

智慧芽化学数据（Patsnap Chemical）库简介

1. Patsnap Chemical 简介

Patsnap Chemical 是智慧芽旗下化学领域垂直产品，于 2017 年 3 月正式上线。Chemical 数据库收录了超过 1 亿个有机和无机化学物质，如小分子有机物、聚合物、盐、混合物及配位化合物等；110 万条的美国专利反应数据；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专利数据进行了关系，为化学研发提供全流程解决方案。

2. Patsnap Chemical 用户价值

- (1) 获取最新技术动态与研究机会；
- (2) 实现可专利性评估及知识产权的利用与保护；
- (3) 进行自由实施尽职调查（FTO）；
- (4) 避免专利侵权及专利无效；
- (5) 追踪竞争对手与合作伙伴；
- (6) 辅助做出正确决策。

3. Patsnap Chemical 已有功能

- (1) 化学物质搜索：
可通过图片、名称、结构（SMILES, InChI, InChI Key 等）进行精确结构、相似结构、子结构等搜索；另外也可利用分子式、理化性质等搜索；
- (2) 药物批准数据搜索：批准日期、申请机构名称、商品名、适应症等；
- (3) 药物临床试验搜索：适应症、临床研究阶段等；
- (4) 化学物质结构联合专利信息搜索, 进一步提高搜索的准确性；

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

摘要 高血压

+ 添加过滤条件

删除过滤条件

选中 全部 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

精确搜索 相似搜索

(5) 多个化学物质同时搜索，可在搜索专利中的多个化合物：

搜索 LabBench 邮件提醒

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

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。

OSIMERTINIB AND AND 点击添加结构

相似 相似

选中 全部 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) 专利中化学物质高亮与提取，更加方便快速的获取专利中的关键信息：

US20170105938A1 COMPOSITIONS AND METHODS FOR DELIVERY OF OMEPRAZOLE PLUS ACETYSALICYLIC ACID

专利详情 图文对照 引用信息 同族专利 法律信息

添加工作空间 化学

1 WO2017161301A1

4 附图

[0342] The subjects underwent the following assessments on the evening of Day 6: [0343] Vital signs (blood pressure, heart rate) [0344] Urine drug screen (including ethanol)

[0345] Day 7. Following an overnight fast and prior to receiving the Day 7 dose of study drug, the pH probe was placed to monitor intragastric pH for a period of 24 hours. In addition, a pre-dose blood sample was collected. Following study drug administration, sequential blood samples were obtained for PK assessments of omeprazole and salicylic acid/ acetylsalicylic acid at approximately 10, 20, 30 and 45 minutes and 1, 1.5, 2, 3, 3.5, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 16, 20 and 24 hours.

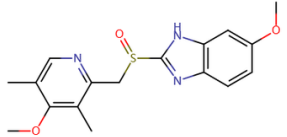
[0346] Study drug was administered to each subject as appropriate during their time in the clinic.

[0347] Day 8. In the morning of Day 8, the final blood sample was collected. Subjects also underwent assessments for AEs and the pH probe was removed. The subjects were discharged from the Phase 1 study.

[0348] For Treatment Period 2, the procedure was as follows: [0349] Washout Period. Subjects underwent a washout period to dissipate all effects of the study medication prior to the beginning of the next treatment cycle. Information regarding AEs that may have occurred during this period and the use of concomitant medications were collected and documented on the eCRFs.

[0350] Final Visit. Upon completion of the Treatment Period 2 and prior to discharge from the Phase 1 unit, the following procedures were performed: vital signs, blood draw for clinical laboratory analyses, urine collection for urinalysis, and AE and concomitant medications assessments. These procedures were also performed for any subject who discontinued early from the study.

[0351] Intragastric pH Measurement. The pharmacodynamic assessment evaluated in this study was 24-hour intragastric pH. The 24-hour pH assessments were performed on Day 7 using a Sandhill ZepHr pH data logger (Sandhill Scientific), which measured the difference in potential between the recording and reference electrodes in the tip of the probe, and stored this value every couple of seconds. A 2-point calibration of the electrode was performed using 0.1M HCl and 0.1M NaOH buffers. The distance of the electrode from the stomach wall was approximately 1 cm.



化合物名称

106 条结构式

全选

103 salicylic acid...
1 次提及
标题 / 摘要 0
权利要求 0
说明书 1

104 sulfuric acid
1 次提及
标题 / 摘要 0
权利要求 0
说明书 1

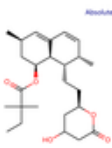
1 条已勾选

提取

https://chemical.zhiiu.com/chemical_data/detail?inchi_key=SUBDBMMJZJIVOS-UHFFFAOYSA-N / -0.05 and pH 4.00 (+/-0.05) buffers. The distance of the electrode from

(7) 化合物邮件提醒，监控化合物专利、相似结构、批准等信息变化：

邮件提醒

 **schembl14307236**

标题 * schembl14307236 Email Alert

类型 * 全部

0 updates for "schembl14307236 Email Alert trial-20180530"

Date Range: 30 May 2018—04 June 2018 [Manage my alerts](#)

Email Alert Title: schembl14307236 Email Alert trial-20180530

Identifier: RYMZZMVNJR MUDD-MAHSCPGXSA-N / 143864642

0 New patents	0 Clinical trials	0 Regulatory App	0 Similar structures
0 Substructures	0 Superstructures		

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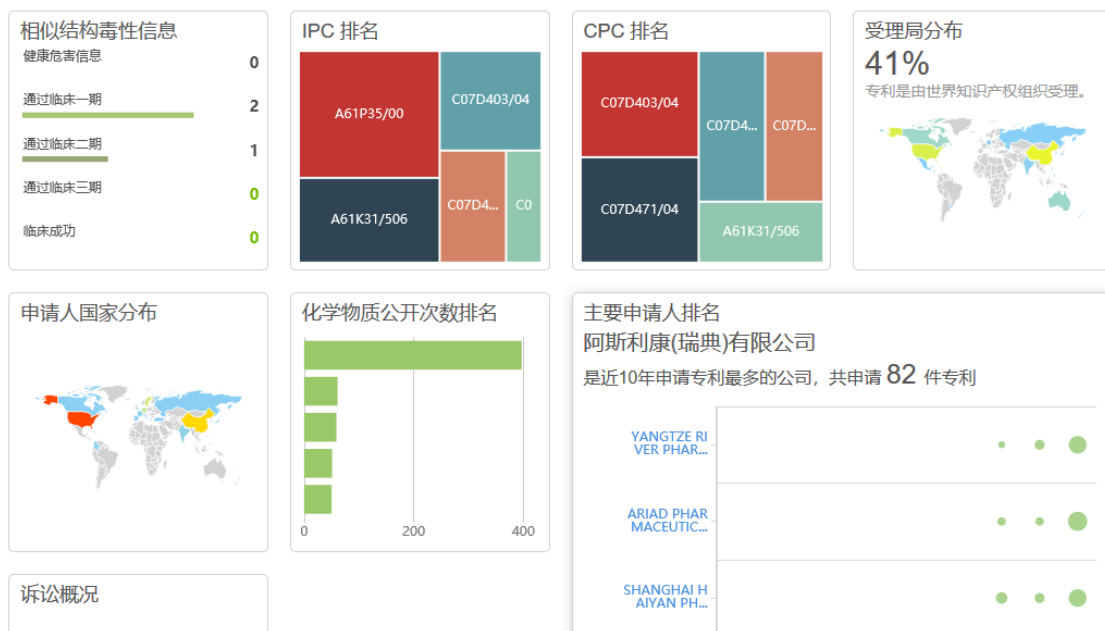
If you need help, please send to support@patSnap.com
PatSnap Chemical team

苏州工业园区百纳谱信息科技有限公司
苏州市工业园区新平街388号 腾飞创新园塔楼C9F

(8) 促进研发和专利人员高效沟通的工作空间 (labbench):

#	别名	化合物名称	物质结构	分子式	分子量	专利总数	注释	中国专利	世界知
1	SIMVASTATIN 79902-63-9 simvastatin simvastatin hydroxy acid zocor mk-733 synvinolin	SIMVASTATIN		C25H38O5	418.574	61462		439	116
2	p-toluenesulfonylsemicarbazide 10306-10-8 1-tosylsemicarbazide p-toluenesulfonyl semicarbazide benzenesulfonic acid, 4-methyl-, 2-(aminocarbonyl)hydrazide p-toluenesulfonyl semicarbazide 1-(p-methylphenylsulfonyl)semicarbazide	p-toluenesulfonylsemicarbazide		CBH11N3O3S	229.25	2970		651	290
3	schemb667703	schemb667703		CBH11N3O3S	229.25	280		3	63

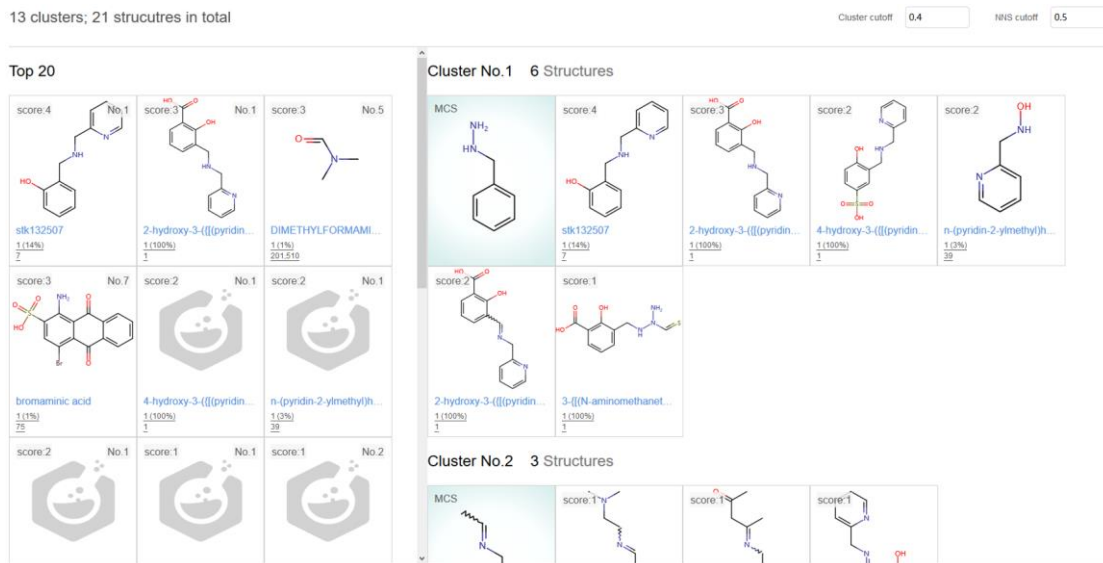
(9) 化学物质关联专利多维度分析, 实现对化合物专利的全面分析:



(10) 更直观的化学物质三维视图分析:



(11) 专利中核心化合物的提取(内侧版本已发布),对专利中的化合物进行分组、打分和排序,识别出最重要的化合物:



4. PatSnap Chemical 正在开发功能

- (1) 美国专利中聚合物 (polymer) 数据的搜索;
- (2) 美国专利中马库什 (Markush) 结构数据的搜索;
- (3) 专利中反应数据的提取与搜索。

5. PatSnap Chemical 解决方案

Chemical 数据库集成了智慧芽 1 亿余件来自全球的专利数据,用户可通过 Chemical 数据库的化学物质高亮功能迅速找到专利中难以发现的化学物质信息,从而提升工作效率。



The screenshot displays the PatSnap Chemical interface. The main content area shows a patent document with chemical structures highlighted in blue. A sidebar on the right lists search results for chemical compounds, including their names and citation counts.

Chemical Compound Search Results:

化合物名称	提及次数	标题 / 摘要	权利要求	说明书
456 条结构式				
28	14 次提及	0	0	14
29	13 次提及	0	0	13
30	11 次提及			

6. PatSnap Chemical 服务模式

Chemical 数据库以网页方式浏览，开通账号以后即可以使用检索、分析、化学物质高亮等数据与功能的使用；试用地址 <https://www.zhahuiya.com/huaxue/>。

7. PatSnap Chemical 服务案例

目前在全球共有客户 100 余家，包括拜耳化学、