

朱传娴

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# 美国化学文摘社(CAS) 持续推动科技创新



课程签到码



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A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

# 大纲

- 为什么需要美国化学文摘社
- CAS主要产品
  - SciFinder Web（简称SciFinder）
  - SciFinder<sup>n</sup>
  - PatentPak
  - MethodsNow

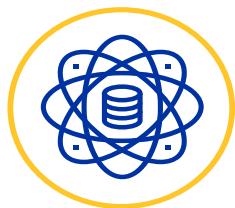


课程签到码

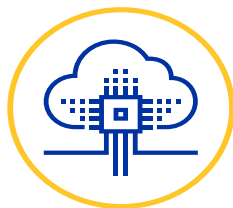


# 美国化学文摘社(CAS)隶属美国化学会(ACS)，致力于追踪、收录、标引科学信息

- 拥有超过110年的经验；创立权威化学索引《化学文摘》(CA)
- 密切追踪、标引和提炼着全球化学相关的文献（包括专利）
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新, 助力于解决科研方面的难题与挑战



**UNPARALLELED**  
SCIENTIFIC CONTENT



**SPECIALIZED**  
TECHNOLOGY



**UNMATCHED**  
HUMAN EXPERTISE



课程签到码



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# CAS数据覆盖学科

- 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



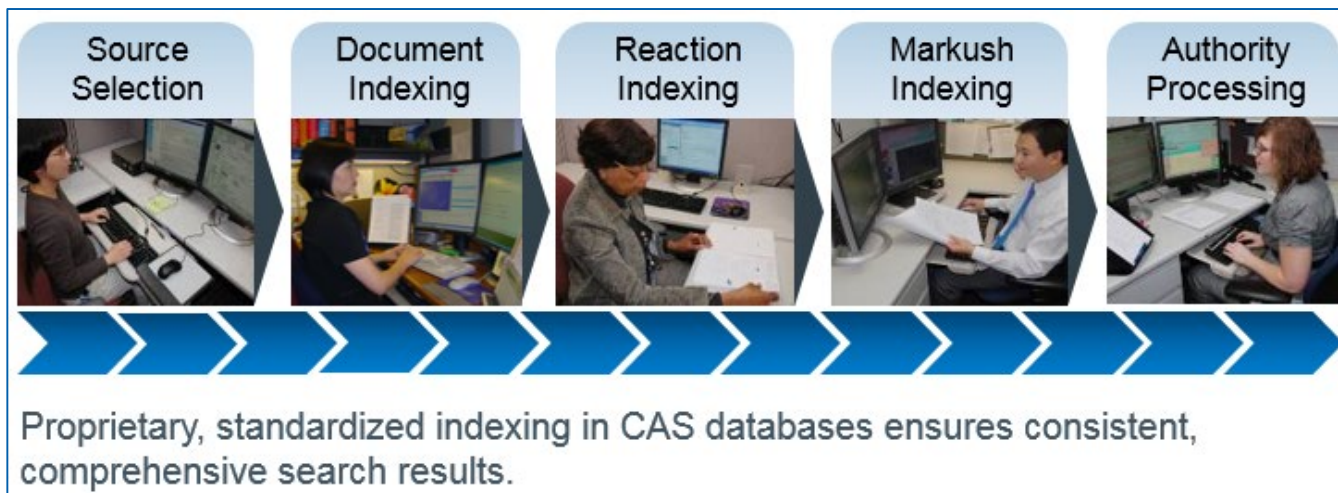
课程签到码



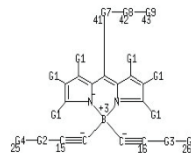
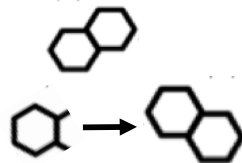
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# CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘



1990  
Smith, M.  
anthracene



Androst-4-en-  
3-one, 17-  
hydroxy-17-  
methyl-, (17β)-



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## CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

- 人工标引——精准揭示关键技术信息
- 数千名科学家组成的编辑团队深刻理解客户的实际需求
- 审阅、筛选、摘要、标引以覆盖并揭示全球所有已公开的化学及相关信息
- CAS登记号——物质的黄金标准
- CAS Roles (CAS物质角色)——生物研究、性能用途、分析检测、合成制备
- CAS Index Terms (CAS技术词语标准)——揭示技术词语相互间的关联
- CA Sections (CAS学科分类，80个类别)——精准定位具体研究领域



课程签到码



# CAS各类科学信息研究工具

STNext™

SCIFINDER™  
A CAS SOLUTION

PATENTPAK™  
A CAS SOLUTION

FORMULUS™  
A CAS SOLUTION

SCIFINDER<sup>n</sup>  
A CAS SOLUTION

CHEMZENT™  
A CAS SOLUTION

More coming!

METHODSNOW™  
A CAS SOLUTION

NCI™ GLOBAL  
A CAS SOLUTION



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# LIMITLESS POSSIBILITIES 无限可能

## 定制服务应对挑战.



### CONTENT SERVICES 内容服务

- 定制数据集合  
Content licensing
- 数据结构  
Data structure
- 数据平台  
Data platforms



### TECHNOLOGY SERVICES 技术服务

- 数据架构  
Data architecture
- 平台整合  
Platform integration
- 检索引擎  
Search engines
- 定制解决方案  
Custom solutions



### KNOWLEDGE SERVICES 知识服务

- 外包IP检索  
Outsourced IP search
- 数据分析  
Analytics
- 机会分析  
Opportunity exploration
- 技术评估  
Technical Assessment



### PROFESSIONAL SERVICES 专业服务

- 人员派遣  
Talent augmentation
- 咨询  
Consulting
- Technical writing  
科技写作
- Scientific analysis  
科研分析





# 大纲

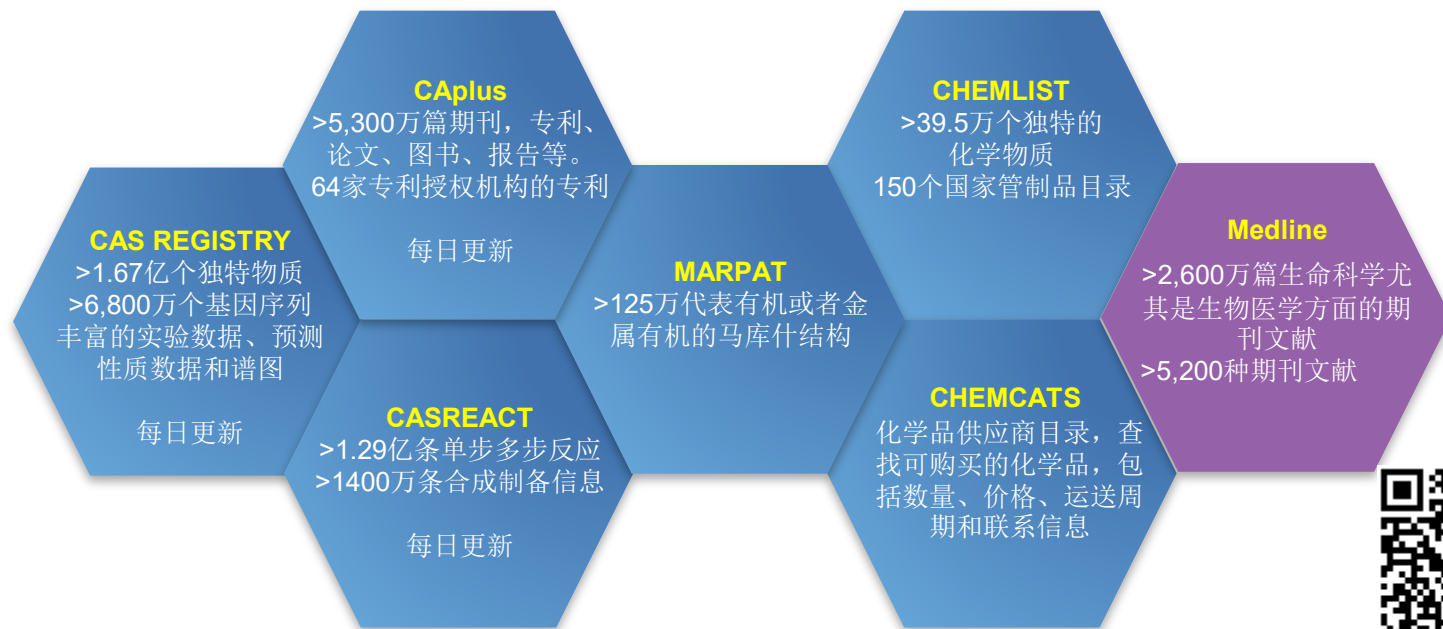
- 为什么需要美国化学文摘社
- CAS主要产品
  - SciFinder Web（简称SciFinder）
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  - PatentPak
  - MethodsNow



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# SciFinder覆盖的数据库



SciFinder是提供经CAS科学家人工标引内容的工具型数据库。




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# SciFinder Web登录网址: <https://SciFinder.cas.org>




Log In to SciFinder®

Username or Email Address

Next

[Can't log in?](#)



Log In to SciFinder®

Welcome, scicas7521 [Not You?](#)

Password

Log In

Keep me signed in

[Can't log in?](#)



课程签到码

每个用户必须注册后才能使用

# SciFinder Web主界面

The screenshot shows the SciFinder web interface with several callout boxes in Chinese:

- 文献检索** (Literature Search): Points to the left sidebar menu.
- 物质检索** (Substance Search): Points to the 'SUBSTANCES' section in the sidebar.
- 反应检索** (Reaction Search): Points to the 'REACTIONS' section in the sidebar.
- 工具栏** (Toolbar): Points to the top navigation bar containing 'Explore', 'Saved Searches', and 'SciPlanner'.
- 已保存的结果集** (Saved Results Sets): Points to the 'SAVED ANSWER SETS' panel on the right.
- 定题追踪** (Topic Tracking): Points to the 'KEEP ME POSTED' section at the bottom right.

The interface includes a search bar with a 'Search' button and an 'Advanced Search' link. The sidebar lists search criteria under three categories: REFERENCES, SUBSTANCES, and REACTIONS. The right sidebar shows a list of saved answer sets and a 'KEEP ME POSTED' section.

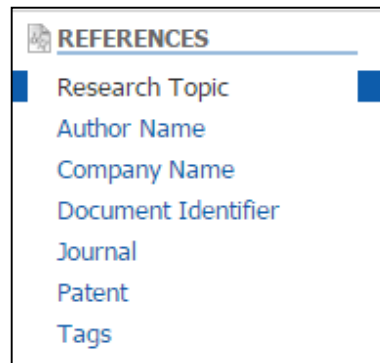
# SciFinder Web检索——文献检索

## 文献检索方法

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

## 检索策略推荐

- 关注某特定领域的文献：主题检索
- 关注物质有关的文献：先获得物质，再获得文献
- 关注某科研人员的文献：作者名检索
- 关注某机构科研进展：机构名检索



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# SciFinder Web检索——文献检索

The screenshot displays the SciFinder web interface. The top navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows a search for 'nano with immunotherapy of cancer' with a 'Search' button and an 'Advanced Search' link. Below the search, a list of 11 research topic candidates is shown, each with a checkbox and a reference count.

Research Topic Candidates Selected	References
<input checked="" type="checkbox"/> 744 references were found containing all of the concepts "nano", "immunotherapy" and "cancer" closely associated with one another.	744
<input type="checkbox"/> 2734 references were found where all of the concepts "nano", "immunotherapy" and "cancer" were present anywhere in the reference.	2734
<input type="checkbox"/> 1697 references were found containing the two concepts "nano" and "immunotherapy" closely associated with one another.	1697
<input type="checkbox"/> 4144 references were found where the two concepts "nano" and "immunotherapy" were present anywhere in the reference.	4144
<input type="checkbox"/> 63058 references were found containing the two concepts "nano" and "cancer" closely associated with one another.	63058
<input type="checkbox"/> 109454 references were found where the two concepts "nano" and "cancer" were present anywhere in the reference.	109454
<input type="checkbox"/> 50122 references were found containing the two concepts "immunotherapy" and "cancer" closely associated with one another.	50122
<input type="checkbox"/> 97303 references were found where the two concepts "immunotherapy" and "cancer" were present anywhere in the reference.	97303
<input type="checkbox"/> 2318356 references were found containing the concept "nano".	2318356
<input type="checkbox"/> 187476 references were found containing the concept "immunotherapy".	187476
<input type="checkbox"/> 4775515 references were found containing the concept "cancer".	4775515

输入关键词检索，之后根据检索要求勾选候选项

# SciFinder Web检索——文献检索

The screenshot displays the SciFinder web interface. At the top, there are navigation tabs: "Get Substances", "Get Reactions", "Get Related Citations", and "Tools". Below these, the search results are listed, with the first result selected. The main content area shows the details of the first article: "Greener solid state synthesis of a ternary lanthanum complex at room temperature".

Overlaid on the interface are three panels:

- Analyze Panel:** Shows a list of fields to analyze, including Author Name, CAS Registry Number, CA Section Title, Company-Organization, Database, Document Type, Index Term, CA Concept Heading, Journal Name, Language, Publication Year, and Supplementary Terms. A "Show More" button is at the bottom.
- Refine Panel:** Provides options to refine the search by Research Topic, Author, Company Name, Document Type, Publication Year, Language, or Database.
- Categorize Panel:** Contains a table for selecting a heading and category, and index terms of interest.

**Table 1: Categorize Panel**

Category Heading	Category	Index Terms	Selected Terms
All	Substances (20113)		
Technology	Topics (391)		
General chemistry			
Biology			
Physical chemistry			
Genetics & protein chemistry			
Synthetic chemistry			
Biotechnology			
Polymer chemistry			
Environmental chemistry			
Analytical chemistry			
Catalysis			

Buttons: OK, Cancel

对于文献结果集进行筛选  
Analyze、Refine、Categorize



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# SciFinder Web检索——文献记录

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

By: Peyman, Gholam A.  
Assignee: USA

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

### Patent Information

Patent No.	PatentPak Options	Kind	Language	Date	Application No.	Date
US 20170172932	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	A1		Jun 22, 2017	US 2016-15143981	May 2, 2016
US 9849092	<a href="#">PDF</a>	B2	English	Dec 26, 2017		
US 20170173191	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	A1	English	Jun 22, 2017	US 2015-14976321	Dec 21, 2015

### Priority Application

US 2015-14976321	A2	Dec 21, 2015
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### Indexing

Immunochemistry (Section15-3)
Section cross-references: 1, 8, 14, 63
<b>Concepts</b> <b>重要概念</b>
Clustered regularly interspaced short palindromic repeat
CRISPRi; early cancer detection and enhanced immunotherapy/thermotherapy/ optionally gene delivery combination
Therapeutic use; Biological study; Uses
Virus-like particle

### Substances

1425049-49-5 Cas9 nuclease	Page 21 in PATENTPAK
CRISPR/cas9 complex; early cancer detection and enhanced immunotherapy/thermotherapy/ optionally gene delivery combination	
Therapeutic use; Biological study; Uses	

### CAS Role

### QUICK LINKS

0 Tags, 0 Comments

### PATENT INFORMATION

Jun 22, 2017  
US 20170172932  
A1

### APPLICATION

May 2, 2016  
US 2016-15143981

### PRIORITY

Dec 21, 2015  
US 2015-14976321

### SOURCE

U.S. Pat. Appl. Publ. No. 2017/0172932, 22pp., Cont.-in-part of U.S. Pat. No. 976,321.  
Patent  
2017  
CODEN:USXXCO

### ACCESSION NUMBER

2017:1034814  
CAN167:99362  
CAPLUS

### LANGUAGE

English

文献详情界面包括:

- 标题
- 摘要
- 文献中重要的技术术语
- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
- 参考文献
- 链接原文



CAS

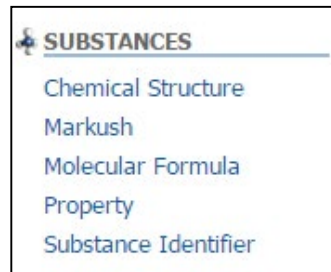
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# SciFinder Web检索——物质检索

## 物质检索方法

- 结构式检索
- 分子式检索
- 理化性质（物质属性）检索
- 物质标识符检索：化学名称，CAS RN
- 从文献或反应结果获得



## 物质检索策略推荐

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



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# SciFinder Web检索——物质检索

The screenshot displays the SciFinder web interface for substance search. It is divided into several sections:

- Navigation:** Explore, Saved Searches, SciPlanner.
- Left Panel:** REFERENCES (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), SUBSTANCES (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), REACTIONS (Reaction Structure).
- Main Search Area:** Substance Identifier "Aspirin" > substances (1). Input field contains "Aspirin". Search button is visible.
- Analyze/Refine Panel:** Analyze by: Substance Role, Bioactivity Indicators, Commercial Availability, Elements, Reaction Availability, Substance Role (selected), Target Indicators, Commercial Availability. Formation, Nonpreparative: 1; Miscellaneous: 1; Occurrence: 1; Preparation: 1; Process: 1; Properties: 1; Prophetic in Patents: 1. Show More button.
- Results Panel:** Substance Identifier "Aspirin" > substances (1). Sort by: CAS Registry Number. 0 of 1 Substance Selected. Result 1: 50-78-2. Chemical structure of Aspirin is shown. Key Physical Properties: C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> Benzoic acid, 2-(acetyloxy)-. Regulatory Information, Spectra, Experimental Properties.
- Refined Results Panel:** Opened saved answer set "Ak limited" (5358). Sort by: CAS Registry Number. 0 of 5358 Substances Selected. Refine by: Chemical Structure (selected), Isotope-Containing, Metal-Containing, Commercial Availability, Property Availability, Property Value, Reference Availability, Atom Attachment. Structure Editor: Java, Non-Java. Search type: Substructure. Only retrieve substances that: Have references, Are commercially available, Are a single component, Are in specific substance classes, Are in specific types of studies. Results list includes: 1. 2437834-71-2, 5. 2426690-81-3, 9. 2426690-67-5. Key Physical Properties: C<sub>6</sub>H<sub>6</sub> Benzene, (4-methylene-2-tetradecyn-1-yl)-; C<sub>6</sub>H<sub>6</sub> Benzene, (3-methyl-5-octen-7-yn-1-yl)-; C<sub>14</sub>H<sub>18</sub> INDEX NAME NOT YET ASSIGNED.

当物质结果集多时依然通过  
Analyze、Refine进行筛选

# SciFinder Web检索——物质记录

CAS Registry Number 50-78-2

~46,629   ~140 

**C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>**

Benzoic acid, 2-(acetyloxy)-

**Molecular Weight**

180.16

**Melting Point (Experimental)**

Value: 135 °C

**Boiling Point (Experimental)**

Value: 197-200 °C | Condition: Press: 7 Torr

**Density (Experimental)**

Value: 1.40 g/cm<sup>3</sup>

**pKa (Predicted)**

Value: 3.48±0.10 | Condition: Most Acidic Temp: 25 °C

**Other Names**

Rhodine (7CI)

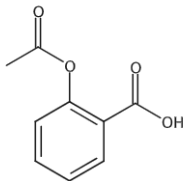
Salicylic acid acetate (8CI)

2-(Acetyloxy)benzoic acid

2-Acetoxybenzoic acid

2-Carboxyphenyl acetate

[View more...](#)



▶ EXPERIMENTAL PROPERTIES

实验属性

▶ EXPERIMENTAL SPECTRA

实验谱图

▶ PREDICTED PROPERTIES

预测属性

▶ PREDICTED SPECTRA

预测谱图

▶ REGULATORY INFORMATION

管制信息

▶ BIOACTIVITY INDICATORS

生物活性指示剂

▶ TARGET INDICATORS

生物靶点指示剂

▶ CAS REFERENCE ROLES

文献研究类别

▶ ADDITIONAL DETAILS

其他



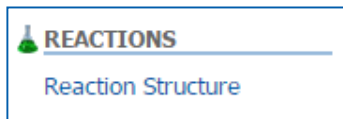
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# SciFinder Web检索——反应检索

- 反应检索方法

结构式



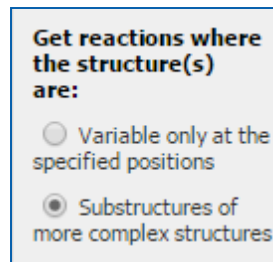
- 常用获取方法

已知物质：由物质获取反应

已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索



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# SciFinder Web检索——反应检索

The Structure Editor window displays a chemical reaction where nitrobenzene (reactant) is converted to aniline (product). The interface includes a toolbar on the left, a central drawing area, and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has three radio buttons: 'Structure', 'Reaction' (selected), and 'Markush'. Below these, a section titled 'Get reactions where the structure(s) are:' contains two options: 'Variable only at the specified positions' and 'Substructures of more complex structures' (selected). At the bottom, there are 'OK' and 'Cancel' buttons. The status bar at the bottom shows the chemical formula  $C_7H_7NO_2 \cdot C_7H_7N$  and the coordinates 137.14 . 107.16.

The REACTIONS search results interface shows a list of reactions and a reagent analysis table. The table lists reagents and their counts:

Reagent	Count
H <sub>2</sub>	≥ 8274
Fe	≥ 2235
HCl	≥ 2174
SnCl <sub>2</sub>	≥ 2074
NH <sub>4</sub> Cl	≥ 1851
Zn	≥ 1240
N <sub>2</sub> H <sub>4</sub> ·H <sub>2</sub> O	≥ 1154
NaOH	≥ 1135
NaHCO <sub>3</sub>	≥ 797
AcOH	≥ 697

The interface also shows a list of reactions, each with a 'View Reaction Detail' link and a 'Similar Reactions' link. The first reaction is highlighted, showing a chemical structure of nitrobenzene reacting to form aniline with a 100% yield. The interface includes a 'Show More' button and a 'Send to SciPlanner' button.

当反应结果集多时通过  
Analyze、Refine进行筛选

# SciFinder Web检索——反应记录

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

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

COc1ccc([N+](=O)[O-])cc1 → COc1ccc(N)cc1

100%

**Overview**

**Steps/Stages**

1.1  $\text{RiH}_2$ ,  $\text{R:Cs}_2\text{CO}_3$ , C:1610424-70-8, C:1034343-98-0 (oxide), Si:PhMe, 2 h, 100°C, 1 atm

**Notes**

palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, solid-supported catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions  
Quick View [or Other Sources](#)  
By Sabater, Sara et al  
From ACS Catalysis, 4(6), 2038-2047; 2014

**Experimental Procedure**

**Catalysis** **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of  $\text{H}_2$  to a mixture of nitroarene (0.3 mmol),  $\text{Cs}_2\text{CO}_3$  (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO ( $6 \times 10^{-3}$  mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with  $\text{H}_2$  in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

**METHODSNow™**

**Procedure**

1. Add molecular hydrogen with a balloon filled with 1 atm of  $\text{H}_2$  to a mixture of nitroarene (0.3 mmol),  $\text{Cs}_2\text{CO}_3$  (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO ( $6 \times 10^{-3}$  mmol, based on metal) in toluene (5 mL).
2. Then evacuate and backfill the system with  $\text{H}_2$  in cycles three times before putting the reaction vessel in an oil bath at 100 °C for 2 h.

[View more...](#)

[View with MethodsNow](#)

反应式

概览：步骤、反应试剂、溶剂、催化剂、温度、文献来源等

实验详情：来自原文

操作步骤：CAS编辑根据原文进行加工整理



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# SciFinder<sup>n</sup>是来自美国化学文摘社（CAS）的全新产品

- 基于用户习惯、需求、检索策略和革新技术，采用新方法将CAS内容传递给研究人员
- 先进的平台不仅需要实现信息的获取，还要帮助用户发现最佳起点
- CAS的化学信息历史积累、系统知识和人工智力能够加速您的工作

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# SciFinder<sup>n</sup>登录网址: <https://SciFinder-n.cas.org>




Log In to SciFinder<sup>n</sup>

Username or Email Address

Next

[Create an account.](#) | [Can't log in?](#)



Log In to SciFinder<sup>n</sup>

Welcome, scicas7521 [Not You?](#)

Password

Log In

Keep me signed in

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账号与SciFinder Web相同



# 简化的界面，快速执行检索

灵活的检索选项

快速运行之前的检索项目

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Search: treatment of cancer

Recent Searches

March 28, 2017

11:55 AM  
References: high temperature low density plasma (424K)

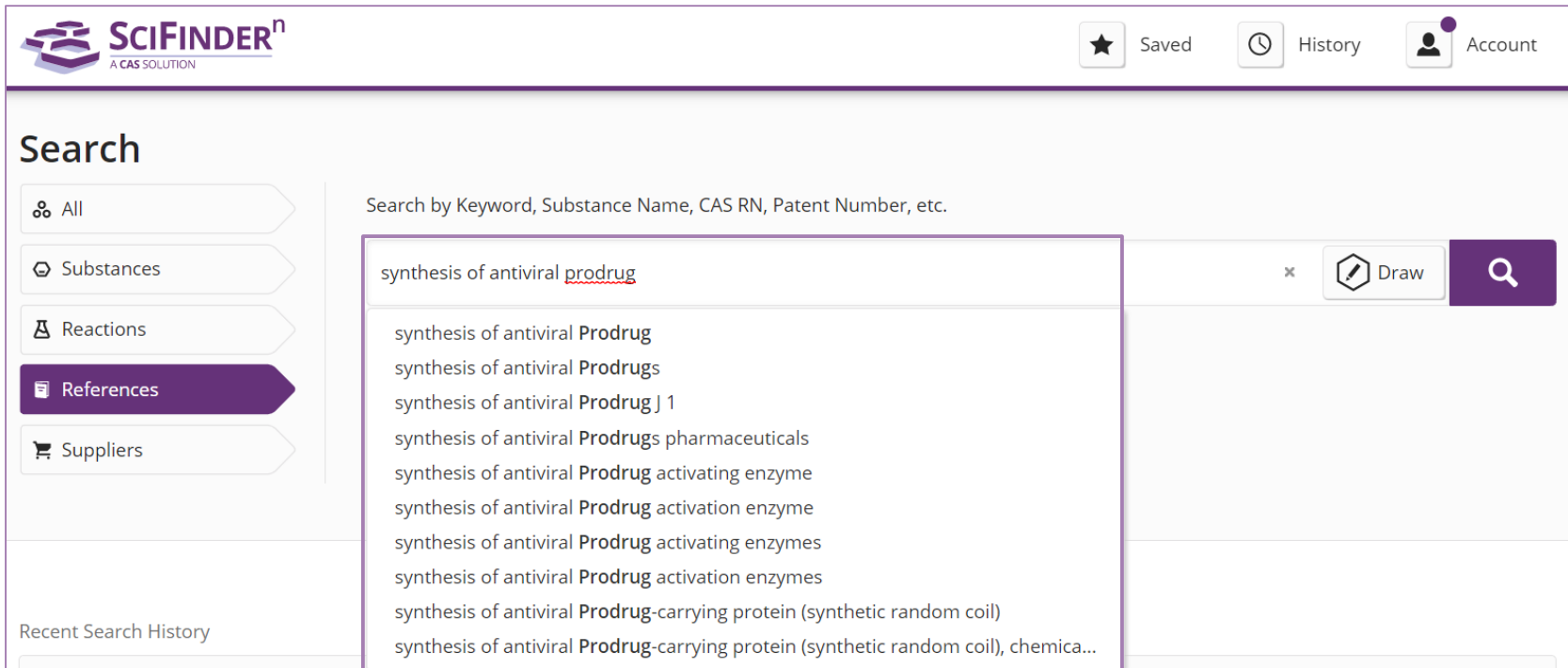
10:14 AM  
References: Advanced Search (6)  
Organization: Memorial Sloan-Kettering Cancer Ctr.

March 27, 2017

5:33 PM  
Reactions: Cc1c(Cl)c(Cl)c(Cl)c1Cl As Drawn (9), Substructure (39)

便捷地合并文本与结构检索

# 自动提示词，启发灵感；同时支持自然语言和布尔逻辑运算符



The screenshot displays the SciFinder search interface. At the top left is the SciFinder logo with the tagline 'A CAS SOLUTION'. On the top right, there are navigation icons for 'Saved', 'History', and 'Account'. The main search area is titled 'Search' and includes a sidebar with filters: 'All', 'Substances', 'Reactions', 'References' (highlighted), and 'Suppliers'. Below the filters is a 'Recent Search History' section. The search input field contains the text 'synthesis of antiviral prodrug'. A dropdown menu is open, showing a list of suggestions: 'synthesis of antiviral Prodrug', 'synthesis of antiviral Prodrugs', 'synthesis of antiviral Prodrug J 1', 'synthesis of antiviral Prodrugs pharmaceuticals', 'synthesis of antiviral Prodrug activating enzyme', 'synthesis of antiviral Prodrug activation enzyme', 'synthesis of antiviral Prodrug activating enzymes', 'synthesis of antiviral Prodrug activation enzymes', 'synthesis of antiviral Prodrug-carrying protein (synthetic random coil)', and 'synthesis of antiviral Prodrug-carrying protein (synthetic random coil), chemica...'. To the right of the search input is a 'Draw' button with a chemical structure icon and a search button with a magnifying glass icon.

# 支持布尔逻辑运算符及双引号，提高检索准确性

The screenshot shows the SciFinder search results page. The search query is "synthesis and antiviral prodrug". The results are sorted by Relevance and viewed as Partial Abstracts. The first result is titled "Metabolism, Biochemical Actions, and Chemical Synthesis of Anticancer Nucleosides, Nucleotides, and Base Analogs" by Shelton, Jadd; Lu, Xiao; Hollenbaugh, Joseph A.; Cho, Jong Hyun; Amblard, Franck; Schinazi, Raymond F. The abstract mentions that more than 20% of patients on antiviral treatment are treated with one or more of these analogs. The second result is titled "Synthesis and biological evaluation of prodrugs of zidovudine" by Aggarwal, Sunil K.; Gogu, Sudhir R.; Rangan, S. R. S.; Agrawal, Krishna C. The interface includes filters for Document Type and Language, and options to load more results or view full text.

synthesis and antiviral prodrug  
remdesivir or cinanserin  
antiviral prodrug not antitumor drug  
synthesis and (remdesivir or cinanserin)  
“total synthesis” of taxol

# 直观的结果页面，丰富的聚类分析

直观、丰富的聚类分析，  
助于快速分析和筛选

The screenshot shows the SciFinder interface with search results for 'synthesis and antiviral prodrug'. The page features a left sidebar with filters for Document Type, Language, Publication Year (with a histogram), Author, Organization, Publication Name, Concept, CAS Solutions, Formulation Purpose, Database, and Search Within Results. The main content area displays two search results. Result 1 is titled 'Metabolism, Biochemical Actions, and Chemical Synthesis of Anticancer Nucleosides, Nucleotides, and Base Analogs' by Shelton, Jadd, Lu, Xiao, Hollenbaugh, Joseph A.; Cho, Jong Hyun; Amblard, Franck; Schinazi, Raymond F. Result 2 is titled 'Synthesis and biological evaluation of prodrugs of zidovudine' by Aggarwal, Sunil K.; Gogu, Sudhir R.; Rangan, S. R. S.; Agrawal, Krishna C. Both results include abstracts and options for full text, substances, reactions, and citations.

# Citation Map: 引文地图, 发现相关的研究方向

## Citation Map

Synthesis and evaluation of novel amidate prodrugs of PMEA and PMPA

By: Ballatore, C.; McGuigan, C.; De Clercq, E.; Balzarini, J. *Bioorganic & Medicinal Chemistry Letters* (2001), 11(8), 1053-1056 | Language: English, Database: CAplus

[Full Text](#) ▾

**Abstract:** Some novel amidate prodrugs of PMEA and PMPA have been synthesized and tested in vitro for their biol. activity. Compound I in particular showed greatly enhanced antiviral potency compared with the parent nucleotide analog. In vitro enzymic studies and structure-activity relationships indicate that the degradation mechanism of such prodrugs may be the same as that described for the phosphoramidate triesters of nucleotide analogs.

### Filter by

Document Type

- Journal (68)
- Patent (3)
- Review (30)
- Conference (1)
- Editorial (1)

Author

Concept

- Antiviral agents (44)
- Prodrugs (33)
- Homo sapiens (28)
- Human (28)
- Human immunodeficiency virus 1 (19)

[View All](#)

### References This Document Cites

- Aryl Phosphoramidate Derivatives of d4T Have Improved Anti-HIV Efficacy in Tissue Culture and May Act by an Entirely New Mechanism of Reverse Transcriptase Inhibition  
*Journal of Medicinal Chemistry* (1996)  
Cited By 230 [Map](#)
- HPMPC (cidofovir), PMEA (adefovir) and related acyclic nucleoside phosphonate analogs: a review of their pharmacology and clinical potential in the treatment of viral infections  
*Antiviral Chemistry & Chemotherapy* (1997)  
Cited By 229 [Map](#)
- Mechanism of anti-HIV action of masked alaninyl d4T-MP derivatives  
*Proceedings of the National Academy of Sciences of the United States of America* (1996)  
Cited By 134 [Map](#)
- Characterization of the activation pathway of phosphoramidate triester prodrugs of stavudine and zidovudine  
*Molecular Pharmacology* (1999)  
Cited By 125 [Map](#)

### References Citing This Document

- Prodrugs of Phosphates and Phosphonates  
*Journal of Medicinal Chemistry* (2008)  
Citing 291 [Map](#)
- Phosphonomethoxyalkyl analogs of nucleotides  
*Current Pharmaceutical Design* (2003)  
Citing 220 [Map](#)
- Synthesis of Nucleoside Phosphate and Phosphonate Prodrugs  
*Chemical Reviews* (Washington, DC, United States) (2014)  
Citing 212 [Map](#)
- Aryloxy phosphoramidate triesters as protides  
*Mini-Reviews in Medicinal Chemistry* (2004)  
Citing 168 [Map](#)
- Aryloxy Phosphoramidate Triesters: a Technology for Delivering Monophosphorylated Nucleosides and Sugars into Cells  
*ChemMedChem* (2009)  
Citing 140 [Map](#)

Copyright © 2009 American Chemical Society. All rights reserved. Synthesis and Antiviral Evaluation of Alkoxyalkyl Derivatives of 9-(5)-(3-Hydroxy-2-phosphonomethoxypropyl)adenine against Cytomegalovirus and

# Retrosynthesis: 高效获取逆合成反应路线

## Retrosynthesis

Powered by ChemPlanner®

Overview Steps Scoring

Step Key

- ⇒ Experimental
- ⇨ Predicted

Plan Options

Synthetic Depth: 3  
Predicted Rules: Common  
Break & Protect Bonds: No  
[Edit Plan Options](#)

Plan Information

Estimated Yield: 76%  
Overall Price: \$41,403.90  
(USD per 100 grams)

Reaction scheme showing a target molecule (A) being broken down into precursors (B, C, D, E, F, G, H, I, J, K, L) with associated yields and supplier counts.

- A: Suppliers (29), Max. Yield: 92%
- B: Suppliers (41), Max. Yield: 96%
- C: Suppliers (24), Max. Yield: 85%
- D: Suppliers (60), Max. Yield: 95%
- E: Suppliers (115)
- F: Suppliers (63)
- G: Suppliers (41), Max. Yield: 91%
- H: Suppliers (8), Max. Yield: 91%
- I: Suppliers (60), Max. Yield: 100%
- J: Suppliers (40), Max. Yield: 91%
- K: Suppliers (58)
- L: Suppliers (158)

Reset

对已知化合物，Retrosynthesis既可以获取其已经报道的逆合成实验路线，也可以查看其预测的路线

# 预测的逆合成实验路线结果

**Retrosynthesis** Powered by ChemPlanner®

Overview Steps **Scoring** [Download] [Email] [Save]

Scoring Profiles

- Complexity Reduction
- Convergence
- Evidence
- Yield
- Atom Efficiency

Apply Reset Scoring

Avg. Yield: 61%

Avg. Yield: 66%

Suppliers (379)

Suppliers (7)

Max. Yield: 99%

Suppliers (67)

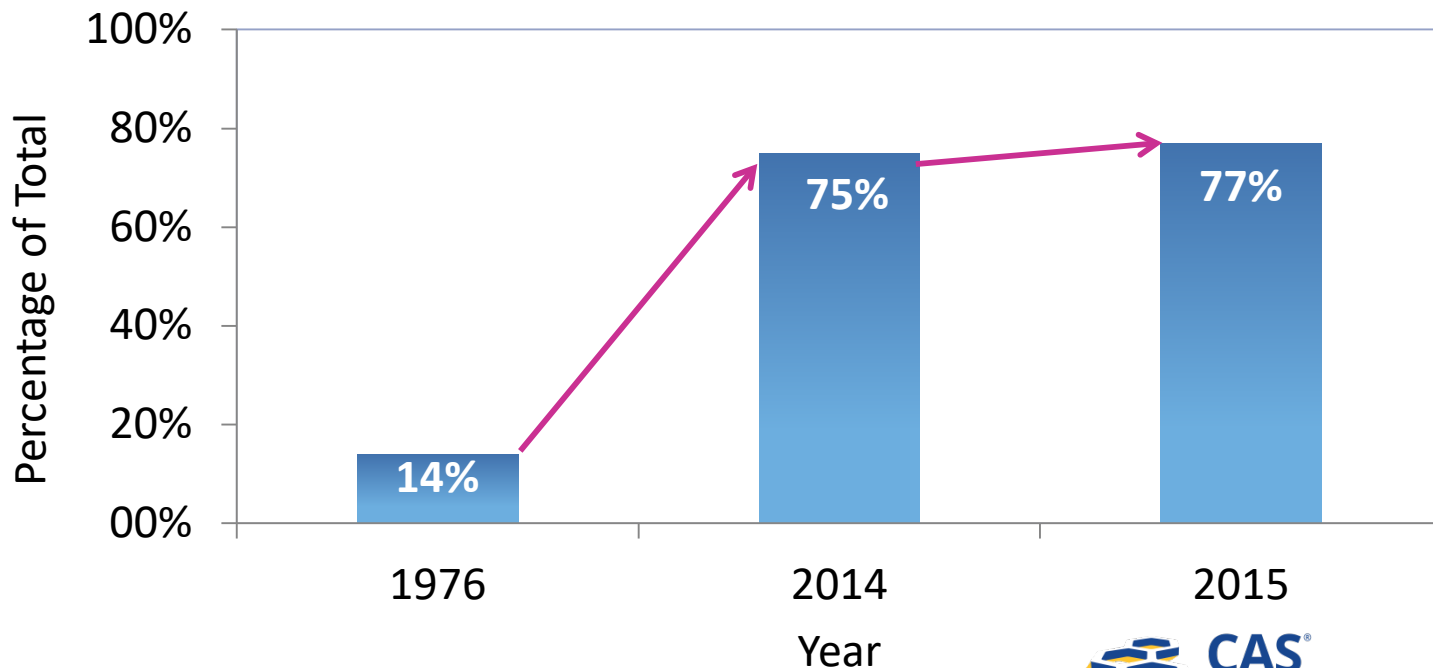
Reset

Feedback

预测新化合物的合成路线后，可继续通过Scoring灵活调整预测参数

# 越来越多的新化合物倾向于首先通过专利公布

## Percentage of New Compounds from Patents





# PatentPak™是唯一提供快速定位物质相关化学信息的工具

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- 在CAS**专利族文献**中找到你所熟悉语言的专利



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# PatentPak——专利工作流程解决方案

PatentPak浏览器

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专利PDF文件

By Orhan, Ilkay Erdogan; Kartal, Murat  
From Turkish Journal of Pharmaceutical Sciences (2015), 12(2):279-286. | Language: English, Database: CAPLUS

PATENTPAK  
A CAS SOLUTION

Key Substances in Patent

CAS RN 25953-19-9  
Search in SciFinder | View Detail  
Analyst Markup Locations (1)  
page 2

CAS RN 1404-90-6  
Search in SciFinder | View Detail  
Analyst Markup Locations (1)  
page 2

5. 根据权利要求4所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的应用,其特征在于,所述耐药性的革兰氏阳性致病菌是对头孢唑啉、万古霉素和/或达托霉素产生耐药性的革兰氏阳性致病菌。

6. 根据权利要求4或5所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的应用,其特征在于,所述耐药性革兰氏阳性致病菌为耐药的金黄色葡萄球菌和/或表皮葡萄球菌。

7. 权利要求1至6所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的化学合成方法,其特征在于,包括以下步骤:

S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

S2. 合成4,4-二甲基-3,5-二羟基-2,6-二丁酰基-2,5-环己二烯酮;

S3. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-2,5-环己二烯酮;

S4. 合成2,4,6-三甲氧基苯甲醚;

S5. 合成2-甲基,3,5-二甲氧基苯甲醚;

S6. 合成3'-甲基-2',4',6'-三甲氧基苯丁酮;

S7. 合成3'-甲基-2',4',6'-三羟基苯丁酮;

S8. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-6-(5-甲基-2,4,6-三羟基-3-丁酰基苯基)-2,5-环己二烯酮。

8. 权利要求7所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的化学合成方法,其特征在于,包括以下步骤:

S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

Jz, Jians; Liang, Ying; Xu, Junqiang  
Molecular Research (2015), 3(1), 1-8. | Language: English, Database: CAPLUS

在PatentPak浏览器中点击物质下面的紫色灯泡,快速定位到PDF文件中的物质信息。也可从PDF文件中与PatentPak进行互动

# PatentPak——专利工作流程解决方案

28. Flavaspidic acid BB of phloroglucinol derivatives of Dryopteris fragrans and antibacterial application

**PATENTPAK**  
A CAS SOLUTION

PAGE 2 / 12 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 2216756-37-3

Search in SciFinder | View Detail

Structure Markush Reactions

CAS RN 108-73-6

Search in SciFinder | View Detail

Analyst Markup Locations (2)

page 2 page 8

5. 根据权利要求4所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的应用,其特征在于,所述耐药性的革兰氏阳性致病菌是对头孢唑啉、万古霉素和/或达托霉素产生耐药性的革兰氏阳性致病菌。

6. 根据权利要求4或5所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的...于,所述耐药性革兰氏阳性致病菌为耐药的金黄色葡萄球菌和/或表皮葡萄菌

7. 权利要求1至6所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的化学...在于,包括以下步骤:

S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

S2. 合成4,4-二甲基-3,5-二羟基-2,6-二丁酰基-2,5-环己二烯酮;

S3. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-2,5-环己二烯酮;

S4. 合成2,4,6-三甲氧基苯甲醚;

S5. 合成2-甲基,3,5-二甲氧基苯甲醚;

S6. 合成3'-甲基-2',4',6'-三甲氧基苯丁酮;

S7. 合成3'-甲基-2',4',6'-三羟基苯丁酮;

S8. 合成4,4-二甲基-3,5-二羟基-2-丁酰基-6-(5-甲基-2,4,6-三甲氧基)-2,5-环己二烯酮。

8. 权利要求7所述香鳞毛蕨间苯三酚类化合物黄绵马酸BB的化学合...于,包括以下步骤:

S1. 合成2',4',6'-三羟基-3'-丁酰基苯丁酮;

green and high efficient conditions

**SciFINDER**  
A CAS SOLUTION

Explore Saved Searches SciPlanner

Opened saved answer set "phloroglucinols" (14942)

REFERENCES

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

STANCES

Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

REACTIONS

Reaction Structure

Structure Editor:

Java Non-Java

Search Type:

Allow variability only as specified

Substructure

Click image to change structure or view detail.

Import CXF

Search

可在PatentPak浏览器中直接返回  
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# MethodsNow 是一个完整的 CAS 解决方案



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# 一个产品，两个界面

The screenshot shows the SciFinder interface. At the top, there's a navigation bar with 'SciFinder' logo and user information. Below it, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area displays a chemical reaction scheme. On the left, there's a sidebar with 'REAGENTS' and 'ANALYZE' options. The reaction scheme shows a starting material reacting with a reagent to form a product. Below the reaction, there's a section titled 'Overview' with a 'MethodsNow™' logo and a 'Procedure' section. The procedure lists the reagents and conditions for the reaction. The yield is indicated as 79%.

The screenshot shows the MethodsNow Analysis interface. At the top, there's a navigation bar with 'METHODSNOW' logo and user information. Below it, there's a search bar with the text 'Enter keyword, matrix, analyte, etc.' and a search button. Below the search bar, there's a section titled 'Advanced Search'. Below that, there's a section titled 'Browse Method Categories' with a grid of categories including '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', and 'Water Analysis'. Below the categories, there's a section titled 'Recent Searches' with a search bar and a button.

MethodsNow Synthesis 嵌在 SciFinder 中

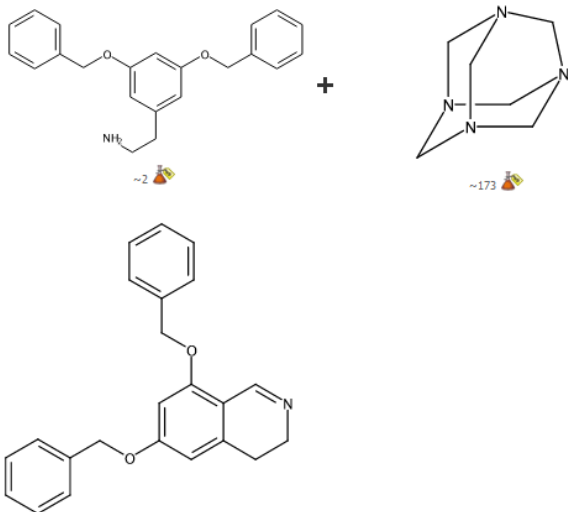
MethodsNow Analysis 有独立平台  
[www.methodsnow.com](http://www.methodsnow.com)

## MethodsNow

### Asymmetric formal synthesis of schulzeines A and C

By Jang, Jaebong; Jung, Jong-Wha; Ahn, Jaeseung; Sim, Jaehoon; Chang, Dong-Jo; Kim, Dae-Duk; Suh, Young-Ger  
From Organic & Biomolecular Chemistry, 10(27), 5202-5204; 2012  
Published by Royal Society of Chemistry

Reaction Steps 1 2 3 4 5 6 7 8 9 10 11



<b>Products</b>	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
<b>Reactants</b>	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
<b>Solvents</b>	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
<b>Procedure</b>	1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethylamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon. 2. Stir the mixture for 3 hours at 90°C. 3. Dilute the reaction mixture with H <sub>2</sub> O. 4. Basify with potassium carbonate and extract with CH <sub>2</sub> Cl <sub>2</sub> . 5. Wash the combined organic layers with brine. 6. Dry over MgSO <sub>4</sub> and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
<b>Scale</b>	gram
<b><sup>1</sup>H NMR</b>	(CDCl <sub>3</sub> , 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, J = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
<b><sup>13</sup>C NMR</b>	(CDCl <sub>3</sub> , 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
<b>IR</b>	(thin film, neat) ν <sub>max</sub> 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm <sup>-1</sup>
<b>HRMS</b>	(FAB+) calcd for C <sub>23</sub> H <sub>27</sub> NO <sub>2</sub> (M+H <sup>+</sup> ) 344.1651; found 344.1658
<b>Mass Spec</b>	(FAB+) m/z 344 (M+H <sup>+</sup> )
<b>Physical</b>	yellow solid
<b>Pub ID</b>	3-614-CAS-200055

物质信息  
名称、角色

实验过程

图谱信息

保存/导出

MethodsNow Synthesis中的实验详情不仅包含原文中描述的实验内容，还包括 supporting information中涉及的实验内容

多步反应中，原文没有描述的实验过程以灰色展示

Print/Export

Close

# 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!

# MethodsNow – Analysis (www.methodsnow.com)

## Analysis of Nitric oxide in Blood plasma by Electrochemical biosensors

CAS MN: 2-114-CAS-117192

Method Category: Biomolecule Isolation Assay; Gas Analysis  
Technique: Electrochemical biosensors

Materials	Role
Nitric oxide	analyte
Blood plasma	matrix
Catheters	material
Nitric oxide (NO) sensor (700 µm in diameter at the detection tip)	material
4-French (4-Fr) catheter (1,200 mm long)	material
7-Fr JR catheter	material
Doppler guide wire	material
Silicon	reagent
Isosorbide dinitrate	reagent
Acetylcholine	reagent
Ketamine	reagent
N <sup>ω</sup> -Methyl-L-arginine	reagent
Heparin	reagent
Pentobarbital sodium	reagent
Physiological saline solutions	reagent
Polyurethanes	reagent

实验的材料

改写的标题

### Source

Evaluation of bioavailability of nitric oxide in coronary circulation by direct measurement of plasma nitric oxide concentration

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Full Text -

Abstract -

Although bioavailability of NO in the coronary circulation is commonly evaluated by acetylcholine (ACh) relation to the flow response after injection of ACh are still unknown. Thus, the authors directly measured NO sensor for coronary sinus. An NO-sensitive sensor was located and fixed in a 4-Fr catheter with a pure water, the catheter-type NO sensor was located in the coronary sinus in anesthetized dogs. The intracoronary injection of ACh (0.4 and 1.0 µg/kg) increased plasma NO concentration in a dose-dependent manner. The intracoronary injection of ACh (0.4 and 1.0 µg/kg) increased plasma NO concentration in a dose-dependent manner. After ACh, the peak value of plasma NO concentration decreased basal NO concentration by 3 nM and suppressed the ACh-induced NO concentration. These results indicate that production of NO in the coronary circulation can be evaluated in the coronary sinus. A NO concentration in terms of magnitude and time course. Direct measurement of plasma NO concentration in the coronary circulation.

### Equipment Used

Nitric oxide (NO) monitor, iNO-T, Innovative Instruments, Tampa, FL

Respirator pump, VS-600, Instrumental Development, Pittsburgh

Strain gauge pressure transducer, TP-400T, Nihon Kohden, Tokyo

实验仪器

文献信息

### Instructions

#### Preparation of animals

1. Sedate the adult mongrel dogs (n = 7) with ketamine (200 mg i.m.).
2. Anesthetize with pentobarbital sodium (30 mg/kg i.v.).
3. Heparinize the each dog by injecting 100 units/kg of heparin.
4. Ventilate the animals by using a respirator pump (model VS-600, Instrumental Development, Pittsburgh).
5. Place the NO sensor in the coronary sinus through a 7-Fr JR catheter (Bright Chip, Cordis, Miami) from the right jugular vein.
6. Place a doppler guide wire (FloWire, JoMed, Rancho Cordova, CA) in the left anterior descending artery through another 7-Fr JR catheter inserted in the right carotid artery under cinefluorography.

#### Preparation of nitric oxide (NO) sensor

1. Mount the NO sensor (amiNO-700 XL, Innovative Instruments, Tampa, FL; 700 µm in diameter at the detection tip) in a 4-Fr catheter (1,200 mm long; Hirakawa Hewtech, Tokyo).
2. Fix with silicon adhesive.
3. Attach soft protection tip of polyurethane at the edge of the detection tip to protect the vessel wall.
4. Attach two metal wires along the detection tip to protect the detection tip.
5. Monitor oxidative current of NO by using an NO monitor (model iNO-T, Innovative Instruments).
6. Calibrate each sensor by using an NO-saturated pure water.
7. Prepare NO-saturated pure water by bubbling pure NO gas in oxygen-free pure water.
8. Inject 5 µL into a well stirred saline solution (50 mL) using a gas-tight syringe and immerse NO sensor (final NO concentration: 190 nM).

#### Determination of nitric oxide (NO)

1. Monitor plasma NO concentration in the coronary sinus using NO sensor, phasic coronary blood flow by the doppler guide wire in the left anterior descending artery and aortic pressure by a strain gauge pressure transducer (model TP-400T, Nihon Kohden, Tokyo).
2. Measure average peak velocity (APV) as coronary flow velocity.
3. Inject saline (vehicle) and acetylcholine (ACh) of 0.4 µg/kg and 1.0 µg/kg from the left coronary artery (LCA) for 20 s.
4. Dilute each solution to 5 mL with saline.
5. Administrate N<sup>ω</sup>-methyl-L-arginine (L-NAME, 10 µg/kg/min) into the LCA for 20 min to inhibit NO synthesis.
6. Repeat the ACh injection at two doses (0.4 µg/kg and 1.0 µg/kg).
7. Inject NO donor, isosorbide dinitrate (ISDN, 0.5 mg).

### Validation

Sensitivity	366 ± 122 pA/nM
Concentration	1.9 ± 0.6 nM vs. 5.0 ± 2.7 nM (After L-NAME vs. control) at 0.4 µg/kg 2.8 ± 0.8 nM vs. 7.3 ± 3.5 nM (After L-NAME vs. control) at 1.0 µg/kg

详细步骤

数据有效性



# 使用注意事项

- 一人注册一个帐号
- 实名注册，需提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（以电子形式存储不超过5,000条记录）
- 不得账号分享
- 不得将账号用于非学术研究



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