

# Patsnap 智慧芽

化学专利搜索系统用户手册

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## Chapter 1

# 一/ 系统入门

1.1 系统简介

1.2 功能介绍

1.3 浏览器推荐

1.4 账号登录与登出

1.5 联系客服



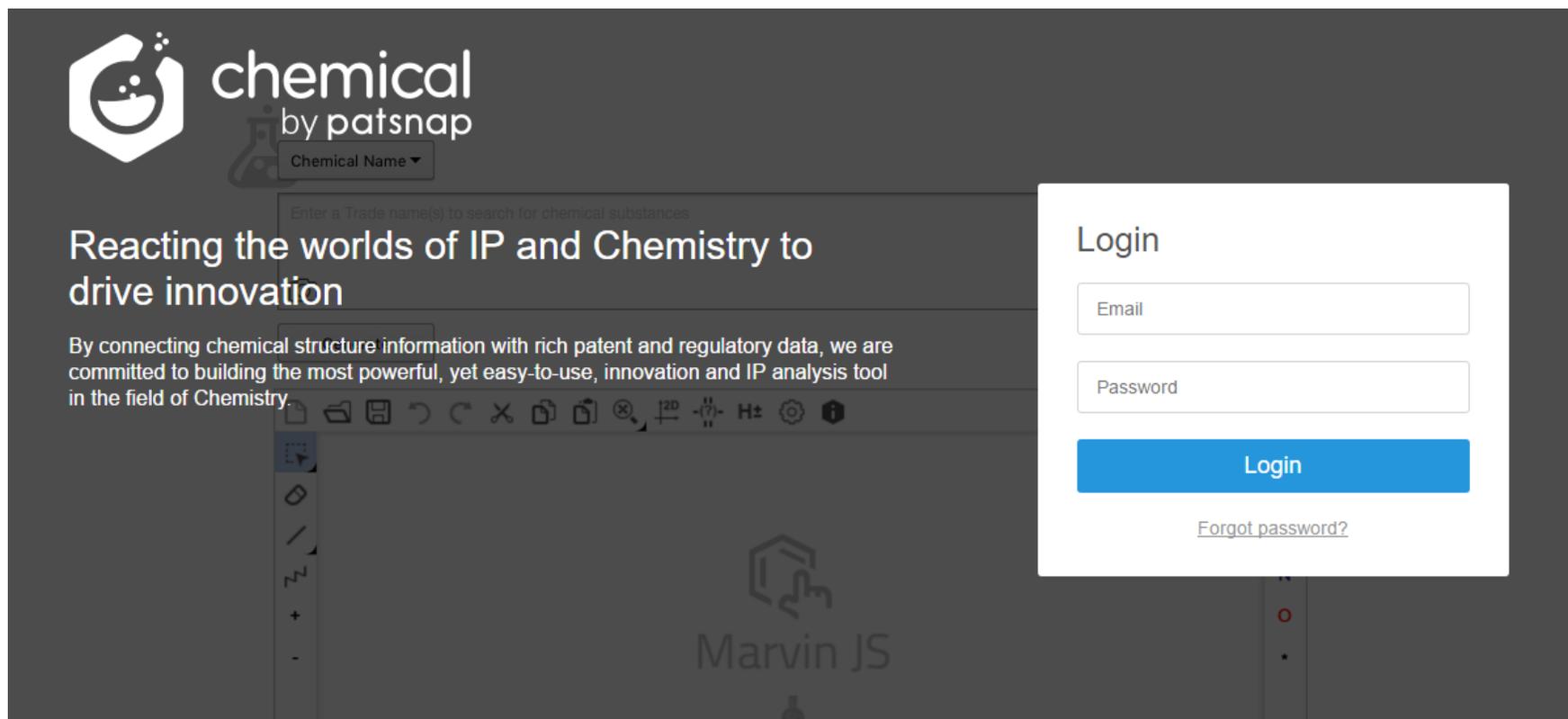
## 1.1 系统简介

- PatSnap Chemical 化学专利搜索为PatSnap旗下产品，历经多年精心打造和优化，成为众多企业、律所、代理机构、大学、政府与科研院所研发人员的推荐工具。
- 专注于基础全面的化学专利信息。数据库涵盖欧专、世界知识产权组织、美国、中国、德国、日本、台湾等7个地区或组织的全文以及100+个国家地区的摘要数据，总数超过1亿余条；支持英语全文搜索；根据用户使用习惯设计了多种搜索方式和阅读模式，新用户可以快速掌握使用方法，得心应手。
- 追求于创新，借助于图形化分析作出最佳决策。首创3D专利地图显示专利关联度分布，专利分析可以如此简单而强大；将冗长的权利要求书自动整理出每个保护点，每个关键都不会被忽略；用图片搜索专利，为费尽心思收集关键词的您擦一把汗；每个月至少有一次功能上新，我们在追求更好的路上一路奔跑。
- 更强调体验，易于上手，学习成本低。简单的功能界面配合细节设置的功能，能满足专业化的需求而不复杂；搜索结果多种图文方式呈现，贴合不同用户的习惯和需要；多处助手设置，完成一项操作无需跳转页面；零培训即能应用自如，任何疑问24小时内提供回复。
- 侧重于应用，是方便易用的协作工具。只要有网络，身处任何地方都可以随时搜索专利或查阅已保存的信息；集搜索和分析于一体，既纵览全局，预测趋势变化，又不错过细节；多种搜索途径，无论您是资深的IP工程师，还是技术控，都会找到适合自己的使用方式。

# 一/ 系统入门

## 1.2 功能介绍

- 提供四种不同的化学检索入口：结构检索入口、属性检索入口、批量检索入口、专利检索入口
- 专业的化学结构式绘制插件，自带丰富的绘制及展示小功能
- 多种不同的检索结果展示视图：标准视图、网格视图、表格视图、高级分析视图
- 高级分析视图提供多维度的数据统计和趋势分析
- 提供全文检索，基于检索结果可进行二次多级过滤
- 专利分析检索系统和三维地图分析链接跳转
- 提供邮件提醒、历史记录操作，方便用户使用



chemical  
by patSnap

Chemical Name ▾

Enter a Trade name(s) to search for chemical substances

Reacting the worlds of IP and Chemistry to drive innovation

By connecting chemical structure information with rich patent and regulatory data, we are committed to building the most powerful, yet easy-to-use, innovation and IP analysis tool in the field of Chemistry.

Marvin JS

### Login

Email

Password

Login

[Forgot password?](#)

## 1.3 浏览器推荐

支持火狐、谷歌和IE11以上版本浏览器，可保证更好的使用体验；

## 1.4 登录与登出

### 1.4.1 登陆网址：

<https://chemical.zhuhuiya.com/>（中国）；

### 1.4.2 账号登录：

- 1) 输入您的会员账号密码，即可登录系统；
- 2) 如果忘记密码，可通过“忘记密码？”设置新的密码重新登录系统；

Enter a chemical name or identifier of interest and search for it below Search

Marvin JS  
ChemAxon

All Database 🇦🇺 🇨🇦 🇨🇭 🇨🇳 🇩🇪 🇪🇺 🇫🇷 🇬🇧 🇮🇳 🇮🇹 +12 Chemical Preview

Search: Exact Structures Similar Structures Substructures Superstructures Direct to Patents ⚙️

### 1.4.3 账号登出:

如图右上角 **F** 显示当前登录用户名的大写首字母, 点击此按钮出现用户菜单, 选择点击 **Logout** 即可登出;

fangjuan  
fangjuan@patsnap.com

- Email Alerts
- History
- Logout

### 给我们留言

请输入关键字进行筛选帮助文档, 如登录、下载

下一步

云客服提供的服务

### 1.5 联系客服

点击 **?** 输入相应关键词筛选帮助文档, 解答检索中遇到困惑; 若无, 可将疑问发送到智慧芽官方邮箱, 有专门客服为您解答;

## Chapter 2

# 二/ 检索结果入口

2.1 结构检索入口

2.2 属性检索入口

2.3 InChI Keys批量检索入口

2.4 专利检索入口



## 二/ 检索结果入口

### 2.1 结构检索入口

The screenshot shows the chemical search interface with the following numbered callouts:

- 1: Top navigation menu (Structure, Properties, Bulk, Patents)
- 2: Search input field with placeholder text "Enter a chemical name or identifier of interest and search for it below"
- 3: Image upload icon
- 4: Search button
- 5: Marvin JS chemical drawing tool
- 6: Database selector (All Database)
- 7: Language selector (Australia, Canada, Switzerland, China, Germany, India, Finland, France, UK, Italy, etc.)
- 8: Exact Structures button
- 9: Similar Structures button
- 10: Substructures button
- 11: Superstructures button
- 12: Direct to Patents button
- 13: Settings icon



此页面是登录系统成功显示的首页

【1】页面上方一级菜单是化学检索的四种入口 (Structure、Properties、Bulk) 以及专利检索入口 ( Patents )

【2】文本输入框：化合物名称、分子式 等任意属性值

【3】化合物图片上传

【4】搜索按钮

【5】化学绘制插件Marvin JS

【6】数据库选择器

【7】化合物预览

【8】结构精确检索入口

【9】结构相似度检索入口

【10】子结构检索入口

【11】父结构检索入口

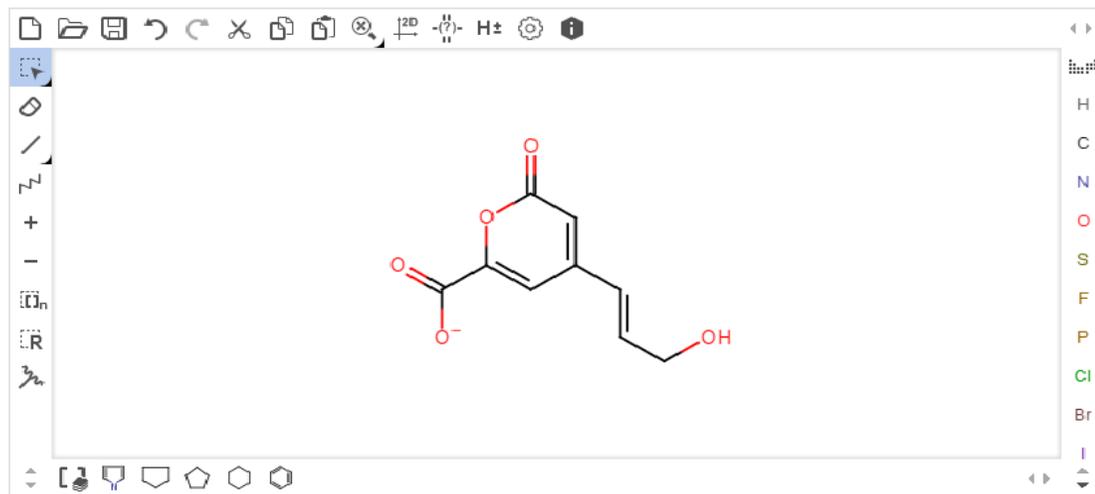
【12】专利分析检索系统入口

【13】检索相关设置



Please chose 1 from the top 5 most relevant results

Chemical Name	Chemical Formula	Synonym Name
<input type="radio"/> ALCOHOL	C2H6O	ALCOHOL; ethanol; ethyl alcohol; alcoh...
<input checked="" type="radio"/> arabidopyl alcohol	C9H7O5-	arabidopyl alcohol
<input type="radio"/> Vinyltelluro alcohol	C2H4OTe	Vinyltelluro alcohol
<input type="radio"/> (?)-Solidago alcohol	C20H30O2	(?)-Solidago alcohol
<input type="radio"/> Pentafluorophenylpentafluoroethylphos...	C8HF10OP	Pentafluorophenylpentafluoroethylphosp...



No exact match

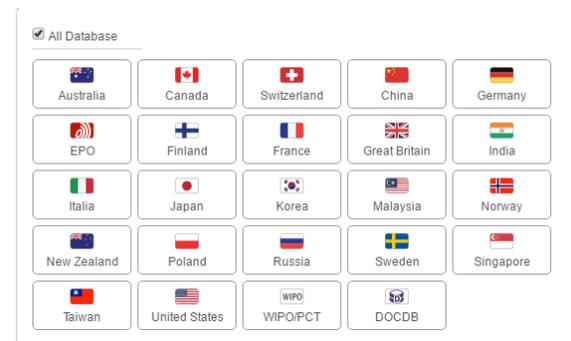
Try another search type

All Database Chemical Preview

Search:

## 2.1.1 结构精确检索

1. 这里以手动输入化合物信息为例，输入化合物的名称、分子式以及其他任一信息，例如：alcohol或C2H6O或InChI Key等，点击“Search”按钮；
2. 在显示的top5列表选取一个化合物，Marvin JS面板中实时显示选取的化合物结构式；
3. 点击“Chemical Preview”，预览化合物的信息；
4. 点击 进入全局设置，具体操作见章节3.3，这里的设置和检索结果页面的全局设置保持同步一致；
5. 点击数据库选择器“**All Database**”，选择数据库来源；



如果数据库选择其中未选择任何一个，底部五个Search入口

Search:

5. 点击检索入口，例如“Exact Structures”，以精确检索跳转至化学检索页面，也可以选择其他检索方式跳转。

6. 如图检索结果页面显示符合条件的结果；

The screenshot displays the search results for 'arabidopyl alcohol'. The main search bar contains the text 'Search through structural, regulatory and clinical trial information' and 'AND'. Below it, there is a search bar for 'Search through patent information' with a search icon. The interface includes navigation options like 'Standard', 'Grid', 'Table', and 'Analysis', along with a 'Molecular Weight' dropdown menu. A 'Select page' section shows '1-1 chemicals, 1 chemicals in total'. The search results list 'arabidopyl alcohol' with its synonyms and a 'Search with Structure' link. The chemical structure is shown in a box. The interface also features a 'Refine by' section with options like 'Single Compo...', 'Regulatory Approvals', 'Top Std. Assignees', 'CPC', and 'Molecular Weight(Da)'. A 'Refine' button is located at the bottom left. A pagination bar at the bottom center shows '<< 1 >>'. The top right corner has a 'Chemical Landscape' widget.

Enter a chemical name or identifier of interest and search for it below Search

Chemical Name	Chemical Formula	Synonym Name
TOLUENE	C7H8	TOLUENE; toluene; methylbenzene; toluol;...

All Database +12 Chemical Preview

Search: Exact Structures Similar Structures Substructures Superstructures Direct to Patents

## 2.1.2 结构相似度检索

1. 这里以手动绘制化合物为例，在Marvin JS面板中绘制化学结构式：在工具框中选择分子式点击在面板中，用线条加以连接，例如结果为甲苯C7H8；
2. 点击“Chemical Preview”，预览化合物的信息；
3. 点击检索入口，例如“Similar Structures”，以相似检索跳转至检索结果页面，例如当前的相似度为图中所示，相似度的具体设置将在章节3.3中讲述；

### Similarity Search

Tanimoto threshold

4. 如图检索结果页面显示符合条件的结果；

Search through structural, regulatory and clinical trial information AND

Search through patent information Q

Standard Grid Table Analysis Similarity Email Alert Structures to Patents Analyze Chemical Space

Select page 1-20 chemicals, 4,501 chemicals in total

**TOLUENE**  
 Synonyms: TOLUENE; toluene; methylbenzene; toluol; Benzene, methyl-; 108-88-3; Phenylmethane; methylbenzol; Toluene; methacide; anisal 1a; tolu-sol; monomethyl benzene; Methane, ph...  
**1,959,633 Refined Patents (100%)**  
**1,959,633 Total Patents**  
 Similarity Score: 1  
[Search with Structure](#)

**benzyl**  
 Synonyms: benzyl; Benzyl radical; Methyl, phenyl-; 2154-56-5; Methylphenyl-; phenyl(2H2)methyl; 2154-54-3; AC1L3VYC; DTXSID50175878  
**810,215 Refined Patents (100%)**  
**810,215 Total Patents**  
 Similarity Score: 1  
[Search with Structure](#)

Similar structures search (0.7): TOLUENE

AND Molecular Formula

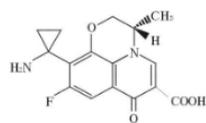
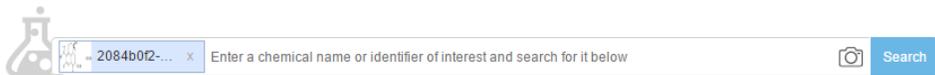
Information Refine

Refine by

- Metal-Contain... 2313
- Single Compo... 502
- Isotope-Conta... 259
- Chemical Prop... 70
- Commercially ... 20

Regulatory Approvals

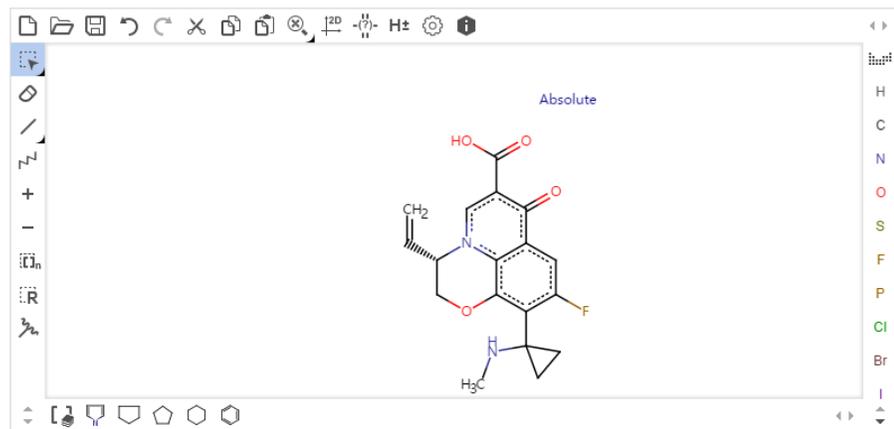
Top Std. Assignees



Chemical Image Search

Image size:  
602 x 230

· CH<sub>3</sub>SO<sub>3</sub>H



All Database +12 Chemical Preview

Search: **Exact Structures** Similar Structures Substructures Superstructures Direct to Patents

## 2.1.3 子结构检索

1. 这里以上传化合物图片为例，点击 ，从本地上传一个化合物图片 (png/jpg/...etc.)，下方显示该图片及其尺寸大小， Marvin JS面板中也该化合物结构式；
2. 点击“Chemical Preview”，预览化合物的信息；
3. 点击检索入口，例如“Substructures”，以子结构检索跳转至检索结果页面；
4. 如图检索结果页面显示符合条件的结果；

Structure Properties Bulk Patents

Search through structural, regulatory and clinical trial information AND

Search through patent information

Standard Grid Table Analysis Molecular Weight Email Alert Structures to Patents Analyze Chemical Space

Substructures search: AND Molecular Formula

Information Refine

Refine by

No results were returned

Regulatory Approvals

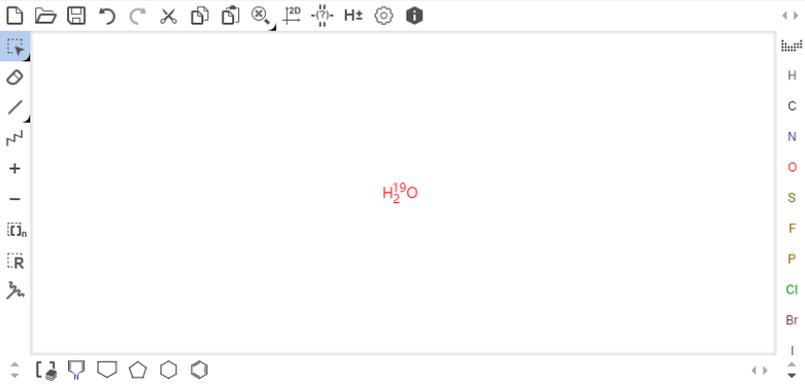
Top Std. Assignees

Hmm... we didn't find anything...  
[Try another Structure](#)

H2O 

Please chose 1 from the top 5 most relevant results

Chemical Name	Chemical Formula	Synonym Name
<input type="radio"/> oxidane	H2O	<a href="#">oxidane</a>
<input type="radio"/> AC1L3F0A	H2O	<a href="#">AC1L3F0A</a>
<input type="radio"/> ( <sup>16</sup> O)water	H2O	<a href="#">(<sup>16</sup>O)water</a>
<input type="radio"/> Water (D,T)	H2O	<a href="#">Water (D,T)</a>
<input checked="" type="radio"/> oxygen-19	H2O	<a href="#">oxygen-19; CHEBI:36933; IN010689; (1...</a>

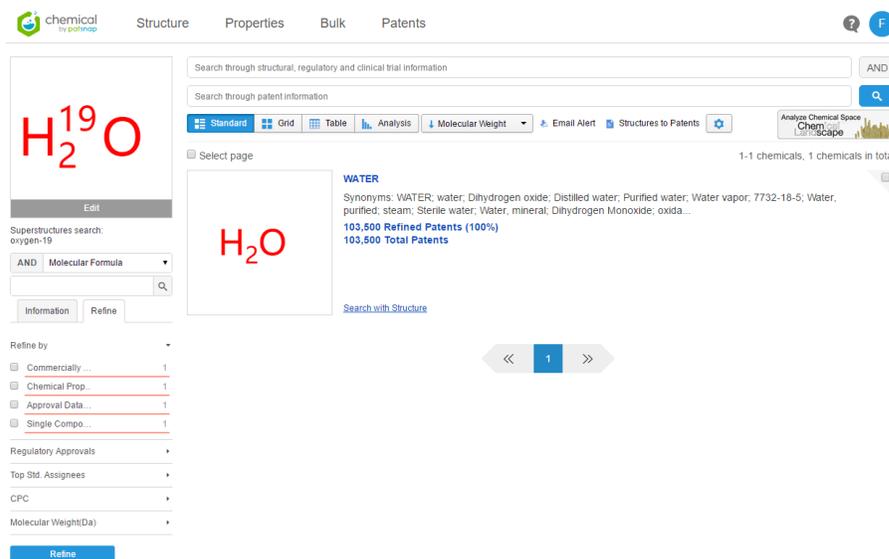


All Database 

Search:      

## 2.1.4 父结构检索

1. 这里以手动输入化合物信息为例，输入化合物的名称、分子式以及其他任一信息，例如：H2O，点击“Search”按钮；
2. 在显示的top5列表选取一个化合物，Marvin JS面板中实时显示选取的化合物结构式；
3. 点击数据库选择器“All Database”，选择数据库源为“China”；
5. 点击检索入口，例如“Superstructures”，以父结构检索跳转至化学检索页面；
6. 如图检索结果页面显示符合条件的结果；



Structure Properties Bulk Patents

Search through structural, regulatory and clinical trial information

Search through patent information

1-1 chemicals, 1 chemicals in total

Select page

**H<sub>2</sub><sup>19</sup>O**

Edit

Superstructures search: oxygen-19

AND | Molecular Formula

Information Refine

Refine by

- Commercially ... 1
- Chemical Prop... 1
- Approval Data... 1
- Single Compo... 1

Regulatory Approvals

Top Std. Assignees

CPC

Molecular Weight(Da)

**H<sub>2</sub>O**

WATER

Synonyms: WATER; water; Dihydrogen oxide; Distilled water; Purified water; Water vapor; 7732-18-5; Water, purified; steam; Sterile water; Water, mineral; Dihydrogen Monoxide; oxida...

**103,500 Refined Patents (100%)**

**103,500 Total Patents**

[Search with Structure](#)

<< 1 >>

## 二/ 检索结果入口

### 2.2 属性检索入口

The screenshot displays the search interface for chemical structures and patents. At the top, there are navigation tabs for Structure, Properties, Bulk, and Patents. The Properties tab is active, showing a list of filters: Structure Properties (Molecular Formula, Molecular Species, Molecular Weight), Patent Properties, Approval Properties, and Clinical Trial Properties. Each filter has a plus sign to expand it. Below the filters, there are buttons for 'Create New Search Query' and 'Clean'. The main search area is divided into 'Search for Chemical Structures' and 'Patent Query'. The 'Chemical Query' field contains the text 'MOL\_FORMULA:(ss)'. Below the search fields, there is a row of flags representing different databases, and a 'Search' button at the bottom. Numbered callouts (1-11) point to various UI elements: 1 points to the Structure Properties header, 2 to the Molecular Weight filter, 3 to the Patent Properties header, 4 to the Approval Properties header, 5 to the 'Create New Search Query' button, 6 to the 'Clean' button, 7 to the 'Chemical Query' input field, 8 to the 'Patent Query' input field, 9 to the database selection row, 10 to the 'Search' button, and 11 to the 'Search helper' link.

【1】 结构属性栏：属性项默认有3个

【2】 专利属性栏：属性项默认有4个

【3】 审核属性栏：属性项默认有3个

【4】 临床试验属性栏：属性项默认有4个

【5】 生成Query按钮

【6】 清除Query按钮

【7】 化合物查询条件框

【8】 专利查询条件框

【9】 数据库选择器

【10】 化学专利检索入口

【11】 搜索帮助

This screenshot shows the 'Patent Properties' section of the search interface. It features four filter items, each with a plus sign to expand it. The first item is 'Title' with a text input field. The second is 'Assignee(s)' with a text input field. The third is 'Application Date' with two date input fields separated by 'TO'. The fourth is 'IPC' with a dropdown menu.

This screenshot shows the 'Approval Properties' section of the search interface. It features three filter items, each with a plus sign to expand it. The first is 'USFDA Applicant Company' with a text input field. The second is 'USFDA Approval Date' with two date input fields separated by 'TO'. The third is 'USFDA Current Status' with a dropdown menu.

This screenshot shows the 'Approval Properties' section of the search interface, which is identical to the previous one. It features three filter items: 'USFDA Applicant Company', 'USFDA Approval Date', and 'USFDA Current Status'.

Structure Properties (1) Search helper

AND Molecular Formula

AND Molecular Species

AND Molecular Weight  TO

Patent Properties (1)

AND Title

AND Assignee(s)

AND Application Date  TO

AND IPC

Approval Properties

Clinical Trial Properties

Corporate tree allows you to select assignees based on their corporate parent and subsidiaries structure. You will have access to reliable and accurate global corporate tree data covering over 1.5 million companies.

Corporate Tree

Search for Chemical Structures

Chemical Query

MOL\_FORMULA: (H2O)

chemical by patmap Structure Properties Bulk Patents

Patent Query

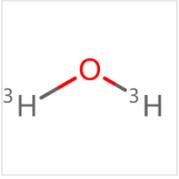
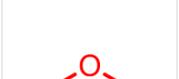
TTL: (water)

Property search

Molecular Formula

1-6 chemicals, 6 chemicals in total

Select page

	<p><b>TRITIATED WATER</b></p> <p>Synonyms: TRITIATED WATER; Tritiated water; Tritium oxide; Water, tritiated; ditritium oxide; Tritiated water (HTO); C HEBI:29374; 13670-17-2; 14940-65-9; Water, heavy; Water-t2; 3H...</p> <p><b>192 Refined Patents (8%)</b> <b>2,440 Total Patents</b></p> <p><a href="#">Search with Structure</a></p>
	<p><b>DEUTERIUM OXIDE</b></p> <p>Synonyms: DEUTERIUM OXIDE; Water-d2; Heavy water; 7789-20-0; Deuterated water; Dideuterium oxide; Heavy water-d2; Water(sup 2)-H2; Water, heavy (D2-O); UNII-J65BV539M3; Deuterium o...</p> <p><b>1,480 Refined Patents (7%)</b> <b>21,057 Total Patents</b></p>

1. 在页面上方一级菜单中点击“Properties”；
2. 在结构属性栏中输入需要检索的化合物的信息，如图C7H8，  
1) 点击  增加属性项；2) 点击  删除属性项；3) 在下拉列表框里选择合适的属性；

只要有一个属性项输入值，下方的Chemical Query文本框就能生成query，也可手动输入查询条件的query；

2. 在专利属性栏输入专利相关信息，同样可以点击  和  增删属性项；

3. 输入专利属性栏某个属性值的时候，右边提供帮助窗口快速查询，只要有一个属性项输入值，下方的Patent Query文本框就能生成query，也可手动输入查询条件的query；

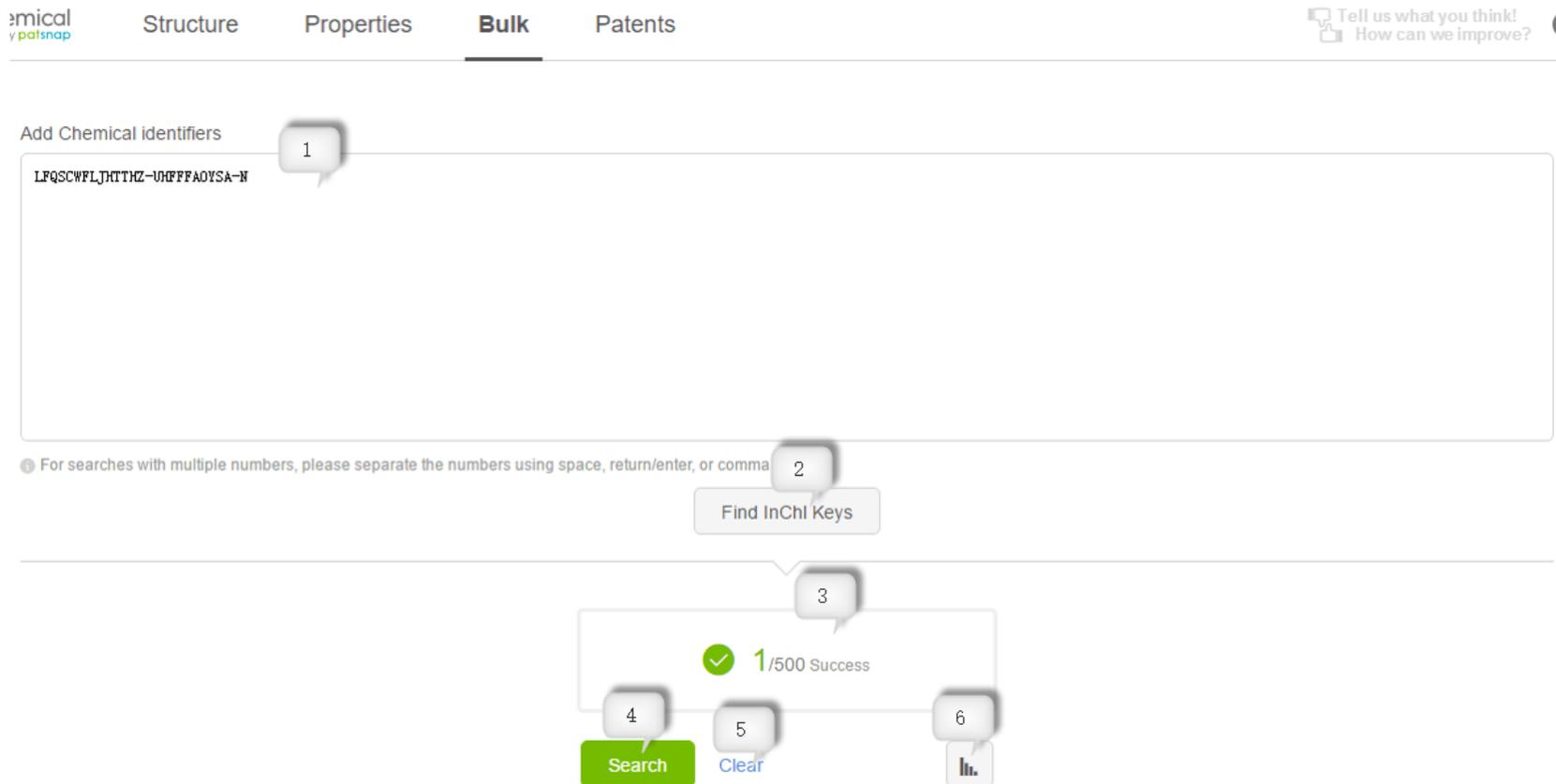
4. Chemical Query和Patent Query两个文本框中至少有一个有查询query语句，“Search”按钮即可高亮点击；

5. 点击数据库选择器“All Database”，选择数据库源；

6. 点击检索入口“Search”按钮，跳转至检索结果页面；

## 二/ 检索结果入口

### 2.3 InChI Keys批量检索入口



The screenshot shows the 'Bulk' search interface on the chemical by patSnap website. The interface includes a navigation bar with 'Structure', 'Properties', 'Bulk', and 'Patents'. A search input field contains the InChI Key 'LFQSCWFLJHTTHZ-UHFFFAOYSA-N'. Below the input field is a 'Find InChI Keys' button. At the bottom, there are 'Search' and 'Clear' buttons, and a '1/500 Success' status indicator. A bar chart icon is also visible.

Numbered callouts highlight the following features:

- 1: Add Chemical identifiers input field
- 2: Find InChI Keys button
- 3: Search results area (1/500 Success)
- 4: Search button
- 5: Clear button
- 6: Bar chart icon for advanced analysis

Additional text in the interface: "For searches with multiple numbers, please separate the numbers using space, return/enter, or comma"

【1】化合物Inchl Keys输入框：  
多个InChl Key之间以空格、逗号、回车为分隔符

【2】Find InChl Keys 查询按钮：当  
【1】为空时被置灰不能使用

【3】查询结果数统计

【4】检索结果入口

【5】清除文本框所有Inchl Keys

【6】高级分析入口

Add Chemical Identifiers

```
HUNXMJYCHXQEGX-UHFFFAOYSA-N ULGZDMOVFRHVEP-RWJQBGP  
RISDZDVHYCURHD-BFYHYZMSA-N MGSQSKXKPCMD-UHFFFAOYSA-N  
FXHGMSSSGDXY-UHFFFAOYSA-N HXVZVITUCIVKZ-UHFFFAOYSA-N  
PNIDMLOPMSWEU-ZCNSNBSA-M LFGSCWFLJHTTIZ-UHFFFAOYSA-N
```

For searches with multiple numbers, please separate the numbers using space, return/enter, or comma.

Find InChI Keys

9/500 Success

Search Clear

Imported Compounds:

HUNXMJYCHXQEGX-UHFFFAOYSA-N  
SA-N  
ULGZDMOVFRHVEP-RWJQBGP  
GSA-N  
JYIKNQVWKBUSNH-OGZDCFRISA-N  
A-N  
RISDZDVHYCURHD-BFYHYZMSA-N

Search through structural, regulatory and clinical trial information

AND

Search through patent information

Q

Standard Grid Table Analysis Molecular Weight

Email Alert

Structures to Patents

Settings

Analyze Chemical Space  
Chemical Landscape

Bulk search

AND Molecular Formula

Information Refine

Refine by

Single Compo... 9  
Commercially ... 5  
Approval Data... 5  
Chemical Prop... 4

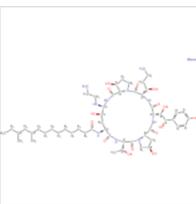
Regulatory Approvals

Top Std. Assignees

CPC

Molecular Weight (Da)

Refine

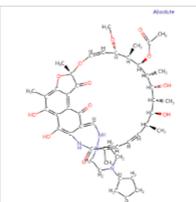


CASPOFUNGIN

Synonyms: CASPOFUNGIN; Caspofungin; Cancidas; Capsfungin; Caspofungin (INN); AC1MCVUN; CHEMB  
L499808; CHEBI:474180; AR-1K4318; LS-187303; D07626; MK-0991; SCHEMBL6726364; JYIKNQVWK...

6,259 Refined Patents (100%)  
6,259 Total Patents

Search with Structure



RIFAPENTINE

Synonyms: RIFAPENTINE; 61379-65-5; MolPort-035-395-832; HY-B0269; AC-729; AKOS015961203; CS-22  
58; BC206226

Search with Structure

1. 在页面上方一级菜单中点击“Bulk”；

2. 在Bulk文本框中输入多个InChI Key，例如图中输入了9个InChI Key；

3. 点击“Find InChI Keys”，下方显示搜索到的符合输入InChI key的结果以及条目数；

4. 点击检索入口“Search”按钮，跳转至检索结果页面；

5. 检索结果页面显示Bulk中输入的9个InChI Key关联的9个化合物信息；

6. 高级分析详见章节4；

## 二/ 检索结果入口

### 2.4 专利检索入口

1. 在页面上方一级菜单中点击“Patents”；
2. 浏览器中打开一个新的窗口跳转至专利检索页面，在字段文本框中输入检索字段如“C7H8”，点击“搜索”；
3. 在检索结果页面中选择若干专利信息，右下角出现对话框，点击“提取化学结构式”，选择要显示的字段，点击“提取”，跳转至检索结果页面，显示检索结果；

Chemical Extraction from Patents

Search through structural, regulatory and clinical trial information

Search through patent information

Extracted from: Title, Abstract, Claims, Description

Imported Patents: EP0643685B1, FR2589876A1

Select page

1-20 chemicals, 120 chemicals in total

AND Molecular Formula

Information Refine ?

Refine by

- Single Compo... 117
- Chemical Prop... 87
- Commercially ... 80
- Approval Data... 15
- Metal-Contain... 3

Regulatory Approvals

Top Std. Assignees

CPC

Molecular Weight(Da)

Refine

ALCOHOL

Synonyms: ALCOHOL; ethanol; ethyl alcohol; alcohol; Methylcarbinol; grain alcohol; Ethyl hydroxide; Ethyl hydrate; Algrain; Anhydrol; Tecsol; Alkohol; Denatured alcohol; Jaysol S; ...

3,756,904 Refined Patents (100%)

3,756,904 Total Patents

Search with Structure

Silica

Synonyms: Silica; SILICON DIOXIDE; Quartz; Cristobalite; Dioxosilane; Diatomaceous earth; Tridymite; Silicic anhydride; Diatomaceo us silica; Sand; Infusorial earth; Diatomite; Sili...

3,138,024 Refined Patents (100%)

3,138,024 Total Patents

Search with Structure

## Chapter 3

# 三/ 检索结果展示

- 3.1 检索结果页面说明
- 3.2 检索结果视图模式
- 3.3 检索结果全局设置
- 3.4 检索结果二次过滤
- 3.5 检索结果的排序及跳转专利检索
- 3.6 单个化合物信息详情



## 三/ 检索结果展示

### 3.1 检索结果页面说明

The screenshot shows the search results for Benzene on the chemical by patSnap platform. The interface includes a search bar with the query 'MOL\_FORMULA:(C6H6)', a navigation menu with 'Structure', 'Properties', 'Bulk', and 'Patents', and a results list. The results list shows three entries for Benzene, each with a chemical structure and associated patent information. Callouts 1-18 point to various UI elements: 1 (Structure), 2 (Search filters), 3 (Date range), 4 (Information), 5 (Refine), 6 (Search bar), 7 (Search through), 8 (View options), 9 (Molecular Weight), 10 (Email Alert), 11 (Structures to Patents), 12 (Settings), 13 (Chemical Space map), 14 (Compound Name), 15 (Synonyms), 16 (Patent counts), 17 (Refined Patents), 18 (Search with Structure).

此页面为检索结果的首页，文中提到的所有入口都将跳转至此页面

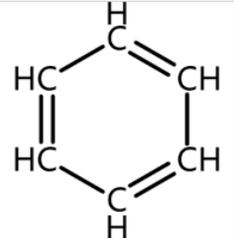
- 【1】 检索入口信息
- 【2】 自由组合逻辑运算符AND/OR/NOT
- 【3】 二次过滤设置
- 【4】 化合物信息
- 【5】 二次过滤“Refine”设置
- 【6】 二次过滤条件检索式
- 【7】 视图选项：Standard、Grid、Table
- 【8】 高级分析
- 【9】 排序选项
- 【10】 邮件提醒
- 【11】 结构专利检索入口
- 【12】 全局设置
- 【13】 三维专利地图入口
- 【14】 化合物信息-Compound Name
- 【15】 化合物信息-Synonyms
- 【16】 化合物信息-关联专利数（百分比）
- 【17】 化合物信息-专利总数
- 【18】 结构检索入口返回

## 三/ 检索结果展示

### 3.2 检索结果视图模式

Standard Grid Table Analysis Molecular Weight Email Alert Structures to Patents

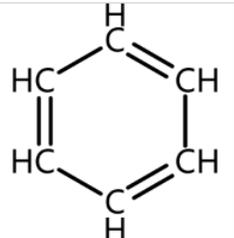
Select page 1-4 chemicals, 4 chemicals in total



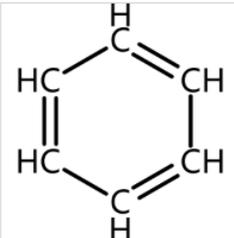
**BENZENE**  
Synonyms: BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phene; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; Be...  
**1,402,479 Refined Patents (100%)**  
**1,402,479 Total Patents**  
[Search with Structure](#)

Standard Grid Table Analysis Molecular Weight Email Alert Structures to Patents

Select page 1-4 chemicals, 4 chemicals in total



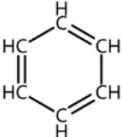
**BENZENE**  
Synonyms: BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phene; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; Be...  
**1,402,479 Refined Patents (100%)**  
**1,402,479 Total Patents**  
[Search with Structure](#)



**benzene**  
Synonyms: benzene  
**1 Refined Patents (100%)**  
**1 Total Patents**  
[Search with Structure](#)

Standard Grid Table Analysis Molecular Weight Email Alert Structures to Patents

4 result(s)

#	Chemical Name	Structure	Molecular Formula	Total Patents	US Patents	Top Assignee
1	<a href="#">BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phene; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; Benzin; Bicarburet of hydrogen;...</a>		C6H6	<a href="#">1,402,479</a>	<a href="#">383,061</a>	<a href="#">BASF</a>

#### 3.1.1 标准视图-Standard

- 在检索结果首页中点击 **Standard**，检索结果以标准视图展示：每行显示一个化合物信息，方便用户查看

#### 3.1.2 缩略视图-Grid

- 在检索结果首页中点击 **Grid**，检索结果以缩略视图展示：每行显示两个化合物信息，方便用户查看进行对比；

#### 3.1.3 表格视图-Table

- 在检索结果首页中点击 **Table**，检索结果以缩略视图展示：每行显示两个化合物信息，方便用户查看；

## 三/ 检索结果展示

### 3.3 检索结果全局设置

Preferences for displaying structure search results

Table Search Preferences

Fields Available

- Molecular Weight
- EP Patents
- WO Patents
- CN Patents

Fields Displayed 7/8

- Chemical Name
- Similarity Score
- Structure
- Molecular Formula
- Total Patents
- US Patents
- Top Standardized Assignee

Save Cancel Reset

Preferences for displaying structure search results

Table Search Preferences

Exact Search Matching

- Match with complete structural identity to query structure
- Match structural identity, but allow stereoisomers

Fuzzy Search Results

- Allow alternative atomic masses (Isotopes)
- Allow alternative atomic charges
- Allow Tautomers
- Ignore Stereo Information in Tautomer Region

Similarity Search

Tanimoto threshold 0.8

Records per page 20

Default display Standard

Save Cancel Reset

1. 在检索结果首页中，点击  进入设置对话框；
2. 对话框默认显示“Table”设置框，所有字段支持用鼠标在两个选项框中往返拖拽以及排序；
3. 左侧“Fields Available”中显示可选化合物信息字段；
4. 右侧“Fields Displayed”中显示已选化合物信息字段（最多支持8个，右上角显示其个数），其中“Fields Displayed”中的“Chemical Name”和“Similarity Score”不可用鼠标操作；
5. 点击“Save”保存设置，设置在“Table”表格视图中立即生效：检索结果表格字段及顺序与上述设置一致；
6. 对话框点击选择“Search Preferences”设置框，在此设置框中设置检索匹配：精确检索匹配方式、模糊检索结果、相似度系数、每页显示数量、默认显示视图；

## 三/ 检索结果展示

### 3.4 检索结果二次过滤

The screenshot displays the chemical search interface for Benzene. At the top, the navigation bar includes 'Structure', 'Properties', 'Bulk', and 'Patents'. The search bar contains the query: MOL\_FORMULA:(C6H6) AND MOL\_FORMULA:(C6H6) AND MOL\_FORMULA:(C6H6) AND MOL\_FORMULA:(C6H6) AND MOL\_FORMULA:(C6H6). Below the search bar, there are options for 'Standard', 'Grid', 'Table', and 'Analysis', along with a 'Molecular Weight' dropdown and 'Email Alert' and 'Structures to Patents' buttons. The search results show a single result for Benzene, with a chemical structure and a list of synonyms: BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phene; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; Be... The results also indicate 378,334 Refined Patents (27%) and 1,402,479 Total Patents. A 'Refine' sidebar on the left shows filters for 'Chemical Property Data' (CPC C07D401/14) and 'Regulatory Approvals'. The 'Refine by' section includes 'Commercially ...' (1), 'Chemical Prop...' (1), and 'Single Compo...' (1). The 'Regulatory Approvals' section includes 'CPC' (1) and 'Molecular Weight(Da)'. A 'Refine' button is at the bottom of the sidebar.

1. 以结构精确检索入口跳转到检索结果首页，可以看到左上角入口信息：结构式以及“Edit”，点击可以返回结构检索入口；
2. 在二次过滤条件中选择设置过滤条件，点击 **AND**，选择“or”、“not”逻辑词，在方框内输入想过滤出来或者过滤出去的关键词，对检索结果页面进行过滤，可以多次点击 **Q**，增加多个过滤条件；
3. 上述设置的过滤条件以检索式显示在页面上方文本框中，如图显示，上行是关于化合物的过滤条件，下行是关于专利的过滤条件，也可手动输入符合格式的检索式；
4. 在二次过滤“Refine”中设置过滤条件，设置结果显示在如图Refine框中，点击“Refine”按钮；
5. 页面按照检索式和Refine过滤条件显示符合条件的检索结果；

## 三/ 检索结果展示

### 3.5 检索结果排序及跳转专利检索

The screenshot displays the search results for Benzene on the chemical by patSnap platform. The interface includes a search bar, navigation tabs (Structure, Properties, Bulk, Patents), and a list of results. A dropdown menu for sorting is open, showing options like 'Molecular Weight', 'Compound Name', and 'Number of Patents'. A 'Structures to Patents' dialog box is open, allowing the user to select a range of records (1 to 4) for patent search. The results list shows 'BENZENE' with 1,402,479 refined patents and 1,402,479 total patents. Other results include 'benzene' with 1 refined patent and 1 total patent.

1. 鼠标移动至 **↓ Molecular Weight** ，支持的排序字段和方式如图所示；

2. 点击“Structures to Patents”，在弹出的对话框中选择化合物的范围，点击“Submit”跳转至专利检索结果首页；

Search through structural, regulatory and clinical trial information  AND

Search through patent information

Standard Grid Table Analysis Molecular Weight Email Alert Structures to Patents Analyze Chemical Space

Select page 1-4 chemicals, 4 chemicals in total

Exact structures search:  
BENZENE

AND Molecular Formula

Information Refine

Chemical Name

BENZENE

Chemical Formula

C6H6

Synonym Name

BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phene; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; B e...

InChI Key

UHOVQNZJYSORNB-UHFFFAOY S.A.N

**BENZENE**

Synonyms: BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phene; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; B e...

**1,402,479 Refined Patents (100%)**  
**1,402,479 Total Patents**

[Search with Structure](#)

**benzene**

Synonyms: benzene

**1 Refined Patents (100%)**  
**1 Total Patents**

[Search with Structure](#)

**benzene**

Synonyms: benzene

3. 也可选择某个化合物点击“Search with Structure”返回结构检索入口;

4. 选择其中若干个, 右下角弹出selected对话框, 点击“Structures to Patents”可跳转至专利检索结果首页;

patsnap INCHI\_KEY:(UHOVQNZJYSORNB-UHFFFAOYSA-N)

AND 二次搜索

1-20条专利, 共1,402,479条专利 定制完整检索语句

#	公开(公)物号	标题	公开(公)日	申请(专)利人	申请号	发明人	申请日
1	JP602014175105A1	錠剤を以てした抗酸剤を用いた胃酸抑制剤、胃酸抑制剤およびその製剤	2017-02-23	日高信康株式会社 住友薬品株式会社	JP2015513688	秋田 誠 太田 敦之 斎藤 幸也 +2	2014-04-14
2	DE3853906T2	Mehrschichtresistmaterial und Bildaufzeichnungsverfahren damit	1995-10-12	FUJITSU LTD,JP	DE3853906	KOBAYASHI KOICHI,JP OHSHIO SHUZO,JP	1988-10-28
3	DE69622571T2	ZUSAMMENSETZUNGEN UND VERFAHREN ZUR SYNTHESE VON ORGANOPHOSPHORUS DERIVATEN	2003-03-27	POLSKA AKADEMIA NAUK: CENTRUM BADAN MOLEKULARNYCH I MAKROMOLEKULARNYCH IODZ	DE69622571	STEC J WOZNIAK LUCYNA	1996-08-29
4	DE2529017A1	VERFAHREN ZUR HERSTELLUNG VON N,N'-BIS-(1-HYDROXYBUTYL)-ZL-AETHYLENDIAMIN	1976-07-08	CHINONIN GYOGYSZER-ES VEGETSZETI TERMEKEK GIARA RT	DE2529017	ECSEVY ZOLTAN HERMANN GER VOERGES JUDITH DR KOVACS GER MINDLER VERA DR +2	1975-12-29
5	EP0183448B1	Silver halide color photo-sensitive material	1991-10-23	KONICA CORPORATION	EP1985308302	NAKAYAMA NORITAKA KAWAKATSU SATOSHI KATOH KATSUNORI +1	1985-11-14
6	EP0840736A1	IMPROVED SYNTHONS FOR THE SYNTHESIS AND DEPROTECTION OF PEPTIDE NUCLEIC ACIDS UNDER MILD CONDITIONS	1998-05-13	PERSEPTIVE BIOSYSTEMS, INC.	EP19969	EGHOLM MICHAEL HODGE RICHARD P +2	
7	CH332481A	Verfahren zur Herstellung organischer Verbindungen	1958-09-15	CIBA AKTIENGESELLSCHAFT	CH332481DA	FERDINAND HUEBNER PLAHRER	1954-05-03

2 selected

Structures to Patents

unselect all

# 三/ 检索结果展示

## 3.6 单个化合物信息详情

检索结果首页中点击某个化合物进入详情页面;

UHOVQNZJYSORNB-UHFFFAOYSA-N BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phe...

Overview Reaction Data Human Approvals Clinical Trial Data Sources

[Search with structure](#) 1,402,479 Total Patents

Compound Name BENZENE

Synonyms BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phene; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; Benzene; Benzeen; More >>

Trade Names -

Molecular Formula C6H6

IUPAC Name benzene

Standard InChI Key UHOVQNZJYSORNB-UHFFFAOYSA-N

Standard InChI InChI=1S/C6H6

Canonical SMILES C1=CC=CC=C1

Isometric SMILES C1=CC=CC=C1

Polymers

[poly\(p-dichlorobenzene\)](#) 304 patents

IUPAC Source Name(s) poly(p-dichlorobenzene)

IUPAC Structure Name(s) poly(1,4-phenylene)

Other Name(s) -

Polymer Group Polyphenylenes

Polymerization Reaction Polycondensation

Monomer Reagents benzene

ChemSpider [ChemSpider:UHOVQNZJYSORNB-UHFFFAOYSA-N](#)

DailyMed [BENZENE](#)

Wikipedia [BENZENE](#)

Atlas [BENZENE](#)

BindingDB [50167939](#)

ChEBI [16716](#)

eMolecules [479848](#)

EPA CompTox Dashboard [DTXSID3039242](#)

FDA SRS [J64922108F](#)

Human Metabolome Database [HMDB01505](#)

Mcule [MCULE-4899719484](#)

Nikkaji [J2.375B](#)

NMRShiftDB [7901](#)

PubChem [241](#)

ZINC [ZINC00967532](#)

Identifiers

Cross-References

Structural Properties

Molecular Weight	78.114 g/mol
XLogP3	1.6866
Hydrogen Bond Donor Count	0
Hydrogen Bond Acceptor Count	0
Rotatable Bond Count	0
Exact Mass	78.047 g/mol
Monoisotopic Mass	78.047 g/mol
Topological Polar Surface Area	0
Heavy Atom Count	6
Formal Charge	0
Complexity	15
Isotope Atom Count	0
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Covalently-Bonded Unit Count	1
#Ro5 Violations	0
ACD LogP	2.18
ACD LogD pH7.4	2.18
QED Weighted	0.44

### 1. Overview信息:

1) Identifiers---唯一标识信息 2) Cross-References---参照信息 3) Structural Properties---结构属性;

2. 点击“Search with Structure”可返回结构检索入口;

patSnap POLYMER (P210001) fangjuan@patSnap.c...

AND 二次搜索

过滤 分析

申请人 发明人 时间分析 分类分析 国家/地区 代理机构 法律状态 自定义分析

概览

申请趋势

IPC分类排名

申请人排名

The Binding Database

3. 所有标蓝色字体提供数据来源的官方链接，如图所示：

- 1) 点击Overview-> [poly\(p-dichlorobenzene\)](#) 304 patents
- 2) 点击Cross-References-> [BindingDB](#) 50167939
- 3) 点击Cross-References-> [McuLe](#) MCULE-4899719484

myBDB login

Search and Browse

Target

Sequence

Name &

Ki IC50 Kd EC50

Rate constants

$\Delta G^\circ$   $\Delta H^\circ$   $-T\Delta S^\circ$

pH (Enzymatic Assay)

pH (ITC)

Substrate or Competitor

Compound Mol. Wt.

Chemical Structure

Pathways

Source Organism

Number of Compounds

Monomer List in csv

Het List in SDF

Compound

FDA Drugs

Important Compounds

Chemical Structure

Name

SMILES

Number of Data / Targets

Special tools

3D Structure Series

Find My Compound's Targets

Find Compounds for My Targets

Do Virtual Screening

SCOP

Citation

Author

Journal/Citation

Institution

Home Info Download About us Email us Contribute data Web Services

BDBM50167939 3,4-DNH-5-Hydroxy Tryptamine; BM 613; Benzen; Benzine; Benzol; Bicarburet of hydrogen; CHEMBL277500; Cc-34 (+/-); Coal naphtha; Mineral naphtha; Phenol; Pyrobenzol; Pyrobenzole; [6]annulene; benzene; benzole; cyclohexatriene; erythro-Phenyl-2-piperidyl-carbinol (-); phenyl hydride; trans-N, N-Dimethylphenylcyclopropylamine; trans-N-Methylphenylcyclopropylamine

InChI string: InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H

SMILES: c1ccccc1

InChI Key: InChIKey=UHOVQNZJYSORNB-UHFFFAOYSA-N

Data: 11 Ki 1 Kd

PDB links: 2 PDB IDs match this monomer.

Find this compound or compounds like it in BindingDB or PDB:

Substructure

Similarity at least: 0.85 must be >= 0.5

Exact match

Activity Spreadsheet -- Enzyme Inhibition Constant Data

Found 12 hits for monomerid = 50167939

Target (Institution)	Ligand	Target Links	Ligand Links	Trg + Lig Links	Ki nM
Thromboxane (HUMAN)	BDBM50167939			Purchase	1.40
University of Li&eagrove.ge		GoogleScholar	KEGG	Article	
Curated by PDSP K <sub>i</sub> Database	(3,4-DNH   5-Hydroxy Tryptamine   BM 613   Benzen   ...)	AfnyNet	KEGG	PubMed	
Thromboxane Alpha (HUMAN)	BDBM50167939		KEGG	Article	2.10
		GoogleScholar	KEGG	PubMed	

mcule

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MCULE-4899719484

Compound [Show structure](#)

ADD TO COLLECTION Share

InChIKey: UHOVQNZJYSORNB-UHFFFAOYSA-N

SMILES: C1C=CC=CC=C1

Formula: C6H6

Amount	Price	Purity (%)	Delivery time	
1 mg	76 USD	90	10 working days	GET QUOTE
5 mg	76 USD	90	10 working days	GET QUOTE
10 mg	119 USD	90	10 working days	GET QUOTE

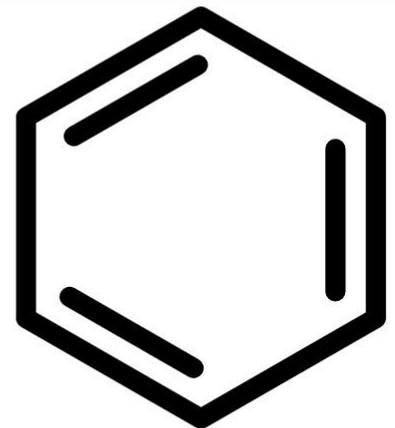
New customers are eligible for 10% discount if indicated at the time of ordering.

GET QUOTE FOR MULTIPLE COMPOUNDS GET CUSTOM QUOTE

Actions Downloads Product availability Basic properties

1-Click Docking Predict the binding orientation and affinity of the ligand to a target.

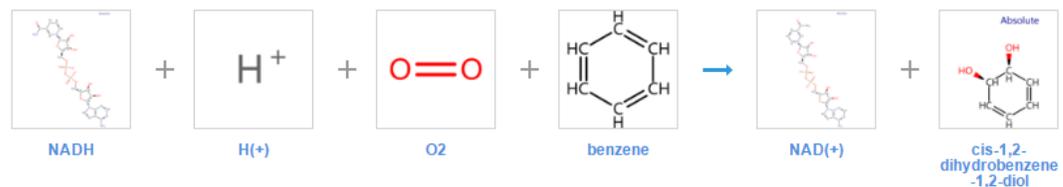
1-Click Scaffold Hop Find novel active ligands structurally different from the ligand.



UHOVQNZJYSORNB-UHFFFAOYSA-N BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phe...

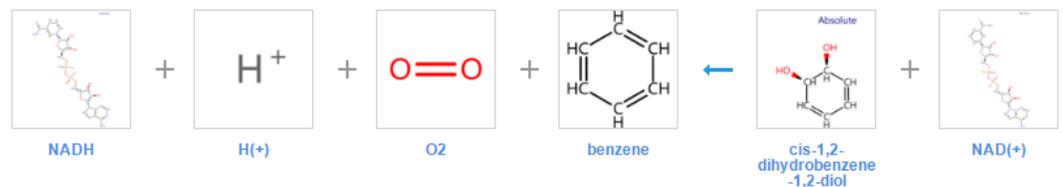
Overview **Reaction Data** Human Approvals Clinical Trial Data Sources

As Reactant (1)



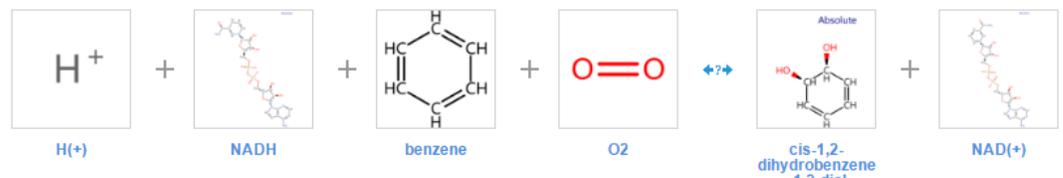
Details

As Products (1)



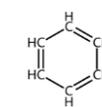
Details

Bidirectional (2)



Rhea

1. Reaction Data 分别展示前面检索的“苯环”



在化学反应中三种不同角色的反应式信息:

- 1) 作为反应物;
  - 2) 作为生成物;
  - 3) 作为双向化合物;
2. 点击任一图片可跳转至结构检索入口;
  3. 点击标蓝色的任一分子式可跳转至苯环的 Overview 信息;

chemical by patSnap

Structure Properties Bulk Patents

UHOVQNZJYSORNB-UHFFFAOYSA-N BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phe...

Overview Reaction Data **Human Approvals** Clinical Trial Data Sources

FDA (USA) EMA (Europe) CFDA (China) **ECHA REACH**

European Chemicals Agency – Registration, Evaluation, Authorisation and Restriction of Chemicals

### Benzene

GHS02: Flammable, GHS08: Serious Health Hazard, GHS07: Health hazard

Other Safety Notes

Danger! According to the harmonised classification and labelling (CLP00) approved by the European Union, this substance may be fatal if swallowed and enters airways, may cause genetic defects, may cause cancer, causes damage to organs through prolonged or repeated exposure, is a highly flammable liquid and vapour, causes serious eye irritation and causes skin irritation.

Additionally, the classification provided by companies to ECHA in REACH registrations identifies that this substance is harmful to aquatic life with long lasting effects.

#### Active Manufacturer(s)

AFKEM AG, Erdmannstr. 10 22765 Hamburg Germany

Arsol Aromatics GmbH & Co. KG, Uferstr. 105 45881 Gelsenkirchen Germany

Ashland Services BV (OR2), Pesetastraat 5 2991 XT Barendrecht Netherlands

B-Lands Consulting (8111117-5), World Trade Center, 5 Place Robert Schuman - BP1510 38025 Grenoble France France

BASF Antwerpen N.V., Haven 725, Scheldelaan 600 2040 Antwerpen 4 Antwerpen Belgium

BASF SE, Carl-Bosch-Str. 38 67056 Ludwigshafen am Rhein Rheinland-Pfalz Germany

Belgium Marketing Services N.V., Britselei 23 - box 201 2000 Antwerpen Belgi?? Belgium

Borealis AG, Wagramerstrasse 17-19 1220 Wien Austria

Borealis Polymers Oy, P.O. Box 330 06101 Porvoo Finland

BP Chemical NV/SA, Amerselbaan 2 2440 Geel Belgium

Human Approvals 展示不同国家监督管理机构的批准信息:

- 1) FDA(USA)---美国食品药品监督管理局
- 2) EMA(Europe)---欧洲药品管理局
- 3) CFDA(China)---中国食品药品监督管理局
- 4) ECHA REACH---欧洲化学品管理署REACH检测

Structure Properties Bulk Patents

UHOVQNZJYSORNB-UHFFFAOYSA-N BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phe...

Overview Reaction Data Human Approvals **Clinical Trial Data** Sources

Total (1)

Collaborators	
Brief Title	LSH Silicone Hydrogel Soft Hydrophilic Contact Lens for Daily Wear
Conditions	Myopia;
Interventions	Device: Lagado LSH (mangofilcon A) Soft (hydrophilic) Contact Lens; Device: Benz 3GX (hioxifilcon B) Soft (hydrophilic) Contact Lens;
CT.gov Identifier	NCT01735045
Study Type	Interventional
Study Phase	Phase 3
Enrollment	76
Ages	18
Gender	All

**Completed** First received 11 Jun 2012  
Last updated 25 Nov 2012

**ClinicalTrials.gov**

Try our beta test site

**IMPORTANT:** Listing of a study on this site does not reflect endorsement by the National Institutes of Health. Talk with a trusted healthcare professional before volunteering for a study. Read more...

Find Studies About Clinical Studies Submit Studies Resources About This Site

Home > Find Studies > Study Record Detail

Text Size

### LSH Silicone Hydrogel Soft Hydrophilic Contact Lens for Daily Wear

**This study has been completed.**

**Sponsor:**  
Szabocsik and Associates, Inc.

**Information provided by (Responsible Party):**  
Szabocsik and Associates, Inc.

**ClinicalTrials.gov Identifier:**  
NCT01735045  
First received: June 11, 2012  
Last updated: November 25, 2012  
Last verified: November 2012  
History of Changes

Full Text View Tabular View **No Study Results Posted** Disclaimer How to Read a Study Record

#### Purpose

This study is to evaluate the performance of the LSH (mangofilcon A) silicone hydrogel soft contact lenses when used as a daily wear contact lens for the correction of myopia.

Condition	Intervention	Phase
Myopia	Device: Lagado LSH (mangofilcon A) Soft (hydrophilic) Contact Lens Device: Benz 3GX (hioxifilcon B) Soft (hydrophilic) Contact Lens	Phase 3

Study Type: Interventional  
Study Design: Allocation: Randomized  
Intervention Model: Parallel Assignment  
Masking: Open Label  
Primary Purpose: Treatment

Official Title: LSH Silicone Hydrogel Soft Hydrophilic Contact Lens for Daily Wear

1. Clinical Trial Data 展示应用于临时试验的数据;
2. 点击标蓝色的字体 CT.gov Identifier NCT01735045可跳转至临床试验数据的来源官方链接;

Example: "Heart attack" AND "Los Angeles"

Search for studies:  Search

Advanced Search | Help | Studies by Topic | Glossary

1. Sources 展示检索化合物的食品来源以及气味;

2. 点击“Learn more at” 标金色粗体字  
可跳转至数据的来源官方链接;

Dr. Duke's Phytochemical and Ethnobotanical Databases

UHOVQNZJYSORNB-UHFFFAOYSA-N BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzene; Phenyl hydride; Pyrobenzol; Benzen; Phe...

Overview Reaction Data Human Approvals Clinical Trial Data Sources

Food Sources

Odors

### Safflower

Phytochem Chemical Name	BENZENE
Plant Part	Flower
Content Range	0.13 - 0.25 ppm
Learn more at	<b>Dr. Duke's Phytochemical and Ethnobotanical Databases</b>

### Ma Huang, Chinese Ephedra

Phytochem Chemical Name	BENZENE
Plant Part	Shoot
Learn more at	<b>Dr. Duke's Phytochemical and Ethnobotanical Databases</b>

### Lovage

Phytochem Chemical Name	BENZENE
Plant Part	Root
Learn more at	<b>Dr. Duke's Phytochemical and Ethnobotanical Databases</b>

**Dr. Duke's Phytochemical and Ethnobotanical Databases**

Search Help About Contact Us Disclaimer

Search for  in

Hint: To browse or limit your search, select an entity type from the dropdown list next to the search box. Help

49,788 entities found (Showing items 1 through 20) Click on an entity to view details

1 2 3 4 5 6 7 8 9 10 .. 2490 Next

Key: **A**=Biological Activity **C**=Chemical **E**=Ethnobotany Plant **P**=Plant **S**=Syndrome **U**=Ethnobotany Use

- P** Abelmoschus esculentus (Okra)
- P** Abelmoschus manihot (Manioc Hibiscus)
- P** Abelmoschus moschatus (Ambrette; Musk Okra; Tropical Jewel Hibiscus; Muskmallow)
- P** Abies alba (Silver-Fir)
- P** Abies balsamea (Balsam Fir)
- P** Abies sachalinensis (Japanese Fir; Shin-Yo-Yu)
- P** Abrus precatorius (Crab's Eye; Jequerity; Coral Beadplant; Indian Licorice; Licorice Vine; Love Bean; Lucky Bean; Minnie-Minnies; Prayer Be)
- P** Acacia catechu (Black Cutch; Catechu)
- P** Acacia decurrens (Green Wattle)
- P** Acacia farnesiana (Cassie; Huisache; Sweet Acacia; Opopanax; Popinac)
- P** Acacia lenticularis
- P** Acacia leucophloea (Pilang Bast)
- P** Acacia melanoxylon (Blackwood)

## Chapter 4

# 四/ 高级分析

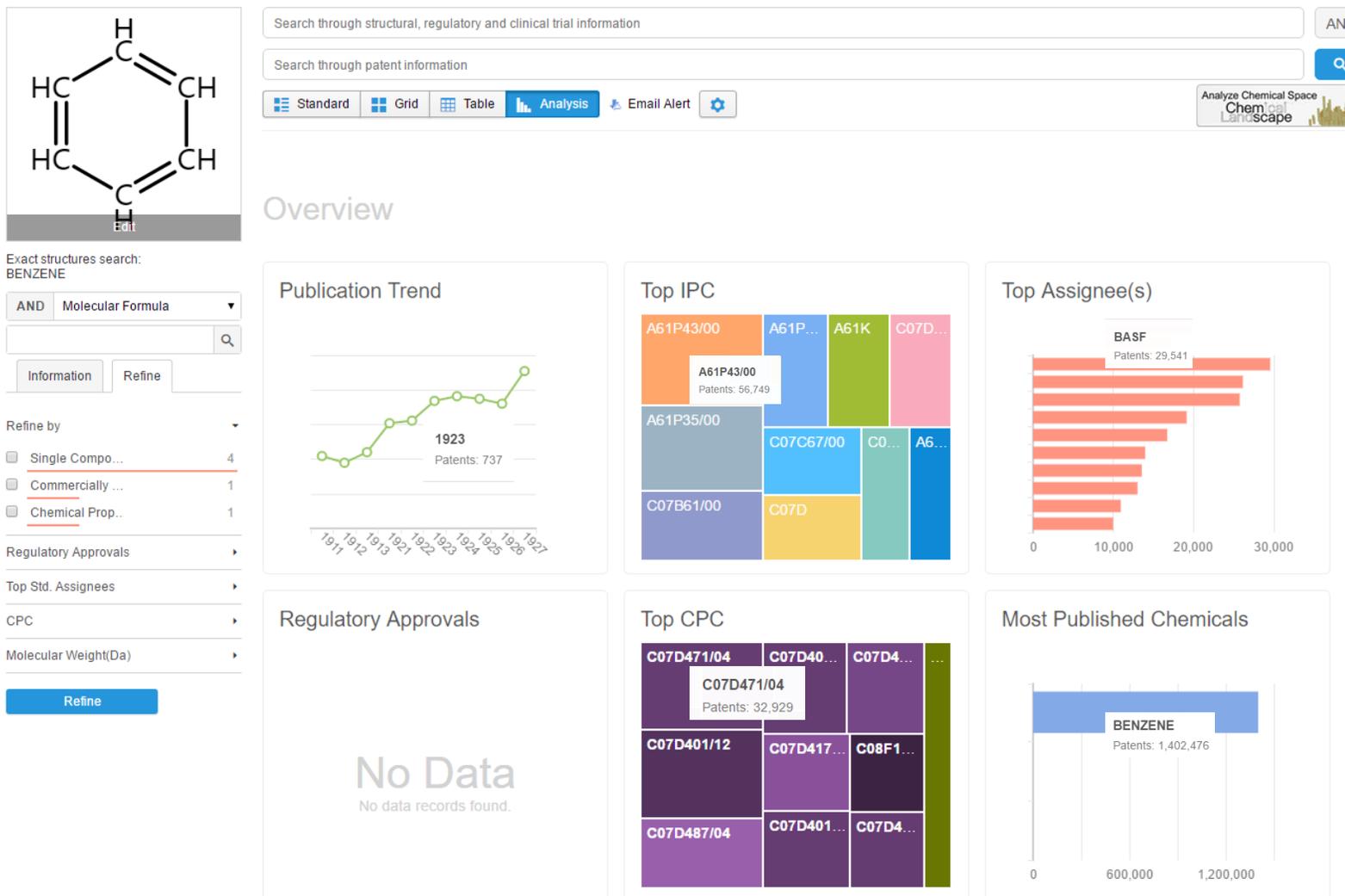
4.1 分析结果概览

4.2 分类详情



## 四/ 高级分析

### 4.1 分析概览



1. 点击 **Analysis**，进入高级分析页面，此分析为定量分析概览，主要数据来源为化合物相关的专利数据；
2. 同三种视图一样，支持左侧的二次过滤和“Refine”过滤；
3. 所有图表均以Top 10内显示数据，点击其中任一分析统计图表头，可进入详情页面；
4. 矩形图表中，矩形面积表示关联专利数量大小，面积越大表示专利数越多，点击某个图表中的最小统计单位，如坐标点、矩形图、柱形图等，可进入单个化合物的检索结果页面。

## 四/ 高级分析

### 4.2 分析详情



Publication Trend

- All
- Last 20 years
- Last 10 years

1911 To 2017

Apply

1. 点击分析图表“Publication Trend”可进入详情页面；
2. 默认时间跨度为“Last 20 years”，可自定义时间跨度查看分析图表；
3. 下方底部显示默认图表类型，如图为曲线图，可以选择其他图表类型；

Search through structural, regulatory and clinical trial information

Search through patent information

Standard Grid Table Analysis Molecular Weight Email Alert Structures to Patents Analyze Chemical Space ChemEscape

Select page 1-1 chemicals, 1 chemicals in total

Exact structures search: BENZENE

AND Molecular Formula

Information Refine

Publication Year 2003

Refine by

- Commercially ... 1
- Chemical Prop... 1
- Single Compo... 1

Regulatory Approvals

Top Std. Assignees

CPC

Molecular Weight(Da)

Refine

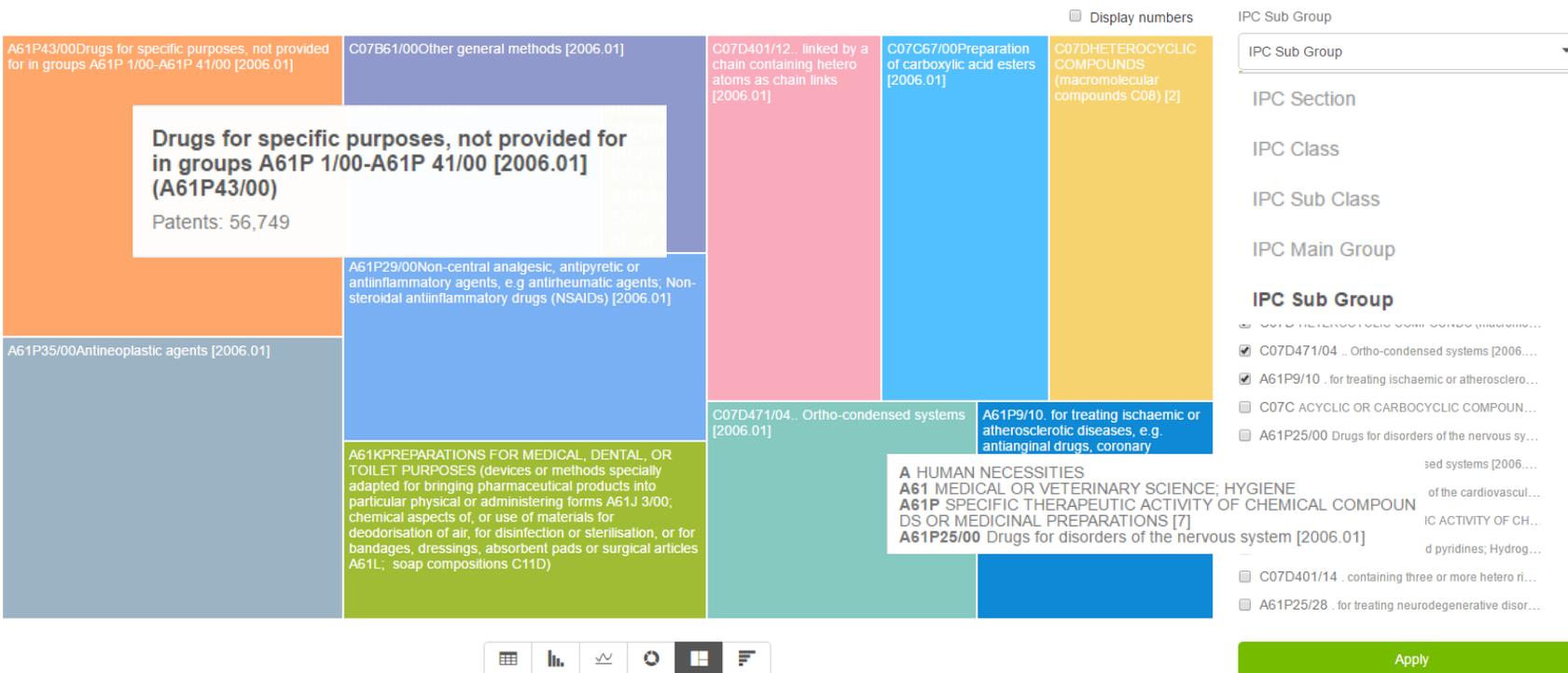
BENZENE

Synonyms: BENZENE; benzene; benzo; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phene; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; Be...

43,402 Refined Patents (3%)

1,402,476 Total Patents

Search with Structure



1. 点击分析图表“Top IPC”可进入详情页面;
2. 右侧下拉列表框中可选择IPC分类级别, 下面按级别显示该级别的具体分类;
3. 下方底部显示默认图表类型, 如图为矩形图, 可以选择其他图表类型;

Search through structural, regulatory and clinical information

Search through patent information

Standard | OK | Table | Analysis | Molecular Weight | Email Alert | Structures to Patents

Select page

Exact structures search: BENZENE

AND | Molecular Formula

Information | Refine

Refine by

- Commercially 1
- Chemical Prop. 1
- Single Compo. 1
- Regulatory Approvals
- Top IRL Assignees
- CPC
- Molecular Weight(Dal)

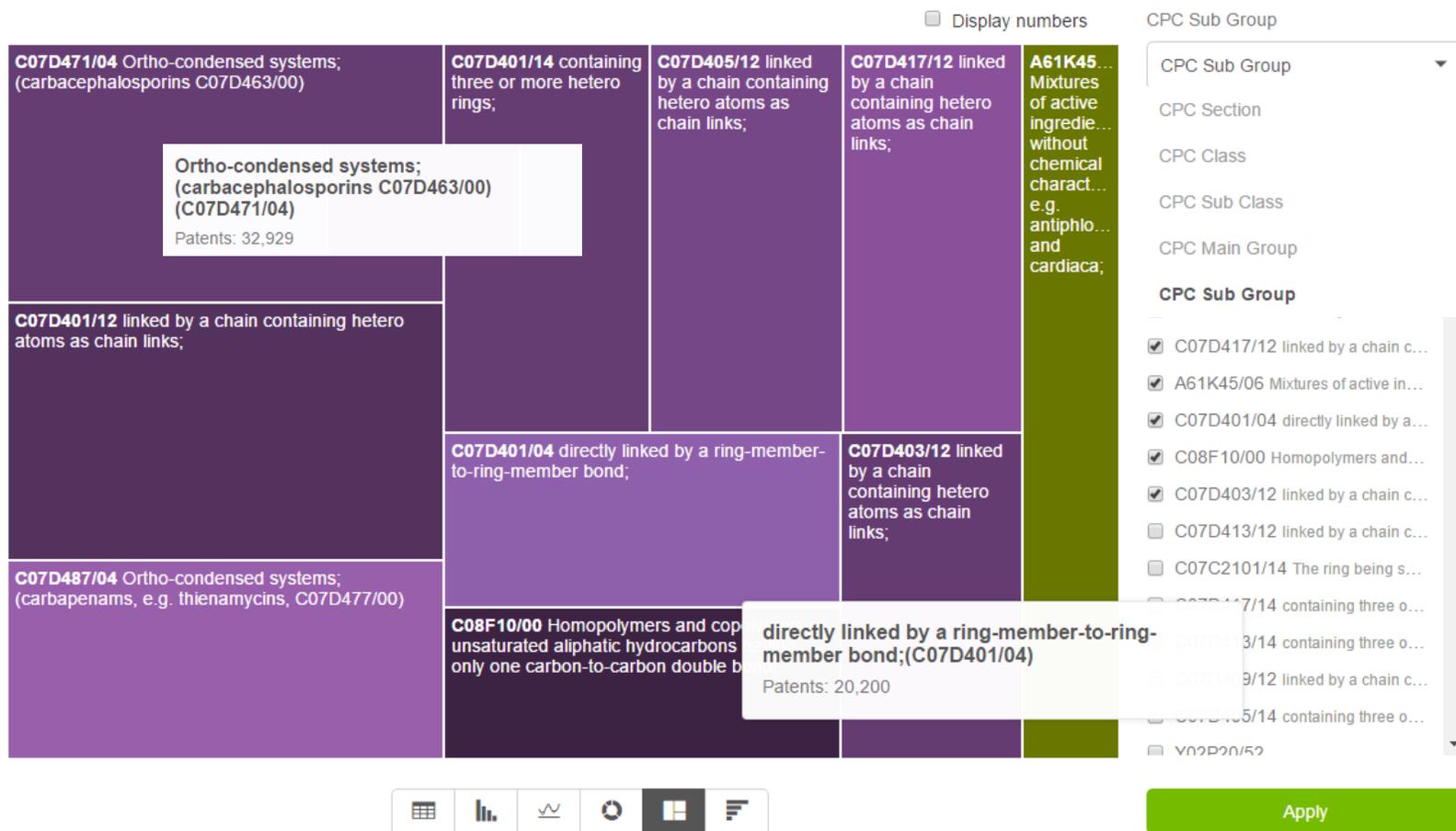
Refine

1-1 chemicals, 1 chemicals in total

**BENZENE**  
Synonyms: BENZENE; benzene; benzol; benzole; Cyclohexatriene; Pyrobenzole; Benzine; Phenyl hydride; Pyrobenzol; Benzen; Phenol; Mineral naphtha; Coal naphtha; 71-43-2; Benzolene; Be...  
56,749 Refined Patents (4%)  
1,462,474 Total Patents

Search with Structures

# Top CPC



1. 点击分析图表“Top CPC”可进入详情页面;
2. 右侧下拉列表框中可选择CPC分类级别, 下面按级别显示该级别的具体分类;
3. 下方底部显示默认图表类型, 如图为矩形图, 可以选择其他图表类型;



1. 点击分析图表 “Most Published Chemicals” 可进入详情页面;
2. 右侧选项可选择要显示的化合物;
3. 下方底部显示默认图表类型, 如图为横向柱形图, 可以选择其他图表类型;

## Chapter 5

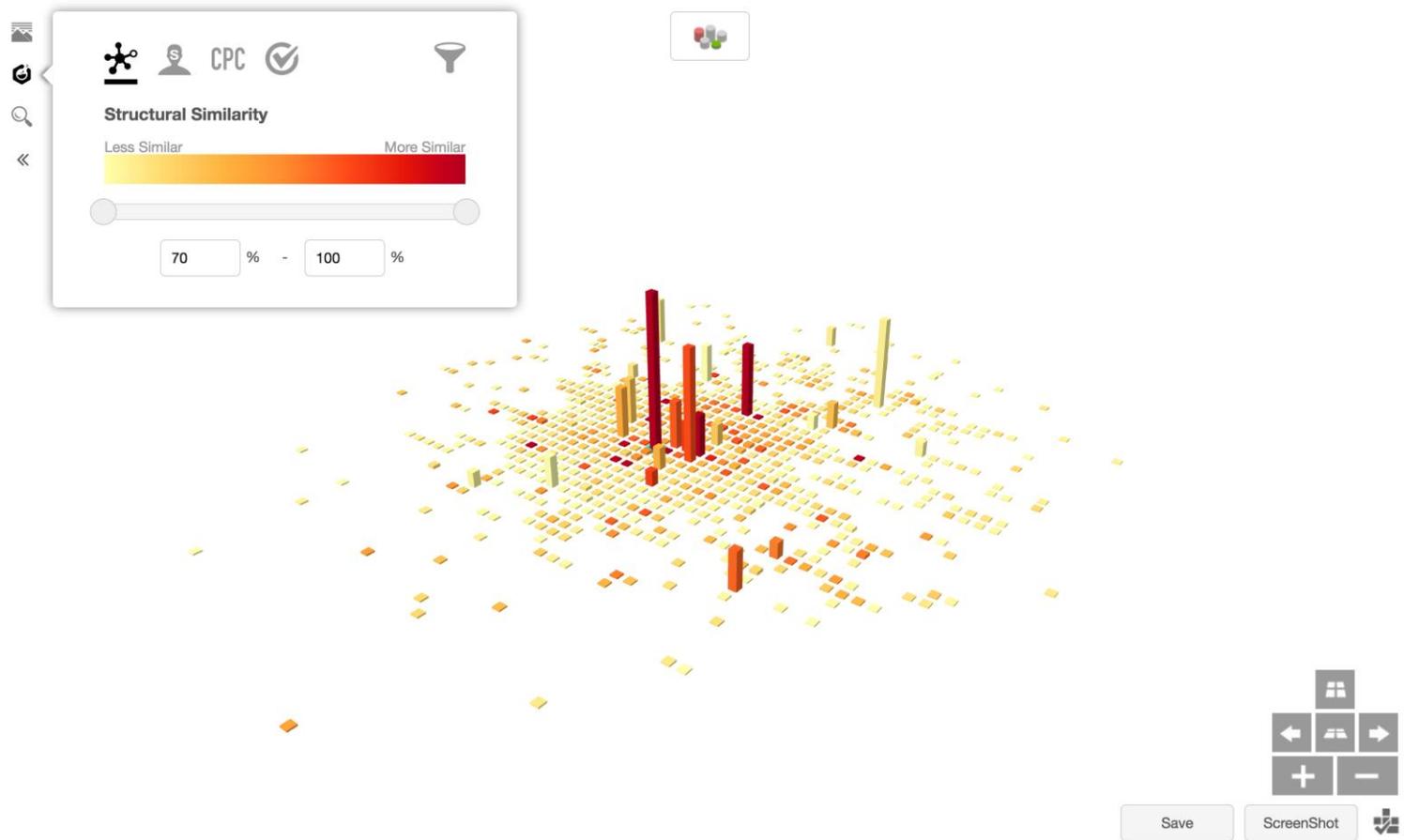
# 五/ 三维化学地图

- 5.1 生成三维化学地图
- 5.2 在三维化学地图中过滤
- 5.3 在三维化学地图中搜索
- 5.4 保存及恢复三维化学地图



## 五/ 三维专利地图

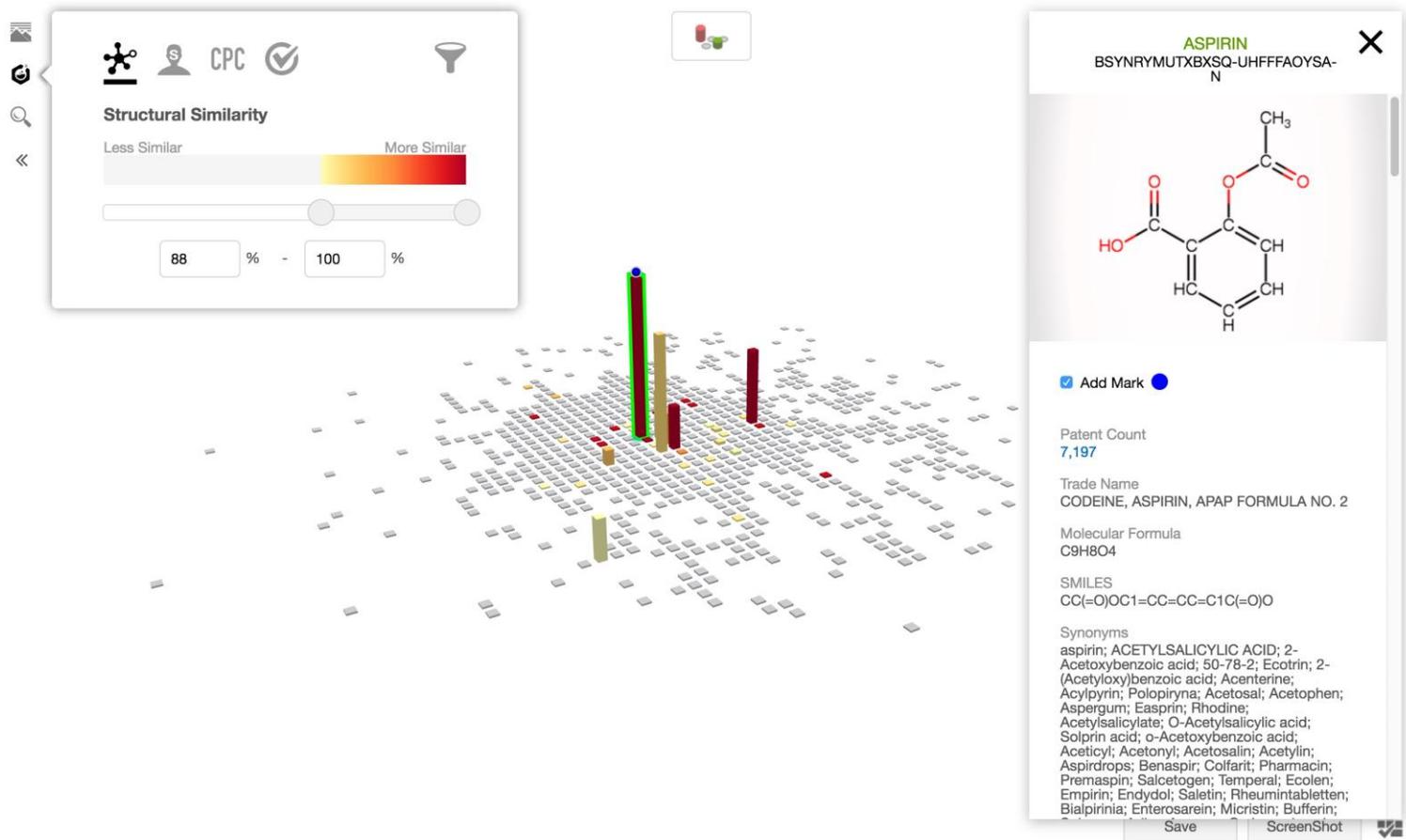
### 5.1 生成三维化学地图



1. 在“Structure”入口中输入化合物名称，例如：simvastatin，选择一种搜索方式后跳转至检索结果页面；
2. 在检索结果页面点击 ，进入三维化学地图页面；
3. 等待分析完毕，分析结果显示出来。
4. 用户可以使用鼠标左右拖动，缩放三维化学地图。也可以使用右下角的控制方向面板进行操作。
5. 上方中央的  图标提供了几种显示方式，用户可以按自己的需求切换成自己喜欢的方式。

## 五/ 三维专利地图

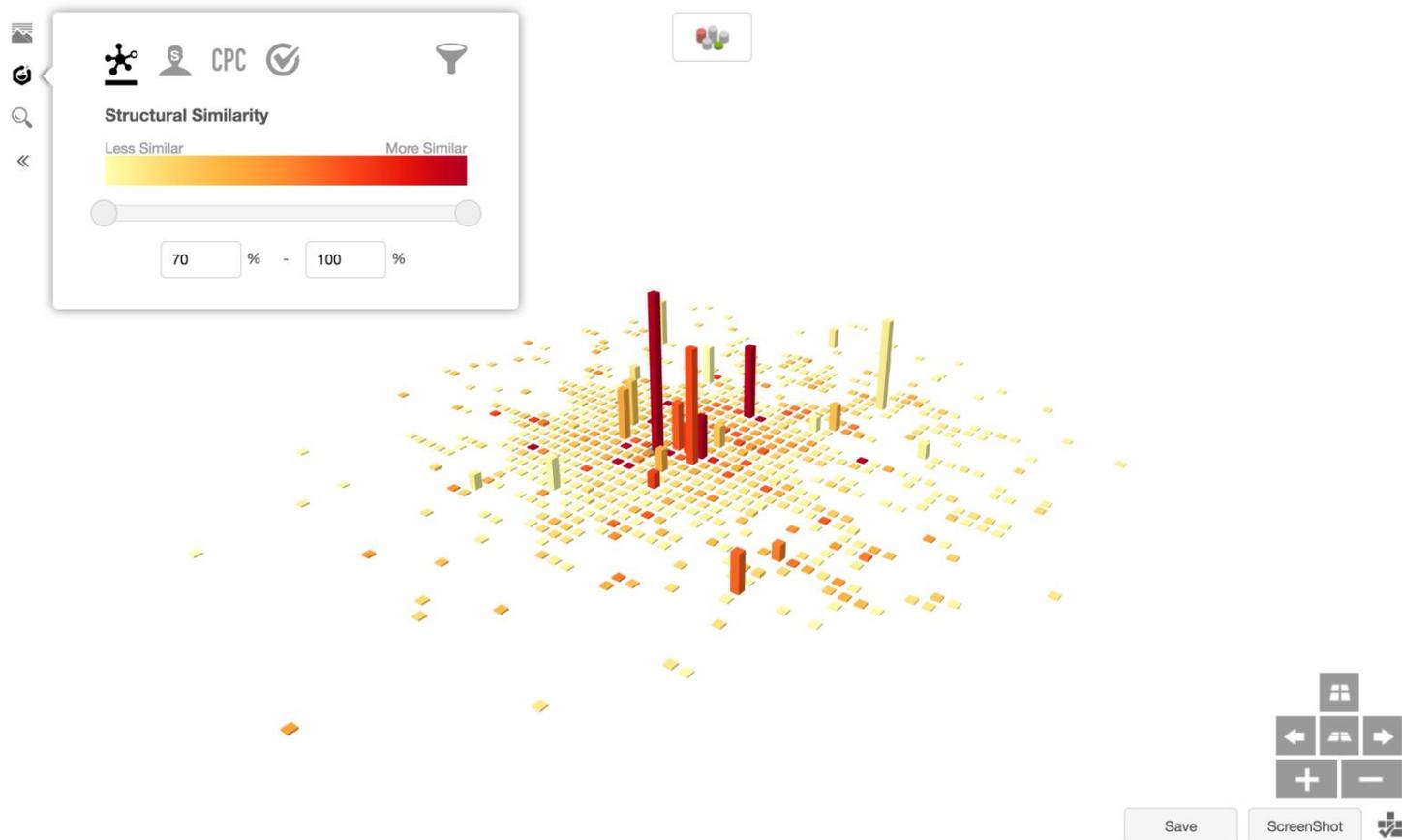
### 5.1 生成三维化学地图



1. 点击图中的每一个化学结构式可以查看该化学式的详细信息。
2. 在化学式详情面板用户可以勾选“Add Mark”给当前选中的化学结构式加上标记。
3. 点击“Patent Count”下面的数字链接，可以在智慧芽专利数据库中查看含有该化学结构式的相关专利。

## 五/ 三维化学地图

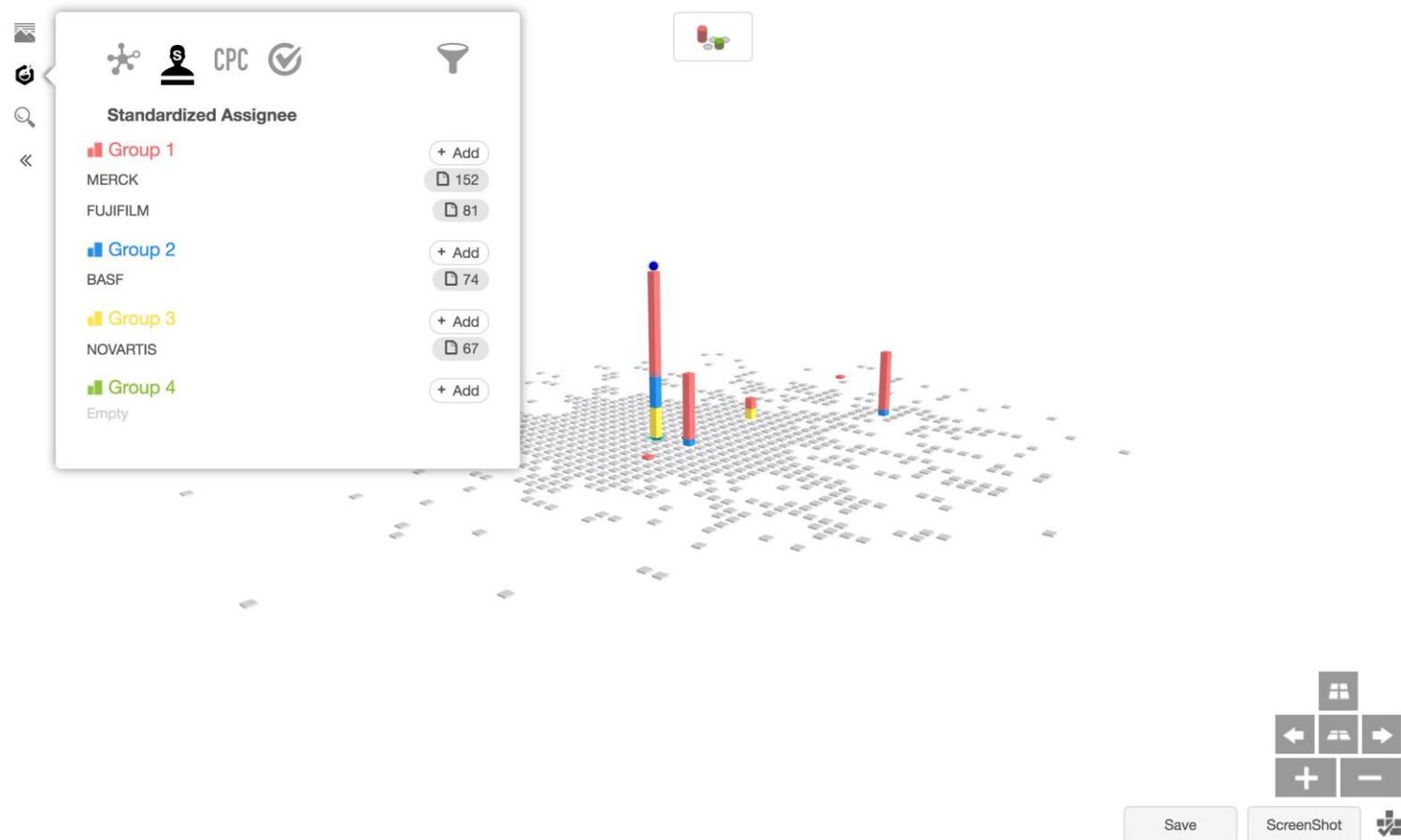
### 5.2 在三维化学地图中过滤



1. 三维化学地图提供了多种按化学式或相应专利属性进行过滤的功能，点击左侧  可以进入过滤功能面板。
2. 从左至右的过滤功能依次为：“结构式相似度”，“专利标准化申请人”，“专利联合分类号”和“药监局审核”过滤功能。
3. 最右侧的  提供了一个全局的按化学式对应的专利条目数过滤功能。

## 五/ 三维化学地图

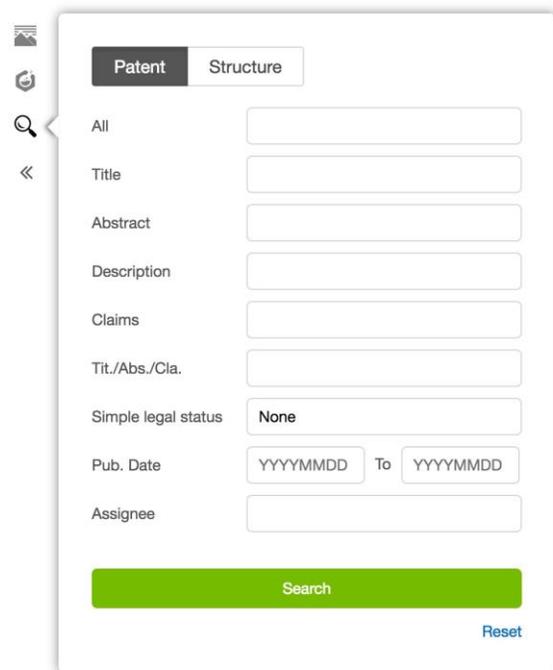
### 5.2 在三维化学地图中过滤



1. “专利标准化申请人”和“专利联合分类号”过滤功能允许用户将不同的申请人或分类号添加到预定义的分组中。分组的颜色将也会被标在相应的化学结构上对应的柱子上；
2. 当不同组内的数据对应相同的化学结构式时，柱子会按专利数量的比例染成多段颜色。

## 五/ 三维化学地图

### 5.3 在三维化学地图中搜索



Patent Structure

All

Title

Abstract

Description

Claims

Tit./Abs./Cla.

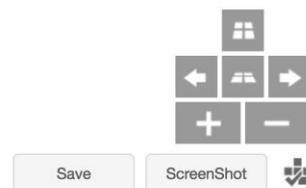
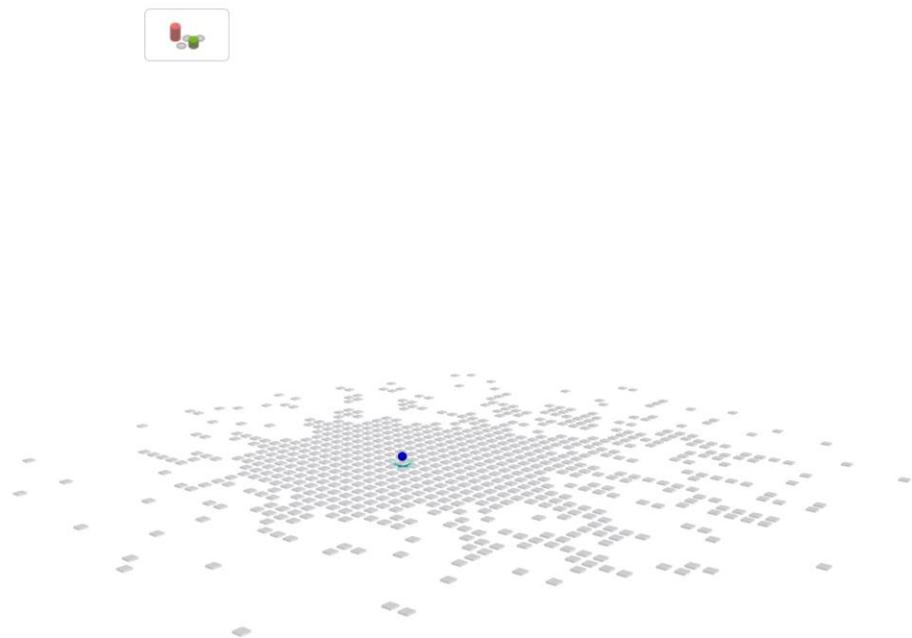
Simple legal status

Pub. Date  To

Assignee

Search

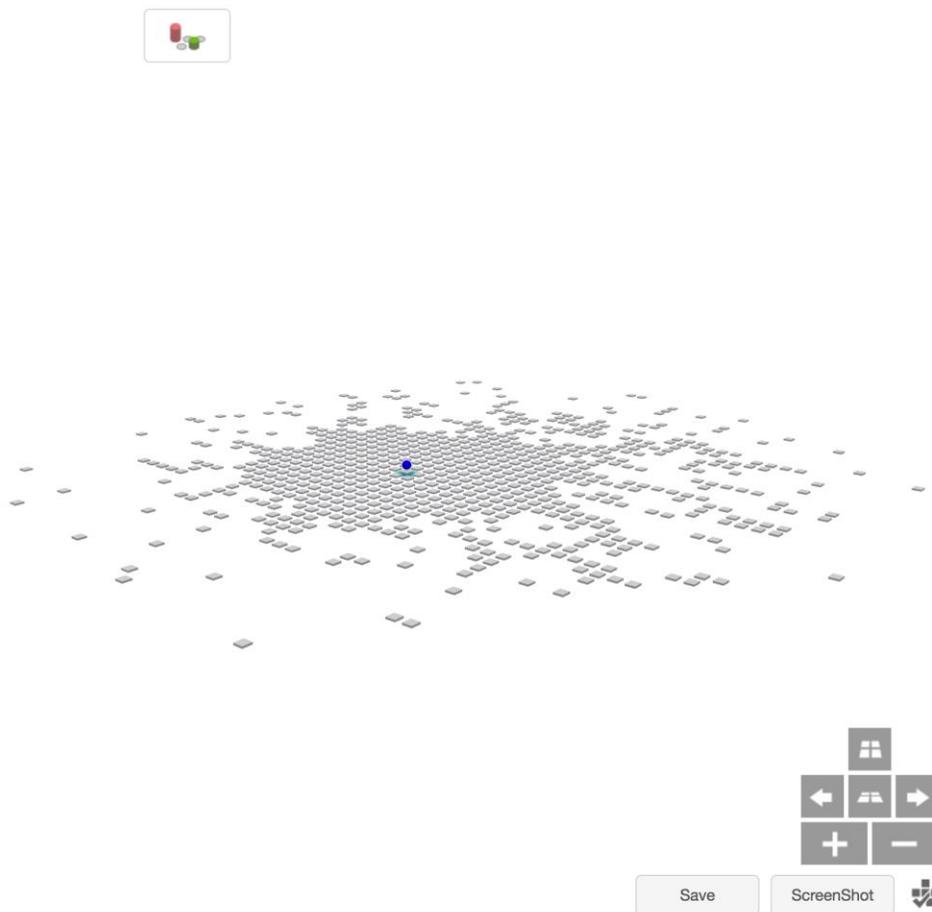
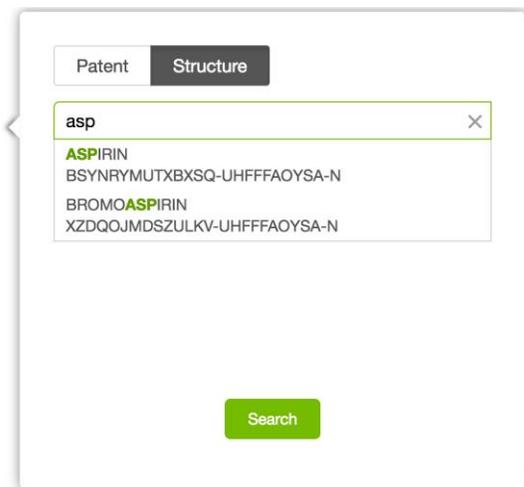
Reset



1. 三维化学地图提供了两种搜索方式，分别是“按专利字段搜索结构式”和“按结构式名称搜索结构式”；
2. 使用专利字段检索时，用户在希望搜索的字段输入框中填上期望搜索的内容，点击搜索按钮进行搜索；
3. 如果有匹配的结构式，相应的结构式会在地图上被高亮标示出来；

## 五/ 三维化学地图

### 5.3 在三维化学地图中搜索



1. 用户点击“Structure”标签页可以切换到按化学式名称精确搜索功能；
2. 可以根据用户的输入提示在当前分析中存在的化学结构式；
3. 用户点击名称后，相应的结构式就会在三维地图上高亮显示出来；

## 五/ 三维化学地图

### 5.4 保存及恢复三维化学地图



1. 在三维化学地图上，点击左下角的Save按钮，输入标题和描述，就可以将当前的分析结果保存下来；
2. 点击左边栏的  图标可以进入我的化学地图页面，可以查看和搜索过往保存过的化学地图；
3. 点击任何一个地图可以恢复之前的分析结果；
4. 鼠标移至地图上，点击出现的  按钮，再选择  ，可以删除该条已保存的记录；

## Chapter 6

# 六/ 用户中心

6.1 邮件提醒设置

6.2 历史操作记录



## 5.1 邮件提醒设置

Structure Properties Bulk Patents

fangjuan  
fangjuan@patsnap.com

Email Alerts History Logout

Active Inactive Edit

**Chemical Email Alert**

Aspirin - SYOKIDBDQMKNQDQ-HHUWHTLVSA-N

New compounds from Similarity Search  
3,450 Similar Compounds

Send to  
fangjuan@patsnap.com (myself)  
+1 more user(s)  
(1 user(s) has unsubscribed)

Execute  
Send on every Sunday  
Last alert: 14 Oct 2016  
Next alert: 21 Oct 2016

Edit Email Alert

Aspirin  
Similarity Search (0.8):  
SYOKIDBDQMKNQDQ-HHUWHTLVSA-N

Title \*  
Aspirin Similarity

Type

- All
- New Similar Compound (Similarity Threshold 0.8)
- New Superstructure
- New Regulatory Approval
- Change in Regulatory Approval
- Expired Regulatory Approval
- New Clinical Trial
- Change in Clinical Trial Phase
- Clinical Trial Result Publication

Send to  
fangjuan@patsnap.com (myself)

Unsubscribed  
rbansal@globalbloodt.com 15 Oct 2016 15 Oct 2016  
The user(s) above have unsubscribed from the email alert.

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Alert when there are no update

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Up to 1,000 records will be included in the email attachment  
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Aspirin  
Similarity Search (0.8):  
SYOKIDBDQMKNQDQ-HHUWHTLVSA-N

Title \*  
Untitled Email Alert

Type

- All
- New Similar Compound (Similarity Threshold 0.8)
- New Superstructure
- New Regulatory Approval
- Change in Regulatory Approval
- Expired Regulatory Approval
- New Clinical Trial
- Change in Clinical Trial Phase
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Frequency  
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1. 点击用户中心邮件提醒 或者在检索结果首页点击
2. 邮件提醒操作:
  - 1) 支持对邮件提醒的启动和暂停;
  - 2) 支持对邮件提醒的修改;
  - 3) 支持对邮件提醒的删除;

## 5.2 历史操作记录

Structure Properties Bulk Patents

Chemical History

20170415 To 2017

fangjuan  
fangjuan@patsnap.com

Email Alerts History Logout

All	Time	Action
All Searches	Today	
Exact Search	11:40 AM	ChemScape: [ChemScape]77ab858fe9624ed292d60d0bfb98184
Similarity Search	11:39 AM	ChemScape: [ChemScape]77ab858fe9624ed292d60d0bfb98184
Substructure Search	11:39 AM	Exact Search: UHOVONZJYSORNB-UHFFFAOYSA-N - BENZENE; benzene, benzol, benzole, Cyclohexatriene, Pyrobenzole, Benzine, Phenyl hydride, Pyrobenzol, Benzen, Phene, Mineral naphtha, Coal naphtha, 71-43-2, Benzolene, Benzin, Bicarbonate of hydrogen, Motor benzol, Carbon oil, Benzeen, Benzolo, Fenzen; [6]Annulene, Benzol; [6]Annulene, Benzol 90, Nitration benzene, Benzen [Dutch], Benzen [Czech], Rcr waste number U019, Benzolo [Italian], Benzine (Obs.), Benzin (Obs.), NCI-C55276; Caswell No. 077; Annulene, Benzinum; Benzolium; Benzol diluent; Benzene, pure; CCRIS 70; NSC 67315; HSDB 35; UN 1114; [6]Annulene; CHEBI:16716; UNII-J64922108F; 1,3,5-cyclohexatriene; EINECS 200-753-7; UN1114; EPA Pesticide Chemical Code 008801; Benzene (including benzene from gasoline); A13-00808; CHEMBL277500; UHOVONZJYSORNB-UHFFFAOYSA-N; MFC000003009; BNZ; Benzene-UL-14C; 26181-88-4; RNG; 2,5-cyclohexadien-1,4-yiene, Aromatic alkane; benzene-1-thy; 1sw; Benzene, anhydrous; Benzene, ACS min; Benzene-U-14C; Benzene, HPLC Grade; Z299; 47; BENZENE, ACS; ACMC-2095nd; Benzene + aniline combo; DSSTox_Cli_135; Benzene, labeled with carbon-14 and tritium; WLN: RH; EpiRpe ID:116867; AC1L185P; DSSTox_RID_79433; DSSTox_GSID_39242; ghi.PD_Mitscher_Jego 503; 48503; SUPELCO; 270709; ALDRICH; 32212; RIEDEL; 401765; ALDRICH; 676985; ALDRICH; DTXSID3039242; 12540_FLUKA; 12553; FLUKA; HMD01505; 3,4-DNH; Benzene, labeled with carbon-14; Benzene, Spectrophotometric Grade; 183; 220; 223; 311955; SIGMA; 322644; SIGMA; MolPort-000-971-944; 12553; SIAL; 32212; SIAL; ZINC96753; trans-N-Methylphenylcyclopropanamine; 154628; SIAL; 276709; SIAL; 319953; SIAL; 401765; SIAL; 676985; SIAL; ACT07832; NSC67315; ZX-47016050; Tox21_202487; 1,3-Cyclohexadiene-5,6-diyne radical; ANW-41399; BDBM50167939; BM 613; NSC-67315; STL264205; AKOS008967253; FCH2258263; LG-1605; MOULE-4899719484; OR40181; RL04726; RTR-002195; Benzene [UN1114] [Flammable liquid]; CAS-71-43-2; Benzene [UN1114] [Flammable liquid]; erythro-Phenyl-2-piperidyl-carbinol (-); NCGC00090744-01; NCGC00090744-02; NCGC00163890-01; NCGC00163890-02; NCGC00260036-01; trans-N, N-Dimethylphenylcyclopropanamine; 8030-30-6; AJ-24530; AN-23800; AN-24993; BBV-36966095; Cc-34 (+/-); KB-47520; OR028055; SC-74481; ZB015460; AB1007259; B0020; FT-0680146; FT-0622636; FT-0622667; FT-0656867; FT-0657604; J64922108F; 00038; 00042; S0631; 3945-EP0930075A1; 3945-EP1441224A2; 3945-EP2269977A2; 3945-EP2269978A2; 3945-EP2269985A2; 3945-EP2269986A1; 3945-EP2269987A1; 3945-EP2269988A2; 3945-EP2269989A1; 3945-EP2269990A1; 3945-EP2269991A2; 3945-EP2269992A1; 3945-EP2269993A1; 3945-EP2269994A1; 3945-EP2270000A1; 3945-EP2270006A1; 3945-EP2270008A1; 3945-EP2270010A1; 3945-EP2270113A1; 3945-EP2270114A1; 3945-EP2272516A2; 3945-EP2272537A2; 3945-EP22727813A2; 3945-EP22727817A1; 3945-EP2272822A1; 3945-EP2272825A2; 3945-EP2272828A1; 3945-EP2272832A1; 3945-EP2272839A1; 3945-EP2272840A1; 3945-EP2272841A1; 3945-EP2272849A1; 3945-EP2272935A1; 3945-EP2272972A1; 3945-EP2272973A1; 3945-EP2272974A1; 3945-EP2272975A2; 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