

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



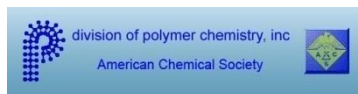
arXiv.org

Aldrichimica ACTA

ACS  
chemical  
biology



BEILSTEIN JOURNAL  
OF ORGANIC CHEMISTRY



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

ACS Chemical  
Neuroscience

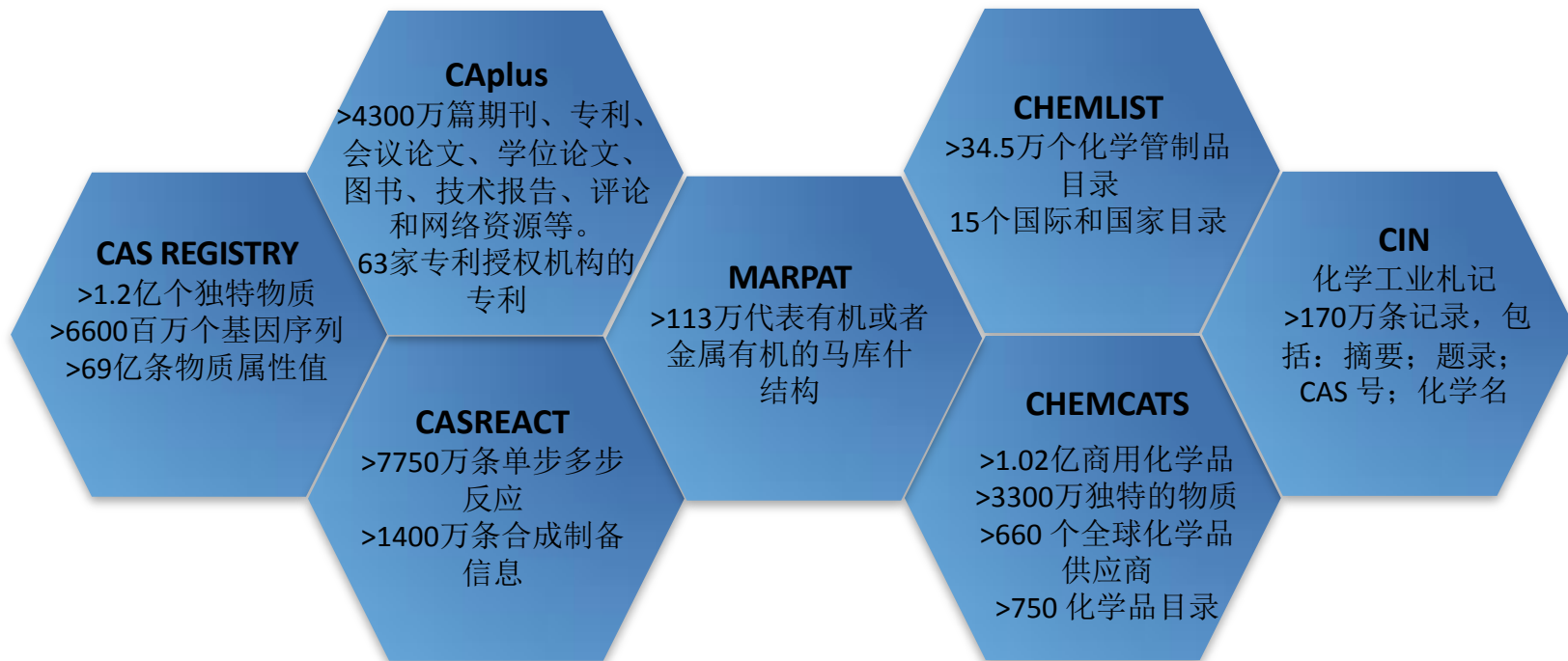


THE JOURNAL OF  
PHYSICAL CHEMISTRY  
Letters



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

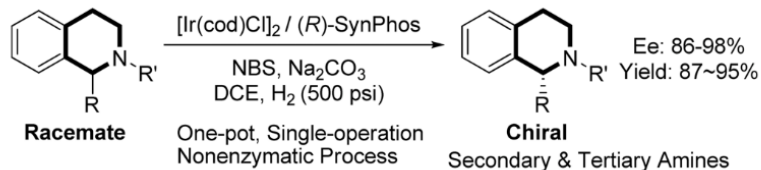
- **生物化学：**
  - 农化产品管控信息,生化遗传学,发酵,免疫化学,药理学
- **有机化学各领域：**
  - 氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇
- **大分子化学各领域：**
  - 纤维素、木质素、造纸;涂料、墨水
  - 染料、有机颜料 ;合成橡胶 ;纺织品、纤维
- **应用化学各领域：**
  - 大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金
- **物理、无机、分析化学各领域：**
  - 表面化学,催化剂,相平衡,核现象,电化学

# 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-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  
CAN15:233236

### 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/>



## Sign In

Username

Password

Remember me  
(Do not use on a shared computer)

Sign In

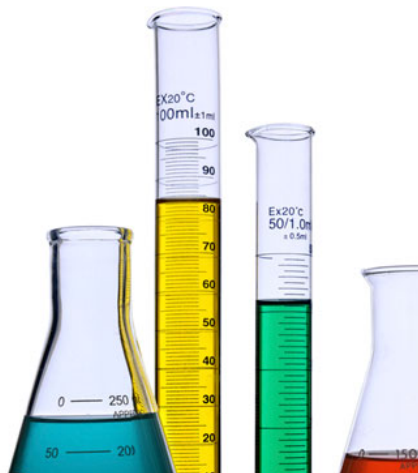
[Forgot Username or Password?](#)

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

## New to SciFinder?

[Learn more about gaining access to SciFinder.](#)

输入SciFinder账号和密码



## News & Updates

### Welcome to SciFinder

#### Did you notice our new look?

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

#### Apply for the 2016 SciFinder Future Leaders Program!

Build your career, help shape the future of research information and attend one of the most respected scientific meetings in the world. Apply for the 2016 SciFinder Future Leaders program by April 10!

#### A New Way to Explore Synthetic Preparations in SciFinder!



CAS<sup>®</sup>

A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

# SciFinder主界面

检索完，请点击退出

CAS Solutions



工具栏

Preferences | SciFinder Help

Sign Out

Welcome Cyrene Qian

Explore

Saved Searches

SciPlanner

## REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

## SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

## REACTIONS

- Reaction Structure

## REFERENCES: RESEARCH TOPIC

Examples:

The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

Search

Advanced Search

已保存的结果集

## SAVED ANSWER SETS

- S2
- S1
- importment MNS
- for jwkyb
- for jwkyb
- for vwusq
- lung cancer
- methodsnow
- pincer2
- pincer crystal
- Autosaved Reference Set

View All | Import

检索入口

定题追踪

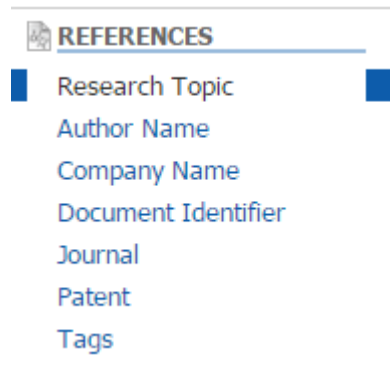
## KEEP ME POSTED

- C-N bond activation
- Mar 12, 2016(1)
- Mar 05, 2016(2)
- Feb 27, 2016(2)

12

# SciFinder检索——文献检索

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



# 文献检索——主题: Suzuki催化反应

- 检索式: Suzuki reaction with catalyst

The screenshot displays the CAS SciFinder search interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. On the left side, there is a sidebar menu with three main categories: 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. Under 'REFERENCES', options include Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', options include Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. Under 'REACTIONS', the option is Reaction Structure. The main search area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field containing the text 'Suzuki reaction with catalyst'. Below the input field, there are 'Examples:' listed as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the search area, there is a link for 'Advanced Search'.

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

Advanced Search  Always Show

Publication Years   
Examples: 1995, 1995-1999, 1995-, -1995

Document Types

<input type="checkbox"/> Biography	<input type="checkbox"/> Historical
<input type="checkbox"/> Book	<input type="checkbox"/> Journal
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Letter
<input type="checkbox"/> Commentary	<input type="checkbox"/> Patent
<input type="checkbox"/> Conference	<input type="checkbox"/> Preprint
<input type="checkbox"/> Dissertation	<input type="checkbox"/> Report
<input type="checkbox"/> Editorial	<input type="checkbox"/> Review

Languages

<input type="checkbox"/> Chinese	<input type="checkbox"/> Japanese
<input type="checkbox"/> English	<input type="checkbox"/> Polish
<input type="checkbox"/> French	<input type="checkbox"/> Russian
<input type="checkbox"/> German	<input type="checkbox"/> Spanish
<input type="checkbox"/> Italian	

Author

Last Name *	First	Middle
<input type="text"/>	<input type="text"/>	<input type="text"/>

Company   
Examples:  
Minnesota Mining and Manufacturing  
DuPont

## 主题检索的候选项

### 1 of 5 Research Topic Candidates Selected

- 85 references were found containing "Suzuki reaction with catalyst " as entered.
- 8603 references were found containing the two concepts "Suzuki reaction" and "catalyst" closely associated with one another.
- 10489 references were found where the two concepts "Suzuki reaction" and "catalyst" were present anywhere in the reference
- 18337 references were found containing the concept "Suzuki reaction".
- 2563534 references were found containing the concept "catalyst".

[Get References](#)

“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

检索结果处理工具

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

Sort by:

0 of 7906 References Selected

Page: 1 of 80

1. **Highly efficient palladium(II) hydrazones as catalysts for Suzuki-Miyaura coupling reaction in aqueous medium**

Quick View Other Sources

By Muthumari, Subramanian, Kamesh, 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  $[PdCl(PPh_3)_2(L)]$  (where HL = thiophene) incorporating  $PPh_3$  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- $\beta$ -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- $\beta$ -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- $\beta$ -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-Jiu; 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

The screenshot displays a web interface for searching and analyzing chemical literature. At the top, there are navigation buttons: 'Get Substances', 'Get Reactions', 'Get Related Citations', 'View Only CHEMZENT', and 'Tools'. Below these, a 'Sort by:' dropdown menu is open, showing five options: 'Accession Number', 'Author Name', 'Citing References', 'Publication Year', and 'Title'. The 'Citing References' option is highlighted in blue. To the left of the main results area, there is a sidebar with 'Analyze by:' options, including 'Author Name', 'Accession Number', 'Author Name', 'Citing References', 'Publication Year', and 'Title'. The main results area shows two entries, each with a checkbox, a search icon, and a title. The first entry is titled 'Palladium(II) hydrazone based catalysts for the Suzuki coupling reaction' and the second is 'Highly Water-dispersible Magnetite Nanoparticles Supported-Palladium-β-Cyclodextrin'. Each entry includes the authors' names and a brief abstract snippet.

Author	Count
Zhou Mingjie	146
Wang Ping	114
Zhang Zhenhua	81
Molander Gary A	54
Liu Chun	48
Langer Peter	43
Zhang Juanjuan	42

Sort by: Accession Number  
Accession Number  
Author Name  
Citing References  
Publication Year  
Title

Analyze by: Author Name

1. **Palladium(II) hydrazone based catalysts for the Suzuki coupling reaction**  
By Muthumari, Subramanian; Ramesh, Rengan  
From RSC Advances (2016), Ahead of Print. | Language: English, Database: CAPLUS

2. **Highly Water-dispersible Magnetite Nanoparticles Supported-Palladium-β-Cyclodextrin**  
By Kaboudin, B.; Salemi, Hadi; Kazemi, Foad; Yokomatsu, Tsutomu  
From RSC Advances (2016), Ahead of Print. | Language: English, Database: CAPLUS

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

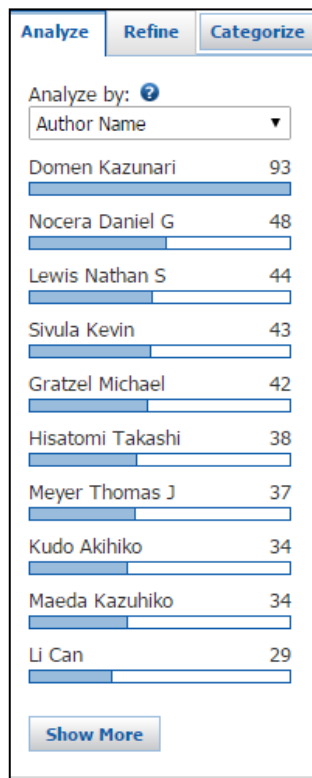
## 12种文献分析选项

Analyze Refine Categorize

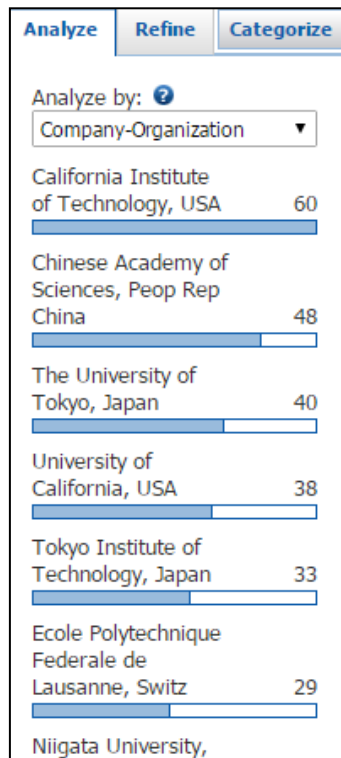
Analyze by: ?

- Author Name
- CAS Registry Number
- CA Section Title
- Company-Organization
- Database
- Document Type
- Index Term
- CA Concept Heading
- Journal Name
- Language
- Publication Year
- Supplementary Terms

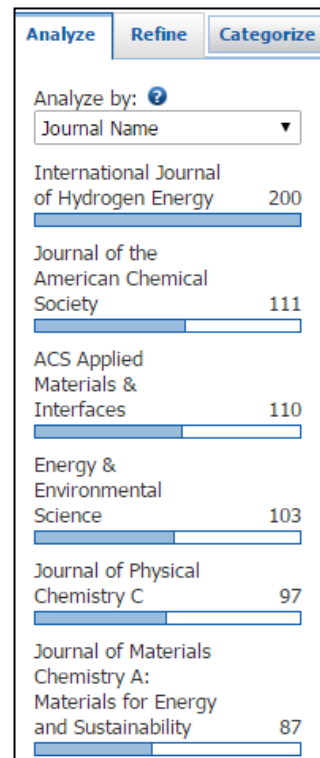
## 主要研究人员



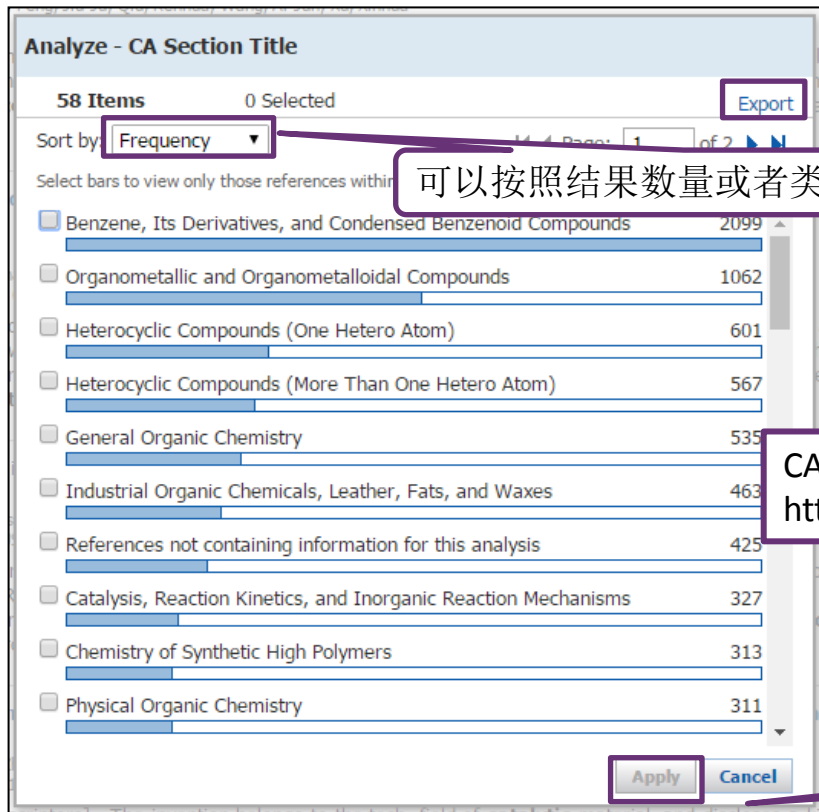
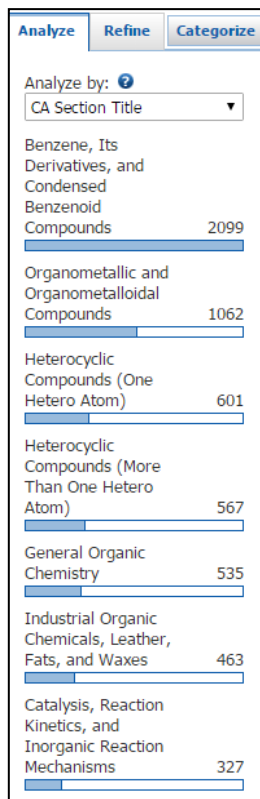
## 主要研究机构, 合作伙伴, 竞争对手



## 主要发表期刊



# 文献检索结果: Analyze



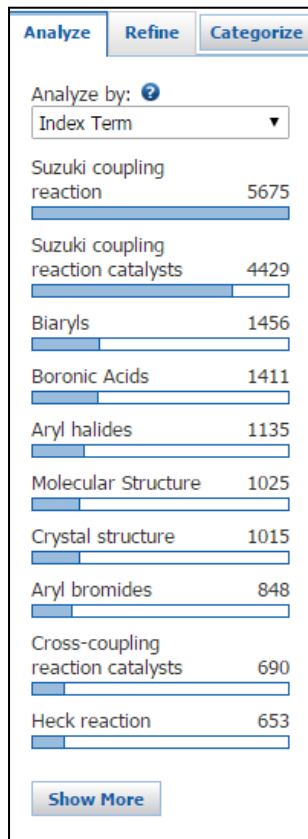
可以将分析结果导出xls文件

可以按照结果数量或者类别字母顺序排序

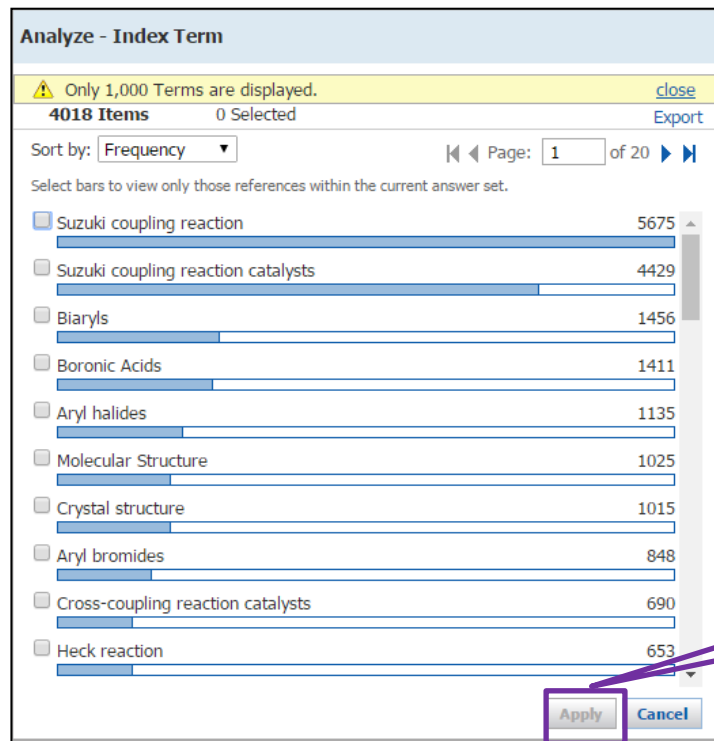
CAS把收录的信息分为5个大类80个小类:  
<http://www.cas.org/content/ca-sections>

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

Research Topic "Suzuki reaction with catalyst" > references (7906)

REFERENCES

Analyze **Refine** Categorize

Sort by: Accession Number

0 of 7906 References Selected

Refine by:

- Research Topic
- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic

1. **Highly efficient palladium(II) hydrazone based catalysts for the Suzuki coupling reaction in aqueous media**  
   
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)hydrazone complexes of the general formula...  
incorporating...  
means...  
coordin...

2. **Highly Water-dispersible Magnetite Nanoparticles Supported-Palladium- $\beta$ -Cyclodextrin as Efficient Catalyst**  
   
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- $\beta$ -sonogashira carbon-carbon **coupling reactions**. Magnetite nanoparticles supported **catalyst** was characterized. The **catalyst** displayed excellent activity for wide range of substrates in aq. soln. under mild **reaction** conditions. The **nanocatalyst** was successfully examined 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**

在结果中筛选主题带有“nanoparticles”的文献

# 文献检索结果: Refine

Analyze Refine Categorize Sort by: Accession Number ↓

0 of 7906 References Selected

Refine by:

- Research Topic
- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Preprint
- Report
- Review

Refine

1. **Highly efficient palladium(II) hydrazone based catalysts for the Suzuki coupling 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(PPH<sub>3</sub>)(L)] (where HL = thiophene aldehyde benzhydrazones) incorporating PPH<sub>3</sub> 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. **Cu Nanowires Catalyst through a simple wet-chemical strategy for ligand-free Suzuki cross coupling reaction**  
Quick View Other Sources  
By Jiu, Renhua; Wang, Ai-Jun; Xu, Xinhua  
From RSC Advances (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 **catalytic** activity.

4. **Pd immobilized on modified magnetic Fe<sub>3</sub>O<sub>4</sub> nanoparticles: Magnetically recoverable and reusable Pd nanocatalyst for Suzuki-Miyaura coupling reactions and Ullmann-type N-arylation of indoles**

在结果中筛选综述文献



CAS<sup>®</sup>

A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

# 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

**Categorize**

1. Select a heading and category.

Category Heading	Category
All	Catalysts (10816)
General chemistry	Catalysis (245)
Synthetic chemistry	
<b>Catalysis</b>	
Physical chemistry	
Technology	
Biotechnology	
Polymer chemistry	
Genetics & protein chemistry	
Environmental chemistry	
Biology	
Analytical chemistry	

2. Select index terms of interest.

Page: 1 of 109

Select All Deselect All

- Palladium dichloride
- Transition metal complexes
- Triphenylphosphine
- Silica
- Ligands
- Phosphines
- PdCl2(dppf)
- 2-Dicyclohexylphosphino-2',6'-dimethoxybiphenyl
- N-Heterocyclic carbenes
- Carbon
- Tricyclohexylphosphine
- Metallacycles
- Gold
- Tri-tert-butylphosphine

Selected Terms

Click 'X' to remove the category from 'Selected Terms'

- Catalysis > Catalysts (1 Terms)

Catalysis > Catalysts > 1 Index Term(s) Selected

OK Cancel

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

### Categorize

1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Prepared substances (90040)	Page: 1 of 6 <b>Select All</b> <b>Deselect All</b>	Click 'X' to remove the category from 'Selected Terms'
General chemistry	Reactants & reagents (48653)	<input type="checkbox"/> Suzuki coupling reaction 5689	<input checked="" type="checkbox"/> Catalysis > Catalysts (1 Terms)
<b>Synthetic chemistry</b>	<b>Reactions (578)</b>	<input type="checkbox"/> Cross-coupling reaction 655	
Catalysis	Manufactured substances (5001)	<input type="checkbox"/> Heck reaction 655	
Physical chemistry	Purified substances (765)	<input type="checkbox"/> Coupling reaction 478	
Technology	Bio-prepared substances (418)	<input type="checkbox"/> Sonogashira coupling reaction 453	
Biotechnology		<input type="checkbox"/> Arylation 363	
Polymer chemistry		<input type="checkbox"/> Stille coupling reaction 292	
Genetics & protein chemistry		<input type="checkbox"/> Cyclization 218	
Environmental chemistry		<input type="checkbox"/> Solvent effect 205	
Biology		<input type="checkbox"/> Stereoselective synthesis 203	
Analytical chemistry		<input type="checkbox"/> Enantioselective synthesis 181	
		<input type="checkbox"/> Reduction 181	

Synthetic chemistry > Reactions

**OK**   **Cancel**

# 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CPlus<sup>SM</sup>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)-

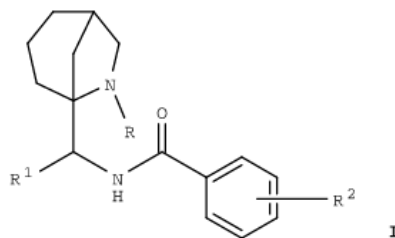
## Quick View

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

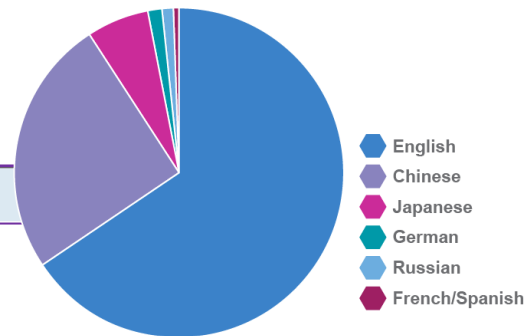
By Dargazani, Ghad; Estenne-Bouhtou, Genevieve; Medaisko, Florence  
From PCT Int. Appl. (2010), WO 2010092287 A1 Aug 19, 2010. | Language: French, Database: CAPLUS

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



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



# 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-Bu)<sub>3</sub>P as a ligand.

**Process for synthesis of substituted secondary amines via condensation of aniline with aryl halides with a palladium catalyst and (t-Bu)<sub>3</sub>P 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-Bu)<sub>3</sub>P 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-Bu)<sub>3</sub>P 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



**PATENTPAK**<sup>TM</sup>  
A CAS SOLUTION

- 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



**CAS**<sup>®</sup>

A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

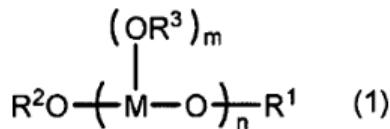
# 点击PatentPak, 一键获得专利pdf文件, 快速定位到关键物质

## 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



A compd. represented by the formula  $\text{R}^2\text{O}(\text{M}(\text{OR}^3)_m\text{O})_n\text{R}^1$  (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;  $\text{R}^1$ ,  $\text{R}^2$  and  $\text{R}^3$  each independently represent a  $\text{C}_{1-16}$  alkyl group which is optionally substituted with one or more fluorine atoms, or a  $\text{C}_{2-17}$  acyl group which is optionally substituted with one or more fluorine atoms, represent, and when a plurality of  $\text{R}^3$  are present, the plurality of  $\text{R}^3$  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 optoelectronic devices employing the organic compounds as electroluminescent hosts

Quick View **PATENTPAK**

By Lee, Han-Il; Song, In, Soo-Hyun; Cho, Eun-Gun; Jung, Ho-Kuk

From Eur. Pat. Appl. No. EP 2947071

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

点击PatentPak, 获取PatentPak Viewer

istics employing the

From Eur. Pat. Appl. No. EP 2947071

... are org. compd. represented by Formula (I), where X,  $\text{L}^{1-6}$ ,  $\text{R}^{1-22}$ , 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**



CAS<sup>®</sup>

A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

# 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

The screenshot displays the PatentPak interface. At the top left, the logo 'PATENTPAK A CAS SOLUTION' is visible. The top navigation bar includes 'PAGE 33 / 65', 'ZOOM' controls, and a 'DOWNLOAD PDF' button with a location pin icon. On the left sidebar, 'Key Substances in Patent' lists two entries: 'CAS RN 1830362-23-6' and 'CAS RN 1830362-24-7', each with a chemical structure and a 'Search in SciFinder | View Detail' link. The main content area shows a chemical reaction between intermediate I-1 and 4-bromobenzimidamide hydrochloride, catalyzed by NaOH in EtOH, to form product I-2. Below the reaction, patent text [0093] describes the procedure. A purple callout box points to a location pin icon on the reaction scheme, with an arrow pointing to the 'DOWNLOAD PDF' button. Another callout box points to a lightbulb icon below the chemical structure of I-2, with an arrow pointing to the 'View Detail' link in the sidebar.



# PatentPak——专利工作流程解决方案

The screenshot displays the PatentPak interface. At the top, there are navigation controls: 'PAGE 45 / 65', 'ZOOM' (with minus and plus buttons), and 'DOWNLOAD PDF'. The main content area shows a patent document with line numbers 45, 50, and 55. The text describes the deposition of various layers for an organic light emitting diode. Chemical structures are shown in the left sidebar, including a quinoline derivative and a complex metal-organic complex. The interface includes search options like 'Search in SciFinder' and 'View Detail' for both the structures and the patent text. A purple arrow points from a text box to the 'Search in SciFinder' link in the left sidebar.

Key Substances in Patent

Search in SciFinder | View Detail

Analyst Markup Locations (2)

- page 44
- page 45

CAS RN 2085-33-8

Search in SciFinder | View Detail

Analyst Markup Locations (2)

- page 44
- page 45

45 phosphorescent dopant based on 100 wt% of the total amount of the emission layer.

45 [0199] On the emission layer, a 50 Å-thick hole blocking layer was formed by depositing bis (2-methyl-8-quinolinolate)-4-(phenylphenolato)aluminium (BALq) under the same vacuum deposition condition. Subsequently, a 250 Å-thick electron transport layer (ETL) was formed by depositing tris (8-hydroxyquinolino)aluminium (Alq3) under the same vacuum deposition condition. LiF and Al were sequentially deposited to form a cathode on the electron transport layer (ETL), manufacturing an organic light emitting diode.

50 [0200] The organic light emitting diode has a structure of ITO/BNTPD 60nm/HT-1 30 nm/EML (a compound 1 (93 wt%) + Ir(pq)2acac (7 wt%), 30nm)/Balq (5 nm)/Alq3 25 nm/LiF (1 nm)/Al (100 nm).

Example 2

55 [0201] An organic light emitting diode was manufactured according to the same method as Example 1 except for using the compound 2 according to Synthesis Example 22 instead of the compound 1 according to Synthesis Example 21.

44

也可实现PDF文件与  
PatentPak Viewer互动

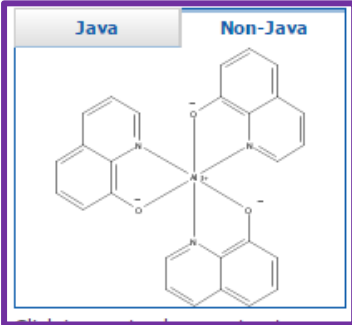
可在PatentPak Viewer中直接返回  
SciFinder进行结构、马库什和反应检索

# PatentPak——专利工作流程解决方案

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF


**Search**

Advanced Search

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

 ChemDraw  
Launch a SciFinder subst  
More

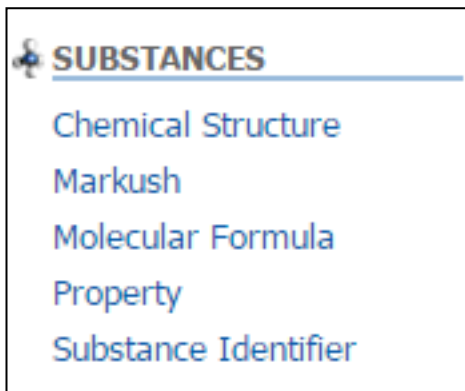
从PatentPak Viewer直接跳转到结构检索界面，同时无需绘制，系统会自动将相应的结构直接导入到绘图面板，点击Search即开始SciFinder检索，拓展新的研究方向

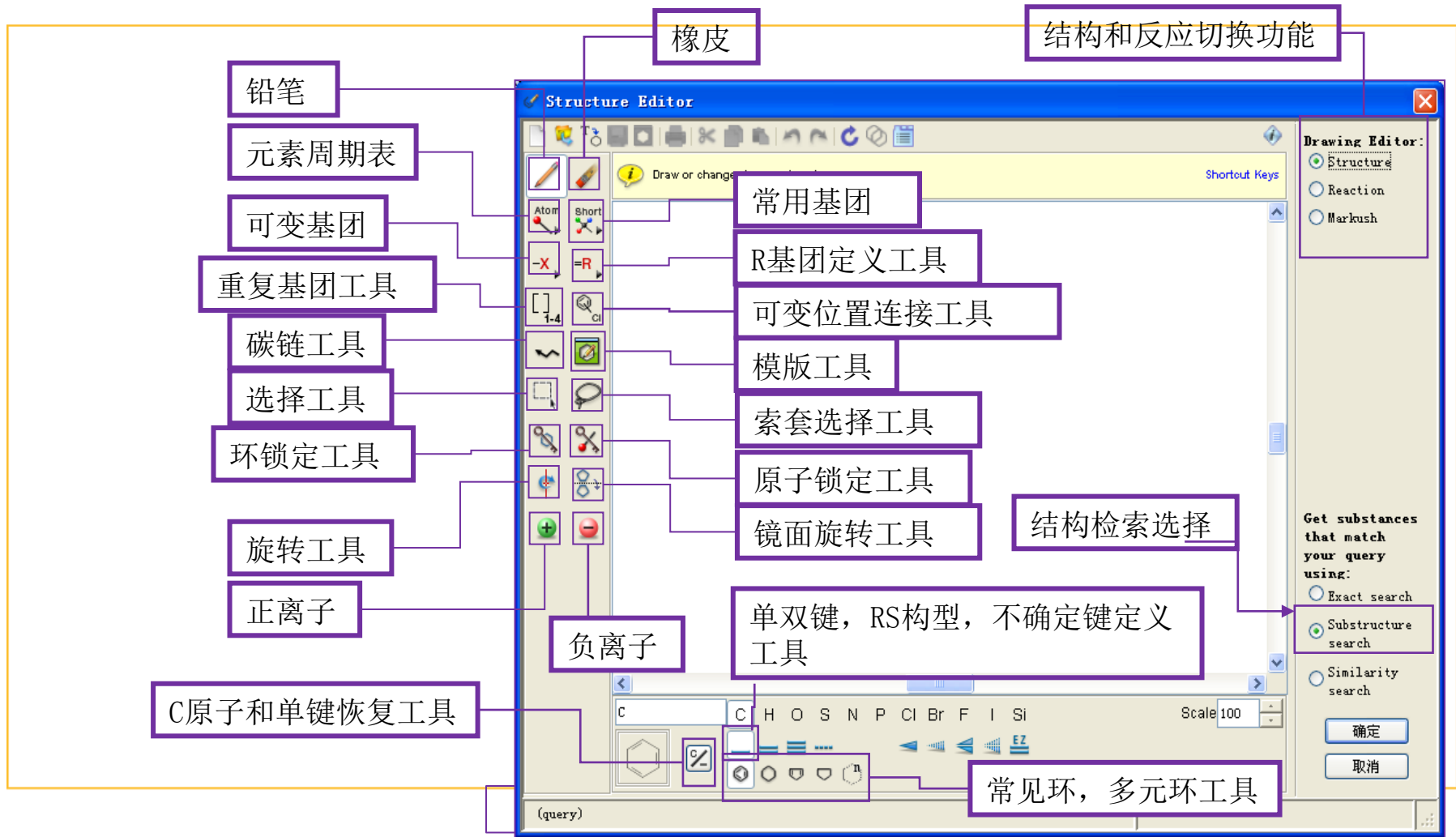
# 提纲

- 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

C原子和单键恢复工具

负离子

常用基团

R基团定义工具

可变位置连接工具

模版工具

索套选择工具

原子锁定工具

镜面旋转工具

单双键, RS构型, 不确定键定义工具

结构检索选择

常见环, 多元环工具

# 举例：不固定位置取代

The image displays two screenshots of the CAS Structure Editor interface, illustrating the process of adding a chlorine atom to a benzene ring at a non-fixed position.

**Left Screenshot:** Shows a benzene ring with a methyl group (CH<sub>3</sub>) attached. The chemical formula is Cc1ccccc1Cl. The interface includes a toolbar with various drawing tools, a search bar, and a drawing editor panel on the right with options for Structure, Reaction, and Markush. The bottom status bar shows the formula C7H7Cl and the number 92.14 . 36.46.

**Right Screenshot:** Shows the same benzene ring with a methyl group, but now a chlorine atom (Cl) is being added to the ring. The interface is similar to the left screenshot, but the drawing editor panel on the right has the "Structure" option selected. The bottom status bar shows the formula C7H7Cl and the number 126.59.

直接导入已保存的.cxf或者.mol文件

将绘制结构存为模板

**Shortcuts**

CH	CH <sub>2</sub>	Me	OMe	Et	OEt	Pr-n	Pr-i	OPr-n
OPr-i	Bu-n	Bu-i	Bu-s	Bu-t	OBu-n	OBu-i		
OBu-s	OBu-t	Ph	OPh	o-C <sub>6</sub> H <sub>4</sub>	m-C <sub>6</sub> H <sub>4</sub>			
p-C <sub>6</sub> H <sub>4</sub>	CF <sub>2</sub>	CF <sub>3</sub>	CCl <sub>2</sub>	CCl <sub>3</sub>	CBr <sub>2</sub>	CBr <sub>3</sub>	Cl <sub>2</sub>	
Cl <sub>3</sub>	CHO	CN	C(O)CH <sub>3</sub>	CO <sub>2</sub> H	COOH	COSH		
CS <sub>2</sub> H	CSSH	NH	NH <sub>2</sub>	NH <sub>3</sub>	NO <sub>2</sub>	OH		
OPO <sub>3</sub> H <sub>2</sub>	OSO <sub>3</sub> H	PO <sub>3</sub> H <sub>2</sub>	SH	SO <sub>2</sub>	SO <sub>3</sub> H			

Close

常用基团



环锁定工具



原子锁定工具

**Structure Editor**

Select and draw structures with templates.

常用模板

**Templates**

Enter 3 or more characters...

- Alkaloid (9)
- Amino Acid (25)
- Bicarboyclic (8)
- Carbohydrate (7)
- Coordination (14)
- Cycloalkane (13)
- Miscellaneous (6)
- Monocarboyclic (19)
- N-containing (19)
- NOS-containing (10)
- Nucleic Acid (5)
- O-containing (11)
- Polycarboyclic (13)
- Rings (4)
- S-containing (6)
- Steroid (7)
- User-Defined (0)

Close



**CAS**  
A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

# 化学结构检索: 精确结构检索

Structure Editor

Click and drag to select objects. Ctrl-click to select or deselect individual objects.

Atom Short

-X =R

1-4

Structure Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK

Cancel

酒石酸二苄酯

C H O S N P Cl Br F I Si

C<sub>12</sub>H<sub>18</sub>O<sub>6</sub> 330.34

结构式中的原子和环  
全部被锁定,不可被取代



# 物质结构结果集

0 of 20 Substances Selected

<p><input type="checkbox"/> 1. <b>622-00-4</b> <b>手性化合物</b></p> <p>~105   ~53 </p> <p>Absolute stereochemistry.,Rotation (+).</p> <p><b>C<sub>18</sub> H<sub>18</sub> O<sub>6</sub></b> Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester</p> <p>▶ <b>Key Physical Properties</b> Experimental Properties</p>	<p><input type="checkbox"/> 2. <b>4136-22-5</b> </p> <p>~18   ~39 </p> <p>Absolute stereochemistry.,Rotation (-).</p> <p><b>C<sub>18</sub> H<sub>18</sub> O<sub>6</sub></b> Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2<i>S</i>,3<i>S</i>)-</p> <p>▶ <b>Key Physical Properties</b></p>	<p><input type="checkbox"/> 3. <b>93993-87-4</b> <b>非手性化合物</b></p> <p>~9   ~4 </p> <p><b>C<sub>18</sub> H<sub>18</sub> O<sub>6</sub></b> Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester</p> <p>▶ <b>Key Physical Properties</b></p>
<p><input type="checkbox"/> 4. <b>4079-56-5</b> </p> <p>~5  </p> <p>Relative stereochemistry.</p> <p><b>C<sub>18</sub> H<sub>18</sub> O<sub>6</sub></b> Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2<i>R</i>,3<i>R</i>)-<i>rel</i>.</p> <p>▶ <b>Key Physical Properties</b></p>	<p><input type="checkbox"/> 5. <b>4079-57-6</b> </p> <p>~5   ~1 </p> <p>Relative stereochemistry.</p> <p><b>C<sub>18</sub> H<sub>18</sub> O<sub>6</sub></b> Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2<i>R</i>,3<i>S</i>)-<i>rel</i>.</p> <p>▶ <b>Key Physical Properties</b></p>	<p><input type="checkbox"/> 6. <b>89960-73-6</b> <b>聚合物单体的组合物</b></p> <p>~2 </p> <p>622-00-4 <b>C<sub>18</sub> H<sub>18</sub> O<sub>6</sub></b></p> <p>Absolute stereochemistry.,Rotation (+).</p> <p>101-68-8 <b>C<sub>15</sub> H<sub>10</sub> N<sub>2</sub> O<sub>2</sub></b></p>

# 高级检索——提前限定

**Search**

[Advanced Search](#)  Always Show

Characteristics  **Single component**  
 Commercially available  
 Included in references

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

Studies  Analytical  
 Biological  
 Preparation  
 Reactant or reagent



0 of 7 Substances Selected

1. **622-00-4** 🔍

~105 ~57

Absolute stereochemistry.,Rotation (+).

**C<sub>18</sub> H<sub>18</sub> O<sub>6</sub>**  
Butanedioic acid, 2,3-dihydroxy- (2*R*,3*R*)-, 1,4-bis(phenylmethyl) ester

▶ **Key Physical Properties**  
Experimental Properties

4. **4079-56-5** 🔍

~5

Relative stereochemistry.

**C<sub>18</sub> H<sub>18</sub> O<sub>6</sub>**  
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2*R*,3*R*)-*rel*

▶ **Key Physical Properties**

3. **93993-87-4** 🔍

~9 ~7

Absolute stereochemistry.

**C<sub>18</sub> H<sub>18</sub> O<sub>6</sub>**  
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester

▶ **Key Physical Properties**

6. **896448-46-7** 🔍

~2 ~3

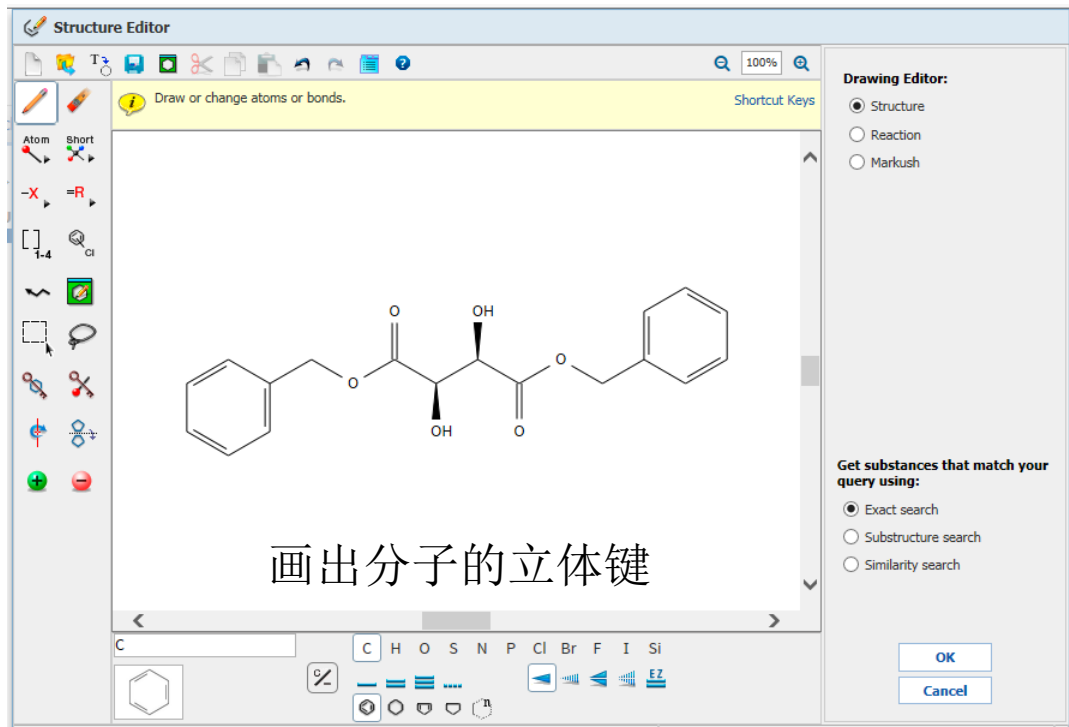
Absolute stereochemistry.

**C<sub>18</sub> H<sub>18</sub> O<sub>6</sub>**  
Butanedioic acid, 2,3-dihydroxy-, 1,4-bis(phenylmethyl) ester, (2*S*,3*R*)-

▶ **Key Physical Properties**

去除混合物，组合物，配合物，盐等

## 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

1 of 5 Stereo Candidates Selected		Substances
<input checked="" type="checkbox"/>	Absolute stereo match	1
<input type="checkbox"/>	Absolute stereo mirror image	1
<input type="checkbox"/>	Relative stereo match	1
<input type="checkbox"/>	Stereo that doesn't match query	3
<input type="checkbox"/>	No stereo in answer structure	1


Get Substances

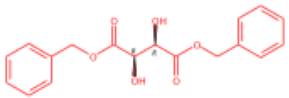
选择绝对立体构型完全匹配的结果



0 of 1 Substance Selected

1. **622-00-4** 🔍

~105 📄  ~57 🧪



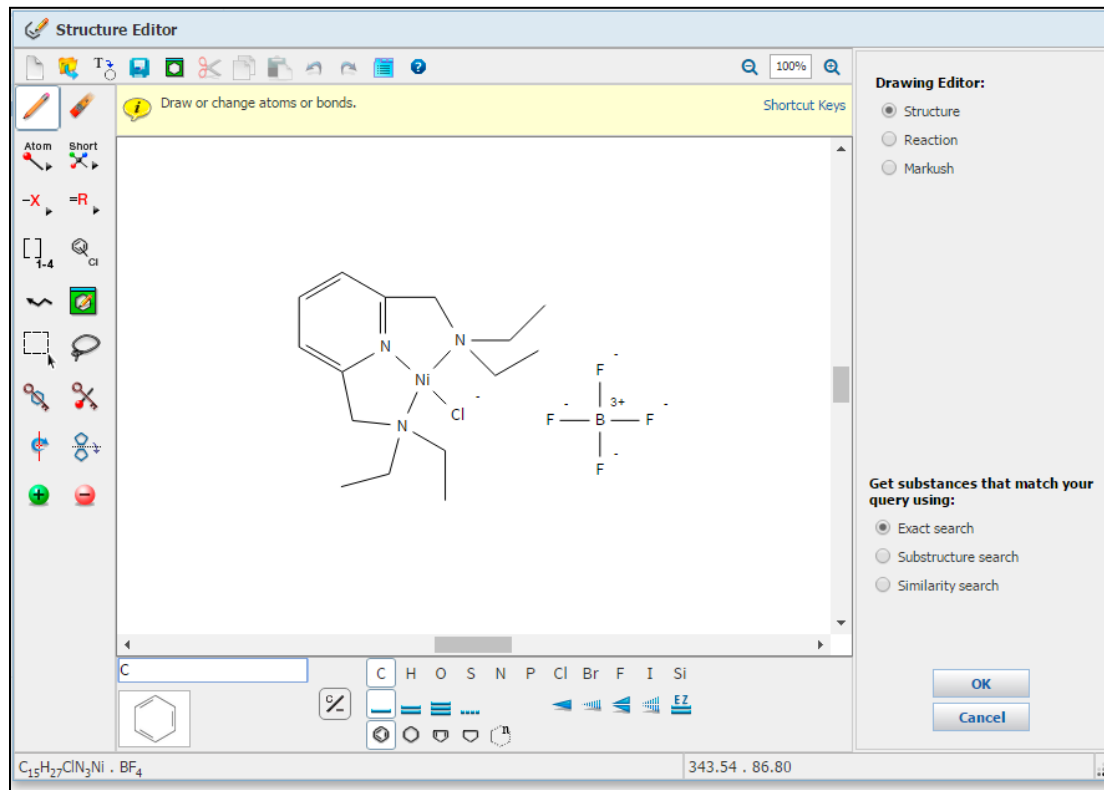
Absolute stereochemistry., Rotation (+).

**C<sub>18</sub> H<sub>18</sub> O<sub>6</sub>**  
Butanedioic acid, 2,3-dihydroxy- (2*R*,3*R*)-, 1,4-bis(phenylmethyl) ester

▶ **Key Physical Properties**  
Experimental Properties



# 精确结构检索配合物



# 获得精确结构检索结果

Characteristics	<input checked="" type="checkbox"/>	Single component
	<input type="checkbox"/>	Commercially available
	<input type="checkbox"/>	Included in references
Classes	<input type="checkbox"/>	Alloys
	<input checked="" type="checkbox"/>	Coordination compounds
	<input type="checkbox"/>	Incompletely defined
	<input type="checkbox"/>	Mixtures
	<input type="checkbox"/>	Polymers
	<input type="checkbox"/>	Organics, and others not listed
Studies	<input type="checkbox"/>	Analytical
	<input type="checkbox"/>	Biological
	<input type="checkbox"/>	Preparation
	<input type="checkbox"/>	Reactant or reagent

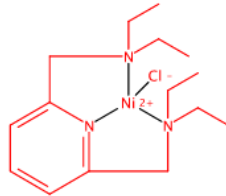
Sort by: CAS Registry Number

0 of 1 Substance Selected

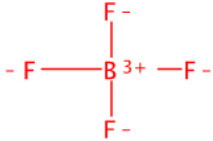
1. 1955541-98-6

~1

1955541-97-5  
C<sub>15</sub> H<sub>27</sub> Cl N<sub>3</sub> Ni



14874-70-5  
B F<sub>4</sub>



C<sub>15</sub> H<sub>27</sub> Cl N<sub>3</sub> Ni · B F<sub>4</sub>  
INDEX NAME NOT YET ASSIGNED

# 物质检索结果——Analyze

## 六种分析选项

Analyze Refine

Analyze by: ?

- Bioactivity Indicators
- Bioactivity Indicators
- Commercial Availability
- Elements
- Reaction Availability
- Substance Role
- Target Indicators

## 生物活性

Analyze Refine

Analyze by: ?

Bioactivity Indicators

Nervous system agents (all) 2

Show More

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

Analyze Refine

Analyze by: ?

Substance Role

Preparation 30

Analytical Study 21

Properties 13

Biological Study 11

Reactant or Reagent 10

Uses 9

Formation, Nonpreparative 8

Occurrence 3

Process 3

Miscellaneous 2

Show More

## 靶点

Analyze Refine

Target Indicators

DNA-binding proteins (all) 1

Enzymes (all) 1

Growth factors, animal (all) 1

Neuropeptides (all) 1

Opioid peptides (all) 1

Phosphoproteins (all) 1

Prolactin (all) 1

Pro-opiomelanocortin (all) 1

Proteins 1

Receptors (all) 1

Show More

# 物质检索结果——Refine

Analyze Refine

Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

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

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
  - Alloys
  - Coordination compounds
  - Incompletely defined
  - Mixtures
  - Polymers
  - Organics, and others not listed
- Are in specific types of studies
  - Analytical
  - Biological
  - Preparation
  - Reactant or reagent

Refine

Analyze Refine

Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Retrieve substances with:

- Any property
- Any predicted property
- Any experimental property
- Any selected experimental property

Refine



CAS<sup>®</sup>

A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY



# SciFinder中的物质记录

点击CAS RN 获得物质详细信息

1. **50-36-2** 🔍

~21151 ~26

Absolute stereochemistry.,Rotation (-).

**C<sub>17</sub>H<sub>21</sub>N O<sub>4</sub>**  
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*,2*R*,3*S*,5*S*)-

▶ **Key Physical Properties**  
Regulatory Information  
Spectra  
Experimental Properties

2. **53-21-4** 🔍

**CAS Registry Number: 50-36-2**

- » View Substance Detail
- 🔍 Explore by Structure ▶
- Synthesize this...
- Get Reactions where Substance is a ▶
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile
- Send to SciPlanner

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<sub>17</sub>H<sub>21</sub>N O<sub>4</sub>**

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)

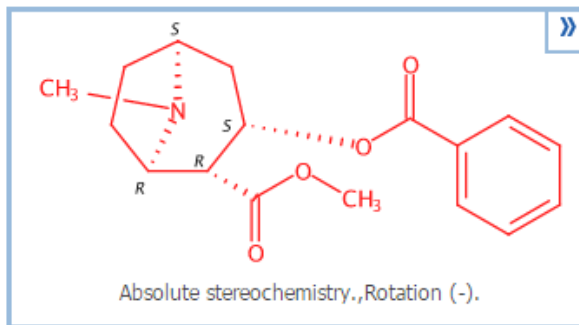
Value: 187 °C | Condition: Press: 0.1 Torr

### Density (Predicted)

Value: 1.22±0.1 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr

### pKa (Predicted)

Value: 8.97±0.60 | Condition: Most Basic Temp: 25 °C



物质信息详情

**EXPERIMENTAL PROPERTIES**

实验数据与实验谱图

**EXPERIMENTAL SPECTRA****<sup>1</sup>H NMR** IR Mass Raman UV and Visible

<sup>1</sup> H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	<a href="#">See spectrum</a>		(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	273.33		(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

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

1-4 Cl

Get substances that match your query using:

Exact search

Substructure search

Similarity search

OK

C H O S N P Cl Br F I Si

# 浏览亚结构检索结果

0 of 63231 Substances Selected

1. 525-82-6

~3509 ~78

**C<sub>15</sub> H<sub>10</sub> O<sub>2</sub>**  
4H-1-Benzopyran-4-one, 2-phenyl-

▶ **Key Physical Properties**  
Regulatory Information  
Spectra  
Experimental Properties

2. 54849-75-1

~6

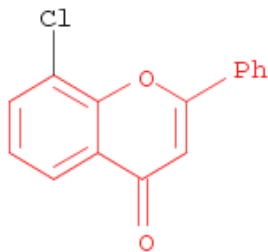
**C<sub>15</sub> H<sub>5</sub> D<sub>5</sub> O<sub>2</sub>**  
4H-1-Benzopyran-4-one, 2-(phenyl-*d*<sub>5</sub>)-

Spectra

# 浏览亚结构检索结果

251. Substance Detail  
1148-20-5

取代物

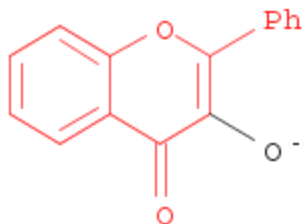


**C<sub>15</sub> H<sub>9</sub> Cl O<sub>2</sub>**

4#1-Benzopyran-4-one, 8-chloro-2-phenyl-

261. Substance Detail  
85481-91-0

离子



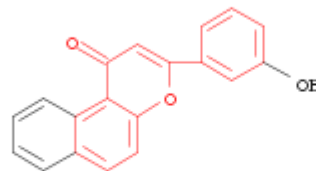
**C<sub>15</sub> H<sub>9</sub> O<sub>3</sub>**

4#1-Benzopyran-4-one, 3-hydroxy-2-phenyl-, ion

Experimental Properties

273. Substance Detail  
136116-17-1

稠环物质



**C<sub>19</sub> H<sub>12</sub> O<sub>3</sub>**

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

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

母体骨架结构不变，  
母体中的氢可以被取代

Search

Advanced Search  Always Show

Characteristics  Single component  
 Commercially available  
 Included in references

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

Studies  Analytical  
 Biological  
 Preparation  
 Reactant or reagent

将两个活性分子片段  
限定在同一物质中

# 两个分子片段出现在同一物质中

Chemical Structure substructure with limiters > substances (49240)

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sample Analysis: Substance Role

Preparation ≥ 6761

Biological Study ≥ 5629

Uses ≥ 4822

Prophetic in Patents ≥ 1649

Reactant or Reagent ≥ 1241

Properties ≥ 369

Process ≥ 49

Combinatorial Study ≥ 25

Analytical Study ≥ 17

Occurrence ≥ 7

Show More

Sort by: CAS Registry Number

0 of 49240 Substances Selected

Page: 1 of 3283

1. **1997357-70-6**

CC(=O)Nc1ccc(cc1)Nc2ccc(O)c3ccccc23

**C<sub>20</sub> H<sub>18</sub> N<sub>4</sub> O<sub>3</sub> S<sub>2</sub>**  
Acetamide, *N*-[4-[3-[[[(1-methyl-1*H*-indol-4-yl)sulfonyl]amino]phenyl]-2-thiazolyl]-

▶ **Key Physical Properties**

2. **1997357-68-2**

CC(=O)Nc1ccc(cc1)Nc2ccc(O)c3ccccc23

**C<sub>20</sub> H<sub>18</sub> N<sub>4</sub> O<sub>3</sub> S<sub>2</sub>**  
Acetamide, *N*-[4-[3-[[[(1-methyl-1*H*-indol-5-yl)sulfonyl]amino]phenyl]-2-thiazolyl]-

▶ **Key Physical Properties**

3. **1995871-38-9**

Cc1ccc(cc1)Nc2ccc(O)c3ccccc23

**C<sub>30</sub> H<sub>26</sub> N<sub>5</sub> S**  
Pyridinium, 4-[2-[6-[[[2-(2-benzothiazolyl)hydrazinylidene]methyl]-9-ethyl-9*H*-carbazol-3-yl]ethenyl]-1-methyl-

4. **1995847-80-7**

Cc1ccc(cc1)Nc2ccc(O)c3ccccc23

Absolute stereochemistry.

**C<sub>40</sub> H<sub>58</sub> N<sub>6</sub> O<sub>7</sub> S**  
1*H*-Indole-3-pentanoic acid,  $\gamma$ -[[[2-[(1*R*,3*R*)-1-(acetyloxy)-4-

5. **1995846-52-0**

Cc1ccc(cc1)Nc2ccc(O)c3ccccc23

Absolute stereochemistry.

**C<sub>30</sub> H<sub>47</sub> N<sub>5</sub> O<sub>5</sub> S**

6. **1995844-98-8**

Cc1ccc(cc1)Nc2ccc(O)c3ccccc23

Absolute stereochemistry.



# 物质检索——相似结构检索

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

1-4 Cl

HS NH N COOH

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search



Select All Deselect All

## 相似结构检索候选项

1 of 6 Similarity Candidates Selected

Substances

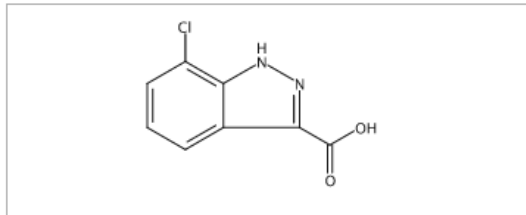
<input type="checkbox"/>	≥ 99 (most similar)	0
<input type="checkbox"/>	95-98	0
<input type="checkbox"/>	90-94	0
<input type="checkbox"/>	85-89	11
<input checked="" type="checkbox"/>	80-84	34
<input type="checkbox"/>	75-79	82
<input type="checkbox"/>	70-74	254
<input type="checkbox"/>	65-69	633
<input type="checkbox"/>	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



$C_8H_5ClN_2O_2$   
1H-Indazole-3-

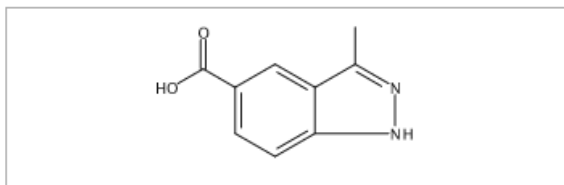
Key Physical

取代基变化

Score: 79

3. 885223-58-5

~11 ~34



$C_9H_8N_2O_2$   
1H-Indazole-5-carboxylic acid, 3-methyl-

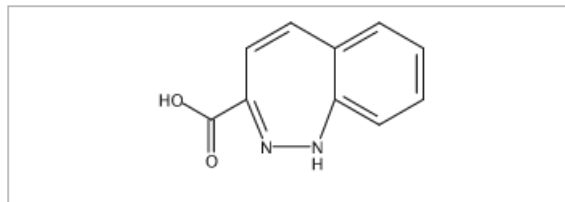
Key Physical Properties

取代基位置变化

Score: 71

117. 72119-92-7

~1



$C_{10}H_8N_2O_2$   
1H-1,2-Benzodiazepine-3-carboxylic acid

Key Physical Properties  
[Experimental Properties](#)

母体结构变化

## 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

The screenshot displays the CAS SciFinder web interface. At the top left, there is a 'CAS Solutions' dropdown menu and the SciFinder logo with the tagline 'A CAS SOLUTION'. Below this is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. On the left side, there is a sidebar menu with three main categories: 'REFERENCES', 'SUBSTANCES', and 'REACTIONS'. Under 'REFERENCES', options include Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', options include Chemical Structure, Markush, Molecular Formula, Property (which is highlighted with a blue bar), and Substance Identifier. Under 'REACTIONS', the option is Reaction Structure. The main content area is titled 'SUBSTANCES: PROPERTY' and features a radio button for 'Experimental'. Below this is a dropdown menu for 'Select Property...' with a list of properties: Boiling Point (°C), Density (g/cm<sup>3</sup>), Electric Conductance (S), Electric Conductivity (S/cm), Electric Resistance (ohm), Electric Resistivity (ohm\*cm), Glass Transition Temp. (°C), Magnetic Moment (μB), Median Lethal Dose (LD50) (mg/kg), Melting Point (°C), Optical Rotatory Power (degrees), Refractive Index, and Tensile Strength (MPa). To the right of the dropdown menu are two input fields with example text: 'Examples: 44, 25-35, >125'.

# 物质检索——性质检索

The screenshot displays the SciFinder web interface. On the left, there are navigation menus for REFERENCES, SUBSTANCES, and REACTIONS. The SUBSTANCES menu is expanded, showing options like Chemical Structure, Molecular Formula, and Property. The main search area has a dropdown menu for 'Select Property...' with 'Molecular Weight' selected. Below the dropdown, there are input fields for search criteria, with 'Examples: 44, 25-35, >125' shown. A blue 'Search' button is visible at the bottom of the search area.

寻找分子量在250-400之间的物质

# 物质检索——分子式检索

**REFERENCES**

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

**SUBSTANCES**

- Chemical Structure
- Markush
- Molecular Formula**
- Property
- Substance Identifier

**REACTIONS**

**REACTANTS**

**SUBSTANCES: MOLECULAR FORMULA ?**

Examples:  
H4SiO4  
(C3H6O.C2H4O)x

**Search**

无机金属盐：金属离子和阴离子间用点（.）分开

40. **151-21-3**

(Component: 151-41-7)

~79363 ~283

**C<sub>12</sub>H<sub>26</sub>O<sub>4</sub>S . Na**  
Sulfuric acid monododecyl ester sodium salt (1:1)

**Key Physical Properties**

- Regulatory Information
- Spectra
- Experimental Properties

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

# 物质检索——标识符检索

**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: SUBSTANCE IDENTIFIER ?

Enter one per line.  
Examples:  
50-00-0  
999815  
Acetaminophen

**Search**

**提示:**

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

# 提纲

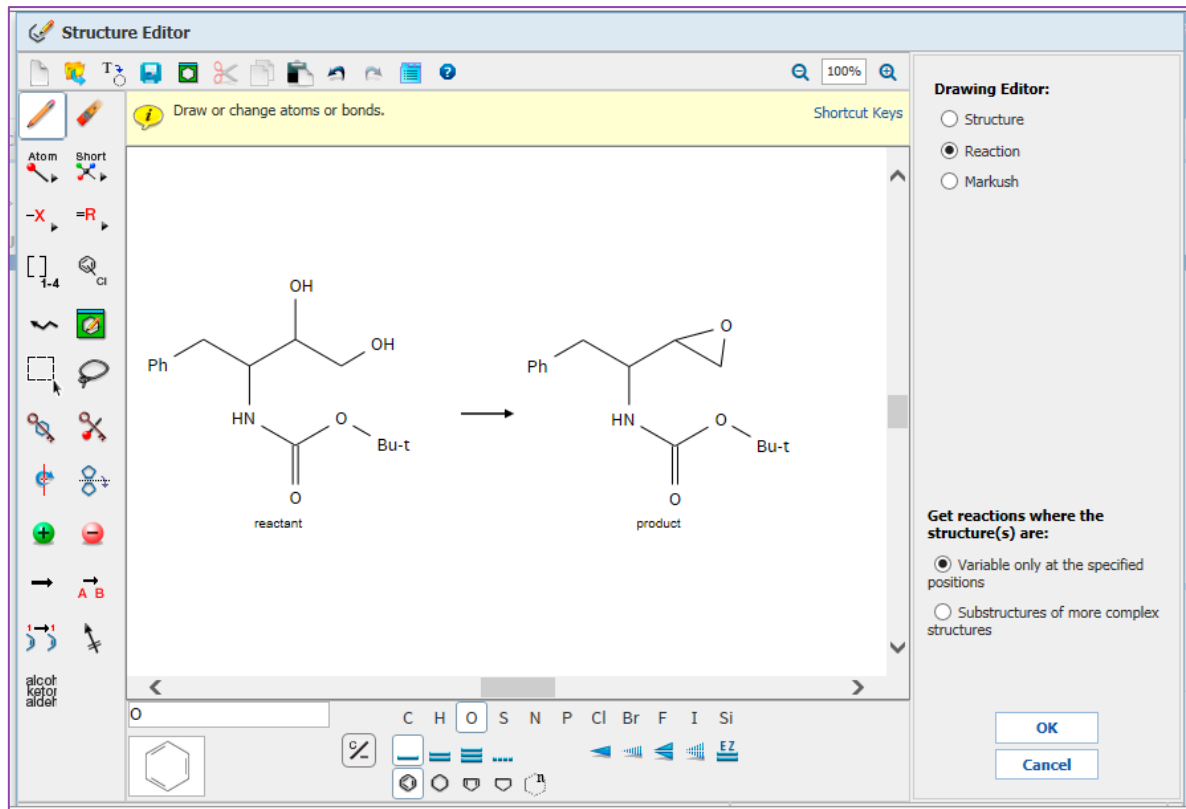
- 美国化学文摘社简介
- **SciFinder简介及检索方式**
  - 文献检索
  - 物质检索
  - **反应检索**
  - 分析方法查询
- SciFinder常见问题及解决



# 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



# 反应结果集

点击Transformation,  
获得反应类型的分类

**REACTIONS**

Analyze Refine

Analyze by: Reagent

Et <sub>3</sub> N	6
PPh <sub>3</sub>	6
EtO <sub>2</sub> CN=NCO <sub>2</sub> Et	4
MeSO <sub>2</sub> Cl	4
1H-Imidazole	3
Bu <sub>4</sub> N <sup>+</sup> •F <sup>-</sup>	3
K <sub>2</sub> CO <sub>3</sub>	3
NaOMe	3
t-BuSiMe <sub>2</sub> Cl	3
C <sub>5</sub> H <sub>5</sub> N	2

Show More

Get References Tools

Group by: No Grouping Document Transformation

Sort by: Relevance

0 of 18 Reactions Selected

1. Conversion of Alcohols to Ether / Mitsunobu Etherification  
12 Reactions

$$R-OH + R^1-OH \longrightarrow R-O-R^1$$

2. Multi-Step Reactions  
6 Reactions

16. View Reaction Detail

2 Steps Hover over any structure for more options.

**Overview**

**Steps/Stages**

1.1 R:Et<sub>3</sub>N, S:(t-Pr)<sub>2</sub>O  
2.1 R:NaOMe, S:AcOEt, S:MeOH

**Notes**

1) ice-cooling for 1 h, 2) ice-cooling for 10 min, Reactants: 2, Reagents: 2, Solvents: 3, Steps: 2, Stages: 2, Most stages in any one step: 1

**References**

Process for producing optically active threo-3-amino-1,2-epoxy compounds  
Quick View PATENTPAK  
By Sagawa, Yukihiro et al.  
From PCT Int. Appl., 9938855, 05 Aug 1999

# 反应结果处理：分析

## 13种分析选项

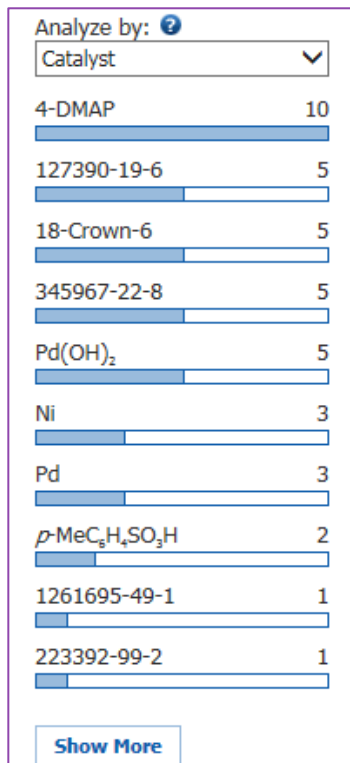
Analyze Refine

Analyze by: ?

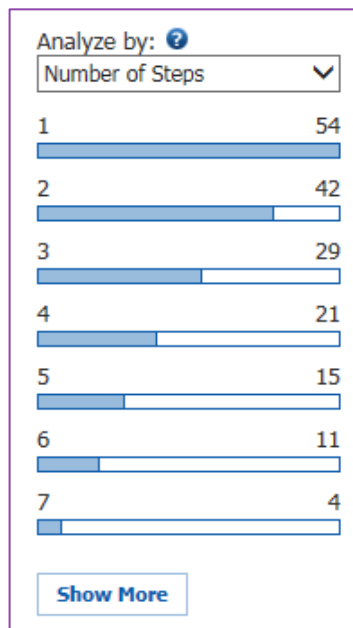
- Author Name
- Catalyst
- Company-Organization
- Document Type
- Experimental Procedure
- Journal Name
- Language
- MethodsNow
- Number of Steps
- Product Yield
- Publication Year
- Reagent
- Solvent



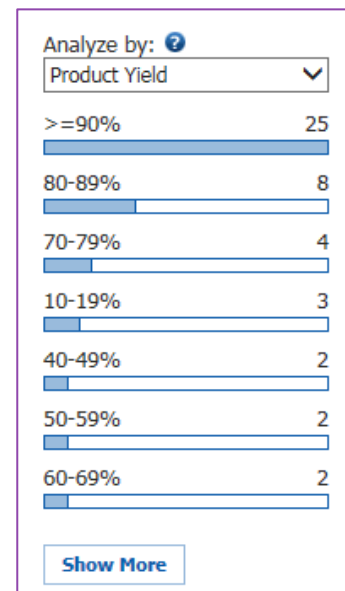
## 催化剂



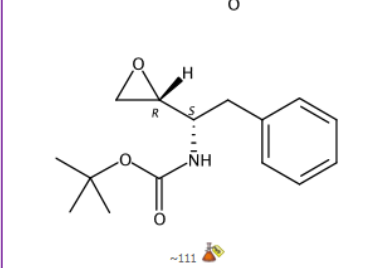
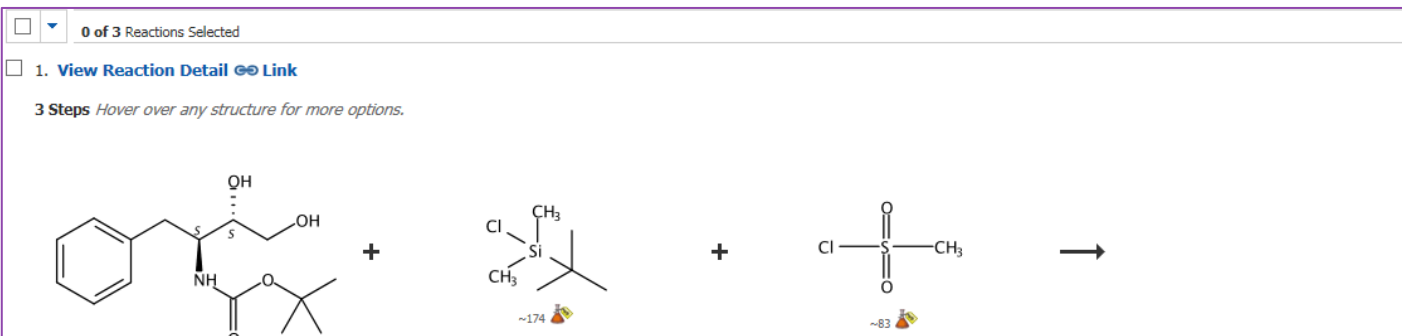
## 反应步数



## 产率



# 针对感兴趣的反应查看实验详情



## Overview

### Steps/Stages

- 1.1 R:Et<sub>3</sub>N, R:4-DMAP, S:PhMe
- 1.2
- 2.1 R:(NH<sub>4</sub>)F, R:AcOH, S:MeOH
- 3.1 R:t-BuOK, S:Me<sub>2</sub>CHOH, S:THF

### Notes

3) key step, stereoselective, Reactants: 3, Reagents: 5, Solvents: 4, Steps: 3, Stages: 4, Most stages in any one step: 2

### References

Process Research and Development for an Efficient Synthesis of the HIV Protease Inhibitor BMS-232632

[Quick View](#) [Other Sources](#)

By Xu, Zhongmin et al

From Organic Process Research & Development, 6(3), 323-328; 2002

▶ [Experimental Procedure](#)

▶ [METHODSNOW™](#)

# Experimental Procedure

## Experimental Procedure

OPR&D

### Step 1

[3-tert-Butyl-dimethylsilyloxy-2(S)-[(methylsulfonyl)-oxy]-1(S)-(phenylmethyl)propyl]-carbamic Acid, 1,1-Di-methylethyl Ester (12). A solution of diol 10 (544 g, 1.034 mol) in 1.2 L of toluene was heated to 88 °C, and a clear solution was obtained. The solution was then cooled to 50 °C. Dimethylamino pyridine (23.6 g, 0.195 mol) and triethylamine (325 mL, 2.32 mol) were charged followed by the slow addition of tert-butyl-dimethylsilyl chloride (350 g, 2.32 mol) while keeping the internal temperature around 50 °C. The reaction mixture was cooled to 0 °C over 3 h. Triethylamine (417 mL) was added followed by the slow addition of trifluoromethanesulfonyl chloride (198 mL), keeping the internal temperature under 5 °C. The resulting mixture was stirred at 0 °C for about 3 h. The solid was filtered through Celite and washed with toluene (2 × 700 mL). The filtrate was washed with water (4 L), 1 N HCl (4 L), and brine (4 L), in that order, and then concentrated in a vacuum to afford 1.04 kg of product 12. Product 12 was subjected to the next step without further purification.

### Step 2

[3-Hydroxy-2(S)-[(methylsulfonyl)oxy]-1(S)-(phenyl-methyl)propyl]-carbamic Acid, 1,1-Dimethylethyl Ester (13). Into a reactor was charged ammonium fluoride (358 g, 9.67 mol), a solution of the crude mesylate 12 (1.04 kg, 1.034 mol) in methanol (5.6 L), and acetic acid (550 mL). The mixture was stirred at ambient temperature for 11 h. The reaction mixture was concentrated to dryness to afford a solid, which was dissolved in 11 L of methyl tert-butyl ether. The resulting solution was washed with water (5 L), 5% sodium bicarbonate (3 × 4 L), and brine (4 L) and then dried over MgSO<sub>4</sub> (300 g). Filtration and partial concentration afforded 5 L of solution. The concentrated solution was then cooled to 4 °C and stirred at this temperature for 18 h to give a slurry. The solid was filtered, washed with cold MTBE (200 mL) and dried under partial pressure to afford 489.1 g of 13. The filtrate was concentrated to 1 L, cooled to 4 °C, and stirred at this temperature for 18 h to give a slurry. Another 61.7 g of solid was obtained after filtration and drying. Thus, a total of 550.8 g of product 13 was obtained as a white solid (80% yield, AP 98).

### Step 3

N-(tert-butyloxycarbonyl)-2(S)-amino-1-phenyl-3(R)-3,4-epoxy-butane (6). To a clear solution of hydroxy mesylate 13 (629.9 g, 1.75 mol) in a mixture of IPA (6.3 L) and THF (1.8 L) at 17 °C, was added KO<sup>t</sup>Bu (207 g, 95%, 1.75 mol) over 20 min. The mixture was stirred for 1.5 h followed by addition of 30 mL of acetic acid over 15 min. The resulting solution was concentrated under vacuum to dryness to afford a white solid. The solid was dissolved in MTBE (9.0 L), and the resulting solution was washed with water (4.5 L), saturated sodium bicarbonate solution (4.5 L), and brine (4.5 L), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated to give an oil (455.2 g). The oil was diluted with hexane (1.3 L) followed by addition of water (200 mL). The mixture was cooled to -4 °C, and solid was obtained. The solid was collected by filtration, washed with 700 mL of cold hexane (0 °C), and dried under vacuum for 18 h to give epoxide 6 as a white solid (400.5 g, 88% yield, AP 97).

冗长的化学名称

数字标记

整段文字  
描述实验步骤

数字标记

字母简写



CAS<sup>®</sup>

A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

# MethodsNow窗口

## MethodsNow

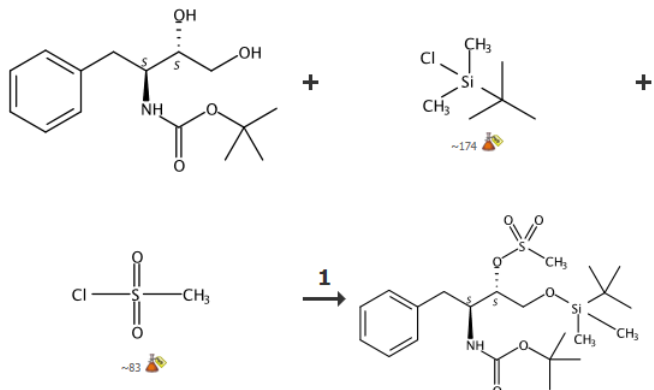
### Process Research and Development for an Efficient Synthesis of the HIV Protease Inhibitor BMS-232632

By Xu, Zhongmin; Singh, Janak; Schwinden, Mark D.; Zheng, Bin; Kissick, Thomas P.; Patel, Bharat; Humora, Michael J.; Quiroz, Fernando; Dong, Lin; Hsieh, Dau-Ming et al

From Organic Process Research & Development, 6(3), 323-328; 2002  
Published by American Chemical Society

#### Reaction Steps

1 2 3



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

## CAS RN即时查看物质

### MethodsNow

<b>Products</b>	Carbamic acid, [(1 <i>S</i> ,2 <i>S</i> )-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-[(methylsulfonyl)oxy]-1-(phenylmethyl)propyl]-, 1,1-dimethylethyl ester, CAS RN: 437713-03-6
<b>Reactants</b>	Carbamic acid, <i>N</i> -[(1 <i>S</i> ,2 <i>S</i> )-2,3-dihydroxy-1-(phenylmethyl)propyl]-, 1,1-dimethylethyl ester, CAS RN: 149451-80-9 <i>tert</i> -Butyldimethylsilyl chloride, CAS RN: 18162-48-6 Methanesulfonyl chloride, CAS RN: 124-63-0
<b>Reagents</b>	Triethylamine, CAS RN: 121-44-8 4-(Dimethylamino)pyridine, CAS RN: 1122-58-3
<b>Solvents</b>	Toluene, CAS RN: 108-88-3
<b>Procedure</b>	<ol style="list-style-type: none"> <li>Heat the solution of chiral diol (544 g) in 1.2 L of toluene to 88 °C.</li> <li>Cool the solution to 50 °C.</li> <li>Charge the dimethylamino pyridine (23.6 g, 0.195 mol) and triethylamine (325 mL, 2.32 mol) followed by the slow addition of <i>tert</i>-butyl-dimethylsilyl chloride (350 g, 2.32 mol) while keeping the internal temperature around 50 °C.</li> <li>Cool the reaction mixture to 0 °C over 3 hours.</li> <li>Add triethylamine (417 mL) followed by the slow addition of trifluoromethanesulfonyl chloride (198 mL) while keeping the internal temperature under 5 °C.</li> <li>Stir the resulting mixture at 0 °C for about 3 hours.</li> <li>Filter the solid through Celite.</li> <li>Wash the solid with toluene (2 x 700 mL).</li> <li>Wash the filtrate with water (4 L), 1 N HCl (4 L) and brine (4 L).</li> <li>Concentrate the filtrate in a vacuum.</li> </ol>
<b>Scale</b>	gram
<b>CAS Method Number</b>	3-008-CAS-1545731

PDF或XLS格式

Print/Export

Close



# 亚结构检索：酮基的还原反应

Structure Editor

Drag the reaction arrow to specify reaction direction.

Atom Short

-X =R

1-4

reactant

product

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

Variables

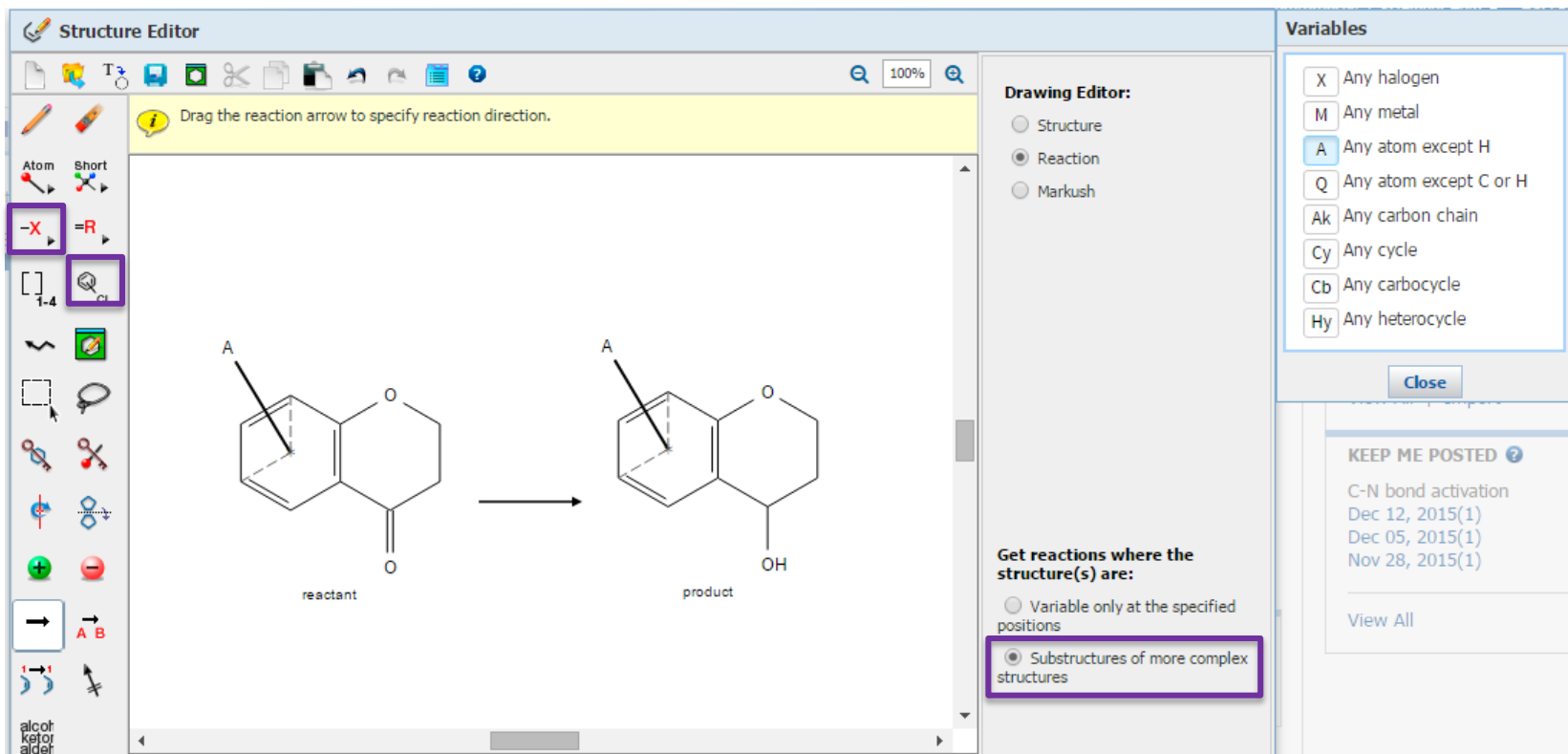
- X Any halogen
- M Any metal
- A Any atom except H
- Q Any atom except C or H
- Ak Any carbon chain
- Cy Any cycle
- Cb Any carbocycle
- Hy Any heterocycle

Close

KEEP ME POSTED

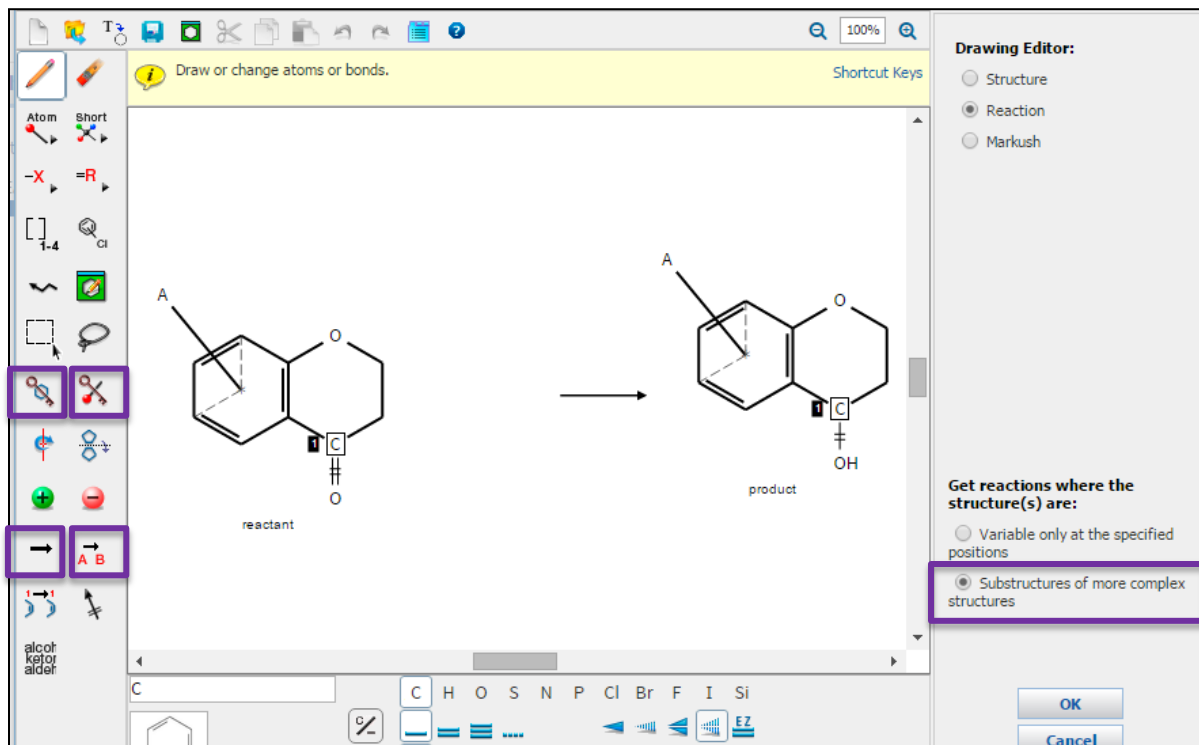
C-N bond activation  
Dec 12, 2015(1)  
Dec 05, 2015(1)  
Nov 28, 2015(1)

View All





## 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

Analyze by: [?](#)  
Reagent

NaBH <sub>4</sub>	529
HCl	425
K <sub>2</sub> CO <sub>3</sub>	387
Et <sub>3</sub> N	367
H <sub>2</sub>	353
NaOH	299
NaHCO <sub>3</sub>	235
Et <sub>3</sub> N •HCl	228
LiBH <sub>4</sub>	190
13289-97-9	149

[Show More](#)

Group by:  Sort by:  [↓](#)

of 1107 Reactions Selected Display Options  of 23 [▶](#)

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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

~43

→

~5

**Overview**

Steps/Stages	Notes
1.1 R:NaBH <sub>4</sub> , S:MeOH, overnight, rt	Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

# 亚结构反应检索结果

Analyze Refine

Group by: No Grouping Sort by: Accession Number

0 of 30 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~5 ~3

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups**

Non-participating Functional Group(s)

View: All 217

1 Selected Clear Selections

- Acetal
- Acetyl
- Acid Halide
- Acyclic Alkene
- Acyclic Ketone
- Acylmetal
- ALCOHOLS

Reactions must have

- all selections**
- any selection

**Overview**

**Steps/Stages**

1.1 R:NaBH<sub>4</sub>, S:MeOH, rt

**Notes**

Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

Identification of 3-hydroxy-4[3,4-dihydro-3-oxo-2H-1,4-benzoxazin-4-yl]-2,2-dimethyldihydro-2H-benzopyran derivatives as potassium channel activators and anti-inflammatory agents

Quick View Other Sources

**限定某官能团参与**

# 亚结构反应检索结果

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

2. View Reaction Detail [Link](#) [Similar Reactions](#)

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

~89

~10

**Overview**

**Steps/Stages**

1.1 S:Me<sub>2</sub>CO, 9 d, rt

**Notes**

biotransformation, enzymic, stereoselective, 100% ee, 100% conversion, Chaetomium sp.1 used, Reactants: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

[selective reduction of 4-chromanone and its derivatives by selected filamentous](#)

[View](#) [Other Sources](#)

ko, Tomasz et al  
Journal of Molecular Catalysis B: Enzymatic, 97, 278-282; 2013

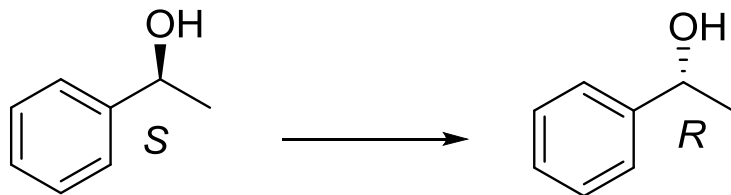
反应分类：生物转化反应，催化/非催化反应，光化学，电化学，顺反选择，手性立体选择等等）

# 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

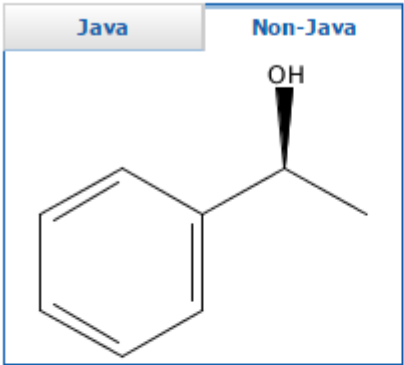


思路：通过物质检索，分别获得起始物和产物的一步反应，再对结果集进行交集。

# 在物质检索中通过精确结构检索起始物

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF


**Search**

Search Type:

- Exact Structure
- Substructure
- Similarity

---

Show precision analysis

 ChemDraw<sup>®</sup>

Launch a SciFinder substance  
More

Select All Deselect All

1 of 4 Stereo Candidates Selected

- Absolute stereo match
- Absolute stereo mirror image
- Relative stereo match
- Stereo that doesn't match query
- No stereo in answer structure

**Get Substances**

# 精确检索S构型物质，获得其为“起始物”的反应

**SUBSTANCE DETAIL** Retrieve reaction information for this record.

[Return](#)

**1. CAS Registry Number 1445-91-6**

~3,350 ~99

**C<sub>8</sub> H<sub>10</sub> O**  
Benzenemethanol, α-methyl-, (αS)-

**Molecular Weight**  
122.16

**Boiling Point (Experimental)**  
Value: 93 °C | Condition: Press: 14 Torr

**Density (Predicted)**  
Value: 1.013±0.06 g/cm<sup>3</sup> | 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



# 将反应结果集限定为一步反应

REACTIONS

Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Accession Number

0 of 7373 Reactions Selected

1. View Reaction Detail Link

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

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Number of Steps:   
Examples: 1, 1 - 3, 1 -, - 3

O=C(O)c1ccccc1[N+](=O)[O-] + O=C(O)

~114

将所得结果集保存为“answer1”

Save This Answer Set

\* Required

Save:

- All answers
- Only selected answers

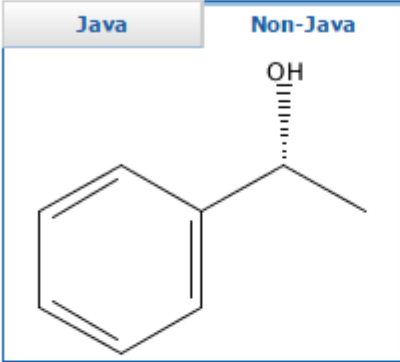
Title: \*

Description:

# 在物质检索中通过精确结构检索产物

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF


**Search**

Search Type:

- Exact Structure
- Substructure
- Similarity

---

Show precision analysis

 ChemDraw®  
Launch a SciFinder substance  
More

Select All Deselect All

1 of 4 Stereo Candidates Selected

- Absolute stereo match
- Absolute stereo mirror image
- Relative stereo match
- Stereo that doesn't match query
- No stereo in answer structure

**Get Substances**

# 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<sub>8</sub>H<sub>10</sub>O**

Benzenemethanol, *o*-methyl-, (*α*,*R*)-

### Molecular Weight

122.16

### Melting Point (Experimental)

Value: 9-11 °C

### Boiling Point (Experimental)

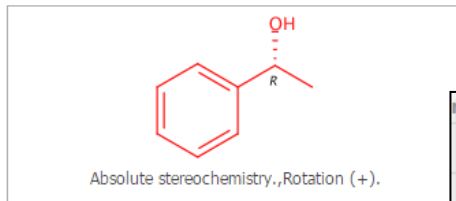
Value: 98 °C

### Density (Predicted)

Value: 1.013±0.06 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr

### pKa (Predicted)

Value: 14.43±0.20 | Condition: Most Acidic Temp: 25 °C



## 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

REACTIONS ?

Get References Tools

Analyze **Refine**

Group by: No Grouping Sort by: Accession Number

0 of 3991 Reactions Selected

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Number of Steps:   
Examples: 1, 1 - 3, 1 -, - 3

**Refine**

1. **View Reaction Detail** [Link](#) [Similar Reactions](#)

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

CC(=O)c1ccccc1 →

~127

**Overview**

将所得结果集保存为“answer2”

3991) **Save This Answer Set**

\* Required

**Save:**

- All answers
- Only selected answers

**Title: \***

**Description:**

**OK** **Cancel**

## 将answer1和answer2合并取交集

**Combine Answer Sets**

2 of 30 Reaction Answer Sets Selected    **References (13)**    **Substances (1)**    **Reactions (30)**

- answer2 (3629)  
Chemical Structure exact > substances (54) > 151
- answer1 (678)  
Chemical Structure exact > substances (52) > 144

**Combine Answer Sets**

Select an option for combining the two selected saved answer sets:

- Combine**    Include all reactions from both sets
- Intersect**    Include only reactions that appear in both sets
- Exclude**    Include only answers from answer2 that are not in answer1
- Exclude**    Include only answers from answer1 that are not in answer2

# 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 ▾ ↓

0 of 16 Reactions Selected

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

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

~99 ~127 ~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

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Primary Alcohol reactant

Secondary Alcohol non-reacting

Aldehyde product

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

OK




Cancel

Formula is not available


C H O S N P Cl Br F I Si

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

REACTIONS   Get References  Tools



Analyze Refine

Analyze by:  Reagent

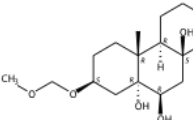
NaHCO <sub>3</sub>	1891
Et <sub>3</sub> N	1836
1H-Imidazole	1222
Bu <sub>4</sub> N <sup>+</sup> • F <sup>-</sup>	1154
NH <sub>4</sub> Cl	1104
2,6-Lutidine	1005
Martin's reagent	976

Group by: No Grouping Sort by: Accession Number ↓


0 of 5067 Reactions Selected

1. View Reaction Detail  Link  Similar Reactions

Single Step *Hover over any*



> reactions (5067) > reactions with transformation "Oxidation or Dehydrogenation o..." (1448)

Get References  Tools

Group by: Transformation Sort by: Frequency ↓

0 of 5067 Reactions Selected

1. Oxidation or Dehydrogenation of Alcohols to Aldehydes and Ketones  
1448 Reactions

$$\begin{array}{ccc} \text{OH} & & \text{O} \\ | & \longrightarrow & || \\ \text{R}-\text{C} & & \text{R}-\text{C}-\text{R}^1 \\ | & & \\ \text{R}^1 & & \end{array}$$



Reaction Structure substructure > reactions (5067) > reactions with transformation "Oxidation or Dehyd

REACTIONS

Analyze Refine

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Get References

Structure Editor

Group by: No Grouping

0 of 1448 Reactions Selected

1. View Reaction Detail [Similar Reactions](#)

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

Atom Short

Click a ring system to block it from

Chemical structure: CC=O

Overview

Steps/Stages

Continue using "acetaldehyde" structure to refine results.

REACTIONS

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

Get References

Tools

Group by: No Grouping Sort by: Relevance

0 of 369 Reactions Selected

1. View Reaction Detail [Similar Reactions](#)

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

Chemical structure: CC(O)CO

Reaction Classification(s):

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Overview

Steps/Stages

1.1 C:CeO<sub>2</sub>, 425°C

Refine

Use limiting functions to select reactions by type.

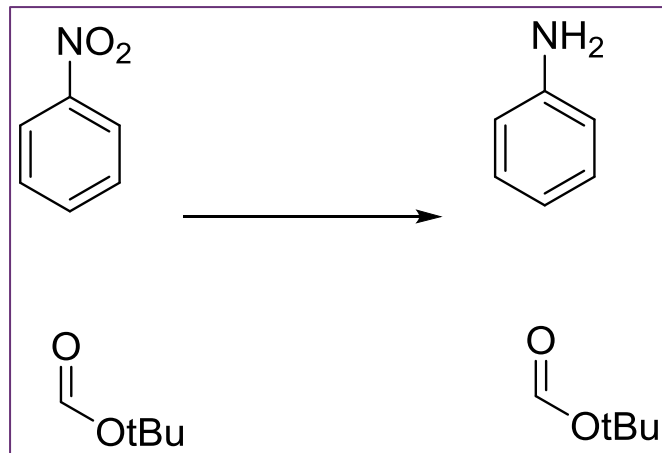
# 提纲

- 反应检索

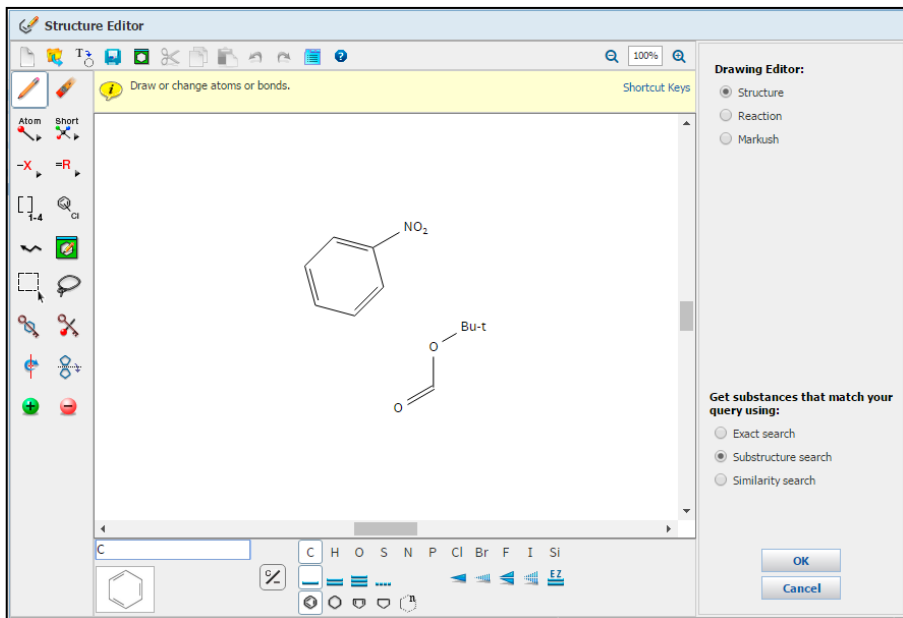
- 反应检索绘制工具及反应信息详情
- 如何通过Analyze、Refine来精选反应
- 亚结构反应检索
  - 手性反转反应
  - 在非反应仲醇存在的条件下，将伯醇转换为乙醛
  - 片段反应

## 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



Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Import CXF

Search

Advanced Search Always Show

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw®  
Launch a SciFinder substance  
More

Characteristics

- Single component
- Commercially available
- Included in references


# 获得亚结构检索结果，并获得这些物质作为反应物的反应

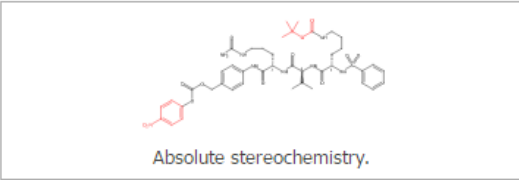
Get References **Get Reactions** Retrieve reactions for selected substances.

Sort by: CAS Registry Number

0 of 35896 Substances Selected

1. **1884208-13-2** 🔍


--1 

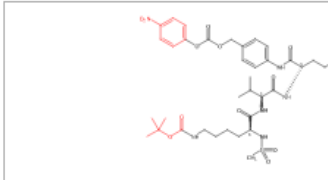


Absolute stereochemistry.

**C<sub>42</sub> H<sub>56</sub> N<sub>8</sub> O<sub>13</sub> S**  
INDEX NAME NOT YET ASSIGNED  
▶ **Key Physical Properties**

2. **1884208-09-6** 🔍

--1 



Absolute stereochemistry.

**C<sub>37</sub> H<sub>54</sub> N<sub>8</sub> O<sub>13</sub> S**  
INDEX NAME NOT YET ASSIGNED  
▶ **Key Physical Properties**

### Get Reactions

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

- Product
- Reactant
- Reagent
- Reactant or reagent
- Catalyst
- Solvent
- Any role

# 限定反应步数为一步反应

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Chemical Structure substructure with limiters > substances (35896) > get reactions (374800) > get reactions (374800)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Accession Number ↓

0 of 374800 Reactions Selected Page: 1 of 7496

Refine by: ⓘ

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Number of Steps:  Examples: 1, 1 - 3, 1 -, - 3 Refine

1. View Reaction Detail ⓘ Link

4 Steps Hover over any structure for more options.

[Step 2.1] ~38

[Step 3.1] ~74

[Step 4.1]

# 反应结构限定

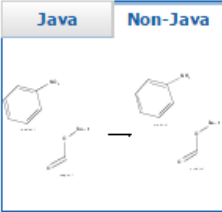
Analyze Refine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Structure Editor:

Java Non-Java

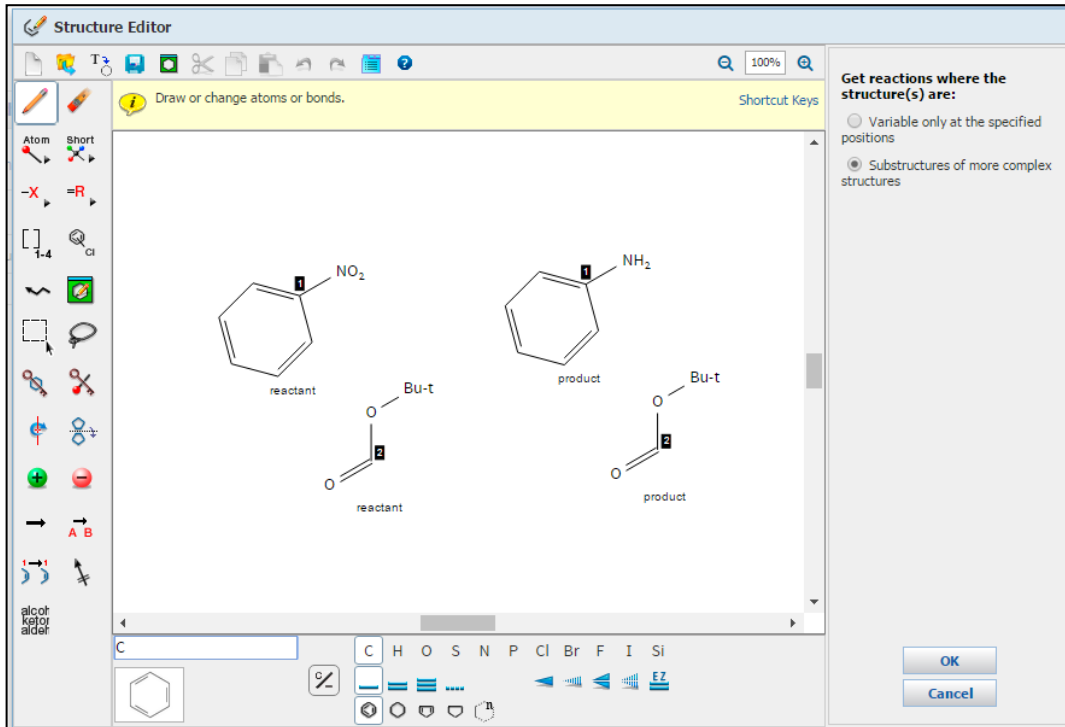


Click image to change structure or view detail.  
Search type: **Substructure**

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

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.*

~31      100%      ~112

**Overview**

**Steps/Stages**

1.1 R:H<sub>2</sub>, 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](http://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



Your single source to search and compare  
the latest published scientific methods.

Log In with your CAS Username

[Learn more](#)

Username

Password

Log In

[Forgot Username or Password?](#)

Use of this product means that you agree to the [Terms & Conditions](#).

# MethodsNow Analysis (www.methodsnow.com)

保存结果集

检索/高级检索



方法分类



历史检索



The screenshot shows the MethodsNow Analysis website interface. At the top, there is a navigation bar with the logo 'METHODSNOW A CAS SOLUTION' and user options 'Saved' and 'Account'. Below the navigation bar is a search section with a search bar and a magnifying glass icon. Underneath the search bar is an 'Advanced Search' link. The main content area is titled 'Browse Method Categories' and lists various categories such as 'Agricultural Applications / Analysis', 'Bioassays', 'Biomolecule Isolation', 'Environmental Analysis', 'Food Analysis', 'Pharmacology / Toxicology', 'Polymer Analysis', and 'Water Analysis'. At the bottom of the page, there is a 'Recent Searches' section with a search history entry 'hplc lycopene analysis' and a close button (X).

Click a browse category to view related methods

Click historical search to re-run search

Click "X" to delete search history

# 高级检索



[Return to Home](#)

## Advanced Search

Keyword

AND  Matrix

AND  Analyte

逻辑运算符: and, or, not

删除一条检索条件

Add Search Criteria



增加一条检索条件



[Return to Home](#)

## Advanced Search

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



Results (1704)

目前手性化合物拆分的文献量

Sort Relevance

[← 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**



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 $\mu$ m Whatman filter paper; Acetyl- $\beta$ -cyclodextrin
Method Category	Chiral Separation
Technique	Liquid chromatography spectrometric detectors; Capillary zone electrophoresis
Equipment Used	Capillary electrophoresis system; Diode array detector
Source	<b>Determination of the R-enantiomer of valsartan in pharmaceutical formulation by capillary electrophoresis</b> 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	<a href="#">View Structure</a>	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	<a href="#">View Structure</a>	67-56-1
Diethylamine	reagent	<a href="#">View Structure</a>	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<sup>-1</sup> 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  $\mu\text{g}$  as limit of detection (LOD) and 0.015  $\mu\text{g}$  as limit of quantification (LOQ) for (R,R)-sertraline, for 10  $\mu\text{L}$  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 ( $1000 \mu\text{g mL}^{-1}$ ) 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 solution of sertraline hydrochloride 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 afflow rate of  $0.7 \text{ mL min}^{-1}$ .
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 $\mu\text{g}$ , of 100 $\mu\text{g mL}^{-1}$ analyte concentration, (R, R) - sertraline
Limit of Quantitation	0.015 $\mu\text{g}$ , of 100 $\mu\text{g mL}^{-1}$ analyte concentration, (R, R) - sertraline
Recovery	98.3%, RSD 0.7%, 0.075 $\mu\text{g}$ spiked bulk drug sample, (R, R) - sertraline (sample 1) 100.1%, RSD 0.4%, 0.150 $\mu\text{g}$ spiked bulk drug sample, (R, R) - sertraline (sample 2) 101.4%, RSD 0.8%, 0.225 $\mu\text{g}$ spiked bulk drug sample, (R, R) - sertraline, (sample 3) 100.8%, RSD 0.5%, 0.150 $\mu\text{g}$ spiked dosage sample, (R, R) - sertraline, (sample 4) 98.5%, RSD 0.8%, 0.075 $\mu\text{g}$ spiked dosage sample, (R, R) - sertraline, (sample 5) 101.8%, RSD 0.8%, 0.225 $\mu\text{g}$ 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

## Search

Enter keyword, matrix, analyte, etc.

- lubricating oil additives
- lubricating oil additives, antioxidants
- lubricating oils**

Browse Method Categories

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

Recent Searches



## 选中分析物和基质

### ^ Analyte

- Copper (31)
- Nickel (20)
- Iron (16)
- Lead (16)
- Chromium (14)

[View All](#)

### ^ Matrix

- Lubricating oils (41)
- Petroleum (14)
- Gasoline (12)
- Gas oils (11)
- Petroleum refining residues (11)

[View All](#)

## 选中技术手段

### ^ Technique

- Flame atomic absorption spectroscopy (12)
- Inductively coupled plasma mass spectrometry (9)
- Electrothermal atomic absorption spectroscopy (8)
- Inductively coupled plasma atomic emission spectrometry (7)
- Ore genesis (7)

[View All](#)



## 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	<a href="#">View Structure</a>	7440-66-6
Lubricating oils	matrix		
Hollow cathode lamp (HCL)	material		
Titanium ultrasound probe	material		
High density polypropylene bottles	material		
Hydrogen peroxide	reagent	<a href="#">View Structure</a>	7722-84-1
Hydrochloric acid	reagent	<a href="#">View Structure</a>	7647-01-0
Nitric acid	reagent	<a href="#">View Structure</a>	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<sub>2</sub>O<sub>2</sub>, 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<sup>-1</sup> 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<sup>-1</sup>.

# 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<sub>3</sub>.
2. Store in high density polypropylene bottles.

## 结果有效性数据

### Validation

Limit of Detection	17.6 $\mu\text{g/L}$
Recovery	92 - 119%
Precision	4% (RSD)
Concentration	0.881 $\pm$ 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

[← Return to Home](#)

**^ Analyte**

- Nickel (18)
- Copper (17)
- Chromium (14)
- Iron (14)
- Lead (14)

[View All](#)

**^ Matrix**

- Lubricating oils (41)
- Petroleum (14)
- Gasoline (12)
- Gas oils (11)
- Petroleum refining residues (11)

[View All](#)

**∨ Method Category**

## Results (41)

[Analysis of Zinc in Lubricating oils by Ultrasonic extraction](#)  
CAS MN: 1-135-CAS-1225564

[View Details & Instructions](#) [Remove from Compare](#)

Analyte	Zinc
Matrix	Lubricating oils
Other Materials	Reagent: Hydrochloric acid; Hydrogen peroxide
Method Category	Petroleum Product Analysis; Element Detection
Technique	Ultrasonic extraction; Inductively coupled plasma atomic emission spectrometry
Equipment Used	ultrasonic bath; thermostatic bath; ICP-OES spectrometer
Source	Voltammetric Determination of Zinc in Lubricating Oils

Sort Relevance ▾  
Compare Results

[Compare \(1/3\)](#)

# 方法对比

		1	2	3	
Title	Analysis by Example	Other Materials	Hydrochloric acid; 18-Crown-6; Ethanol; Hexane; Acetone; 4-Bromomethyl-7-methoxycoumarin; Potassium bicarbonate; <a href="#">View All</a>	Acetonitrile; Boric acid (H <sub>3</sub> BO <sub>3</sub> ); Sodium hydroxide; Ethanol; Spherisorb ODS-2 (250 mm × 4.6 mm i.d., 5 μm); ODS guard <a href="#">View All</a>	Nitric acid; Acetone; Hydrogen peroxide
CAS Method Number	1-106	Equipment Used	Liquid chromatograph, 1100, Agilent Technologies, Waldbronn, Germany; Quaternary pump, Agilent Technologies. <a href="#">View All</a>	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, <a href="#">View All</a>
Method Category	Archaeology	Conditions	<b>Instrument:</b> Mobile phase: mixture of methanol-water; flow rate 1.5 mL/min; Detection wavelength: excitation at 325 nm <a href="#">View All</a>	<b>Instrument:</b> Mobile phase: mixture of acetonitrile (A) and water (B); flow rate 1.1 mL/min; Detection wavelength: excitation at <a href="#">View All</a>	<b>Instrument:</b> Radio frequency power: 1200 W; plasma gas flow: 13 L/min; auxiliary gas flow: 0.75 L/min; nebulizer gas flow: 0.87 <a href="#">View All</a>
Technique	Fluorescence Spectroscopy	Source	<b>Identification of lipid binders in old oil paintings by separation of 4-bromomethyl-7-methoxycoumarin derivatives of fatty</b> <a href="#">View All</a>	<b>Effect of calibration standards on the quantification of hydroxy products from can coatings</b> <a href="#">View All</a>	<b>Quantitative lead determination in coating paint on children's outwear by LA-ICP-MS: A practical calibration strategy for solid</b> <a href="#">View All</a>
Analyte	Oleic Acid, Stearic Acid				
Matrix	Coatings, Poppy Seed Oil				

# 所有方法详情都可以进行对比

Method	Extraction and derivatization 1. Place solid parts scalpered from the nitrocellulose disk (0.5–1 cm) in a <a href="#">View All</a> ▾	Determination of BADGE-2H <sub>2</sub> O and BFDGE-2H <sub>2</sub> O by LC-FLD 1. Perform the analysis on a LC system <a href="#">View All</a> ▾	Microwave-assisted acid digestion 1. Prepare the calibration curve in 2% HNO <sub>3</sub> by incremental amount as 0 <a href="#">View All</a> ▾	
Linearity Range	1.0 × 10 <sup>-7</sup> to 1.8 × 10 <sup>-4</sup> mmol for all analytes		0 - 150 ng/mL	
Limit of Detection	6.0 × 10 <sup>-8</sup> mmol for all analytes		0.002 ng/mL	
Recovery	70 ± 10% for 100 µL (poppy seed oil), myr seed		101.3% (EC681k (polyethylene)), 95.3%	
Retention Time 10.8 min, min. <a href="#">View</a>	Concentration		0.884 ± 0.003 µg/mL, BADGE 2H <sub>2</sub> O, 0.966 ± 0.004 µg/mL, BFDGE 2H <sub>2</sub> 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](mailto:china@acsi.info)

中文网站：<http://www.cas-china.org/>

英文网站：<http://www.cas.org/>

