



# CAS SciFinder<sup>n</sup> 快速入门指南

2021 年 12 月

# 目录

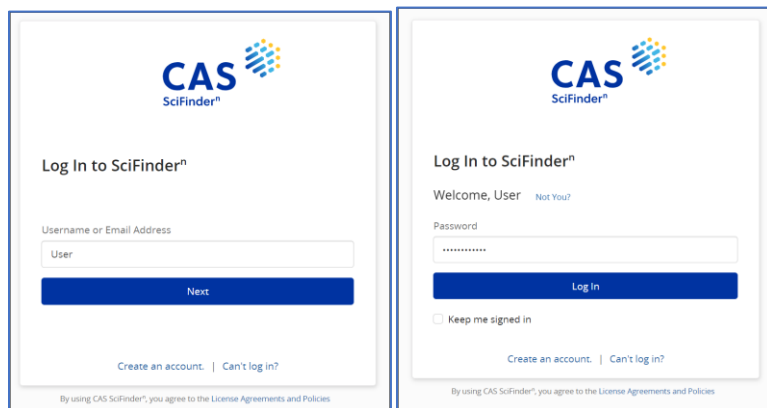
欢迎使用 CAS SciFinder <sup>®</sup> .....	2
检索.....	2
物质结果集.....	4
物质详情.....	5
文献结果集.....	6
文献详情.....	7
反应结果集.....	9
反应详情.....	10
化学品供应商.....	11
供应商详情.....	12
生物序列.....	13
可视化分析生物序列检索结果.....	15
可视化分析结构检索结果.....	15
检索历史.....	16
CAS SciFinder <sup>®</sup> 支持.....	17

## 欢迎使用 CAS SciFinder<sup>®</sup>

本快速指南将展示如何开始使用令人信赖、内容全面的检索引擎 CAS SciFinder<sup>®</sup>。

首先输入 <https://scifinder-n.cas.org> 打开 CAS SciFinder<sup>®</sup> 登录页面。

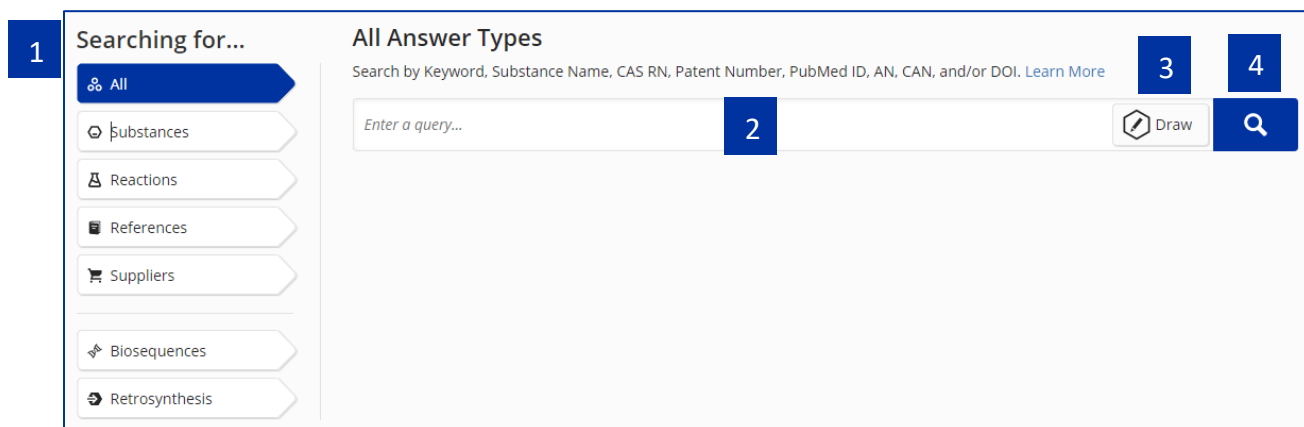
输入用户名和密码。



## 检索

可以通过关键词、物质名称、CAS 登记号、专利号或结构进行检索。

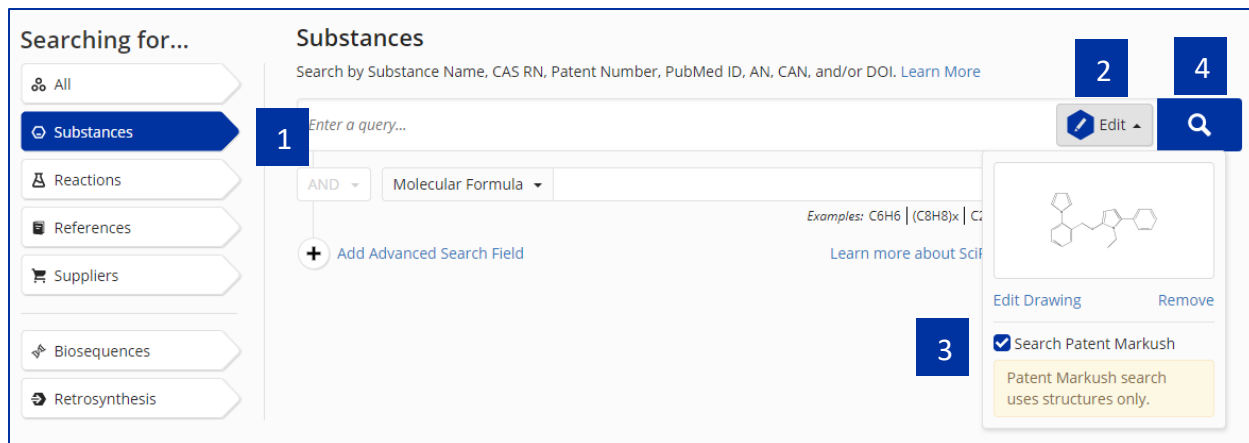
注意：你可以输入文献的 DOI 号在 “All” 或 “References” 中检索。



1. 选择检索类型
2. 输入检索式
3. 打开结构编辑器，绘制（导入）结构或反应式
4. 点击进行检索

在进行 **References** 和 **Substances** 高级检索（**Advanced Search**）时，可以使用逻辑运算符连接不同的字段。

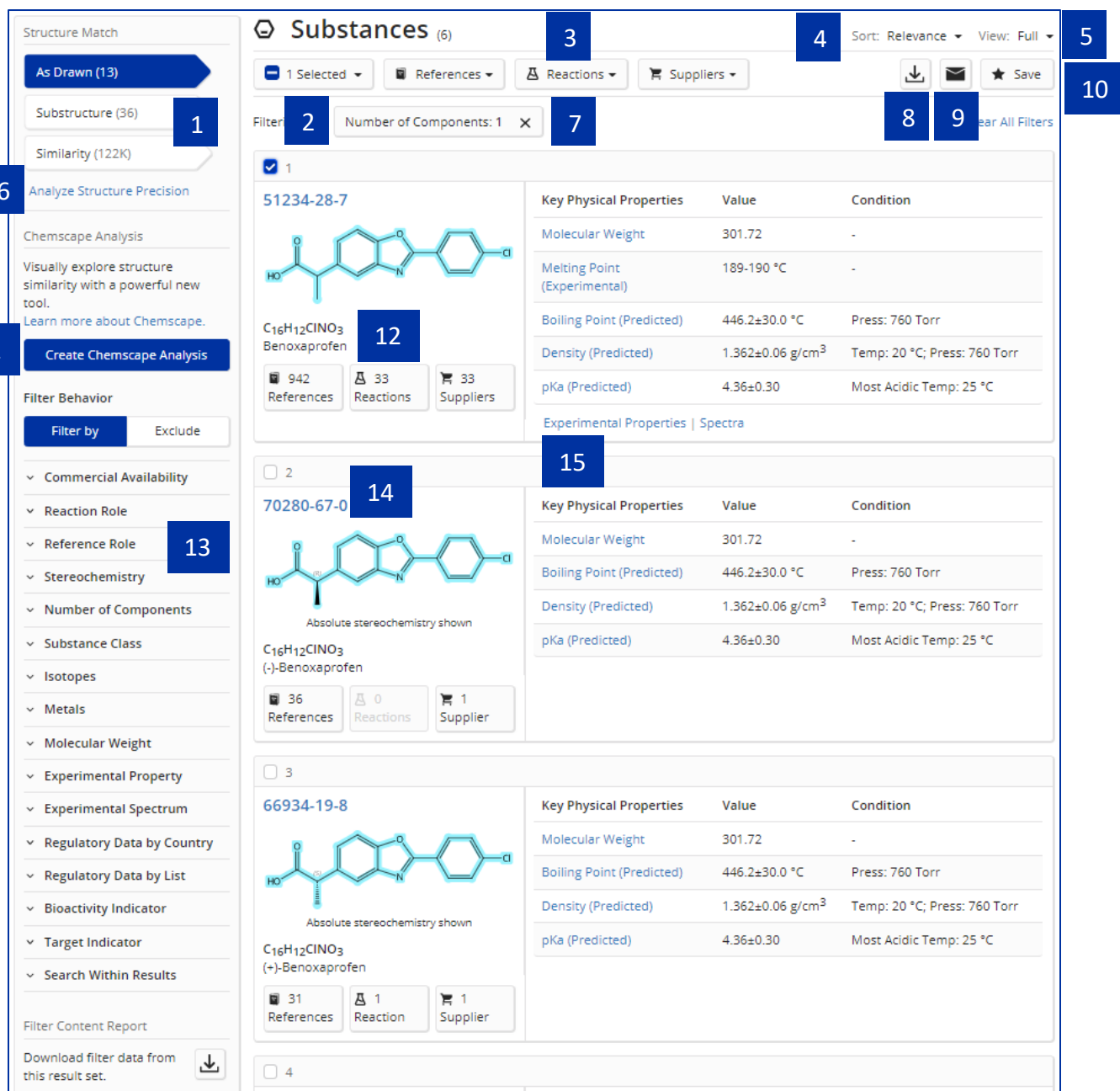
专利 Markush 检索: 进行专利 Markush 检索, 先选择 **Substances**, 然后在结构编辑器中绘制/导入结构, 再勾选 **Search Patent Markush**。



The screenshot shows the CAS SciFinder search interface. On the left, under 'Searching for...', the 'Substances' option is selected (indicated by a blue arrow and a '1' in a blue box). The main search area is titled 'Substances' and includes a search bar with the placeholder 'Enter a query...' (indicated by a '2' in a blue box). Below the search bar, there are options for 'AND' and 'Molecular Formula'. A chemical structure drawing tool is visible on the right, with a '3' in a blue box pointing to the 'Search Patent Markush' checkbox, which is checked. A '4' in a blue box points to the search button (magnifying glass icon). A note below the checkbox states: 'Patent Markush search uses structures only.'

1. 选择 Substances
2. 点击打开结构编辑器, 绘制或导入结构
3. 选择 “**Search Patent Markush**”
4. 点击执行检索

## 物质结果集



The screenshot displays the CAS SciFinder search results page for Benoxaprofen. The interface is annotated with numbered callouts (1-15) highlighting key features and actions:

- 1:** Structure Match filter options: As Drawn (13), Substructure (36), Similarity (122K).
- 2:** Filter button.
- 3:** Substances (6) header.
- 4:** Sort: Relevance, View: Full dropdown.
- 5:** Download, Email, Save icons.
- 6:** Analyze Structure Precision button.
- 7:** Filter: Number of Components: 1 X button.
- 8:** Clear All Filters button.
- 9:** Clear All Filters button.
- 10:** Clear All Filters button.
- 11:** Create Chemscape Analysis button.
- 12:** 942 References, 33 Reactions, 33 Suppliers buttons for the first result.
- 13:** Filter Behavior sidebar with various filters like Commercial Availability, Reaction Role, Reference Role, Stereochemistry, etc.
- 14:** 36 References, 0 Reactions, 1 Supplier buttons for the second result.
- 15:** 31 References, 1 Reaction, 1 Supplier buttons for the third result.

The results table shows the following data for the three entries:

Entry	Chemical Name	Formula	Key Physical Properties	Value	Condition
1	Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Molecular Weight	301.72	-
1	Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Melting Point (Experimental)	189-190 °C	-
1	Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Boiling Point (Predicted)	446.2±30.0 °C	Press: 760 Torr
1	Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Density (Predicted)	1.362±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
1	Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	pKa (Predicted)	4.36±0.30	Most Acidic Temp: 25 °C
2	(-)-Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Molecular Weight	301.72	-
2	(-)-Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Boiling Point (Predicted)	446.2±30.0 °C	Press: 760 Torr
2	(-)-Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Density (Predicted)	1.362±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
2	(-)-Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	pKa (Predicted)	4.36±0.30	Most Acidic Temp: 25 °C
3	(+)-Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Molecular Weight	301.72	-
3	(+)-Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Boiling Point (Predicted)	446.2±30.0 °C	Press: 760 Torr
3	(+)-Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	Density (Predicted)	1.362±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
3	(+)-Benoxaprofen	C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>	pKa (Predicted)	4.36±0.30	Most Acidic Temp: 25 °C

1. 选择结构匹配类型
2. 保留或者去除选中结果
3. 获得物质结果集的文献、反应和供应商信息
4. 改变结果集排序方式
5. 改变物质信息展示方式
6. 获取两性离子、异构体等
7. 点击 X 去除筛选选项
8. 下载结果

9. 发送电子邮件分享物质结果集
10. 保存结果及设置定题跟踪
11. 对结构检索结果进行专利可视化分析
12. 获取该物质的文献、反应和供应商信息
13. 物质结果集筛选或排除选项
14. 点击物质的 CAS 登记号查看物质详细信息
15. 物质基本属性

## 物质详情

**Substance Detail** (1 of 6)

References (942) Reactions (33) Suppliers (33) **1**

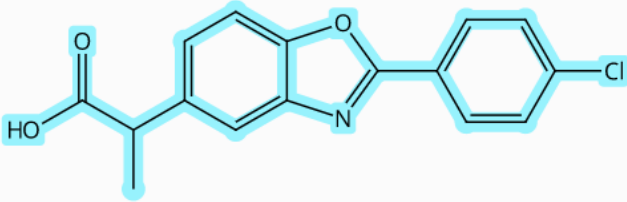
← Prev Next →

↓ ✉ ★ Save

CAS Registry Number **2 3 4**

51234-28-7

**5**



**C<sub>16</sub>H<sub>12</sub>ClNO<sub>3</sub>**

5-Benzoxazoleacetic acid, 2-(4-chlorophenyl)-α-methyl- (9CI, ACI)

Key Physical Properties <b>6</b>	Value	Condition
Molecular Weight	301.72	-
Melting Point (Experimental)	189-190 °C	-
Boiling Point (Predicted)	446.2±30.0 °C	Press: 760 Torr
Density (Predicted)	1.362±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	4.36±0.30	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

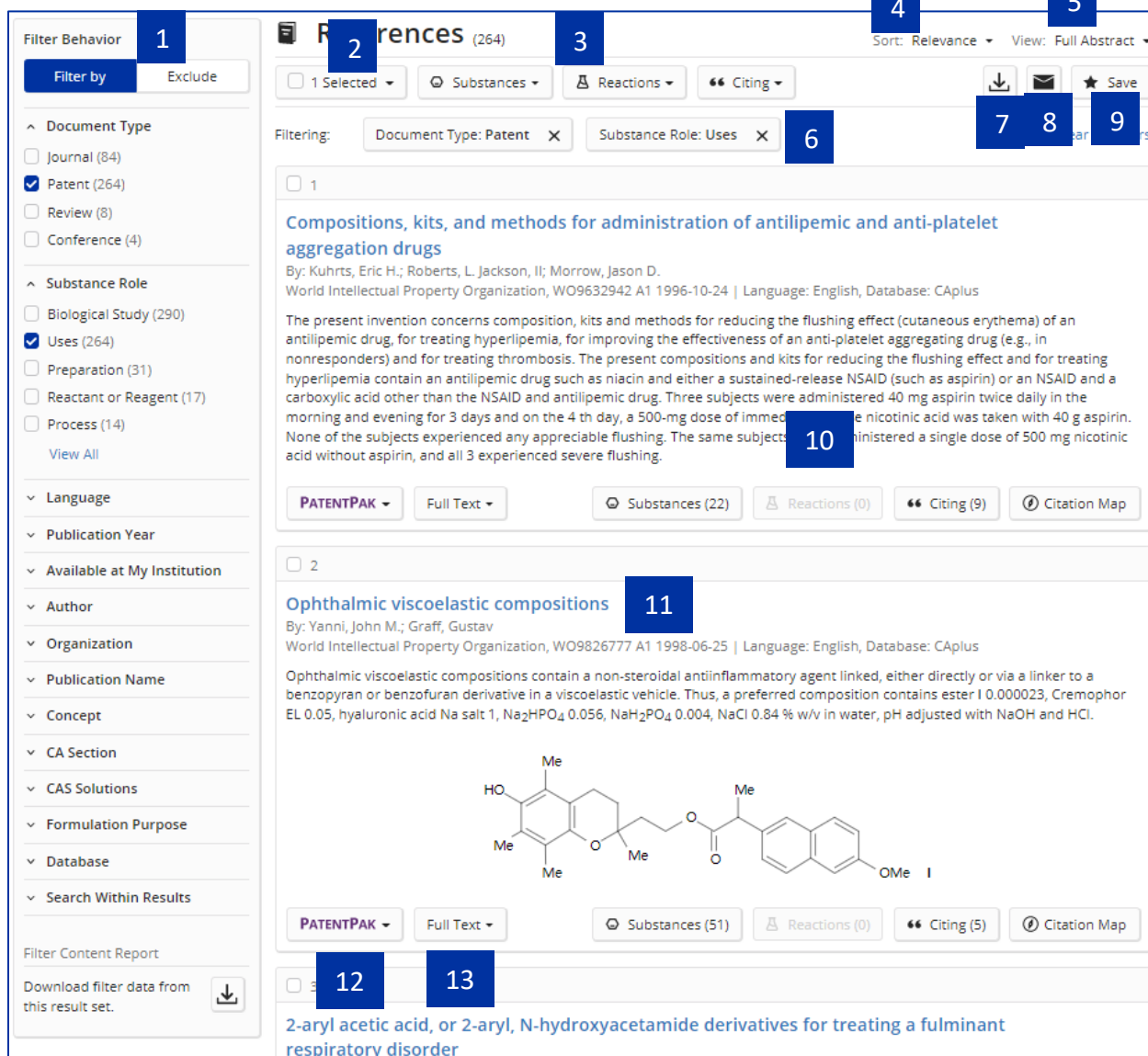
**8** Expand All | Collapse All

- ▼ Other Names and Identifiers
- ▼ Experimental Properties
- ▼ Experimental Spectra **7**
- ▼ Predicted Properties
- ▼ Predicted Spectra
- ▼ Bioactivity Indicators
- ▼ Target Indicators
- ▼ Regulatory Information
- ▼ Additional Details

1. 获取物质的文献、反应和供应商信息

2. 下载信息详情
3. 发送电子邮件分享物质信息详情
4. 保存信息详情
5. 点击结构图片，展示物质信息窗口，可以获得物质详情、生成逆合成路线、编辑或下载结构文件
6. 物质基本属性
7. 物质详细性质信息
8. 展开或折叠所有分类

## 文献结果集



The screenshot shows the CAS SciFinder interface with the following numbered callouts:

- 1**: Filter Behavior section, including Filter by and Exclude buttons.
- 2**: Results list header, showing 'References (264)'.
- 3**: Filter buttons for Substances, Reactions, and Citing.
- 4**: Sort and View options (Sort: Relevance, View: Full Abstract).
- 5**: Download, Email, and Save icons.
- 6**: Filtering section showing selected filters: Document Type: Patent, Substance Role: Uses.
- 7**: Search icon.
- 8**: Filter icon.
- 9**: Save icon.
- 10**: Abstract text for 'Compositions, kits, and methods for administration of antilipemic and anti-platelet aggregation drugs'.
- 11**: Abstract text for 'Ophthalmic viscoelastic compositions'.
- 12**: Abstract text for '2-aryl acetic acid, or 2-aryl, N-hydroxyacetamide derivatives for treating a fulminant respiratory disorder'.
- 13**: Chemical structure image of a complex organic molecule.

1. 包含或排除选中的筛选项
2. 保留或删除选中的文献
3. 获得文献结果集的物质、反应和引文信息

4. 文献结果排序标准
5. 改变文献信息展示方式
6. 点击 X, 移除筛选选项
7. 下载文献结果
8. 发送电子邮件分享文献结果
9. 保存结果及设置定题跟踪
10. 获取该文献的物质、反应、引文和引文地图
11. 点击查看文献详情
12. 点击 PatentPak 查看专利同族及获取专利全文
13. 点击获取原文链接

## 文献详情

☰
Reference Detail
(1 of 159)

2
3
4
5
6

PATENT

**Patent Number**  
WO9632942

**Publication Date**  
1996-10-24

**Application Number**  
WO1996-US5398

**Application Date**  
1996-04-19

**Kind Code**  
A1

**Assignee**  
Vital Therapeutics, L.L.C., United States  
Vanderbilt University, United States  
Kuhrts, Eric H.  
Roberts, L. Jackson, II  
Morrow, Jason D.

**Source**  
World Intellectual Property Organization  
CODEN: PIXXD2

**Database Information**  
AN: 1996:743696  
CAN: 126:1198  
CAplus

**Language**  
English

Compositions, kits, and methods for administration of antilipemic and anti-platelet aggregation drugs

By: Kuhrts, Eric H.; Roberts, L. Jackson, II; Morrow, Jason D.

The present invention concerns composition, kits and methods for reducing the flushing effect (cutaneous erythema) of an antilipemic drug, for treating hyperlipemia, for improving the effectiveness of an anti-platelet aggregating drug (e.g., in nonresponders) and for treating thrombosis. The present compositions and kits for reducing the flushing effect and for treating hyperlipemia contain an antilipemic drug such as niacin and either a sustained-release NSAID (such as aspirin) or an NSAID and a carboxylic acid other than the NSAID and antilipemic drug. Three subjects were administered 40 mg aspirin twice daily in the morning and evening for 3 days and on the 4<sup>th</sup> day, a 500-mg dose of immediate-release nicotinic acid was taken with 40 g aspirin. None of the subjects experienced any appreciable flushing. The same subjects were administered a single dose of 500 mg nicotinic acid without aspirin, and all 3 experienced severe flushing.

Keywords: NSAID antilipemic platelet aggregation; antithrombotic carboxylate sustained release

7
PATENTPAK PDF
Full Text
8

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO9632942	English	A1	PDF	1996-10-24	WO1996-US5398	1996-04-19
					US1995-425060	1995-04-19
US5773453	Undetermined	A		1998-06-30	US1995-425057	1995-04-19
					US1995-548822	1995-10-26
CA2218696	Undetermined	A1		1996-10-24	CA1996-2218696	1996-04-19
AU9657879	Undetermined	A		1996-11-07	AU1996-57879	1996-04-19
EP821587	Undetermined	A1		1998-02-04	EP1996-914555	1996-04-19
US5981555	English	A	PDF   PDF+   Viewer	1999-11-09	US1997-937669	1997-09-26

Expand All | Collapse All

∨ IPC Data 10

∨ Concepts 11

∨ Substances 12

∨ Formulations

∨ Cited Documents 14

1

Substances (22)

Reactions (0)

Citing (9)

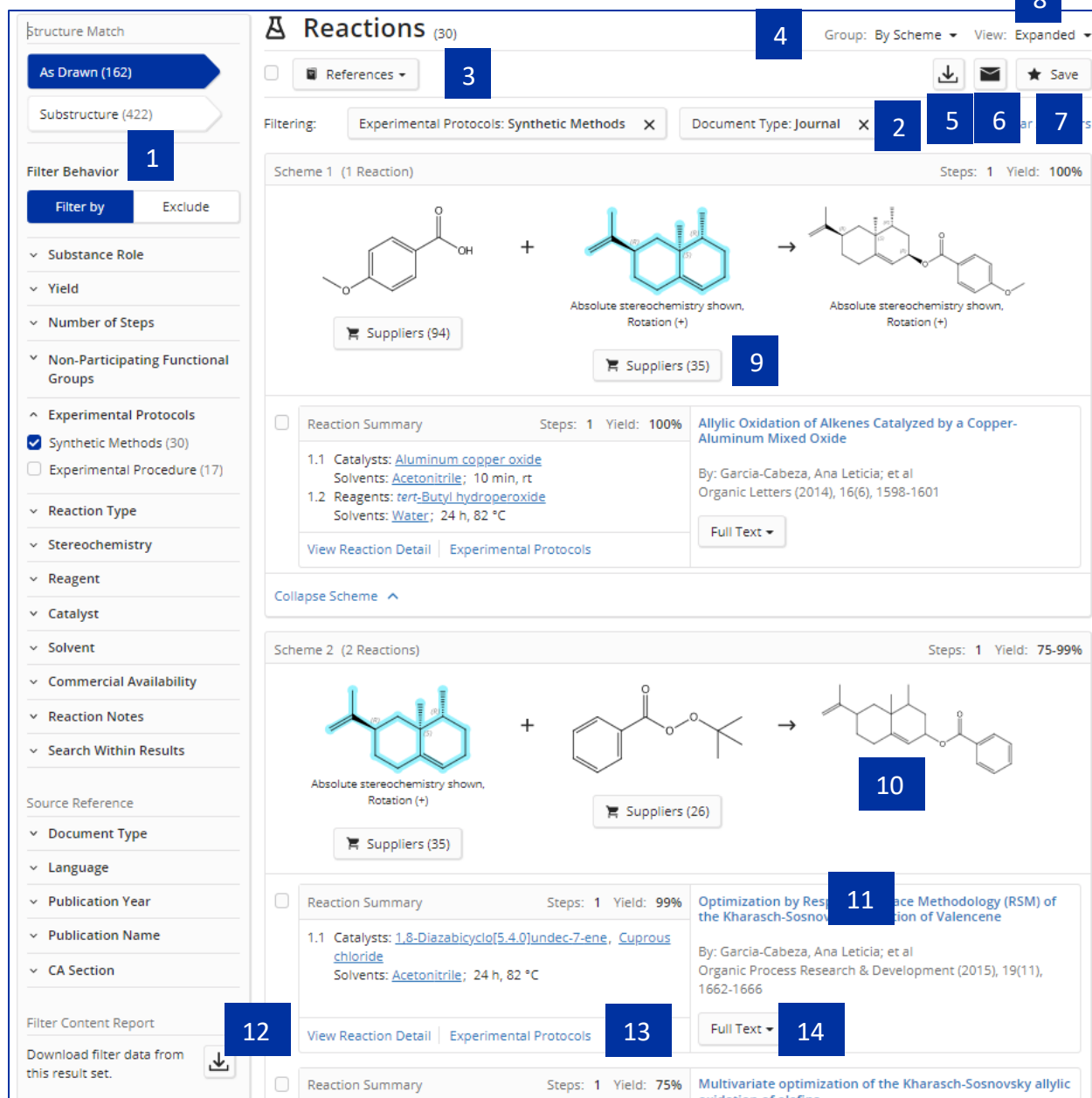
Citation Map

↓
✉
★ Save



1. 获取该文献报道的物质
2. 查看哪些文献引用了该文献
3. 查看该文献的引文地图
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6. 保存文献详情
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10. 该专利的 IPC
11. 文献中的重要技术术语
12. 文献中报道的物质及 CAS 为该物质添加的标引信息
13. 该文献披露的制剂/配方信息
14. 该文献的参考文献

## 反应结果集

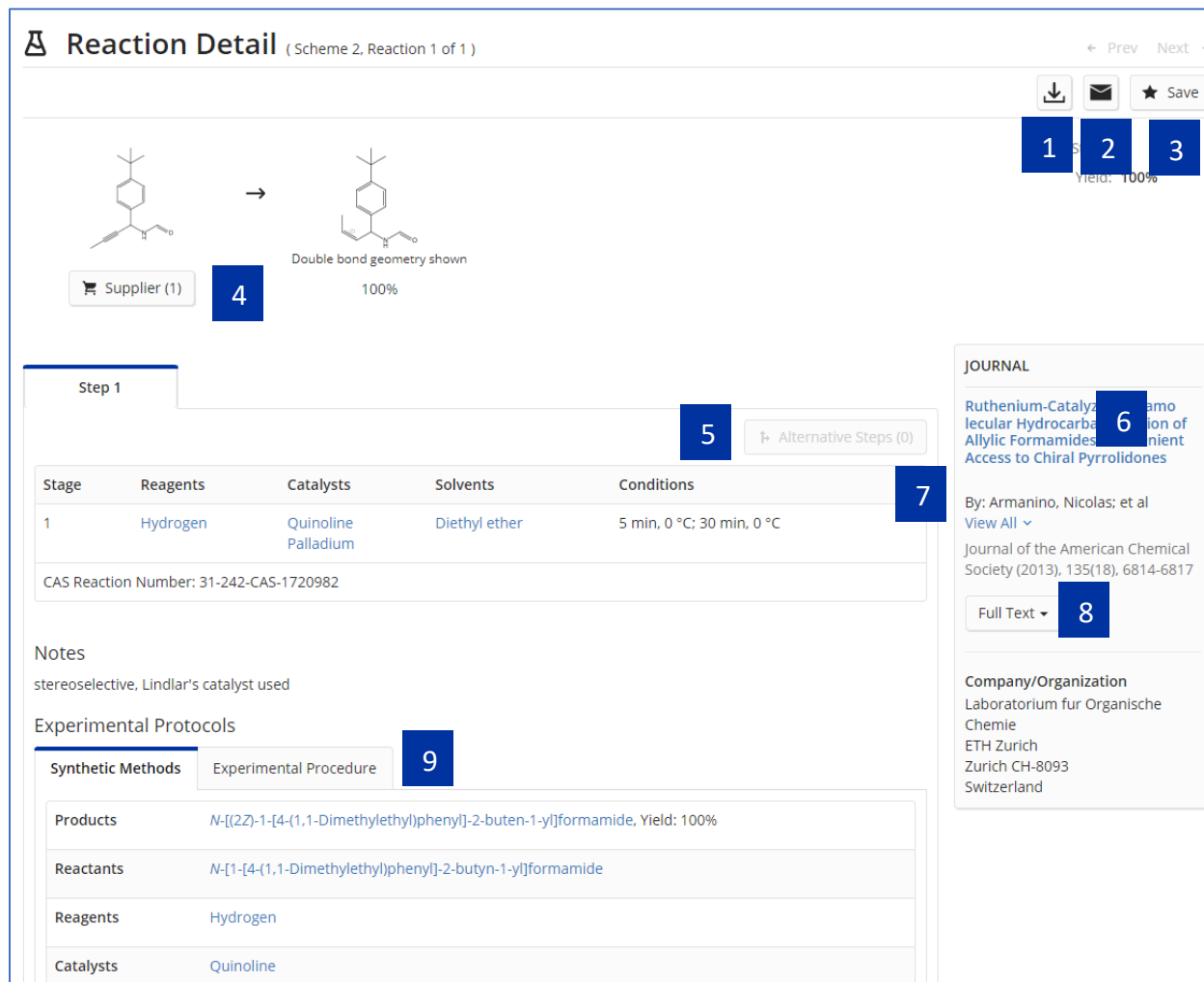


The screenshot displays the CAS SciFinder interface for reaction search results. On the left is a sidebar with various filters. The main area shows a list of reactions, with two examples highlighted. Each reaction entry includes a chemical scheme, a reaction summary, and a source reference. Numbered callouts (1-14) point to specific UI elements: 1. Filter Behavior section; 2. Filtering options (Experimental Protocols: Synthetic Methods, Document Type: Journal); 3. References button; 4. Group and View dropdowns; 5. Download icon; 6. Email icon; 7. Save icon; 8. Reaction information display mode; 9. Suppliers button; 10. Reaction scheme; 11. Reaction summary; 12. Filter Content Report; 13. View Reaction Detail button; 14. Full Text button.

1. 包含或者排除筛选选项
2. 点击 X 去除筛选选项
3. 获得反应的文献信息
4. 改变结果排序方式
5. 下载结果
6. 发送电子邮件分享反应检索结果
7. 保存结果及设置定题追踪
8. 改变反应信息展示方式

9. 获得该物质的供应商信息
10. 点击结构图片或物质名称，展示物质信息窗口，可以获得物质详情、生成逆合成路线、编辑或下载结构文件
11. 点击查看该反应的文献信息
12. 打开反应详情页面
13. 展示反应方法详情
14. 查看原文链接

## 反应详情



**Reaction Detail** (Scheme 2, Reaction 1 of 1)

← Prev Next →

Download Email Save

1 2 3  
Yield: 100%

Supplier (1) 4

Double bond geometry shown  
100%

Step 1

Alternative Steps (0) 5

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrogen	Quinoline Palladium	Diethyl ether	5 min, 0 °C; 30 min, 0 °C

CAS Reaction Number: 31-242-CAS-1720982

Notes  
stereoselective, Lindlar's catalyst used

Experimental Protocols

Synthetic Methods Experimental Procedure 9

Products	<i>N</i> -[(2 <i>Z</i> )-1-[4-(1,1-Dimethylethyl)phenyl]-2-buten-1-yl]formamide, Yield: 100%
Reactants	<i>N</i> -[1-[4-(1,1-Dimethylethyl)phenyl]-2-buten-1-yl]formamide
Reagents	Hydrogen
Catalysts	Quinoline

**JOURNAL**

Ruthenium-Catalyzed Asymmetric Hydrocarbonylation of Allylic Formamides: Convenient Access to Chiral Pyrrolidones 6

By: Armanino, Nicolas; et al  
View All

Journal of the American Chemical Society (2013), 135(18), 6814-6817

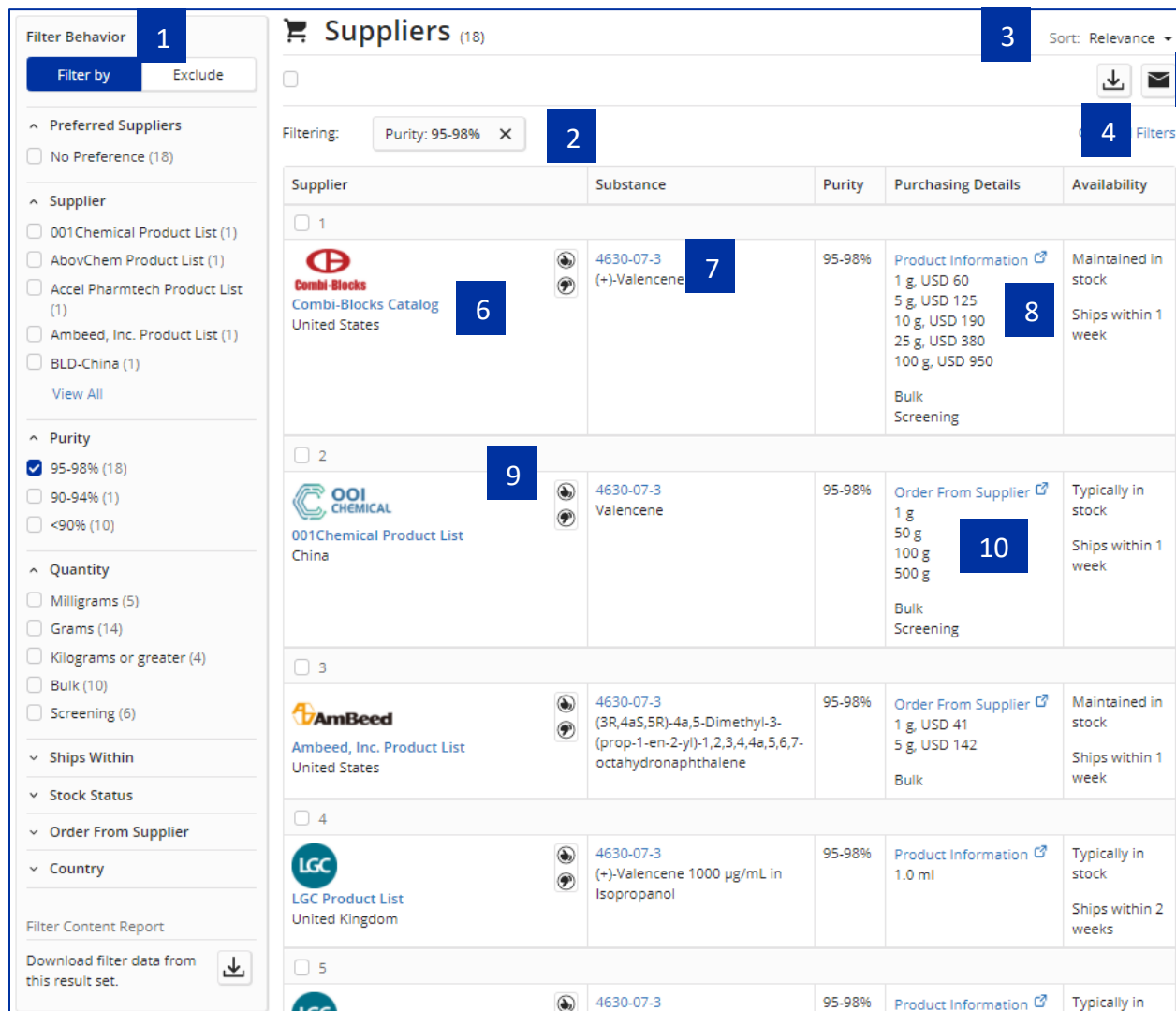
Full Text 8

**Company/Organization**  
Laboratorium für Organische Chemie  
ETH Zurich  
Zurich CH-8093  
Switzerland

1. 下载反应详情
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5. 查看该产物的其他可行反应
6. 点击获得反应的文献信息详情页面
7. 查看文献的全部作者

8. 全文链接
9. 反应实验方法

## 化学品供应商



The screenshot shows the 'Suppliers' interface with the following callouts:

- 1: Filter Behavior section
- 2: Purity filter: 95-98%
- 3: Sort: Relevance
- 4: Filters button
- 5: Download and Email icons
- 6: Combi-Blocks supplier details
- 7: Substance name: (+)-Valencene
- 8: Product information link
- 9: OOI Chemical supplier details
- 10: Order From Supplier link



Supplier	Substance	Purity	Purchasing Details	Availability
Combi-Blocks Combi-Blocks Catalog United States	4630-07-3 (+)-Valencene	95-98%	Product Information 1 g, USD 60 5 g, USD 125 10 g, USD 190 25 g, USD 380 100 g, USD 950 Bulk Screening	Maintained in stock Ships within 1 week
OOI CHEMICAL 001Chemical Product List China	4630-07-3 Valencene	95-98%	Order From Supplier 1 g 50 g 100 g 500 g Bulk Screening	Typically in stock Ships within 1 week
AmBeed AmBeed, Inc. Product List United States	4630-07-3 (3R,4aS,5R)-4a,5-Dimethyl-3-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene	95-98%	Order From Supplier 1 g, USD 41 5 g, USD 142 Bulk	Maintained in stock Ships within 1 week
LGC LGC Product List United Kingdom	4630-07-3 (+)-Valencene 1000 µg/mL in Isopropanol	95-98%	Product Information 1.0 ml	Typically in stock Ships within 2 weeks
LGC	4630-07-3	95-98%	Product Information	Typically in

1. 筛选结果
2. 点击 X 去除筛选选项
3. 重新排列结果
4. 下载结果
5. 发送电子邮件分享供应商信息
6. 查看供应商详情
7. 点击打开物质信息窗口，查看物质信息、生成逆合成路线，编辑/下载结构
8. 打开供应商网站产品信息页面
9. 点击设置优选或非优选供应商
10. 打开产品订购页面

## 供应商详情

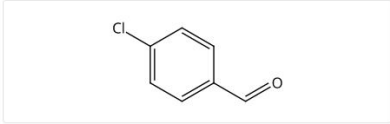

**Supplier Detail** (1 of 77) ← Prev Next →

**1** 2 3

BIONET Screening and Fragments Library  

Web	<a href="https://www.keyorganics.net">https://www.keyorganics.net</a>	Substance Information	
Email	<a href="mailto:enquiries@keyorganics.net">enquiries@keyorganics.net</a>	CAS Registry Number	104-88-1 <b>4</b>
Phone	+44(0) 1840 212137	CAS Name	4-Chlorobenzaldehyde

Item Details

Chemical Name	4-Chlorobenzaldehyde	 <b>5</b>
Order Number	PS-9029	
Purity	97%	
Quantity, Price	1mg, GBP 30.00 5mg, GBP 37.00 10mg, GBP 51.00	
	Bulk Available Screening Available	
Stock Status	Typically in stock	
Ships Within	1 week	
Pricing Information	4 May 2021	
Last Updated		
Order From Supplier 	<b>6</b>	

Additional Contact Information

BIONET/Key Organics Ltd.  
Highfield Road Industrial Estate  
Camelford, Cornwall, PL32 9RA  
United Kingdom

Fax +44(0) 1840 213712

1. 点击设置为优选或非优选供应商
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4. 点击获得物质详情页面
5. 点击结构图片，打开物质信息窗口，可以查看物质信息、生成逆合成路线，编辑/下载结构
6. 进入供应商网站打开物质采购页面

## 生物序列

Substances

Draw
Search
Star
Clock
User

[Return to Home](#)

**BLAST Search Details**

Sequence Type: Protein  
Search Within: Proteins  
BLAST Algorithm: BLASTp  
NCBI Included: Yes  
Alignment Identity: -  
Query Coverage: 90%  
E-Value: 10  
Match with Gaps?: No  
Gap Costs: Existence 11  
Extension 1  
Word Size: 3

**Bioscape Analysis**

Visually explore sequence similarity with a new tool.  
[Learn more about Bioscape.](#)

5 Create Bioscape Analysis

## Biosequences (58)

2
Sort: Subject Coverage
View: Expanded

**References** 4 Download

Query Details MSGRHREPTT SNVSVAKIAFTGAVLGGGGI AMAAQATAATDGEWDQVARCESGGNWSINTGNGYLGLQFTQSTWAAHGGGEPAPSAQLAS... 1 More

1 Alignment Identity: 100%

Query 1

407

Subject 1

407

Matches: 407  
Mismatches: 0

View Less

Alignment Subject References 7 8 References

Alignment Data  
BLAST Score: 2148  
E-Value: 0

Q	1	MSGRHREPTT	SNVSVAKIAF	TGAVLGGGGI	AMAAQATAAT	DGEWDQVARC	ESGGNWSINT	GNGYLGLQF	70
S	1	MSGRHREPTT	SNVSVAKIAF	TGAVLGGGGI	AMAAQATAAT	DGEWDQVARC	ESGGNWSINT	GNGYLGLQF	70
Q	71	TQSTWAAHGG	GEFAPSAQLA	SREQQIAVGE	RVLATQGRGA	WPVCGRGLSN	ATPREVLPAS	AAMDAPLDA	140
S	71	TQSTWAAHGG	GEFAPSAQLA	SREQQIAVGE	RVLATQGRGA	WPVCGRGLSN	ATPREVLPAS	AAMDAPLDA	140
Q	141	AVNGEPAPLA	PPPADPAPPV	ELAANDLPAP	LGEPLPAAPA	DPAPPADLAP	PAPADVAPPV	ELAVNDLPAP	210
S	141	AVNGEPAPLA	PPPADPAPPV	ELAANDLPAP	LGEPLPAAPA	DPAPPADLAP	PAPADVAPPV	ELAVNDLPAP	210

2 Alignment Identity: 99.75%

Query 1

407

Matches: 406  
Mismatches: 1

Alignment
Subject
References

References

CAS Registry Number: 935175-75-0

NCBI Identifier: [CCC63477.1](#), [KAN93036.1](#), [ALA77280.1](#), [CAL70905.1](#), [AET18174.1](#), [ALV10075.1](#), [AGE66835.1](#), [A0A7S8HJL9](#), [A0A7U4BSU5](#), [A0A0H3M8Z9](#), [AKO23866.1](#), [WP\\_011799137.1](#), [AMO09483.1](#) 9

Length: 407 aa

Sequence

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1 MSGRHRKPTT SNVSVAKIAF TGAVLGGGGI AMAAQATAAT DGEWDQVARC ESGGNWSINT GNGYLGLQF TQSTWAAHGG
81 GEFAPSAQLA SREQQIAVGE RVLATQGRGA WPVCGRGLSN ATPREVLPAS AAMDAPLDA AVNGEPAPLA PPPADPAPPV
161 ELAANDLPAP LGEPLPAAPA DPAPPADLAP PAPADVAPPV ELAVNDLPAP LGEPLPAAPA DPAPPADLAP PAPAEAPPAA
241 PADLAPPAPA DLAPPVELAV NDLAPLGEF LPAAPAEELAP PADLAPASAD LAPPAPADLA PPAPAEAPP APADLAPPAA
321 VNEQTAPGDQ PATAPGCPVG LATDLELPEP DPQPADAPP GDWTEAPAET PQVSNIAATK KLWQAIRAQD WCGNDALDSL
401 AQPYYVIG

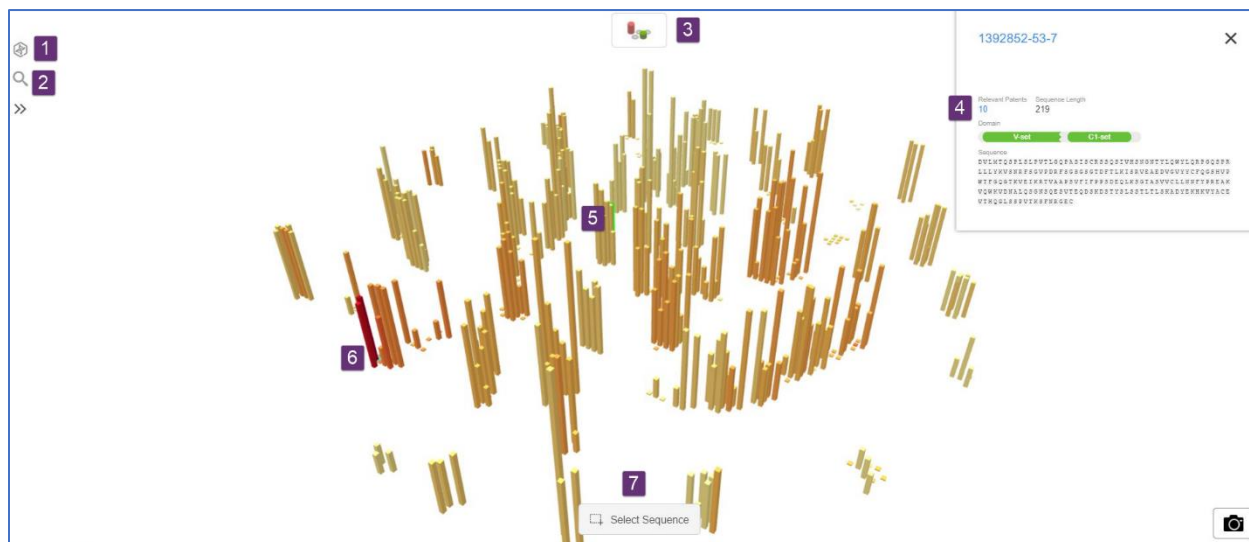
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13

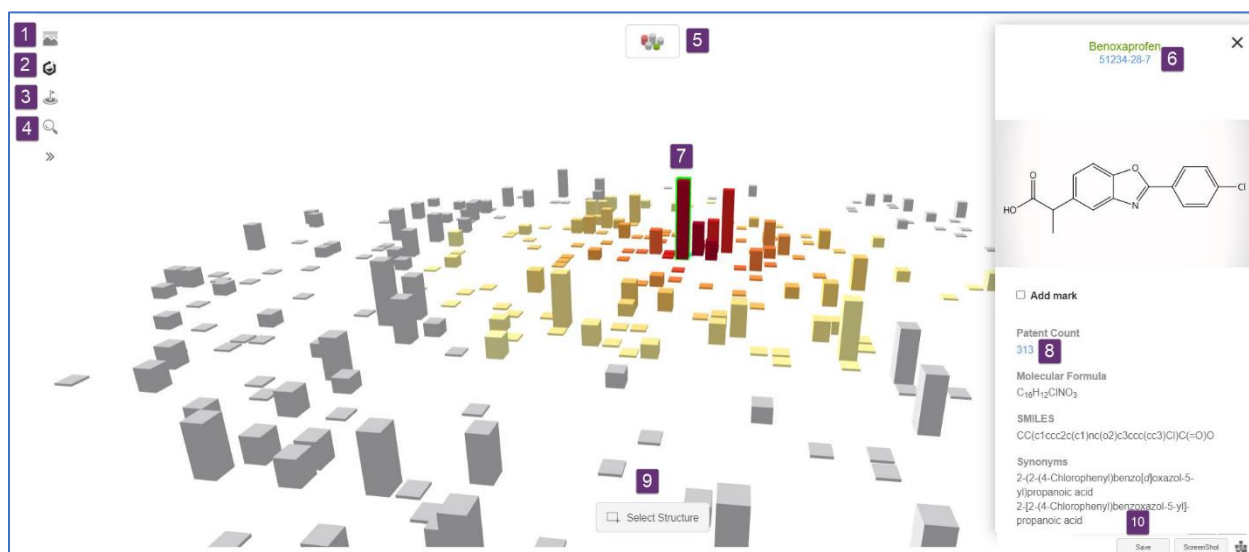
1. 检索序列
2. 重排结果
3. 改变结果展示方式
4. 下载结果
5. 可视化分析序列专利
6. 筛选序列结果
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9. 点击进入 **NCBI** 查看序列详细信息

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1. 点击通过相似性筛选序列
2. 通过专利关键词或者简单法律状态筛选序列
3. 点击改变序列结果的展示方式
4. 点击查看序列的相关专利
5. 点击查看该序列的专利数量和序列长度
6. 查询序列
7. 点击 Select Sequence 选中序列

## 可视化分析结构检索结果

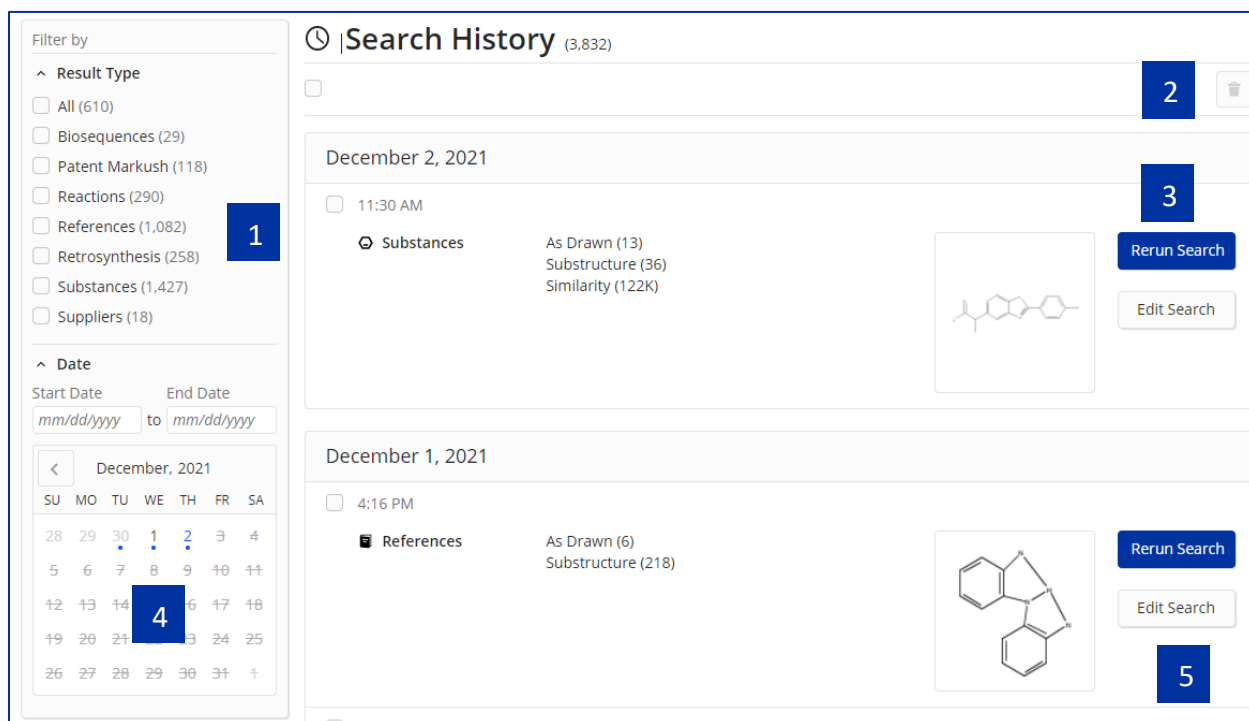


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2. 点击筛选或对结构进行分组
3. 点击添加结构，并识别其在可视化视图中的位置



4. 点击通过关键词或结构来筛选物质
5. 更改结果展示方式
6. 点击查看物质信息详情
7. 点击查看该物质的结构及其专利量
8. 点击查看物质的相关专利
9. 点击 **Select Structure**，选中多个结构
10. 点击保存 Chemscape，稍后可以在 My Chemscape 中访问

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1. 选择结果类型，查看检索历史
2. 在检索历史中删除
3. 重新运行检索，获得最新检索结果
4. 选择特定的日期范围展示检索历史
5. 点击 **Edit Search** 重新编辑，并运行检索

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