

Pharmaceutical Substances  
数据库介绍与平台使用指南

## 您将会了解到…

1. Thieme 出版社
2. Pharmaceutical Substances 数据库内容
3. Pharmaceutical Substances 平台使用
  - 文本检索
  - 结构检索

## 1. Thieme 出版社介绍



- 德国著名的医学与科学出版社，成立于1886年；
- 总部位于斯图加特，在全球共有900多名员工。
- 致力于为临床医师、教师、学生和科研人员提供高品质的出版物，包括图书、期刊和数据库等。
- 出版内容主要专注于**医学、药学和有机合成化学**领域资源。

Pharmaceutical Substances (药物物质)

<http://www.thieme-chemistry.com/ps/prod/>

## 2. Pharmaceutical Substances 数据库

Pharmaceutical Substances (药物物质) 数据库, 简称PS, 是关于FDA许可药物的工业合成和商业应用一站式信息来源。通过PS 可以快速查询2600多种药物活性成分 (API, 原料药) 及其中间体的合成路线、专利文献、商业应用信息。

由Axel Kleemann, Jürgen Engel, Bernhard Kutscher三位教授和Dietmar Reichert 博士通过从大量文献和专利数据中搜集评估原料药相关信息编著而成。

化学研发与工艺科学家; 医药化学领域教师学生; 从事药物研究、开发、市场评估工作人员最重要的必备参考工具。

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## Pharmaceutical Substances 数据库内容

**Thieme Pharmaceutical Substances**

Query Results About

Welcome to **Pharmaceutical Substances**

- Syntheses
- Patents
- Applications

Now with new Interface

**Search for term**

Enter search term [Search](#)

**Search for structure/reaction**

CONTACT AND SUPPORT

If you have any questions, feedback or need technical support please contact us via E-Mail.

- 2659种FDA许可药物活性成分 (API)
- 每年更新2次，添加FDA许可的新的API
- 文本检索、(亚)结构、反应式
- 在线浏览，不需安装软件

Pharmaceutical Substances 数据库中一条完整的API记录包括:

# 1. Factual Data 事实数据

Help | About Pharmaceutical Substances | About Thieme Chemistry

Thieme Pharmaceutical Substances

Query Results About

1 Results

> Atorvastatin calcium

**Atorvastatin calcium**

Synonyms: CI-981, YM-548  
 ATC: C10AA05  
 Use: hypolipidemic, HMG-CoA-reductase inhibitor

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

Formula: C<sub>66</sub>H<sub>68</sub>CaF<sub>2</sub>N<sub>4</sub>O<sub>10</sub>  
 MW: 1155.36 g/mol  
 CAS-RN: 134523-03-8

Derivatives  
**free acid**

Formula: C<sub>33</sub>H<sub>35</sub>FN<sub>2</sub>O<sub>5</sub>  
 MW: 558.65 g/mol  
 CAS-RN: 134523-00-5

Substance Classes

> Anilides  
 > Fluorocarboxylic acids

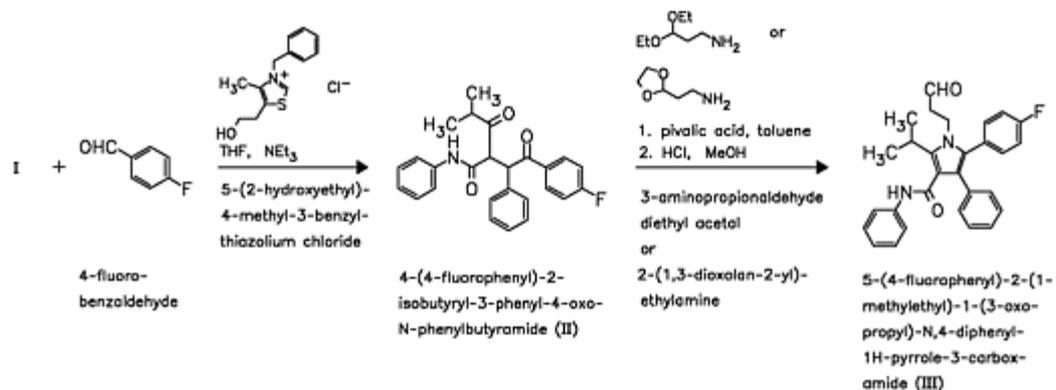
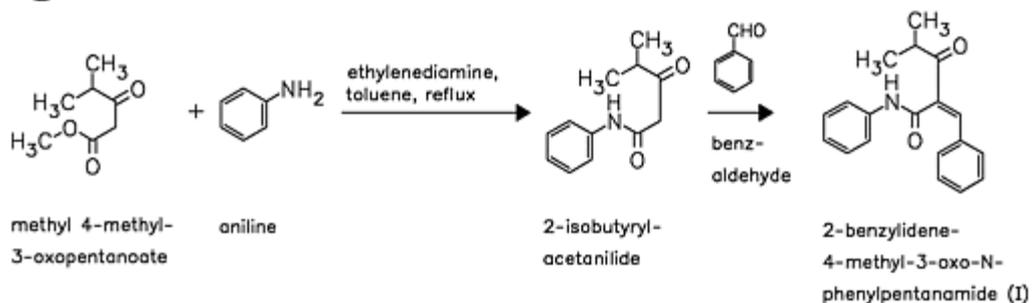
- INN号、商品名、俗名
- 化学名称（IUPAC）
- ATC代码
- CAS号、EINECS号
- 分子式、分子量、急性毒性
- 主要应用
- 医疗用途/治疗分类

## 2. Synthetic Pathway 合成路线

### Synthesis Path

ⓐ early synthetic methods

ⓐ1



- 工业全合成路线  
(可实现规模生产的可靠路线, 解读自专利等技术文章)
- 中间体合成路线

## 3. All intermediates 中间体信息

Substances Referenced in Synthesis Path			
CAS-RN	Formula	Chemical Name	CAS Index Name
77-76-9	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	acetone dimethyl acetal	Propane, 2,2-dimethoxy-
95061-51-1	C <sub>22</sub> H <sub>20</sub> O <sub>3</sub>	(S)-(+)-2-acetoxy-1,1,2-triphenylethanol	1,2-Ethandiol, 1,1,2-triphenyl-, 2-acetate, (S)-
41365-75-7	C <sub>7</sub> H <sub>17</sub> NO <sub>2</sub>	3-aminopropionaldehyde diethyl acetal	1-Propanamine, 3,3-diethoxy-
62-53-3	C <sub>6</sub> H <sub>7</sub> N	aniline	Benzenamine
100-52-7	C <sub>7</sub> H <sub>6</sub> O	benzaldehyde	Benzaldehyde
4568-71-2	C <sub>13</sub> H <sub>16</sub> ClNOS	3-benzyl-5-(2-hydroxyethyl)-4-methylthiazolium chloride	
125971-57-5	C <sub>19</sub> H <sub>19</sub> NO <sub>2</sub>	2-benzylidene-4-methyl-3-oxo-N-phenylpentanamide	Pentanamide, 4-methyl-3-oxo-N-phenyl-2-(phenylmethylene)-
434935-49-6	C <sub>4</sub> H <sub>7</sub> BrO <sub>3</sub>	(S)-4-bromo-3-hydroxybutanoic acid	
540-88-5	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	<i>tert</i> -butyl acetate	Acetic acid, 1,1-dimethylethyl ester
125995-13-3	C <sub>14</sub> H <sub>27</sub> NO <sub>4</sub>	<i>tert</i> -butyl (4 <i>R</i> ,6 <i>R</i> )-2-[6-(2-aminoethyl)-2,2-dimethyl-1,3-dioxan-4-yl]acetate	1,3-Dioxane-4-acetic acid, 6-(2-aminoethyl)-2,2-dimethyl-, 1,1-dimethylethyl ester, (4 <i>R</i> - <i>cis</i> )-

- CAS号
- 分子式
- 化学名称
- CAS索引名称

## 4. Marketing Data 市场信息

### Trade Names

Country	Trade Name	Vendor	Annotation
D	Sortis	Parke DavisGödeckePfizerMack, Illert.	
F	Caduet	Pfizer	comb.
	Tahor	Pfizer	
GB	Lipitor	Pfizer	
	Lipitor	Warner-Lambert	
I	Torvast	Pfizer	
	Totalip	Guidotti	
J	Lipitor	Astellas	
USA	Lipitor	Parke DavisPfizer	

### Formulations

tabl. 5 mg, 10 mg, 20 mg, 40 mg, 80 mg

- 上市国家（全球6大市场）
- 商品名
- 供应商名称
- 上市剂型

## 5. Patents 专利文献/综述/优先权信息

- 制备专利/工艺专利

- 晶型专利

- 制剂专利

### References

US 4 681 893 (Warner-Lambert; 21.7.1987; appl. 30.5.1986).  
 US 5 273 995 (Warner-Lambert; 28.12.1993; appl. 26.2.1991; USA-prior. 21.7.1989).  
 EP 409 281 (Warner-Lambert; appl. 23.1.1991; USA-prior. 21.7.1989, 26.2.1991).  
 DE 1 061 073 (Warner-Lambert; appl. 20.7.1990; USA-prior. 21.7.1989).

### review:

Roth, B.D. et al.: J.  
 Nanninga, T. et al.:  
 Li, J.J.; Johnson, D.:

**a1** US 4 647 576 (Wa  
 US 5 124 482 (Wa  
 US 5 149 837 (Wa

### alternative synth

WO 2 003 004 457  
**a2a3** US 5 273 99

### improved process

WO 2 005 087 723  
 CA 2 460 935 (Apo

**a4** US 4 681 893 (

**bc1** US 5 155 251

**c1** US 5 103 024 (

US 6 433 213 (Wa

US 6 596 879 (Wa

US 6 962 994 (Wa

**c2** US 5 248 793 (

**(S)-3,4-dihydrox**

**d1** US 5 292 939 (

US 5 319 110 (Hol

US 5 374 773 (Hol

US 6 239 311 (Hol

US 5 998 633 (Wa

### **crystalline forms of atorvastatin calcium:**

US 5 959 156 (Warner-Lambert; 19.10.1999; appl. 29.9.1997; USA-prior. 17.7.1995).

WO 9 703 959 (Warner-Lambert; appl. 8.7.1996; USA-prior. 17.7.1995).

WO 9 703 958 (Warner-Lambert; appl. 6.2.1997; USA-prior. 17.7.1995).

US 6 528 661 (Teva; 4.3.2003; appl. 24.10.2001; prior. 16.11.2000, 13.8.2001, 1.10.2001).

### **crystalline forms I – III:**

US 5 969 156 (Warner-

### **crystalline form III:**

US 6 121 461 (Warner-

### **crystalline forms V –**

US 6 605 729 (Warner-

### **factory process for cr**

US 6 600 051 (Warner-

### **production scale proc**

US 6 605 728 (Warner-

### **crystalline form VII:**

US 6 605 636 (Teva; 12

### **stable oral formulation:**

US 5 686 104 (Warner-Lambert; 11.11.1997; appl. 20.5.1994; USA-prior. 19.1.1993).

US 6 126 971 (Warner-Lambert; 3.10.2000; appl. 2.7.1997; USA-prior. 19.1.1993, 4.8.1994).

WO 9 416 693 (Warner-Lambert; appl. 4.8.1994; USA-prior. 19.1.1993).

### **aerosol formulation:**

US 2 001 006 656 (Univ. Washington; 5.7.2001, appl. 17.2.1999).

### **novel formulation:**

US 2 001 006 658 (Abbott; 5.7.2001; appl. 31.3.1999).

### **combination therapy with amlodipine:**

US 2 002 025 981 (Pfizer; 28.2.2002; appl. 10.10.2001; WO-prior. 10.8.1998).

### **use for prevention of BPH:**

US 2 002 004 521 (M.Goldberg; 10.1.2002; appl. 5.1.2001).

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## ➤ Example 索非布韦 (Sofosbuvir)

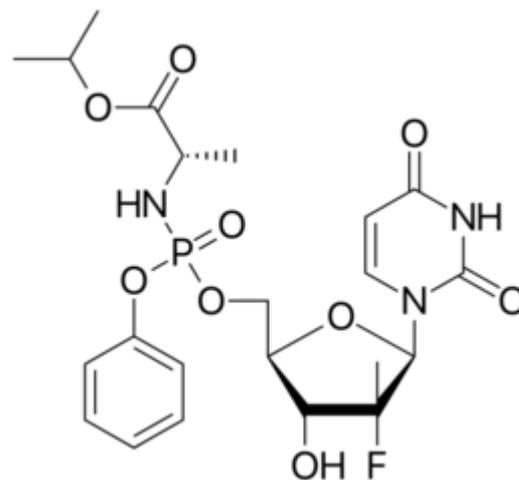
Question: 如何在PS中查找索非布韦的相关信息(合成方法、生产厂家、专利等)

产品名称: 索非布韦

英文名称: Sofosbuvir

用途: 首个无需联合干扰素就能安全有效

治疗某些类型丙肝的药物。



## Pharmaceutical Substances 检索平台-PS4.0版

Thieme Pharmaceutical Substances

Query Results About

Welcome to **Pharmaceutical Substances**

- Syntheses
- Patents
- Applications

Now with new Interface

**Search for term**

Enter search term [Search](#)

**Search for structure/reaction**

CONTACT AND SUPPORT

If you have any questions, feedback or need technical support please contact us via E-Mail.

**News**

**Pharmaceutical Substances 4.0 is online now!**  
Find industrial syntheses and commercial applications of pharmaceutical compounds even faster! This version features a new interface, improved structure searching and 20 new APIs. Enjoy!  
[Read more ...](#)

**Catalytic Transformations via C-H Activation**  
Teach yourself about this and other hot fields with Science of Synthesis! The online tool provides reliable synthetic organic transformations in context of each other and helps to speed up your research.  
[Read more ...](#)

### 解决方案:

- 主题词检索
- 结构式检索

## 检索：1.主题词检索

Thieme Pharmaceutical Substances

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Search for term

Sofosbuvir

Search

Search for structure/reaction

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> Read more ...

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> Read more ...

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1 输入主题词

2 点击Search

## 检索：1.主题词检索结果

2 Results

Sort by Title ▾

> Ledipasvir

> Sofosbuvir



结果列表

### Sofosbuvir

Synonyms: PSI-7977, GS-7977

ATC: J05AB

Use: antiviral, treatment of Hepatitis C, Nucleotide polymerase inhibitor

Chemical name: Isopropyl (2S)-2-[[[(2R,3R,4R,5R)-5-(2,4-dioxypyrimidin-1-yl)-4-fluoro-3-hydroxy-4-methyl-tetrahydrofuran-2-yl]methoxy-phenoxy-phosphoryl]amino]propanoate

Formula: C<sub>22</sub>H<sub>29</sub>FN<sub>3</sub>O<sub>9</sub>P

MW: 529.5 g/mol

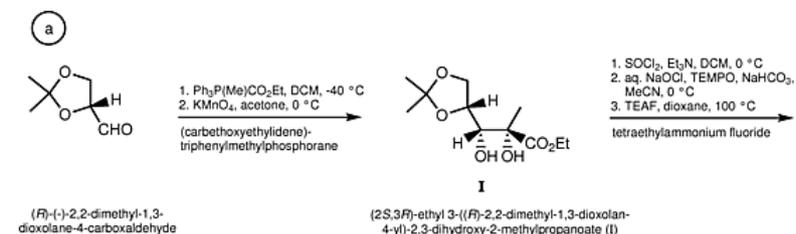
CAS-RN: 1190307-88-0

物质信息

### Substance Classes

- > Cytidines
- > Fluorine compounds

### Synthesis Path

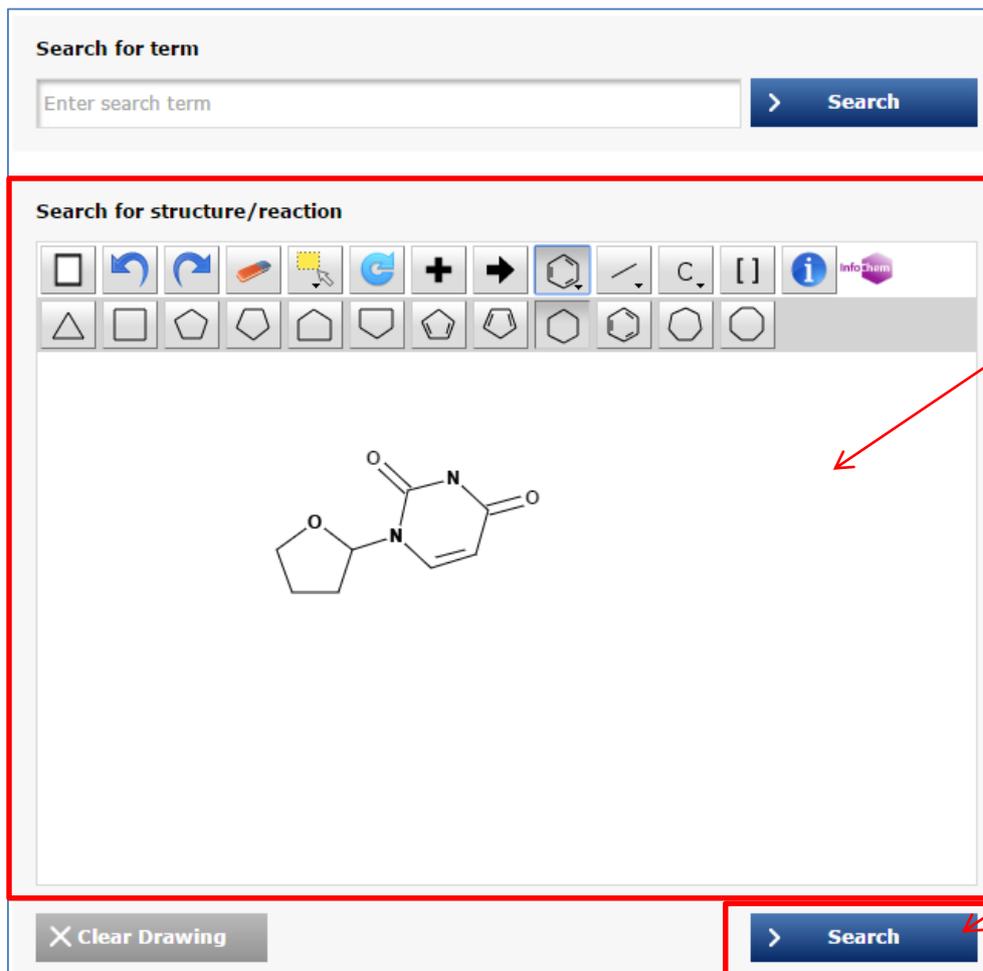


## 检索：2. 结构式检索

Search for term

Enter search term > Search

Search for structure/reaction



Clear Drawing > Search

The image shows a software interface for chemical structure search. At the top, there is a search bar labeled 'Search for term' with a 'Search' button. Below it is a section labeled 'Search for structure/reaction' which contains a toolbar with various drawing tools (like rings, lines, and atoms) and a central canvas. The canvas displays a chemical structure of a fused ring system, specifically a 2-(furan-2-yl)pyridin-4(1H)-one. At the bottom of this section, there is a 'Clear Drawing' button and a 'Search' button. Red arrows point from the text annotations to the 'Search' button in the bottom right and the toolbar area.

1 画图  
(仅需绘制  
一个简单的  
核心结构)

2 点击Search

## 检索：2. 结构式检索（可选）

1 上传结构式

Thieme Pharmaceutical Substances

Query Results About

**FUNCTIONS**

- > Upload MOL/RXN...
- > Upload CDX...
- > Reset Query

Enter your query

**Search for term**

Enter search term **> Search**

**Search for structure/reaction**

**> Search**

X Clear Drawing

2 点击Search

## 检索: 2. 结构式检索结果

[Help](#) | [About Pharmaceutical Substances](#) | [About Thieme Chemistry](#)

**Thieme** Pharmaceutical Substances

Query
Results
About

### 检索结果

14 Results

Sort by Title ▾

- › Brivudine
- › Capecitabine
- › Cytarabine
- › Doxifluridine
- › Idoxuridine
- › Nelarabine
- › Sofosbuvir
- › Sorivudine
- › Stavudine
- › Tegafur
- › Telbivudine
- › Trifluridine
- › Zalcitabine
- › Zidovudine

### Sofosbuvir

Synonyms: PSI-7977, GS-7977

ATC: J05AB

Use: antiviral, treatment of Hepatitis C, Nucleotide polymerase inhibitor

Chemical name: Isopropyl (2S)-2-[[[(2R,3R,4R,5R)-5-(2,4-dioxypyrimidin-1-yl)-4-fluoro-3-hydroxy-4-methyl-tetrahydrofuran-2-yl]methoxy-phenoxy-phosphoryl]amino]propanoate

Formula: C<sub>22</sub>H<sub>29</sub>FN<sub>3</sub>O<sub>9</sub>P

MW: 529.5 g/mol

CAS-RN: 1190307-88-0

---

Substance Classes

- › Cytidines
- › Fluorine compounds

---

Synthesis Path

CHO

1. Ph<sub>3</sub>P(Me)CO<sub>2</sub>Et, DCM, -40 °C

2. KMnO<sub>4</sub>, acetone, 0 °C

(carboxymethyldene)

1. SOCl<sub>2</sub>, Et<sub>3</sub>N, DCM, 0 °C

2. aq. NaOCl, TEMPO, NaHCO<sub>3</sub>, MeCN, 0 °C

3. TEAF, dioxane, 100 °C

(sotroathalammonium fluoride)

物质信息，包括化学信息、合成路线、商品名称、生产厂家、专利信息、文献信息.....

更多信息，请联系我们：

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