

# SciFinder<sup>n</sup>快速入门指南

## SciFinder<sup>n</sup>——最全面的化学及相关学科信息资源，加速实现科学突破

SciFinder<sup>n</sup>是一个研发应用平台，由美国化学会（American Chemical Society，简称“ACS”）旗下的美国化学文摘社（Chemical Abstracts Service, 简称“CAS”）出品，提供全球最大、最权威的化学及相关学科文献、物质和反应信息。SciFinder<sup>n</sup>涵盖了化学及相关领域如生物医药、工程、材料科学、农业科学等多学科、跨学科的科技信息。SciFinder<sup>n</sup>收录的文献类型包括期刊、专利、会议论文、学位论文、图书、技术报告、评论和网络资源等。

SciFinder<sup>n</sup>收录所有已经公开披露、高质量且来自可靠信息源的信息，由CAS科学家分析文献的每一个细节并加以标引，您无需担心遗漏任何关键信息。



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## 登陆进入 SciFinder<sup>n</sup>

(https://SciFinder-n.cas.org)

SciFinder<sup>n</sup> is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.

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## 开始检索

SciFinder<sup>n</sup> 具有全新的简洁界面。

1

All

Substances

Reactions

References

Suppliers

2

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

Enter a query...

3

4

1. 选择需要的检索选项：选择 All，进行全面的检索（包括物质，反应，文献和供应商）
2. 输入检索信息：关键词，CAS 登记号，专利号等

3. 点击 Draw，绘制检索结构
4. 点击放大镜，开始检索

## All 检索结果展示

1

2

3

1. 显示检索的结果集：物质，反应，文献，供应商及对应的结果数，点击任何一项即可进入对应的结果界面
2. 点击 Substances，即可进入物质结果集界面
3. 点击 Reactions，即可进入反应结果集界面

## 文献检索

文献检索使用了全球最高级的化学智能算法。结果页面可视化、动态化，并且显示布局便于使用。

1. 选择 References，进行文献检索
2. 输入检索信息：关键词、物质名称、CAS 登记号和专利号等
3. 点击 Draw，绘制检索结构
4. 点击 Advanced Search，进行作者、期刊或组织机构检索
5. 点击放大镜，开始检索

## 文献检索结果展示

1. 点击 **Sort** 右侧小箭头，对结果进行重新排序
2. 点击 **View** 右侧小箭头，选择结果展示的详略
3. 全面的文献结果分类
4. 下载检索结果
5. 分享检索结果
6. 保存检索结果，并可同时设定信息更新提醒
7. 查看文献详情
8. 获取全文链接
9. 获取相关的物质
10. 获取相关的反应
11. 获取被引用文献
12. 引文地图，获取引用及被引用文献
13. 回到首页界面

# 文献详情

1. Return to Results

2. Reference Detail (7 of 1,187)

3. Substances (9) Reactions (10) Cited By (4) Citation Map

4. Prev Next

5. Patent

6. Patent Information

7. Patent Number: WO2008087666

8. Publication Date: 2008-07-24

9. Application Number: WO2008-IN39

10. Application Date: 2008-01-21

11. Kind Code: A1

12. Assignee: Almet Corporation, India

Source: World Intellectual Property Organization

Database Information: AN: 2008:890825, CAN: 149:201074, CAplus

Language: English

Preparative process for ether derivative of artemisinin

By: Degani, Mariam S.; Narkhede, Sachin S.; Pedgaonkar, Yogesh Y.; Chavan, Sunil S.

Abstract: A process was disclosed for the preparation of therapeutically useful antimalarial artemisinin ether derivatives, such as I [R<sup>10a</sup> = H, R<sup>10b</sup> = alkyloxy], and comprised reducing artemisinin I [R<sup>10a</sup>R<sup>10b</sup> = O] to dihydroartemisinin I [R<sup>10a</sup> = H, R<sup>10b</sup> = OH] using a mixture of sodium borohydride and a dihydroxy compound, followed by etherification in presence of an acid catalyst and an alc. α/β-Arteether I [R<sup>10a</sup> = H, R<sup>10b</sup> = OEt] was prepared with 92% overall yield using sodium borohydride, HOCH<sub>2</sub>CH(OH)Me and Me<sub>2</sub>CHOH in hexane for the reduction of artemisinin and H<sub>2</sub>SO<sub>4</sub> and EtOH in hexane for the etherification of the intermediate α/β-dihydroartemisinin.

Chemical structure I: C[C@H]1[C@@H]2[C@H](OC)[C@H](OC)[C@@H](OC)[C@H]2[C@@H](OC)[C@H]1O

PATENTPAK Viewer Full Text

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2008087666	English	A1	PDF   PDF+   Viewer	2008-07-24	WO2008-IN39	2008-01-21
IN2007MU00122	English	A		2008-10-03	IN2007-MU122	2007-01-19
WO2008087667	English	A1				

Substances (9)

478287-92-2: C17H24O5 α/β-Arteether

131175-87-6: C15H24O5 (3R,5aS,6R,8aS,9R,12R,12aR)-Decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-...

82638-05-9: C18H26O5 (3R,5aS,6R,8aS,9R,12R,12aR)-Decahydro-10-methoxy-3,6,9-trimethyl-3,12-epoxy-12H-...

1. 返回至文献结果集界面
2. 文献书目信息
3. 文献相关信息：物质、反应、引文
4. 点击左右箭头，查看上一篇或下一篇文献详情
5. PatentPak 浏览器快速阅读专利全文
6. 全文链接
7. PDF: 获取专利 PDF 全文
8. PDF+: 获取附有物质标引信息的专利 PDF 全文



9. Viewer: PatentPak 浏览器，在线快速阅读专利全文
10. 概念词语
11. 文献中报道的物质
12. 引文信息

## 专利文献的获取——PatentPak 的使用

The screenshot shows the SciFinder interface with the search results for 'PCSK9 inhibitors'. The left sidebar contains filters for Document Type and Substance Role. The main area displays a list of patent results with columns for Patent, Language, Kind Code, and actions (PDF, PDF+, Viewer). The 'PATENTPAK' dropdown menu is open, showing options for PDF, PDF+, and Viewer. The 'Viewer' option is highlighted, indicating the next step in the process.

1. 选择文献类型为 Patent
2. 点击 PatentPak 旁的小箭头，查看专利族
3. PDF: 获取专利 PDF 全文
4. PDF+: 获取附有物质标引信息的专利 PDF 全文
5. Viewer: PatentPak 浏览器，在线快速阅读专利全文

The screenshot displays the PATENTPAK interface. At the top, there are navigation controls for PAGE (218 / 234), ZOOM, and DOWNLOAD (PDF, PDF+). The main content area shows a patent document with the title "WO 2012/101252" and "PCT/EP2012/051320". The page number "217" is visible. The text describes various conditions and treatments, including "(x) persons suffering from hypothyroidism;" and "(xiv) persons taking one or more of the following medicines: medicines altering the way the immune systems works (e.g. cyclosporin or antihistamines), antibiotics or antifungal medicines (e.g. erythromycin, clarithromycin, ketoconazole, itraconazole, rifampicin, fusidic acid), medicines regulating lipid levels (e.g. gemfibrozil, colestipol), calcium channel blockers (e.g. verapamil, diltiazem), medicines regulating the heart rhythm".

On the left sidebar, there are sections for "Key Substances in Patent". The first section shows "CAS RN 59865-13-3" with a chemical structure and a purple box containing the number "3". Below it, "Analyst Markup Locations (3)" are listed: Page 50, Page 55, and Page 218 (highlighted with a purple box containing "1"). The second section shows "CAS RN 9028-35-7" for "Hydroxymethylglutaryl coenzyme A reductase (NADPH)" with "Analyst Markup Locations (2)": Page 60 and Page 223.

In the main text area, there are purple boxes with numbers "2" and "5" highlighting specific parts of the text.

1. 物质位置信息：点击页码定位符号，右侧 PDF 全文快速跳转该物质出现的页码处，同时对应物质的位置符号由蓝色变为紫色。
2. PDF 全文中对应的物质位置符号
3. 点击 CAS 登记号，获取物质详情
4. 下载专利全文：PDF: 获取专利 PDF 全文；PDF+: 获取附有物质标引信息的专利 PDF 全文。

## 分析实验详情的获取——MethodsNow 的使用

References - purification of sofosbuvir

2000 to 2017  
No Min to No Max Apply  
View Larger

Available at My Institution  
Author  
Organization  
Publication Name  
Concept  
CAS Solutions  
MethodsNow: Analysis (4,278)  
Database  
Search Within Results

View More

Full Text

Substances (2) Reactions (0) Cited By (8) Citation Map

**RP-HPLC Method for Simultaneous Determination of Sofosbuvir and Ledipasvir in Tablet Dosage Form and Its Application to In Vitro Dissolution Studies**

By: Zaman, Bakht; Siddique, Faisal; Hassan, Waseem  
Chromatographia (2016), 79(23-24), 1605-1613 | Language: English, Database: CAPlus  
View Reference Detail | MethodsNow: Analysis

**Abstract:** A reversed-phase high-performance liquid chromatog. method was developed for the simultaneous determination of sofosbuvir and ledipasvir in tablet dosage form. The anal. was performed on Luna anal. column 250 × 4.6 mm, 5 μm, octyl silica packing (Si-[CH<sub>2</sub>]<sub>7</sub>-CH<sub>3</sub>) C8, using ammonium acetate buffer solution pH 7.0 and acetonitrile 35:65 % volume/volume as mobile phase at flow rate of 0.7 mL min<sup>-1</sup> for isocratic elution. Detection of sofosbuvir and ledipasvir was performed on a UV detector at 245 nm. The retention times of sofosbuvir and ledipasvir were 4.468 ± 0.013 min and 8.242 ± 0.012 min, resp.

View More

Full Text

Substances (3) Reactions (0) Cited By (7) Citation Map

**A UHPLC-MS/MS method for the quantification of direct antiviral agents simeprevir, daclatasvir, ledipasvir, sofosbuvir/GS-331007, dasabuvir, ombitasvir and paritaprevir, together with ritonavir, in human plasma**

By: Ariaudo, Alessandra; Favata, Fabio; De Nicolo, Amedeo; Simiele, Marco; Paglietti, Luca; Boglione, Lucio; Cardellino, Chiara Simona; Carcieri, Chiara; Di Perri, Giovanni; D'Avolio, Antonio  
Journal of Pharmaceutical and Biomedical Analysis (2016), 125, 369-375 | Language: English, Database: CAPlus  
View Reference Detail | MethodsNow: Analysis

1. 选择 CAS Solutions 中的 MethodsNow: Analysis
2. 点击 MethodsNow: Analysis 获取实验方法详情

Journal

Source  
Chromatographia  
Volume: 79  
Issue: 23-24  
Pages: 1605-1613  
Journal  
2016  
DOI: 10.1007/s10337-016-3179-9

Database Information  
AN: 2016:1599543  
CAN: 165:581014  
CAPlus

Company/Organization  
Institute of Chemical Sciences  
University of Peshawar  
Khyber Pakhtunkhwa 25120  
Pakistan

Publisher  
Springer

Language  
English

**RP-HPLC Method for Simultaneous Determination of Sofosbuvir and Ledipasvir in Tablet Dosage Form and Its Application to In Vitro Dissolution Studies**

By: Zaman, Bakht; Siddique, Faisal; Hassan, Waseem

**Abstract:** A reversed-phase high-performance liquid chromatog. method was developed for the simultaneous determination of sofosbuvir and ledipasvir in tablet dosage form. The anal. was performed on Luna anal. column 250 × 4.6 mm, 5 μm, octyl silica packing (Si-[CH<sub>2</sub>]<sub>7</sub>-CH<sub>3</sub>) C8, using ammonium acetate buffer solution pH 7.0 and acetonitrile 35:65 % volume/volume as mobile phase at flow rate of 0.7 mL min<sup>-1</sup> for isocratic elution. Detection of sofosbuvir and ledipasvir was performed on a UV detector at 245 nm. The retention times of sofosbuvir and ledipasvir were 4.468 ± 0.013 min and 8.242 ± 0.012 min, resp., and the total run time was 20 min. The method was validated according to the requirements of the USP (category I). The overall recovery of both analytes was 100 ± 1 %; the relative standard deviation for precision and intraday precision was less than 2.0 %. The method was linear with correlation coefficient (r) >0.9999, limits of detection 0.485 and 0.175 μg mL<sup>-1</sup>, and limits of quantification was 1.619 and 0.586 μg mL<sup>-1</sup> for sofosbuvir and ledipasvir, resp. The method was successfully applied to the assay and in vitro dissolution studies of sofosbuvir and ledipasvir in tablet dosage form.

Full Text

Expand All | Collapse All

Concepts  
Substances  
MethodsNow: Analysis

Title	CAS Method Number
Analysis of Sofosbuvir in Pharmaceutical tablets by Reversed-phase HPLC	1-101-CAS-288134

3. 点击 CAS 方法号，获取实验方法详情  
 获得 CAS 科学家深度标引的、全面、有条理的实验详情。

CAS Solutions  
**METHODSNow**  
A CAS SOLUTION

Analysis of Sofosbuvir in Pharmaceutical tablets by Reversed-phase HPLC  
 CAS MN: 1-101-CAS-288134

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis  
 Technique: UV-visible spectroscopy; Reversed-phase HPLC

Materials	Role	Image	CAS RN
Ledipasvir	analyte	<a href="#">View Structure</a>	1256388-51-8
Sofosbuvir	analyte	<a href="#">View Structure</a>	1190307-88-0
Pharmaceutical tablets	matrix		
0.45 µm nylon filter paper	material		
Luna analytical column 250 × 4.6 mm, 5 µm, octyl silica packing (Si-[CH <sub>2</sub> ]-CH <sub>3</sub> ) <sub>2</sub> C <sub>8</sub>	material		
Vacuum filtration assembly,	material		
0.2 µm nylon membrane filter	material		
Monopotassium phosphate	reagent	<a href="#">View Structure</a>	7778-77-0
2,6-Di-tert-butyl-4-methylphenol	reagent	<a href="#">View Structure</a>	128-37-0
Polyoxyethylene sorbitan monooleate	reagent		9005-65-6

**Source**  
 RP-HPLC Method for Simultaneous Determination of Sofosbuvir and Ledipasvir in Tablet Dosage Form and Its Application to In Vitro Dissolution Studies  
 Zaman, Bakht; Siddique, Faisal; Hassan, Waseem  
 Chromatographia (2016), 79 (23-24), 1605 - 1613. Springer  
 CODEN: CHRGB7 | ISSN: 00095893 | DOI: 10.1007/s10337-016-3179-9

[Full Text](#)

**Abstract**  
 A reversed-phase high-performance liquid chromatog. method was developed for the simultaneous determination of sofosbuvir and ledipasvir in tablet dosage form. The anal. was performed on Luna anal. column 250 × 4.6 mm, 5 µm, octyl silica packing (Si-[CH<sub>2</sub>]-CH<sub>3</sub>)<sub>2</sub> C<sub>8</sub>, using ammonium acetate buffer solution pH 7.0 and acetonitrile 35:65 % volume/volume as mobile phase at flow rate of 0.7 mL min<sup>-1</sup> for isocratic elution. Detection of sofosbuvir and

**Equipment Used**  
 HPLC system  
 Pump, Adept CE-4104, Cecil Instruments Limited, UK  
 UV detector, Adept CE 4200, Cecil Instruments Limited, UK  
 Electronic balance, AW220, Shimadzu, Japan  
 Ultrasonic bath, SONOREX, Bandelin, Germany

**Conditions**  
**Instrument**  
 Column: Luna analytical column 250 × 4.6 mm, 5 µm, octyl silica packing (Si-[CH<sub>2</sub>]-CH<sub>3</sub>)<sub>2</sub> C<sub>8</sub>; mobile phase: ammonium acetate buffer pH 7.0 and acetonitrile in the ratio 35:65% v/v ; flow rate: 0.7 mL/min  
 wavelength: 245 nm

**Instructions**  
**Preparation of dissolution medium**  
 1. Prepare potassium dihydrogen orthophosphate 0.01 M solution by dissolving 8.16 g in about 4.0 L purified water using a 6.0-L volumetric flask.  
 2. Add 90 g of polysorbate 80 to the solution and dissolve by mechanical shaking and heat to 37 °C.  
 3. Adjust the pH of the solution to 6.0 ± 0.5 by using 0.0075 mg/mL solution of butylated hydroxytoluene (BHT) and adjust the volume to 6.0 L using purified water.  
**Preparation of pharmaceutical tablets**  
 1. Prepare sample solution of tablet dosage form by dissolution of 10 tablets in 1 L dissolution medium.  
 2. Dilute ten milliliters of the solution with ammonium acetate buffer pH 7.0 and acetonitrile in the ratio 35:65% v/v to a composite sample stock solution containing sofosbuvir 0.4 mg/mL and ledipasvir 0.09 mg/mL using 100 mL amber-colored volumetric flasks and filter through 0.45 µm nylon filter paper from Millipore.  
**Preparation of stock solutions**  
 1. Prepare the stock solutions by dissolving equivalent to 20.0 mg of sofosbuvir (SOF) and 4.5 mg ledipasvir (LED) separately in 30 mL of acetonitrile in 50-mL amber-colored volumetric flasks and dilute to volume with ammonium acetate buffer pH 7.0.  
 2. Store the reference and sample stock solutions at 2 - 8 °C, protect from light and further dilute.  
**Reversed phase high-performance liquid chromatography (RP-HPLC)**  
 1. Use the HPLC system consisting of a Cecil Adept CE-4104 low pressure quaternary gradient pump, Adept CE 4200 variable wavelength UV detector (Cecil Instruments Limited UK), controlled by PowerStream chromatography manager software version 4.2.  
 2. Carry out the separation on Luna analytical column (Phenomenex USA) 250 × 4.6 mm, 5 µm, octyl silica packing (Si-[CH<sub>2</sub>]-CH<sub>3</sub>)<sub>2</sub> C<sub>8</sub>.  
 3. Prepare the mobile phase by mixing ammonium acetate buffer pH 7.0 and acetonitrile in the ratio 35:65% v/v and filter through a 0.2 µm nylon membrane filter using a Millipore vacuum filtration assembly.  
 4. Set the flow rate at 0.7 mL/min.  
 5. Set the detector at 245 nm.

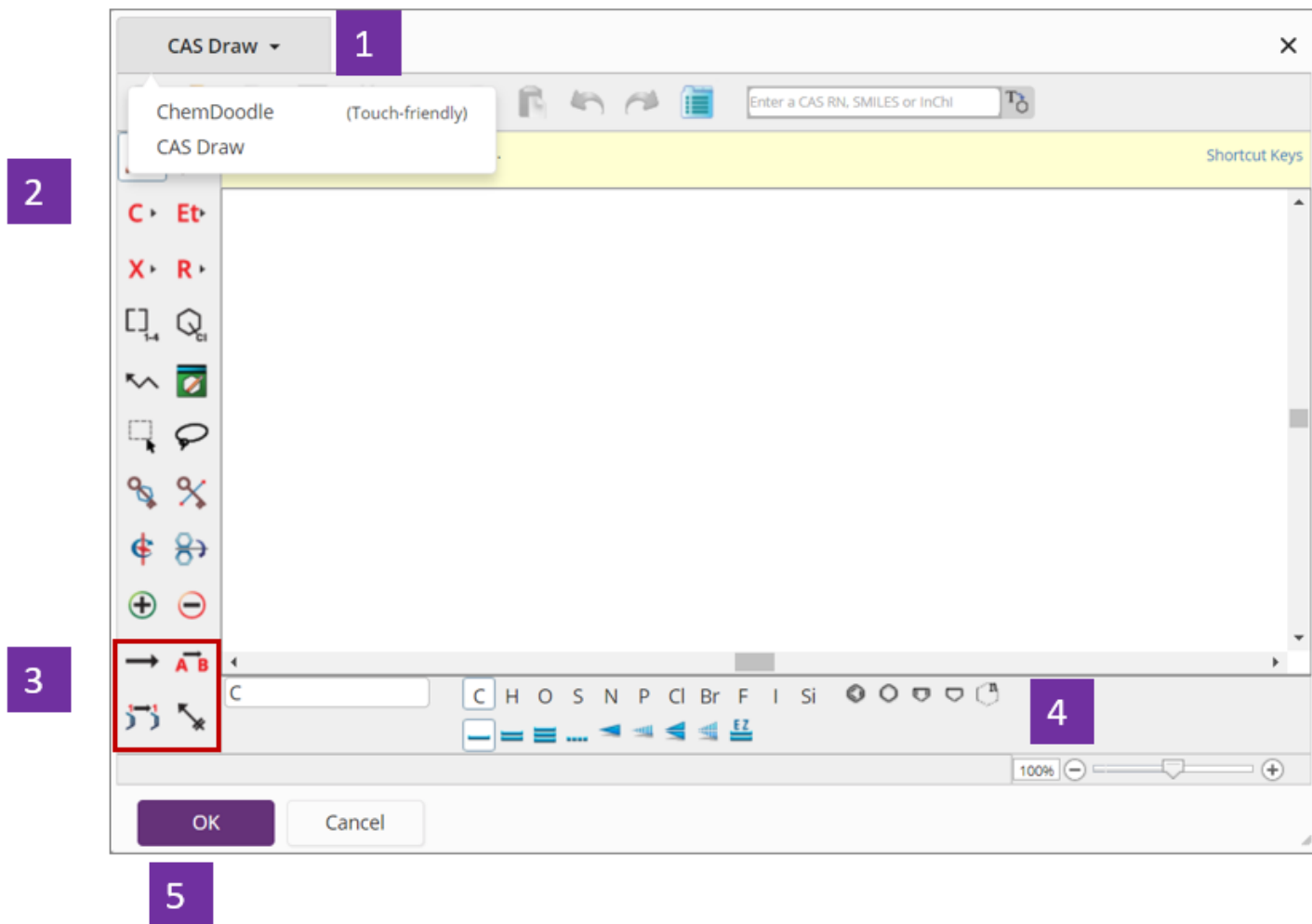
Validation	
Limit of Detection	0.485 µg/mL, Sofosbuvir 0.175 µg/mL, Ledipasvir
Limit of Quantitation	1.619 µg/mL, Sofosbuvir 0.586 µg/mL, Ledipasvir
Recovery	99.67 ± 0.40, 100.05 ± 0.65, 99.39 ± 0.55, 99.71 ± 0.58, 99.31 ± 0.41 and 98.95 ± 0.61% in 120, 100, 80, 60, 40 and 20% concentrations, respectively, Sofosbuvir 99.88 ± 0.69, 99.76 ± 0.59, 99.04 ± 0.78, 99.19 ± 0.54, 100.08 ± 0.4 and 99.33 ± 0.51% in 120, 100, 80, 60, 40 and 20% concentrations, respectively, Ledipasvir
Accuracy	0.33, -0.05, 0.61, 0.29, 0.69 and 1.05% (RE) in 120, 100, 80, 60, 40 and 20% concentrations, respectively, Sofosbuvir 0.12, 0.24, 0.96, 0.81, -0.08 and 0.67% (RE) in 120, 100, 80, 60, 40 and 20% concentrations, respectively, Ledipasvir
Precision	0.669, 0.727 and 0.872% (RSD, peak area) in 96 µg/mL concentration, Sofosbuvir 0.955, 0.975 and 0.492% (RSD, peak area) in 3.2 µg/mL concentration, Ledipasvir
Retention Time	4.468 ± 0.013 min, Sofosbuvir 8.242 ± 0.012 min, Ledipasvir

## 物质检索

The screenshot shows the SciFinder search interface. On the left, a navigation menu is highlighted with a purple bar, and a callout '1' points to the 'Substances' option. The main search area has a callout '2' pointing to the search input field. Below the input field, a callout '4' points to the 'Advanced search' link. On the right side of the search bar, there is a 'Draw' button with a callout '3' and a search magnifying glass icon with a callout '5'. The top right corner contains 'Saved', 'History', and 'Account' buttons.

1. 选择 Substances，进行物质检索
2. 输入检索信息：物质名称、CAS 登记号、专利号等
3. 点击 Draw，绘制结构
4. 点击 Advanced Search，进行分子式和物质属性检索
5. 点击放大镜，开始检索

## 结构编辑器的使用



1. 结构编辑器的两种模式：ChemDoodle 支持触摸屏模式，CAS Draw 为普通的绘图模式。
2. 绘制结构需要的一系列工具
3. 绘制反应需要的工具
4. 常用的原子、环和键
5. 点击 OK，开始检索

## 物质结果界面

物质检索以直观的布局展示结果。结果展示页面突出了最相关的结果，关键属性信息，以及高分辨率结构图。

The screenshot displays the CAS SciFinder search results page. On the left, a sidebar (1) offers filtering options under 'Structure Match' (As Drawn (1), Substructure (6), Similarity (4,072)), 'Analyze Structure Precision', and 'Filter by' (Commercial Availability, Reaction Role, Reference Role, Number of Components, Substance Class, Isotopes, Metals, Molecular Weight). The main area (4) shows search results for 'Substances (6)'. The first result (7) is '1219937-98-0', 1-[[[4-Fluorophenyl]amino]carbonyl]cyclopropanecarbonyl chloride, with its chemical structure and associated data (47 References, 123 Reactions, 4 Suppliers). The second result (9) is '1416321-38-4', Cyclopropanecarbonyl chloride, 1-[[[3-chloro-4-fluorophenyl]amino]carbonyl]-, with its chemical structure and associated data (1 Reference, 2 Reactions, 0 Suppliers). On the right, a table (8) lists 'Key Physical Properties' for each substance, including Molecular Weight, Boiling Point (Predicted), Density (Predicted), and pKa (Predicted). At the top right, options for 'Sort: Relevance' (5) and 'View: Full' (6) are visible, along with a 'Save' button.

1. 结果结构匹配程度：As Drawn 精确结构，Substructure 亚结构，Similarity 相似结构
2. 点击 Analyze Structure Precision，对精确结构和亚结构的检索结果进行更细化的结构分类
3. 全面的物质结果聚类
4. 和物质结果集相关的文献、反应和供应商
5. 重新排序
6. 选择结构信息展示的详略
7. 点击 CAS 登记号，查看物质详情
8. 关键的物理属性
9. 此物质相关的文献、反应和供应商

# 物质详情界面

← Return to Results

## Substance Detail (1 of 11)

← Prev Next →

References (223) Reactions (9) Suppliers (8)

Download Email Save

CAS Registry Number  
3327-64-8

Relative stereochemistry shown

$C_6H_{10}O_6$   
Gulonic acid,  $\gamma$ -lactone

Key Physical Properties	Value	Condition
Molecular Weight	178.14	-
Boiling Point (Predicted)	467.9±18.0 °C	Press: 760 Torr
Density (Predicted)	1.766±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.06±0.60	Most Acidic Temp: 25 °C

Expand All | Collapse All

- Other Names
- Predicted Properties
- Predicted Spectra
- Additional Details

1. 点击左右箭头，查看前一个或后一个物质详情
2. 此物质相关的文献、反应和供应商
3. 下载、分析及保存物质详情
4. 关键的物理属性
5. 名称、预测属性、预测谱图及其他信息



## 物质 Markush 结构检索

Search

All

Substances

Reactions

References

Suppliers

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

Enter a query...

Use [Advanced search](#) for Molecular Formula and Substance Property

Edit

Search Patent Markush

Edit Drawing Remove

1. 选择 Substances，进行 Markush 结构检索
2. 点击 Draw，绘制检索结构
3. 勾选 Search Patent Markush
4. 点击放大镜，开始检索

## 物质 Markush 结构检索结果展示

Patent Markush Match

As Drawn (1)

Substructure (33)

Filter by

Patent Office

Japan (1)

Patent Markush (1)

References

JP2003261514

View Reference Detail

Patent claim 1

PATENTPAK Full Text

831,833,835,837: opt. substd. by 1 or more G12

1015,1017,1019,1020: opt. substd. by 1 or more G12

G4

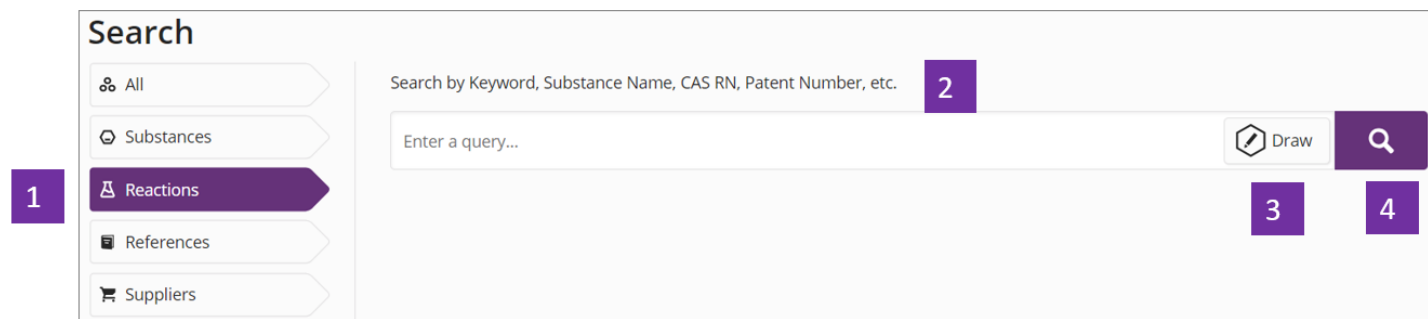
G1

G12

1. Markush 结构检索的匹配程度：As Drawn 精确结构，Substructure 亚结构
2. 点击专利号，获取专利文献详情
3. 匹配的 Markush 结构在专利中出现的位置
4. PatentPak: 高效获取经 CAS 科学家深度标引的专利全文
5. 全文链接

## 6. Markush 结构的描述

### 反应检索



1. 选择 Reactions，进行反应检索
2. 输入检索信息：关键词、物质名称、CAS 登记号和专利号等
3. 点击 Draw，绘制反应式
4. 点击放大镜，开始检索

### 反应检索结果展示

反应检索显示了相关的结果，以及关键合成信息。

The screenshot displays the CAS Reactions search results page. On the left, a 'Structure Match' sidebar (1) offers filters for 'As Drawn (176)', 'Substructure (418K)', and 'Similarity (78K)'. Below this, a 'Filter by' section (2) includes options for Yield (90-100% to 30-49%), Number of Steps (1), Reaction Mapping, Experimental Protocols, Reaction Type, Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes, and Search Within Results. The main area shows 'Reactions (176)' with a 'View Expanded' dropdown (3). The selected reaction, 'Scheme 1 (1 Reaction) View', shows the conversion of benzoic acid to benzyl alcohol with 100% yield. A 'Reaction Summary' table (4) lists reagents (Triethyl borate, Dimethyl sulfide, trihydroboron, Methanol), solvents (Dichloromethane, Tetrahydrofuran), and conditions (2 stages). A 'References' section (5) provides the citation: 'Well-Defined Silica-Supported Zirconium-Benzyl Cationic Species: Improved Heterogenization of Single-Site Polymerization Catalysts' by Popoff, Nicolas; et al, European Journal of Inorganic Chemistry (2014), 2014(5), 888-895. A 'Full Text' link (6) is also present. 'Scheme 2 (11 Reactions) View All' is shown below, with 'Suppliers (15)' and 'Suppliers (9)' buttons.

1. 反应结果集的匹配程度: As Drawn 精确结构, Substructure 亚结构, Similarity 相似结构
2. 全面的反应结果集聚类
3. 选择结果展示的详略
4. 反应条件概述
5. 获取文献详情
6. 文献全文链接

## 反应详情

1

← Return to All Reaction Schemes

## Reaction Detail (Scheme 1, Reaction 1 of 1)

← Prev Next →

📄 📧 ⭐ Save

Steps: 1  
Yield: 100%

100%

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Triethyl borate (Dimethyl sulfide)trihydroboron	-	Dichloromethane Tetrahydrofuran	rt; overnight, reflux
2	Methanol	-	-	0 °C

CAS Reaction Number: Not assigned

Experimental Protocols

MethodsNow™

Products: Benzenemethanol, labeled with carbon-13  
Yield: 100%

Reactants: Benzoic acid, labeled with carbon-13

Reagents: Triethyl borate  
(Dimethyl sulfide)trihydroboron  
Methanol

Solvents: Dichloromethane  
Tetrahydrofuran

Procedure

1. Add a solution of benzoic acid  $\alpha$ - $^{13}\text{C}$  labeled at 100% (5.000 g, 40.940 mmol, purchased from E uniso-T op) in dry tetrahydrofuran (THF, 100 mL) dropwise to a solution of  $\text{BH}_3\text{-Me}_2\text{S}$  (82 mL, 81.900 mmol, 1M in  $\text{CH}_2\text{Cl}_2$ ) and  $\text{B}(\text{OEt})_3$  (14 mL, 81.900 mmol) in dry THF (300 mL).
2. Stir the resulting solution overnight at reflux, after  $\text{H}_2$  evolution.
3. Quench the mixture with  $\text{MeOH}$  (100 mL) at 0 °C, when cold.
4. Evaporate the volatiles.
5. Dissolve the residue again in  $\text{MeOH}$  (100 mL).
6. Evaporate the solvent to obtain benzyl alcohol.

Scale: gram

Characterization Data

Benzenemethanol, labeled with carbon-13

Proton NMR Spectrum ( $\text{C}_6\text{D}_6$ , 300 MHz, 298 K):  $\delta = 4.06$  (d,  $^1J_{\text{H-C}} = 150$  Hz, 2H,  $\text{CH}_2$ ), 7.00 (m, 5H, Ar-H) ppm

State: clear oil

CAS Method Number 3-614-CAS-3359623

Reference

Well-Defined Silica-Supported Zirconium-Benzyl Cationic Species: Improved Heterogenization of Single-Site Polymerization Catalysts

View Reference Detail

By: Popoff, Nicolas; et al  
View All

European Journal of Inorganic Chemistry (2014), 2014(5), 888-895

Full Text

Company/Organization

C2P2 (CNRS-UMR 5265), ESCPE  
Lyon  
Universite Lyon 1  
Villeurbanne 69626  
France

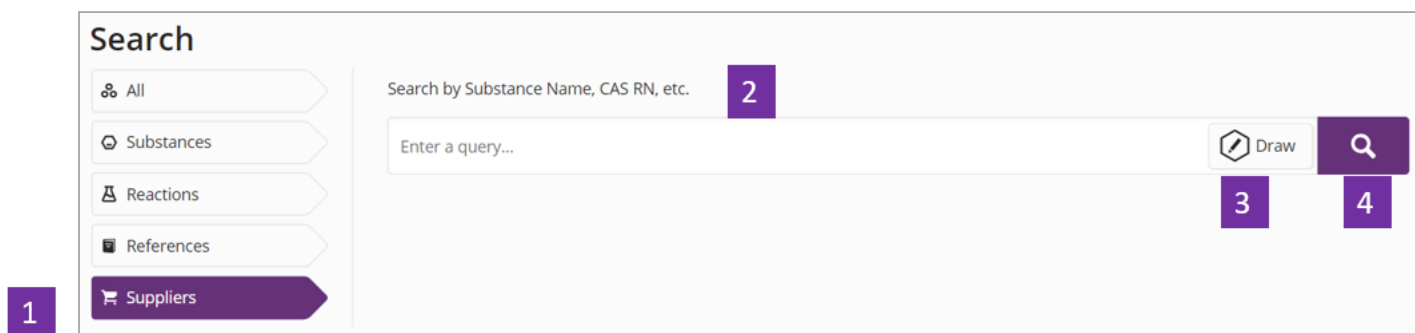
2

5

6

1. 返回至反应结果集界面
2. 下载、分享并保存检索结果
3. 反应步骤概述
4. MethodsNow, 获取全面有条理的实验详情
5. 查看文献详情
6. 文献全文链接

## 供应商检索



1. 选择 Suppliers，进行供应商检索
2. 输入检索信息：物质名称、CAS 登记号等
3. 点击 Draw，绘制检索结构
4. 点击放大镜，开始检索

## 供应商检索结果展示

The screenshot shows the SciFinder search results page for Suppliers. The page title is 'Suppliers (98)'. On the left, there is a filter sidebar with sections: Preferred Suppliers, Supplier, Purity, Quantity, Ships Within, Stock Status, Order From Supplier, and Country. The 'Supplier' section is expanded, showing various product lists. On the right, there is a table of search results. The table has columns: Supplier, Substance, Purity, Purchasing Details, and Availability. The first row is highlighted with a '3' in a purple box. The 'Substance' column contains '63968-64-9 Artemisinin' with a '4' in a purple box. The 'Purchasing Details' column contains 'Product Information' with a '5' in a purple box. The 'Availability' column contains 'Limited or intermittent availability' and 'Ships within 2 weeks'. The second row is also highlighted, showing 'A&A Life Science Product Listing United States' as the supplier, '63968-64-9 Artemisinin' as the substance, and 'Order From Supplier' as the purchasing detail. The third row shows 'AB PharmaTech Product List United States' as the supplier, '63968-64-9 Artemisinin' as the substance, and 'Order From Supplier' as the purchasing detail. The fourth row shows 'AB PharmaTech Product List United States' as the supplier, '63968-64-9 Artemisinin' as the substance, and 'Order From Supplier' as the purchasing detail. The fifth row shows 'AB PharmaTech Product List United States' as the supplier, '63968-64-9 Artemisinin' as the substance, and 'Order From Supplier' as the purchasing detail. The sixth row shows 'Chem Scene' as the supplier, '63968-64-9 Artemisinin' as the substance, and 'Order From Supplier' as the purchasing detail.

1. 全面的结果集聚类
2. 下载、分享检索结果

3. 点击供应商名，获取供应商信息
4. 点击 CAS 登记号，获取物质详情
5. 点击进入购买页面

## 保存的结果

The screenshot shows the SciFinder interface with the following elements highlighted by numbered callouts:

- 1:** The 'Saved' section header and the alert notification.
- 2:** The 'Filter by' sidebar on the left.
- 3:** The 'Migrate Saved Answers & Alerts (Keep Me Posted)' button.
- 4:** The 'No Alerts' notification and the 'View Alert Results' dropdown menu.
- 5:** The alert notification details, including dates and a 'Mark All As Viewed' button.
- 6:** The 'Rerun Search' button at the bottom right.

1. 查看保存的及信息更新提醒的结果集
2. 结果集的类型
3. 删除或分享结果
4. 点击铃铛旁的箭头，更改提醒设置
5. 查看设置的信息更新结果
6. 重新进行检索

## 检索历史

SciFinder<sup>n</sup> 动态跟踪您的检索记录，并帮助您快速找到之前的检索。您还可以很容易地进行保存并设置检索提醒。

The screenshot displays the SciFinder search history page. At the top, there is a search bar with a 'Reactions' dropdown and a search icon. On the left, a 'Filter by' sidebar includes 'Search Type' (All, Substances, Reactions, References, Suppliers) and 'Date' (Start/End Date, calendar). The main area shows a 'Search History' section with a clock icon and '(1,437)' results. A '1 Selected' filter is active. The history is organized by date, with 'June 27, 2018' selected. Three search entries are visible, each with a time stamp and a 'Rerun Search' button. The first entry is for 'Reactions' at 5:27 AM, showing a chemical reaction scheme. The second is for 'Substances' at 5:14 AM, showing a complex polycyclic structure. The third is for 'Substances' at 5:08 AM, showing a bicyclic structure with a hydroxyl group. Numbered callouts 1 through 6 are placed on the interface: 1 on the search bar, 2 on the Search Type filter, 3 on the Date filter, 4 on the '1 Selected' filter, 5 on the Rerun Search button for the first entry, and 6 on the user profile icon.

1. 检索历史
2. 检索类型
3. 检索日期
4. 筛选检索结果
5. 重新开始检索
6. 退出检索

美国化学文摘社（Chemical Abstracts Service, 简称“CAS”）是美国化学会（American Chemical Society, 简称“ACS”）旗下的分支机构，是全球提供化学及相关信息解决方案的权威机构。秉承美国化学会“运用化学的力量改善人们的生活”的愿景，美国化学文摘社专业的科学家团队致力于发现、收集及管理所有公开的化学物质信息，创建了世界上对于创新至关重要的、最具价值的内容集合。全球的科研人员及从事专利的专业人士依靠美国化学文摘社提供的研究解决方案实现其科研发现并完成工作流程。

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