



智慧芽化学数据库快速入门指南

智慧芽化学数据库

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1. 简介

智慧芽化学数据库（Patsnap Chemical）是智慧芽旗下化学领域垂直产品，于 2017 年 3 月份正式上线。Chemical 数据库收录了超过 1 亿个有机和无机化学物质，包括小分子有机物、聚合物、盐、混合物及配位化合物等；另外还收录了近 2 万条的药品批准信息及 8 万余条临床实验数据。Chemical 数据库将上述收录数据与智慧芽的上亿条专利数据进行了打通，并提供基于化学物质与专利的可视化分析图表，为化学知识产权及研发工作提供全流程解决方案。

2. 化合物搜索

2.1 结构式绘制

利用截图中的四种方式可以在化学结构编辑框中绘制结构式。

The screenshot shows the Patsnap Chemical search interface. At the top, there is a navigation bar with icons for home, search, LabBench, and notifications. Below the navigation bar, there are four search tabs: '普通绘制界面' (General Drawing Interface), '结构式搜索' (Structure Search), '组合结构式搜索' (Advanced Structure Search), '关键词搜索' (Keyword Search), and '性质搜索' (Property Search). The '结构式搜索' tab is selected.

In the center, there is a chemical structure drawing area with a toolbar on the left containing various drawing tools like selection, zoom, and drawing primitives. A red box highlights the text '④ 导入化学结构式的其他文件数据' (Import chemical structure data from other files).

To the right of the drawing area, there is a panel for searching by name or formula. It includes a text input field '输入化学物质名称或别名' (Enter chemical substance name or alias) with a placeholder '(2) 物质名称或别名进行搜', a '上传化学结构式图片' (Upload chemical structure image) button with a placeholder '③ 上传图片', and a scrollable list of substances. The list includes OSIMERTINIB, ENTECAVIR, GEFTINIB, OSIMERTINIB, SIMVASTATIN, and ASPIRIN. There is also a '化合物预览' (Compound Preview) toggle switch and a detailed view for OSIMERTINIB.

At the bottom, there are buttons for '精确搜索' (Exact Search), '相似搜索' (Similar Search), and a more options menu.

2.2 添加搜索条件

(1) 选择专利来源及专利文献范围

chemical by patsnap 搜索 LabBench 邮件提醒

« 普通绘制界面 **结构式搜索** 组合结构式搜索 关键词搜索 性质搜索 批量搜索

选择数据库

全部数据库

欧洲专利局	WIPO/PCT	美国	中国	日本	英国
法国	德国	俄罗斯	瑞士	韩国	中国台湾
澳大利亚	加拿大	中国香港	芬兰	印度	意大利
中国澳门	荷兰	挪威	新西兰		
新加坡	DOCB				

① 化合物相关专利来源范围的选择

② 化学物质所在专利文献范围

精确搜索 相似搜索 ...

(2) 添加专利字段及检索设置

« 普通绘制界面 **专利名称/摘要/权利要求** 邮件提醒

说明书 标准化申请人 分子量 法律状态 专利信息 结构信息 药物批准信息 临床试验信息

专利名称/摘要/权利要求 AND 专利名称/摘要/权利要求 + 添加过滤条件

通过专利文献关键词及化合物信息获得更准确的搜索结果 ③

删除过滤条件 搜索全局设置

相似搜索 (Tanimoto) 0.8 每页显示数目 50

④ 设置搜索条件

精确搜索 相似搜索 ...

2.3 搜索方式

The screenshot shows the patsnap Chemical search interface. At the top, there are tabs for '普通绘制界面' (General Drawing Interface), '结构式搜索' (Structure Search), '组合结构式搜索' (Advanced Structure Search), '关键词搜索' (Keyword Search), '性质搜索' (Property Search), and '批量搜索' (Batch Search). Below the tabs is a drawing tool with various chemical structure building blocks. A chemical structure of a complex organic molecule is drawn in the center. To the right of the structure is a vertical legend for element colors: H (light blue), C (grey), N (dark blue), O (red), S (yellow), F (orange), P (purple), Cl (green), Br (brown), and I (pink). Below the drawing tool are buttons for '选中 全部 数据库' (Select All Database), '专利名称/摘要/权利要求/说明书' (Patent Name/Abstract/Claims/Specification), and '+ 添加过滤' (Add Filter). At the bottom are two search buttons: '精确搜索' (Exact Search) and '相似搜索' (Similar Search). A red box highlights the '相似搜索' button. To the right of the search buttons is a tooltip for '相似搜索' which says '搜索包含当前化合物的专利' (Search patents containing the current compound). Other numbered options shown in the tooltip are: ③ 子结构搜索 (Substructure search), ④ 超结构搜索 (Supersubstructure search), ⑤ 配方搜索 (Formula search), and ⑥ 专利搜索 (Patent search).

上述⑤和⑥是基于精确结构进行的搜索。

3. 搜索结果页及功能

3.1 结果页功能概览

The screenshot shows the patsnap search results page for the compound OSIMERTINIB. At the top, it displays the search term 'OSIMERTINIB' and various filtering options: '通过关键词、临床信息等过滤搜索结果' (Filter by keywords, clinical information, etc.), '通过结构式过滤搜索结果' (Filter by structure), '结果数目' (Number of results: 941), '邮件监控化合物' (Email monitoring compounds), '搜索结果专利分析' (Patent analysis of search results), and '修改相似度过滤搜索结果' (Modify similarity filter). Below these are detailed search filters for '全部数据库' (All databases), '全部字段' (All fields), and specific filters for 'OSIMERTINIB' such as '单一组分' (Single component: 896), '商业来源数据' (Commercial source data: 15), '包含同位素' (Contains isotopes: 7), '包含可用的批准信息' (Contains available approval information: 1), '法律状态' (Legal status), '临床研究阶段' (Clinical trial stage), '权利要求类型' (Claim type), '药物批准信息' (Drug approval information), '[已]申请(专利权)人' (Applicant/Assignee), 'ATC 代码' (ATC code), and 'IPC 分类号' (IPC classification number). On the right, detailed results for OSIMERTINIB (#1) and chemb3353412 (#2) are shown, including similarity scores, patent counts, applicants, and别名 (onyms). A sidebar lists related compounds: Targeting Amino Phenyl, OSIMERTINIB, Tumor Treating Cancer, Compounds and Salts, Diatomaceous Earth, Organic Solutions, Purification by FCC, Methanolic Ammonia, Amino pyrimidin-2-amine Intermediate 23, and Polymorphic Form. A button at the bottom right says '查看397条相关专利(100%)' (View 397 related patents (100%)).

3.2 过滤搜索结果

(1) 用结构式过滤

The screenshot shows the patsnap chemical search interface. A red box highlights the "在结果中添加结构式过滤" (Add structural filter to results) button. The left sidebar shows various filters like "单一组分" (Single component) selected, with a count of 896. The main area is titled "添加一个结构式过滤" (Add a structural filter) and features the Marvin JS interface. A tooltip says: "添加结构式，通过精确、相似搜索对搜索结果进行过滤" (Add structure, filter search results through precise and similar search). Below the Marvin JS interface are buttons for "保存" (Save) and "取消" (Cancel).

(2) 通过关键词、临床信息等过滤搜索结果

The screenshot shows the patsnap chemical search interface with a red box highlighting the "通过技术或创新关键词、临床信息、批准信息、结构式信息进行二次搜索" (Perform a secondary search using technical or innovative keywords, clinical information, approval information, and structural information) button. Step ① is indicated by a red circle around this button. Step ② is indicated by a red circle around the "AND" operator. Step ③ is indicated by a red circle around the "摘要" (Abstract) dropdown menu. Step ④ is indicated by a red circle around the "添加过滤内容" (Add filter content) button. Step ⑤ is indicated by a red circle around the "提交" (Submit) button at the bottom right. The Marvin JS interface is also visible at the bottom.

3.3 邮件监控化合物

化合物邮件监控可以跟踪化合物的专利信息、相似结构信息批准数据等数据的变化。

The screenshot shows the patsnap search results page for compound OSIMERTINIB. On the left, there is a list of results with a detailed view for OSIMERTINIB, including its chemical structure, patent count (397), and application status (Granted). On the right, a modal window titled '邮件提醒' (Email Alert) is open, allowing users to customize alert settings for this compound. The '标题' (Title) field is set to 'OSIMERTINIB 邮件提醒'. The '类型' (Type) section includes checkboxes for '全部' (All) and '选择邮件提醒内容' (Selected email alert content), which are both checked. Under '选择邮件提醒内容' (Selected email alert content), several options are listed: '新专利 (名称/摘要/权利要求)' (New patent (name/abstract/right requirements)), '新的相似化合物 (> 相似分数)' (New similar compounds (> similarity score)), '新的子结构' (New substructures), '新的超结构' (New superstructures), '批准信息更新' (Approval information update), and '临床信息更新' (Clinical information update). The '发送到' (Send to) field contains the email address 'sunxingrong@patsnap.com(我自己)'. Below this, there is a note about accepting terms of service and frequency settings ('每周' (Weekly) and '周一' (Monday)). A checkbox for '没有更新也发送提醒' (Send alerts even if no updates) is also present.

3.4 化合物检索结果导出

可将需要的化合物导出到本地。

The screenshot shows the patsnap search results page for compound OSIMERTINIB. On the left, there is a list of results with a detailed view for OSIMERTINIB. On the right, a modal window titled '导出' (Export) is open, allowing users to export the search results. The '选择搜索结果的导出范围' (Select search results export range) section has a radio button selected for '已勾选的化学结构 (1个化学结构)' (Selected chemical structures (1 chemical structure)). The '选择导出文件格式' (Select export file format) dropdown is set to 'Excel (*.xlsx)'. The '选择导出内容' (Select export content) dropdown is expanded, showing options like '物质基本信息' (Basic material information), '物质性质信息' (Material property information), '临床试验信息' (Clinical trial information), '药物批准信息' (Drug approval information), and '药物批准信息及相关文献信息' (Drug approval information and related literature information). There are also checkboxes for '包含化学结构式图片' (Include chemical structure diagrams) and '完成后邮件通知我' (Notify me after completion). At the bottom of the dialog is a large blue '导出' (Export) button.

3.5 化合物检索结果保存到 LabBench

LabBench 是 Chemical 一个线上工作空间，用户可以利用 LabBench 进行本地及线上化学物质的管理。

The screenshot shows the patsnap Chemical interface with the following steps highlighted:

- ① 点击保存到LabBench**: A tooltip points to the "保存到LabBench" button in the top right corner of the search results page.
- ② 可保存到新的文件夹或者保存到已有文件夹**: A tooltip points to the "新建LabBench" option in the save dialog.
- ③ 点击自定义保存项目 高级选项**: A tooltip points to the "高级选项" link in the save dialog.
- ④ 点击进入LabBench**: A tooltip points to the "我的LabBenches" link in the navigation bar.
- ⑤ 自己创建文件夹**: A tooltip points to the "新建LabBench" folder icon in the LabBenches list.
- ⑥ 同事分享文件夹**: A tooltip points to the "同事分享" section at the bottom of the LabBenches list.

Key visible elements include the search bar, filter options like "精确搜索" and "临床信息", and the detailed search results for compound #1: 10-(3-chloropropyl)-2-(methylsulphonyl)-10h-phenothiazine. The save dialog also shows options for selecting specific structures and saving to existing or new projects.

#	化合物名称	物质结构	分子式	分子量	专利总数	注释	别名
1	TETRAFLUOROETHYLENE		C2F4	100.016	242035		
2	LOVASTATIN		C24H36O5	404.547	97441		
3	PRAVASTATIN		C23H36O7	424.534	72946		
4	disioxane, hexamethyl-		C6H18OS2	162.379	64757		

4. 专利中化合物高亮与提取

首先在化学数据库中绘制结构式搜索，找到相应专利，再利用化学物质高亮与定位功能迅速找到专利中难以发现的化学物质信息。

4.1 化合物检索结果页跳转专利

通过技术或创新关键词、临床信息、批准信息、结构式信息进行二次搜索

共1个结果

勾选当前页

#1 10-(3-chloropropyl)-2-(methylsulphonyl)-10h-phenothiazine

专利数 8 (100%) / 8 ① 点击专利数目跳转到结果页面

申请(专利权)人: TYCHE IND S

别名 10-(3-chloropropyl)-2-(methylsulphonyl)-10h-phenothiazine | 40051-30-7 | 10-(3-chloropropyl)-2-(met)

显示全部

通过该结构式搜索

② 点击专利标题进入当前专利详情页

序号	公开(公告)号	法律状态/事件	化学结构式	标题	申请(专利权)人	发明人	申请日	公开(公告)日
<input type="checkbox"/> 1	IN201641043070A			A NOVEL PROCESS FOR THE PREPARATION OF METOPIMAZINE	SURANA COLLEGE MICRO LABS LIMITED	SAMIELSON, SAKUNTALA PIJAKKALA, JEEVITHA KESHAV, KUMAR, PRAMOD +2	2016-12-16	2017-02-03
<input checked="" type="checkbox"/> 2	CN10583752B	授权		一种2-(甲基氨基)-10H-吩噻嗪的制备方法	大连理工大学	张华, 孟海霞	2016-05-30	2018-04-27
<input checked="" type="checkbox"/> 3	IN4431CHE2014A			PROCESS FOR THE PREPARATION OF PHENOTHIAZINE DERIVATIVES	TYCHE INDUSTRIES LIMITED	NARAYANA RAO, MUTYALA, RAMADAS CHAVAKULA, VIJAYA RAJU MADDALA +1	2014-09-10	2016-07-01
<input checked="" type="checkbox"/> 4	IN567CHE2014A			IDENTIFICATION, SYNTHESIS AND STRUCTURAL STUDIES OF NEW REARRANGED IMPURITY IN METOPIMAZINE	TYCHE INDUSTRIES LIMITED	NARAYANA RAO, MUTYALA, RAMADAS CHAVAKULA, VIJAYA RAJU MADDALA +1	2014-01-28	2016-08-31
<input checked="" type="checkbox"/> 5	IN5689CHE2013A			NOVEL POLYMORPH OF METOPIMAZINE	MSN LABORATORIES PRIVATE LIMITED	SRINIVASAN, THIRUMALAI RAJAN, SAJAI ESWARIAH, MUMMADI VENKATESH +1	2013-12-10	2015-06-12
<input checked="" type="checkbox"/> 6	IN361CHE2013A			NOVEL CRYSTALLINE FROM OF AN ANTI-EMETIC DRUG	TYCHE INDUSTRIES LIMITED	NARAYANA RAO, MUTYALA, RAMADAS CHAVAKULA, VIJAYA RAJU MADDALA +1	2013-01-29	2015-02-13
<input checked="" type="checkbox"/> 7	IN360CHE2010A			PROCESS FOR THE PREPARATION OF METOPIMAZINE	MSN LABORATORIES LIMITED	MARINE, SATYANARAYANA REDDY, SAJAI ESWARIAH, KOMATI, SATYANARAYANA +1	2010-02-15	2011-08-19

4.2 从专利中提取化合物并跳转到化合物检索结果页

点击“化学”图标提取专利中的化学物质

④ 光标浮在高亮物质显示化学结构

提取化合物跳转到化合物结果页面，可进行该化合物的专利分析

(INCHI_KEY:((BQDBKDMTJBJLA-UHFFFAOYSA-N)) AND (PN:(IN201641043070A))

共1个结果

勾选当前页

#1

METOPIMAZINE

专利数 1 (1%) / 3,836

申请(专利权)人: SURANA COLLEGE

别名 METOPIMAZINE | 14008-44-7 | 14170-03-7 | exp-999 | metopimazine | vogalene | nortrip | exp 9 显示全部

通过该结构式搜索 创建邮件提醒

5. 多化学物质联合搜索

5.1 搜索两个化合物集合的交集

组合结构式搜索 关键词搜索 性质搜索 批量搜索

添加多个结构进行相似/子结构/配方搜索；或者搜索包含所添加结构的专利。

① 绘制结构式，只能绘制2个

OSIMERTINIB INDOLE

② 选择搜索方式，只支持相似、子结构和超结构

③ 点击搜索上述两个化合物相似/子结构/超结构集合中的公共化合物

精确 相似 子结构 超结构

数据库 专利名称/摘要/权利要求/说明书 + 添加过滤条件 全局设置

搜索专利 搜索配方 搜索化合物

5.2 用多个化合物搜索专利及专利中的其他化合物

组合结构式搜索 关键词搜索 性质搜索 批量搜索

添加多个结构进行相似/子结构/配方搜索；或者搜索包含所添加结构的专利。

① 绘制结构式，可绘制最多5个

GEFITINIB OSIMERTINIB

② 选择搜索方式 精确

③ 点击搜索同时包括上面化合物的专利

④ 点击搜索包括上述两个化合物专利中的其他化合物

精确 相似 子结构 超结构

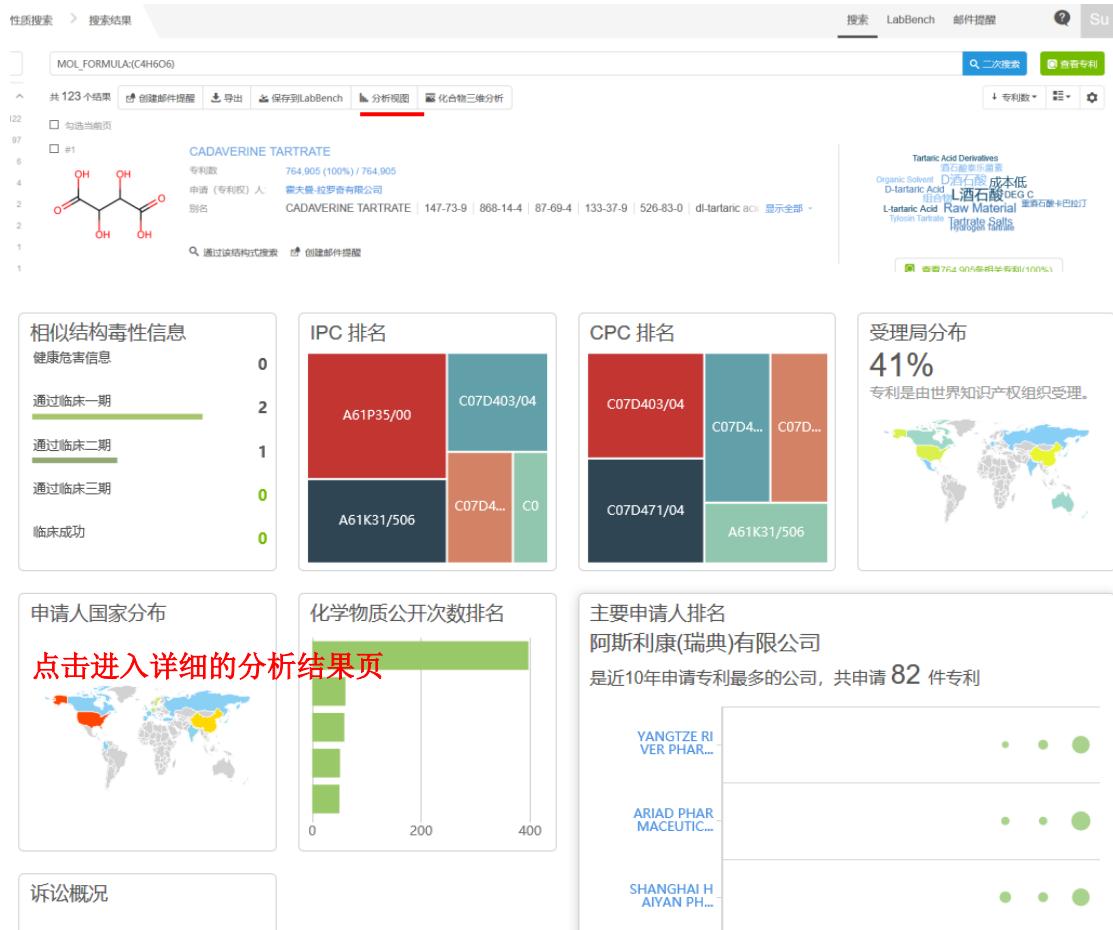
数据库 专利名称/摘要/权利要求/说明书 + 添加过滤条件 全局设置

搜索专利 搜索配方 搜索化合物

6. 搜索结果分析

6.1 化合物搜索结果关联专利分析

点击检索结果页面的分析视图进入到检索结果相关专利的可视化分析视图页面, 点击图表打开详细的分析图。



6.2 化合物地图分析



The screenshot shows the patsnap interface with several key features:

- Structural Similarity:** A color scale from yellow (Less Similar) to red (More Similar) with a midpoint at 100%. Below it are two input fields: "80" and "100" with percentage signs.
- 3D Structure Cloud:** A 3D plot where each cube represents a chemical substance. A specific cluster of cubes is highlighted in green.
- Text Labels:**
 - ② 分子量分析 (Molecular Weight Analysis)
 - ③ 专利权人分析 (Patent Holder Analysis)
 - ④ CPC分类法分析 (CPC Classification Method Analysis)
 - ⑤ CPC分类法分析 (CPC Classification Method Analysis)
 - ⑥ 化合物关联专利申请年分析 (Compound Associated Patent Application Year Analysis)
 - ⑦ 化合物关联专利申请地域分析 (Compound Associated Patent Application Geographic Analysis)
 - ⑧ 药物批准信息分析 (Drug Approval Information Analysis)
 - ⑨ 药物临床实验阶段分析 (Drug Clinical Trial Stage Analysis)
- 化合物详情:** A detailed view for OSIMERTINIB (DUYJMQNPNNNFPI-UHFFFAOYSA-N). It includes:
 - SMILES: CN1C=CC2=C1CC=C2C1C3=NC(=NC=C3)N4C=CC=C(C=C4)N5C(=O)C=C5N6C=C7C=CC=C7C=C6N
 - Trade Name: TAGRISSO
 - Molecular Formula: C28H33N7O2
 - Synonyms: Osimertinib, Tagrisso, Tagrisso (osimertinib)

7. 性质搜索

The search interface includes the following tabs:

- 搜索 (Search)
- LabBench
- 邮件提醒 (Email Reminders)
- 性质搜索 (Property Search)** (selected)
- 关键词搜索 (Keyword Search)
- 批量搜索 (Batch Search)

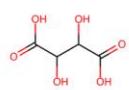
The search filters are organized into four main sections:

- ① 通过专利数据搜索化合物** (Search compounds through patent data)
 - 专利特征 (Patent Features):
 - AND: 专利名称 (Patent Name)
 - AND: 申请 (专利权) 人 (Applicant)
 - AND: 申请日 (Application Date) (from YYYYMMDD to YYYYMMDD)
 - AND: IPC 分类号 (IPC Classification Number)
- ② 通过结构特征搜索** (Search by structural features)
 - AND: 分子式 (Molecular Formula) (e.g., C4H6O6)
 - AND: 酸碱性 (Acidity/Basicity)
 - AND: 分子量 (Molecular Weight) (from to)
- ③ 通过药物批准特征搜索** (Search by drug approval features)
 - AND: USFDA 申请公司/机构 (USFDA Application Company/Institution)
 - AND: USFDA 批准日期 (Approval Date) (from YYYYMMDD to YYYYMMDD)
 - AND: USFDA 当前临床阶段 (Current Clinical Phase)
- ④ 通过药物临床试验数据搜索** (Search by drug clinical trial data)
 - AND: 主要责任人 (Principal Investigator)
 - AND: 首次收到日期 (First Received Date) (from YYYYMMDD to YYYYMMDD)
 - AND: 研究对象最小年龄 (Age of Minimum Subject) (from to)
 - AND: 临床研究阶段 (Clinical Trial Phase)

共 123 个结果 [创建邮件提醒](#) [导出](#) [保存到LabBench](#) [分析视图](#) [化合物三维分析](#)

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#1



CADAVERINE TARTRATE

专利数 764,905 (100%) / 764,905

申请 (专利权) 人: 霍夫曼-拉罗奇有限公司

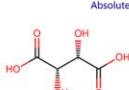
别名 CADAVERINE TARTRATE | 147-73-9 | 868-14-4 | 87-69-4 | 133-37-9 | 526-83-0 | dl-tartaric acid 显示全部 ~

[通过该结构式搜索](#) [创建邮件提醒](#)

Tartaric Acid Derivatives
酒石酸衍生物
Organic Solvent
D-tartaric Acid
L-tartaric Acid DEG C
L-tartaric Acid Raw Material
Tartaric Tartrate
Hydrogen Tartrate

[查看764,905条相关专利\(100%\)](#)

#2



Absolute TARTARIC ACID

专利数 9,383 (100%) / 9,383

申请 (专利权) 人: 默克专利股份有限公司

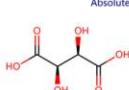
别名 TARTARIC ACID | 147-71-7 | 1150316-16-7 | e334 | tartaric acid | d-(+)-tartaric acid | d-tartaric acid 显示全部 ~

[通过该结构式搜索](#) [创建邮件提醒](#)

Pharmaceutical Compositions Containing
Salt Form Selective Crystallization
Process for Preparation
Nucleic Acid Tartaric Acid 2-thiethyl
Amine D-tartaric Acid D-酒石酸
L-tartaric Acid Novel Salts Lubricant
Crystalline Compound

[查看9,383条相关专利\(100%\)](#)

#3



Absolute TARTRATE

专利数 9,159 (100%) / 9,159

申请 (专利权) 人: 益森药业有限公司

别名 TARTRATE | 87-69-4 | 133-37-9 | 138508-61-9 | 1039646-76-8 | 1334703-49-9 | 1336-18-1 | 1- 显示全部 ~

[通过该结构式搜索](#) [创建邮件提醒](#)

Glass Composition
Oral Care Composition
膏状物 oil L-Tartaric Acid 化合物
Process for Preparation
葡萄糖 Component Tartaric Acid
Pharmaceutical Compositions Containing
个人呼吸区 Personal Breathing Zone

[查看9,159条相关专利\(100%\)](#)

通过分子式搜索可以查到化合物全部的构型与异构体，其他信息可以对检索结果进行排除。