

# SciFinder 最新进展及专利检索

2015年8月20日



## 议程

- SciFinder 2014-2015最新进展
- 专利检索举例



## SciFinder®

- 全球最全面、最权威化学及相关学科信息
- 广泛用于查找科研至关重要的文献、物质和反应信息的直观工具
- PatentPak - 专利工作流程解决方案。即时获取专利中难以发现的化学信息及熟识语言专利族成员

SciFinder——最全面、最高质量的化学研究工具，有助于节省时间与费用

全面、时效和质量的行业领先者

训练有素的科学家编写的专业内容

 SciFinder®

广泛用于各种科学研究

功能强大、易于使用



## SciFinder 2014-2015最新进展

- 为用户提供最有价值的资源：时间
- 更便捷的访问商品来源信息
- 可阅读性和用户体验都得到了改进

## 为用户提供最有价值的资源：时间

### ■ PatentPak™ : 专利工作流程解决方案

- 为用户检索和获取专利中关键化学信息节省时间
  - 来自11个主要专利局的PDF专利全文
  - 多语言专利族PDF文件
  - 定位标引的重要化学物质所在专利页码
- 在SciFinder中可直接使用

### ■ SciFinder 和ChemDraw® 整合

- 从ChemDraw开始物质或反应检索，然后在SciFinder中获得相应的检索结果
- 从ChemDraw的结构或反应无缝传输到SciFinder

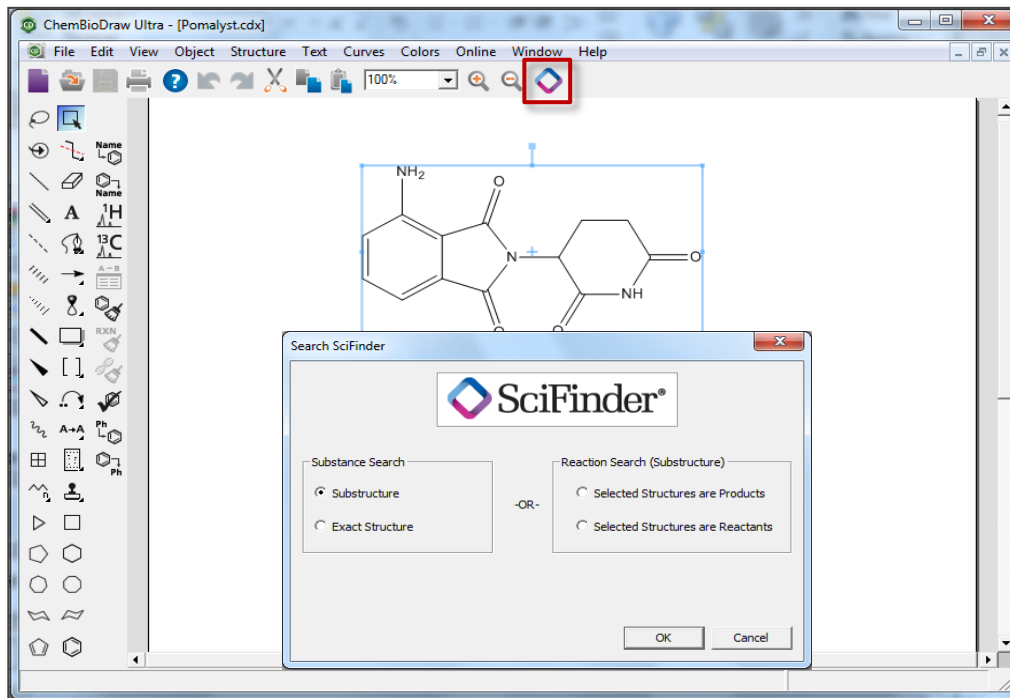
### ■ Analyze功能的改进

- 对文献分析不再限制数量。互动分析条和Show More功能现在能分析任意多的文献量
- 默认分析数量已经从1000条增加到20000条



## SciFinder 和 ChemDraw 整合

- 从ChemDraw开始物质或反应检索，然后在SciFinder中获得相应的检索结果
- 无缝传输一个ChemDraw结构或反应到SciFinder





## 改进—Analyze功能

- 分析的文献数量不再有限制
  - 互动分析条和Show More功能可以分析任意数量的文献
- 默认分析数量也已经从1000条提高到了20000条

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Research Topic "sleep aids" > references (373) > get substances (3692)

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Analyze | Refine

Sort by: CAS Registry Number

0 of 3689 Substances Selected

Page: 1 of 74

Substance Role	Preparation	Biological Study	Uses	Reactant or Reagent	Properties	Process	Prophetic in Patents	Analytical Study	Occurrence	Formation, Nonpreparative
3361	2852	2818	1743	1160	889	851	842	664	615	

Show More

1. 1323190-03-9  
CCOC(=O)C1=NC2=CC=CC=C2N1C3=CC=CC=C3  
 C<sub>22</sub> H<sub>18</sub> N<sub>6</sub> O<sub>3</sub>  
 Pyrido[2,3-c]pyridazine-3-carboxylic acid, 1,4-dihydro-1-[(6'-methyl[2,3'-bipyridin]-5-yl)methyl]-4-oxo-, ethyl ester

2. 1323189-82-7  
CCOC(=O)C1=NC2=CC=CC=C2N1C3=CC=CC=C3  
 C<sub>22</sub> H<sub>18</sub> N<sub>6</sub> O<sub>3</sub> S  
 Pyrido[2,3-c]pyridazine-3-carboxylic acid, 1,4-dihydro-1-[(6'-methyl[2,3'-bipyridin]-5-yl)methyl]-4-thioxo-, ethyl ester

3. 1323189-59-8  
CCOC(=O)C1=NC2=CC=CC=C2N1C3=CC=CC=C3  
 C<sub>17</sub> H<sub>14</sub> I N<sub>3</sub> O<sub>3</sub>  
 Pyrido[2,3-c]pyridazine-3-carboxylic acid, 1,4-dihydro-1-[(4-iodophenyl)methyl]-4-oxo-, ethyl ester

4. 1323188-86-8  
CCOC(=O)C1=NC2=CC=CC=C2N1C3=CC=CC=C3  
 C<sub>20</sub> H<sub>18</sub> N<sub>6</sub> O<sub>2</sub> S  
 Pyrido[2,3-c]pyridazine-3-carboxylic acid, 1,4-dihydro-1-[[6-(1-methyl-1H-pyrazol-4-yl)-3-pyridinyl]methyl]-4-thioxo-, ethyl ester

5. 1253115-21-7  
CCOC(=O)C1=NC2=CC=CC=C2N1C3=CC=CC=C3  
 C<sub>9</sub> H<sub>8</sub> Cl N<sub>2</sub> O<sub>2</sub> S  
 2-Thiophenepropanoic acid, 3-chloro-α-hydrazinylidene-β-oxo-, ethyl ester, (α,Z)

6. 1253115-20-6  
CCOC(=O)C1=NC2=CC=CC=C2N1C3=CC=CC=C3  
 C<sub>6</sub> H<sub>12</sub> N<sub>2</sub> O  
 Cyclohexanol, 2-diazenyl-, (1R,2R)-ref



## 更便捷地访问商业来源信息

- 以表格形式呈现商业来源信息
- 在答案集页面，设置首选或非首选商业来源
- 可通过” sort by Number of Commercial Source” 按每个物质的  
    供应商排列检索结果
  - 可快速定位起始原料、试剂及其他有兴趣的化合物

## 表格形式呈现商业来源信息

- 经常被查询的商业信息会被置于答案集的前端
  - 供应商信息
  - 纯度
  - 规格
  - 库存状态
  - 运输信息
- 可按供应商信息、纯度、规格、库存状态和运输信息重排结果集以方便快捷的获取到有价值的商业来源信息

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Chemical Structure exact > substances (3) > 32018-88-5 > commercial sources (57)

COMMERCIAL SOURCES

Analyze

Analyze by: Commercial Source

Ryan Scientific HTS and Building Blocks Product List 7

AKos Building Blocks Product List 2

Alchem Pharmtech Product List 2

Ark Pharm Product List 2

Aurum Pharmatech Product List 2

Beta Pharma Scientific Product List 2

Bide Pharmatech Product List 2

ChemPur Product List 2

Fluorochem Product List 2

Sunshine Chemlab Product List 2

Sort by: Commercial Source

0 of 57 Commercial Sources Selected

Commercial Source	Substance	Purity	Quantity	Purchasing Details	Stock Status	Ships Within
1. AB Chem Product List Canada	32018-88-5 5-Amino-1-naphthoic acid	95-98%			Synthesis on demand	2 weeks
2. abcr GmbH Product List Germany	32018-88-5 5-Amino-naphthalene-1-carboxylic acid		Grams	1 g		
3. Accel Pharmtech Product List United States	32018-88-5 5-amino-naphthalene-1-carboxylic acid	95-98%	Grams	25G, contact source 500g, contact source		
4. AKos Building Blocks Product List Germany	32018-88-5 1-Naphthalenecarboxylic acid, 5-amino-		Milligrams	500MG, EUR190 Screening	Typically in stock	2 weeks
5. AKos Building Blocks Product List Germany	32018-88-5 1-Naphthalenecarboxylic acid, 5-amino-		Grams	1G, EUR230 5G, EUR740 Screening	Typically in stock	2 weeks
6. Alchem Pharmtech Product List United States	32018-88-5 5-aminoNaphthalene-1-carboxylic acid	95-98%	Grams	1g 5g 10g 25g		

## 可阅读性和用户体验的改进

- 物质详情查看
  - 物理性质被置于显示页的顶端，便于快捷获取需要的物理性质数据
  - 展开/隐藏菜单便于快捷查找到自己需要的内容
  - 可自行勾选所需要的打印或导出的内容
- 更易于阅读的格式显示管制品信息，可快速定位感兴趣的内容
- 物质答案集展示
  - 管制信息、实验理化性质和图谱信息都以链接形式呈现
  - 在商业来源图标旁显示了供应商数量

## 物质详情显示页排列的改进提高了结果可读性

- 常用的物理性质被置于显示页的顶端，用户更易于获取所需的信息
- 可勾选需要打印或导出的内容

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Chemical Structure exact > substances (3) > 32018-88-5

**SUBSTANCE DETAIL** Get References Get Reactions Get Commercial Sources Send to SciPlanner

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**1. CAS Registry Number** 32018-88-5

$C_{11}H_9NO_2$   
1-Naphthalenecarboxylic acid, 5-amino-

**Molecular Weight**  
187.19

**pKa (Predicted)**  
Value: 2.79±0.10 | Condition: Most Acidic Temp: 25 °C

**Melting Point (Experimental)**  
Value: 201-202 °C

**Boiling Point (Predicted)**  
Value: 447.5±20.0 °C | Condition: Press: 760 Torr

**Density (Predicted)**  
Value: 1.352±0.06 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr

**Other Names**  
1-Naphthoic acid, 5-amino- (6CI,7CI,8CI)  
1-Aminonaphthalene-5-carboxylic acid  
5-Amino-1-naphthoic acid

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- EXPERIMENTAL PROPERTIES
- PREDICTED PROPERTIES
- PREDICTED SPECTRA
- CAS REFERENCE ROLES
- ADDITIONAL DETAILS

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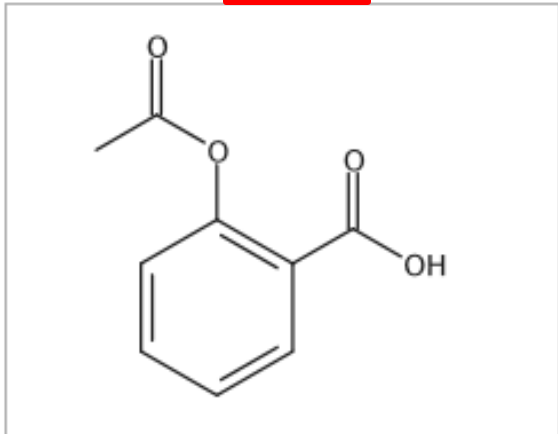
利用展开/隐藏菜单更易于获取到所需的信息

## 显示物质

商业来源图标包括了  
供应商数量

1. 50-78-2

~35308    ~146

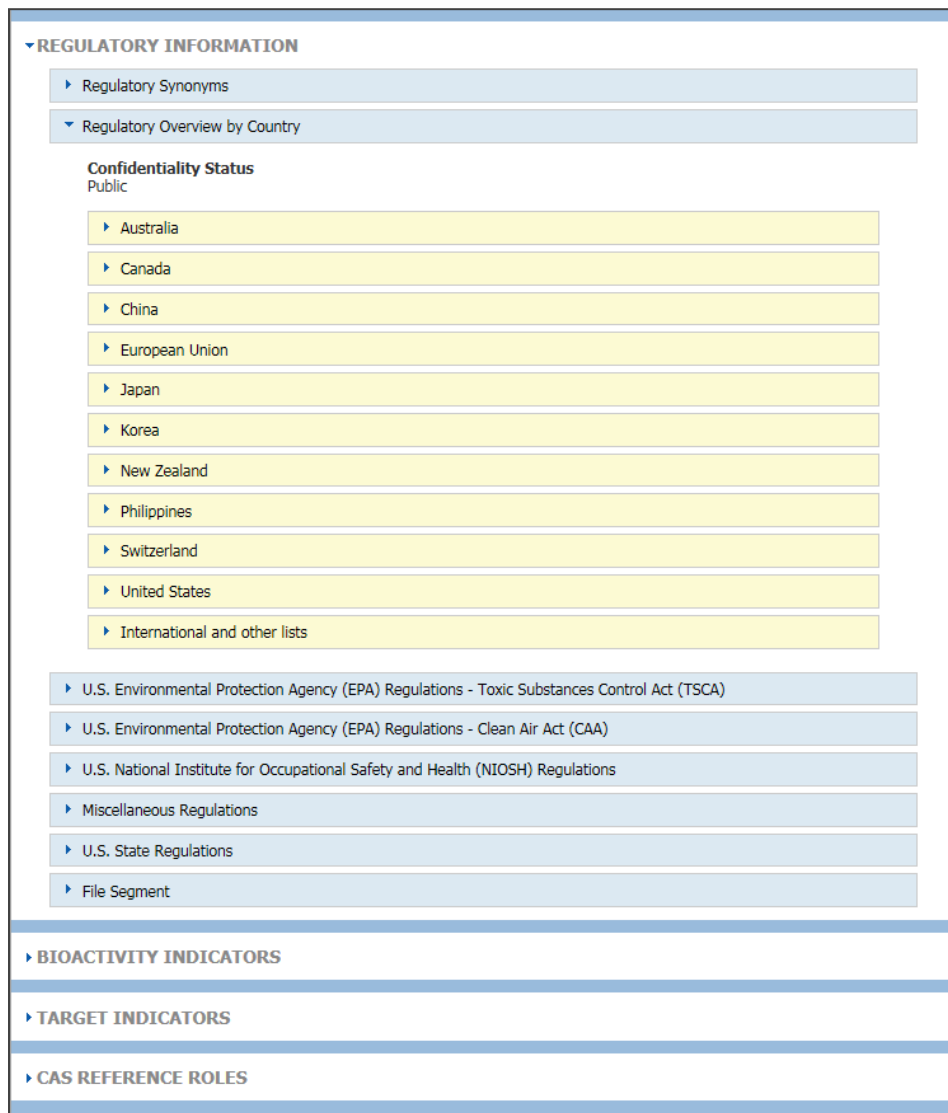


**C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>**  
Benzoic acid, 2-(acetyloxy)-

[Regulatory Information](#)  
[Spectra](#)  
[Experimental Properties](#)

管制信息、实验理化性质和图谱  
信息都以链接形式呈现

管制信息显示格式的改进，更便于用户快速获取所需信息，甚至可以按照国家进行获取



▼ REGULATORY INFORMATION

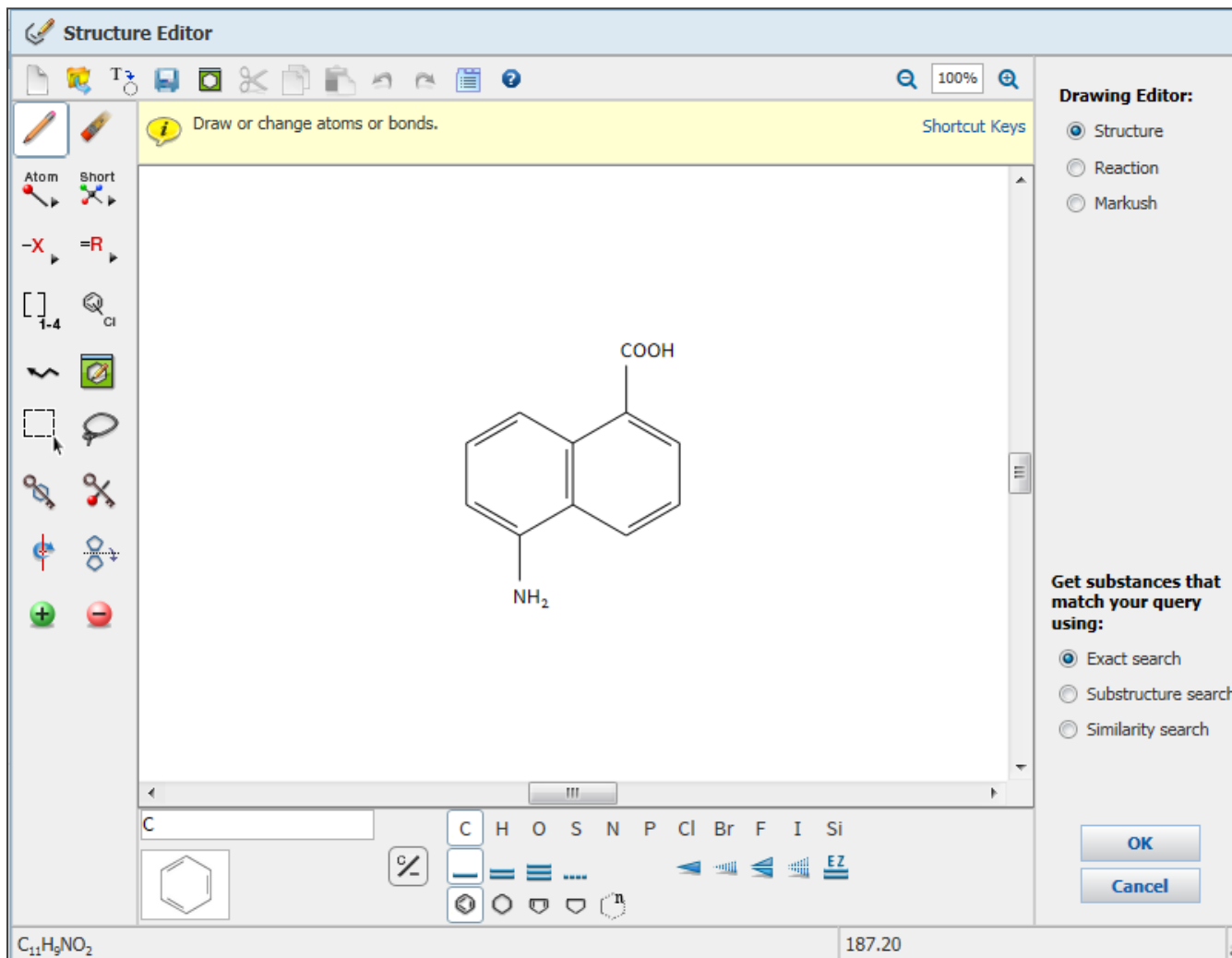
- ▶ Regulatory Synonyms
- ▼ Regulatory Overview by Country
  - Confidentiality Status**  
Public
  - ▶ Australia
  - ▶ Canada
  - ▶ China
  - ▶ European Union
  - ▶ Japan
  - ▶ Korea
  - ▶ New Zealand
  - ▶ Philippines
  - ▶ Switzerland
  - ▶ United States
  - ▶ International and other lists
- ▶ U.S. Environmental Protection Agency (EPA) Regulations - Toxic Substances Control Act (TSCA)
- ▶ U.S. Environmental Protection Agency (EPA) Regulations - Clean Air Act (CAA)
- ▶ U.S. National Institute for Occupational Safety and Health (NIOSH) Regulations
- ▶ Miscellaneous Regulations
- ▶ U.S. State Regulations
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▶ BIOACTIVITY INDICATORS

▶ TARGET INDICATORS

▶ CAS REFERENCE ROLES

## Non-Java结构编辑器







## 议程

- SciFinder® 2014-2015最新进展
- 专利检索举例
  - 获取立普妥合成、制备最具影响力的专利文献
  - 如何从结构式出发获取完整的专利文献

# CAS科学家理解并人工标引文献，使化学信息更易被发现

## Source Selection



### Title

**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**

### Bibliographic Information

**Inventor:** Nakashima, Harue; Kawakami, Sachiko  
**Patent Assignee:** Semiconductor Energy Laboratory Co., Ltd., Japan (JP)  
**Source:** PCT Int. Appl. pp.21 *In English*  
 CODEN: PIXXD2

### Abstract

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 through 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).

### Indexing

#### Index Terms:

19606-98-5P  
 Device Component Use (DEV) Industrial Manufacture (IMF) Preparation (PREP) Synthetic Preparation (SPN) Uses (USES)

(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 to be used as an electroluminescence source for display devices)

29344-72-7P

36809-26-4P

Industrial Manufacture (IMF) Preparation (PREP) Reactant (RCT) Reactant or Reagent (RACT) Synthetic Preparation (SPN)

(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 to be used as an electroluminescence source for display devices)

## Authority Processing



(54) Title: METHOD FOR

(57) Abstract: One embod  
 reaction of aniline with aryl

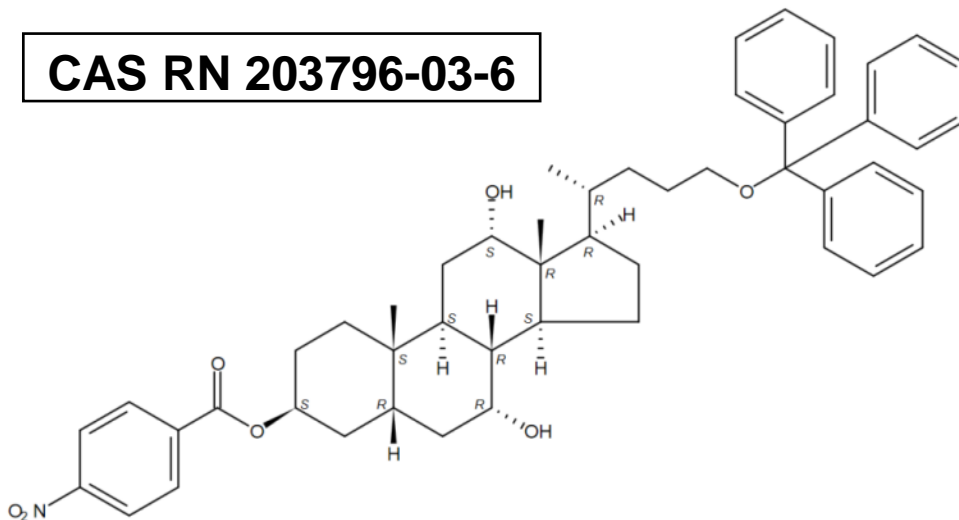
ne by the

## 该处披露了详细的标引过程，如文中容易被遗漏的结构信息

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste.

Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding NaHCO<sub>3</sub> solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO<sub>2</sub> chromatography (Et<sub>2</sub>O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529, 1489, 1448, 1345 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 144.70, 136.79, 130.77, 128.88, 127.86, 126.98, 123.70, 64.22, 47.79, 46.79, 42.15, 39.76, 37.47, 35.52, 35.34, 32.87, 28.74, 27.71, 26.85, 26.30, 25.16, 23.41, 17.98, 12.77; ESI-MS (thioglycerol+Na<sup>+</sup> matrix) m/e: ([M+Na]<sup>+</sup>) 808.4203 (53.1%)

**CAS RN 203796-03-6**



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SciPlanner

Chemical Structure exact &gt; substances (3)

## 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 ?

Lipitor

Enter one per line.

Examples:

50-00-0

999815

Acetaminophen

Search

## SAVED ANSWER SETS ?

OILS

POLYSICON

nifelat

drug for cancer

CHO AND C2H2

oled-substance

20140317 by LJ

CHO

C2H2

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degradation of Nifelat  
No results

## 物质详细信息

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(Component: 134523-00-5)

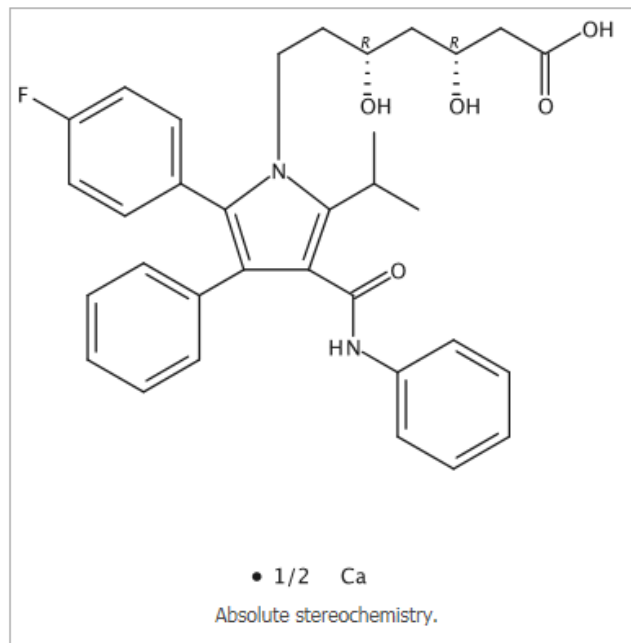
~1,626  ~154  **C<sub>33</sub>H<sub>35</sub>F N<sub>2</sub>O<sub>5</sub> · 1/2 Ca**1*H*-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1), (β*R*,δ*R*)-**Other Names**1*H*-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1), [*R*-(*R*<sup>6</sup>,*R*<sup>6</sup>)]-

Atacor

Atoraz

Atorvastatin calcium

Atorvastatin hemicalcium

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## ▶ EXPERIMENTAL PROPERTIES

## ▶ EXPERIMENTAL SPECTRA

## ▶ REGULATORY INFORMATION

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Substance Identifier "Lipitor" > substances (1) > 134523-03-8

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<input type="checkbox"/> Analytical Study	<input checked="" 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 checked="" 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	

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

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**CAS Registry Number** 134523-03-8

(Component: 134523-00-5)

~1,626 ~154


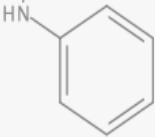
**C<sub>33</sub>H<sub>35</sub>FN<sub>2</sub>O<sub>5</sub> · 1/2 Ca**

1*H*-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1) (β,δ,δ*R*)-

**Other Names**

1*H*-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1) [*R*-(*R*<sup>\*</sup>,*R*<sup>\*</sup>)]-

Atocor  
Atoraz  
Atorvastatin calcium  
Atorvastatin hemicalcium  
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100%

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- Publication Year
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Document Type(s)

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

Refine

 1. Oral pharmaceutical compositions for use in dyslipidemias Quick View **PatentPak**

By Barranco Hernandez, Gustavo; Senosiain Pelaez, Juan Pablo; Garcia-Salgado Lopez, Enrique Raul; Luna Guiza, Maria del Coral  
From Mex. Pat. Appl. (2014), MX 2013006332 A 20141219. | Language: Spanish, Database: CAPLUS

The invention relates to a solid oral pharmaceutical compn. contg. a statin and another antilipidemic agent, to a method for the prodn. of said compn., and to the use of said combination for producing a pharmaceutical formulation that can be used to treat metabolic syndrome, type II diabetes, or other diseases. The invention further relates to the use of a pharmaceutical combination formed by atorvastatin and fenofibrate, for producing a medicament that can be used to increase the levels of HDL2a and HDL2b, and to reduce the levels of HDL3a, HDL3b and HDL3c.

 2. Simple and rapid method for preparation of atorvastatin hemi-calcium Quick View **PatentPak**

By Duan, Yuqiang; Wang, Liye; Jia, Yuxiang; Luo, Ming  
From Faming Zhuanli Shenqing (2015), CN 104447487 A 20150325. | Language: Chinese, Database: CAPLUS

The present invention discloses a method of atorvastatin hemi-calcium prepn., which consists of six steps to obtain atorvastatin hemi-calcium pure product. The special thing is that on the one hand the hydrolysis of atorvastatin ester and transformation into calcium salt are simultaneously carried out in one step in one-pot, on another aspect obtained crude atorvastatin hemi-calcium can be purified by heat refluxing in Et acetate, Pr acetate, or Bu acetate, cooling, and crystn. The present invention simplifies the process steps, shortens the reaction time, makes the reaction more thorough, c...

 3. An improved kilogram-scale preparation of atorvastatin calcium

Quick View Other Sources

By Novozhilov, Yuri V.; Dorogov, Mikhail V.; Blumina, Maria V.; Smimov, Alexey V.; Krasavin, Mikhail  
From Chemistry Central Journal (2015), 9, 7. | Language: English, Database: CAPLUS

A high-yielding synthesis of atorvastatin calcium salt on 7 kg scale is developed, that affords >99.5% product purities by introducing the following key improvements: i. isolating the pure product of the ketal deprotection step as cryst. solid, and ii. using a convenient Et acetate extn. procedure to isolate the pure atorvastatin calcium at the ester hydrolysis and counter-ion exchange step.

 4. Preparation of atorvastatin derivatives Quick View **PatentPak**

By Wu, Feihong; Wang, Zhonghua; Li, Bing; Yu, Xiaodong; Wu, Fulong; Zhu, Yanbin; Li, Yuanmei

# 获取最具影响力的专利文献

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Substance Identifier "Lipitor" > substances (1) > 134523-03-8 > get references (305) > refine "Patents only" (245) > refine "china" (35)

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Aronhime Judith	7
Anon	6
De Lange Ben	6
Kumar Yatendra	6
Mathew Joy	6
Kumar Saridi Madhava Dileep	5
Suri Sanjay	5

1. **al compositions for use in dyslipidemias**  
 Q Quick View PatentPak ▾  
 By Barranco Hernandez, Gustavo; Senosiain Pelaez, Juan Pablo; Garcia-Salgado Lopez, Enrique Raul; Luna Guiza, Maria del Coral  
 From Mex. Pat. Appl. (2014), MX 2013006332 A 20141219. | Language: Spanish, Database: CAPLUS

The invention relates to a solid oral pharmaceutical compn. contg. a statin and another antilipemic agent, to a method for the prodn. of said compn., and to the use of said combination for producing a pharmaceutical formulation that can be used to treat metabolic syndrome, type II diabetes, or other diseases. The invention further relates to the use of a pharmaceutical combination formed by atorvastatin and fenofibrate, for producing a medicament that can be used to increase the levels of HDL2a and HDL2b, and to reduce the levels of HDL3a, HDL3b and HDL3c.

2. **Simple and rapid method for preparation of atorvastatin hemi-calcium**  
 Q Quick View PatentPak ▾  
 By Duan, Yuqiang; Wang, Liye; Jia, Yuxiang; Luo, Ming  
 From Faming Zhuanli Shenqing (2015), CN 104447487 A 20150325. | Language: Chinese, Database: CAPLUS

The present invention discloses a method of atorvastatin hemi-calcium prepn., which consists of six steps to obtain atorvastatin hemi-calcium pure product. The special thing is that on the one hand the hydrolysis of atorvastatin ester and transformation into calcium salt are simultaneously carried out in one step in one-pot, on another aspect obtained crude atorvastatin hemi-calcium can be purified by heat refluxing in Et acetate, Pr acetate, or Bu acetate, cooling, and crystn. The present invention simplifies the process steps, shortens the reaction time, makes the reaction more thorough, c...

3. **Preparation of atorvastatin derivatives**

100%



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Sambasivam 9

Aronhime Judith 7

Anon 6

De Lange Ben 6

Kumar Yatendra 6

Mathew Joy 6

Kumar Saridi 5

Madhava Dileep 5

Suri Sanjay 5

1. Oral pharmaceutical compositions for use in dyslipidemias

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By Barranco Hernandez, Gustavo; Senosiain Pelaez, Juan Pablo; Garcia-Salgado Lopez, Enrique Raul; Luna Guiza, Maria del Coral  
From Mex. Pat. Appl. (2014), MX 2013006332 A 20141219. | Language: Spanish, Database: CAPLUS

The invention relates to a solid oral pharmaceutical compn. contg. a statin and another antilipidemic agent, to a method for the prodn. of said compn., and to the use of said combination for producing a pharmaceutical formulation that can be used to treat metabolic syndrome, type II diabetes, or other diseases. The invention further relates to the use of a pharmaceutical combination formed by atorvastatin and fenofibrate, for producing a medicament that can be used to increase the levels of HDL2a and HDL2b, and to reduce the levels of HDL3a, HDL3b and HDL3c.

2. Simple and rapid method for preparation of atorvastatin hemi-calcium

Quick View PatentPak ▾

By Duan, Yuqiang  
From Faming Zhu  
Patent No. Kind Language  
CN 104447487 A Chinese 150325. | Language: Chinese, Database: CAPLUS

The present invention provides a simple and rapid method for preparing atorvastatin hemi-calcium prepn., which consists of six steps to obtain atorvastatin hemi-calcium pure product. The special thing is that on the one hand the hydrolysis of atorvastatin ester and transformation into calcium salt are simultaneously carried out in one step in one-pot, on another aspect obtained crude atorvastatin hemi-calcium can be purified by heat refluxing in Et acetate, Pr acetate, or Bu acetate, cooling, and crystn. The present invention simplifies the process steps, shortens the reaction time, makes the reaction more thorough, c...

3. Preparation of atorvastatin derivatives

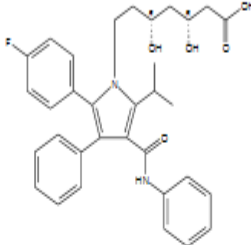
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CAS RN 134523-03-8



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page 4

CAS RN 1305-62-0

HO—Ca—OH


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page 4

CAS RN 134395-00-9

PatentPak Viewer

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(12) 发明专利申请

(10) 申请公布号 CN 104447487 A  
(43) 申请公布日 2015. 03. 25

(21) 申请号 201410732761. 6  
(22) 申请日 2014. 12. 07  
(71) 申请人 河南豫辰药业股份有限公司  
地址 461100 河南省许昌市许昌县张潘镇前汪村  
(72) 发明人 段玉强 王利叶 贾玉香 罗明  
(51) Int. Cl.  
C07D 207/34(2006. 01)

njay 5 3. Preparation of atorvastatin derivatives

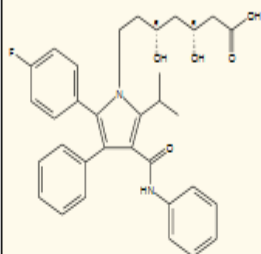
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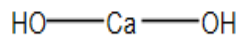


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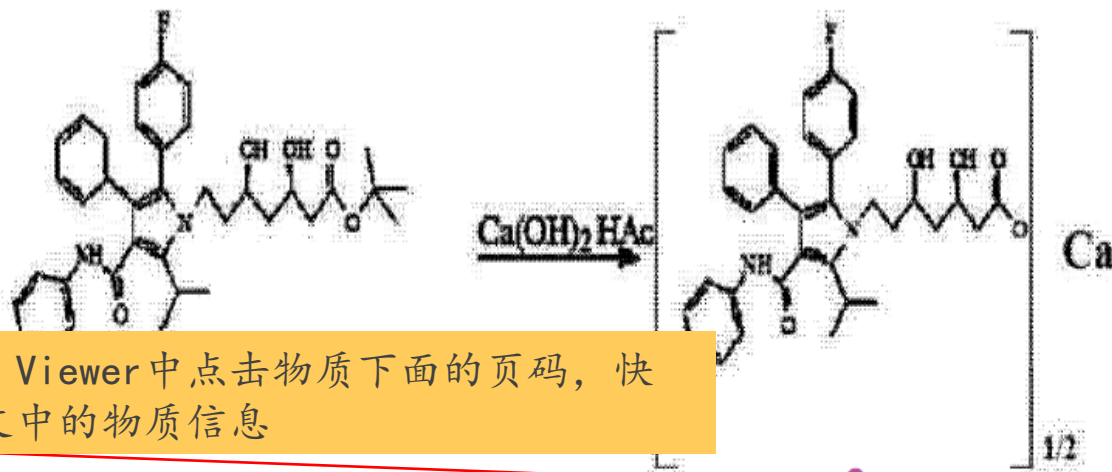
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CAS RN 134395-00-9

[0015] 下面结合实施例对本发明做详细说明,而不是限定本发明的保护范围。

[0016] 本发明的合成路线如下:



在PatentPak Viewer中点击物质下面的页码,快速定位到原文中的物质信息

## 实施例 1

向反应瓶中加入 100 ml 水、15ml 乙醇、20 g R-(R\*, R\*)-2-(4-氟基苯)-β, δ-二羟基-5-(1-异丙基)-3-苯基-4-((苯胺)羰基)-1H-吡咯-1-庚酸叔丁酯(0.03mol)以及 4 g 氢氧化钙(0.10mol),将混合物搅拌并加热混合物至 45℃,然后继续搅拌并向混合物中滴加 5g (0.08mol)醋酸,用 HPLC 跟踪反应,7 小时左右反应即可进行完毕。反应结束后,

# PatentPak—专利工作流程解决方案

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CAS RN 1305-62-0

HO—Ca—OH

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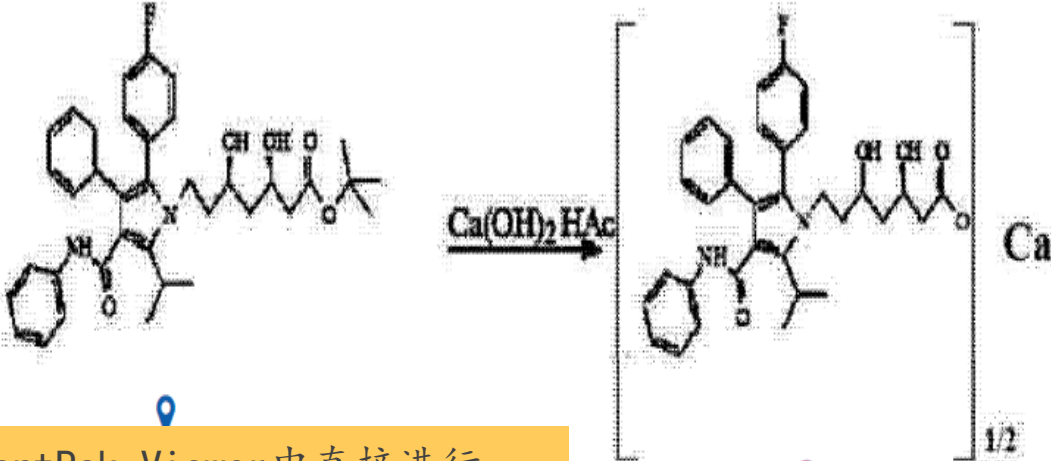
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Structure Markush Reactions

[0015] 下面结合实施例对本发明做详细说明,而不是限定本发明的保护范围。

[0016] 本发明的合成路线如下:



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向反应瓶中加入 100 ml 水、15ml 乙醇、20 g R-(R\*, R\*)-2-(4-氟基苯)-β, δ-二羟基-5-(1-异丙基)-3-苯基-4-((苯胺)羰基)-1H-吡咯-1-庚酸叔丁酯(0.03mol)以及 4 g 氢氧化钙(0.10mol),将混合物搅拌并加热混合物至 45℃,然后继续搅拌并向混合物中滴加 5g (0.08mol)醋酸,用 HPLC 跟踪反应,7 小时左右反应即可进行完毕。反应结束后,

3. Preparation of atorvastatin derivatives

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Author Name  
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Document Identifier  
Journal  
Patent  
Tags

## SUBSTANCES

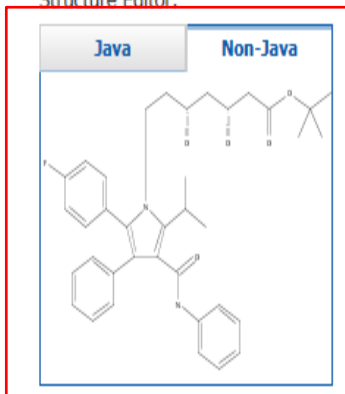
Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

## REACTIONS

Reaction Structure

## SUBSTANCES: CHEMICAL STRUCTURE ?

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 Substructure  
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Show precision analysis



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nifelat

drug for cancer

CHO AND C2H2

oled-substance

20140317 by LJ

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C2H2

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degradation of Nifelat  
No results



## 议程

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- 专利检索举例

--获取立普妥合成、制备最具影响力的专利文献

--如何从结构式出发获取完整的专利文献

## 在专利中表示物质的方式

- 确定物质 [Specific Substance]:
  - 以确定的化学结构所表示的物质
- 预测性物质 [Prophetic Substance]:
  - 使用Markush结构表示的预测物质，一个Markush可以表示上百或上千个化学物质

## 专利中的确定物质 [Specific Substance]

- 在专利权利要求书 (claim) 中所描述的确定的化学物质会被Registry数据库收录
- 对于专利中其他确定物质，只有有充分的证据证明此物质存在，（有详尽的实验数据，一般为实施例中的物质），才会被Registry收录

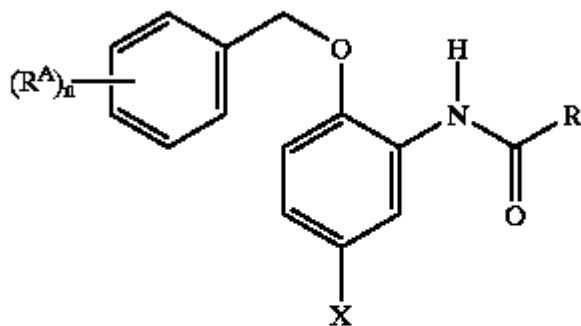


# 专利中所收录的预测性物质1

(57)

## ABSTRACT

Disclosed is a compound comprising a 2-benzyloxy-5-haloacylanilide having the structural formula I:



Formula I

wherein

R is hydrogen or an alkyl group,

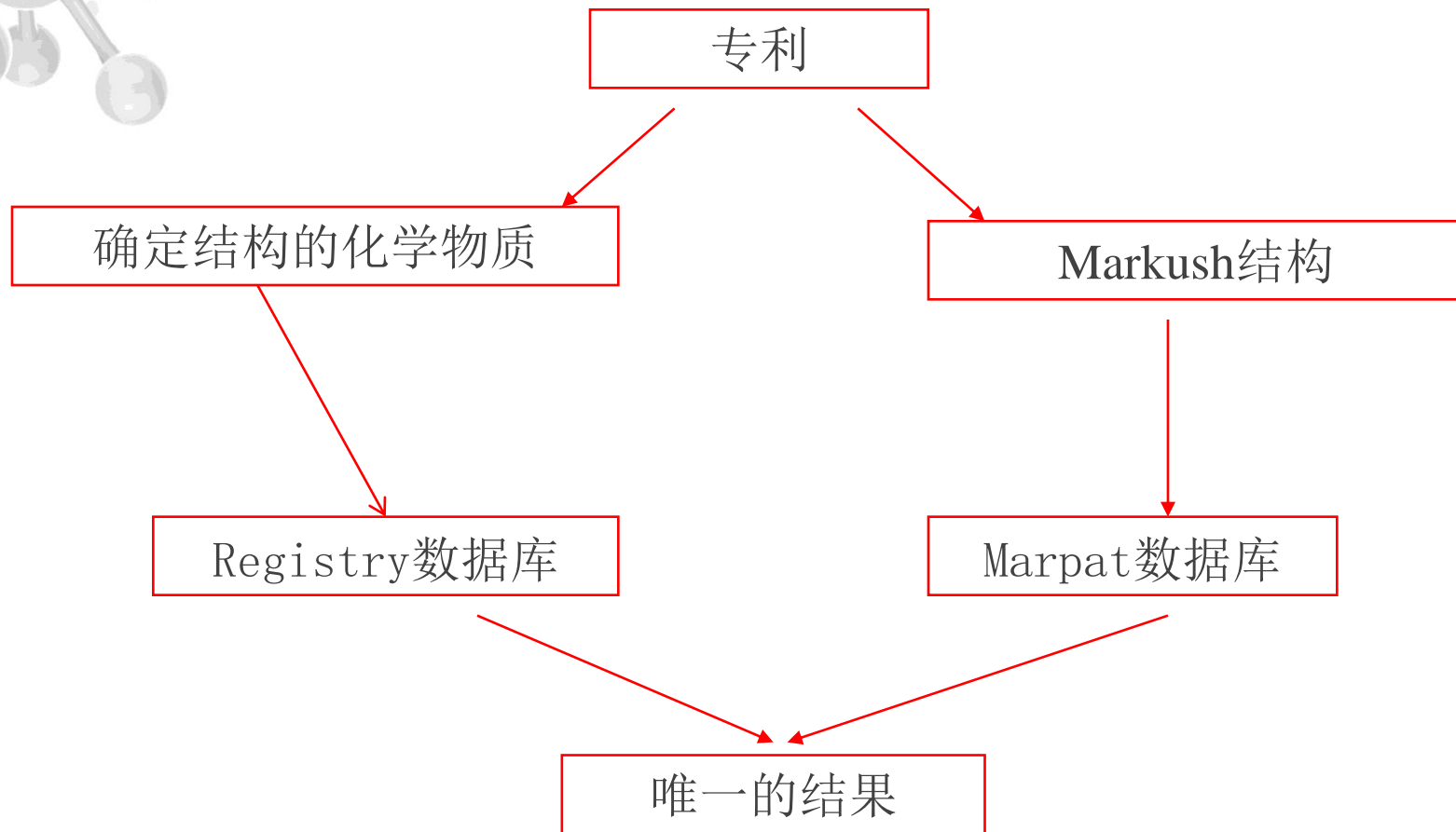
R<sup>A</sup> is a substituent and n is 0-5; and

X is a halogen.

Also disclosed is a method for preparing a coupler using the compound. The compound and method simplify the preparation of photographic couplers.

**5 Claims, No Drawings**

## 获取完整化合物文献信息途径

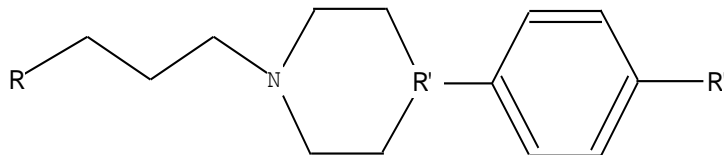




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查询报道具有如下结构特征专利文献:



要求:

- R = 任意杂环
  - R' = C, N, P
  - R'' = C, N
  - 6 圆环均为单环
  - 价键不饱和的地方均允许有取代
- 
-

# 绘制结构，并检索文献中报道的确定结构的物质

Structure Editor

Click a ring system to block it from further ring fusion. Click a chain to block it from ring formation.

Atom Short

-X =R

[ ] 1-4 Cl

Hy

R1

R2

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C H O S N P Cl Br F I Si

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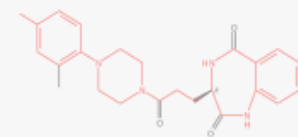
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re substructure &gt; substances (2916)

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 0 of 2916 Substances Selected 1. 1797637-65-0 🔍~0 **C<sub>17</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>S**  
Piperazine, 1-(4-nitrophenyl)-4-[3- 4. 1795186-49-0 🔍~0  5. 1794933-03-1 🔍~0  3. 1795736-35-4 🔍~0 

Absolute stereochemistry.

**C<sub>24</sub>H<sub>28</sub>N<sub>4</sub>O<sub>3</sub>**  
1H-1,4-Benzodiazepine-2,5-dione, 3-[3-[4-(2,6-dimethylphenyl)-1-piperazinyl]-3-oxopropyl]-3-(3R)- 6. 1794918-10-7 🔍~0 

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Document Type(s)

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



## 1. Method for the preparation of piperazinylalkyltriazole by regioselective 1,3-dipolar cycloaddition reaction

Quick View PatentPak

By Ko, Hun Yeong; Kwak, Ju Myeong; Choi, Jae I.; Moon, Ji Su

From *Repub. Korean Kongkae Taeho Kongbo* (2015), KR 2015024156 A 20150306. | Language: Korean, Database: CAPLUS

Disclosed is a prepn. method of I, characterized by 1,3-dipolar cycloaddn. reaction of II with  $R^2-C\equiv CH$  in the presence of a copper catalyst [ $n = 1$  or  $2$ ;  $R^1 = H$ , halo, alkyl, etc.;  $R^2 =$  alkyl, (un)substituted benzyl, (un)substituted aryl, etc.]. For example, a mixt. of 1-(3-azidopropyl)-4-phenylpiperazine (0.4 mmol), phenylacetylene (0.6 mmol) and Cu/C (2 mol%) in dioxane was reacted under irrads. of microwave [ $60^\circ$ , 10 min] and chromatographed to give 1-phenyl-4-(3-(4-phenyl-1,2,3-triazol-1-yl)propyl)piperazine (76% yield). And, regioselective prepn. of III [ $n$ ,  $R^1$ ,  $R^2 =$  same as above] using a...



## 2. Synthesis and antimicrobial activity of novel benzoxazine sulfonamide derivatives

Quick View Other Sources

By Konda, Saidulu; Raparathi, Srujana; Bhaskar, K.; Munaganti, Rajesh Kumar; Guguloth, Vijayacharan; Nagarapu, Lingaiah; Akkewar, Dattatray M.

From *Bioorganic & Medicinal Chemistry Letters* (2015), 25(7), 1643-1646. | Language: English, Database: CAPLUS

A new series of benzoxazine-6-sulfonamide derivs., e.g., I, were synthesized in excellent yields and the resulting compds. were evaluated for their antimicrobial activities. All the synthesized compds. were assessed for their antibacterial and antifungal activities. Several compds. showed low inhibitory concn. (MIC of 31.25 and 62.5  $\mu\text{g/mL}$ ) against Gram-pos. bacteria, Gram-neg. bacteria and fungi, which are comparable to the inhibitory effect of std. drugs.

3. 2-Butyl-4-chloroimidazole based substituted piperazine-thiosemicarbazone hybrids as potent inhibitors of *Mycobacterium tuberculosis*

Quick View Other Sources

By Jallapally, Anvesh; Addla, Dinesh; Yogeewari, Perumal; Sriram, Dharmarajan; Kantevari, Srinivas

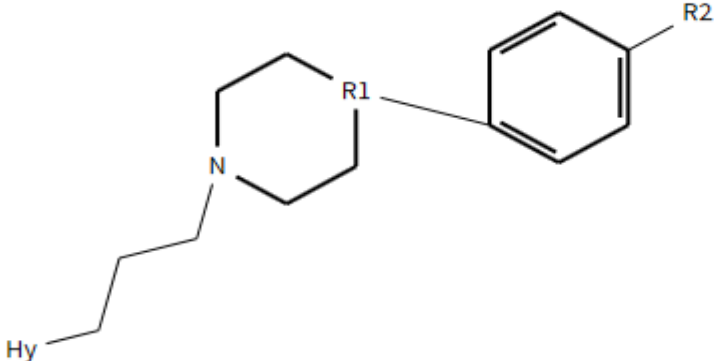
From *Bioorganic & Medicinal Chemistry Letters* (2014), 24(23), 5520-5524. | Language: English, Database: CAPLUS

A series of 2-butyl-4-chloroimidazole based substituted piperazine-thiosemicarbazone hybrids was designed by combining three different pharmacophoric fragments in single mol. architecture. 2-Butyl-4-chloro-1-((3-(4-substituted)piperazin-1-yl)propyl)-1H-imidazole-5-carbaldehydes were prepd. by reacting carboxaldehydes with N-alkylpiperazines and were subsequently condensed with thiosemicarbazide to give the desired compds. in very good yields. Among all sixteen compds. screened for in vitro antimycobacterial

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- Reaction
- Markush

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

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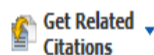
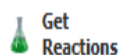
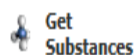
C H O S N P Cl Br F I Si

Chemical structure editor interface showing a Markush structure (a benzene ring with a substituent R2, connected via a methylene group to a piperidine ring with a substituent R1, which is further connected via a propyl chain to a hydrogen atom (Hy)). The interface includes a toolbar with drawing tools, a search bar, and a drawing editor panel with options for Structure, Reaction, and Markush (selected). The Markush options are further detailed with radio buttons for "Variable only at the specified positions" and "Substructures of more complex structures" (selected).

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Jain Sanjay 13

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Van Broeck Didier 11

Emonds Alt Xavier 10

Proietto Vincenzo 10

Saxena Anil Kumar 10

 1. Preparation of functionalized and substituted indoles as anticancer agents

[Quick View](#) [PatentPak](#)

By James, Ian; Dixon, Ian; Bu, Xian

From PCT Int. Appl. (2015), WO 2015074124 A1 20150528. | Language: English, Database: CAPLUS

The invention relates substituted indoles as tropomyosin inhibitors; processes for their prepn., and methods for treating or preventing proliferative diseases, preferably cancer, using compds. of the invention. Compds. of formula I wherein R<sup>1</sup> is substituted Ph, substituted piperazinyl, substituted pyrazolyl, etc.; R<sup>2</sup> is Me, substituted Ph, substituted pyridyl, etc.; R<sup>3</sup> is NH<sub>2</sub> and derivs., piperazinyl, morpholinyl, etc.; R<sup>4</sup> is H and methyl; R<sup>5</sup> is H, alkyl, alkoxy; X<sup>1</sup> is (CH<sub>2</sub>)<sub>0-5</sub>; X<sup>2</sup> = X<sup>3</sup> = O, NH, CO, etc.; X<sup>4</sup> is O, NH and derivs.; and pharmaceutically acceptable drugs and prodrugs thereof, are...

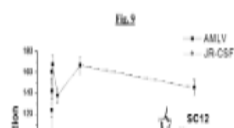
 2. Novel compositions useful for inhibiting HIV-1 infection and methods using same

[Quick View](#) [PatentPak](#)

By Cocklin, Simon

From PCT Int. Appl. (2015), WO 2015051230 A1 20150409. | Language: English, Database: CAPLUS

The present invention includes novel compns. useful for preventing or treating an HIV-1 infection in a subject in need thereof. The present invention further includes a novel method of preventing or treating an HIV-1 infection in a subject in need thereof, the method comprising administering to the subject an effective amt. of a compd. of the invention. In certain embodiments, the subject is further administered at least one addnl. therapeutic agent.





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Select saved answer set(s) to combine with your current answer set (874):

9 Answer Sets 1 Selected

	Reference Answer Set Details	Date Saved
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<input checked="" type="checkbox"/>	structure1 (286) Chemical Structure substructure > substances (2916) > get references (401) > refine "Patents only" (286)	Jul 16, 2015
<input type="checkbox"/>	Autosaved Reference Set (1) An answer set was automatically saved because the session ended due to inactivity on Wed Jul 01 04:52:53 EDT 2015. Substance Identifier "1786400-23-4" > substances (1) > 1786400-23-4 > get references (1)	Jul 1, 2015
<input type="checkbox"/>	OILS (89)	May 14, 2015

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- Combine** Include all answers from both sets
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1. **Preparation of functionalized and substituted indoles as anticancer agents**

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By James, Ian; Dixon, Ian; Bu, Xian

From PCT Int. Appl. (2015), WO 2015074124 A1 20150528. | Language: English, Database: CAPLUS

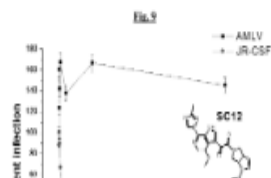
The invention relates substituted indoles as tropomyosin inhibitors; processes for their prepn., and methods for treating or preventing proliferative diseases, preferably cancer, using compds. of the invention. Compds. of formula I wherein R<sup>1</sup> is substituted Ph, substituted piperazinyl, substituted pyrazolyl, etc.; R<sup>2</sup> is Me, substituted Ph, substituted pyridyl, etc.; R<sup>3</sup> is NH<sub>2</sub> and derivs., piperazinyl, morpholinyl, etc.; R<sup>4</sup> is H and methyl; R<sup>7</sup> is H, alkyl, alkoxy; X<sup>1</sup> is (CH<sub>2</sub>)<sub>0-3</sub>; X<sup>2</sup> = X<sup>3</sup> = O, NH, CO, etc.; X<sup>4</sup> is O, NH and derivs.; and pharmaceutically acceptable drugs and prodrugs thereof, are...

2. **Novel compositions useful for inhibiting HIV-1 infection and methods using same**

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By Cocklin, Simon

From PCT Int. Appl. (2015), WO 2015051230 A1 20150409. | Language: English, Database: CAPLUS



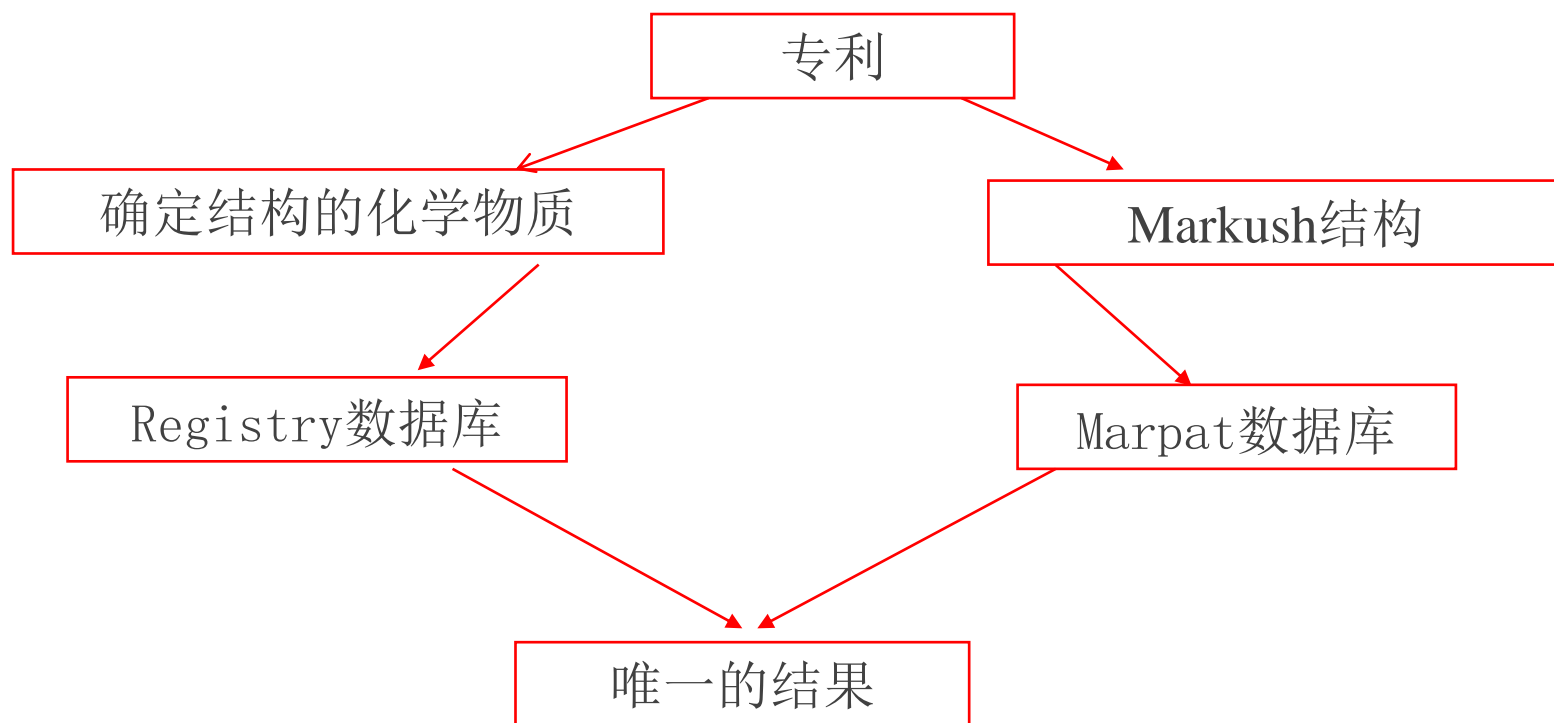
The present invention includes novel compns. useful for preventing or treating an HIV-1 infection in a subject in need thereof. The present invention further includes a novel method of preventing or treating an HIV-1 infection in a subject in need thereof, the method comprising administering to the subject an effective amt. of a compd. of the invention. In certain embodiments, the subject is further administered at least one addnl. therapeutic agent.

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