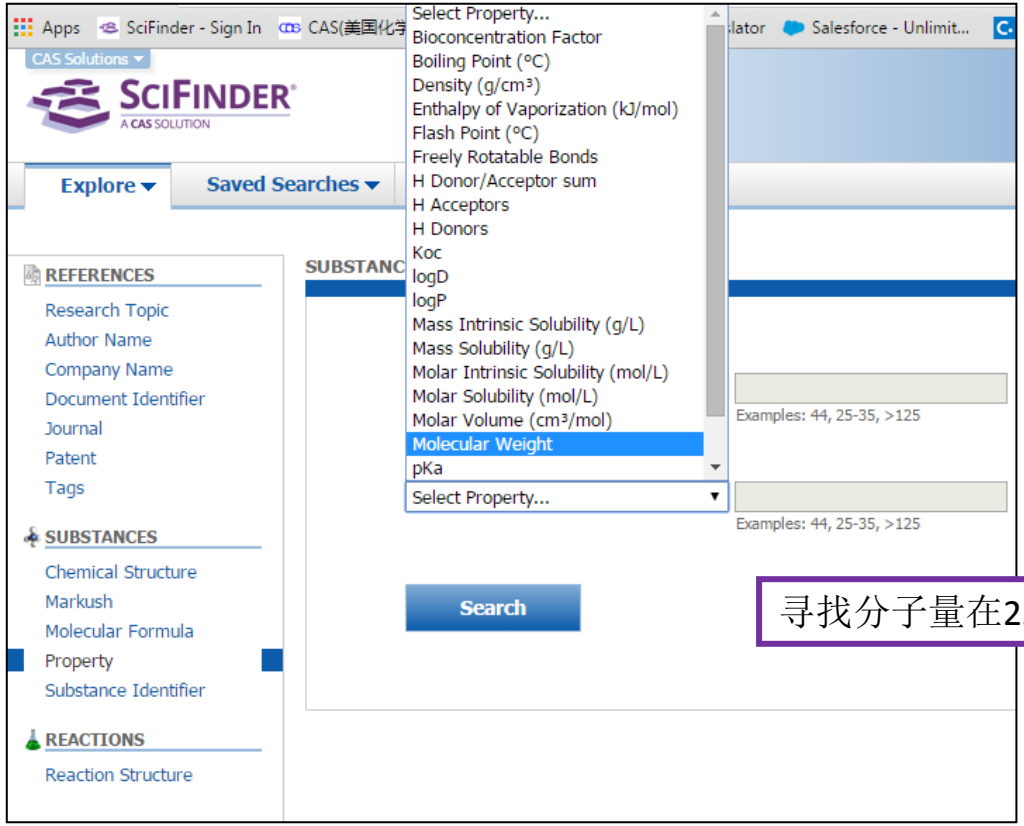
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

物质检索——性质检索



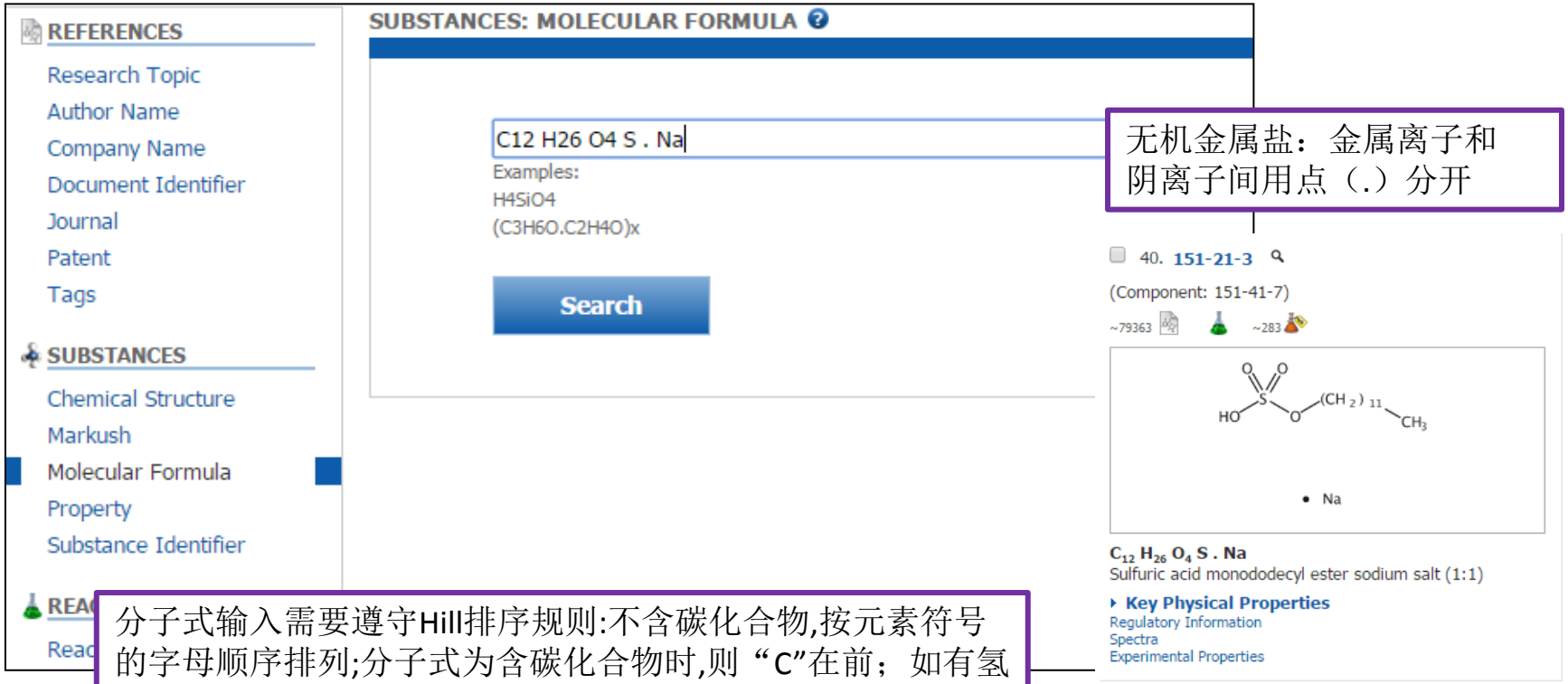
CAS
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

物质检索——性质检索

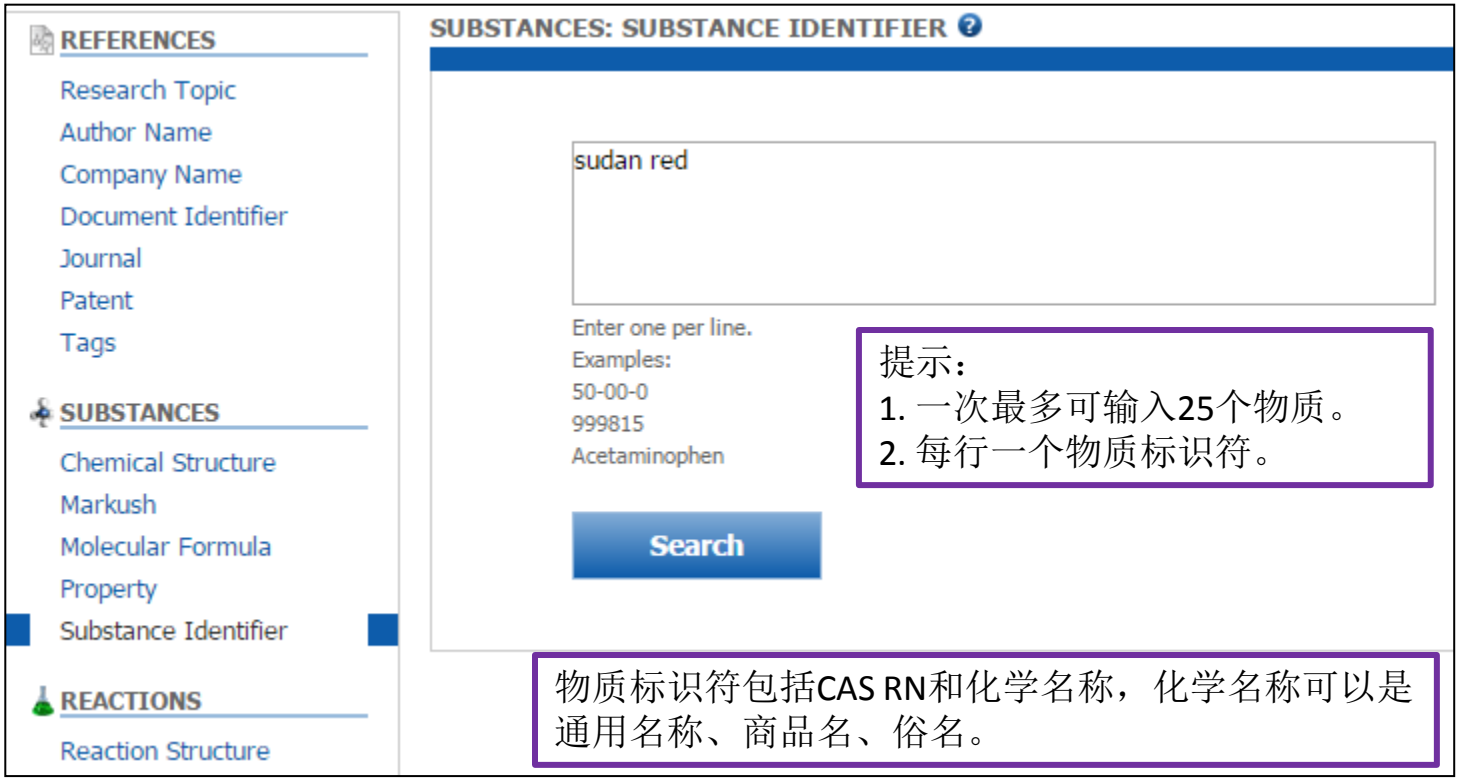


寻找分子量在250-400之间的物质

物质检索——分子式检索



物质检索——标识符检索



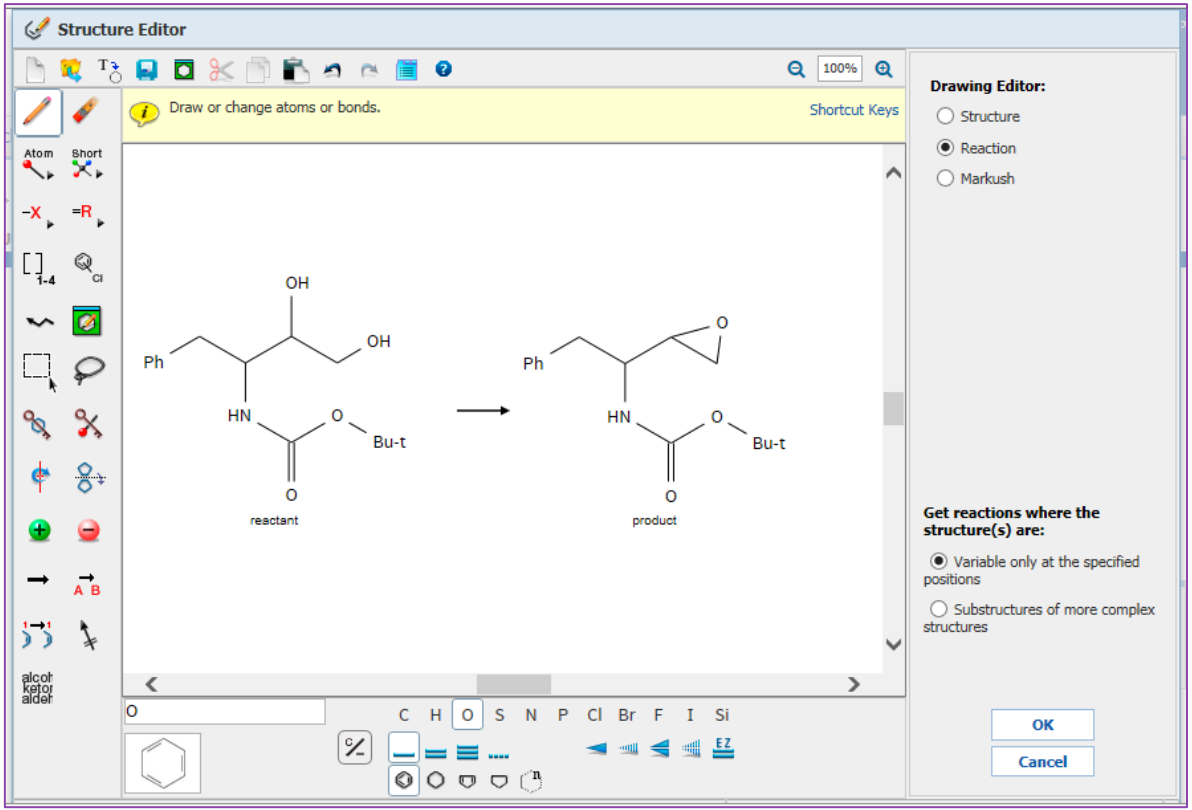
提纲

- 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
  - 分析方法查询
- SciFinder常见问题及解决

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
  - 案例分享

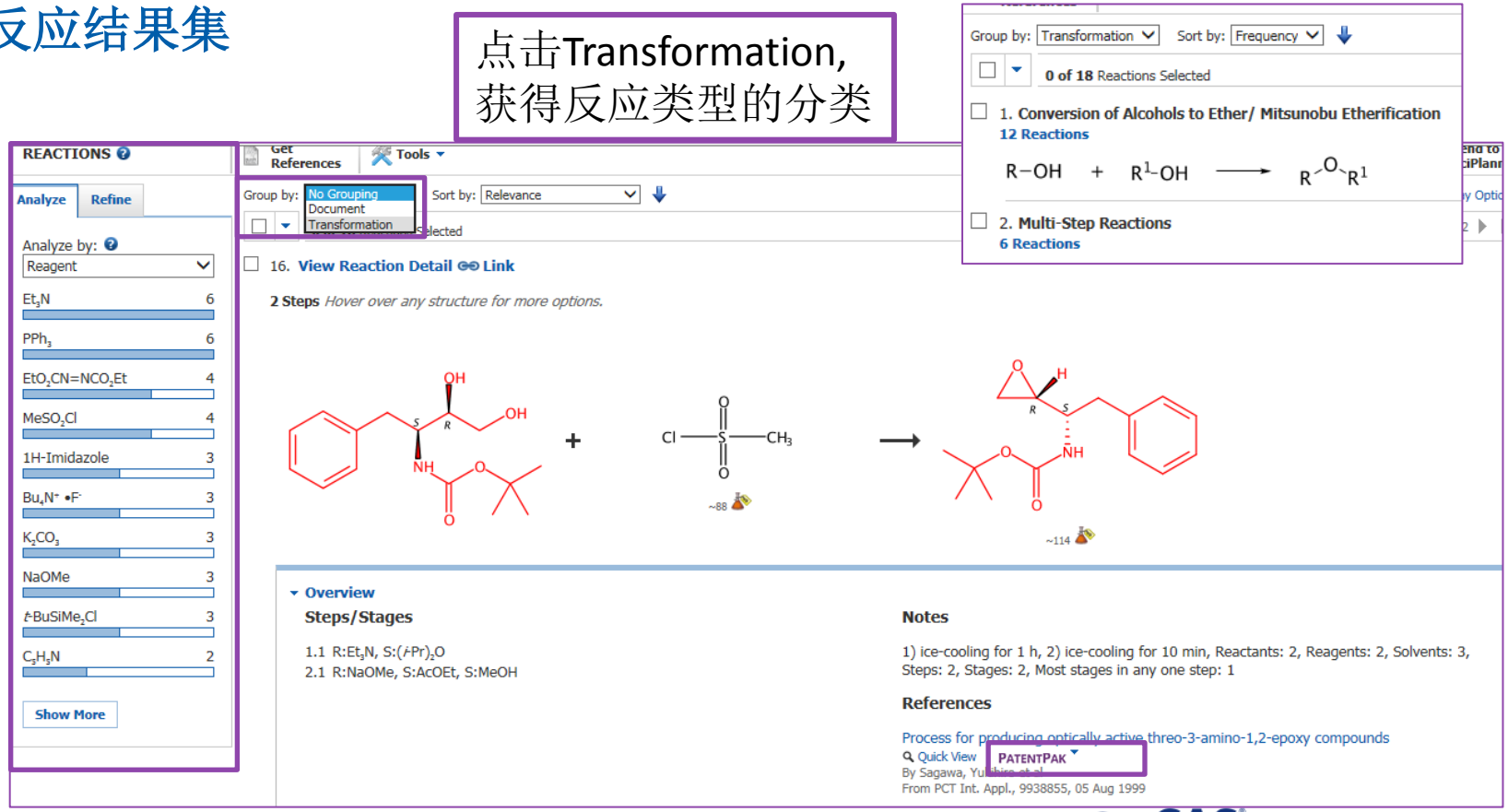
反应检索：精确结构反应检索



CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

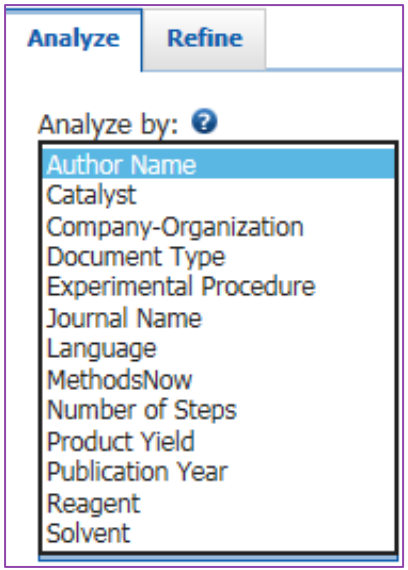
反应结果集

点击Transformation,
获得反应类型的分类

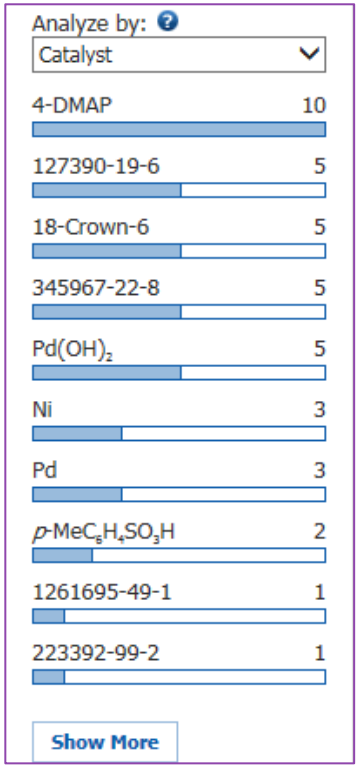


反应结果处理：分析

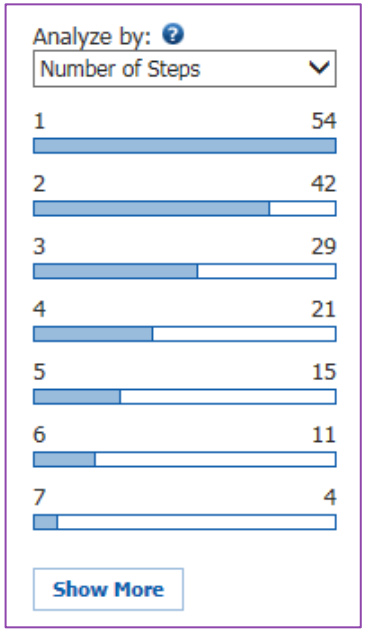
13种分析选项



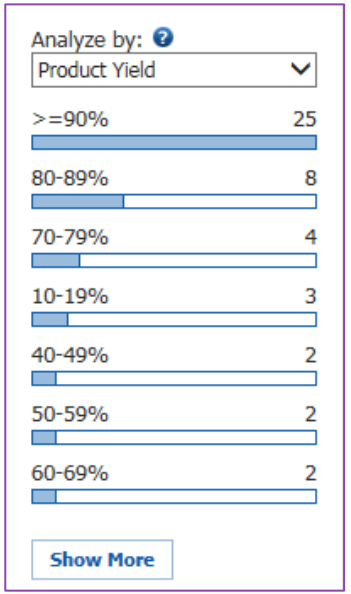
催化剂



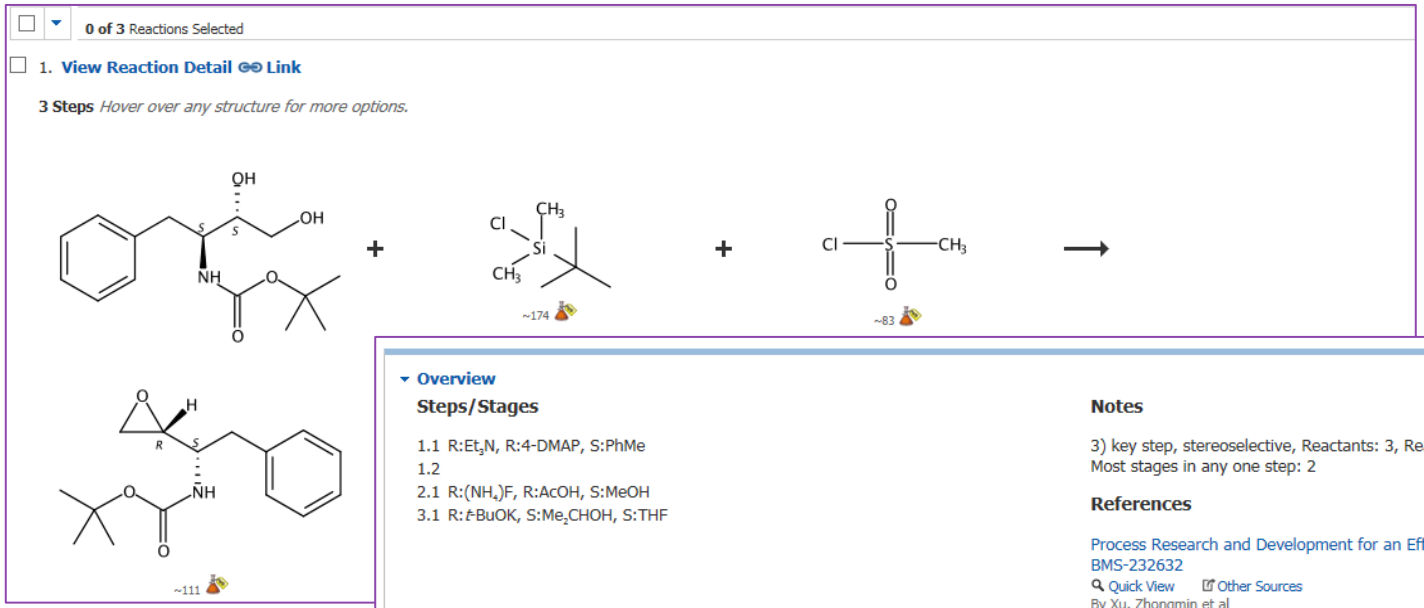
反应步数



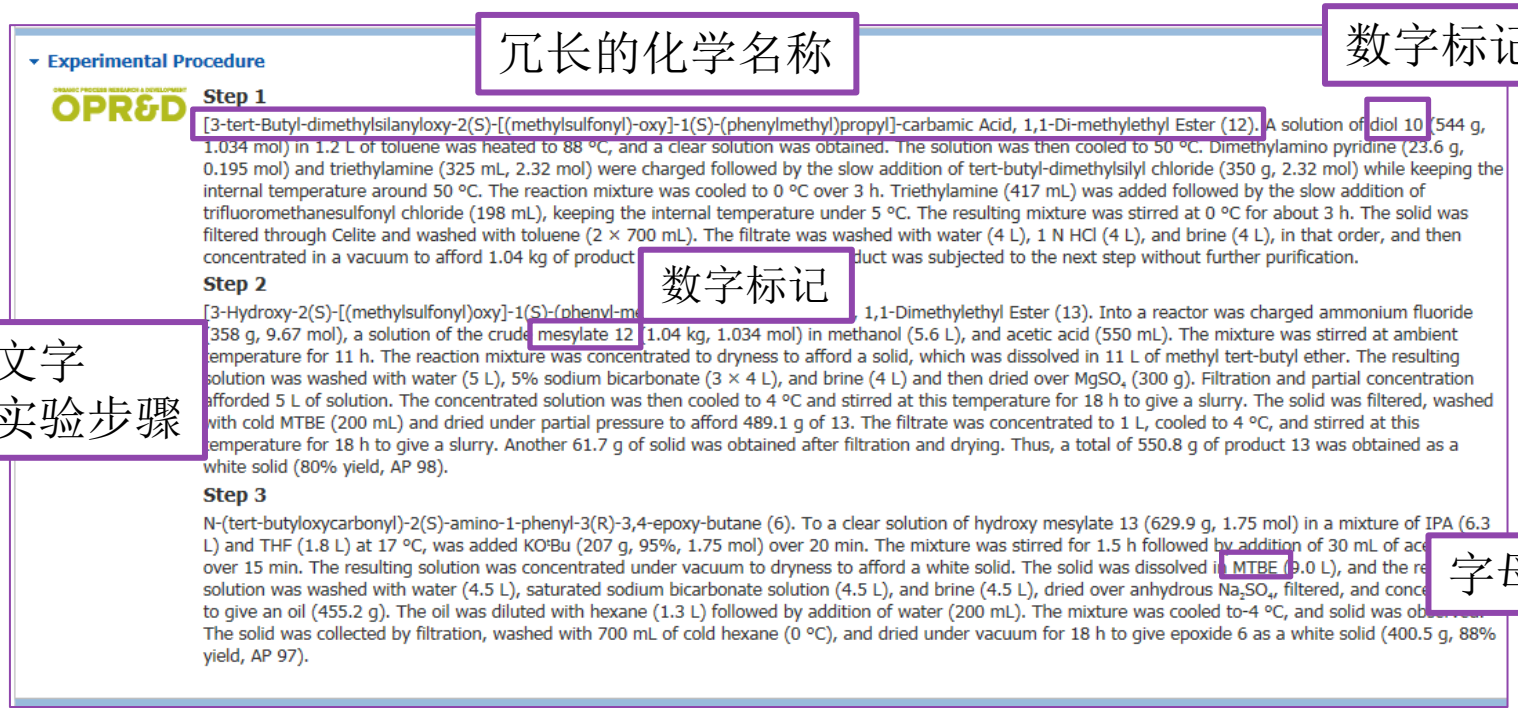
产率



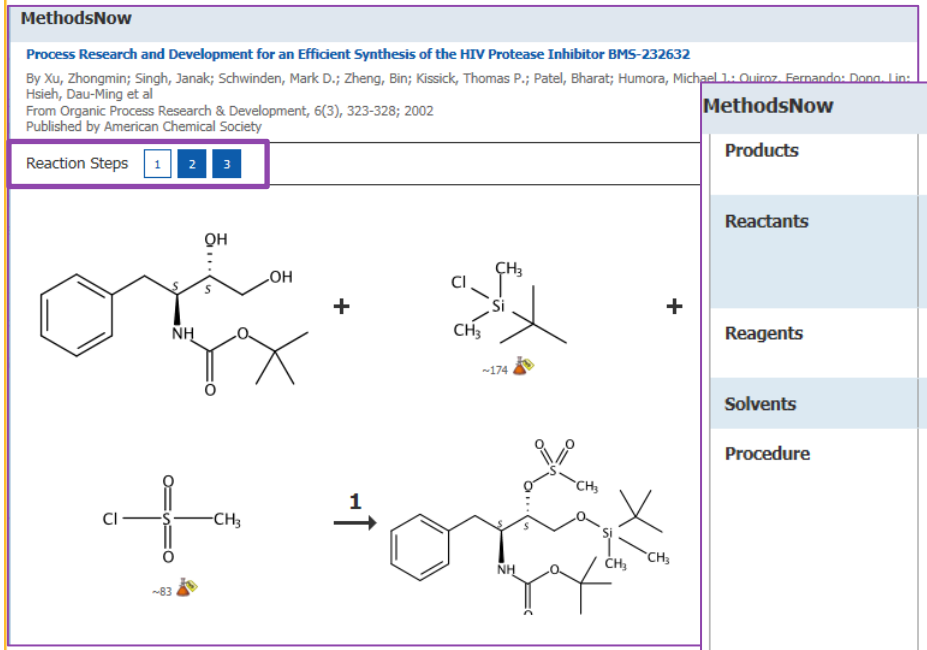
针对感兴趣的反应查看实验详情



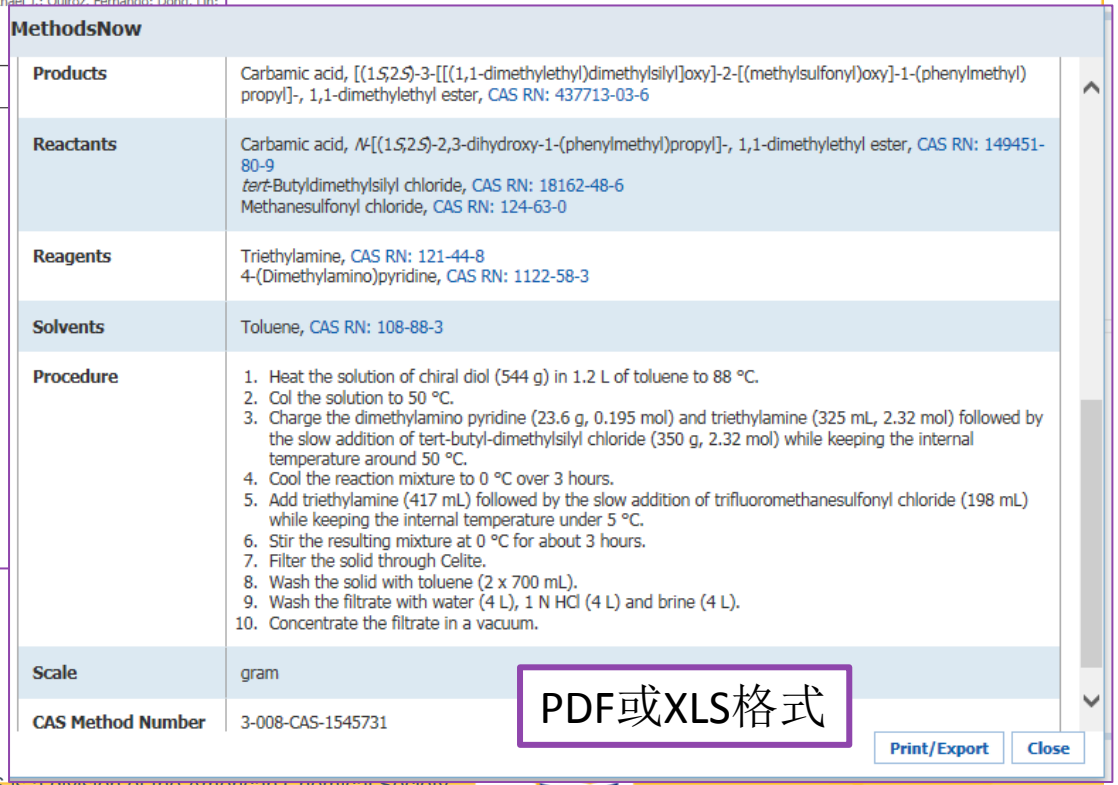
Experimental Procedure



MethodsNow窗口



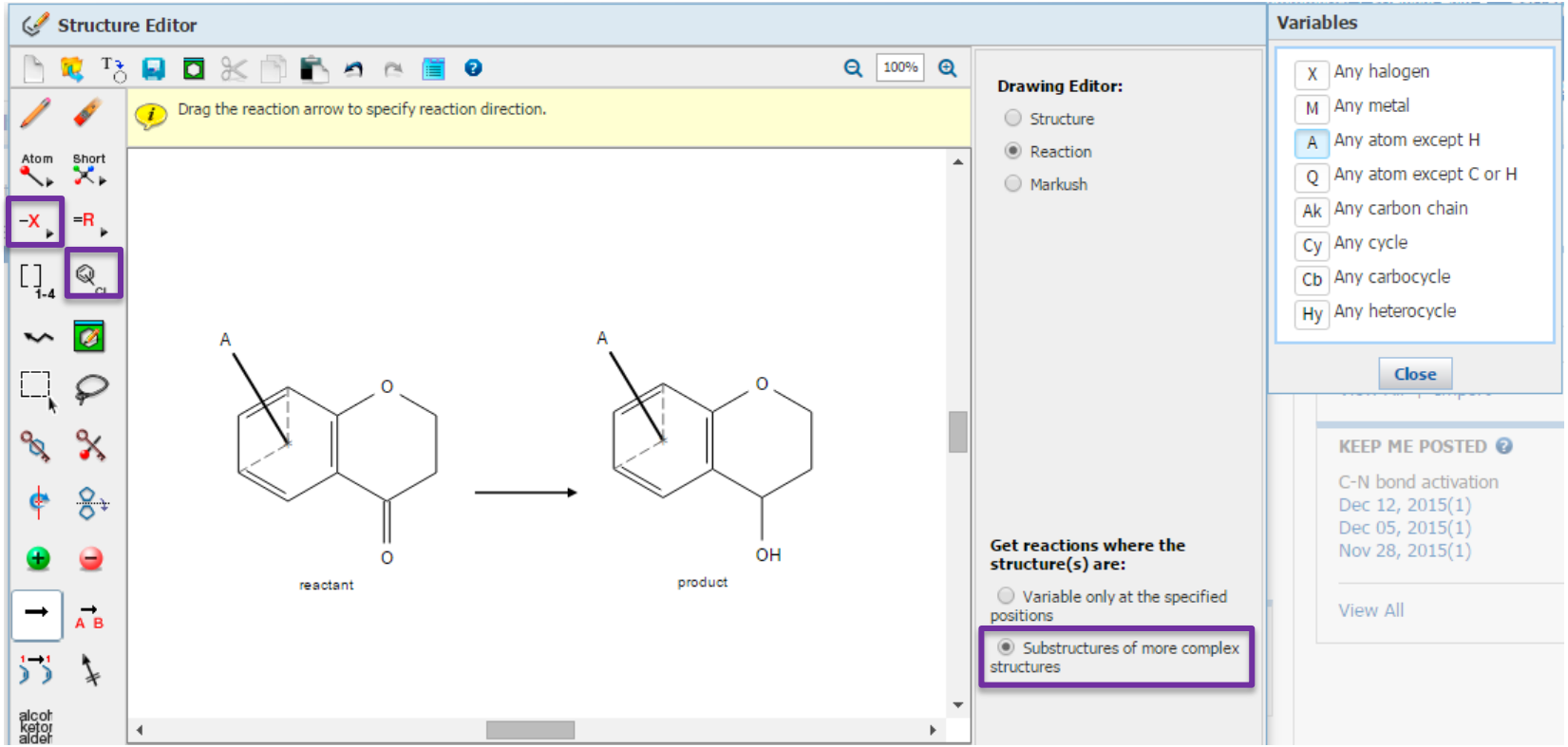
CAS RN即时查看物质



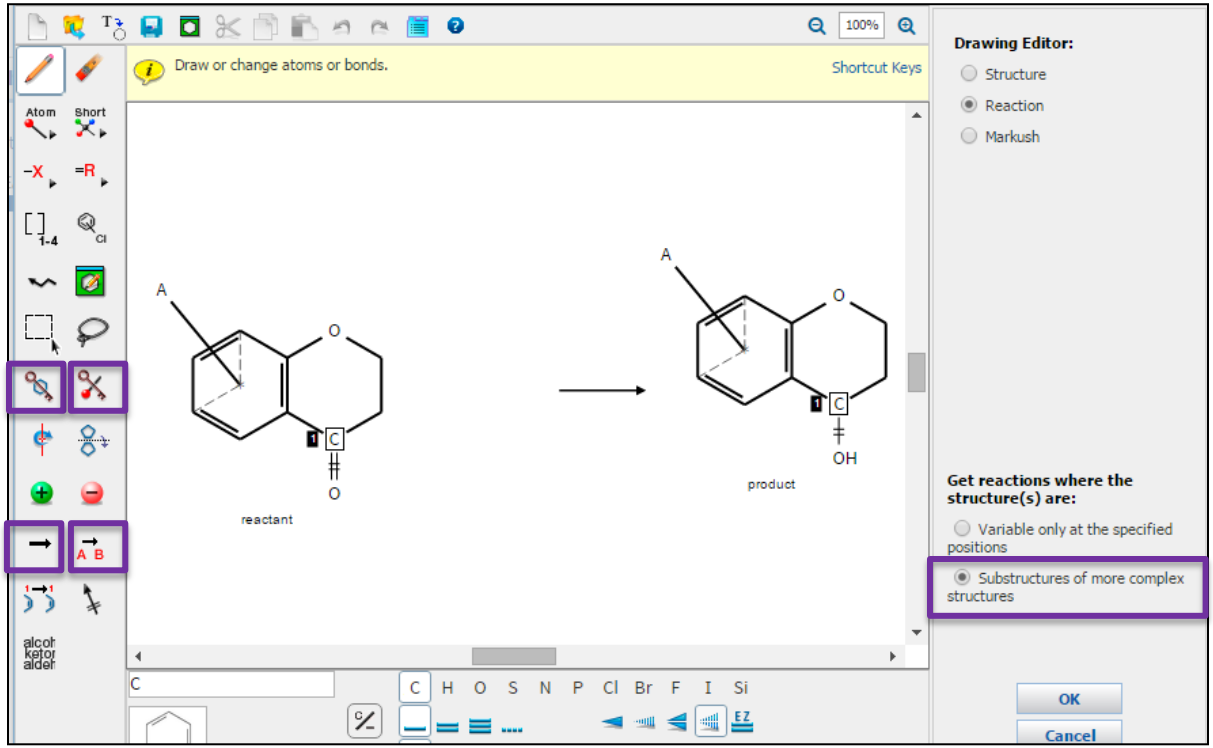
产物，反应物，试剂，溶剂，步骤，
反应类型，规模，产物状态，CAS方法号

PDF或XLS格式

亚结构检索：酮基的还原反应



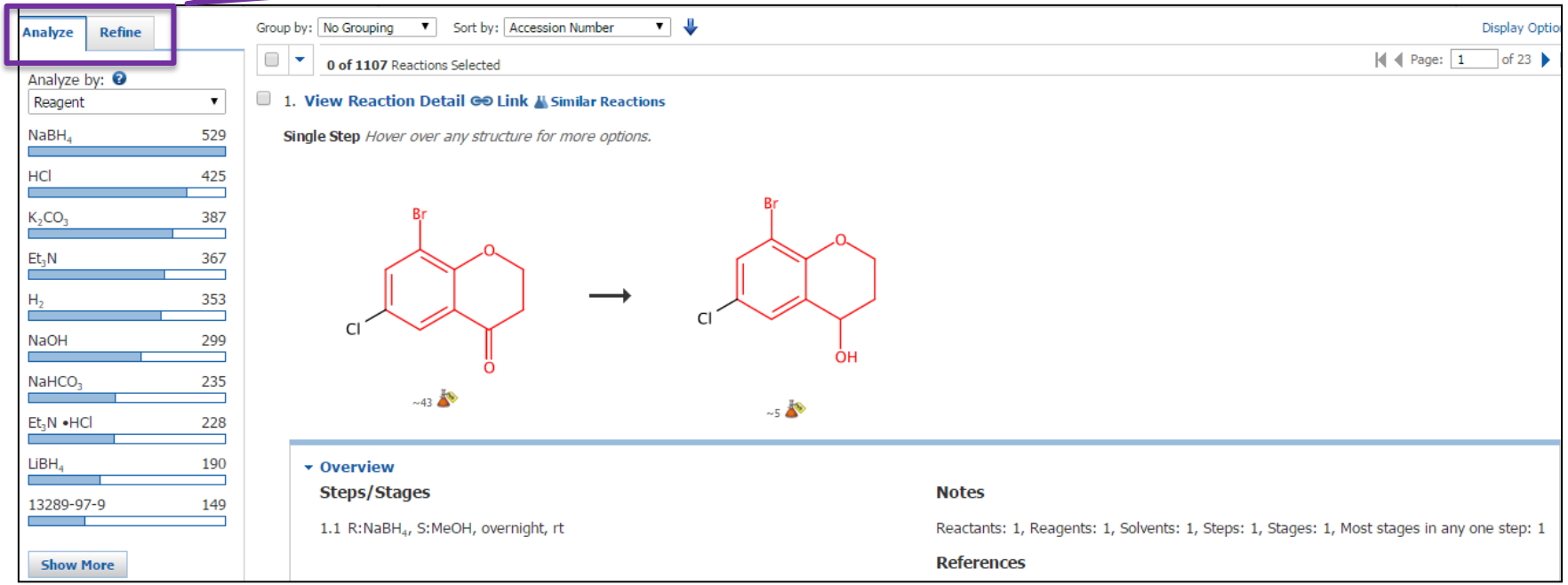
亚结构检索：酮基的还原反应



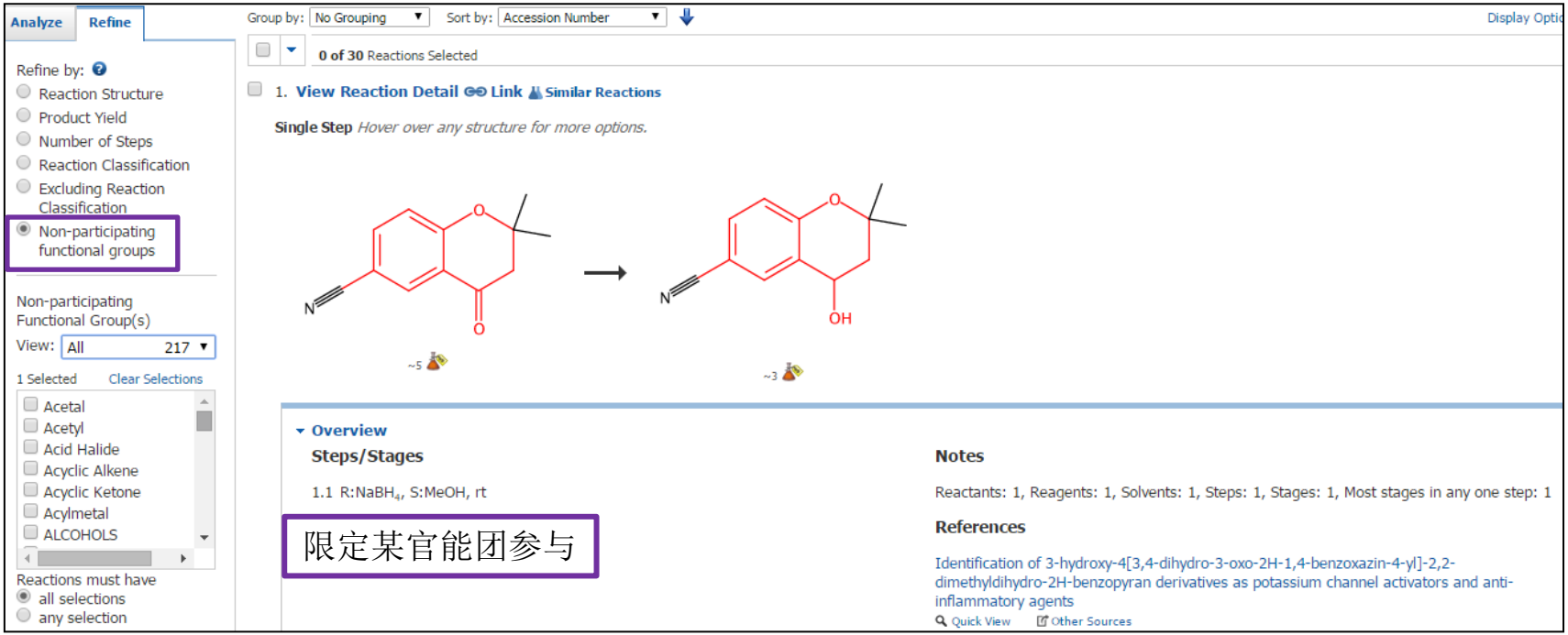
检索酮基的还原反应，需将碳原子锁定

亚结构反应检索结果

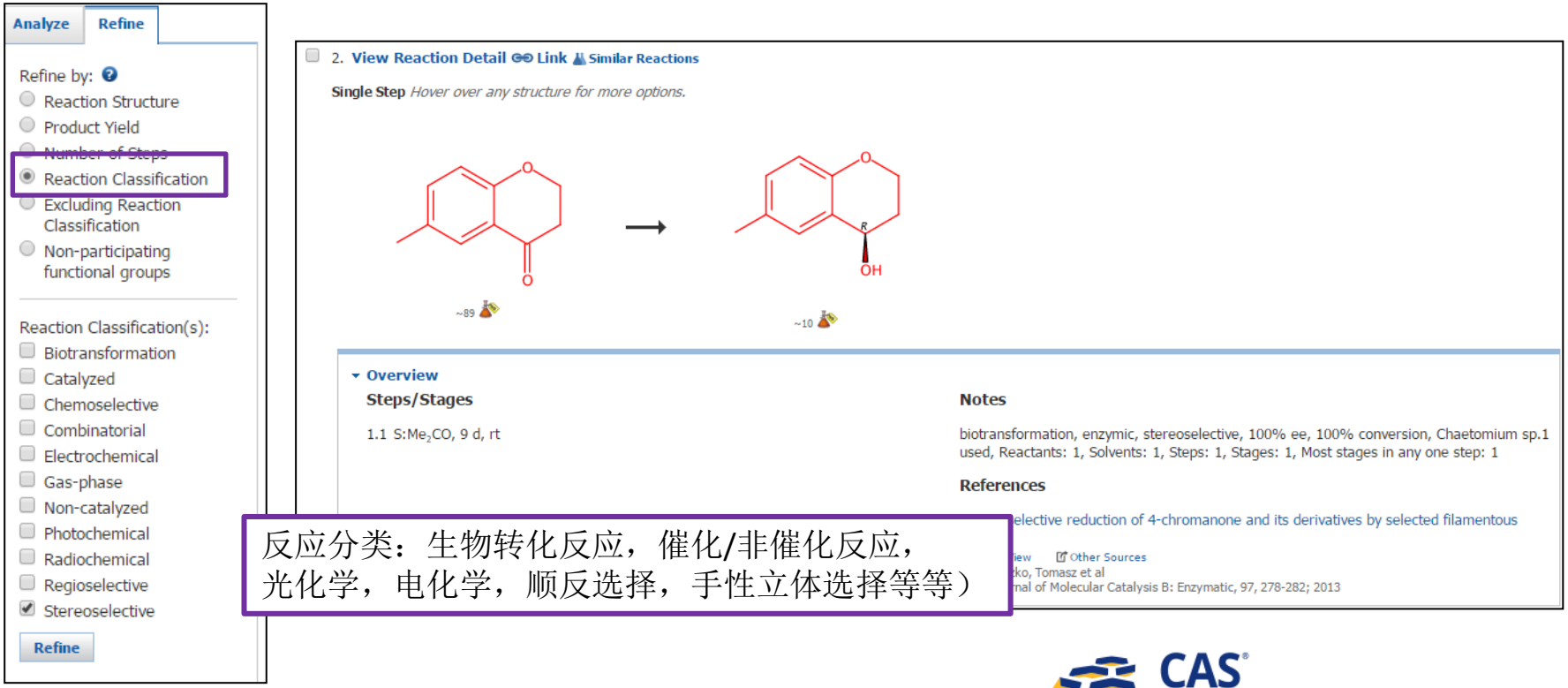
通过Analyze或者Refine处理检索结果



亚结构反应检索结果



亚结构反应检索结果

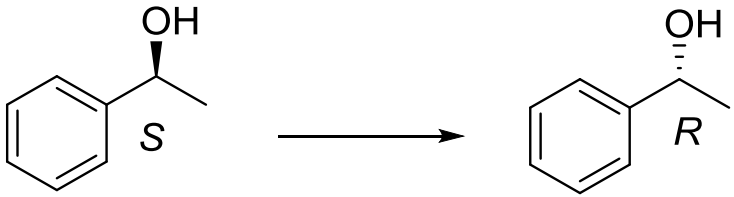


反应分类：生物转化反应，催化/非催化反应，
光化学，电化学，顺反选择，手性立体选择等等）

提纲

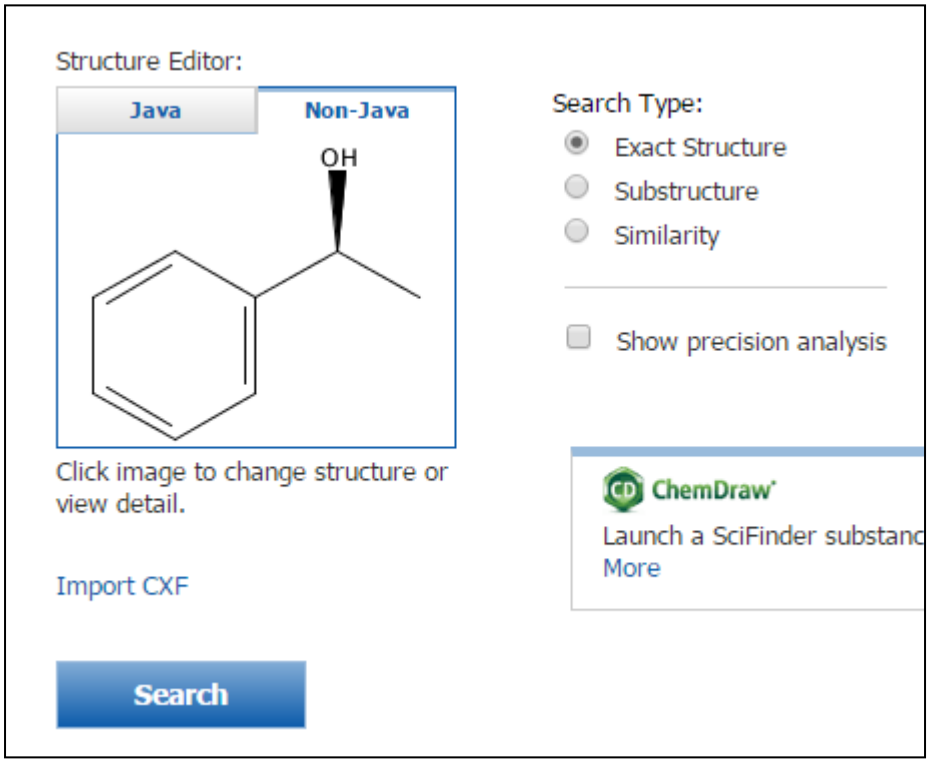
- 反应检索
  - 反应检索绘制工具及反应信息详情
  - 如何通过Analyze、Refine来精选反应
  - 亚结构反应检索
    - 手性反转反应
    - 在非反应仲醇存在的条件下，将伯醇转换为乙醛
    - 片段反应

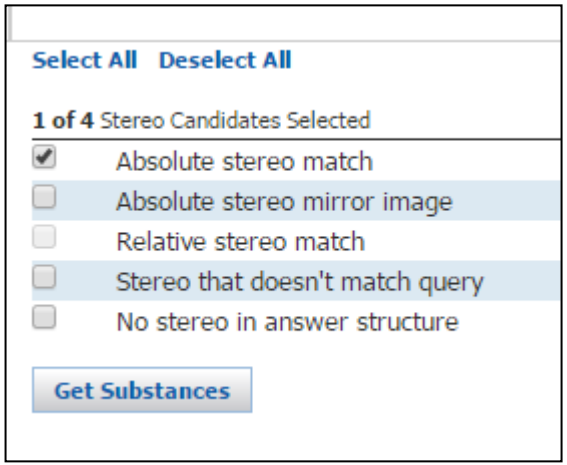
检索如下精确结构的反应



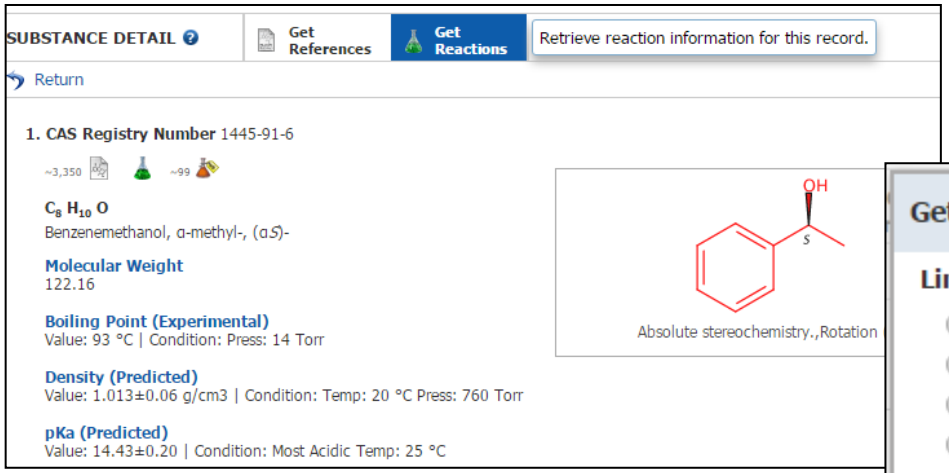
思路：通过物质检索，分别获得起始物和产物的一步反应，再对结果集进行交集。

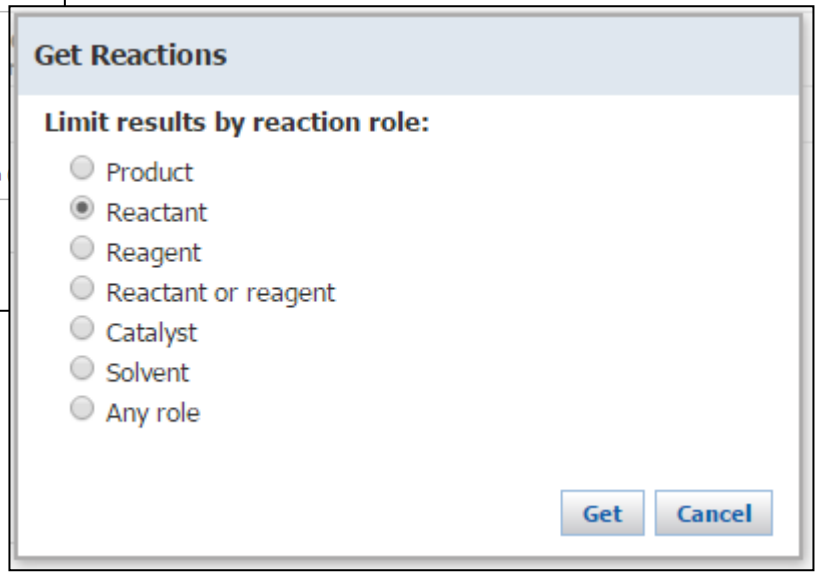
在物质检索中通过精确结构检索起始物



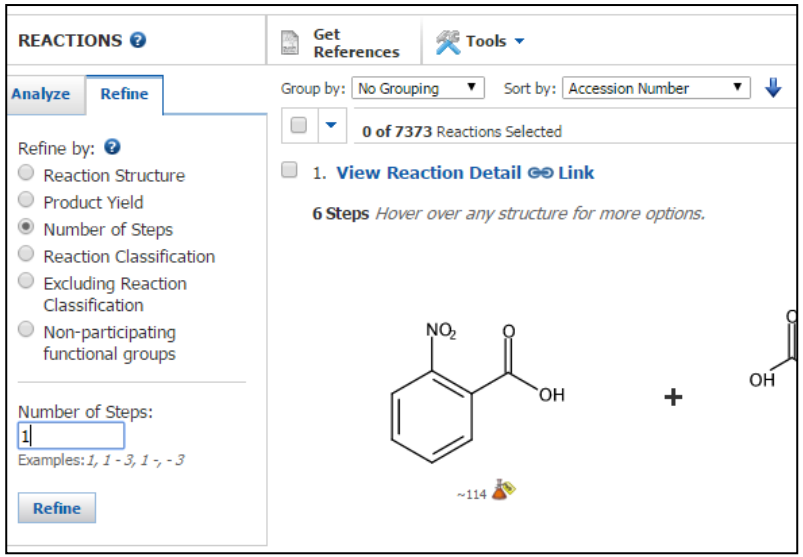


精确检索S构型物质，获得其为“起始物”的反应

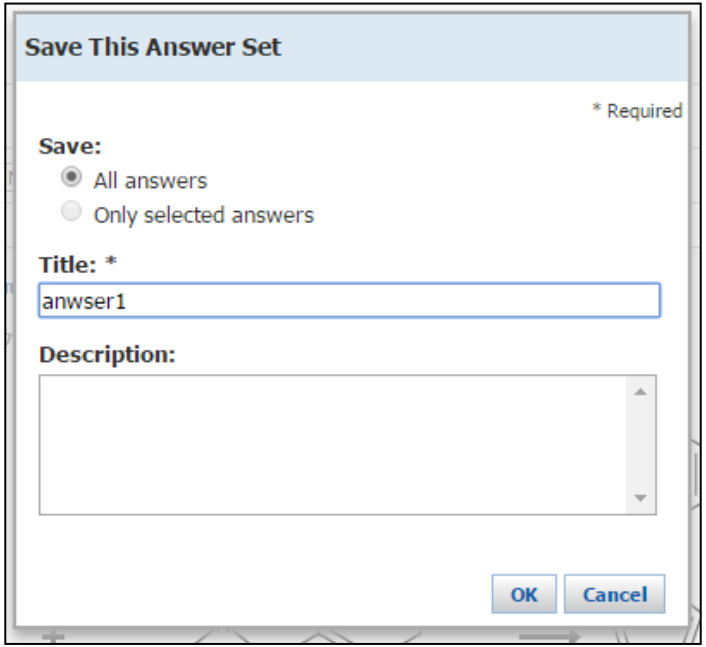




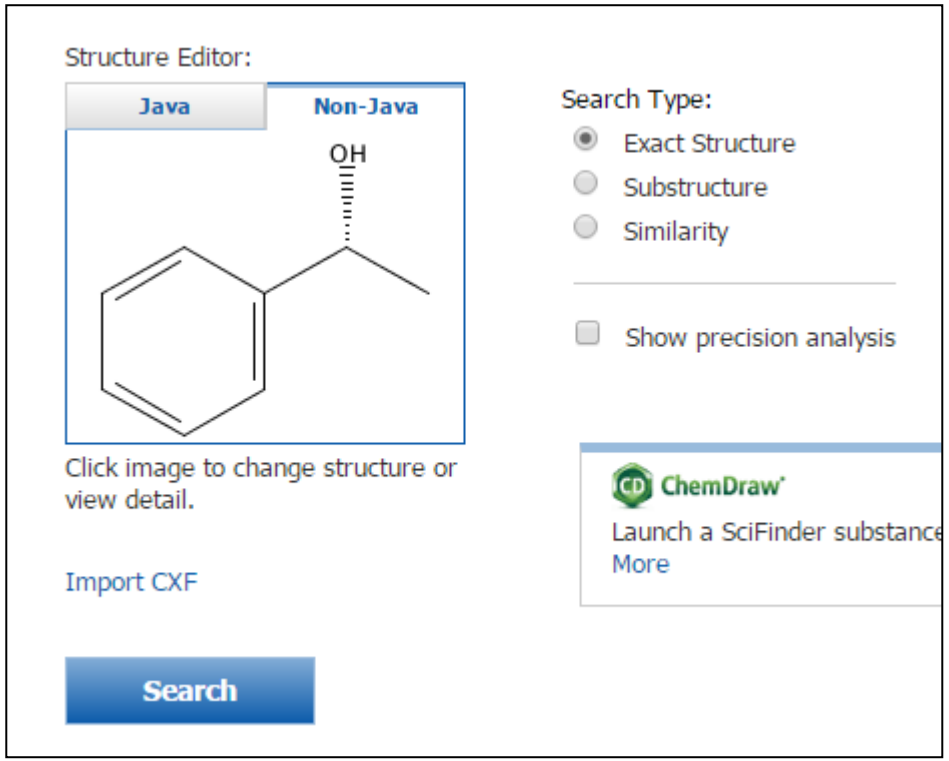
将反应结果集限定为一步反应

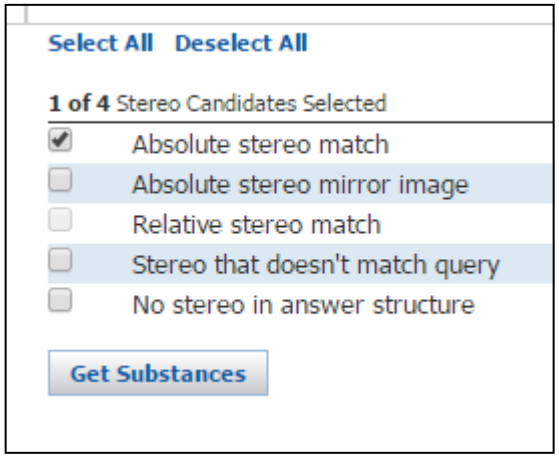


将所得结果集保存为”answer1”



在物质检索中通过精确结构检索产物





精确检索R构型物质，获得其为“产物”的反应

1. CAS Registry Number 1517-69-7

~3,242 ~104

$C_8 H_{10} O$

Benzenemethanol, α-methyl-, (α*R*)-

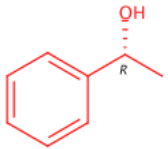
Molecular Weight
122.16

Melting Point (Experimental)
Value: 9-11 °C

Boiling Point (Experimental)
Value: 98 °C

Density (Predicted)
Value: 1.013±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 14.43±0.20 | Condition: Most Acidic Temp: 25 °C



Absolute stereochemistry.,Rotation (+).

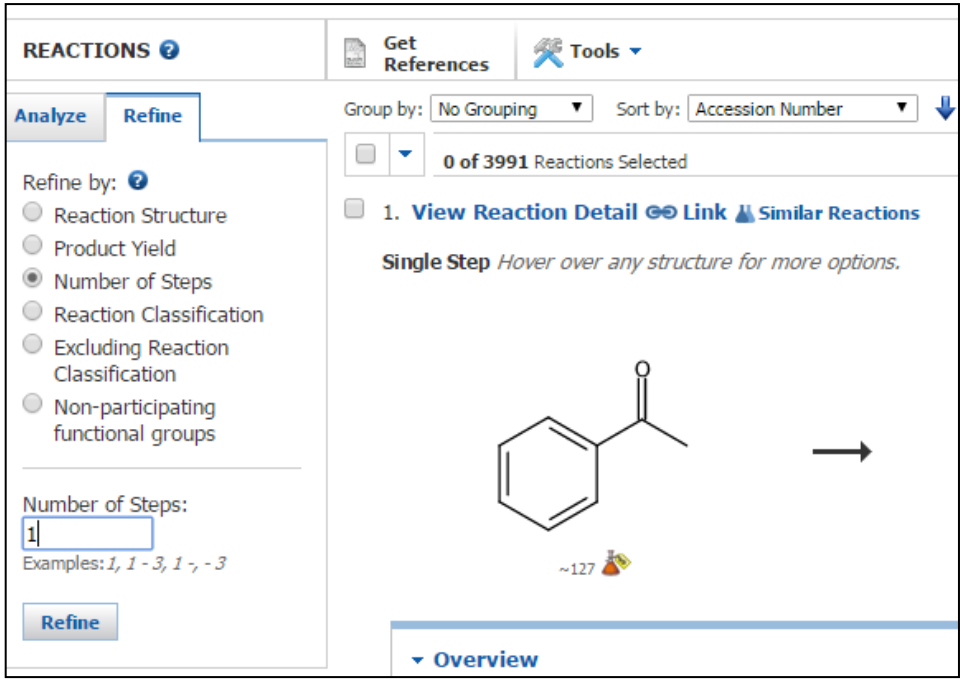
Get Reactions

Limit results by reaction role:

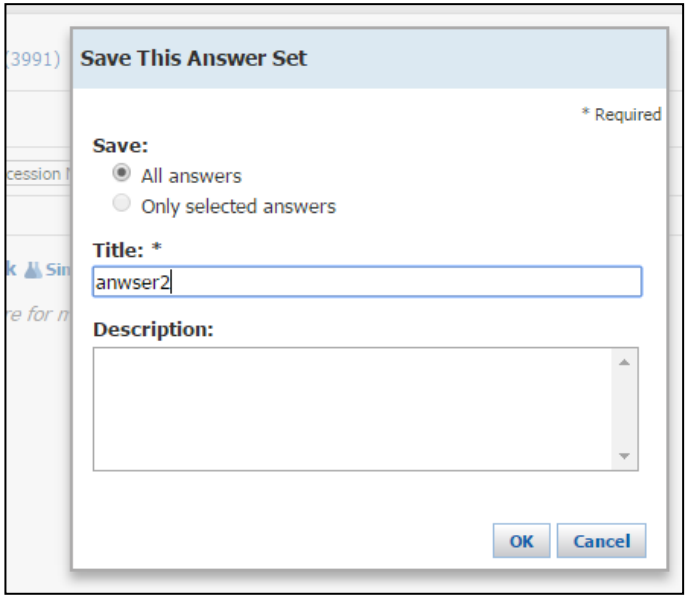
- (•) Product
- ( ) Reactant
- ( ) Reagent
- ( ) Reactant or reagent
- ( ) Catalyst
- ( ) Solvent
- ( ) Any role

Get Cancel

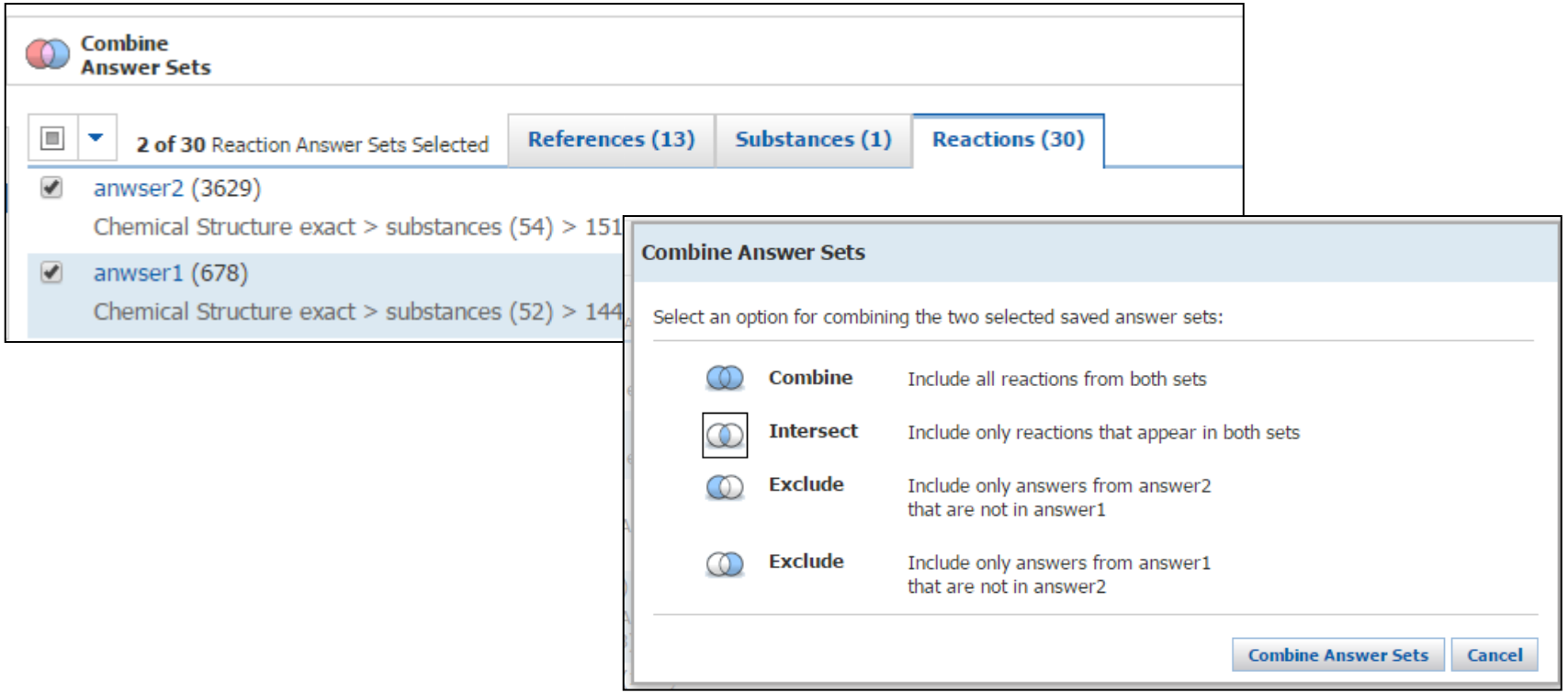
将反应结果集限定为一步反应



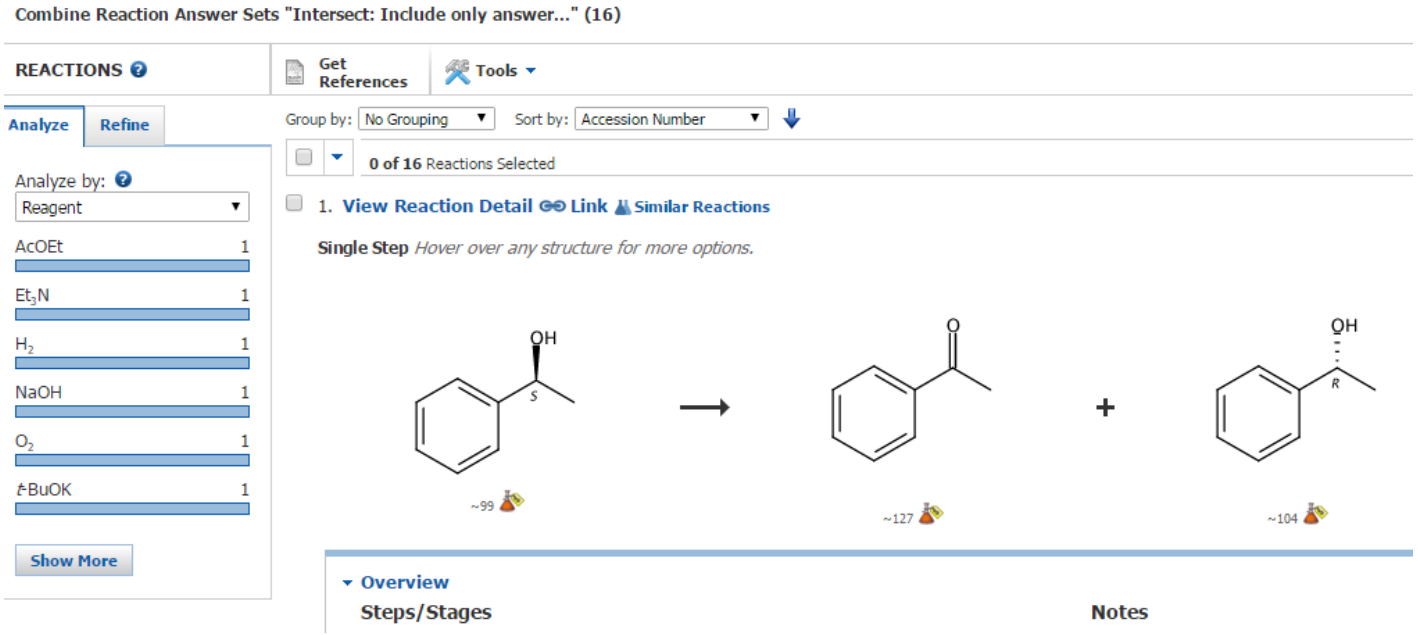
将所得结果集保存为”answer2”



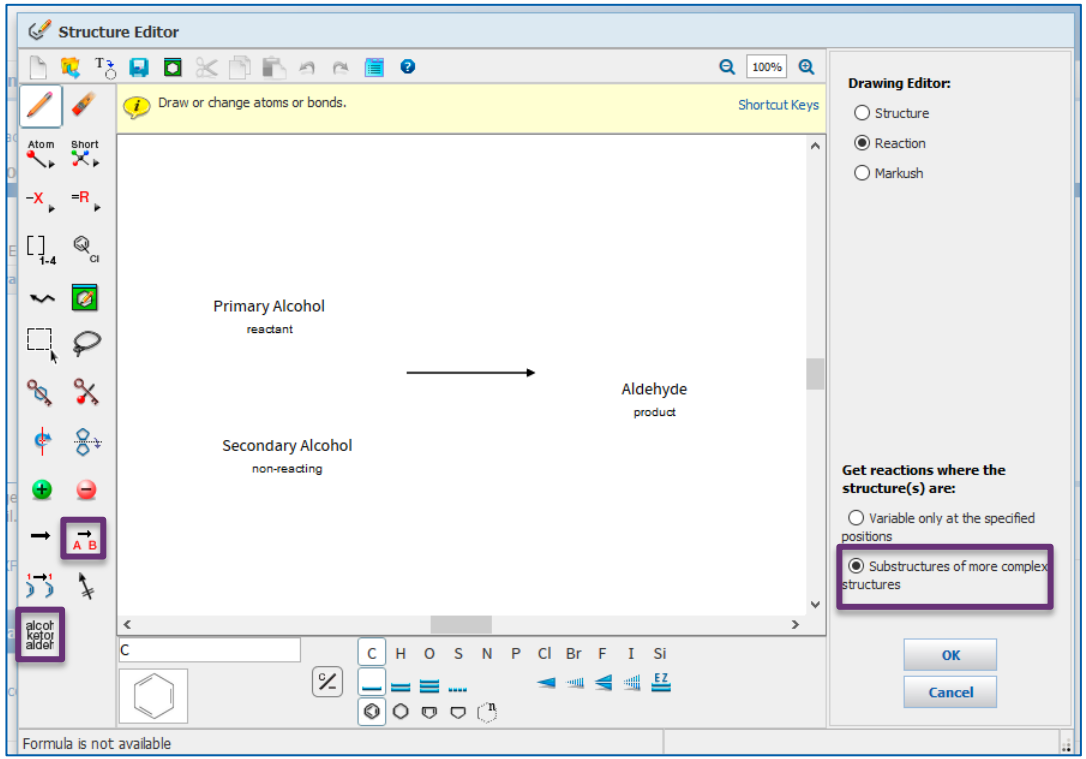
将answer1和answer2合并取交集



获得准确的反应结果

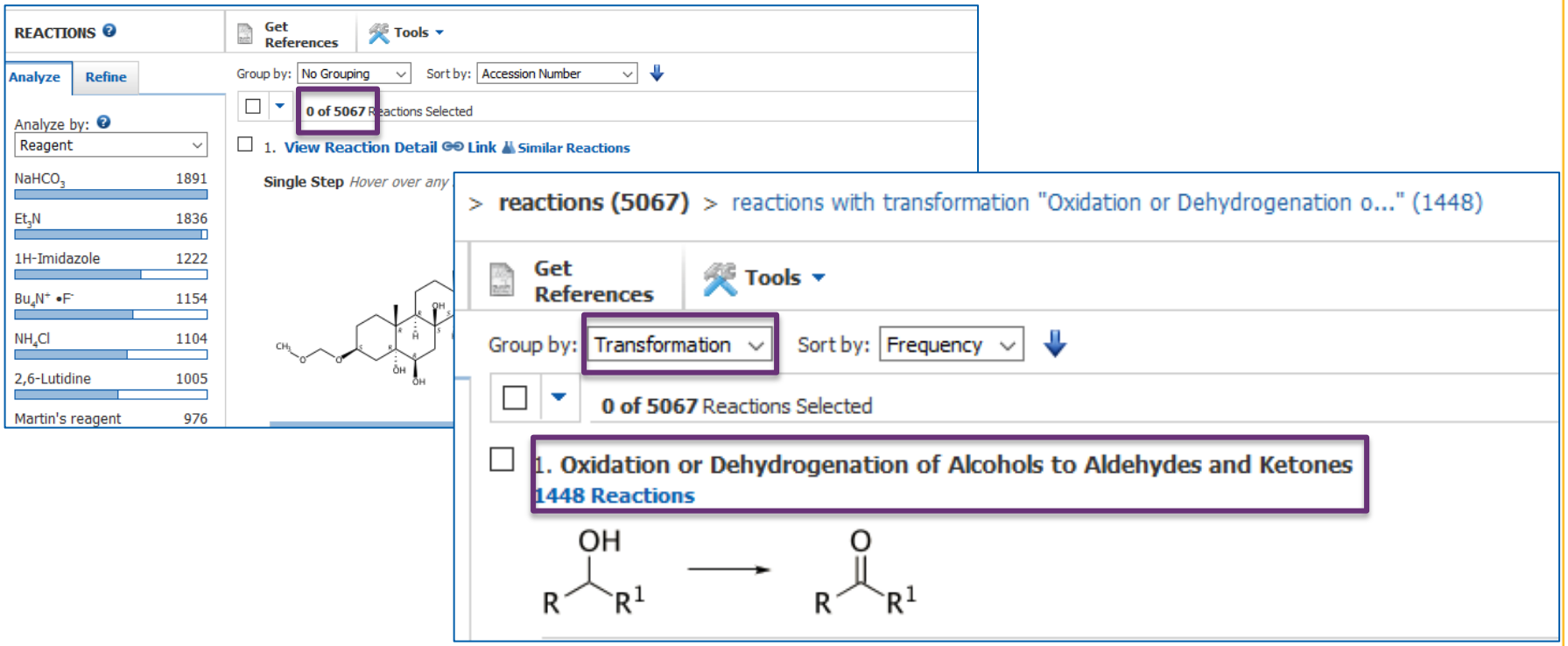

Combine Reaction Answer Sets "Intersect: Include only answer..." (16)
REACTIONS
Get References
Tools
Analyze
Refine
Group by: No Grouping
Sort by: Accession Number
Analyze by:
Reagent
AcOEt 1
Et3N 1
H2 1
NaOH 1
O2 1
t-BuOK 1
Show More
0 of 16 Reactions Selected
1. View Reaction Detail Link Similar Reactions
Single Step Hover over any structure for more options.
OH
S
~99
O
~127
+
OH
R
~104
Overview
Steps/Stages
Notes

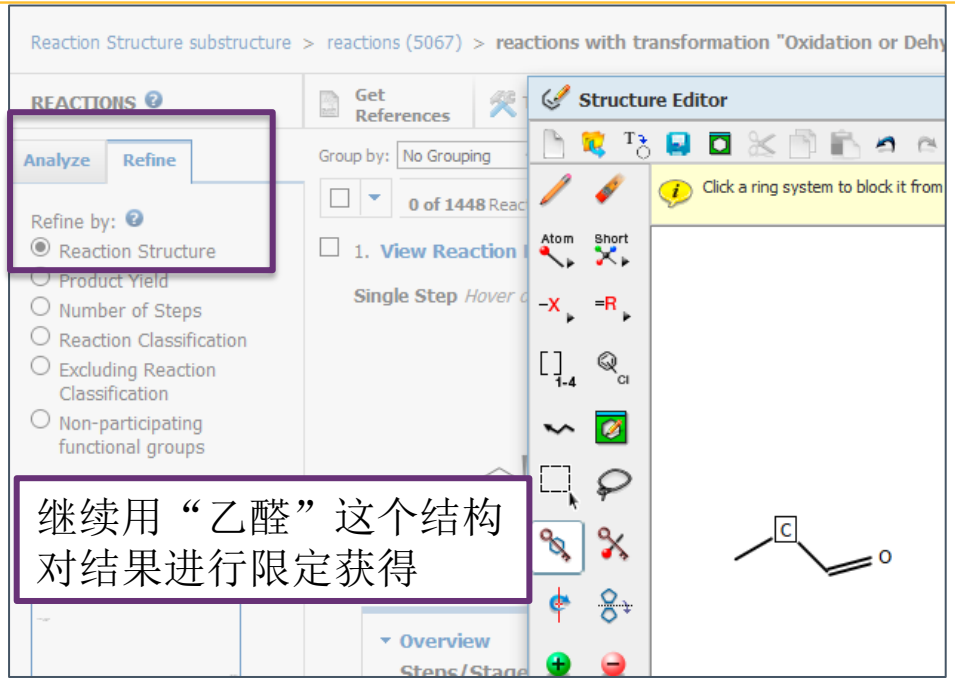
案例：在非反应仲醇存在的条件下，将伯醇转换为乙醛

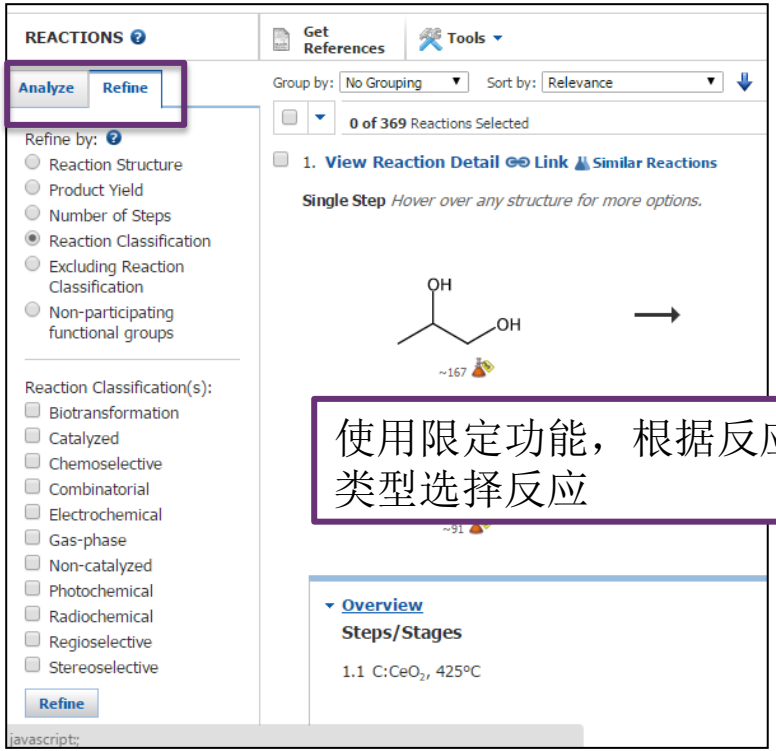


使用反应角色定义工具和官能团列表

案例：在非反应仲醇存在的条件下，将伯醇转换为乙醛




Reaction Structure substructure > reactions (5067) > reactions with transformation "Oxidation or Dehy
REACTIONS
Get References
Structure Editor
Analyze
Refine
Refine by:
Reaction Structure
Product Yield
Number of Steps
Reaction Classification
Excluding Reaction Classification
Non-participating functional groups
Group by: No Grouping
0 of 1448 Reac
1. View Reaction
Single Step Hover
Click a ring system to block it from
Atom
Short
Overview
Steps/Stage
继续用“乙醛”这个结构对结果进行限定获得

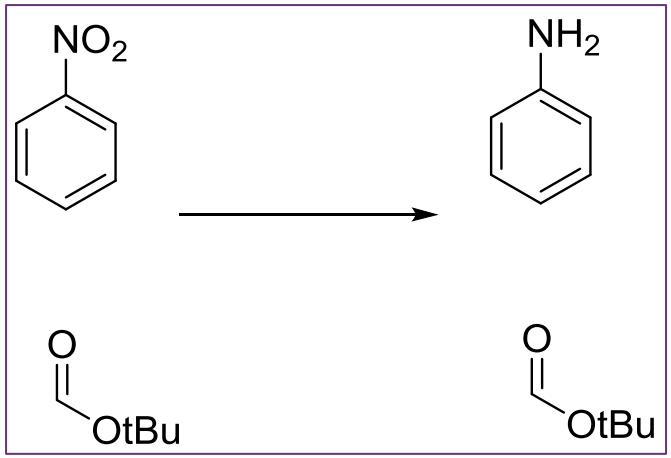

REACTIONS
Get References
Tools
Analyze
Refine
Refine by:
Reaction Structure
Product Yield
Number of Steps
Reaction Classification
Excluding Reaction Classification
Non-participating functional groups
Reaction Classification(s):
Biotransformation
Catalyzed
Chemoselective
Combinatorial
Electrochemical
Gas-phase
Non-catalyzed
Photochemical
Radiochemical
Regioselective
Stereoselective
Refine
Group by: No Grouping
Sort by: Relevance
0 of 369 Reactions Selected
1. View Reaction Detail Link Similar Reactions
Single Step Hover over any structure for more options.
OH
OH
~167
~91
Overview
Steps/Stages
1.1 C:CeO2, 425°C
javascript:;
使用限定功能，根据反应类型选择反应

提纲

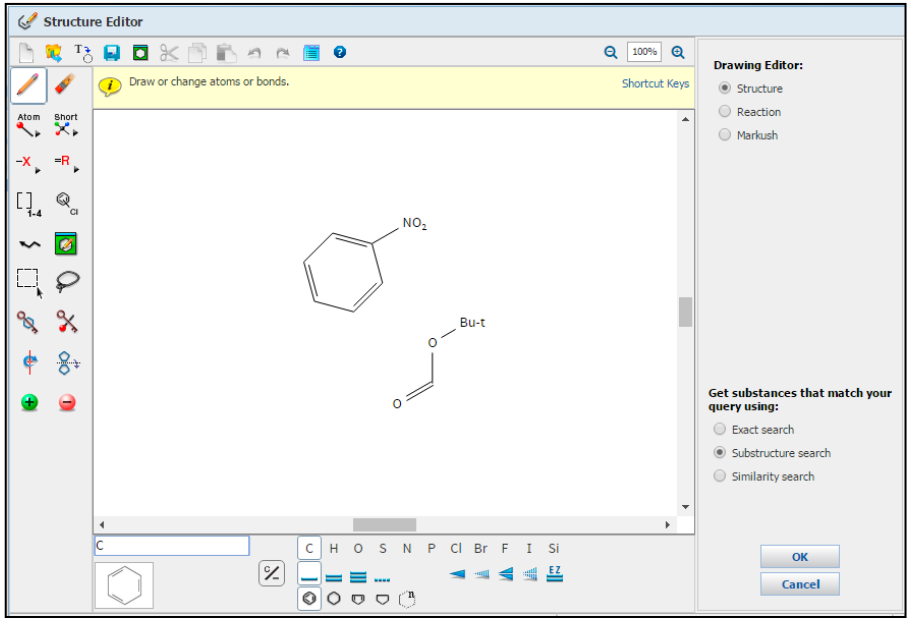
- 反应检索
  - 反应检索绘制工具及反应信息详情
  - 如何通过Analyze、Refine来精选反应
  - 亚结构反应检索
    - 手性反转反应
    - 在非反应仲醇存在的条件下，将伯醇转换为乙醛
    - 片段反应

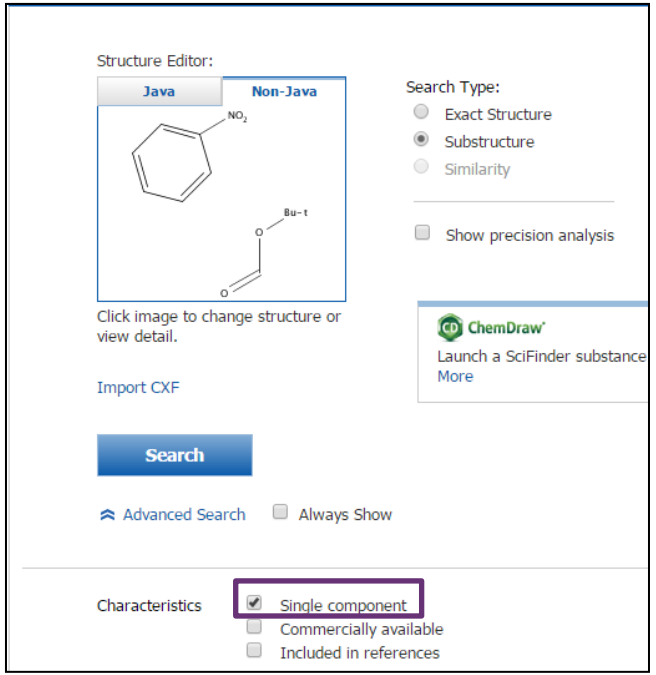
片段反应检索

- 检索要求：
  - 起始物上带有BOC基团
  - 苯环上的硝基还原为氨基
  - BOC基团不变
- 检索思路：
  - 要保证苯环和BOC基团在同一个结构上，需要从物质结构检索开始，通过物质获得反应，再对反应进行限定。

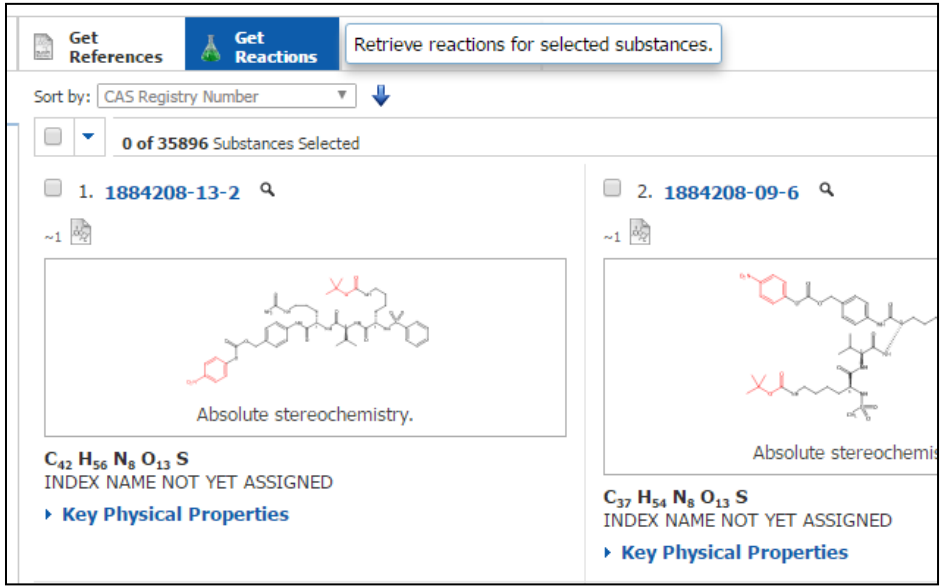


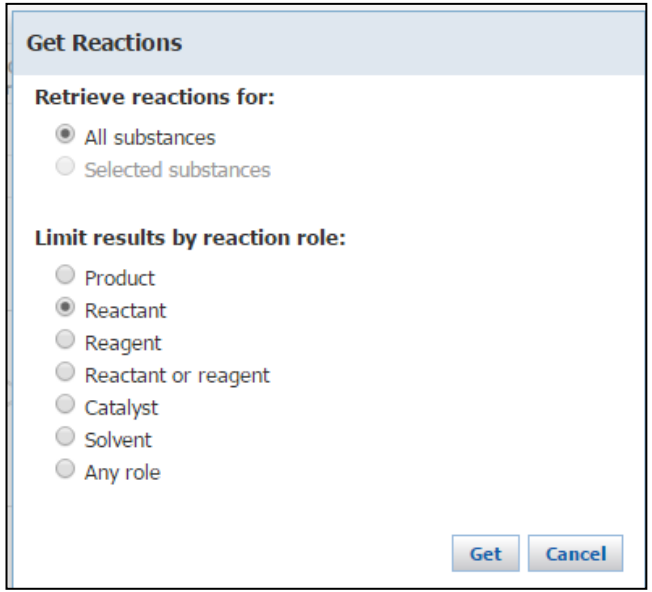
绘制片段结构，选择亚结构反应检索，并定义为单一组分



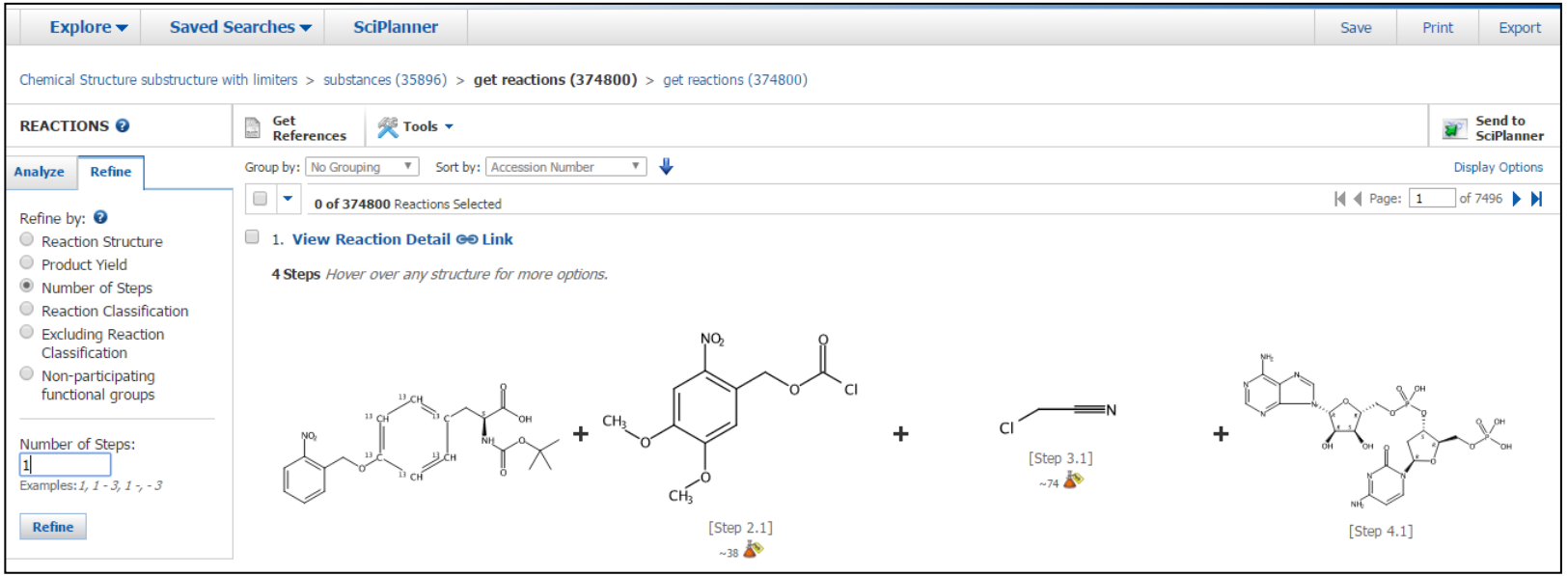


获得亚结构检索结果，并获得这些物质作为反应物的反应

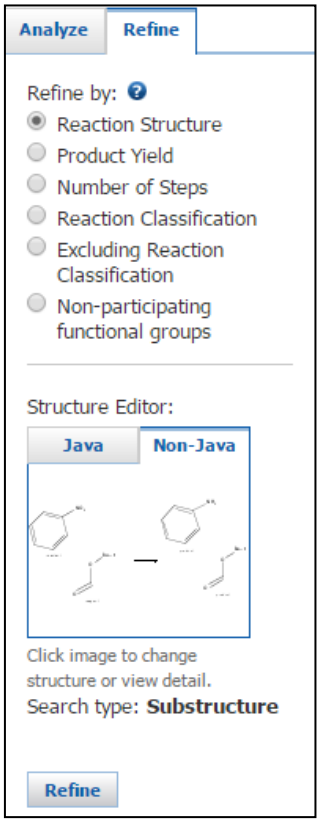


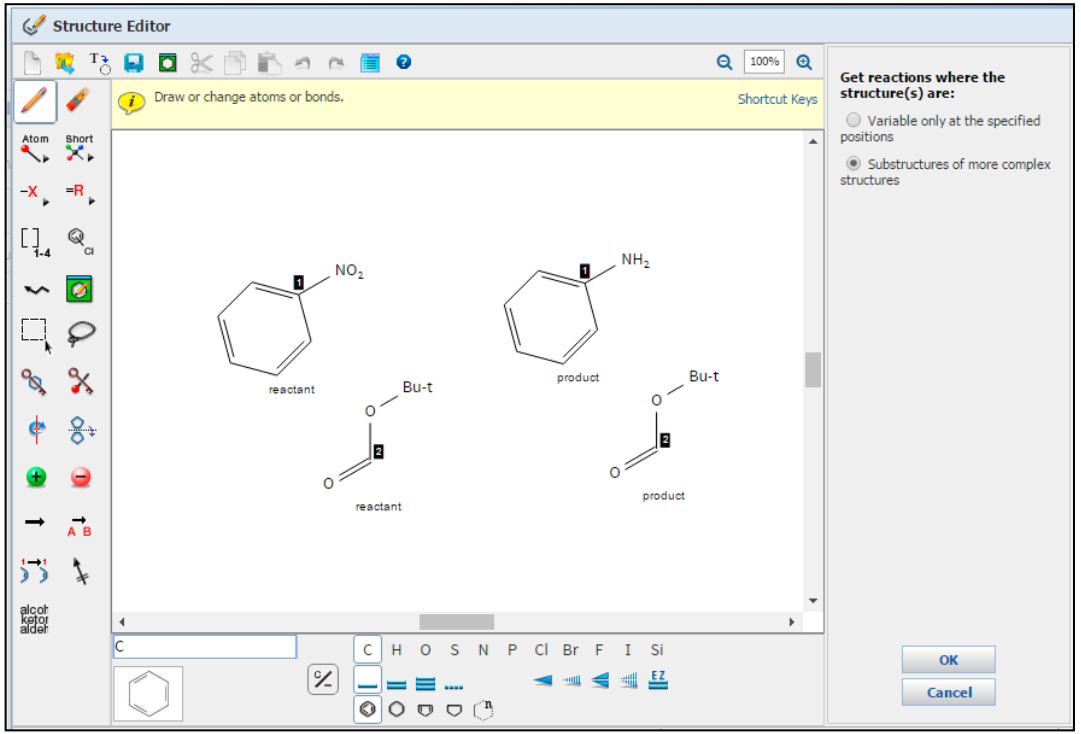


限定反应步数为一步反应

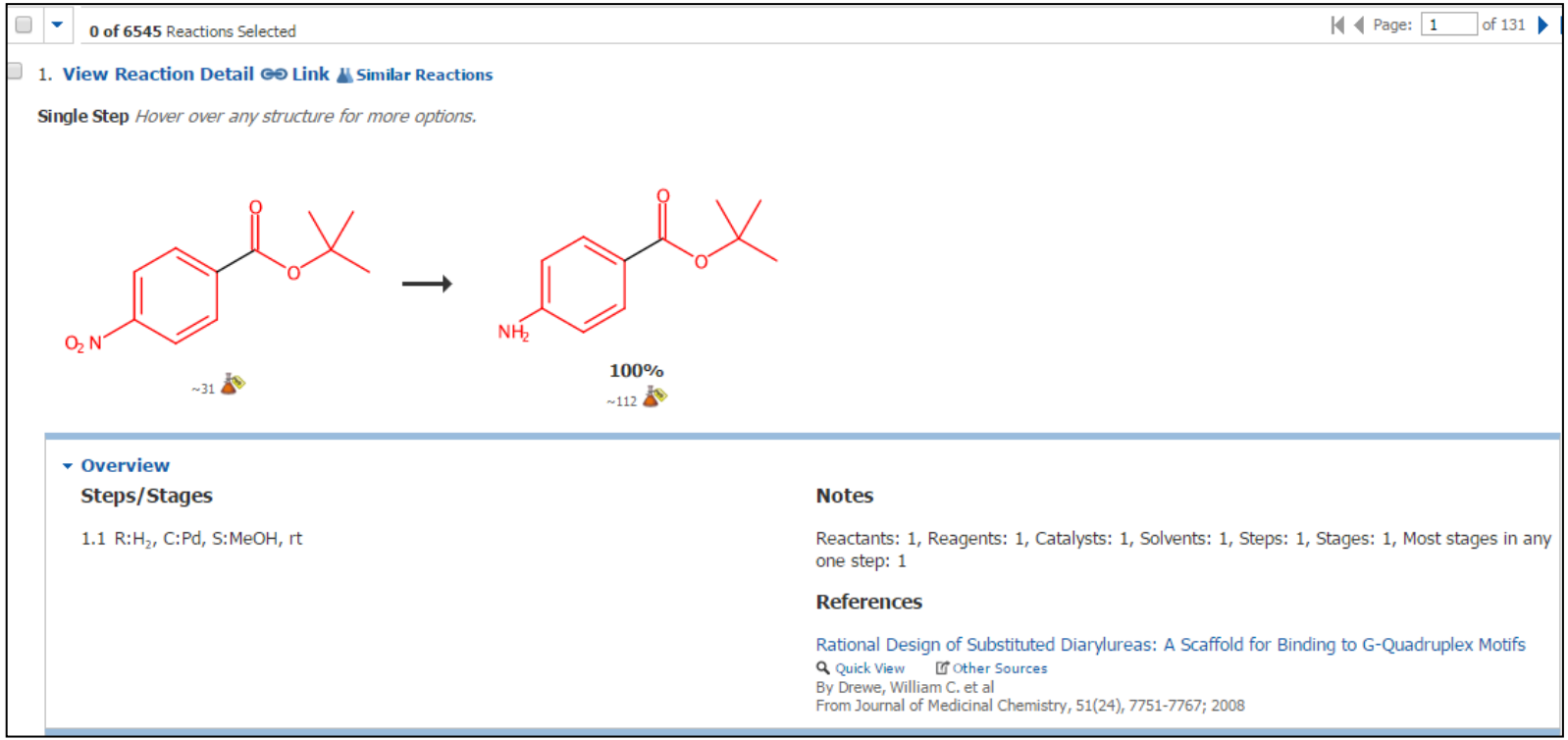


反应结构限定


Analyze
Refine
Refine by:
Reaction Structure
Product Yield
Number of Steps
Reaction Classification
Excluding Reaction Classification
Non-participating functional groups
Structure Editor:
Java
Non-Java
Click image to change structure or view detail.
Search type: Substructure
Refine


Structure Editor
Draw or change atoms or bonds.
Shortcut Keys
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
reactant
product
reactant
product
OK
Cancel

符合检索要求的反应


0 of 6545 Reactions Selected
Page: 1 of 131
1. View Reaction Detail Link Similar Reactions
Single Step Hover over any structure for more options.
O
O
O2N
~31
100%
O
O
NH2
~112
Overview
Steps/Stages
1.1 R:H2, C:Pd, S:MeOH, rt
Notes
Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1
References
Rational Design of Substituted Diarylureas: A Scaffold for Binding to G-Quadruplex Motifs
Quick View
Other Sources
By Drewe, William C. et al
From Journal of Medicinal Chemistry, 51(24), 7751-7767; 2008

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
  - 分析方法查询
- SciFinder常见问题及解决

MethodsNow Analysis 快速获得权威可靠的分析方法

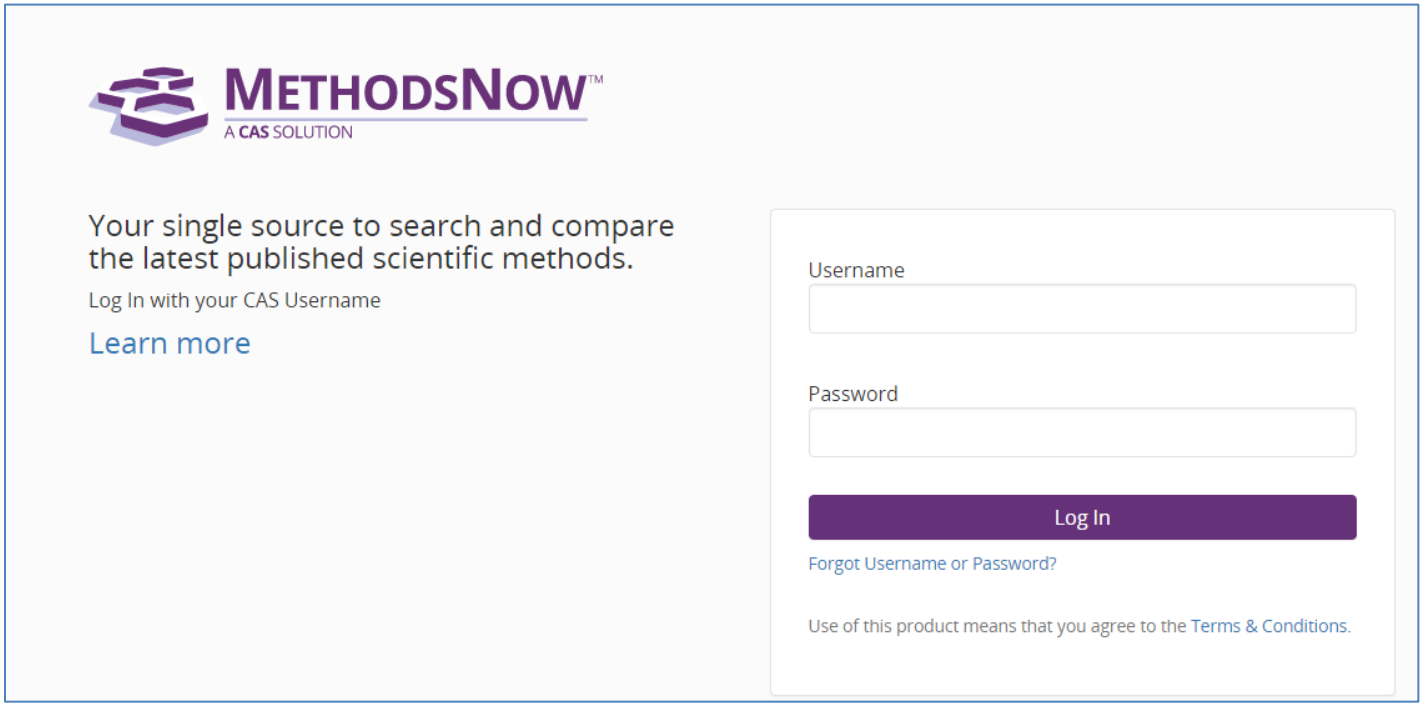
- MethodsNow Analysis 简介
- 案例：查找有关润滑油的分析方法
- 案例：查找手性分析方法

MethodsNow Analysis (www.methodsnow.com)

- **Organic Compound Analysis:** 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…
- **Organometallics / Inorganics:** 地质分析，无机物分析，金属有机化合物分析
- **Pharmacology / Toxicology:** 成瘾药物检测，有毒物检测…
- **Bioassays:** 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定…
- **Water Analysis:** 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析…
- **Historical Analysis / Dating:** 考古分析，同位素分析
- **Environmental Analysis:** 土壤/空气/水分析，农药残留分析
- **Agricultural Applications / Analysis:** 除草剂分析…
- **Food Analysis:** 脂肪酸分析，脂肪酸酯分析，蛋白质分析…
- **Fuels / Geology / Biofuels:** 生物燃料分析，油气分析，石油产品分析，煤炭加工…
- **Miscellaneous:** 化妆品分析，爆炸物分析，纳米材料分析…

目前有13个大类，45个小类。
某些子项目属于多种方法分类！

登录www.methodsnow.com网址，输入用户名和密码

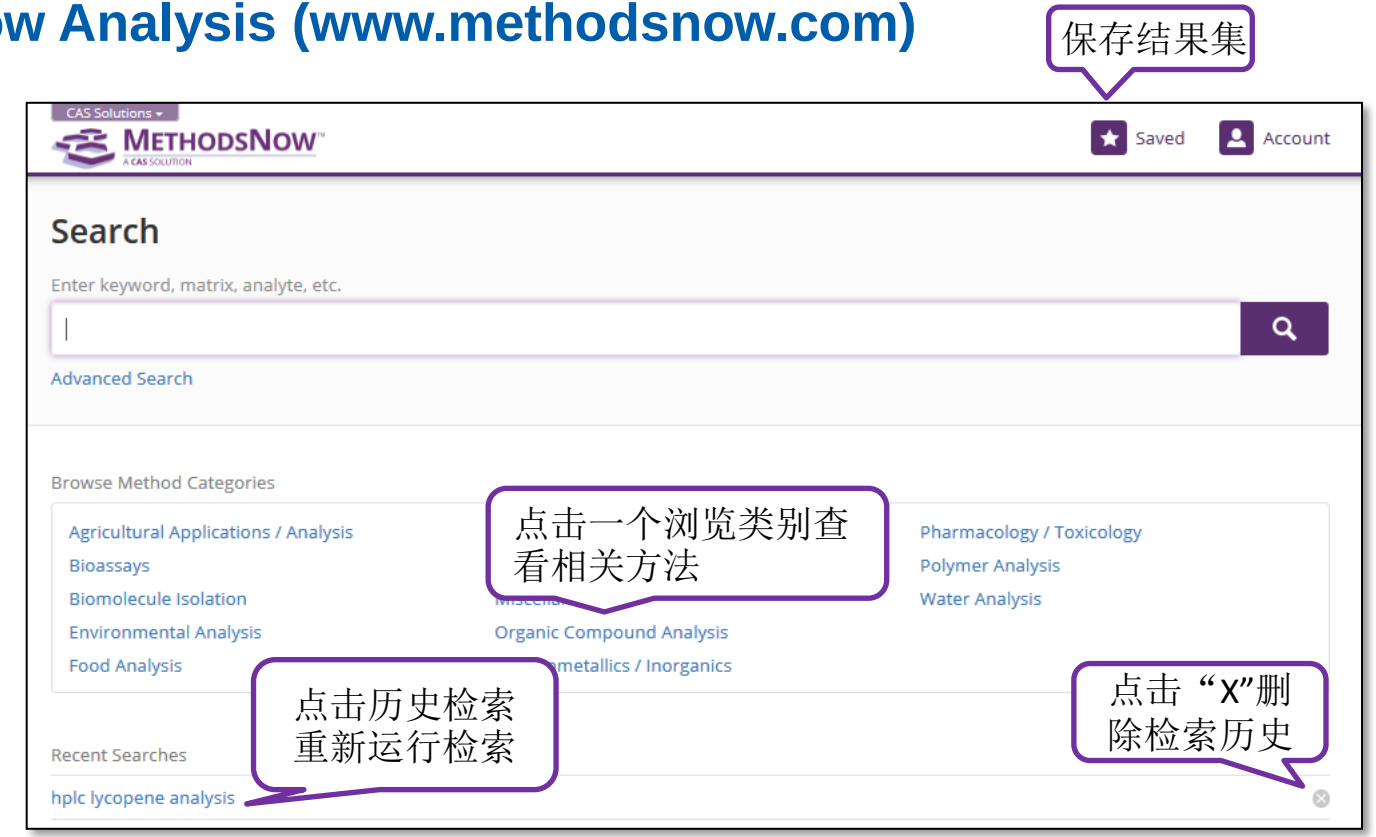


MethodsNow Analysis (www.methodsnow.com)

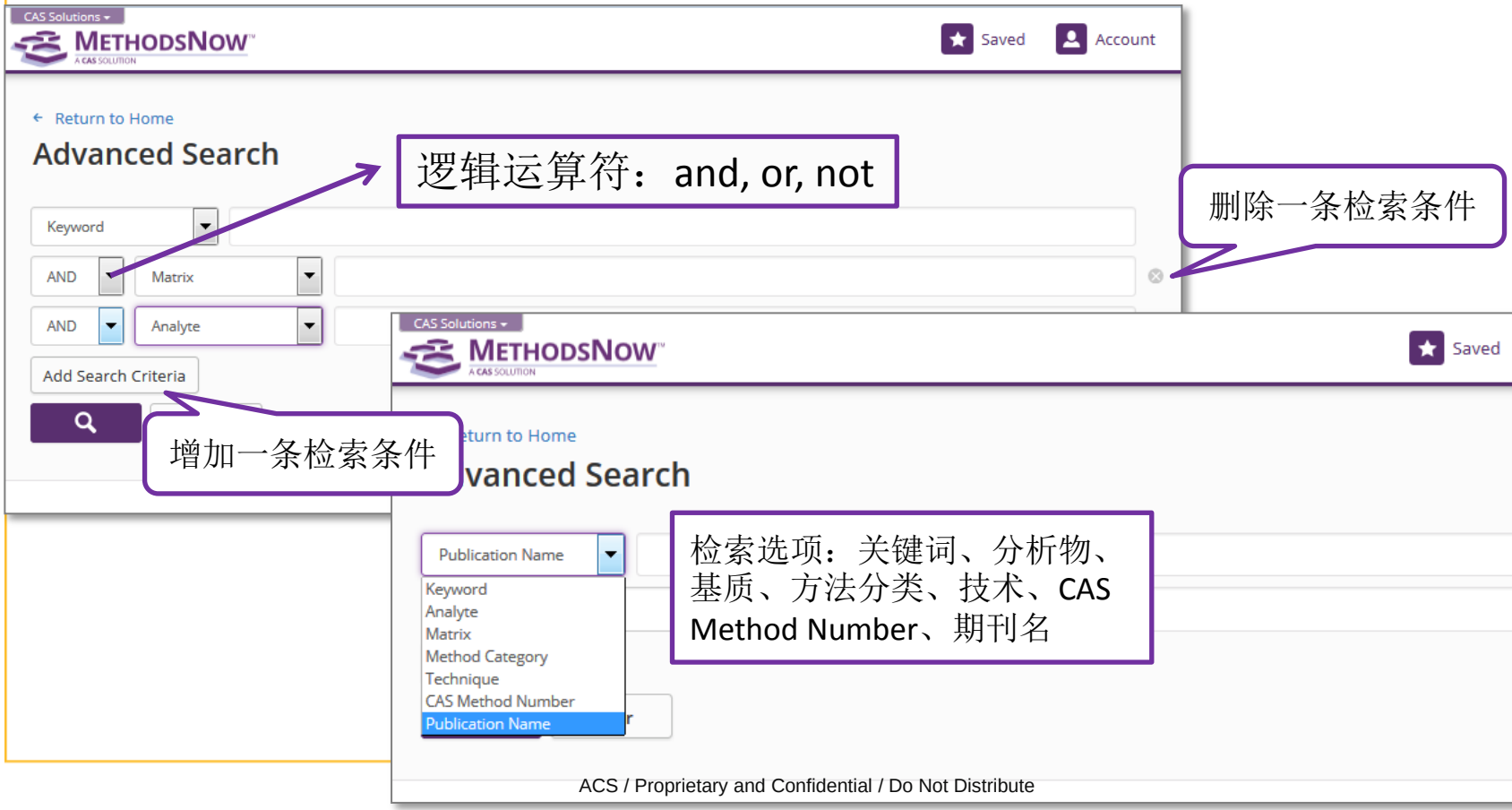
检索/高级检索

方法分类

历史检索



高级检索


CAS Solutions
METHODSNOW
A CAS SOLUTION
Saved
Account
Return to Home
Advanced Search
Keyword
AND
Matrix
AND
Analyte
Add Search Criteria
逻辑运算符：and, or, not
删除一条检索条件
增加一条检索条件
Publication Name
Keyword
Analyte
Matrix
Method Category
Technique
CAS Method Number
Publication Name
检索选项：关键词、分析物、基质、方法分类、技术、CAS Method Number、期刊名

手性化合物拆分

从浏览方法分类开始

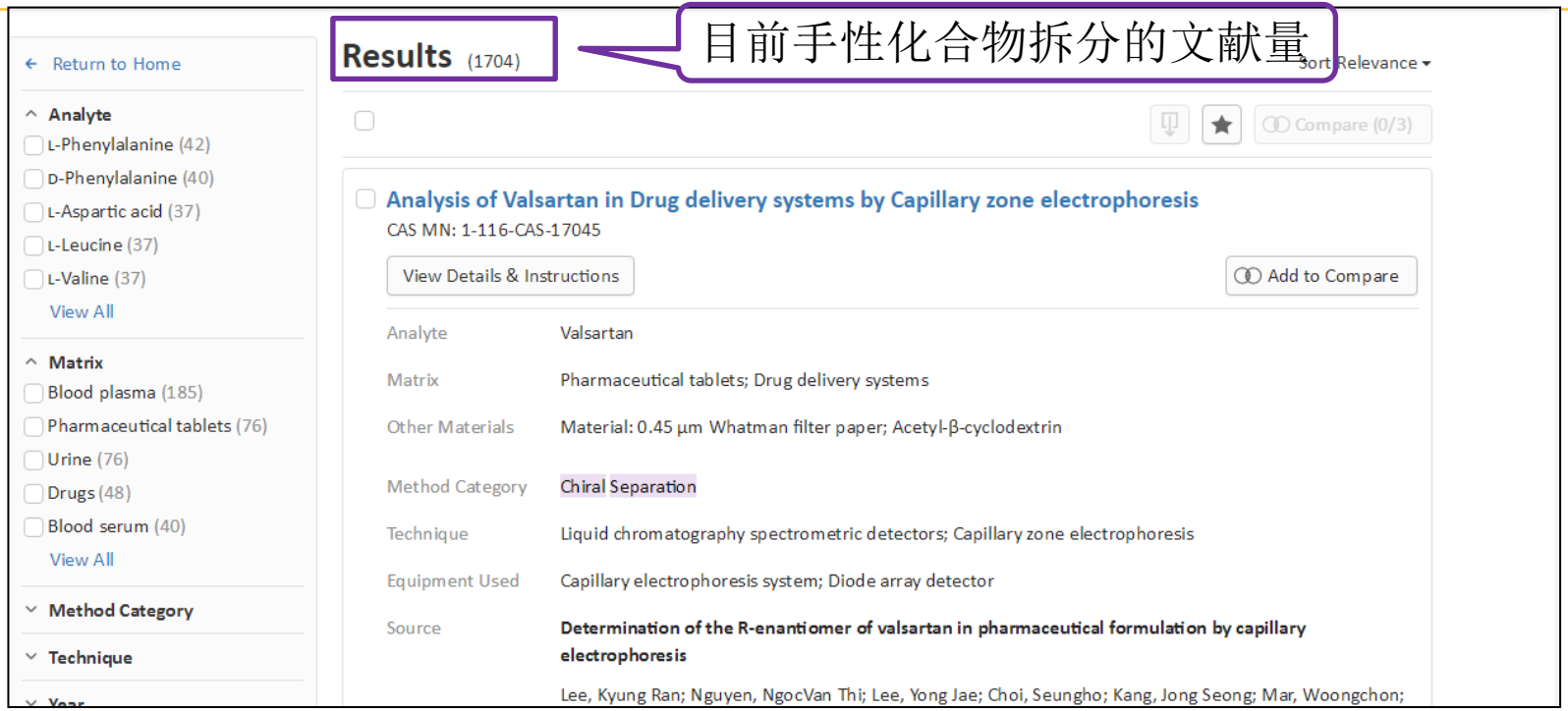
Browse Method Categories

Agricultural Applications / Analysis
Bioassays
Biomolecule Isolation
Environmental Analysis
Food Analysis
Fuels / Geology / Biofuels
Historical Analysis / Dating
Miscellaneous
Organic Compound Analysis
Organometallics / Inorganics
Pharmacology / Toxicology
Polymer Analysis
Water Analysis

Browse Method Categories > Organic Compound Analysis

Active Pharmaceutical Ingredient and Metabolite Analysis
Chiral Separation
Natural Product Isolation Analysis
Organic Compound Analysis

此处有大量手性化合物拆分方法文献


Return to Home
Analyte
L-Phenylalanine (42)
D-Phenylalanine (40)
L-Aspartic acid (37)
L-Leucine (37)
L-Valine (37)
View All
Matrix
Blood plasma (185)
Pharmaceutical tablets (76)
Urine (76)
Drugs (48)
Blood serum (40)
View All
Method Category
Technique
Year
Results (1704)
目前手性化合物拆分的文献量
Sort Relevance
Compare (0/3)
Analysis of Valsartan in Drug delivery systems by Capillary zone electrophoresis
CAS MN: 1-116-CAS-17045
View Details & Instructions
Add to Compare
Analyte Valsartan
Matrix Pharmaceutical tablets; Drug delivery systems
Other Materials Material: 0.45 µm Whatman filter paper; Acetyl-β-cyclodextrin
Method Category Chiral Separation
Technique Liquid chromatography spectrometric detectors; Capillary zone electrophoresis
Equipment Used Capillary electrophoresis system; Diode array detector
Source Determination of the R-enantiomer of valsartan in pharmaceutical formulation by capillary electrophoresis
Lee, Kyung Ran; Nguyen, NgocVan Thi; Lee, Yong Jae; Choi, Seungho; Kang, Jong Seong; Mar, Woongchon;

手性物质拆分方法详情

Analysis of (±)-Sertraline hydrochloride in Pharmaceutical tablets by HPLC

CAS MN: 1-116-CAS-52651

Method Category: Chiral Separation; Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: HPLC

手性分离和活性药物组份和代谢分析

Materials	Role	Image	CAS RN
(±)-Sertraline hydrochloride	analyte	View Structure	79617-89-3
Pharmaceutical tablets	matrix		
Chiralpak IA	material		859767-48-9
Chiracel OD - H column (5 µm particle size in (250 × 4.6) mm)	material		
Chiral AD - H column (5 µm particle size in (250 × 4.6) mm)	material		
Methanol	reagent	View Structure	67-56-1
Diethylamine	reagent	View Structure	109-89-7

手性物质拆分方法详情

Source

A validated chiral LC method for the enantiomeric separation of sertraline hydrochloride in bulk drug samples and pharmaceutical dosage forms

Radhakrishnanand, P.; Rao, D. V. Subba; Surendranath, K. V.

Analytical Chemistry: An Indian Journal (2008), 7 (7), 515 - 520. Trade Science Inc.

CODEN: ACNHAY

Document Sources

Abstract ^

A simple and new isocratic polar mode chiral HPLC method has been developed for the enantiomeric separation of sertraline hydrochloride in bulk drugs and dosage forms with an elution time of about 15 min. The separation was achieved on immobilized amylose based chiral stationary phase (Chiralpak-IA) using 0.1% diethylamine in methanol as mobile phase. The mobile phase was delivered at 0.7 mL/min^{-1} flow and the detection was monitored at 220 nm using UV detection technique. The resolution (R_s) between the sertraline and its (R,R)-enantiomer was found to be more than 4.0. The method shows 0.005 µg as limit of detection (LOD) and 0.015 µg as limit of quantification (LOQ) for (R,R)-sertraline, for 10 µL injection volume The validated method yield good results regarding precision, linearity and accuracy. The developed method shows excellent linearity (R^2 > 0.999) over a range of LOQ to 0.3% for (R,R)-sertraline. The percentage recovery of (R,R)-sertraline ranged from 98.3 to 101.8 in bulk drug samples and in pharmaceutical dosage forms. Robustness studies were also carried out on the develop method. The sertraline hydrochloride sample solution stability and mobile phase stability studies were carried out and the results were found to be satisfactory for a study period of 48 h.

Equipment Used

Liquid chromatography (LC) system, 1100 series, Agilent Technologies, Waldbronn, Germany

方法信息详情

Instructions

样品制备

Sample Preparation

1. Get the weight of twenty tablets individually and powder in mortar.
2. Transfer a sample of the powdered tablets, equivalent to 10 mg of active pharmaceutical ingredient (sertraline hydrochloride) into 100 mL volumetric flask.
3. Add about 75 mL of mobile phase and keep on a rotatory shaker for 10 min for the material to dissolve completely and sonicate for 10 min and dilute to 100 mL.
4. Centrifuge the content for 10 min at 3,000 rpm.
5. Collect the supernatant and filter using 0.45 µnylon 66-membrane filter.
6. Use the filtrate as the stock solution.

Standards Preparation

1. Prepare stock solutions of sertraline hydrochloride and (R, R)-sertraline (1000 µg mL^{-1}) individually by dissolving the appropriate amount of the substances in the mobile phase that contains a 0.1% diethylamine in methanol.
2. Prepare the working solutio ide and (R, R)-sertraline in diluent which is the mobile phase.

实验过程

Method or Procedure

1. Inject 10 µl of the sample into the Agilent 1100 series (Agilent Technologies, Waldbronn, Germany) LC system with a diode array detector (DAD).
2. Monitor the output signal using Chemstation software (Agilent) on Pentium computer (Digital Equipment Co., Hoston, USA.).
3. Use Chiralcel OD-H (cellulose tris (3,5-dimethylphenyl carbamate) coated onto silica-gel), Chiralpak AD-H (amylose tris (3,5-dimethylphenylcarbamate) coated onto silica-gel) and Chiralpak-IA (amylose tris (3,5- dimethylphenylcarbamate) immobilized onto silica- gel) as the chiral column.
4. Optimize the chromatographic conditions using a Chiralpak IA column.
5. Take 0.1% diethylamine in methanol as the mobile phase at aflow rate of 0.7 mL min^{-1}.
6. Maintain the column temperature at 25 °C and monitor the detection at 220 nm.

手性分离有效性

Validation

实验有效性数据

Limit of Detection	0.005 µg, of 100 µg mL^{-1} analyte concentration, (R, R) - sertraline
Limit of Quantitation	0.015 µg, of 100 µg mL^{-1} analyte concentration, (R, R) - sertraline
Recovery	98.3%, RSD 0.7%, 0.075 µg spiked bulk drug sample, (R, R) - sertraline (sample 1) 100.1%, RSD 0.4%, 0.150 µg spiked bulk drug sample, (R, R) - sertraline (sample 2) 101.4%, RSD 0.8%, 0.225 µg spiked bulk drug sample, (R, R) - sertraline, (sample 3) 100.8%, RSD 0.5%, 0.150 µg spiked dosage sample, (R, R) - sertraline, (sample 4) 98.5%, RSD 0.8%, 0.075 µg spiked dosage sample, (R, R) - sertraline, (sample 5) 101.8%, RSD 0.8%, 0.225 µg spiked dosage sample, (R, R) - sertraline, (sample 6)
Precision	3.0%, RSD, (R, R) - sertraline
Retention Time	6.0 min, Sertraline hydrochloride 7.0 min, (R, R) - sertraline

获取手性化合物拆分方法步骤：

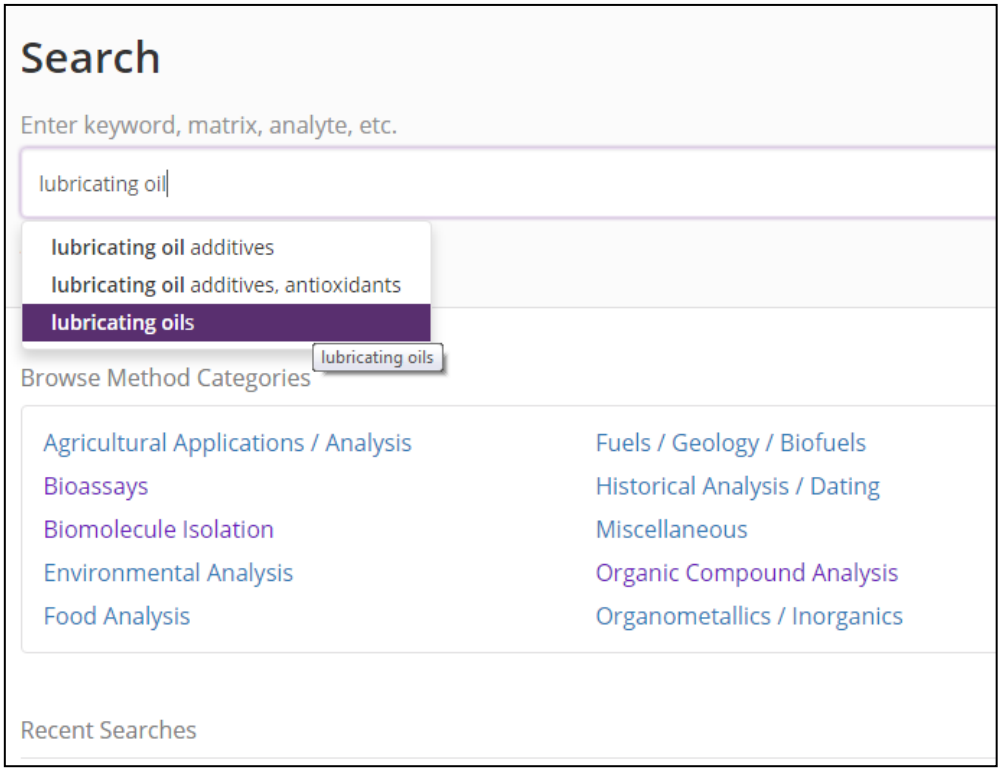
1.从方法分类列表中，选择手性拆分，获得手性拆分的全部文献

2. 根据需要，从基质、分析物、技术手段/仪器筛选项中选择目标条件进行筛选

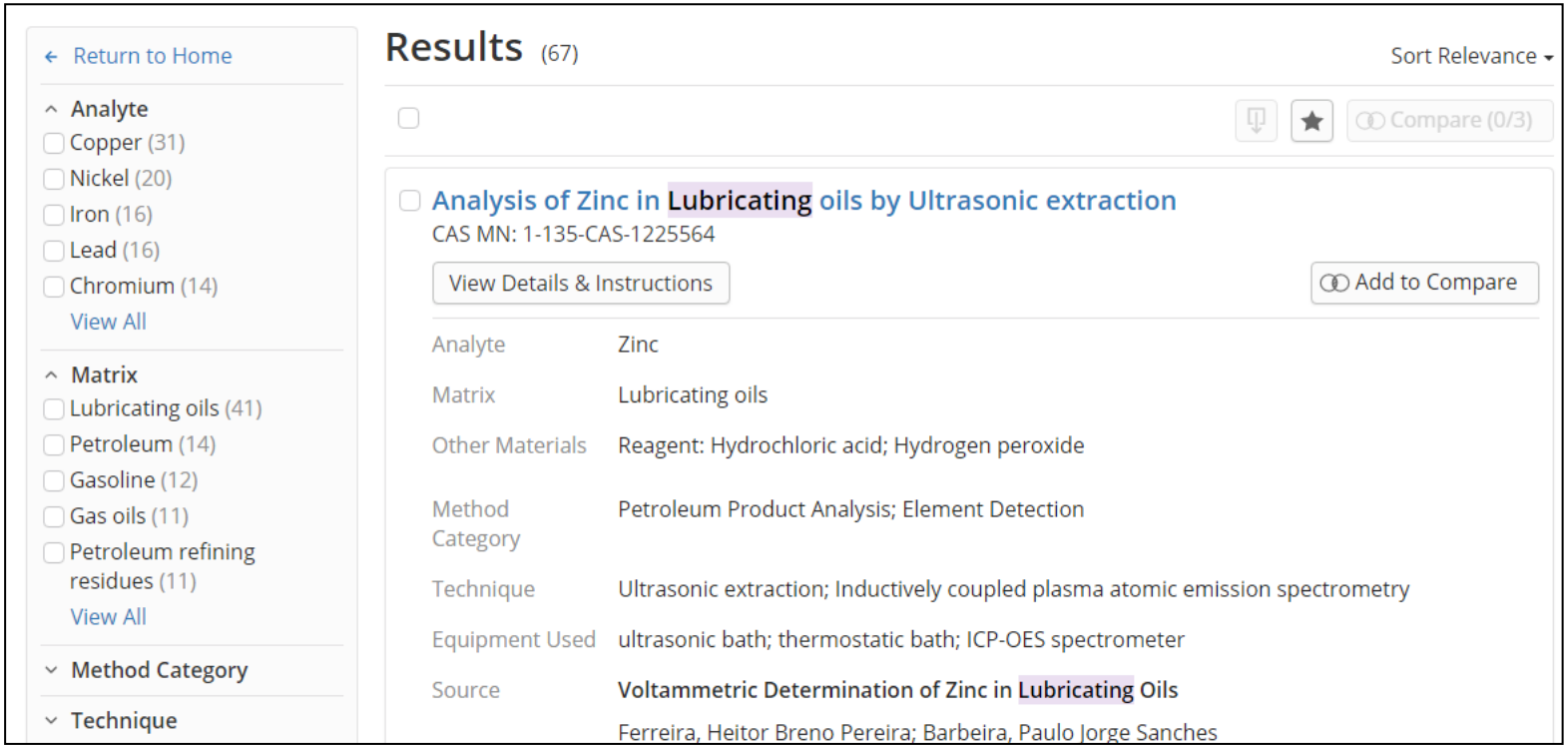
3.展开感兴趣的方法详情

4.对比感兴趣的方法

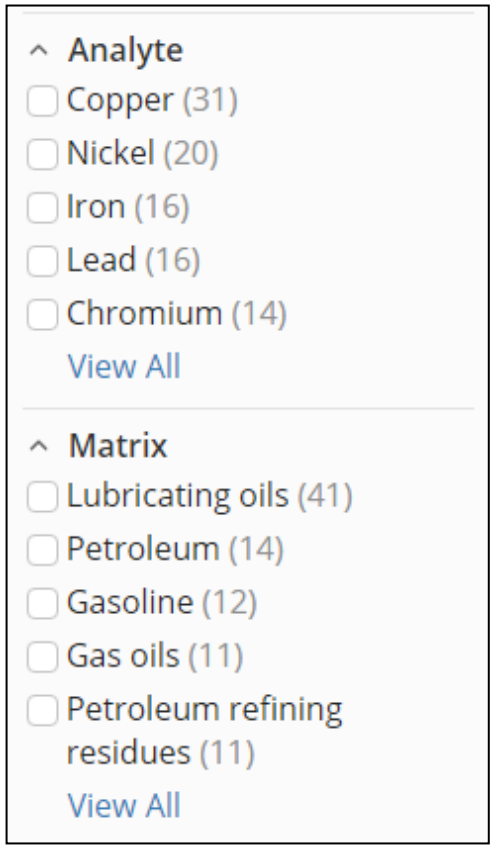
案例：获取润滑油相关的分析方法



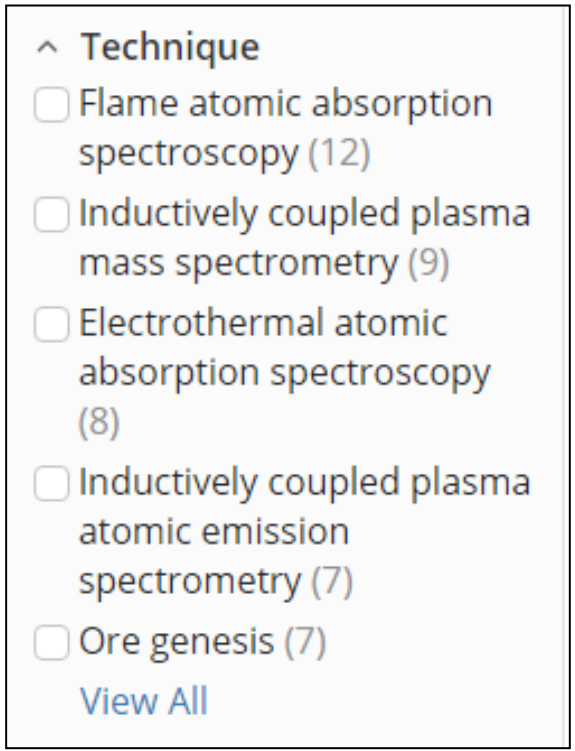
获得全部润滑油分析方法——数量持续增长中



选中分析物和基质



选中技术手段



选择感兴趣的方法，查看方法信息详情

Analysis of Zinc in Lubricating oils by Ultrasonic extraction

CAS MN: 1-119-CAS-125089

Method Category: Element Detection; Petroleum Product Analysis
Technique: Ultrasonic extraction; Flame atomic absorption spectroscopy

Materials	Role	Image	CAS RN
Zinc	analyte	View Structure	7440-66-6
Lubricating oils	matrix		
Hollow cathode lamp (HCL)	material		
Titanium ultrasound probe	material		
High density polypropylene bottles	material		
Hydrogen peroxide	reagent	View Structure	7722-84-1
Hydrochloric acid	reagent	View Structure	7647-01-0
Nitric acid	reagent	View Structure	7697-37-2

方法来源和摘要

Source

Determination of zinc in lubricating oil by flame AAS employing ultrasonic extraction

Sabio, Rafael Miguel; Oliveira, Silvana Ruella; Tognolli, Joao Olimpio; Gomes Neto, Jose Anchieta

Atomic Spectroscopy (2011), 32 (6), 240 - 245. PerkinElmer Inc.

CODEN: ASPND7 | ISSN: 01955373

Document Sources

Abstract

The determination of zinc in lubricating oils by line-source flame at. absorption spectrometry (LS-FAAS) is proposed employing an alternative sample preparation procedure based on ultrasonic wave-assisted acid extraction The chemometric optimization of the main parameters influencing the extraction provided the following conditions: 1.3 mL of HCl, 5.0 mL of H_2O_2, 120 s sonication time, 60 °C heating temperature, and 45% sonication amplitude of the ultrasound probe. Anal. curves in the 0.5 - 4.0 mg L^{-1} Zn range were consistently obtained (R = 0.9990). Com. unused lubricating oil samples were analyzed by the proposed method and by high-resolution continuum source flame AAS (HR-CS FAAS) as the comparative technique. A paired t-test showed that the results between the two techniques were in agreement at the 95% confidence level. The accuracy of the proposed method was evaluated using an alternative sample preparation method based on recovery tests. Recoveries in the 92 - 119% interval were found. The relative standard deviation was 4% and the limit of detection was 17.6 μg L^{-1}.

实验所用仪器/条件/方法步骤

Equipment Used

Flame atomic absorption spectrometer, AAnalyst 100, PerkinElmer, Shelton, CT, USA

Ultrasonic slurry sampler, USS-100, PerkinElmer

Ultrasonic processor, Vibracell VC50-1

Thermostatic water bath, TE 184, Tecnal, SP, Brazil

Conditions

Instrument

Detection wavelength: 213.9 nm; lamp current: 15 mA; fuel gas: acetylene; ratio of air-acetylene: 4:2

Instructions

Collection of the lubricating oil samples

1. Collect the lubricating oil samples.
2. Subject to the extraction procedure.

Preparation of standard solutions

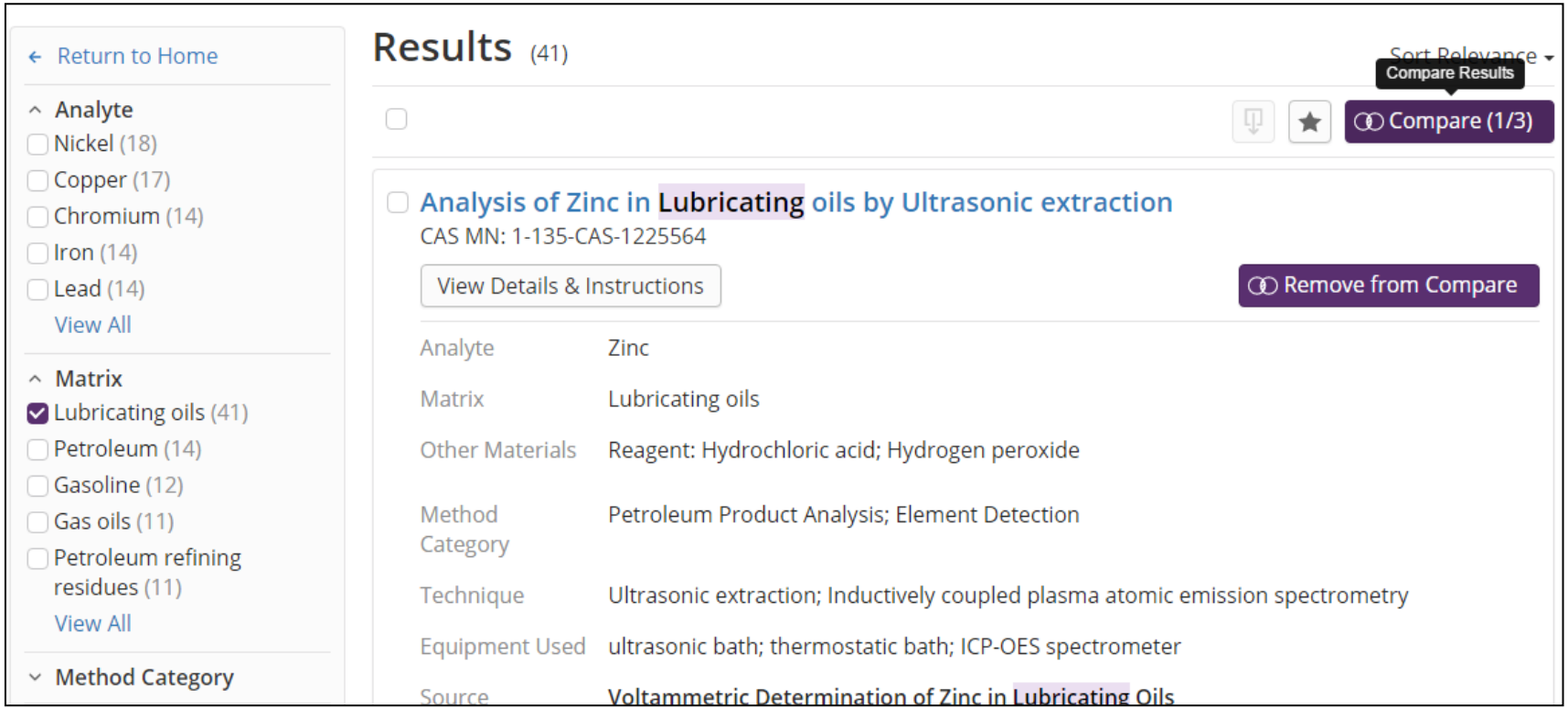
1. Prepare the analytical solutions containing 0.0, 0.5, 1.0, 2.0, 3 0 and 4.0 mg/L Zn daily by appropriate dilutions of the 1000 mg/L stock standard solution and acidify with 1% (v/v) HNO_3.
2. Store in high density polypropylene bottles.

结果有效性数据

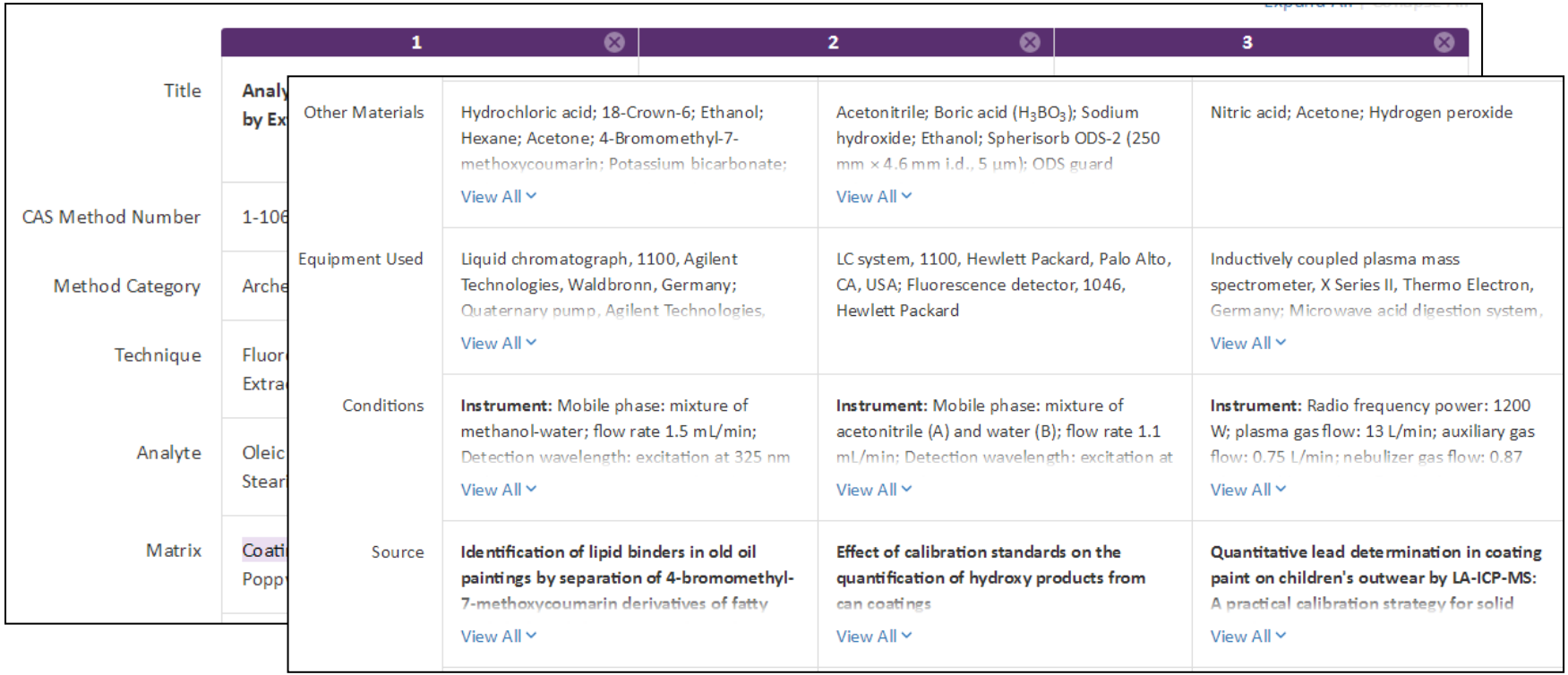
Validation

Limit of Detection	17.6 µg/L
Recovery	92 - 119%
Precision	4% (RSD)
Concentration	0.881 ± 0.034 g/kg (sample data)

MethodsNow Analysis是唯一一个可以对分析方法进行对比的数据库



方法对比



	1	2	3
Title	Analy by Ex		
CAS Method Number	1-106		
Method Category	Arche		
Technique	Fluor Extra		
Analyte	Oleic Stear		
Matrix	Coati Popp		
Other Materials	Hydrochloric acid; 18-Crown-6; Ethanol; Hexane; Acetone; 4-Bromomethyl-7-methoxycoumarin; Potassium bicarbonate; View All	Acetonitrile; Boric acid (H_3BO_3); Sodium hydroxide; Ethanol; Spherisorb ODS-2 (250 mm × 4.6 mm i.d., 5 µm); ODS guard View All	Nitric acid; Acetone; Hydrogen peroxide
Equipment Used	Liquid chromatograph, 1100, Agilent Technologies, Waldbronn, Germany; Quaternary pump, Agilent Technologies, View All	LC system, 1100, Hewlett Packard, Palo Alto, CA, USA; Fluorescence detector, 1046, Hewlett Packard	Inductively coupled plasma mass spectrometer, X Series II, Thermo Electron, Germany; Microwave acid digestion system, View All
Conditions	**Instrument:** Mobile phase: mixture of methanol-water; flow rate 1.5 mL/min; Detection wavelength: excitation at 325 nm View All	**Instrument:** Mobile phase: mixture of acetonitrile (A) and water (B); flow rate 1.1 mL/min; Detection wavelength: excitation at View All	**Instrument:** Radio frequency power: 1200 W; plasma gas flow: 13 L/min; auxiliary gas flow: 0.75 L/min; nebulizer gas flow: 0.87 View All
Source	**Identification of lipid binders in old oil paintings by separation of 4-bromomethyl-7-methoxycoumarin derivatives of fatty** View All	**Effect of calibration standards on the quantification of hydroxy products from** can coatings View All	**Quantitative lead determination in coating paint on children's outwear by LA-ICP-MS:** A practical calibration strategy for solid View All

所有方法详情都可以进行对比

Method	Extraction and derivatization 1. Place solid parts scalpered from the View All	Determination of BADGE-2H$_2$O and BFDGE-2H$_2$O by LC-FLD 1. Perform the analysis on a LC system View All	Microwave-assisted acid digestion 1. Prepare the calibration curve in 2% HNO$_3$ by incremental amount as 0 View All
Linearity Range	1.0 × 10^{-7} to 1.8 × 10^{-4} mmol for all analytes		0 - 150 ng/mL
Limit of Detection	6.0 × 10^{-8} mmol for all analytes		0.002 ng/mL
Recovery	70 ± 10% for 100 µL (poppy seed oil), myri seed		101.3% (EC681k (polyethylene)), 95.3%
Retention Time	10.8 min, min View		
Concentration		0.884 ± 0.003 µg/mL, BADGE 2H$_2$O, 0.966 ± 0.004 µg/mL, BFDGE 2H$_2$O	1539.9 mg/kg (sample data)
Limit of Quantitation			0.005 ng/mL
Accuracy			<3.37% (Bias)
Precision			<4.67% (RSD)

MethodsNow:

- 易于整合到工作流程中
- 快速对比分析方法
- 节省检索及直接获取具体方法的时间——无需通过全文查找方法详情
- 易于阅读的表格形式展示实验详情
- 包括材料、仪器、数据有效性、实验条件及其他更多信息

谢谢关注！

美国化学文摘社北京代表处
电话：010-62508026/7
电子邮箱：china@acsi.info
中文网站：http://www.cas-china.org/
英文网站：http://www.cas.org/

CAS
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY