

汤健钊  
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美国化学文摘社, CAS

# 利用SciFinder助力科研创新和专利保护

# 内容

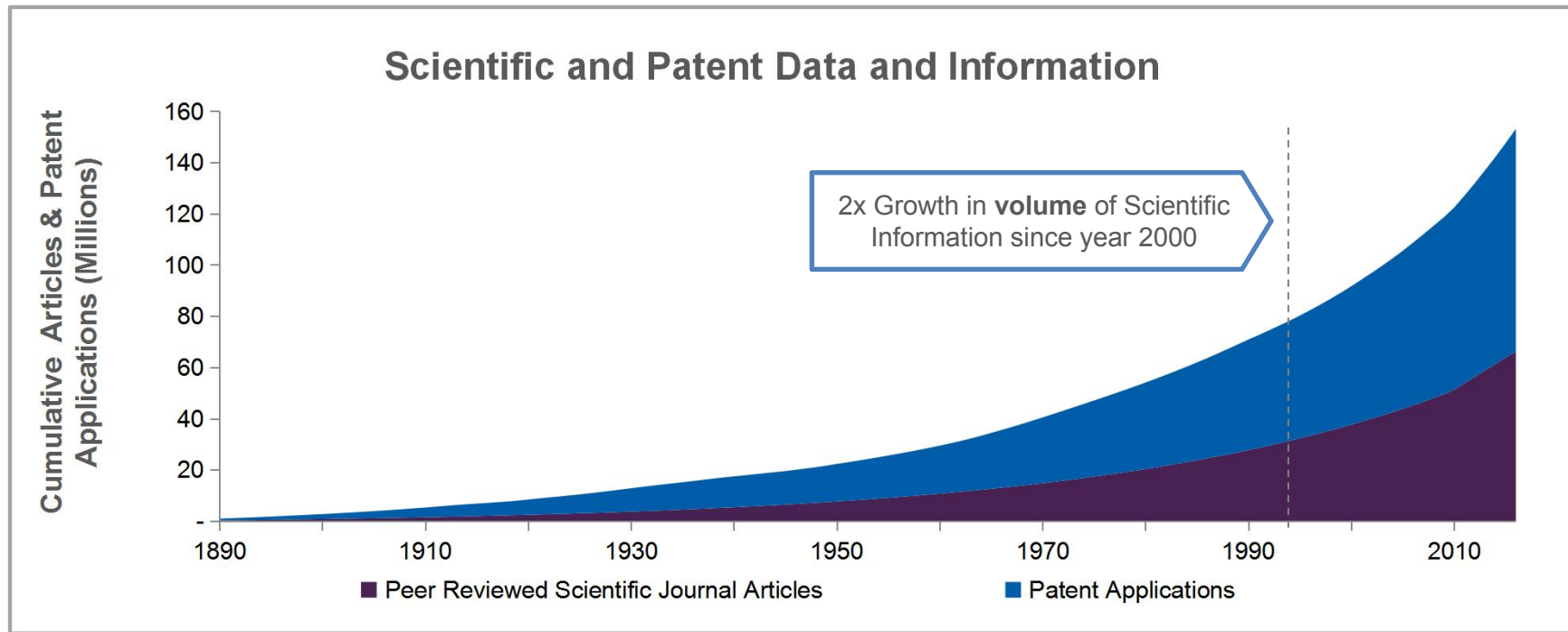
- 为什么需要CAS
- 化合物专利保护策略（以药物研发为例）
- 检索工具的选择和分析
- 案例分享
  - 获取化合物制备专利
  - 获取药物制剂专利
  - 判定化合物结构新颖性和创造性

## 美国化学文摘社（Chemical Abstracts Service）简介

- 成立于1907年，行业领先的科学信息与解决方案提供商，隶属于美国化学会（ACS）。
- 由科学家、技术专家和商业人士组成，追踪、摘要、标引全球化学及相关学科文献，开发、利用最先进的技术，为科学家、专利人士提供权威的信息来源及应用----科学家帮助科学家。
- 全球1,400名员工，包括500多名掌握50多种语言的编辑科学家，400余名技术工程师。

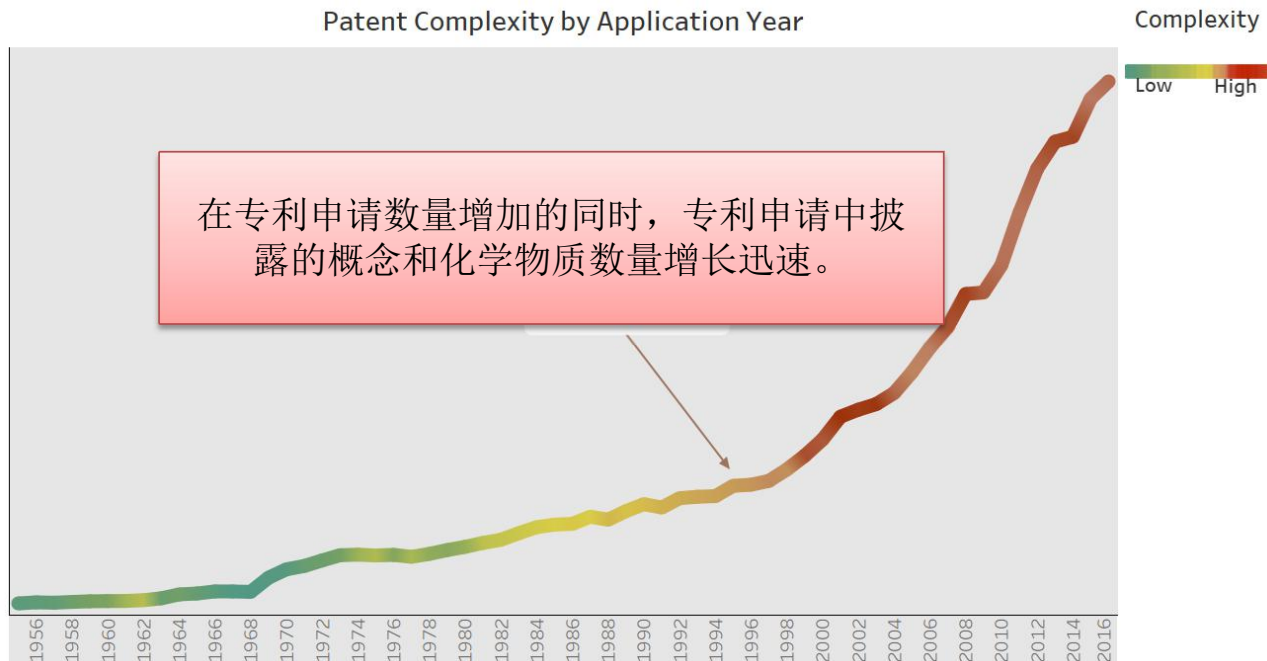


# 科学发现文献和专利数量急剧增长



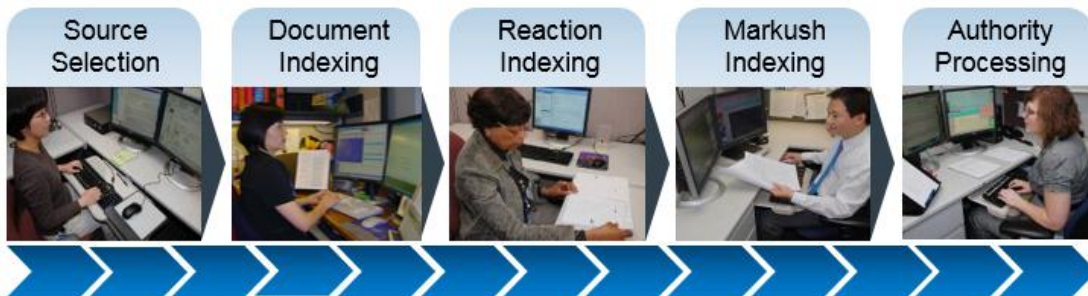
Source: CAS Proprietary data, CAS Analytics & Insights

## 专利包含更多信息，且日益复杂

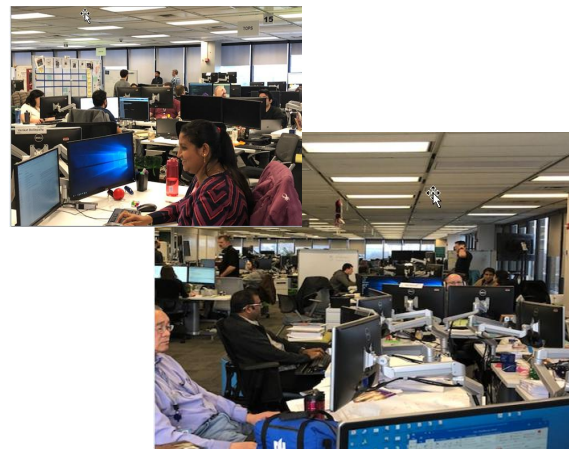


## CAS: 科研信息合作伙伴

- 与全球研发机构合作，提供切实可行的见解(Scientists help scientists)
  - 全面(Comprehensive): Content coverage
  - 智能(Smart): Human intellectual + technology
  - 及时(Timely): Daily update



Proprietary, standardized indexing in CAS databases ensures consistent, comprehensive search results.



# 内容收录&数字化

**Bioactive Constituents from the Termite Nest-Derived Medicinal Fungus *Xylaria nigripes***  
 Jung-Chun Chang,<sup>1</sup> George Hsiao,<sup>1</sup> Bao-Kai Lin,<sup>1</sup> Yuh-Hsiung Kuo,<sup>1,2</sup> Yiu-Min Ju,<sup>3</sup> and Tsong-Hong Lee<sup>1,4</sup>

<sup>1</sup>Institute of Pharmacognosy and Graduate Institute of Medicinal Science and Department of Pharmacology, College of Medicine, Taipei Medical University, Taipei, Taiwan 110  
<sup>2</sup>Department of Chinese Pharmaceutical Sciences and Chinese Medicine Research, China Medical University, Taichung, Taiwan 404  
<sup>3</sup>Department of Botany, Asia University, Taichung, Taiwan 403  
<sup>4</sup>Institute of Plant and Microbial Biology, Academia Sinica, Taipei, Taiwan 115

**Supporting Information**

**ABSTRACT:** Six new entomocyclic-type sesquiterpenes, namely, xylaripenes A–F (**1**–**6**), and one new dihydro-*trans*-cinnamyl 3-hydroxypropylidene-2(1*H*)-pyridin-2(1*H*)-one with *trans*-methyl, -ethyl, and -isobutylpropylamide, and three, and lactonolones were isolated from the dried aerial parts, and bioassays were conducted from the ethyl acetate extracts of the essential bioactive contents and dried termite mycelia, which has long been used as a traditional Chinese medicine for treating insomnia and depression. Their structures were elucidated on the basis of spectroscopic data analysis and compared with the literature. All the new isolates were evaluated against *Trichostema*-induced oxidative stress, cyclic adenosine monophosphate (cAMP), cyclic guanosine monophosphate (cGMP), and cyclic inositol trisphosphate (cIP3) in HEK293 cells. Of the compounds tested, xylaripenes C, D3, and lactonolones showed central agonist inhibitor effects on two induced responses and NEJ production without any significant cell toxicity. The most potent compound 6, exhibited concentration-dependent inhibition on NEJ production and cAMP and cGMP expression with  $IC_{50}$  values of 21.7 ± 4.1, 8.1 ± 2.5, and 3.6 ± 0.5 μM, respectively. These results indicated that the general mechanism of action of xylaripenes C, D3, and lactonolones derived as natural brain-energetic NEJ cells may provide a rationale for the traditional medical uses of *X. nigripes* for treating insomnia and depression.

Item	Number	Chemical Name	Structure
Item 134	6	96650	Lactonolone
Item 136	1,2,5	13612721	3-hydroxy-2-propylpropylamide
Item 140	5	13612721	ethyl-2-hydroxypropylamide
Item 141	1,6	20788628	2-hydroxyethyl-propylamide
Item 142	2	17227716	60-9666
Item 143	4	20448322	60-9666

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</findings>
</document>
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# CAS产品组合

**STNext™**

**SciFINDER<sup>n</sup>**  
A CAS SOLUTION

**PATENTPAK™**  
A CAS SOLUTION

**FORMULUS™**  
A CAS SOLUTION

**METHODSNOW™**  
A CAS SOLUTION

**NCI™ GLOBAL**  
A CAS SOLUTION

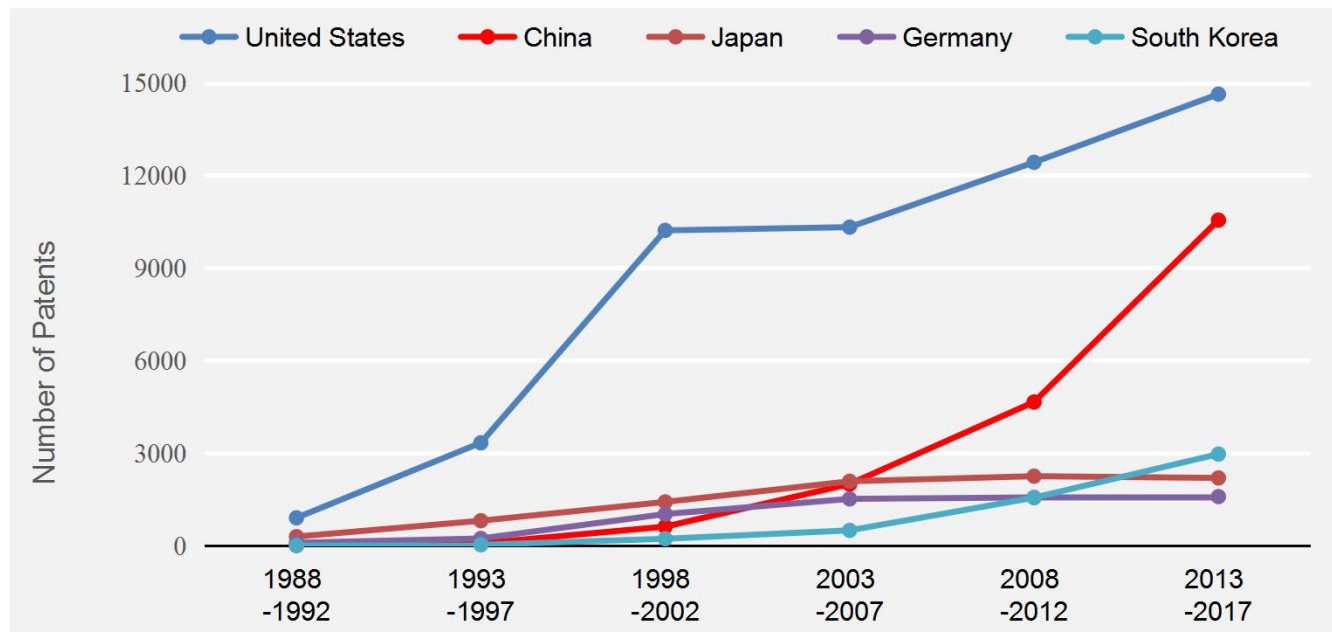
**CHEMZENT™**  
A CAS SOLUTION

More  
Coming!



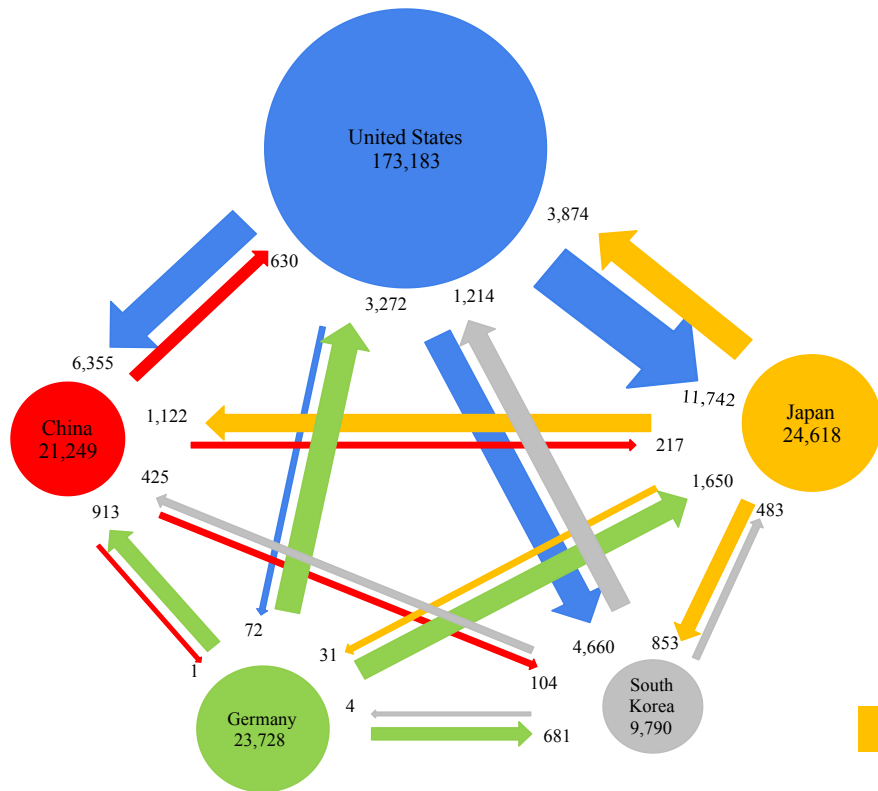


## 全球生物制药领域主要国家专利发展趋势



来源：生物制药研发态势分析报告,中国科学院文献情报中心, 美国化学文摘社

# 生物制药领域主要国家专利技术流向



- 美国、日本、德国非常重视在其他国家的专利输出
- 韩国在美国专利布局较多
- 中国在其他主要国家布局较少，专利仍局限在本国受保护为主

箭头的粗细与专利布局比例呈正相关

来源：生物制药研发态势分析报告,中国科学院文献情报中心, 美国化学文摘社

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# 创新药物研发最关注什么？

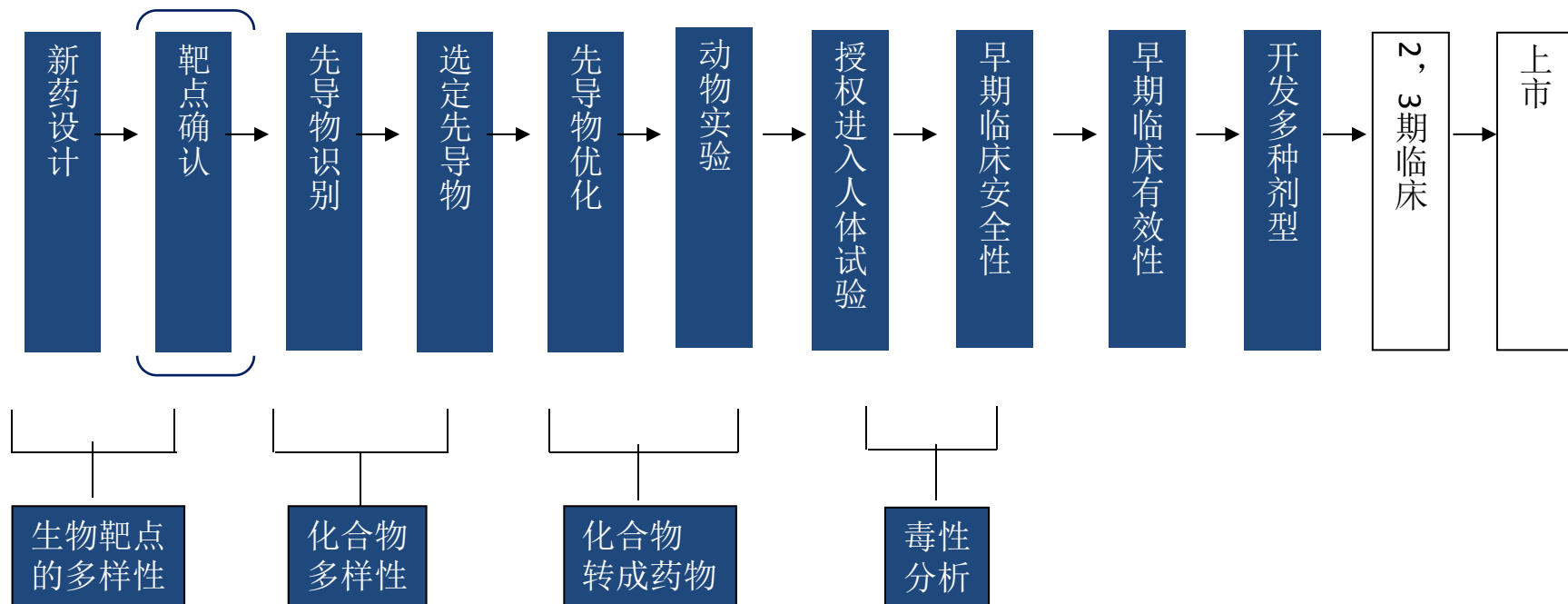
## 规避风险

- “新药”不新
- 项目撞车
- 专利侵权，项目泄密
- 合规

## 领先一步

- 获取及时信息，抢占先机
- 一站式解决方案，提高工作效率
- 科学布局专利，找寻机会，扩大市场份额

# SciFinder是药物研发最高效、最全面的支撑工具



\*Note: 蓝色表示SciFinder可以提供信息支持

## 药物研发专利保护策略

在新药研究的发现阶段申请基本专利保护

- 通式化合物
- 更窄范围的、更加具体定义的、更加有活性的化合物
- 具体的化合物
- 化合物的制备方法
- 含有活性化合物的药物组合物
- 化合物的药物用途

# 药物研发专利保护策略

## 在药物开发阶段申请后续专利保护

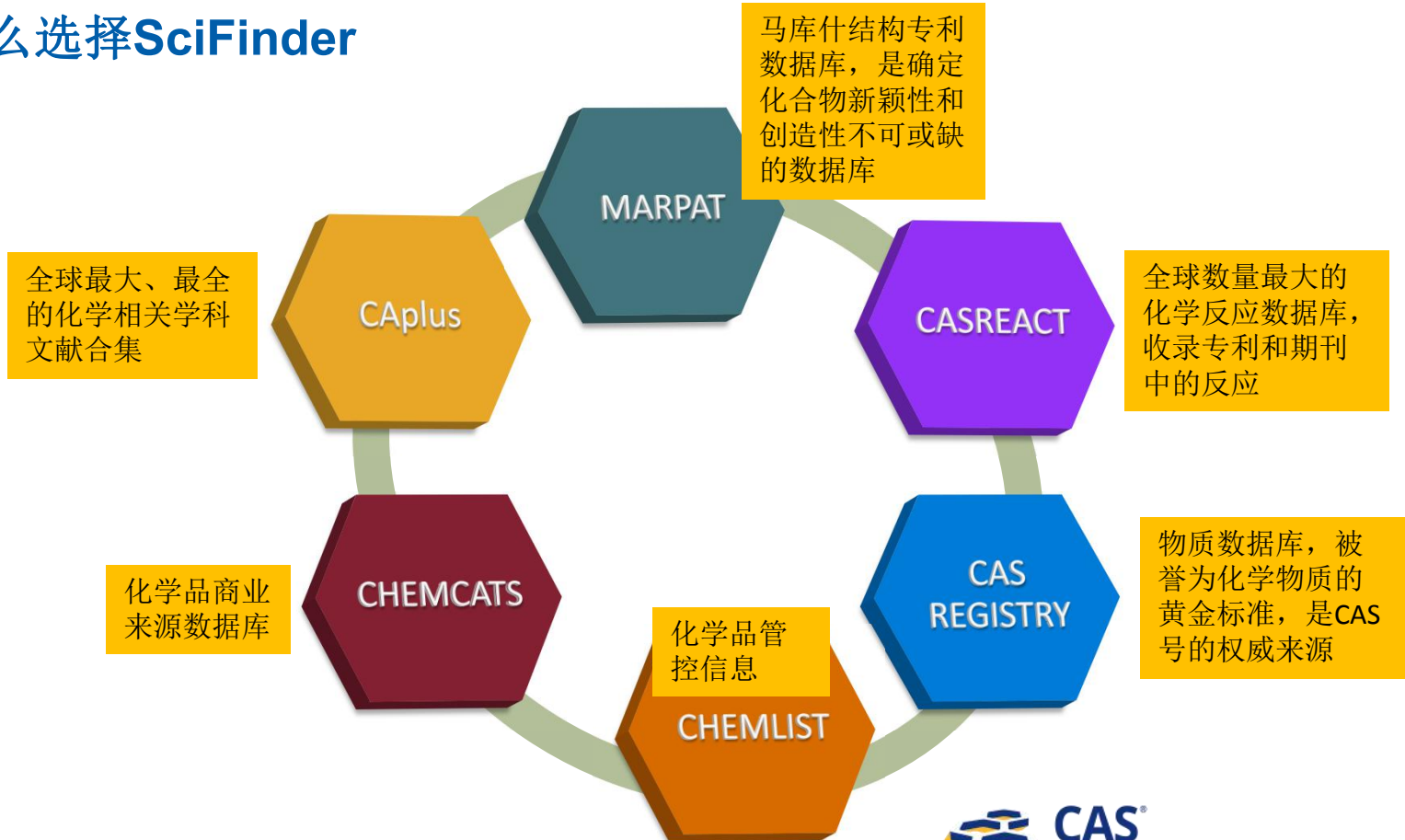
- 要求相对较窄的权利要求的保护范围
- 一个（或多个）对映体专利
- 盐或溶剂化物专利
- 晶形专利
- 前药专利
- 方法专利
- 制剂专利
- 改进的剂型专利
- 联合用药专利

# 内容

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  - 获取药物制剂专利



# 为什么选择SciFinder



## 为什么选择SciFinder

- 内容全面——无需担心遗漏重要信息

时间跨度：19世纪早期至今

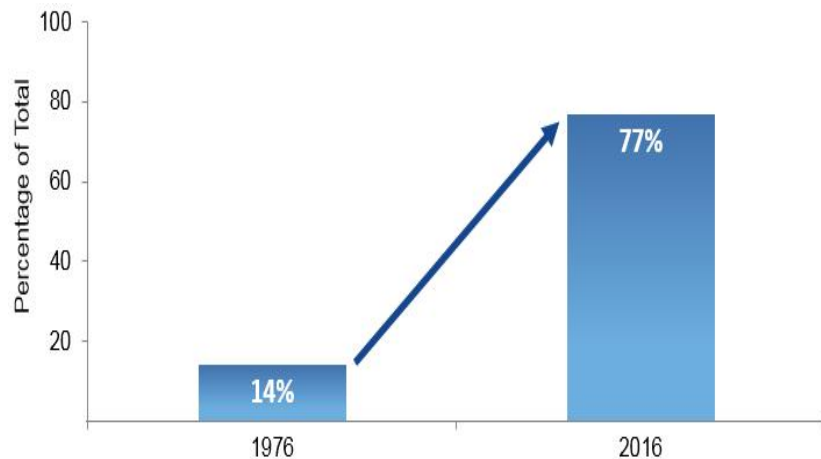
语种：50多种

信息来源国：180多个

收录内容范围：

- 50,000余种科技期刊
- 63家专利授权机构的专利
- 会议论文
- 技术报告
- 图书
- 学位论文
- 产品目录
- 评论
- 会议摘要
- 网络预印本
- 其他网络资源

# 为什么选择SciFinder



化合物首次通过专利披露的比重持续增长



\*Note: 蓝色表示SciFinder收录专利区域

## 为什么选择SciFinder

- 人工标引——精准揭示关键技术信息
  - 全球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

## 只有人工标引才能精准识别：

- 复杂化合物
- 代码类物质（糖类，配合物，功能材料，生物序列...）
- 部分名称化合物
- 表格化合物
- Markush结构
- 专利中的示例部分和现有技术
- ...

# 为什么选择SciFinder

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

CAS科学家重写的标题和摘要

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的科学家对专利进行必要改写，使其更容易被理解和获取



# 为什么选择SciFinder

## High SPF sunscreen composition containing dibenzoylmethane derivatives

By: Duggal, Charu; Gaurav, Kumar; Raut, Janhavi Sanjay  
Assignee: Hindustan Unilever Limited, India

The invention relates to a high SPF sunscreen compn. There is a problem of achieving high SPF while keeping the total amt. of sunscreens in the compns. relatively low. It is desirable, that the enhanced SPF benefit could be achieved through synergistic interaction of commonly used ingredients, thereby the present applicants have been working on solving this problem and have surprisingly found that cosmetic compns. comprising dibenzoylmethane or its deriv. in combination with an oil sol. UV-B sunscreen when incorporated in a sunscreen compn. along with a non-ionic surfactant of a select class meeting certain HLB requirements, provide the enhanced SPF benefits when applied on the substrate of interest. A sunscreen contained stearic acid 15, Parsol MCX 3, Parsol 1789 1.5, Igepal CA210, Carbomer 980 1, niacinamide 1, glycerin 1, iso-Pr myristate 1, titanium dioxide 1, glyceryl stearate 1, mineral oil 1, triethanol amine 0.5, potassium hydroxide 0.5, cetyl alc. 1, silicone oil 1, perfume 0.5, Me paraben + Pr paraben 0.5, and water to 100%.

### Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
<a href="#">IN 2010MU02830</a>	<a href="#">PATENTPAK</a> A		Nov 16, 2012	IN 2010-MU2830	Oct 12, 2010
CA 2813094	A1		Apr 19, 2012	CA 2011-2813094	Sep 12, 2011
<a href="#">WO 2012048972</a>	<a href="#">PATENTPAK</a> A1	English	Apr 19, 2012	WO 2011-EP65756	Sep 12, 2011
CN 103221026	<a href="#">PATENTPAK</a> A	Chinese	Jul 24, 2013	CN 2011-80049663	Sep 12, 2011
CN 103221026	B		Mar 2, 2016		
EP 2627306	A1		Aug 21, 2013	EP 2011-757598	Sep 12, 2011
EP 2627306	<a href="#">PATENTPAK</a> B1	English	Feb 25, 2015		
JP 2013539769	<a href="#">PATENTPAK</a> T	Japanese	Oct 28, 2013	JP 2013-533137	Sep 12, 2011
JP 5851511	<a href="#">PATENTPAK</a> B2	Japanese	Feb 3, 2016		
ZA 2013002505	A		Jun 25, 2014	ZA 2013-2505	Sep 12, 2011
ES 2537616	T3		Jun 10, 2015	ES 2011-757598	Sep 12, 2011
EA 23008	B1		Apr 29, 2016	EA 2013-452	Sep 12, 2011
MX 2013004090	A		Mar 21, 2014	MX 2013-4090	Apr 11, 2013
US 20130280191	<a href="#">PATENTPAK</a> A1	English	Oct 24, 2013	US 2013-13877924	May 28, 2013
US 9034304	<a href="#">PATENTPAK</a> B2	English	May 19, 2015		

### Priority Application

IN 2010-MU2830	A	Oct 12, 2010
EP 2010-192532	A	Nov 25, 2010
WO 2011-EP65756	W	Sep 12, 2011

### QUICK LINKS

0 Tags, 0 Comments

### PATENT INFORMATION

Nov 16, 2012  
[IN 2010MU02830](#)  
A

### APPLICATION

Oct 12, 2010  
IN 2010-MU2830

### PRIORITY

Oct 12, 2010  
IN 2010-MU2830  
Nov 25, 2010  
EP 2010-192532  
Sep 12, 2011  
WO 2011-EP65756

### SOURCE

*Indian Pat. Appl.*  
26pp.; Chemical Indexing  
Equivalent to 156:515015  
(WO)  
[Patent](#)  
2012  
CODEN:INXXBQ

### CLASSIFICATIONS

Main IPC A61K008-04

### ACCESSION NUMBER

2012:1715525



CAS<sup>®</sup>

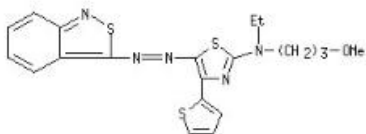
A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

# 为什么选择SciFinder

SciFinder中不但收录专利中报道的确定结构，还收录专利中的通式结构

RN 137784-55-5 REGISTRY  
ED Entered STN: 13 Dec 1991  
CN 2-Thiazolamine, 5-[2-(2,1-benzisothiazol-3-yl)diazenyl]-N-ethyl-N-(3-methoxypropyl)-4-(2-thienyl)- (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 2,1-Benzisothiazole, 2-thiazolamine deriv.  
CN 2-Thiazolamine, 5-(2,1-benzisothiazol-3-ylazo)-N-ethyl-N-(3-methoxypropyl)-4-(2-thienyl)- (9CI)  
MF C20 H21 N5 O S3  
SR CA  
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL

专利中的确定结构

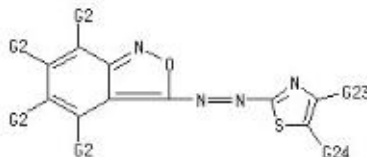


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

MSTR 1 Assembled

专利中的通式结构



Patent location:

claim 1

Note:

and alkali metal, alkaline earth metal salts and tautomers

Note:

substitution is restricted

Note:

additional ring formation also claimed



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## 检索策略

- 物质检索，再获得相应的Preperation文献，保存成结果集1
- 主题检索，“Preparation of 物质名”，Refine至最新文献，保存成结果集2
- 合并结果集1与2

# 获取化合物的制备专利信息

The screenshot shows the CAS SciFinder interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, a breadcrumb trail reads: 'Research Topic "essence extracting with tobacc..." > references (284) > get substances'. The main content area is divided into three sections: 'REFERENCES', 'SUBSTANCES: SUBSTANCE IDENTIFIER', and 'REACTIONS'. The 'SUBSTANCES: SUBSTANCE IDENTIFIER' section is active and contains a search input field with the text 'Solavetivone'. Below the input field, there are instructions: 'Enter one per line. Examples: 50-00-0, 999815, Acetaminophen'. A blue 'Search' button is positioned at the bottom of this section. The left sidebar contains a list of search criteria under three categories: 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (Reaction Structure). The 'Substance Identifier' option is currently selected.

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。

# 获取化合物的制备专利信息

Substance Identifier "solavetivone" > substances (1) > get references (43) > refine "Patents only" (5)



**SUBSTANCES** Get References Retrieve references for selected substances. **Tools**

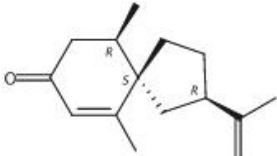
Analyze Refine

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. 54878-25-0

~211  



Rotation (-), Absolute stereochemistry.

**C<sub>15</sub>H<sub>22</sub>O**  
Spiro[4.5]dec-6-en-8-one, 6,10-dimethyl-2-(1-methyl-2-propenyl)-, (2R,5S,10R)-

**Key Physical Properties**  
Spectra

**Get References**

Retrieve references for:

- All substances
- Selected substances

**Limit results to:**

<input type="checkbox"/> Adverse Effect, including toxicity	<input checked="" type="checkbox"/> Preparation
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Process
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Prophetic in Patents
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

**For each sequence, retrieve:**

- Additional related references, e.g., activity studies, disease studies.

**Get** **Cancel**

# 获取化合物的制备专利信息

REFERENCES

Get Substances Get Reactions Get Related Citations Tools

Analyze Refine Categorize

Sort by: Accession Number

0 of 43 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

1. **Solavetivone and 5-epi-beta-*vetivone* as pest repellents and pesticides**  
Quick View PATENTPAK  
By Goldblum, Seth; Warren, Craig B.  
From PCT Int. Appl. (2014), WO 2014099821 A2 20140626. | Language: English  
The claimed pest (mostly insect) repellent and pesticidal (mostly alone or in combinations with one or more addnl. biol. active formers, antioxidants, preservatives, aerosol propellants, colorants, wide variety of application forms for animal, human, and tech. uses...

2. **Isolation and identification of chemical constituents of *Przewalskia tangutica***  
Quick View Other Sources  
By Shao, Jun-jie; Peng, Yong; He, Chun-nian; Xu, Li-jia; Xiao, Xuan; Li, Yu-shan  
From Shenyang Yaokexue Xuebao (2013), 30(11), 840-845. | Language: Chinese  
The chem. constituents of *Przewalskia tangutica* Maxim. were separated by chromatog. and structures were established by ESI-MS, <sup>1</sup>H-NMR ext. and EtOAc ext. of the aerial parts of *P. tangutica* Maxim., and identified as: phenylpropionate (4), tropine (5), thymine (6), cytidine (7), inosine (8), and guanosine (9).

3. **Effect of different preprocessing methods on determination of aroma constituents in aging tobacco, simultaneous distn. and**  
Quick View Other Sources  
By Shen, Jin; Xiao, Zuo-bing; Tian, Huai-xiang; Xu, Ying-bo; Xu, Zhi-qiang; Feng, Shupin  
From Shipin Gongye (Shanghai, China) (2013), 34(9), 209-214. | Language: Chinese  
In order to compare the different preprocessing methods combination of aroma constituents in aging tobacco, simultaneous distn. and these three pretreatment methods were adopted for comparison of SDE detected 105 kinds of aroma compns.; the method of HS-SPME-GC-MS/MS was used to identify the aroma constituents.

0 of 5 References Selected

1. **Solavetivone and 5-epi-beta-*vetivone* as pest repellents and pesticides**  
Quick View PATENTPAK  
By Goldblum, Seth; Warren, Craig B.  
From PCT Int. Appl. (2014), WO 2014099821 A2 20140626. | Language: English, Database: CAPLUS  
The claimed pest (mostly insect) repellent and pesticidal (mostly insecticidal) formulations contain at least one or more addnl. biol. active ingredients. Suitable auxiliary components, antioxidants, preservatives, aerosol propellants, colorants) are selected based on the product wide variety of application forms for animal, human, and tech. uses...

2. **Novel fragrance and methods for production of 5-epi-β-*vetivone*, 2-isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one**  
Quick View PATENTPAK  
By Julien, Bryan N.; Wallace, David M.  
From U.S. Pat. Appl. Publ. (2010), US 20100129306 A1 20100527. | Language: English, Database: CAPLUS  
The present invention relates to 5-epi-β-*vetivone*, 2-isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one for their fragrant qualities, and to novel methods for their prodn. using (-)-premnaspirodiene as starting substrate, such as farnesyl diphosphate, in host cells transformed or transfected with a vector comprising the present invention. Use of the fragrant components or any compn. contg. the component c...

3. **Novel methods for production of 5-epi-β-*vetivone*, 2-isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one**  
Quick View PATENTPAK  
By Julien, Bryan N.; Wallace, David M.  
From PCT Int. Appl. (2008), WO 2008116056 A2 20080925. | Language: English, Database: CAPLUS  
The present invention is directed to novel methods for prodn. of 5-epi-β-*vetivone* (I), 2-isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one (II), which are useful for their fragrant qualities, in one embodiment...

将文献结果集限定为专利，获得所有专利文献



# 获取化合物的制备专利信息

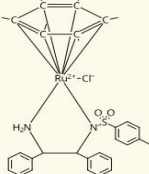
**PATENTPAK**  
A CAS SOLUTION

PAGE 30 / 45 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

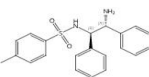
Analyst Markup Locations (1)  
Page 29

CAS RN 310903-41-4



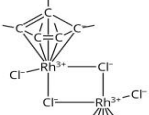
Analyst Markup Locations (1)  
Page 29

CAS RN 144222-34-4



Analyst Markup Locations (1)  
Page 30

CAS RN 12354-85-7



colored oil (5.10 g, 68% area purity by HPLC)

40 step-4: Preparation of N-[(1S)-2-chloro-1-(2-chlorothiazol-5-yl)ethyl]-2-methyl-propane-2-sulfonamide:

a) Preparation of Rhodium catalyst -  $\text{RhCl}[(R,R)\text{-TsDPEN}]\text{Cp}^*$ :

**WO 2018/197541**                      **29**                      **PCT/EP2018/060555**

A 250 mL, three necked flask equipped with Teflon-blade stirrer, nitrogen inlet and thermo-pocket was charged with  $[\text{RhCl}_2\text{Cp}^*]_2$  (2.0g), (1R, 2R)-N-p-toluenesulfonyl-1, 2-diphenylethylenediamine (2.38g), dichloromethane (68 mL) and TEA (1.72 ml) under nitrogen atmosphere. The resulting slurry was stirred for 0.5 h at 22-27 °C and distilled water was added (40 mL). The two phases were separated and the organic phase was washed with water (40 mL). The organic phase was dried over sodium sulphate, filtered and evaporated to get brown coloured solid residue. The brown residue was triturated with n-heptane (20 mL), filtered and dried under nitrogen atmosphere to obtain  $\text{RhCl}[(R, R)\text{-TsDPEN}]\text{Cp}^*$  as red coloured solid (3.4 g).

5

b) Preparation of  $\text{HCOOH}\cdot\text{NEt}_3$  mixture

10 In a 2 L, 3 neck round bottom flask Formic acid (275 mL,  $\geq 99\%$  w/w) was added and cooled to 0 °C. To this, triethylamine 250 mL,  $\geq 99\%$  w/w) was added slowly at 0 °C and used immedi-

化合物制备专利原文

# 获取化合物的制备专利信息

The screenshot shows the SciFinder web interface. At the top, there's a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. A user is logged in as 'James Tang'. A search for 'solavetivone' has been performed, resulting in 48 references. A 'Save This Answer Set' dialog box is open, allowing the user to save the current search results. The dialog box has a 'Save' button highlighted in the background interface. The dialog box contains the following text:

**Save This Answer Set**

Save:  All answers  Only selected answers

Title: \*  
1

Description:

OK Cancel

The background interface shows a list of references under the heading 'REFERENCES'. The first reference is '1. Di-tert-butyl chromate' by Freeman, Fillmore. The second reference is '2. Integration of GC-MS based non-targeted metabolite profiling in tobacco leaves from North Carolina, India and Brazil' by Ma, Dong-Ming; Gandra, Salprasad V. S.; Sharma, Navin; Xie, F. The third reference is '3. Solavetivone and 5-epi-beta-vervetone as pest repellents and potential...' by Goldblum, Seth; Warren, Craig B.

获得所有专利文献后，保存成结果集1

# 获取化合物的制备专利信息

CAS Solutions  
**SciFINDER**  
A CAS SOLUTION

Explore | Saved Searches | SciPlanner

Substance Identifier "solavetivone" > substances (1) > 54878-25-0

**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**

preparation of solavetivone  
Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

Search

Advanced Search

主题检索：“Preparation of 物质名”  
获取最新专利并保存结果集2

Research Topic "preparation of solavetivone" > references (56) > refine "Patents only" (11)

**REFERENCES**

Get Substances | Get Reactions | Get Related Citations | Tools

Analyze | Refine | Categorize

Sort by: Accession Number

0 of 11 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. **Compositions and formulations for preventing and treating of hypertension, as well as for preventing and treating other diseases**  
PATENTPAK \*  
By Reid, Christopher Brian  
From U.S. Pat. Appl. Publ. (2014), US 20140271923 A1 20140918. | Language: En

Patients inflicted with various clustering chronic diseases (CD), cumulative side effects of multiple drugs as well as drug-drug interactions (DDIs) of larger no. of approved drugs during patient treatment. Examined diseases that may be, oncologic, genetic, ischemic, infectious, neurological, and immunological. The invention relates to a method of identifying agents, compounds, or drugs used by the same agents, compounds, or drugs. Thus, solid lipid nanoparticle formulations of an effective amount of other agent(s), and glutathione are dissolved in a 2% poloxamer 407 solution and homogenized for another 30 seconds.

2. **Solavetivone and 5-epi-beta-vetivone as pest repellents and insecticides**  
PATENTPAK \*  
By Goldblum, Seth; Warren, Craig B.  
From PCT Int. Appl. (2014), WO 2014099821 A2 20140626. | Language: En

The claimed pest (mostly insect) repellent and pesticidal (mostly with one or more additional active ingredients. Suitable auxiliary colorants) are selected based on the product application forms (creams, lotions, gels, soaps, powders, for use on skin and hair).

Solavetivone and 5-epi-beta-vetivone can be synthesized by the following process:

3. **Tobacco-derived components and materials**  
PATENTPAK \*  
By Coleman, William Monroe, III; Dube, Michael Francis; Lawson, Darlene M.  
From PCT Int. Appl. (2011), WO 2011088171 A2 20110721. | Language: En

The invention provides a tobacco component, for use in a smoking article, comprising a portion thereof in particulate form or from a flower of the Nicotiana species or in the form of a chemically modified flower, whereby the chemical modification being selected from a wide variety of chemical modifications, including, but not limited to, esterification, acetylation, and enzymatic modification.

**Save This Answer Set**

\* Required

Save:

- All answers
- Only selected answers

Title: \*

2

Description:

OK Cancel



# 获取化合物的制备专利信息

合并结果集1和结果集2专利结果，避免遗漏

Combine Answer Sets

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

- Combine** Include all references from both sets
- Intersect** Include only references that appear in both sets
- Exclude** Include only answers from 2 that are not in 1
- Exclude** Include only answers from 1 that are not in 2

Combine Answer Sets Cancel

# 内容

- 为什么需要CAS
- 化合物专利保护策略（以药物研发为例）
- 检索工具的选择和分析
- 案例分享
  - 获取化合物制备专利
  - 获取药物制剂专利
  - 判定化合物结构新颖性和创造性

# 获取化合物的制剂专利信息

The screenshot displays the CAS SciFinder web interface. At the top, the breadcrumb trail reads: "Substance Identifier 'Aspirin' > substances (1) > get references (87511) > refine 'Patents only' (9435)". The left sidebar contains three main sections: "REFERENCES" with sub-items like Research Topic, Author Name, and Patent; "SUBSTANCES" with sub-items like Chemical Structure and Substance Identifier; and "REACTIONS" with sub-items like Reaction Structure. The "Substance Identifier" option is selected. The main content area is titled "SUBSTANCES: SUBSTANCE IDENTIFIER" and features a search input field containing the text "Plavix". Below the input field, there are instructions: "Enter one per line. Examples: 50-00-0, 999815, Acetaminophen". A blue "Search" button is positioned at the bottom of the input area.

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。

# 获取化合物的制剂专利信息

**SUBSTANCES** Get References Retrieve references for selected substances. Tools ▾

Analyze Refine

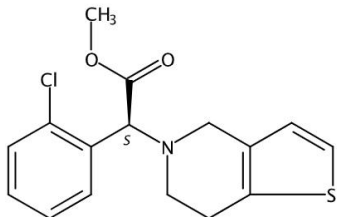
Sort by: CAS Registry Number ▾ ↓

0 of 1 Substance Selected

1. **120202-66-6** 🔍

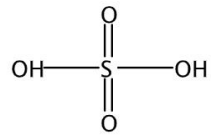
~1213 📄 🧪 ~134 🧪

113665-84-2  
C<sub>16</sub> H<sub>16</sub> Cl N O<sub>2</sub> S



Rotation (+), Absolute stereochemistry.

7664-93-9  
H<sub>2</sub> O<sub>4</sub> S



**C<sub>16</sub> H<sub>16</sub> Cl N O<sub>2</sub> S · H<sub>2</sub> O<sub>4</sub> S**  
Thieno[3,2-c]pyridine-5(4*H*)-acetic acid, α-(2-chlorophenyl)-6,7-dihydro-, methyl ester, (α*S*)-, sulfate (1:1)

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

Show More

## Get References

### Retrieve references for:

- All substances
- Selected substances

### Limit results to:

- Adverse Effect, including toxicity
- Analytical Study
- Biological Study
- Combinatorial Study
- Crystal Structure
- Formation, nonpreparative
- Miscellaneous
- Occurrence
- Preparation
- Process
- Properties
- Prophetic in Patents
- Reactant or Reagent
- Spectral Properties
- Uses

### For each sequence, retrieve:

- Additional related references, e.g., activity studies, disease studies.

**Get** Cancel

# 获取化合物的制剂专利信息

Substance Identifier "Plavix" > substances (1) > get references (1214) > refine "Patents only" (634)

REFERENCES

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Ser Sci

Analyze Refine Categorize

Sort by: Accession Number

0 of 1214 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

0 of 634 References Selected

Sort by: Accession Number

Page: 1 of 32

- 1. Effect of atorvastatin on curative effect in patients with coronary heart disease**  
By A. Rong, Zhang, Yingjun; Han, Di; Liu, Xiumei  
From Jianyan Yixue Yu Linchuang (2016), 13(23), 3317-3319, 3322. | Language: Chinese  
Objective: To investigate the effects of atorvastatin on the treatment of total of 124 patients diagnosed with coronary artery disease by coronary group was given oral clopidogrel bisulfate tablets, the observation group was compared between the two groups. The levels of blood lipids, plaq were compared. Results: The total effective rate of the observation group low-d. lipoprotein cholesterol (LDL-C), plaque area, IMT and levels of cholesterol (HDL-C) and ApoA-I were higher than those of the control group and sP-Selectin in patients with coronary heart disease, reduce atherosclerosis.
- 2. Platelet aggregation inhibitor and preparation method thereof**  
By Bai, Junling; Shao, Qi; Cai, Yijun; Sun, Ningyun; Gu, Miaokai  
From Faming Zhuanli Shengqing (2019), CN 109662948 A 20190423. | Language: Chinese  
The title method comprises: (1) mixing crystal I clopidogrel hydrogen sulfate particles obtained in the step 1 with an anti-sticking agent to obtain mixed coating. According to the prepn. method disclosed by the invention, the configuration conversion of products are solved at the same time. More has low prodn. cost and high efficiency.
- 3. Simple and efficient spherical crystallization of clopidogrel bisulfate form-I crystals**  
By An, Ji-Hun; Kiyonga, Alice Ngunjiri; Lee, Eun Hee; Jung, Kiwon  
From Crystals (2019), 9(1), 53/1-53/13. | Language: English, Database: CAPLUS  
Clopidogrel bisulfate (CLP) form-I crystals are Irregular, rectangular-shaped methods to produce CLP form-I spherical agglomerates with a uniform which produces form-I spherical agglomerates by means of spherical crystallization by using ethanol as solvent and a mixt. of iso-Pr alc. (IPA)/n-Hexane (H size distribution PSD), and polymorphic form, processing parameters ranging from 25 to 40 °C were explored. The effects of these parameters
- 1. Platelet aggregation inhibitor and preparation method thereof**  
By Bai, Junling; Shao, Qi; Cai, Yijun; Sun, Ningyun; Gu, Miaokai  
From Faming Zhuanli Shengqing (2019), CN 109662948 A 20190423. | Language: Chinese, Database: CAPLUS  
The title method comprises: (1) mixing crystal I clopidogrel hydrogen sulfate with a disintegrating agent, adding a binding agent, granulating, drying, and screening to obtain dry granules, (2) mixing the dry particles obtained in the step 1 with an anti-sticking agent to obtain mixed particles, and (3) mixing the mixed particles obtained in the step 2 with a filler, mixing with a glidant and a lubricant, tableting, and coating. According to the prepn. method disclosed by the invention, the problem of sticking and punching in the prodn. process is solved, and the problems of degradn. of active ingredients and stability of configuration conversion of products are solved at the same time. Moreover, the equipment used in the invention is commonly used equipment in the pharmaceutical industry, is suitable for mass prodn., and has low prodn. cost and high efficiency.
- 2. Clopidogrel bisulfate composition, clopidogrel bisulfate tablet and preparation method thereof**  
By Fang, Tonghua; Han, Bing; Cui, Yuhai; Jiang, Min; Jia, Wenjuan  
From Faming Zhuanli Shengqing (2019), CN 109528669 A 20190329. | Language: Chinese, Database: CAPLUS  
The invention discloses a clopidogrel bisulfate compn., clopidogrel bisulfate tablet and prepn. method thereof, which can effectively solve the sticking problem in the process of tableting, and has good stability, and can be stored for a long time without deterioration. The compn. comprises clopidogrel bisulfate,  $\beta$ -cyclodextrin and calcium hydrogen phosphate combined according to a specific proportion.
- 3. Clopidogrel bisulfate lyophilized orally disintegrating tablet**  
By Li, Pengfei; Wu, Longhao; Zhang, Yanyuan  
From Faming Zhuanli Shengqing (2019), CN 109316452 A 20190212. | Language: Chinese, Database: CAPLUS  
The invention provides a prepn. method of clopidogrel bisulfate lyophilized orally disintegrating tablet, which is prepd. by lyophilizing, and ensures the stability of clopidogrel bisulfate.
- 4. Compound aspirin clopidogrel hydrogen sulfate core-encapsulating tablet and its preparation method**  
By Hu, Jiangping; Li, Bing; Feng, Yan; Liu, Jun; Wang, Xiaoyu; Liu, Xin  
From Faming Zhuanli Shengqing (2019), CN 109288805 A 20190201. | Language: Chinese, Database: CAPLUS  
A convenient compd. aspirin clopidogrel hydrogen sulfate core-encapsulating tablet having improved bioavailability, good stability, overcoming drug resistance, avoiding adverse reactions, and rapidly disintegrating the clopidogrel hydrogen sulfate with gastrointestinal release and suitable for treatment of patients with cardiovascular and cerebrovascular diseases is provided. The core-encapsulating tablet comprises the following components in wt. percentage from inside to outside: (1) 21-31.5 of aspirin core, (2) 1.8-3 of enteric coating layer, (3) 64.5-78.5 of clopidogrel hydrogen sulfate layer, and (4) 1.1-2.5 of film coating layer.

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# 获取化合物的制剂专利信息

REFERENCES ⓘ

Analyze Refine **Categorize**

Analyze by: ⓘ  
Author Name ▼

Lannutti Brian	13
Rothbaum Wayne	13
Kaptein Allard	12
Epple Robert	11
Barf Tjeerd	10
Chackalamannil Samuel	10
Covey Todd	10
Hamdy Ahmed	10
Izumi Raquel	10
Johnson Dave	10

Show More

Categorize ⓘ

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

Category Heading	Category	Index Terms	Selected Terms
All	Substances in medicine (14924)	Page: 1 of 25 Select All   Deselect All	Click 'x' to remove the category from 'Selected Terms'
<b>Biotechnology</b>	<b>Medicine (2411)</b>	<input checked="" type="checkbox"/> Pharmaceutical tablets 152	<input checked="" type="checkbox"/> Biotechnology > Medicine (3 Terms)
General chemistry	Substances in adverse effects (2841)	<input type="checkbox"/> Anticoagulants 133	
Physical chemistry	Agriculture (158)	<input type="checkbox"/> Polyethylene glycol 106	
Synthetic chemistry	Substances in biological uses (352)	<input type="checkbox"/> Hydroxypropyl cellulose 101	
Biology	Food (100)	<input type="checkbox"/> Drug delivery systems 98	
Genetics & protein chemistry	Toxicology & forensics (37)	<input type="checkbox"/> Combination chemotherapy 97	
Analytical chemistry	Substances in food chemistry (40)	<input type="checkbox"/> D-Mannitol 90	
Technology	Substances in agriculture (20)	<input type="checkbox"/> Ethanol 86	
Polymer chemistry		<input type="checkbox"/> Cardiovascular agents 77	
Catalysis		<input checked="" type="checkbox"/> Pharmaceutical capsules 72	
Environmental chemistry		<input type="checkbox"/> Ticlopidine 72	
		<input type="checkbox"/> Dipyridamole 62	
		<input checked="" type="checkbox"/> Oral drug delivery systems 63	
		<input type="checkbox"/> Prasugrel 62	

Biotechnology > Medicine > 3 Index Term(s) Selected

OK   Cancel

片剂  
胶囊  
口服药

通过人工索引分类目录(Categorize)  
快速准确定位药物制剂专利文献

# 获取化合物的制剂专利信息

**Categorize** ?

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

Category Heading	Category	Index Terms	Selected Terms
All	Substances in property studies (5952)	Page: 1 of 2 Select All   Deselect All	Click 'x' to remove the category from 'Selected Terms'
Biotechnology	Miscellaneous substances (396)	<input checked="" type="checkbox"/> Pharmaceutical intravenous injections 12	<input checked="" type="checkbox"/> Physical chemistry > Gas, liquid, & solid phenomena (3 Terms)
General chemistry	Substances in processes (343)	<input type="checkbox"/> Crystal structure 11	
<b>Physical chemistry</b>	<b>Gas, liquid, &amp; solid phenomena (116)</b>	<input type="checkbox"/> Pharmaceutical suspensions 11	
Synthetic chemistry	Particle phenomena (43)	<input type="checkbox"/> Enteric-coated drug delivery systems 9	
Biology	Mechanics (40)	<input type="checkbox"/> Freeze drying 0	
Genetics & protein chemistry	Subatomics (31)	<input checked="" type="checkbox"/> Pharmaceutical enteric-coated tablets 9	
Analytical chemistry	Thermodynamics (17)	<input type="checkbox"/> pH 8	
Technology	Surface phenomena (29)	<input type="checkbox"/> Buffers 7	
Polymer chemistry	Spectra & spectroscopy (28)	<input type="checkbox"/> Compression 7	
Catalysis	Electric & magnetic phenomena (18)	<input type="checkbox"/> Impurities 7	
Environmental chemistry		<input checked="" type="checkbox"/> Pharmaceutical injections 7	
		<input type="checkbox"/> Viscosity 7	

Physical chemistry > Gas, liquid, & solid phenomena > 3 Index Term(s) Selected

OK   Cancel

静脉注射  
肠溶片  
注射剂

通过人工索引分类目录(Categorize)  
快速准确定位药物制剂专利文献



# 内容

- 为什么需要CAS
- 化合物专利保护策略（以药物研发为例）
- 检索工具的选择和分析
- 案例分享
  - 获取化合物制备专利
  - 获取药物制剂专利
  - 判定化合物结构新颖性和创造性



## 在专利中表示物质的方式

- 确定物质[Specific Substance]:
  - 具有表征数据的物质（一般为实施例中的物质，会被Registry收录）
  - 专利中其他确定物质（只有有充分的证据证明此物质存在，才会被Registry收录）
- 预测性物质[Prophetic Substance]:
  - 使用通式结构（Markush）表示的预测物质，一个通式结构可以表示上百或上千个化学物质（会被MARPAT数据库收录）
  - 符合Markush结构定义的表格化合物，这些物质并没有在实验室被合成出来，但同样受该专利的保护

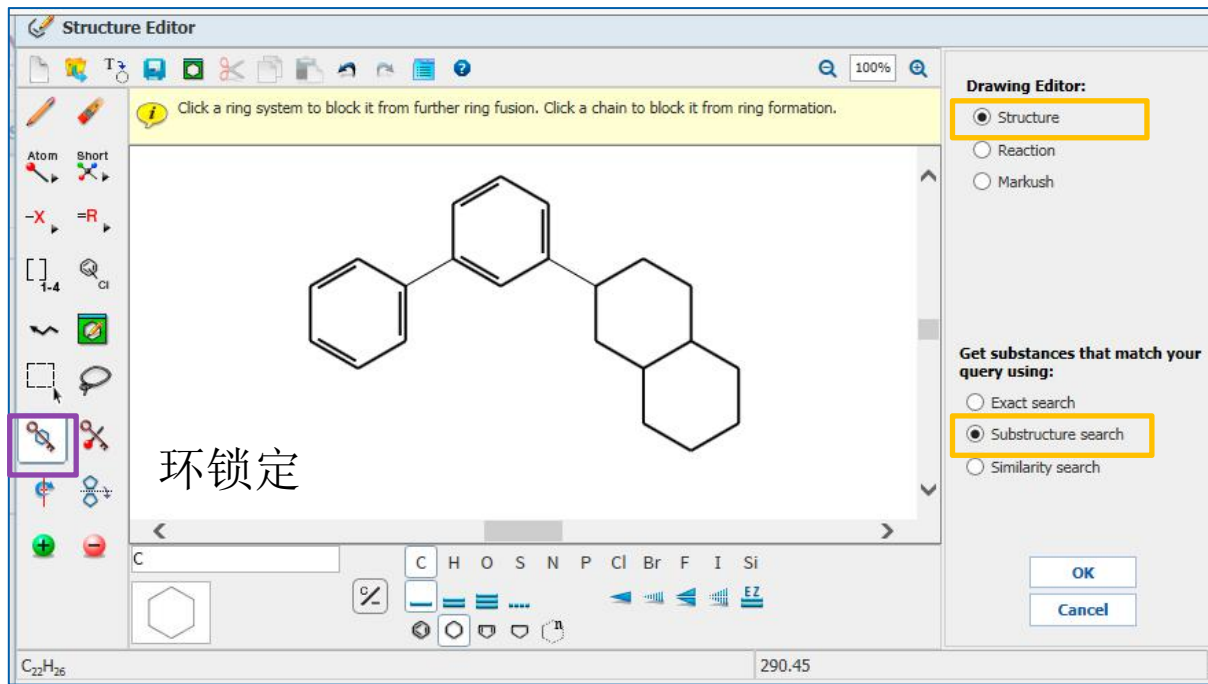
## 检索策略

- 亚结构检索，确定结构的新颖性
- Markush检索，确定结构的创造性

## SciFinder中的Markush检索

- 获取相似物质
- 检索和分析现有技术
- 评估可专利性(新颖性, 创造性)
- 发现相似专利和潜在的侵权风险
- 拓展检索的全面性和完整性
- 补充物质和文献检索

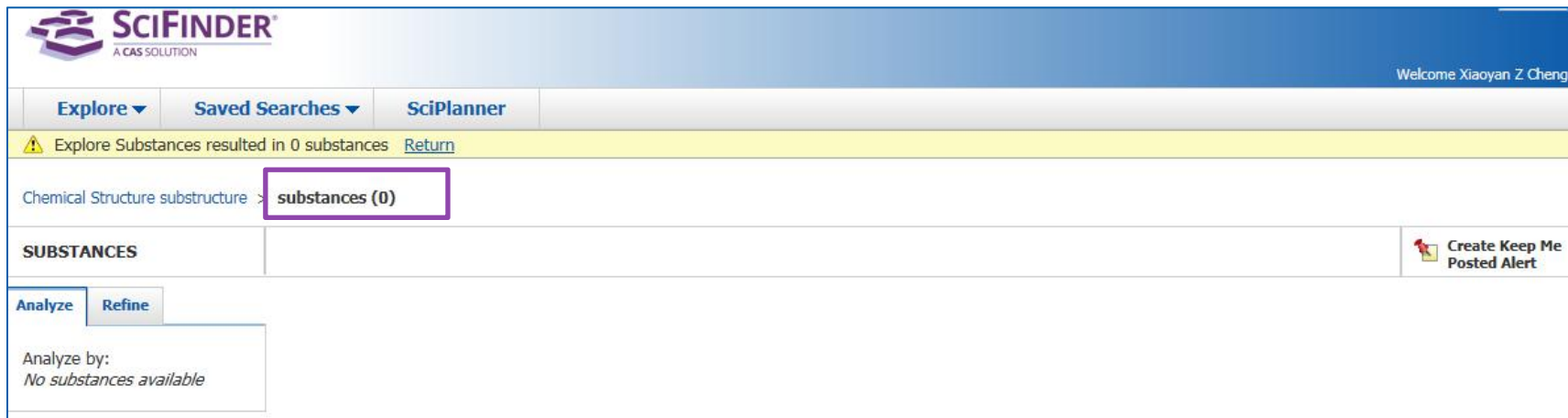
# 判断化合物新颖性及创造性



结构检索

亚结构检索

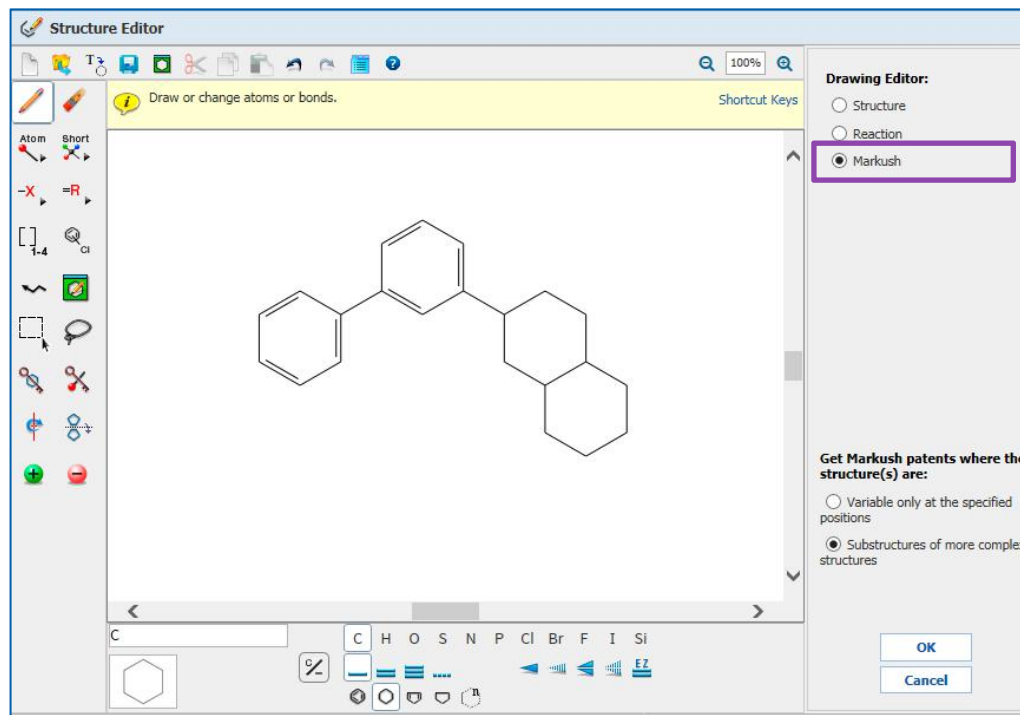
# 判断化合物新颖性及创造性



The screenshot shows the SciFinder interface. At the top left is the SciFinder logo with the text "A CAS SOLUTION". At the top right, it says "Welcome Xiaoyan Z. Cheng". Below the logo are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". A yellow warning banner states: "Explore Substances resulted in 0 substances [Return](#)". Below this, the search input field contains "Chemical Structure substructure" and the results are displayed as "substances (0)". A "SUBSTANCES" section is visible, along with "Analyze" and "Refine" buttons. A "Create Keep Me Posted Alert" button is also present. A message box indicates "Analyze by: No substances available".

物质亚结构检索结果集：零！

# 判断化合物新颖性及创造性



Markush检索

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REFERENCES

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0 of 19 References Selected

## Markush检索结果集：19篇专利文献

Analyze by:

Author Name

Hirata Shinichi	3
Brown Richard James	2
Castro Peter Paul	2
Frasier Deborah Ann	2
Happersett Constance	2
Hsieh Yu Ying	2
Krause Joachim	2
Sternberg Charlene Gross	2
Sudo Go	2
Arita Shusuke	1

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1. Procedure for the preparation of tertiary alcohols, useful as intermediates for liquid crystals, with titanium organic compounds

Quick View Other Sources

By Waechtler, Andreas; Eidenschink, Rudolf; Krause, Joachim; Kurmeier, Hans Adolf  
From Ger. Offen. (1987), DE 3608502 A1 19870917. | Language: German, Database: CAPLUS

A procedure for the prepn. of cyclic compds. I [Ar = (un)substituted aryl or heteroaryl; Q = alicyclic fragment; Z = CO<sub>2</sub>R, CN; Q<sup>3</sup> = alkylene, alkylidene, arom. system, single bond; Y = H, R; R = alkyl; Q<sup>2</sup> and Q<sup>3</sup> are not simultaneous a single bond], useful as liq. crystal intermediates, was characterized in that one reacts oxo compds. II with the corresponding aryltitanium trialkoxide. 4-BrMgC<sub>6</sub>H<sub>4</sub>OMe in THF was treated with TiCl(OCHMe<sub>2</sub>)<sub>3</sub> in THF at 40° and the mixt. stirred 30 min and treated with Et cyclohexanone-4-carboxylate in THF 30-40 min to give Et 4-(4-methoxyphenyl)cyclohexenecarboxylat...

2. Nematic liquid crystal composition with negative dielectric anisotropy, and liquid crystal display element using same

Quick View PATENTPAK

By Sudo, Go; Hirata, Shinichi  
From PCT Int. Appl. (2016), WO 2016006524 A1 20160114. | Language: Japanese, Database: CAPLUS

The nematic liq. crystal compn. contains a compd. R<sup>n1</sup>-Q-Q-R<sup>n2</sup> [R<sup>n1</sup>, R<sup>n2</sup> = (F or Cl-substituted) C<sub>1-10</sub> alkyl, C<sub>1-10</sub> alkoxy, etc., whose one CH<sub>2</sub> group or nonadjacent ≥2 CH<sub>2</sub> groups may be substituted with O or S; Q = p-cyclohexylene] and a compd. I [R<sup>1</sup> = H, O, OH, C<sub>1-12</sub> alkyl whose CH<sub>2</sub> group(s) may be substituted with O, S, CH:CH, etc.; R<sup>2-5</sup> = C<sub>1-8</sub> alkyl whose CH<sub>2</sub> group(s) may be substituted with O, S, CH:CH, etc.; R<sup>2</sup> and R<sup>3</sup>, and/or R<sup>4</sup> and R<sup>5</sup> may be bonded to each other and form ring; R<sup>6</sup>, R<sup>7</sup> = H, C<sub>1-4</sub> alkyl whose CH<sub>2</sub> group(s) may be substituted with O, S, CH:CH, etc.; n<sup>1</sup> = 1-6; M<sup>1</sup> = org. grou...

3. Bicycloalkylidene diphenols for use in polycarbonates

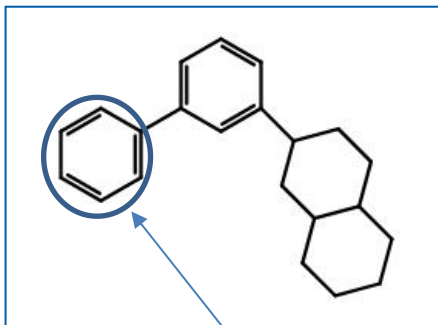
Quick View Other Sources

By Serini, Volker; Westeppe, Uwe; Fengler, Gerd; Hajek, Manfred; Casser, Carl; Waldmann, Helmut  
From Ger. Offen. (1992), DE 4031756 A1 19920409. | Language: German, Database: CAPLUS

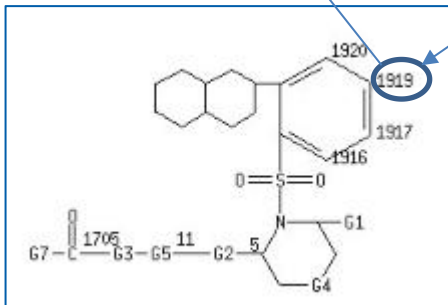
The bisphenols I [R<sup>1</sup>, R<sup>2</sup> = H, halogen, alkyl, cycloalkyl, aryl, arylalkyl; R<sup>3</sup>, R<sup>4</sup> = H, alkyl, aryl, arylalkyl (but ≥1 C atom must bear 2 substituents); m = 4-7], useful in the prepn. of polycarbonates, are prepd. by condensing the appropriate bicycloalkanes and phenols. Stirring PhOH 282, 1,1,4,4-tetramethyl-7-decalinol 104, C<sub>12</sub>H<sub>25</sub>SH 10.1, and 37% HCl 30 g

# Markush检索

检索式



专利文献中匹配的Markush结构



1916, 1917, 1919, 1920: opt. substd. by Ph

Patent location: claim 1

Note: or pharmaceutically acceptable salts, prodrugs, or metabolites

Note: additional oxo-substitution also disclosed

Note: also incorporates claim 35

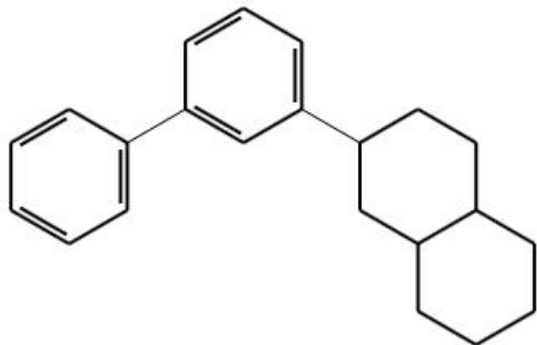


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## 判断化合物新颖性及创造性



亚结构检索结果集：0

Markush检索结果集：19篇专利文献

对于结构查新检索，需要同时进行结构检索和Markush检索，以免漏检

# 谢谢关注！

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