

余敏
syu@acs-i.org

利用SciFinder实现药物专利保护策略

提纲

- 药物研发专利保护策略
- 检索工具的选择和分析
- 案例分享
 - 判定药物结构新颖性和创造性
 - 获取药物制备专利
 - 药物制备方法详情、手性结构拆分方法的获取
 - 药物制剂信息的获取
 - 药理分析方法的获取

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、更加牢固定义的、更加有活性的化合物
- 具体的化合物
- 具体化合物的形式
- 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

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为什么选择SciFinder

■ 我们是CAS

- ACS的分支机构，愿景：运用化学的力量改善人们的生活
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 全面收集、文摘、标引全球化学相关文献
- 总部位于美国俄亥俄州哥伦布市
- 数千名、精通50多种语言的科学家



提供改变世界的解决方案

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

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



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

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)₃P as a ligand.

Process for synthesis of substituted secondary amines via condensation of aniline with aryl halides with a palladium catalyst and (t-Bu)₃P 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)₃P 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)₃P 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
IN 2010MU02830	PATENTPAK A		Nov 16, 2012	IN 2010-MU2830	Oct 12, 2010
CA 2813094	A1		Apr 19, 2012	CA 2011-2813094	Sep 12, 2011
WO 2012048972	PATENTPAK A1	English	Apr 19, 2012	WO 2011-EP65756	Sep 12, 2011
CN 103221026	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	PATENTPAK B1	English	Feb 25, 2015		
JP 2013539769	PATENTPAK T	Japanese	Oct 28, 2013	JP 2013-533137	Sep 12, 2011
JP 5851511	PATENTPAK 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	PATENTPAK A1	English	Oct 24, 2013	US 2013-13877924	May 28, 2013
US 9034304	PATENTPAK 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

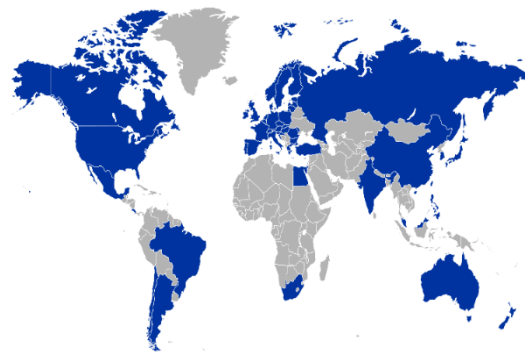
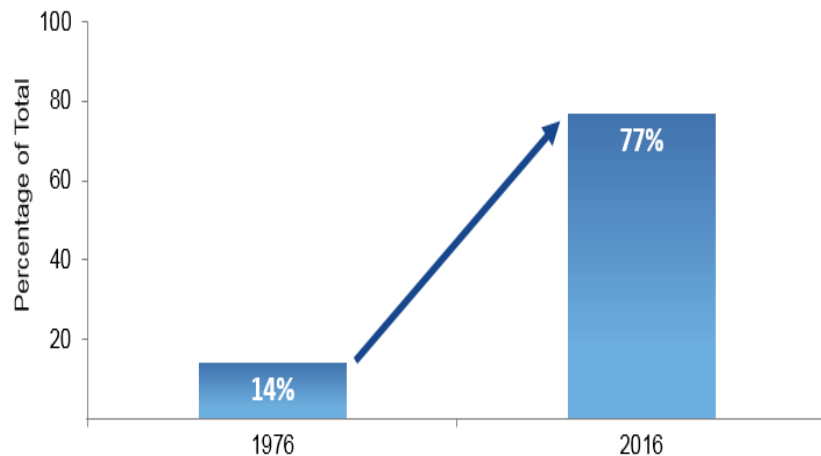


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为什么选择SciFinder

化合物首次通过专利披露的比重持续增长

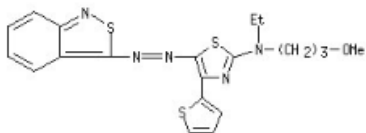


*Note: 蓝色表示SciFinder收录专利区域

为什么选择SciFinder

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

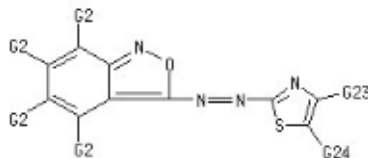


专利中的确定结构

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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

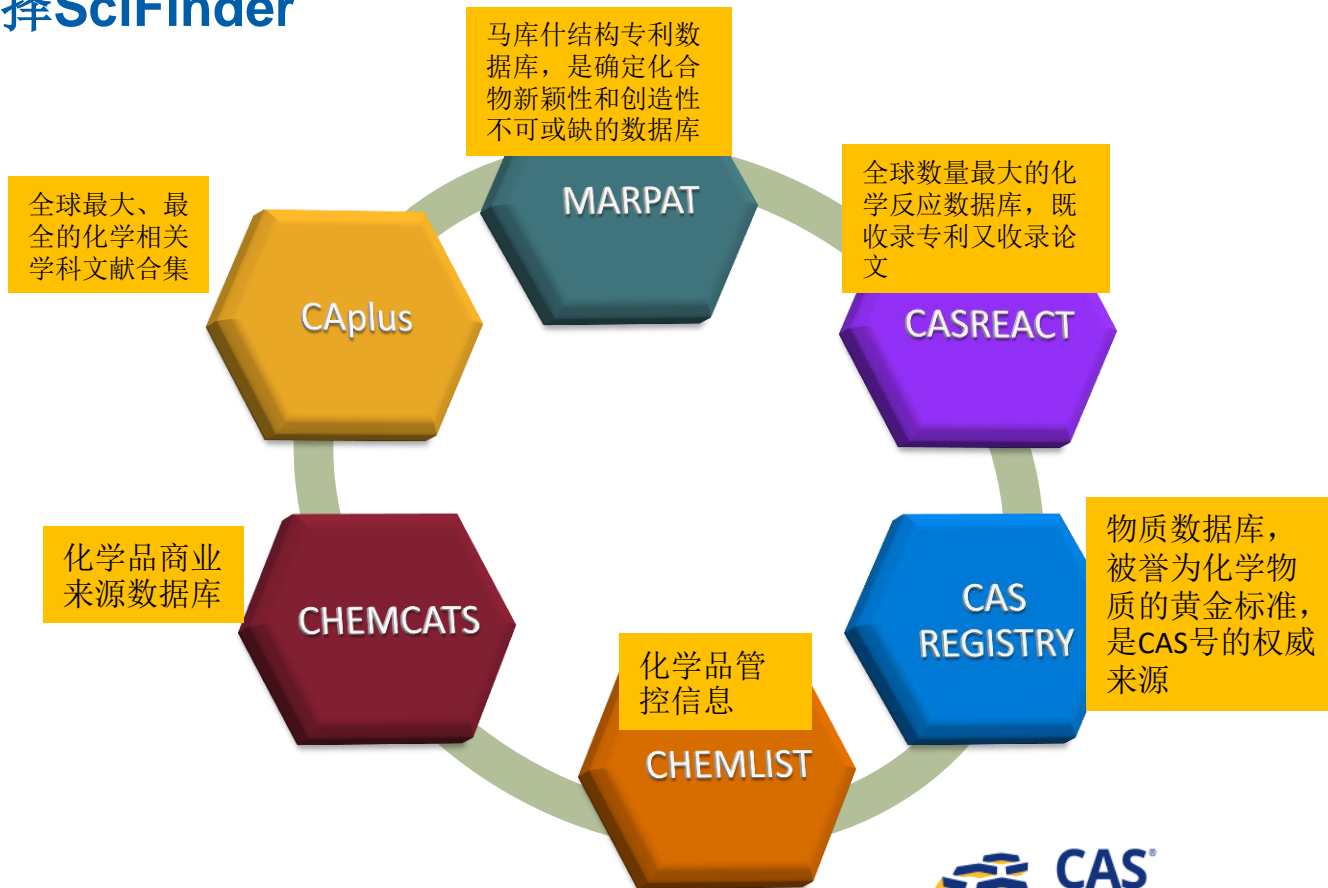
MSTR 1 Assembled



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

为什么选择SciFinder



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 - 药理分析方法的获取
 - 药物制剂信息的获取

在专利中表示物质的方式

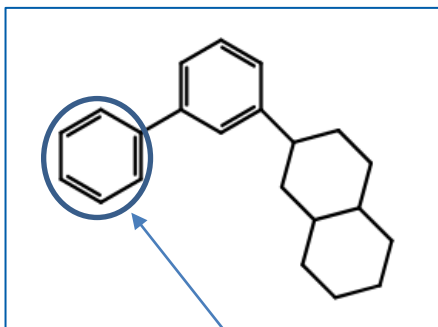
- 确定物质[Specific Substance]:
 - 具有表征数据的物质（一般为实施例中的物质，会被Registry收录）
 - 专利中其他确定物质（只有有充分的证据证明此物质存在，才会被Registry收录）
- 预测性物质[Prophetic Substance]:
 - 使用通式结构（Markush）表示的预测物质，一个通式结构可以表示上百或上千个化学物质（会被MARPAT数据库收录）
 - 符合Markush结构定义的表格化合物，这些物质并没有在实验室被合成出来，但同样受该专利的保护

SciFinder中的Markush检索

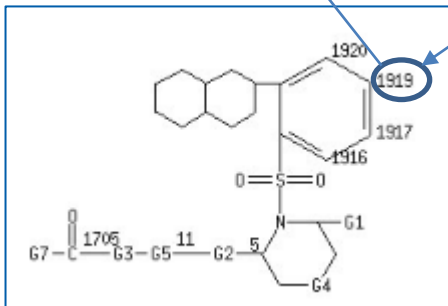
- 获取相似物质
- 检索和分析现有技术
- 评估可专利性
- 发现相似专利和潜在的侵权风险
- 拓展检索的全面性和完整性
- 补充物质和文献检索

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

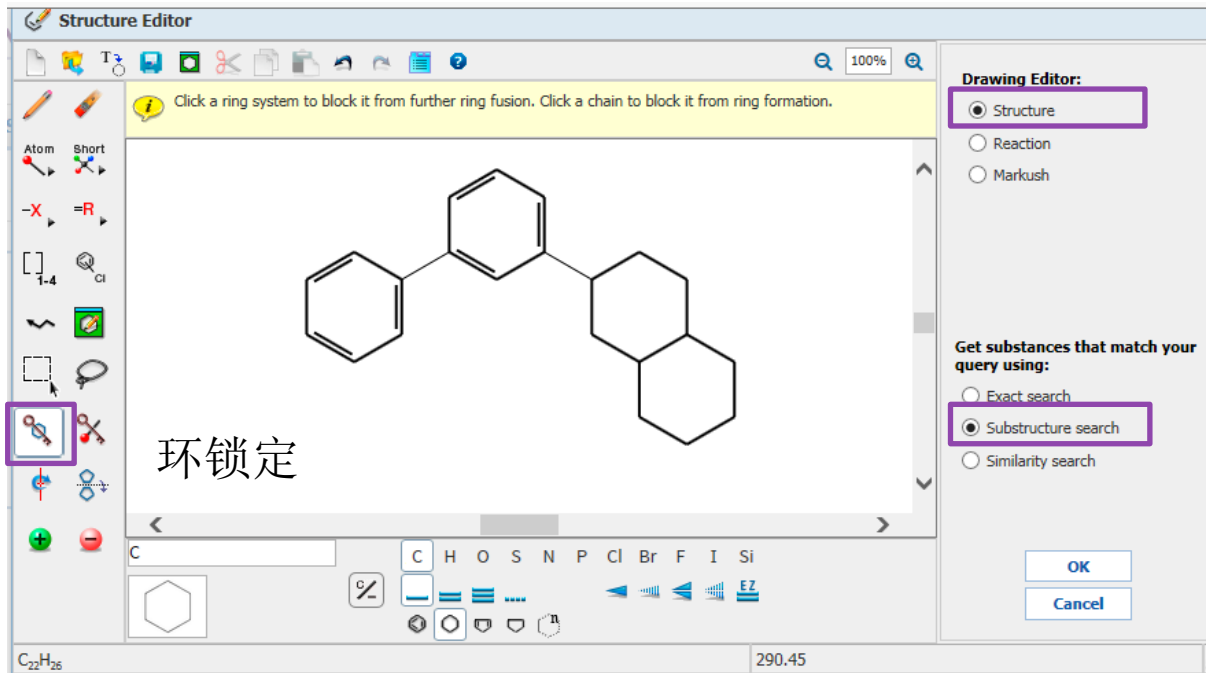
Note: also incorporates claim 35



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判断化合物新颖性及创造性



环锁定

结构检索

亚结构检索

判断化合物新颖性及创造性



Welcome Xiaoyan Z. Cheng

Explore ▾

Saved Searches ▾

SciPlanner

⚠ Explore Substances resulted in 0 substances [Return](#)

Chemical Structure substructure > substances (0)

SUBSTANCES

Create Keep Me Posted Alert

Analyze Refine

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

The screenshot displays the 'Structure Editor' software interface. The central workspace shows a chemical structure consisting of a benzene ring connected to a cyclohexane ring, which is further connected to another benzene ring. The interface includes a toolbar on the left with various drawing and editing tools, a top menu bar with icons for file operations, and a right-hand panel with search options. The 'Drawing Editor' panel has three radio buttons: 'Structure', 'Reaction', and 'Markush', with 'Markush' selected and highlighted by a purple box. Below this, the 'Get Markush patents where the structure(s) are:' section has two radio buttons: 'Variable only at the specified positions' and 'Substructures of more complex structures', with the latter selected and highlighted by a purple box. At the bottom of the right panel are 'OK' and 'Cancel' buttons. The bottom of the interface shows a periodic table with 'C' selected and a search bar.

Markush检索

亚结构检索

判断化合物新颖性及创造性

REFERENCES

Get Substances Get Reactions Get Related Citations Tools Create Keep Me Posted Alert Send to SciPlanner

Analyze **Refine** Categorize

Sort by: Author Name

0 of 19 References Selected Markush检索结果集: 19篇专利文献 [Display Options](#)

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

[Show More](#)

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

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

By Waechter, 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 = CO₂R, CN; Q³ = alkylene, alkylidene, arom. system, single bond; Y = H, R; R = alkyl; Q² and Q³ 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-BrMgC₆H₄OMe in THF was treated with TiCl(OCHMe₂)₃ 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)cyclohexanecarboxylat...

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^{IV1}-Q-Q-R^{IV2} [R^{IV1}, R^{IV2} = (F or Cl-substituted) C₁₋₁₀ alkyl, C₁₋₁₀ alkoxy, etc., whose one CH₂ group or nonadjacent ≥2 CH₂ groups may be substituted with O or S; Q = p-cyclohexylene] and a compd. I [R¹ = H, O, OH, C₁₋₁₂ alkyl whose CH₂ group(s) may be substituted with O, S, CH:CH, etc.; R²⁻⁵ = C₁₋₈ alkyl whose CH₂ group(s) may be substituted with O, S, CH:CH, etc.; R² and R³, and/or R⁴ and R⁵ may be bonded to each other and form ring; R⁶, R⁷ = H, C₁₋₆ alkyl whose CH₂ group(s) may be substituted with O, S, CH:CH, etc.; n¹ = 1-6; M¹ = org. grou...]

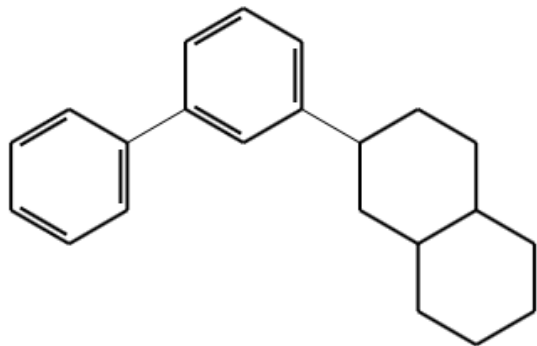
3. **Bicycloalkylidene diphenols for use in polycarbonates**

[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 [R¹, R² = H, halogen, alkyl, cycloalkyl, aryl, arylalkyl; R³, R⁴ = H, alkyl, aryl, arylalkyl (but ≥ 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, C₁₂H₂₅SH 10.1, and 37% HCl 30 g

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

提纲

- 药物研发专利保护策略
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 - 药物制备方法详情、手性结构拆分方法的获取
 - 药物制剂信息的获取
 - 药理分析方法的获取

获取药物的制备专利信息

CAS Solutions

SCIFINDER
A CAS SOLUTION

Explore Saved Searches SciPlanner

Research Topic "essence extracting with tobacc..." > references (284) > get substances

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

Solavetivone

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

Search

提示:

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

获取药物的制备专利信息

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

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

Analyze **Refine**



Analyze by: ?
Substance Role ▾

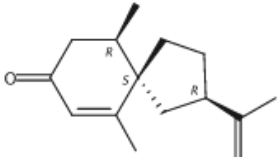
Analytical Study 1
Biological Study 1
Formation, Nonpreparative 1
Occurrence 1
Preparation 1
Process 1
Properties 1
Reactant or Reagent 1

Sort by: CAS Registry Number ▾ ↓

▾ 0 of 1 Substance Selected

1. 54878-25-0 🔍

~211  



Rotation (-), Absolute stereochemistry.

C₁₅H₂₂O
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**

获取药物的制备专利信息

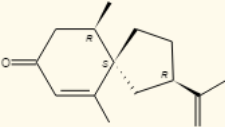
PATENTPAK
A CAS SOLUTION

PAGE 21 / 25 ZOOM DOWNLOAD PDF

药物制备专利原文

Key Substances in Patent

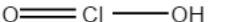
CAS RN 54878-25-0



Search in SciFinder | View Detail

Analyst Markup Location
page 21

CAS RN 7758-19-2



• Na

Search in SciFinder | View Detail

Analyst Markup Location
page 21

medium was prepared by inoculating 50 mL of SDE-ura medium with CALI-5 or ALX7-95 containing YEp-HPS-ura. This culture was grown until early stationary phase (24-48 hr). One mL of this culture was inoculated into 500 mL of SDE-ura medium and grown for 24 hr. A 400-mL aliquot (5% inoculum) was used to inoculate the 8 L of medium.

[0188] The fermentor was maintained at 26° C. The air flow was 4.5 L/min and the dO₂ was maintained above 30% by adjusting the rpm. Furthermore, the pH was maintained at 4.5 using acetic acid and NaOH.

[0189] Once the glucose concentration was below 1 g/L, a feeding regimen was initiated such that the glucose in the fermentor was kept between 0 and 1 g/L. The glucose feed was made by mixing 1400 mL of 60% glucose and 328 mL of 12.5% yeast extract.

[0190] After 5 days, the air and agitation were turned off, and the oil was allowed to rise to the top of the tank and decanted.

Example 3
Preparation of 2-Isopropyl-6,10-dimethyl-spiro[4.5]dec-6-en-8-one (the “(-)-solavetivone”) (5)

[0191] 3,5-Dimethylpyrazole (47 g, 0.49 mol) was dissolved in a mixture of CH₂Cl₂ (650 mL) and t-butyl alcohol (31 mL). The solution was then cooled to ±78° C. Chromyl chloride (CrO₂Cl₂) (13.3 mL) was added over 15 min and stirred for another 15 min before it was allowed to warm to room temperature. Premnaspirodiene (6.69 g, 32.7 mmol) was dissolved in CH₂Cl₂ (650 mL) and added rapidly to the reaction. The dark red solution was stirred for 48 hours. The

Example 5
Preparation of 2-Isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one (3) & 2-Isopropyl-6,10-dimethyl-spiro[4.5]deca-1,6-dien-8-one (4).

[0193] To a solution of (-)-solavetivone (5) (100 mg, 0.46 mmol) dissolved in ethanol (2 mL) was added Amberlyst® IR-15 (150 mg). The suspension was then heated at 105° C. in a sealed reaction flask for 96 hours. The suspension was then filtered through Celite and evaporated under vacuum. The residue was purified on a silica gel column (hexane:ether, 85:15) to afford the mixture as a colorless oil (67 mg, 67%). ESIMS m/z 219 (M+H), 78.7% at 14.71 min; 219 (M+H), 17.1% at 14.89 min.

Example 6
Oxidation of (+)-Valencene to (+)-Nootkatone

[0194] In order to test various reaction conditions for the oxidation of premnaspirodiene to solavetivone, reactions were carried out on commercially available valencene, a compound that is chemically similar to premnaspirodiene and would be expected to oxidized under similar reaction conditions. Reactions were carried out using 250 mg of starting material in a single reaction, using combinations of sodium chlorite and either t-butylhydroperoxide (t-BuOOH) or N-hydroxyphthalimide (NHPI) as described (S. M. Silvestre & I.

SciFinder中的PatentPak

- 即时获得已整合到SciFinder中的专利PDF文件
- 页码信息：准确显示重要物质在专利PDF文件中的位置
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- 33. **An aerosol precursor containing anti-inflammatory medicine pharmacodynamic component and method for dispersing it into nanometer-sized fogdrop**

Quick View **PATENTPAK**

By Chen, Yongkuan; Zhao, Wei; Yang, Liu; Shang, Shanzhai; Tian, Yongfeng; Zhang, Xia; Han, Yi; Han, Jingmei; Yuan, Dalin; Lei, Ping; et al
From Faming Zhuanli Shenqing (2015), CN 104800160 A 20150729. | Language: Chinese, Database: CAPLUS

The present invention relates to an aerosol precursor contg. anti-inflammatory medicine pharmacodynamic component and method for dispersing it into nanometer-sized fogdrop. The aerosol precursor contg. anti-inflammatory medicine pharmacodynamic component contains glycerol, propylene glycol, 1,3-butanediol, **fragrance** matter, and anti-inflammatory medicine **extractum**, and the wt. ratio of glycerol: propylene glycol: 1,3-butylene glycol: **fragrance** matter: anti-inflammatory medicine **extractum** is (40-45) : (20-25) : (0-10) : (0-10) : (1-10). The aerosol precursor

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- 34. **Preparation method of fermentation type buchu crenulata essential oil for tobacco**

Quick View **PATENTPAK**

By Wang, Na; Xi
From Faming Zhuanli Shenqing (2015), CN 104789362. | Language: Chinese, Database: CAPLUS

The invention discloses a preparation method of fermentation type Buchu crenulata essential oil for **tobacco**, comprising the steps: (1) prepg. fermented liq.: grinding Buchu crenulata into Buchu crenulata coarse powder, fermenting buchu crenulata coarse powder, glucose, and water by a wt. ratio of 15~30:1~5:69~85, to obtain fermented liq.; and (2) prepg. Buchu crenulata essential oil for fermn. type **tobacco**: extg. and sepg. the fermented liq. gained in step (1), and collecting obtained oil layer, to obtain fermn. type Buchu crenulata essential oil for **tobacco**. The present invention has simple prepn. te...

- 35. **Aerosol precursor containing medicine for external use active ingredient for treating rhinitis and the method for dispersing into nanometer-sized mist droplets with the same**

Quick View **PATENTPAK**

By Yang, Liu; Zhao, Wei; Shang, Shanzhai; Lei, Ping; Duan, Yuanxing; Yang, Ji; Han, Jingmei; Tian, Yongfeng; Zhu, Donglai; Gong, Xiaowei; et al
From Faming Zhuanli Shenqing (2015), CN 104784391 A 20150722. | Language: Chinese, Database: CAPLUS

The present invention relates to the aerosol precursor contg. medicine for external use active ingredient for treating rhinitis. The aerosol precursor is composed of glycerol, propylene glycol, 1,3-butanediol, **fragrance** matter, the medicine for external use **extractum** for treating rhinitis, and their mass ratio is glycerol: propylene glycol: 1,3 butylene glycol: **fragrance** matter: medicine for external use **extractum** for treating rhinitis=(40-45): (20-25): (0-10): (0-10): (1-10). The medicine for external use **extractum** for treating rhinitis is produced by 1) dissolving the medicine in ethanol, ...

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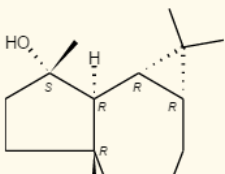
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PAGE 8 / 9 ZOOM DOWNLOAD PDF

Key Substances in Patent

page 8

CAS RN 6750-60-3

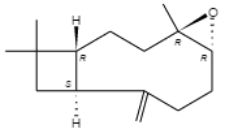


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Analysis Markup Location

page 8

CAS RN 1139-30-6




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10	20.99	α -Bisabolene	甜没药烯	0.17	0.57
11	22.22	Dodecanoic acid	月桂酸	0.30	0.73
12	22.69	Spathulenol	斯巴醇	0.10	0.52
13	22.84	Caryophyllene oxide	氧化石竹烯	0.89	1.06
14	24.46	Juniper camphor	杜松脑	0.43	—
15	26.70	Myristic acid	肉豆蔻酸	1.38	2.75
16	28.27	2-Hydroxycyclopentadecanone	α -羟基环十五酮	0.15	0.92
17	28.41	Perhydrofarnesyl acetone	植酮	2.35	3.55
18	28.72	Pentadecanoic acid	正十五酸	0.33	0.69
19	30.03	Hexadecanoic acid, methyl ester	棕榈酸甲酯	0.21	—
20	30.34	Oxacycloheptadecan-2-one	氧杂环十七烷-2-酮	0.64	1.60
21	30.45	Isophytol	异植物醇	0.53	—
22	31.14	Hexadecanoic acid	棕榈酸	38.49	33.20
23	31.38	Hexadecanoic acid, ethyl ester	棕榈酸乙酯	0.86	0.74
24	32.27	Oleic Acid	油酸	0.36	0.97

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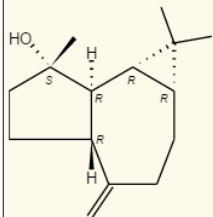
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Key Substances in Patent

page 8

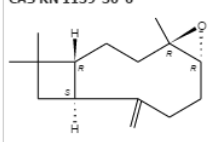
CAS RN 6750-60-3



View Detail

Structure Markush Reactions

CAS RN 1139-30-6



Search in SciFinder | View Detail

10	20.99	-Bisabolene
11	22.22	Dodecanoic acid
12	22.69	Spathulenol
13	22.84	Caryophyllene oxide
14	24.46	Juniper camphor
15	26.70	Myristic acid
16	28.27	2-Hydroxycyclopentadecanone
19	30.03	Hexadecanoic acid, methyl ester
20	30.34	Oxocycloheptadecan-2-one
24	32.27	Oleic Acid

Research Topic "Essences extracting with tobac..." > references (284) > refine "Patents only" (229) > 6750-60-3

SUBSTANCE DETAIL

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Return

CAS Registry Number 6750-60-3

-6,820 -13

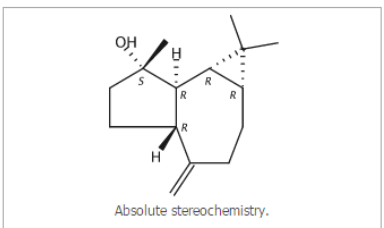
$C_{15}H_{24}O$
 1*H*-Cycloprop[*e*]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1*aR*,4*aR*,7*S*,7*aR*,7*bR*)-

Molecular Weight
220.35

Boiling Point (Experimental)
Value: 284.7 °C

Density (Predicted)
Value: 1.02±0.1 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 15.10±0.40 | Condition: Most Acidic Temp: 25 °C



Absolute stereochemistry.

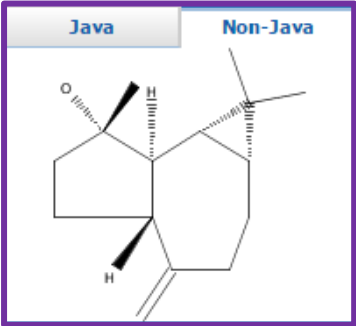
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SciFinder中的PatentPak

SUBSTANCES: CHEMICAL STRUCTURE ?

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

提纲

- 药物研发专利保护策略
- 检索工具的选择和分析
- 案例分享
 - 判定药物结构新颖性和创造性
 - 获取药物制备专利
 - 药物制备方法详情、手性结构拆分方法的获取
 - 药物制剂信息的获取
 - 药理分析方法的获取

在SciFinder中，药物制备信息的获取方式

方法1：在文献检索Research Topic中输入主题（如，preparation of 50-78-2或者synthesis of aspirin）进行检索。

方法2：检索物质后，在物质结果页面，可以由此物质获得制备(preparation)相关文献或者产物为此物质的反应。

方法3：也可以点击物质结构右上角的蓝色双箭头，点击Synthesis this，获得相关反应。

方法4：在SciFinder反应检索编辑器中绘制结构，获得反应。

方法1: 在文献检索Research Topic中输入preparation of ***或者synthesis of ***进行检索

Explore ▼

Saved Searches ▼

SciPlanner

Research Topic "synthesis of aspirin"

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

synthesis of aspirin

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Search

Advanced Search

REFERENCES

Analyze Refine Categorize

Analyze by:

Author Name

Patrono C 4

Valles Juana 4

Dineen Annie E 3

Fahay Jodie T 3

Moscardo Antonio 3

Nizankowska E 3

Pulliam Curtis R 3

Wennmalm A 3

Get Substances Get Reactions Get Related Citations Tools

Sort by: Accession Number

0 of 227 References Selected

1. A kind of method for catalyzed synthesis of aspirin by using choline eutectic solvent [Machine Translation].

Quick View PATENTPAK

By Wang, Yinglei; Li, Wenhuan; Liu, Xueguo; Du, Chaolun; Li, Jin
From Faming Zhanli Shenqing (2017), CN 106928055 A 20170707. | Language: Chinese, Database: CAPLUS

[Machine Translation of Descriptors]. The present invention belongs to environment-friendly org. **synthesis** chem. tech. field, particularly relates to a kind of method for catalyzed **synthesis of aspirin** by using choline eutectic solvent. The method comprises: adding choline eutectic solvent, salicylic acid, acetic anhydride into reaction vessel, after heating reaction 15 ~ 40min at 70 ~ 80 DEG C; purifying the crude products obtained by reaction, obtaining the **aspirin**. The method catalyzed **synthesis of aspirin** by using choline eutectic solvent of the present invention has simple operation, gent...

2. Synthesis of novel aspirin analogs for medicinal testing

Quick View Other Sources

By Albasrawi, Hadeel K.; Timmons, Shannon C.
From Abstracts, 48th Central Regional Meeting of the American Chemical Society, Dearborn, MI, United States, June 6-9 (2017), CERM-66. | Language: English, Database: CAPLUS

Aspirin is a common nonsteroidal anti-inflammatory drug used to treat pain, fever, and inflammation. It is one of the most widely used medications in the world with an estd. 40,000 tons produced and consumed annually. Recent research has shown that this inexpensive age-old drug holds promise as an anticancer agent. Studies have shown that **aspirin** has a remarkable ability to inhibit the proliferation of colorectal cancer cells in vitro, for example. Although the mechanism of action has not yet been established, it is clear that the **synthesis of aspirin** analogs to further probe this finding ...



方法2: 检索物质后, 在物质结果页面, 可以由此物质获得制备 (preparation) 相关文献或者产物为此物质的反应

The screenshot displays a chemical database interface. On the left, a search result for CAS 50-78-2 is shown, including a chemical structure of Benzoic acid, 2-(acetyloxy)- and its molecular formula $C_9H_8O_4$. The structure is CC(=O)Oc1ccccc1C(=O)O. On the right, a 'Get References' dialog box is open, with the 'Preparation' checkbox selected. Below it, a 'Get Reactions' dialog box is also open, with the 'Product' radio button selected. The 'Get Reactions' dialog box has 'Retrieve reactions for:' set to 'All substances' and 'Limit results by reaction role:' set to 'Product'. Buttons for 'Get' and 'Cancel' are visible at the bottom of the dialog boxes.

Get References

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,

Get Reactions

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

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

Get Cancel

方法3: 也可以点击物质结构右上角的蓝色双箭头, 然后点击Synthesis this, 获得反应

Substance Identifier "50-78-2" > substances (1)

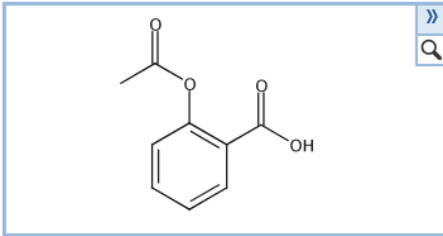
SUBSTANCES Get References Get Reactions Get Commercial Sources Tools ▾

Analyze **Refine** Sort by: CAS Registry Number ▾ ↓

0 of 1 Substance Selected

1. 50-78-2 🔍

~40494 ~119



C₉H₈O₄
Benzoic acid, 2-(acetyloxy)-

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

- View Substance Detail
- Explore by Structure ▶
- Synthesize this...**
- Get Reactions where Substance is a ▶
- Get Commercial Sources
- Get Regulatory Information
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药物合成实验方法详情的获取

SciFINDER
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner Save Print

⚠ 191 reactions with the Document Type **Patent** are displayed [Keep Analysis](#) [Clear](#)

Substance Identifier "tamiflu " > substances (1) > **get reactions (614)** > keep analysis "Document Type" (191)

REACTIONS ⓘ [Get References](#) [Tools ▾](#)

Analyze Refine

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

Group by: No Grouping ▾ Sort by: Accession Number ▾ ↓

0 of 614 Reactions Selected Page: 1

53. [View Reaction Detail](#) [Link](#)

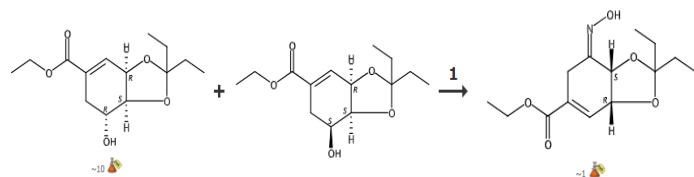
22 Steps *Hover over any structure for more options.*

NC(CS)C(=O)O + Cl + O=Cc1ccccc1 + N=Cc1ccccc1 + CC(C)(C)Si(C)CC=C

• HCl [Step 2.1] ~95 [Step 4.1] ~93

药物合成实验方法详情的获取

MethodsNow



Products	1,3-Benzodioxole-5-carboxylic acid, 2,2-diethyl-3a,6,7,7a-tetrahydro-7-(hydroxyimino)-, ethyl ester, (3aR,7a5)-, 70%, CAS RN: 1234286-93-1
Reactants	Ethyl (3aR,7R,7a5)-2,2-diethyl-3a,6,7,7a-tetrahydro-7-hydroxy-1,3-benzodioxole-5-carboxylate, CAS RN: 943515-58-0 1,3-Benzodioxole-5-carboxylic acid, 2,2-diethyl-3a,6,7,7a-tetrahydro-7-hydroxy-, ethyl ester, (3aR,7S,7a5)-, CAS RN: 1201685-54-2
Reagents	Dess-Martin periodinane, CAS RN: 87413-09-0 Sodium bicarbonate, CAS RN: 144-55-8 Sodium thiosulfate, CAS RN: 7772-98-7 Hydroxylamine hydrochloride, CAS RN: 5470-11-1
Solvents	Dichloromethane, CAS RN: 75-09-2 Water, CAS RN: 7732-18-5 Ethanol, CAS RN: 64-17-5 Pyridine, CAS RN: 110-86-1
Procedure	<ol style="list-style-type: none"> 1. Add Dess-Martin periodinane (392 mg, 0.92 mmol) to a solution of (3aR,7R,7a5)-ethyl 2,2-diethyl-7-hydroxy-3a,6,7,7a-tetrahydrobenzo[d][1,3]dioxole-5-carboxylate (100 mg) in DCM (6 mL) at room temperature for 1 hour. 2. After consumption of the starting material, quench the reaction by adding saturated hypo solution (2 mL) followed by saturated NaHCO₃ (2 mL). 3. Extract the organic layer using DCM (5 mL × 3). 4. Collect all the fractions. 5. Dry the fractions over anhydrous Na₂SO₄. 6. Concentrate the fractions under reduced pressure. 7. Add hydroxylamine hydrochloride (251 mg, 0.74 mmol) followed by pyridine (0.5 mL) to (3aR,7S,7a5)-ethyl 2,2-diethyl-7-hydroxy-3a,6,7,7a-tetrahydrobenzo[d][1,3]dioxole-5-carboxylate (0.37 mmol) in EtOH (1 mL). 8. Stir the reaction mixture at room temperature for 2 hours. 9. Pour the solution into water. 10. Extract the solution with CH₂Cl₂ (3 × 10 mL). 11. Dry the combined organic layers over Na₂SO₄. 12. Filter the combined organic layers.

Scale	milligram
¹H NMR	500 MHz, CDCl ₃ : δ 0.85 (t, 3H, J = 7.5 Hz), 0.93 (t, 3H, J = 7.5 Hz), 1.33 (t, 3H, J = 7.5 Hz), 1.58-1.72 (m, 4H), 3.0 (d, 1H, J = 21.9 Hz), 3.82 (d, 1H, J = 21.9 Hz), 4.25 (q, 2H, J = 6.8 Hz), 4.67 (d, 1H, J = 5.2 Hz), 4.85 (m, 1H), 6.8 (s, 1H).
¹³C NMR	125 MHz, CDCl ₃ : δ 8.1, 8.3, 14.1, 20.8, 29.6, 30.4, 61.1, 73.5, 73.6, 114.4, 126.8, 135.6, 152.7, 166.0.
HRMS	ESI, Orbitrap m/z: calcd for C ₂₂ H ₄₀ O ₃ N 284.1492, found 284.1491.
State	yellow oil.
CAS Method Number	3-614-CAS-3416725



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 - 合成研究工作者可以获取到：详细实验过程、图谱等信息
- 根据需要选择访问界面
 - 合成研究工作者在**SciFinder**中即可获得相关内容
 - 分析研究工作者通过一个全新设计的界面即可获得相关内容
(www.methodsnow.com)

MethodsNow™的两个界面

在SciFinder中，合成方法详情的获取

The screenshot displays the SciFinder interface. At the top, there are navigation tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, a 'REACTIONS' section shows a list of reactions, with '1. View Reaction Detail' selected. The main area features a chemical reaction scheme showing the synthesis of a complex organic molecule from a starting material and a reagent. Below the reaction, an 'Overview' section is visible, and a 'MethodsNow™' section is highlighted with a purple box. This section contains a 'Procedure' with two steps: 1. Stir the mixture of 7-ethyl-4-methyl-2-carboxymethyl-2H-chromen-2-one (400 mg, 1.65 mmol), 1-azidoundecane (358 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), and (+)-sodium L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/15 mL) at room temperature for 4 hours. 2. Add water to the mixture. Below the procedure, there is a section for 'Available Experimental Data' listing ¹H NMR, ¹³C NMR, IR, HRMS, and Mass Spec, with a link to 'View with MethodsNow'.

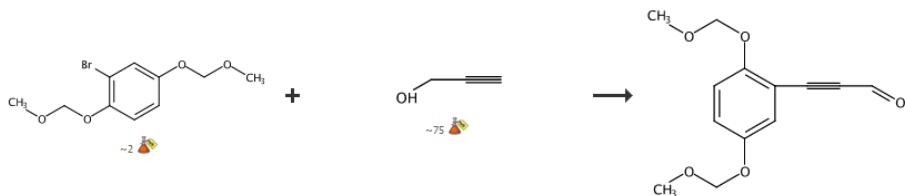
分析方法详情的获取 (www.methodsnow.com)

The screenshot shows the MethodsNow website interface. At the top, there is a 'Search' bar with the placeholder text 'Enter keyword, matrix, analyte, etc.' and a search icon. Below the search bar, there is an 'Advanced Search' section. The main content area is titled 'Browse Method Categories' and lists various analytical methods in a grid format: Agricultural Applications / Analysis, Bioassays, Biomolecule Isolation, Environmental Analysis, Food Analysis, Fuels / Geology / Biofuels, Historical Analysis / Dating, Miscellaneous, Organic Compound Analysis, Organometallics / Inorganics, Pharmacology / Toxicology, Polymer Analysis, and Water Analysis. At the bottom, there is a 'Recent Searches' section with a link to 'Browse: Pesticide Residue Analysis'.

MethodsNow™ — 在SciFinder 中的合成方法详情

6. View Reaction Detail [Link](#)

2 Steps Hover over any structure for more options.



Experimental Procedure: 我们可以做得更好

- 更好的阅读体验?
- 这些数字代表什么?
- 去免费的Supporting Information查? 可能只有图谱。

Experimental Procedure

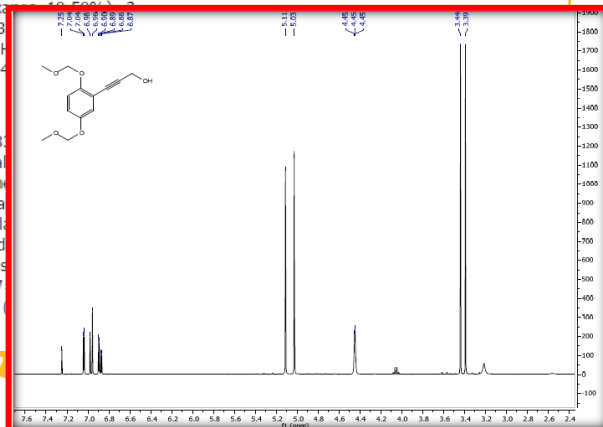
NATURAL PRODUCTS

Step 1

General Procedure for the Sonogashira Coupling.^{8,10,11} Compounds **6a**³¹ and **16**⁸ were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in n-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in n-butylamine (10 mL) and Pd(Ph₃)₄ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured into H₂O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexane). **[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol**² (**8**). Yield 96%; colorless oil. IR (KBr) ν_{max} 3310, 2230 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, *J* = 9 and 3.0 Hz, H-5), 7.03 (1H, d, *J* = 9.0 Hz, H-3), 3.0 Hz, H-3); ¹³C NMR (CDCl₃, 100 MHz) δ 51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.51 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1); HRESIMS *m/z* 275.0900 [M + Na]⁺ (calcd for C₁₃H₁₆O₅ 275.0896).

Step 2

Generation of the Key Aldehyde.¹⁷ Oxalyl chloride (272.3 μ L, 3.12 mmol) in dry CH₂Cl₂ (9 mL) was added to a stirred solution of DMSO (3 mL) in dry CH₂Cl₂ (1.5 mL) under an argon atmosphere at -78 °C. The mixture was stirred for 15 min, and the alcohol **8** (393.5 mg, 1.56 mmol) or **16** (1.56 mmol) in dry CH₂Cl₂ (12 mL) was added dropwise (Note: Swern oxidation could be scaled-up to 1.56 mmol of starting material). After the alcohol was consumed (nearly 2 h), Et₃N (1.88 mL, 7.8 mmol) was added. The reaction mixture was stirred at -78 °C for a further 30 min and was quenched with saturated NH₄Cl and H₂O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was washed with CH₂Cl₂ (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. **Bis(methoxymethoxy)phenyl]prop-2-ynal** (**9**). Yield 91%; colorless oil. IR (KBr) ν_{max} 1660, 2194 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 9.2 and 1.2 Hz, H-3), 9.44 (1H, s, H-9); ¹³C NMR (CDCl₃, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-5), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]⁺ (calcd for C₁₃H₁₄O₅ 273.0739).



MethodsNow™ — 在SciFinder 中的合成方法详情

MethodsNow

Reaction Steps 1 2

Products	2-Propyn-1-ol, 3-[2,5-bis(methoxymethoxy)phenyl]-, 96%, CAS RN: 1214266-55-3
Reactants	Propargyl alcohol, CAS RN: 107-19-7 Benzene, 2-bromo-1,4-bis(methoxymethoxy)-, CAS RN: 131136-47-5

Catalysts	Tetrakis(triphenylphosphine)palladium, CAS RN: 14221-01-3
Solvents	Butylamine, CAS RN: 109-73-9
Procedure	<ol style="list-style-type: none"> 1. Place aryl halide (9.21 mmol) in n-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. 2. Add a mixture of propargyl alcohol (9.21 mmol) in n-butylamine (10 mL) and add Pd(Ph₃)₄ (5% or 3%). 3. Heat the mixture for 21 h at 98 °C and pour into H₂O (80 mL). 4. Extract the product with EtOAc (3 × 80 mL). 5. Wash the combined organic layers with brine, dry over anhydrous Na₂SO₄, and evaporate under reduced pressure. 6. Purify the crude product by silica gel column chromatography (EtOAc/hexanes, 10-50%).
Scale	milligram
¹H NMR	(CDCl ₃ , 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, J = 9 and 3.0 Hz, H-5), 7.03 (1H, d, J = 9.0 Hz, H-6), 7.10 (1H, d, J = 3.0 Hz, H-3)
¹³C NMR	(CDCl ₃ , 100 MHz) δ 51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.19 (C-2), 117.13 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1)
IR	(KBr) ν _{max} 3310, 2230 cm ⁻¹
HRMS	m/z 275.0900 [M + Na] ⁺ (calcd for C ₁₃ H ₁₆ O ₅ 275.0896)
State	colorless oil
CAS Method Number	3-180-CAS-357629

Print/Export Close

化合物7

化合物16

MethodsNow – 分析方法详情(www.methodsnow.com)

Organic Compound Analysis: 天然产物分离分析, 手性分离, 活性药物成分及代谢产物分析…

Organometallics / Inorganics: 地质分析, 无机物分析, 金属有机化合物分析

Pharmacology / Toxicology: 成瘾药物检测, 有毒物检测…

Bioassays: 生物探针, 生物标定细胞实验, 生物标定药物实验, 生物医学材料分析, 生物分子/生物组织分离测定…

Water Analysis: 阴阳离子分析, 元素测定, 痕量元素分析, 废水分析, 生物标记公共卫生分析…

Historical Analysis / Dating: 考古分析, 同位素分析

Environmental Analysis: 土壤/空气/水分析, 农药残留分析…

Agricultural Applications / Analysis: 除草剂分析…

Food Analysis: 脂肪酸分析, 脂肪酸酯分析, 蛋白质分析…

Fuels / Geology / Biofuels: 生物燃料分析, 油气分析, 石油产品分析, 煤炭加工…

Miscellaneous: 化妆品分析, 爆炸物分析, 纳米材料分析…

目前有13个大类, 45个小类。某些子项目属于多种方法分类!

MethodsNow – 分析方法详情

保存结果集

检索/高级检索



方法分类



历史检索



The screenshot shows the MethodsNow web interface. At the top, there is a navigation bar with the logo 'METHODSNOW™ A CAS SOLUTION' and user options 'Saved' and 'Account'. Below the navigation bar is a search section with the heading 'Search' and a text input field labeled 'Enter keyword, matrix, analyte, etc.' with a search icon. Underneath is an 'Advanced Search' link. The main content area is titled 'Browse Method Categories' and contains a grid of category links: 'Agricultural Applications / Analysis', 'Bioassays', 'Biomolecule Isolation', 'Environmental Analysis', 'Food Analysis', 'Pharmacology / Toxicology', 'Polymer Analysis', 'Water Analysis', 'Miscellaneous', 'Organic Compound Analysis', and 'Inorganics / Organometallics / Inorganics'. At the bottom, there is a 'Recent Searches' section with a single entry 'hplc lycopene analysis' and a close button (X).

Click a browse category to view related methods

Click historical search to re-run search

Click "X" to delete search history

MethodsNow – 分析方法详情

从浏览方法分类开始

Browse Method Categories

Agricultural Applications / Analysis

Bioassays

Biomolecule Isolation

Environmental Analysis

Food Analysis

Fuels / Geology / Biofuels

Historical Analysis / Dating

Miscellaneous

Organic Compound Analysis

Organometallics / Inorganics

Pharmacology / Toxicology

Polymer Analysis

Water Analysis

Browse Method Categories > Organic Compound Analysis

Active Pharmaceutical Ingredient and Metabolite Analysis

Chiral Separation

Natural Product Isolation Analysis

Organic Compound Analysis

此处有大量手性化合物拆分方法文献



MethodsNow – 分析方法详情

手性化合物拆分方法

Browse Method Categories

Agricultural Applications / Analysis

Bioassays

Biomolecule Isolation

Environmental Analysis

Food Analysis

Fuels / Geology / Biofuels

Historical Analysis / Dating

Miscellaneous

Organic Compound Analysis

Organometallics / Inorganics

Pharmacology / Toxicology

Polymer Analysis

Water Analysis

Browse Method Categories > Organic Compound Analysis

Active Pharmaceutical Ingredient and Metabolite Analysis

Chiral Separation

Natural Product Isolation Analysis

Organic Compound Analysis

此处有大量手性化合物拆分方法信息



MethodsNow – 分析方法详情

Results (789)

手性化合物拆分方法详情

Sort Relevance ▾

[← Return to Home](#)

^ Analyte

- D-Phenylalanine (22)
- L-Phenylalanine (21)
- D-Alanine (18)
- L-Alanine (17)
- L-Leucine (17)

[View All](#)

^ Matrix

- Blood plasma (135)
- Pharmaceutical tablets (58)
- Urine (44)
- Drugs (30)
- Blood serum (25)

[View All](#)

▾ Method Category

▾ Technique

▾ Year



Compare (0/3)

Analysis of Valsartan in Drug delivery systems by Capillary zone electrophoresis

CAS MN: 1-116-CAS-17045

[View Details & Instructions](#)

Add to Compare

Analyte	Valsartan
Matrix	Pharmaceutical tablets; Drug delivery systems
Other Materials	Material: 0.45 μ m Whatman filter paper; Acetyl- β -cyclodextrin
Method Category	Chiral Separation
Technique	Liquid chromatography spectrometric detectors; Capillary zone electrophoresis
Equipment Used	Capillary electrophoresis system; Diode array detector
Source	Determination of the R-enantiomer of valsartan in pharmaceutical formulation by capillary electrophoresis Lee, Kyung Ran; Nguyen, NgocVan Thi; Lee, Yong Jae; Choi, Seungho; Kang, Jong Seong; Mar, Woongchon; Kim, Kyeong Ho



MethodsNow – 分析方法详情

手性化合物拆分方法详情

Analysis of (±)-Sertraline hydrochloride in Pharmaceutical tablets by HPLC

CAS MN: 1-116-CAS-52651

Method Category: Chiral Separation; Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: HPLC

手性分离和活性药物组份
和代谢分析

Materials	Role	Image	CAS RN
(±)-Sertraline hydrochloride	analyte	View Structure	79617-89-3
Pharmaceutical tablets	matrix		
Chiralpak IA	material		859767-48-9
Chiracel OD - H column (5 µm particle size in (250 × 4.6) mm)	material		
Chiral AD - H column (5 µm particle size in (250 × 4.6) mm)	material		
Methanol	reagent	View Structure	67-56-1
Diethylamine	reagent	View Structure	109-89-7

MethodsNow – 分析方法详情

手性化合物拆分方法详情

Source

A validated chiral LC method for the enantiomeric separation of sertraline hydrochloride in bulk drug samples and pharmaceutical dosage forms

Radhakrishnanand, P.; Rao, D. V. Subba; Surendranath, K. V.

Analytical Chemistry: An Indian Journal (2008), 7 (7), 515 - 520. Trade Science Inc.

CODEN: ACNHAY

Document Sources

Abstract ^

A simple and new isocratic polar mode chiral HPLC method has been developed for the enantiomeric separation of sertraline hydrochloride in bulk drugs and dosage forms with an elution time of about 15 min. The separation was achieved on immobilized amylose based chiral stationary phase (Chiralpak-IA) using 0.1% diethylamine in methanol as mobile phase. The mobile phase was delivered at 0.7 mL/min⁻¹ flow and the detection was monitored at 220 nm using UV detection technique. The resolution (R_s) between the sertraline and its (R,R)-enantiomer was found to be more than 4.0. The method shows 0.005 μg as limit of detection (LOD) and 0.015 μg as limit of quantification (LOQ) for (R,R)-sertraline, for 10 μL injection volume. The validated method yield good results regarding precision, linearity and accuracy. The developed method shows excellent linearity ($R^2 > 0.999$) over a range of LOQ to 0.3% for (R,R)-sertraline. The percentage recovery of (R,R)-sertraline ranged from 98.3 to 101.8 in bulk drug samples and in pharmaceutical dosage forms. Robustness studies were also carried out on the developed method. The sertraline hydrochloride sample solution stability and mobile phase stability studies were carried out and the results were found to be satisfactory for a study period of 48 h.

Equipment Used

Liquid chromatography (LC) system, 1100 series, Agilent Technologies, Waldbronn, Germany

MethodsNow – 分析方法详情

手性化合物拆分方法详情

Instructions

样品制备

Sample Preparation

1. Get the weight of twenty tablets individually and powder in mortar.
2. Transfer a sample of the powdered tablets, equivalent to 10 mg of active pharmaceutical ingredient (sertraline hydrochloride) into 100 mL volumetric flask.
3. Add about 75 mL of mobile phase and keep on a rotatory shaker for 10 min for the material to dissolve completely and sonicate for 10 min and dilute to 100 mL.
4. Centrifuge the content for 10 min at 3,000 rpm.
5. Collect the supernatant and filter using 0.45 µnylon 66-membrane filter.
6. Use the filtrate as the stock solution.

Standards Preparation

1. Prepare stock solutions of sertraline hydrochloride and (R, R)-sertraline ($1000 \mu\text{g mL}^{-1}$) individually by dissolving the appropriate amount of the substances in the mobile phase that contains a 0.1% diethylamine in methanol.
2. Prepare the working solution of sertraline hydrochloride and (R, R)-sertraline in diluent which is the mobile phase.

实验过程

Method or Procedure

1. Inject 10 µl of the sample into the Agilent 1100 series (Agilent Technologies, Waldbronn, Germany) LC system with a diode array detector (DAD).
2. Monitor the output signal using Chemstation software (Agilent) on Pentium computer (Digital Equipment Co., Hoston, USA.).
3. Use Chiralcel OD-H (cellulose tris (3,5-dimethylphenyl carbamate) coated onto silica-gel), Chiralpak AD-H (amylose tris (3,5-dimethylphenylcarbamate) coated onto silica-gel) and Chiralpak-IA (amylose tris (3,5- dimethylphenylcarbamate) immobilized onto silica- gel) as the chiral column.
4. Optimize the chromatographic conditions using a Chiralpak IA column.
5. Take 0.1% diethylamine in methanol as the mobile phase at afflow rate of 0.7 mL min^{-1} .
6. Maintain the column temperature at 25 °C and monitor the detection at 220 nm.

MethodsNow – 分析方法详情

手性化合物拆分方法详情

Validation

实验有效性数据

Limit of Detection	0.005 μg , of 100 $\mu\text{g mL}^{-1}$ analyte concentration, (R, R) - sertraline
Limit of Quantitation	0.015 μg , of 100 $\mu\text{g mL}^{-1}$ analyte concentration, (R, R) - sertraline
Recovery	98.3%, RSD 0.7%, 0.075 μg spiked bulk drug sample, (R, R) - sertraline (sample 1) 100.1%, RSD 0.4%, 0.150 μg spiked bulk drug sample, (R, R) - sertraline (sample 2) 101.4%, RSD 0.8%, 0.225 μg spiked bulk drug sample, (R, R) - sertraline, (sample 3) 100.8%, RSD 0.5%, 0.150 μg spiked dosage sample, (R, R) - sertraline, (sample 4) 98.5%, RSD 0.8%, 0.075 μg spiked dosage sample, (R, R) - sertraline, (sample 5) 101.8%, RSD 0.8%, 0.225 μg spiked dosage sample, (R, R) - sertraline, (sample 6)
Precision	3.0%, RSD, (R, R) - sertraline
Retention Time	6.0 min, Sertraline hydrochloride 7.0 min, (R, R) - sertraline

MethodsNow:

- 易于整合到工作流程中
- 快速对比分析方法
- 节省检索及直接获取具体方法的时间——无需通过全文查找方法详情
- 易于阅读的表格形式展示实验详情
- 包括材料、仪器、数据有效性、实验条件及其他更多信息

提纲

- 药物研发专利保护策略
- 检索工具的选择和分析
- 案例分享
 - 判定药物结构新颖性和创造性
 - 获取药物制备专利
 - 药物制备方法详情、手性结构拆分方法的获取
 - 药物制剂信息的获取
 - 药理分析方法的获取

获取含有Empagliflozin和二甲双胍的制剂信息

检策策略

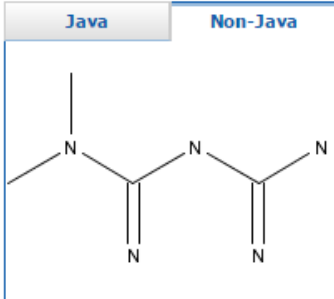
1. 通过结构式检索二甲双胍，得到含有二甲双胍结构式的物质结果集；
2. 在1的结果集中，用Empagliflozin的结构式限定（**Refine by structure**）结果，得到只含Empagliflozin和二甲双胍的混合物；
3. 在2的结果集中点击**Get Reference**，并通过学科领域分类，得到制剂领域文献

绘制“二甲双胍”结构，进行精确结构检索

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



Click image to change structure or view detail.


Import CXF

Search

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

 ChemDraw[®]
Launch a SciFinder substance
[More](#)

限定物质结果：通过化学结构筛选，并限定结果集Mixtures

Opened saved answer set "metformin" (565)

SUBSTANCES

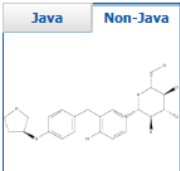
Analyze Refine

Refine by:

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

Structure Editor:

Java Non-Java



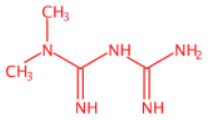
Click image to change structure or view detail.
Search type: **Exact Structure**

Only retrieve substances that:

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

Refine

2. **1115-70-4** (Component: 657-24-9)
~2495 ~135

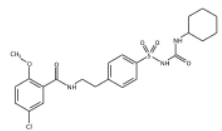


- HCl

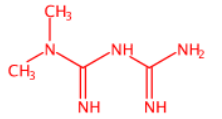
C₄ H₁₁ N₅ · Cl H
Imidodicarbonimidic diamide, *N,N*-dimethyl-, hydrochloride (1:1)
▶ **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

3. **338752-31-1**

10238-21-8
C₂₃ H₂₈ Cl N₃ O₅ S



1115-70-4 (Component: 657-24-9)
C₄ H₁₁ N₅ · Cl H



- HCl



输入限定结构：输入Empagliflozin的CAS号导入结构

The screenshot displays the CAS Structure Editor interface. At the top, a text box contains the text "输入CAS RN 864070-44-0" (Input CAS RN 864070-44-0). Below this, the chemical structure of Empagliflozin is shown. On the right side, a search options dialog is visible, with "Exact search" selected and "Substructure search" unselected. The interface also shows a sidebar with "SUBSTANCES" and "Analyze Refine" options, and a bottom status bar with the molecular formula $C_{27}H_{27}ClO_7$ and a molecular weight of 450.92.

此处选择精确结构检索，
如果可以为Empagliflozin衍生物，
则选择亚结构检索

获得混合物结果集： 只含 “Empagliflozin ” 和 “二甲双胍” 的混合物，并由物质获得文献

STANCES

Get References

Analyze Refine

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **1949774-69-9**

~1

864070-44-0
 $C_{23}H_{27}ClO_7$

Absolute stereochemistry.

1115-70-4 (Component: 657-24-9)
 $C_4H_{11}N_5 \cdot ClH$

• HCl

$C_{23}H_{27}ClO_7 \cdot C_4H_{11}N_5 \cdot ClH$
INDEX NAME NOT YET ASSIGNED

建议:

- 可从物质检索出发，然后从物质获取文献，再选择分析研究领域的文献
- 多浏览CA Section Title，或相关的Index Term进行限定，从而获得符合要求的结果（如制剂，缓释，剂型等）。
- 根据不同的检索要求，灵活结合文献检索和物质（结构或识别号）检索，然后再通过Analyze, Refine,或Categorize获取相关文献。

提纲

- 药物研发专利保护策略
- 检索工具的选择和分析
- 案例分享
 - 判定药物结构新颖性和创造性
 - 获取药物制备专利
 - 药物制备方法详情、手性结构拆分方法的获取
 - 药物制剂信息的获取
 - 药理分析方法的获取

SciFinder中，药理学分析方法的获取

- 方法一：通过物质获得文献，并限定选择结果中**Pharmacology**类别，将新结果集限定为专利文献，再使用 **Categorize**对结果进行分类，选择**Analytical chemistry**,选择其中感兴趣的分析方法，分析物，基质等**Index Term**，从而获得结果。
- 方法二：可以通过物质获得**Analytical Study**文献，并限定选择结果中**Pharmacology**类别，获得相关结果。
- 方法三：如果已知药物作用的某个（或者某几个）靶点，可以由相关靶点获得文献，进而将文献结果限定为 **Pharmacology**类别，后面的操作同方法一所述。
- 方法四：可以通过物质获得文献，在结果中使用相关的**Index Term**或者关键词去限定，从而获得结果。

药理学分析方法的获取

Substance Identifier "Sofosbuvir" > substances (1) > get references (720) >

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

Sofosbuvir

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

Search

Substance Identifier "Sofosbuvir" > substances (1)

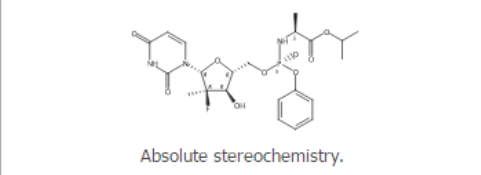
SUBSTANCES **Get References** Retrieve references for selected substances.

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **1190307-88-0**

~720 ~81



Absolute stereochemistry.

C₂₂ H₂₉ F N₃ O₉ P
L-Alanine, *N*-[[*R*(*S*),2'*R*]-2'-deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-, 1-methylethyl ester

Key Physical Properties
Regulatory Information

Analyze by: Substance Role

Analytical Study 1

Biological Study 1

Preparation 1

Process 1

Properties 1

Reactant or Reagent 1

Uses 1

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Get References

Retrieve references for:

All substances
 Selected substances

Limit results to:

<input type="checkbox"/> Adverse Effect, including toxicity	<input 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.

Substance Identifier "sofosbuvir" > substances (1) > get references (746)

REFERENCES ?

Analyze Refine Categorize

Sort by: Accession Number ↓

0 of 746 References Selected

Analyze by: ?

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

Mo Hongmei	17
Younossi Zobair M	15
Dvory Sobol Hadas	14
Jacobson Ira M	14

1. **Antiviral regimens for patients with chronic**
Quick View Other Sources
By Rao, Zhifang; Wang, Wangang; Cheng, Zhenling; Wu
From Zhongguo Yaoshi (Wuhan, China) (2016), 19(2), 3
A review. The efficacy of patients infected with
new drugs against HCV, many new regimens
HCV protease inhibitors telaprevir and boceprevir
such as simeprevir, sofosbuvir and ledipasvir

2. **Guide interpretation of treatment of chronic**
Quick View Other Sources
By Chen, Xinyue; Ren, Shan
From Beijing Yixue (2014), 36(12), 1068-1072. | Language
A review. The paper interprets the choice of
treatment. For patients with GT 1 and 4
Simeprevir (SMV), PEG-IFNα + RBV + Daclatasvir
infection, PEG-IFNα + RBV + SOF for GT 3 and 4

3. **Quantifying antiviral activity optimizes drug**
Quick View Other Sources

选出药理学研究的文献

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500 references with the CA Section Title **Pharmacology** are displayed Keep Analysis Clear Analysis

Substance Identifier "sofosbuvir" > substances (1) > **get references (746)**

REFERENCES ⓘ Get Substances Get Reactions Get Related Citations Tools Create Keep Me Posted Alert Send to SciPlanner

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0 of 746 References Selected

Page: 1 of 5

Analyze by: CA Section Title

Pharmacology 500

Pharmaceuticals	70
Carbohydrates	61
Amino Acids, Peptides, and Proteins	33
Immunochemistry	23
Heterocyclic Compounds (More Than One Hetero Atom)	13

1. Antiviral regimens for patients with chronic hepatitis C virus complicated with cirrhosis
Quick View Other Sources
By Rao, Zhifang; Wang, Wangang; Cheng, Zhenling; Wang, Zhi
From Zhongguo Yaoshi (Wuhan, China) (2016), 19(2), 357-359. | Language: Chinese, Database: CAPLUS

A review. The efficacy of patients infected with hepatitis C virus (HCV) complicated with cirrhosis is not promising after treated with present std. therapy. With more and more new drugs against HCV, many new regimens for the patients with chronic HCV complicated with cirrhosis have come forth. Because the adverse reactions of the first generation HCV protease inhibitors telaprevir and boceprevir are severe, they are not recommended to be used in the patients with chronic HCV complicated with cirrhosis. The other drugs, such as simeprevir, sofosbuvir and ledipasvir show good efficacy in th...

2. Guide interpretation of treatment of chronic hepatitis C in European Association for Study of Liver in 2014
Quick View Other Sources
By Chen, Xinyue; Ren, Shan
From Beijing Yixue (2014), 36(12), 1068-1072. | Language: Chinese, Database: CAPLUS

A review. The paper interprets the choice of therapeutic regimes for the treatment of chronic hepatitis C (CHC), treatment monitoring and regimes adjusting, and individual treatment. For patients with GT 1 and 4 types of HCV infection, the therapeutic regimes include PEGylated interferon α (PEG-IFNα) + ribavirin (RBV), PEG-IFNα + RBV + Simeprevir (SMV), PEG-IFNα + RBV + Daclatasvir (DCV), Sofosbuvir (SOF) + SMV, SOF + DCV, and SOF + RBV. The therapeutic regimes are SOF + RBV for GT 2 type of HCV infection, PEG-IFNα + RBV + SOF for GT 3 type of HCV infection, and PEG-IFNα + RBV for GT 5 and ...

https://scifinder.cas.org/scifinder/view/text/refList.jsf?nav=eNpb85aBtYS8MbGEOcXU1dzIzMXEPMLCzM3Y1MDSKMLczNnjxMDZyDd10NTAyMXZyAWoNKm4iEEwK7EsUS8nMS9dzOvJDU9tUjo0YlI3xvbLZqYGD0ZWMSsC0pTK4oYBBDq_Epzk1KL2tZMleWe...

将文献结果集限定为专利

REFERENCES

Get Substances Get Reactions Get Related Citations Tools

Analyze Refine **Categorize**

Sort by: Accession Number

0 of 500 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. **Antiviral regimens for patients with chronic hepatitis C virus complicated with cirrhosis**
[Quick View](#) [Other Sources](#)
By Rao, Zhifang; Wang, Wangang; Cheng, Zhenling; Wang, Zhi
From Zhongguo Yaoshi (Wuhan, China) (2016), 19(2), 357-359. | Language: Chinese, Database: CAPLUS
A review. The efficacy of patients infected with hepatitis C virus (HCV) complicated with cirrhosis is not pro...
new drugs against HCV, many new regimens for the patients with chronic HCV complicated with cirrhosis ha...
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such as simeprevir, sofosbuvir and ledipasvir show good efficacy in th...

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[Quick View](#) [Other Sources](#)
By Chen, Xinyue; Ren, Shan
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treatment. For patients with GT 1 and 4 types of HCV infection, the therapeutic regimes include PEGylat...
Simeprevir (SMV), PEG-IFN α + RBV + Daclatasvir (DCV), Sofosbuvir (SOF) + SMV, SOF + DCV, and SOF + P...
infection, PEG-IFN α + RBV + SOF for GT 3 type of HCV infection, and PEG-IFN α + RBV for GT 5 and ...

3. **Quantifying antiviral activity optimizes drug combinations against hepatitis C virus infection**
[Quick View](#) [Other Sources](#)
By Koizumi, Yoshiki; Ohashi, Hirofumi; Nakajima, Syo; Tanaka, Yasuhito; Wakita, Takaji; Perelson, Alan S.; Iwami, Shingo; Watashi
From Proceedings of the National Academy of Sciences of the United States of America (2017), Ahead of Print. | Language: English
With the introduction of direct-acting antivirals (DAAs), treatment against hepatitis C virus (HCV) has signif...
disease better, the "best" multidrug treatment is demanded based on scientific evidence. However, there is...
antiviral efficacy and drug-resistance profiles of drug combinations. Based on exptl. anti-HCV profiles in a ce...
potential (IIP), which is the logarithm of the redn. in viral re...

4. **Safety and effectiveness of a 12-week course of sofosbuvir and simeprevir \pm ribavirin in HCV-infected patien**
[Quick View](#) [Other Sources](#)

将所得文献结果集进行分类，选择**Analytical Chemistry**,选择感兴趣的分析手段、分析物或者基质，获得文献结果

0 duplicates were automatically removed.

Substance Identifier "sofosbuvir" > substances

REFERENCES ?

Get Substance

Analyze Refine Categorize

Analyze by: ?

CA Section Title

Pharmacology 66

Show More

Sort by: Accession

1. Com...
By Iyer, ...
From PC...

This i...
one a...
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a par...

2. Met...
By Berns...
From PC...

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Analytes & matrixes (15)
Biotechnology	Analysis (8)
General chemistry	
Genetics & protein chemistry	
Physical chemistry	
Polymer chemistry	
Biology	
Synthetic chemistry	
Technology	
Analytical chemistry	
Environmental chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms	Selected Terms
Select All Deselect All	
<input type="checkbox"/> Biomarkers	3
<input type="checkbox"/> Blood analysis	2
<input type="checkbox"/> Immunohistochemistry	2
<input type="checkbox"/> Therapy monitoring	2
<input type="checkbox"/> Liquid chromatography-mass spectrometry	1
<input type="checkbox"/> Mass spectrometry	1
<input type="checkbox"/> NMR spectroscopy	1
<input type="checkbox"/> Virus plaque assay	1

Analytical chemistry > Analysis

OK Cancel

either interferon or ribavirin, and said at least two direct acting antiviral agents comprise (a) the HC...
a pharmaceutically acceptable salt thereof and (b) the NSSA inhibi...

SciFinder中，药理学分析方法的获取

- 方法一：通过物质获得文献，并限定选择结果中Pharmacology类别，将新结果集限定为专利文献，再使用Categorize对结果进行分类，选择Analytical chemistry,选择其中感兴趣的分析方法，分析物，基质等Index Term，从而获得结果。
- 方法二：可以通过物质获得Analytical Study文献，并限定选择结果中Pharmacology类别，获得相关结果。
- 方法三：如果已知药物作用的某个（或者某几个）靶点，可以由相关靶点获得文献，进而将文献结果限定为Pharmacology类别，后面的操作同方法一所述。
- 方法四：可以通过物质获得文献，在结果中使用相关的Index Term或者关键词去限定，从而获得结果。

使用物质标识符检索到Sofosbuvir并且由物质获得文献

Substance Identifier "Sofosbuvir" > substances (1) > get references (720) >

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

Sofosbuvir

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

Search

Substance Identifier "Sofosbuvir" > substances (1)

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

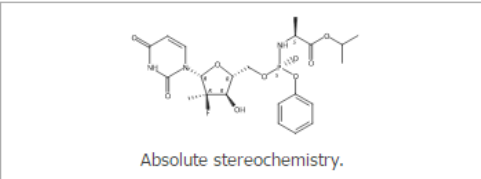
Analyze Refine

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **1190307-88-0**

~720 ~81


Absolute stereochemistry.

C₂₂ H₂₉ F N₃ O₉ P
L-Alanine, *N*-[[*R*(*S*),2'*R*]-2'-deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-, 1-methylethyl ester

Key Physical Properties
Regulatory Information

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获得Analytical Study文献，并使用Analyze by CA Section Title分析结果

Get References

Retrieve references for:

All substances
 Selected substances

Limit results to:

<input type="checkbox"/> Adverse Effect, including toxicity	<input type="checkbox"/> Preparation
<input checked="" 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.

Substance Identifier "sofosbuvir" > substances (1) > get references (10) > keep analysis "CA Section Title" (8)

REFERENCES ⓘ

Analyze Refine Categorize

Sort by: Accession Number ↓

0 of 10 References Selected

Analyze by: ⓘ
CA Section Title

Pharmacology	8
Pharmaceutical Analysis	2

- 1. RP-HPLC Method for Simultaneous Determination of Sofosbuvir and Ledipasvir in Tablet Dosage Form**
[Quick View](#) [Other Sources](#)
By Zaman, Bakht; Siddique, Faisal; Hassan, Waseem
From Chromatographia (2016), 79(23-24), 1605-1613. | Language: English, Database: CAPLUS
A reversed-phase high-performance liq. chromatog. method was developed for the simultaneous determination of sofosbuvir and ledipasvir in tablet dosage form. The method was performed on Luna anal. column 250 × 4.6 mm, 5 μm, octyl silica packing (Si-[CH₂]₇-CH₃) C₁₈ mobile phase at flow rate of 0.7 mL min⁻¹ for isocratic elution. Detection of sofosbuvir and ledipasvir were 4.468 ± 0.013 min and 8.242 ± 0.012 min, resp., and the total ion chromatogram showed a single sharp peak for each compound. The method was validated for linearity, accuracy, precision, and stability. The method was applied to the determination of sofosbuvir and ledipasvir in tablet dosage form. The results were compared with the official method and found to be in good agreement.
- 2. Quantification of sofosbuvir in human serum by liquid chromatography with negative ionization mode and its application to a bioequivalence study**
[Quick View](#) [Other Sources](#)
By Bahrami, Mohammad Taher; Mohammadi, Bahareh; Miraghaei, Shahram; Babaei, Atefeh; Ghaeni, Matin; Behrooz, Amirhossein
From Journal of Separation Science (2016), 39(14), 2702-2709. | Language: English, Database: CAPLUS
In the mass spectrometry of sofosbuvir, a new orally administered antihepatitis C drug, a new source disson. and current methods to its quantification, is based on monitoring of the parent ion. With these methods serum concn. of the drug is quantifiable only up to 4-5 h postdose. HPLC method with a signal intensity of about tenfold compared to the parent ion. ...
- 3. Quantification of sofosbuvir and ledipasvir in human plasma by UPLC-MS/MS method: Application to a bioequivalence study**

SciFinder中，药理学分析方法的获取

- 方法一：通过物质获得文献，并限定选择结果中Pharmacology类别，将新结果集限定为专利文献，再使用Categorize对结果进行分类，选择Analytical chemistry,选择其中感兴趣的分析方法，分析物，基质等Index Term，从而获得结果。
- 方法二：可以通过物质获得Analytical Study文献，并限定选择结果中Pharmacology类别，获得相关结果。
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- 方法四：可以通过物质获得文献，在结果中使用相关的Index Term或者关键词去限定，从而获得结果。

在物质结果页面获得索氟布韦靶点信息，选择感兴趣的靶点，获得文献

CAS Registry Number 1190307-88-0

~743   ~82 

C₂₂H₂₈F N₃O₉P

L-Alanine, N-[[[R(5),2-R]-2'-deoxy-2'-fluoro-2'-methyl-uridylyl]-, 1-methylethyl] ester

Molecular Weight

529.45

Density (Predicted)

Value: 1.41±0.1 g/cm³ | Condition: Temp: 20 °C Pre

pKa (Predicted)

Value: 9.39±0.10 | Condition: Most Acidic Temp: 25

Other Names

GS 7977

Hepcinat

Hepcivir

Isopropyl (2S)-2-[[[2R,3R,4R,5R]-5-(2,4-dioxypyrimidin-3-hydroxy-4-methyl-tetrahydrofuran-2-yl)methoxy-phosphoryl]amino]propanoate

PSI 7977

View more...

▶ BIOACTIVITY INDICATORS

▼ TARGET INDICATORS

Indicators	References
Cytokines (all) > > Interferons	47
Cytokines (all) > > Interleukin 28	25
Enzymes (all) > > > Alanine aminotransferase	33
Enzymes (all) > > > Aspartate aminotransferase	19
Enzymes (all) > > > > DNA-dependent RNA polymerase	12
Enzymes (all) > > > > DNA-dependent RNA polymerase	12
Enzymes (all) > > > > NS3 protease	65
Enzymes (all) > > > > RNA-dependent RNA polymerase	43
Enzymes (all) > > > > RNA-dependent RNA polymerase NS5B	76
Immunophilins (all) > Cyclophilins	10
Interferons (all) > Interferons	47
Viral proteins (all) > > RNA-dependent RNA polymerase NS5B	76
Viral proteins (all) > > Viral nonstructural proteins	91

▶ CAS REFERENCE ROLES

通过学科分类分析，获得药理研究的文献

Substance Identifier "sofosbuvir" > substances (1) > 1190307-88-0 > get references (76) > keep analysis "CA Section Title" (46)

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Analyze by: CA Section Title Pharmacology 46

Amino Acids, Peptides, and Proteins 12

Carbohydrates 9

Heterocyclic Compounds (More Than One Hetero Atom) 3

Pharmaceuticals 2

Biochemical Genetics 1

1. **Preparation method of (2'R)-2'-deoxy-2'-fluoro-2'-methyluridine-3',5'-dibenzoate**
 Quick View PATENTPAK
By Gu, Shihai; Mi, Liang
From Faming Zhuanli Shengqing (2016), CN 106146586 A 20161123. | Language: Chinese, Database: CAPLUS
The present invention provides a synthesis method for prepg. sofosbuvir key intermediate (2'R)-2'-deoxy-2'-fluoro-2'-methyluridine-3',5'-dibenzoate (I). The method comprises: converting 3,5-di-O-benzoyl-2-deoxy-2-methyl-D-ribo- γ -lactone and 2,4-bis(trimethylsiloxy)pyrimidine to I under the effect of catalyst. The invention overcomes the shortcomings of two step synthesis and low yield in prior method. The method has easy and simple processing, low cost, high yield, good product purity, does not need purifn. again, and is conducive to industrialized prodn. Compd. I can be used fo...

2. **Nucleoside analogs for treatment of the flaviviridae family of viruses and cancer**
 Quick View PATENTPAK
By Coats, Steven J.; Amblard, Franck; Mengshetti, Seema; Li, Hao; Schinazi, Raymond F.
From PCT Int. Appl. (2016), WO 2016178876 A2 20161110. | Language: English, Database: CAPLUS
The present invention is directed to compds., compns. and methods for treating or preventing Flaviviridae family of viruses (including HCV, Yellow fever, Dengue, Chikungunya and West Nile virus), RSV, HEV, and influenza infection and cancer in human subjects or other animal hosts.

将所得文献结果集进行分类，选择 **Analytical Chemistry**, 选择感兴趣的分析手段、分析物或者基质，获得文献结果

Substance Identifier "sofosbuvir" > substances

REFERENCES ?

Analyze Refine Categorize

Analyze by: ?
CA Section Title

Pharmacology 46

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Sort by: Acc

Get Substan

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Analysis (4)
General chemistry	Analytes & matrixes (3)
Biotechnology	
Genetics & protein chemistry	
Physical chemistry	
Polymer chemistry	
Biology	
Synthetic chemistry	
Technology	
Analytical chemistry	

2. Select index terms of interest.

Index Terms	Selected Terms
Select All Deselect All	Click 'X' to remove the category from 'Selected Terms'
<input checked="" type="checkbox"/> Liquid chromatography-mass spectrometry 1	<input checked="" type="checkbox"/> Analytical chemistry > Analysis (4 Terms)
<input checked="" type="checkbox"/> Liquid chromatography-quadrupole time-of-flight mass spectrometry 1	
<input checked="" type="checkbox"/> Mass spectrometry 1	
<input checked="" type="checkbox"/> Therapy monitoring 1	

Analytical chemistry > Analysis > 4 Index Term(s) Selected

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From: PCT Int. Appl. (2016) WO/2016/164625 A1 20161013 / Language: English; Database: CASLITE

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- 方法一：通过物质获得文献，并限定选择结果中Pharmacology类别，将新结果集限定为专利文献，再使用Categorize对结果进行分类，选择Analytical chemistry,选择其中感兴趣的分析方法，分析物，基质等Index Term，从而获得结果。
- 方法二：可以通过物质获得Analytical Study文献，并限定选择结果中Pharmacology类别，获得相关结果。
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- 方法四：可以通过物质获得文献，在结果中使用相关的Index Term或者关键词去限定，从而获得结果。

使用物质标识符检索到物质获得文献

Substance Identifier "Sofosbuvir" > substances (1) > get references (720) >

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

Sofosbuvir

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

Search

Substance Identifier "Sofosbuvir" > substances (1)

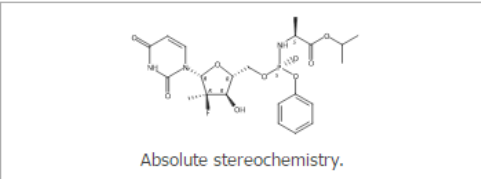
SUBSTANCES **Get References** Retrieve references for selected substances.

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **1190307-88-0**

~720 ~81


Absolute stereochemistry.

C₂₂ H₂₉ F N₃ O₉ P
L-Alanine, *N*-[[*R*(*S*),2'*R*]-2'-deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-, 1-methylethyl ester

Key Physical Properties
Regulatory Information

Analyze **Refine**

Analyze by: Substance Role

Analytical Study 1

Biological Study 1

Preparation 1

Process 1

Properties 1

Reactant or Reagent 1

Uses 1

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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

Substance Identifier "sofosbuvir" > substances (1) > get references (746)

REFERENCES ⓘ

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Analyze Refine Categorize

Sort by: Accession Number ↓

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Analyze by: Author Name

Mchutchison John G	39
Symonds William T	33
Lawitz Eric	25
Pang Phillip S	23
Subramanian G Mani	19
Mo Hongmei	17
Younossi Zobair M	15
Dvory Sobol Hadas	14
Jacobson Ira M	14

- 1. Antiviral regimens for patients with chronic hepatitis C virus complicated with cirrhosis**
Quick View Other Sources
By Rao, Zhifang; Wang, Wangang; Cheng, Zhenling; Wang, Zhi
From Zhongguo Yaoshi (Wuhan, China) (2016), 19(2), 357-359. | Language: Chinese, Database: CAPLUS
A review. The efficacy of patients infected with hepatitis C virus (HCV) complicated with cirrhosis is not prom... new drugs against HCV, many new regimens for the patients with chronic HCV complicated with cirrhosis have HCV protease inhibitors telaprevir and boceprevir are severe, they are not recommended to be used in the pati... such as simeprevir, sofosbuvir and ledipasvir show good efficacy in th...
- 2. Guide interpretation of treatment of chronic hepatitis C in European Association for Study of Liver in 2014**
Quick View Other Sources
By Chen, Xinyue; Ren, Shan
From Beijing Yixue (2014), 36(12), 1068-1072. | Language: Chinese, Database: CAPLUS
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- 3. Quantifying antiviral activity optimizes drug combinations against hepatitis C virus infection**
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Analyze by:

Human 570

Antiviral agents 492

Hepatitis C virus 451

Homo sapiens 410

Hepatitis C 397

Combination chemotherapy 232

Interferons 175

Cirrhosis 148

Genotypes 148

Viral infection 139

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1. Antiviral regimens for patients with chronic hepatitis C virus complicated with cirrhosis

2. Guide interpretation of treatment for patients with chronic hepatitis C virus infection

3. Quantifying antiviral activity in patients with chronic hepatitis C virus infection

4. Safety and effectiveness of treatment for patients with chronic hepatitis C virus infection

Analyze - Index Term

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Select bars to view only those references within the current answer set.

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