

CAS SCIFINDERⁿ

使用技巧手册

2022 年 4 月



CAS SciFinder[®]是美国化学文摘社（CAS）出品的新一代的权威科学研究工具，是化学及相关学科智能研究平台，提供全球全面、可靠的化学及相关学科研究信息和分析工具。CAS SciFinder[®]由国际科学家团队追踪全球科技进展，每日收录汇总、标引、管理着世界上的专利、科技期刊等内容，并通过 CAS SciFinder[®] 平台提供的先进检索技术高效揭示重要的技术信息，确保研究人员及时同步全球重要的研究进展。CAS SciFinder[®] 涵盖了化学及相关领域，如化学、生物、医药、材料、食品、应用化学、化学工程、农学、高分子、物理等多学科、跨学科的科技信息；收录的文献类型包括期刊、专利、会议论文、学位论文、图书、技术报告、评论、预印本和网络资源等。

CAS SciFinder[®] 独特内容和特色：

提升文献检索效率：业界最先进的检索引擎之一，将文献检索时间缩短一半，获得更精确的结果，提高检索效率。

高效设计合成计划：充分利用全球最大的单步和多步反应数据库之一，全面考量反应条件、产率、催化剂和实验步骤，高效设计出合成计划（可节省一半的时间）。

Synthetic Methods 合成方法解决方案：Synthetic Methods 是CAS SciFinder[®]中的模块，是世界上最大合成方法合集之一，涵盖顶级期刊及专利中的合成制备信息，提供合成方法的每步详细操作信息，以易于阅读的表格形式展示实验详情，包括实验操作步骤、实验原料、实验条件、实验量级、反应转化类型、合成产物谱图信息、合成产物形态等

CAS PatentPak[®] 专利分析解决方案：CAS PatentPak 是 CAS SciFinder[®]中的模块，服务于科研人员和知识产权人士。PatentPak 在定位和分析大量专利中的化学结构方面，可以为研究人员节省一半以上的时间。PatentPak 是加速化学专利分析最可靠的工具之一；迄今为止只有 PatentPak 采用人工标引——研究人员可以快速识别专利中难以发现的物质（例如，表格化合物和图形图像内的化合物）。使用 PatentPak 可以访问 CAS REGISTRYSM——世界上最全面的可公开获取的物质信息集合。

逆合成路线设计工具Retrosynthesis: 基于全球最大的化学反应数据合集CAS REACTIONS 结合先进的算法和人工智能, 综合多种因素如原子经济性、收率、绿色、成本等为已被报道分子/未被报道分子提供实验验证或预测的逆合成路线。为合成化学家节省时间并提供新的思路和见解。

支撑生物学研究: 生物序列检索工具Biosequences Search 提供超过12亿条可检索生物序列, 可进行FTO 检索、侵权检索。

可视化检索结果: 用户友好的可视化工具可以帮助用户快速做出更好的决策, 这些工具可以精确定位趋势、模式和异常值, 帮助将信息转化为洞察。

CAS REGISTRY: 全球最大的物质数据合集, 收录自19世纪初至今公开披露的超过1.9亿个独特的物质(包括合金、配合物、矿物、混合物、聚合物和盐), CAS登记号被誉为化学物质的黄金标准, 是向WHO提交INN申请时必须提供的信息, 被广泛地应用在科研界及商务流程中。

CAS Reactions: CAS创立的全球最大化学反应合集, 收录1840年以来源自专利和非专利文献的1.4亿多条单步和多步反应。CAS的科学家在标引化学反应过程中提供了独特的增值信息, 包括: 实验安全信息、反应类型、反应条件及详细的实验操作步骤等, 节省了用户从全文中总结、归纳相关反应信息所花费的时间。

马库什结构: CAS是全球唯一提供专利马库什结构的机构。从全球64家专利授权机构公开的专利中提取超过130万个可检索及浏览的马库什结构。一个马库什结构可能涵盖数千甚至数万个化合物, 提升了用户进行化合物结构新颖性和创造性检索的能力。

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文献检索 90

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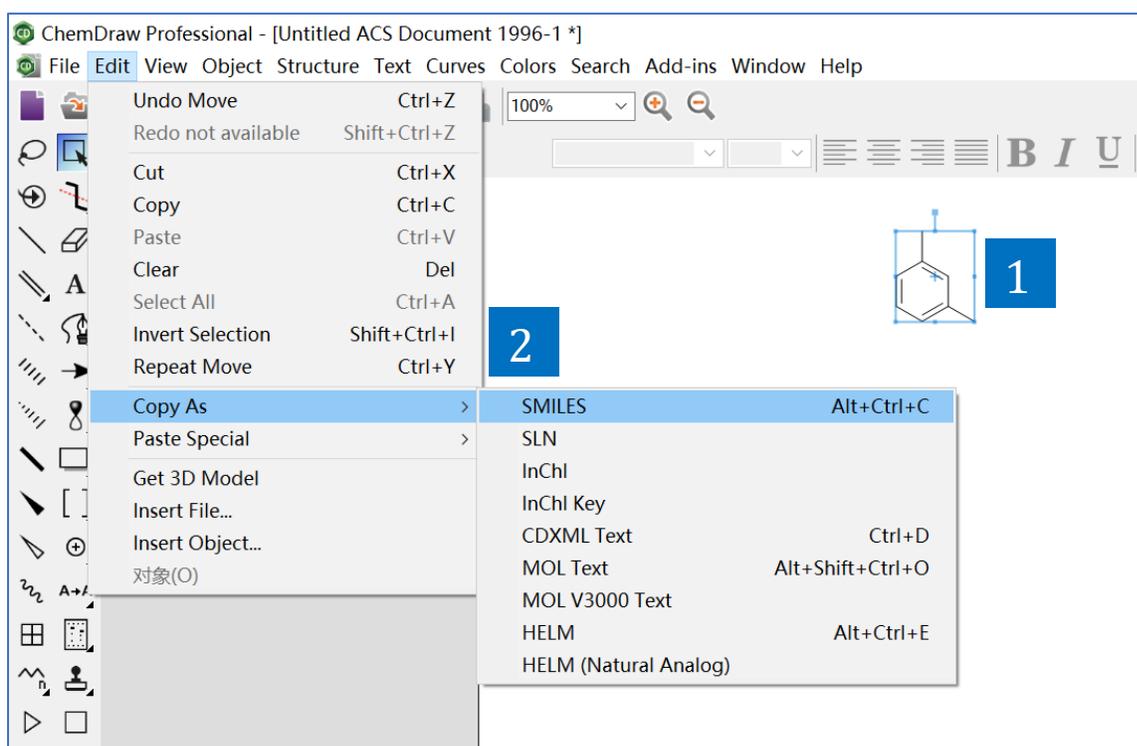
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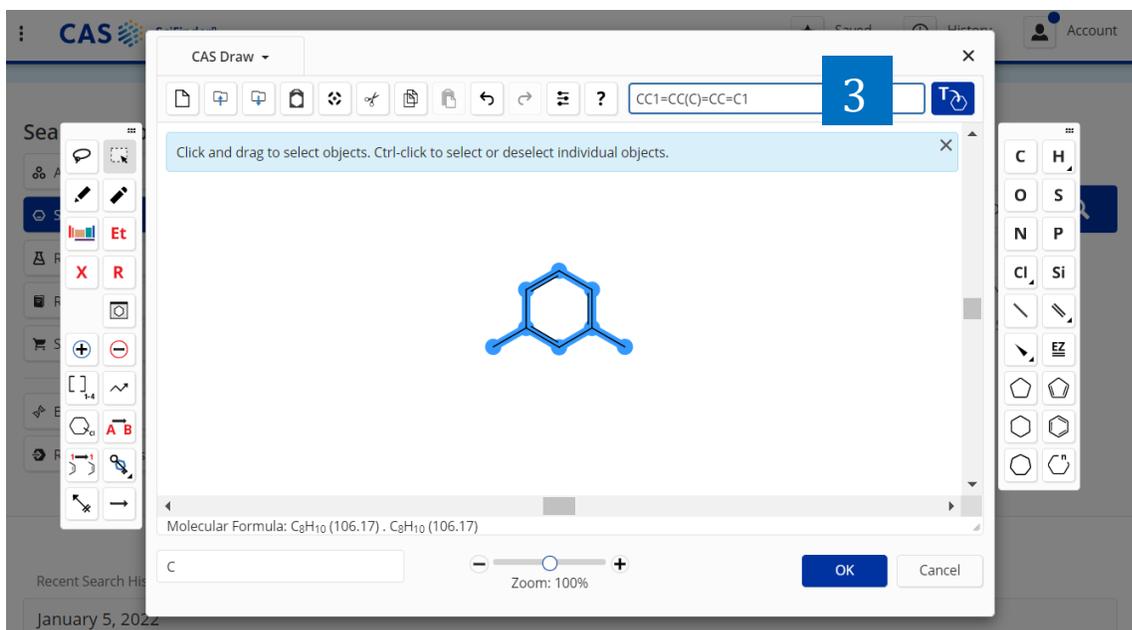
物质检索

与 ChemDraw 联用

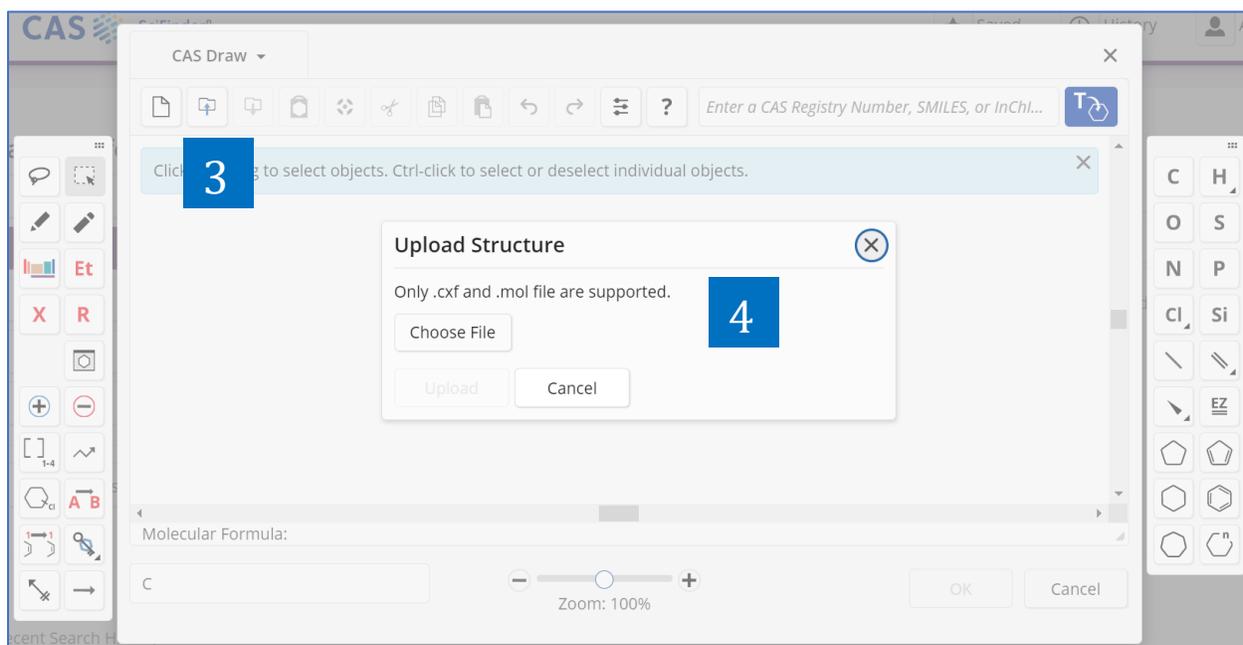
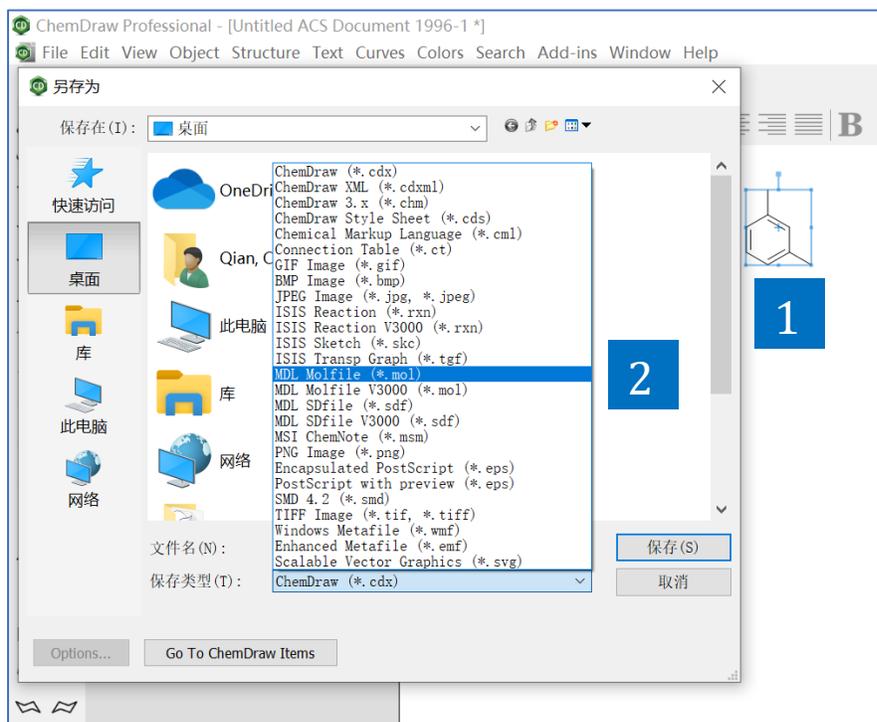
可通过以下三种方式利用 ChemDraw 所绘制的结构在 CAS SciFinder[®] 中进行检索。

- 一. 利用在 ChemDraw 中获得的物质 SMILES、InChI，将结构导入到 CAS SciFinder[®] 的结构编辑器中：





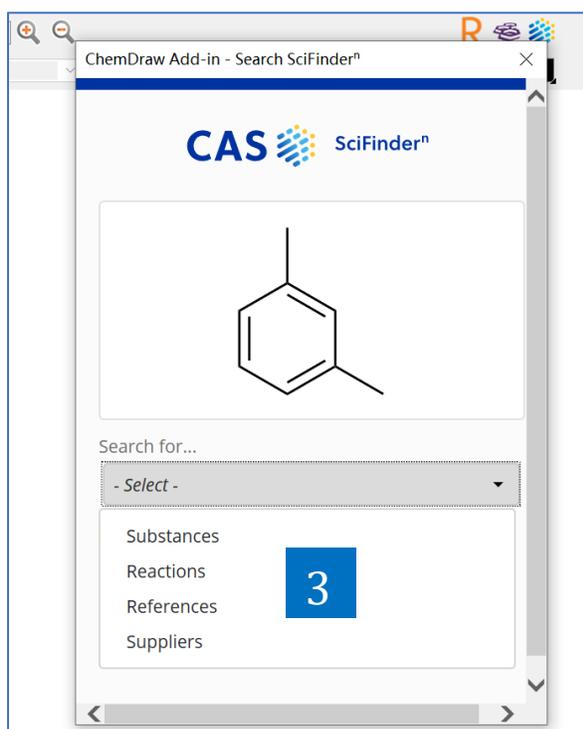
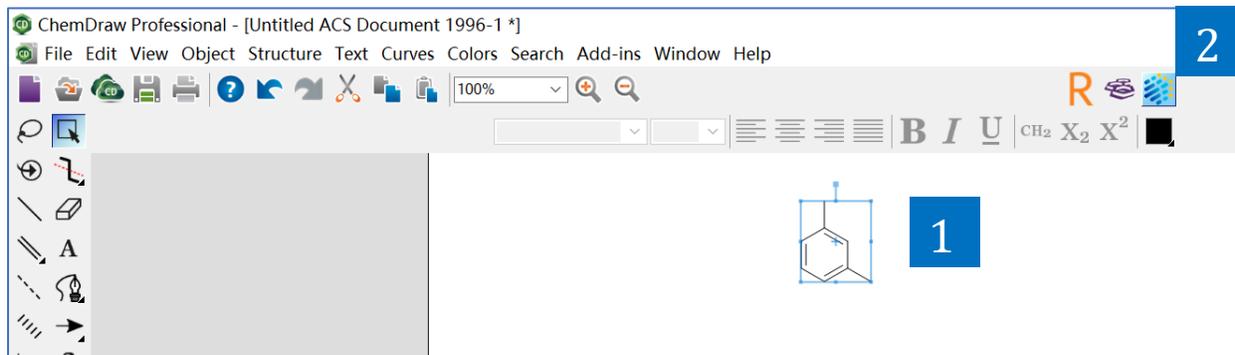
1. 在 ChemDraw 中绘制好结构，并选中。
 2. 点击上方菜单 Edit，选择 Copy As，然后再选择 SMILES 或 InChI。
 3. 在此粘贴在 ChemDraw 中获得的 SMILES 或 InChI，将结构导入到 CAS SciFinder[®] 的结构编辑器中。
- 二. 将 ChemDraw 中绘制的结构保存为 .mol 格式文件，然后再导入到 CAS SciFinder[®] 的结构编辑器中：



1. 在 ChemDraw 中绘制好结构，并选中。
2. 点击上方菜单 File，选择 Save As，将其保存为 MDL Molfile (*.mol)格式的文件。
3. 导入结构。
4. 根据保存的路径，导入.mol 格式的文件。

如需更多 CAS SciFinder[®] 帮助，请联系 china@acs-i.org, 010-63508026/7

三. 直接在 ChemDraw 18.2 以上版本中，点击 Search SciFinder[®] 或点击右上角的 CAS SciFinder[®] 标识图标，则可直接跳转至 CAS SciFinder[®] 中进行检索。



1. 绘制结构并选中。
2. 点击 
3. 选择检索类型，在 CAS SciFinder[®] 中检索 Chemdraw 中绘制的结构。

通过质谱-核磁谱图联用助力物质结构解析

The screenshot displays the CAS SciFinder[®] search interface. At the top, there are navigation options: 'All', 'Substances', 'Reactions', 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'. The search bar is labeled 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More'. A search query is entered: 'total synthesis (5 AND Chemical N AND Concept: stereo*'. A dropdown menu is open, showing 'Molecular Formula' selected, with a sub-menu for 'Chemical Properties' where 'Molecular Weight' is highlighted. The search bar also includes a 'Draw' button and a search icon. Below the search bar, there are examples: 'Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N'. A 'Recent Search History' section shows a search from January 5, 2022, at 9:20 AM. At the bottom right, there are buttons for 'Rerun Search' and 'Edit Search'.

1. 选择 Substances
2. 通过 Advanced Search, 使用 Experimental Spectra, 输入核磁图谱数据
3. 通过 Advanced Search, 使用 Chemical Properties, 选 Molecular Weight 输入分子量数据

Searching for...

- All
- Substances**
- Reactions
- References
- Suppliers
- Biosequences
- Retrosynthesis

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query... Draw 7

Molecular Weight 4 272.38 ×
 Predicted values only. *Examples: 46.07 | 125 to 350 | >300*

AND 5 Carbon-13 NMR 6 155.02, 127 to 129 ×
 Allowance of ± 2 ppm. *Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187*

+ Add Advanced Search Field Learn more about SciFinder[®] Advanced Search.

- 选择分子量，输入具体值或者是区间范围
- 选择逻辑算符（and, or, not）
- 输入核磁数值，可以是具体值或者区间范围
- 开始检索

CAS SciFinder[®] Substances Edit Search Enter a query... × Draw Q ★ 🕒 👤

Substances (6) 8 Sort: Relevance View: Partial

References Reactions Suppliers ↓ ✉ ★ Save And Alerts

Filter Behavior

Filter by Exclude

Commercial Availability

- Available (2)
- Not Available (4)

Reaction Role

- Product (2)
- Reactant (2)
- Reagent (2)
- Catalyst (1)

Reference Role

- Properties (6)
- Adverse Effect (2)
- Agricultural Use (2)
- Analyte (2)
- Analytical Reagent Use (2)
- [View All](#)

Stereochemistry

- Absolute stereochemistry shown

Number of Components

Substance Class

1 221255-16-9 9

 $C_{18}H_{24}O_2$
 (2Z,4E,6E,8E)-8-[(2E)-2-Ethylidene-cyclohexylidene]-3,7-dimethyl-2,4,6-octatrienoic acid
 1 Reference 0 Reactions 0 Suppliers

2 50-28-2

 $C_{18}H_{24}O_2$
 Estradiol
 147K References 955 Reactions 132 Suppliers

3 221315-96-4

 $C_{18}H_{24}O_2$
 (2E,4E,6E,8E)-8-[(2E)-2-Ethylidene-cyclohexylidene]-3,7-dimethyl-2,4,6-octatrienoic acid
 1 Reference 0 Reactions 0 Suppliers

4 57-91-0

 $C_{18}H_{24}O_2$
 Estradiol
 Absolute stereochemistry shown

5 221255-12-5

 $C_{18}H_{24}O_2$
 Double bond geometry shown

6 221315-95-3

 $C_{18}H_{24}O_2$
 Double bond geometry shown

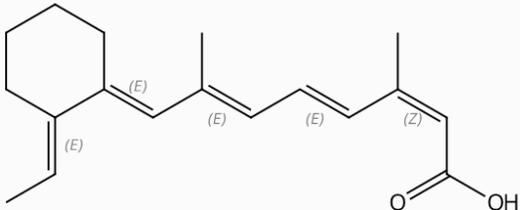
8. 获得的物质结果均满足检索需求
9. 点击物质 CAS 登记号查看物质详情

CAS SciFinder[®] Substances ▾ Edit Search Enter a query... Draw 🔍 ☆ 🕒 👤

Substance Detail (1 of 6) ← Prev Next →

Reference (1) Reactions (0) Suppliers (0) 📄 📧 ☆ Save

CAS Registry Number
221255-16-9



Double bond geometry shown

$C_{18}H_{24}O_2$
2,4,6-Octatrienoic acid, 8-[(2E)-2-ethylidenecyclohexylidene]-3,7-dimethyl-, (2Z,4E,6E,8E)- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	272.38	-
Boiling Point (Predicted)	457.2±14.0 °C	Press: 760 Torr
Density (Predicted)	1.098±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	4.76±0.33	Most Acidic Temp: 25 °C

[Spectra](#)

10. 查看物质分子量

Other Names and Identifiers

Experimental Spectra

¹³C NMR

11

[View Carbon-13 NMR Spectrum](#)

12

Source

(1) ACD

13

Sources

(1) Muccio, D. D.; Magnetic Resonance in Chemistry, (1999), 37(1), 82-85, Cplus

Predicted Properties

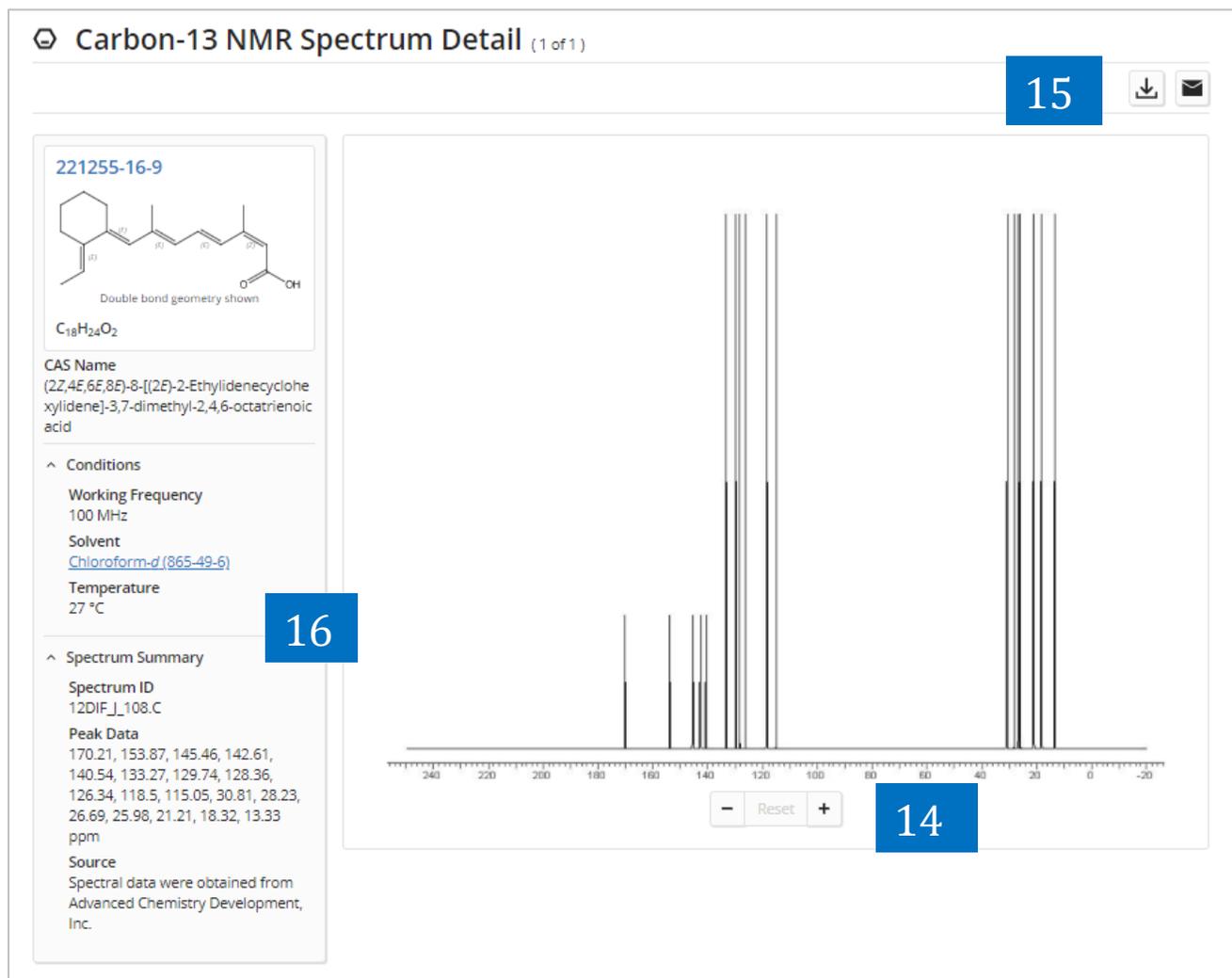
Predicted Spectra

Additional Details

11. 物质详情中的实验谱图

12. 点击超链接，查看核磁谱图

13. 谱图信息的文献来源



14. 缩放谱图

15. 下载谱图图片和谱图详情

16. 测试条件和谱图数据

通过生物活性、靶点筛选物质

The screenshot displays the CAS SciFinder search results page. On the left, there are two filter sections: 'Bioactivity Indicator' (labeled with a blue '1') and 'Target Indicator' (labeled with a blue '2'). The 'Bioactivity Indicator' section includes options like 'Reproductive control agents (58)', 'Hormone antagonists (13)', 'Cardiovascular agents (12)', 'Receptor antagonists (11)', and 'Nervous system agents (9)'. The 'Target Indicator' section includes 'Nuclear proteins (13)', 'Signaling proteins (13)', 'Transcription factors (13)', 'Cell cycle regulatory proteins (2)', 'Enzymes (2)', and 'Membrane proteins (2)'. The main area shows a grid of substance results. Each result includes a CAS number, a chemical structure, the molecular formula, and a list of associated references, reactions, and suppliers. For example, the first result is CAS 1186600-57-6, with molecular formula $C_{26}H_{32}O_3$ and 1 reference, 1 reaction, and 0 suppliers. The second result is CAS 1373991-22-0, with molecular formula $C_{24}H_{32}O_3$ and 2 references, 4 reactions, and 0 suppliers. The third result is CAS 1373991-21-9, with molecular formula $C_{24}H_{32}O_3$ and 2 references, 4 reactions, and 0 suppliers. The fourth result is CAS 1186600-56-5, with molecular formula $C_{25}H_{32}O_3$ and 1 reference, 1 reaction, and 0 suppliers. The fifth result is CAS 1186600-55-4, with molecular formula $C_{25}H_{32}O_3$ and 1 reference, 1 reaction, and 0 suppliers. The sixth result is CAS 1186600-54-3, with molecular formula $C_{26}H_{32}O_3$ and 2 references, 2 reactions, and 0 suppliers.

1. 在物质结果集页面左侧，点击 Bioactivity Indicator，根据适应症筛选物质
2. 点击 Target Indicator，根据靶点筛选物质
3. 点击物质 CAS 登记号，获取物质的生物活性及靶点详情

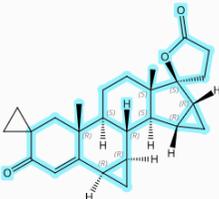
CAS SciFinder[®] Substances Enter a query... Edit Search Star Clock User

Return to Results

Substance Detail (4 of 13) 4

Reference (1) Reaction (1) Suppliers (0) Download Email Save

CAS Registry Number
1186600-57-6



Absolute stereochemistry shown

$C_{26}H_{32}O_3$
Dispiro[cyclopropane-1,2':[2H]dicyclopropa[6,7:15,16]cyclopenta[σ]phenanthrene-17(3'H),2'(5'H)-furan]-3',5''-dione, 1',3'',4'',6',7',8',9',10',11',12',13',14',15',16',20',21'-hexadecahydro-10',13'-dimethyl-, (2'S,6'R,7'R,8'R,9'S,10'R,13'S,14'S,15'R,16'R)- (ACI)

Key Physical Properties	Value	Condition
Molecular Weight	392.53	-
Boiling Point (Predicted)	582.4±50.0 °C	Press: 760 Torr
Density (Predicted)	1.29±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr

- Other Names and Identifiers
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators 5
 - Hormone antagonists
 - Antiprogestins (1)
 - Reproductive control agents
 - Contraceptives (1)
- Target Indicators 6
 - Nuclear proteins
 - Androgen receptors (1)
 - Glucocorticoid receptors (1)
 - Mineralocorticoid receptors (1)
 - Progesterone receptors (1)
 - Signaling proteins
 - Androgen receptors (1)
 - Glucocorticoid receptors (1)
 - Mineralocorticoid receptors (1)
 - Progesterone receptors (1)
 - Transcription factors
 - Androgen receptors (1)
 - Glucocorticoid receptors (1)
 - Mineralocorticoid receptors (1)
 - Progesterone receptors (1)
- Additional Details

4. 点击物质的 CAS 登记号，即可获得物质详情。
5. 在物质详情页面，点击 Bioactivity Indicators 下方的蓝色超链接，即可获得相应适应症的研究文献。
6. 在物质详情页面，点击 Target Indicators 下方的蓝色超链接，即可获得相应靶点的研究文献。

获取物质信息

1. 选择 Substances，进行物质检索
2. 输入检索文本：物质名称、CAS 登记号、专利号等
3. 点击 Draw，绘制结构
4. 点击 Add Advanced Search，用逻辑运算符连接不同字段进行分子式、物质属性和实验谱图等检索
5. 开始检索

CAS SciFinder[®] Substances Enter a query... Edit Search Star Clock User

Return to Home

Structure Match **1**

As Drawn (16)

Substructure (24)

Similarity (24K)

Analyze Structure Precision **2**

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior **3**

Filter by Exclude

Commercial Availability

Substances (16) Sort: Number of References: Descending View: Partial

References Reactions Suppliers **4** Save And Alerts

1 610798-31-7 **8**

C22H21N3O4
Icotinib

2 1204313-51-8

C22H21N3O4.ClH
Components: 2
Component RN: 610798-31-7
[1,4,7,10]Tetraoxacyclododecino[2,3-g]quinazolin-4-amine, N-(3-ethynylphenyl)-7,...

3 1567366-94-2 **7**

C22H16D5N3O4
N-[3-(Ethynyl-2-d)phenyl]-7,8,10,11,13,14-hexahydro-10,11-d₂[1,4,7,10]tetraoxacy...

573 References 133 Reactions 40 Suppliers

61 References 13 Reactions 39 Suppliers

2 References 22 Reactions 0 Suppliers

Filter Behavior

Filter by Exclude

Commercial Availability

Reaction Role

Reference Role

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Bioactivity Indicator

Target Indicator

Search Within Results

Filter Content Report

Download filter data from this result set.

573 References 133 Reactions 40 Suppliers

61 References 13 Reactions 39 Suppliers

2 References 22 Reactions 0 Suppliers

4 1567366-93-1 **9**

C22H8D13N3O4
N-[3-(Ethynyl-2-d)phenyl]-7,8,10,11,13,14-hexahydro-7,8,10,11,13,14-d₆[1,4,7,10]...

2 References 19 Reactions 0 Suppliers

5 1567366-92-0

C22H12D9N3O4
N-[3-(Ethynyl-2-d)phenyl]-7,8,10,11,13,14-hexahydro-7,8,13,14-d₄[1,4,7,10]tetrao...

2 References 19 Reactions 0 Suppliers

6 1567366-91-9

C22H20DN3O4
N-[3-(Ethynyl-2-d)phenyl]-7,8,10,11,13,14-hexahydro[1,4,7,10]tetraoxacyclododeci...

2 References 2 Reactions 0 Suppliers

7 1567366-90-8

8 1567366-82-8

9 1567366-75-9

1. 如果选择了结构检索，则在结果集页面将呈现结构匹配程度：As Drawn 表示被检索结构中的原子和键被锁定后得到的结果；Substructure 表示亚结构检索结果，Similarity 表示相似结构检索结果。

2. 点击 Analyze Structure Precision，对结构检索结果进行更细化的结构分类。
3. 物质结果的聚类分析：商业上可获得性、反应角色、文献角色、立体化学、组份数、物质类型、同位素、金属、分子量、实验属性、实验谱图、管控信息、生物活性、靶点、结构筛选等。
4. 物质结果集中与物质相关的文献、反应和供应商
5. 对物质进行重新排序
6. 选择展示物质信息详略
7. 下载、邮件分享、或保存物质结果并设置提醒
8. 点击 CAS 登记号，查看物质详情
9. 此物质相关的文献、反应和供应商

Substance Detail (1 of 16)

References (558) Reactions (133) Suppliers (39)

CAS Registry Number
610798-31-7

Feedback

C₂₂H₂₁N₃O₄
 [1,4,7,10]Tetraoxacyclododecino[2,3-g]quinazolin-4-amine, N-(3-ethynylphenyl)-7,8,10,11,13,14-hexahydro- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	391.42	-
Boiling Point (Predicted)	581.3±50.0 °C	Press: 760 Torr
Density (Predicted)	1.31±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	5.32±0.20	Most Basic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

- ▼ Other Names and Identifiers
- ▼ Experimental Properties
- ▼ Experimental Spectra

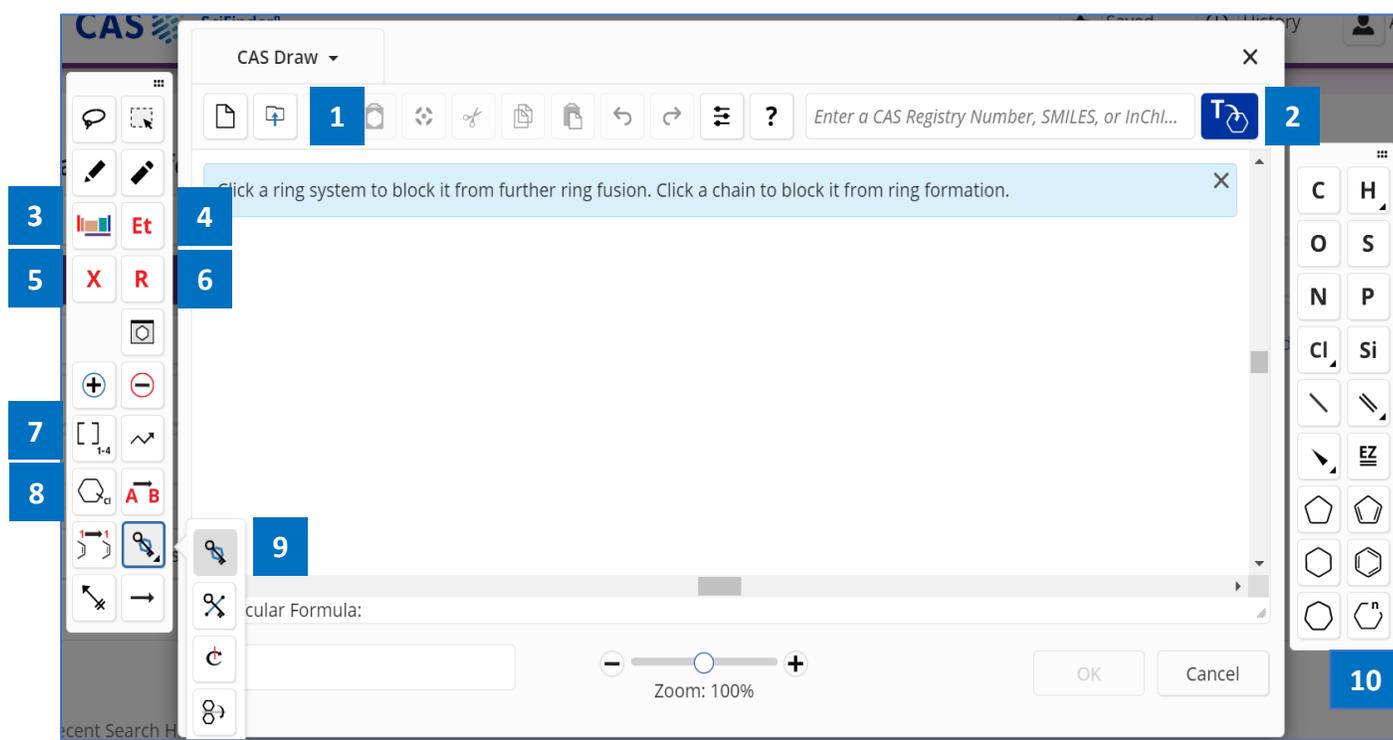
 Feedback

- ▼ Predicted Properties
- ▼ Predicted Spectra
- ▼ Bioactivity Indicators
- ▼ Target Indicators
- ▼ Additional Details

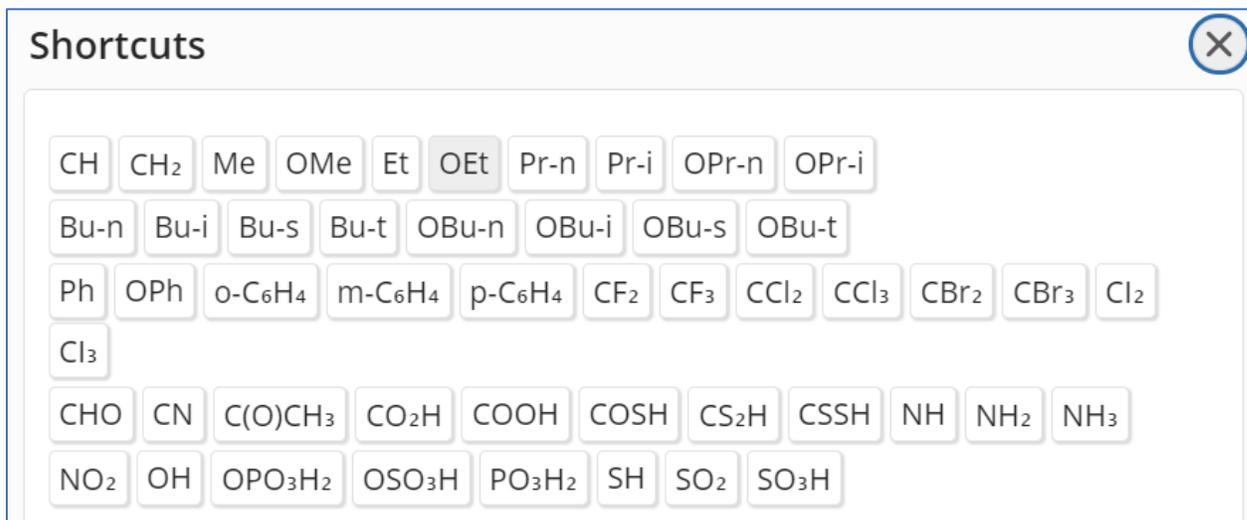
 Feedback

1. 点击左右箭头，查看前一个或后一个物质的详细信息
2. 此物质相关的文献、反应和供应商
3. 下载、分享及保存物质详情
4. 物质的物理属性信息
5. 物质名称、实验属性、实验谱图、预测属性、预测谱图、管控信息及其他信息

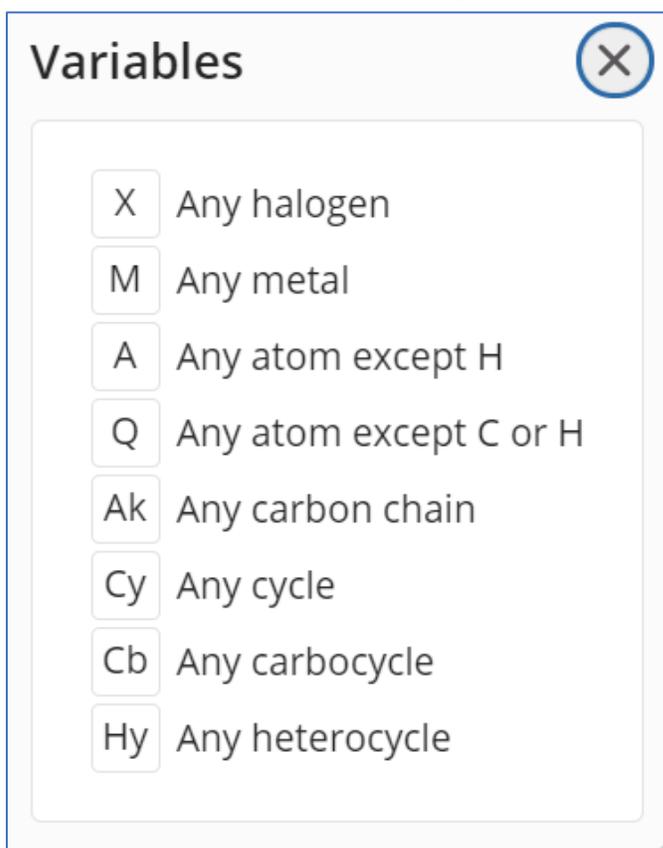
结构编辑器



1. 导入.cxf或者.mol格式文件。
2. 可以直接输入物质的CAS登记号、SMILES或者InChI转化为相应的结构。
3. 元素周期表。
4. 常用官能团列表。



5. 选择可变基团，包括：X: 任意卤素；M: 任意金属；A: 除氢外的任意原子；Q: 除碳/氢外的任意原子；Ak: 任意碳链；Cy: 任意环；Cb: 任意碳环；Hy: 任意杂环。



The image shows a dialog box titled "Variables" with a close button (X) in the top right corner. Inside the dialog, there is a list of variables, each with a small button containing the variable name and a text description to its right:

- X Any halogen
- M Any metal
- A Any atom except H
- Q Any atom except C or H
- Ak Any carbon chain
- Cy Any cycle
- Cb Any carbocycle
- Hy Any heterocycle

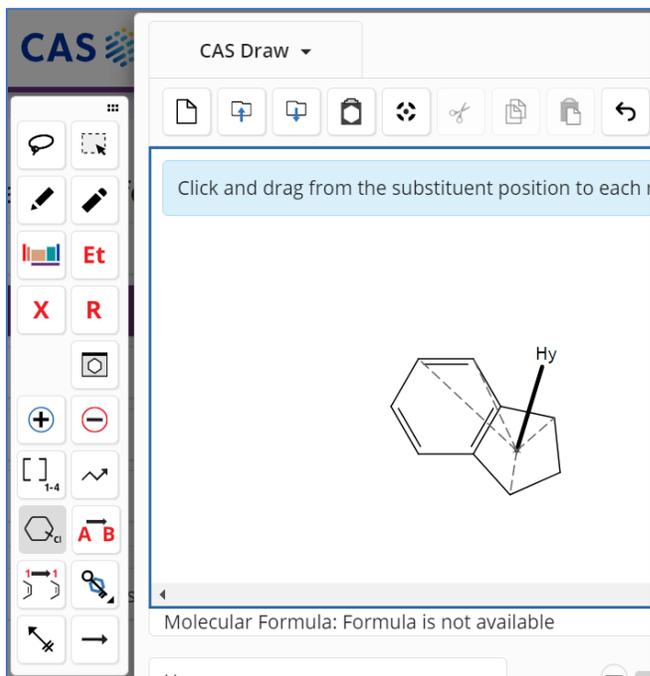
6. 定义R基团。



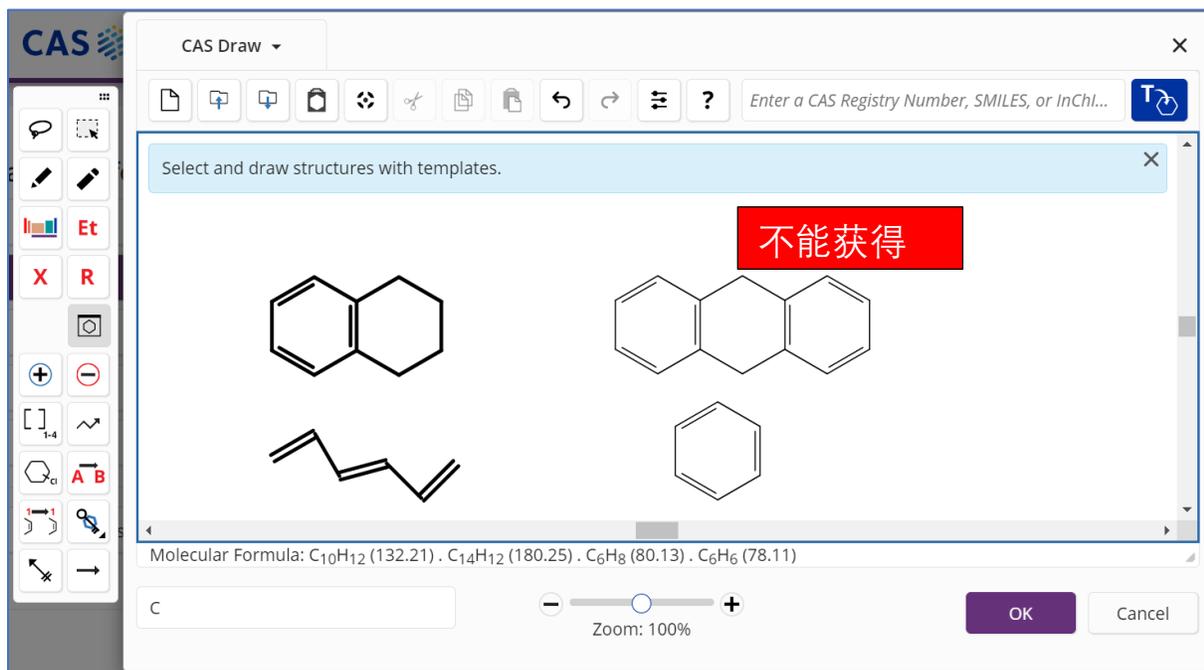
The image shows a dialog box titled "R-Group Definitions" with a close button (X) in the top right corner. At the top, there is a row of buttons labeled R1 through R12, with R1 highlighted in blue and a right-pointing arrow button to the right. Below this is a text input field labeled "R1:". Underneath the input field is a list of expandable categories, each with a right-pointing arrow:

- > Atoms
- > Variables
- > Shortcuts

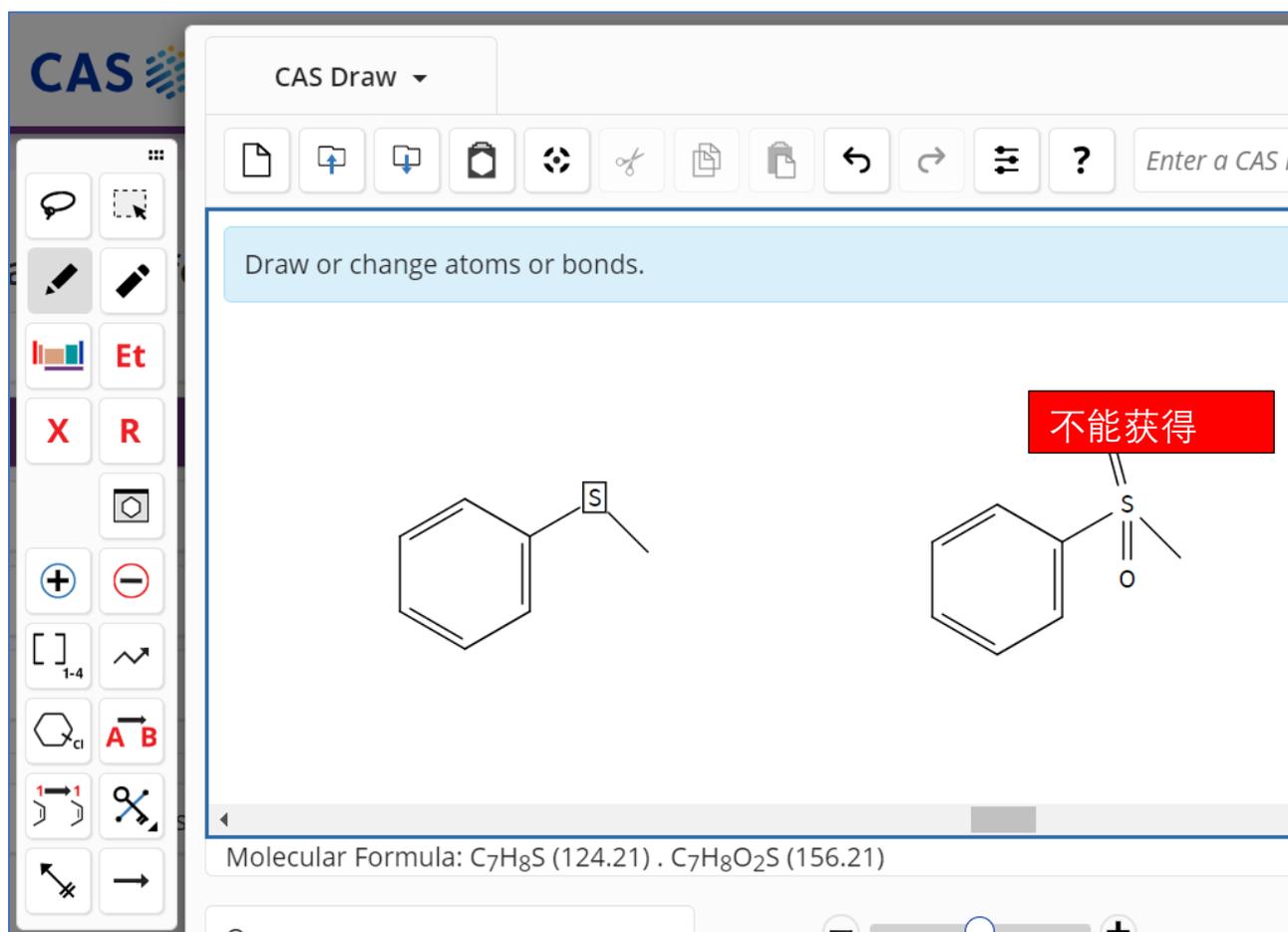
7. 重复原子或者基团。
8. 环上的取代位点不固定。

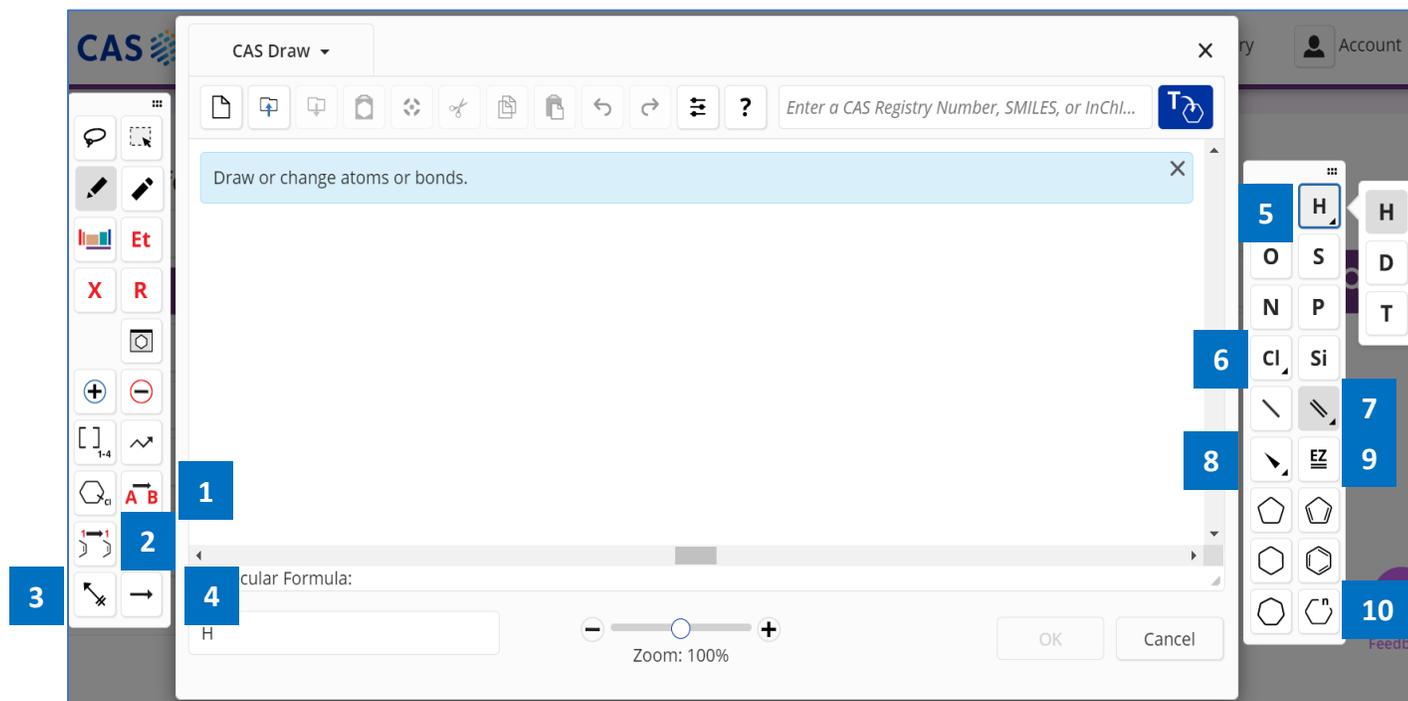


9. 环锁定。当用该功能锁定某个环（系），表示该环（系）不能成为更大环系的一部分；如果用该功能锁定某个链，则表示该链不能成为某个环（系）的一部分。例：

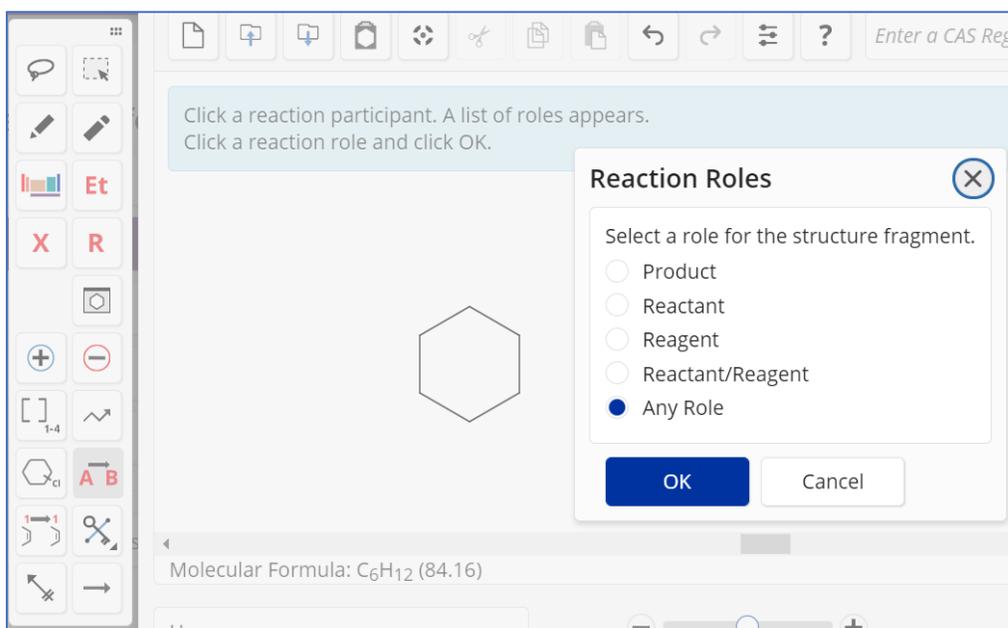


10. 锁定原子。若某原子被锁定，则表明该原子只能连接氢原子。例：





1. 反应角色定义工具，用于定义物质在反应中的角色。



2. 反应原子标记工具。在原料和产物中以相同数字被标记的原子，表明其反应前后为同一原子。
3. 反应键标记工具，起始物的某键被标记，则表明此键在反应过程中发生断开等变化；

产物的某键被标记，则表明此键在反应过程中是新生成的键。

4. 反应箭头。箭头左边的物质是起始物或者试剂，右边为产物。
5. 点击H键，可以选择H原子，或者同位素D或者T。
6. 点击Cl，可以选择卤素：F，Cl，Br，I。
7. 可以选择双键，三键，或者不确定键。
8. 绘制立体键。
9. 用于锁定双键的立体构型，若绘制E构型烯烃，使用此键锁定后，结果集只包含该双键位置为E构型的烯烃，Z构型同理。



10. 绘制指定碳原子个数的碳环。

物质高级检索

The screenshot displays the CAS SciFinder[®] Advanced Search interface. On the left, a sidebar titled "Searching for..." has "Substances" selected, indicated by a blue box with the number "1". Below this, a "Recent Search History" section shows a search from December 28, 2021, at 5:19 PM for "Substances" using "Advanced Search AND Molecular V AND Carbon-13 I".

The main search area is titled "Substances" and includes a search bar with the placeholder "Enter a query...". To the right of the search bar is a "Draw" button (3) and a search icon. Below the search bar, there are dropdown menus for "Molecular Formula" and "AND" (set to "- Select -"). A dropdown menu (2) is open under "Add Advanced Search Field", listing various search criteria: Molecular Formula, CAS Registry Number, Chemical Name, Document Identifier, Patent Identifier, Experimental Spectra, Biological, Chemical Properties, Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, and Thermal.

At the bottom right, a chemical structure of pyridine is shown, along with "Rerun Search" and "Edit Search" buttons.

1. 选择 Substances，然后点击 Add Advanced Search Field。
2. 点击 Select，展示可检索字段。
3. 如果同时还需要检索结构式，则可点击 Draw，绘制结构式。

例 1: 查找符合分子量在 125-350 之间; 核磁碳谱峰值包括 115, 141; 包含吡啶结构片段的物质

The screenshot shows the CAS SciFinder search interface. On the left, a sidebar titled "Searching for..." lists various search categories: All, Substances (highlighted), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main area is titled "Substances" and contains a search bar with the text "Enter a query...". Below the search bar, there are two search criteria: "Molecular Weight" with a range of "125 to 349" and "Carbon-13 NMR" with values "115,141". Both criteria are connected by "AND" operators. A chemical structure of pyridine is shown on the right side of the interface. The interface also includes a "Feedback" button in the bottom right corner and a "Search" button in the top right corner.

1. 选择需要检索的字段（如，Molecular Weight），输入检索式
2. 如果需要其他更多检索字段，则可再次点击 Add Advanced Search Field，添加其他检索字段。不同字段可使用“AND”或“OR”或“NOT”进行连接
3. 输入检索式
4. 绘制好等待检索的结构式
5. 点击检索

获得满足检索需求的物质结果集

例 2：获取玻璃体转化温度在 50-100 摄氏度之间；密度小于 1.5g/cm³ 的聚合物

1. 选择 Substances，然后在文本框输入 poly*（关于星号*的用法，请见 CAS SciFinder[®] 使用技巧之通配符的使用）。
2. 选择 Glass Transition Temperature，输入数值区间。
3. 选择 Density，输入数值区间。
4. 点击检索

获得符合检索需求的结果

如需更多 CAS SciFinder[®] 帮助，请联系 china@acs-i.org, 010-63508026/7

CAS SciFinder[®] Substances Edit Search poly* Draw

Return to Home

Substances (108) Sort: Relevance View: Partial

Filter Behavior

Filter by Exclude

Commercial Availability

Available (98) Not Available (10)

Reaction Role

Product (105) Reactant (100) Reagent (80) Catalyst (66) Solvent (32)

Reference Role

Preparation (108)

References Reactions Suppliers

1 25248-42-4

CCCCC(=O)O

$(C_6H_{10}O_2)_n$
Polycaprolactone

38K References 3,262 Reactions 6 Suppliers

2 9003-39-8

C=CN1CCCC1=O

$(C_6H_9NO)_x$
Poly(vinylpyrrolidone)

152K References 5,885 Reactions 192 Suppliers

3 25322-68-3

HO[CH2CH2O]nH

$(C_2H_4O)_nH_2O$
Polyethylene glycol

398K References 54K Reactions 565 Suppliers

Feedback

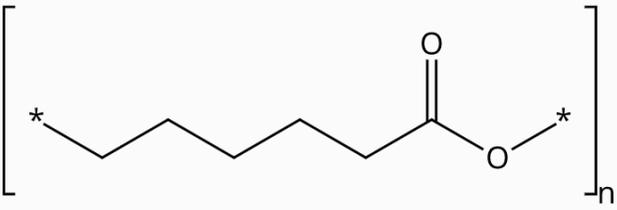
1. 点击物质 CAS 登记号，查看物质信息详情。

可在物质信息详情中查看完整信息。

Substance Detail (1 of 107) ← Prev Next →

References (37K) Reactions (3,067) Suppliers (8) ↓ ✉ ★ Save

CAS Registry Number
25248-42-4



$(C_6H_{10}O_2)_n$ 1

Poly[oxy(1-oxo-1,6-hexanediyl)] (9CI, ACI)

Polymer Class Terms
Polyester

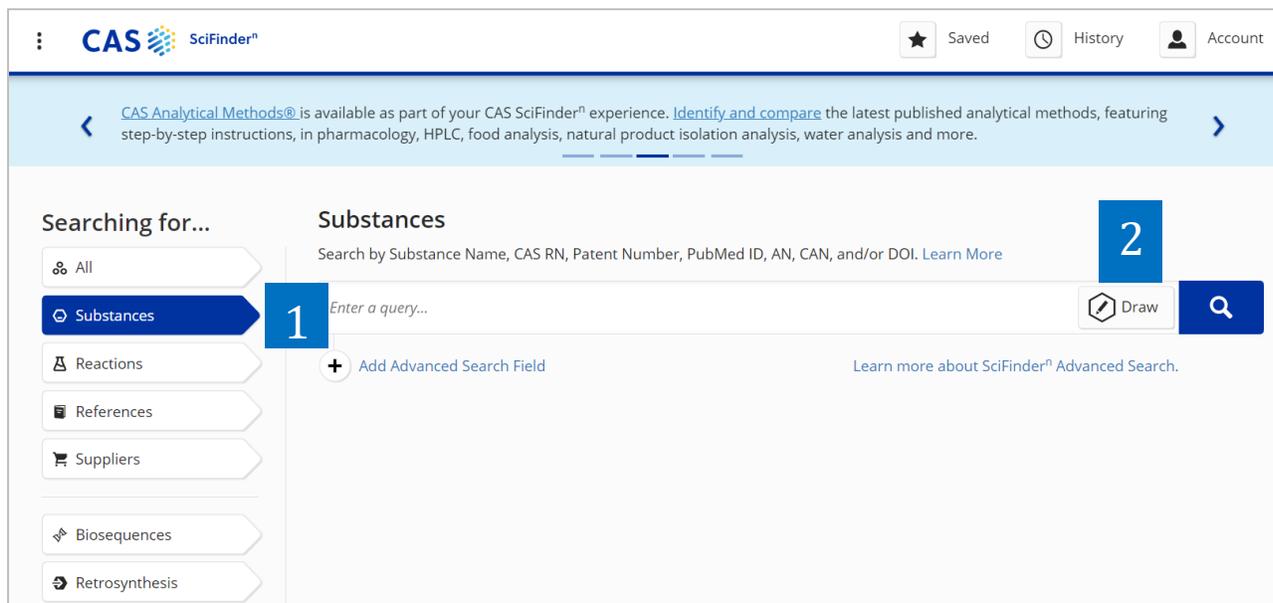
Key Physical Properties	Value	Condition
Melting Point (Experimental)	65.1 °C	-
Density (Experimental)	1.2 g/cm ³	-

Experimental Properties

Property	Value	Condition	Source
Glass Transition Temperature	63.6 °C	-	(1) CAS
Glass Transition Temperature	62.8 °C	-	(1) CAS
Glass Transition Temperature	62.0 °C	-	(1) CAS
Glass Transition Temperature	61.8 °C	-	(1) CAS
Glass Transition Temperature	60.4 °C	-	(1) CAS

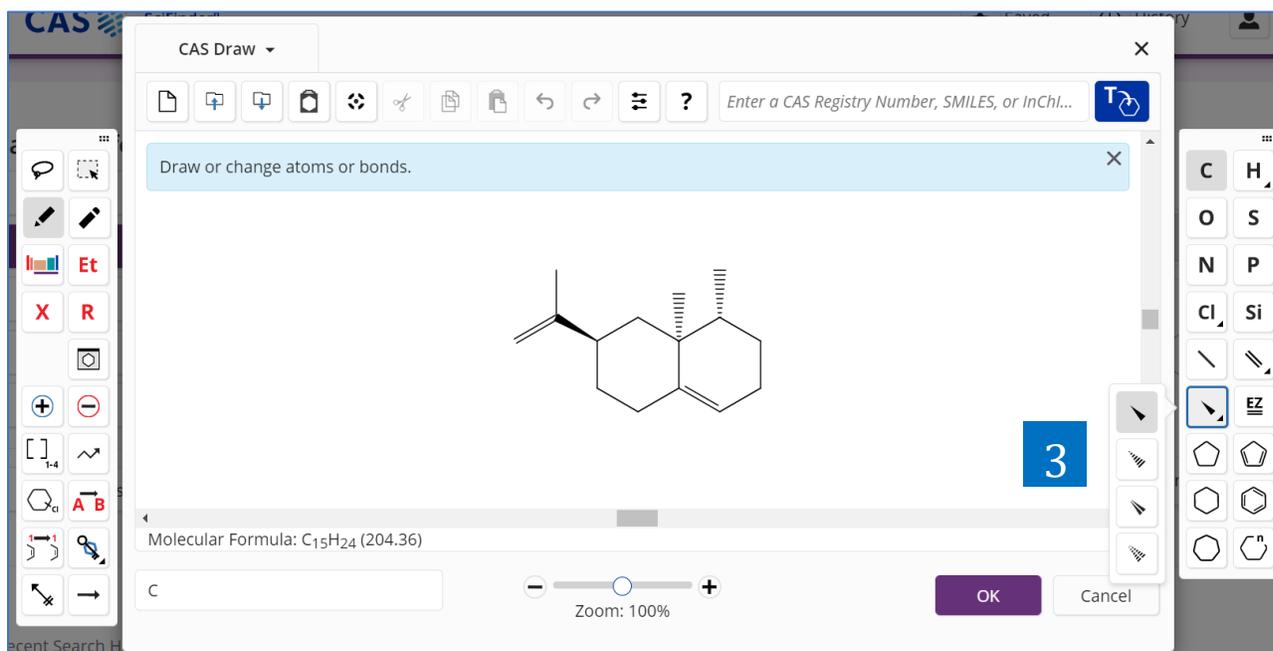
1. 该物质为一种聚酯。
2. 该聚合物的密度为 1.2g/cm³。
3. 该聚合物的玻璃体转化温度。

手性化合物的检索



CAS SciFinder[®] interface showing the search process. The search bar is highlighted with a blue box labeled '1', and the search results section is highlighted with a blue box labeled '2'.

1. 选择 Substances，进行物质检索。
2. 在结构编辑器中绘制出手性化合物的结构。



CAS Draw interface showing the chemical structure editor. The structure is drawn with a wedge bond to indicate stereochemistry. The editor includes a toolbar with various drawing tools, a search bar for CAS Registry Number, SMILES, or InChI, and a zoom control. A blue box labeled '3' is positioned near the structure.

3. 绘制结构时，使用手性异构键标注结构中的手性特征。

The screenshot displays the CAS SciFinder search results page. The search criteria are 'Stereochemistry: Absolute Stereo Match'. The results are presented in a grid format, showing chemical structures and their associated CAS numbers and details. A blue box with the number '4' highlights the 'Stereochemistry' filter section on the left sidebar.

Structure Match

- As Drawn (22)
- Substructure (5,432)
- Similarity (22K)
- Analyze Structure Precision

Chemscap Analysis

Visually explore structure similarity with a powerful new tool. [Learn more about Chemscap.](#)

Filter Behavior

Filter by Exclude

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry**
 - Absolute Stereo Match (11)
 - Absolute Stereo Mirror Image (1)
 - Relative Stereo Match (1)
 - Stereo that Doesn't Match Query (8)
 - No Stereo in Answer Structure (1)

Substances (11)

References Reactions Suppliers

Filtering: Stereochemistry: Absolute Stereo Match

1 2 3 4 5 6

4630-07-3
 Absolute stereochemistry shown, Rotation (-)
 $C_{15}H_{24}$
 Valencene
 3,069 References 156 Reactions 35 Suppliers

1174496-34-4
 Absolute stereochemistry shown
 $C_{15}H_{19}D_5$
 (1R,7R,8aS)-1,2,3,5,6,7,8,8a-Octahydro-1,8a-dimethyl-7-[1-(methyl- d_3)ethenyl]-2,2...
 2 References 2 Reactions 0 Suppliers

2279054-76-9
 Absolute stereochemistry shown, Rotation (-)
 $(C_{15}H_{24}\cdot C_3H_3N)_x$
 Components: 2
 1 Reference 1 Reaction 0 Suppliers

225114-69-2

2374919-94-3
 9012-76-4
 Image Not Available

2279054-69-0

4. 在物质结果集中，通过左侧 Stereochemistry 浏览并选择需要的手性物质。

检索同位素标记的化合物

可通过输入分子式或绘制结构式获取同位素标记的化合物。

方法一： 输入分子式获取同位素标记的化合物（此方法只适用于 H 的同位素 D 和 T 标记的分子）。

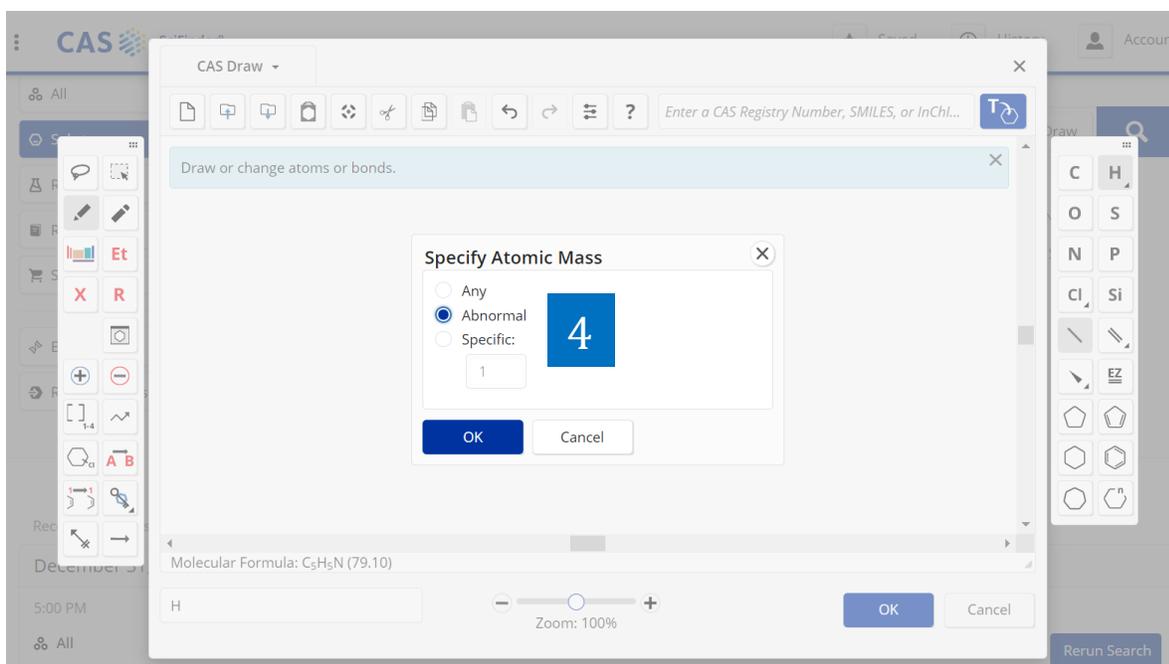
The screenshot shows the SciFinder search interface. On the left, under 'Searching for...', there is a list of search categories: All, Substances, Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The 'Substances' category is selected and highlighted with a blue arrow and a red callout '1'. The main search area is titled 'Substances' and contains a search bar with the placeholder text 'Enter a query...'. Below the search bar, there is a dropdown menu for 'Molecular Formula' with 'C6D6' entered. A red callout '2' points to the 'Add Advanced Search Field' button. To the right of the search bar, there is a 'Draw' button and a search button with a magnifying glass icon. A red callout '3' points to the search button. Below the search bar, there are examples of molecular formulas: 'Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N' and a link to 'Learn more about SciFinder[®] Advanced Search.'

1. 点击 Substances
2. 点击 Add Advanced Search Field, 选择 Molecular Formula, 然后输入分子式（如可直接输入 H 的同位素 D 或 T）。
3. 开始检索

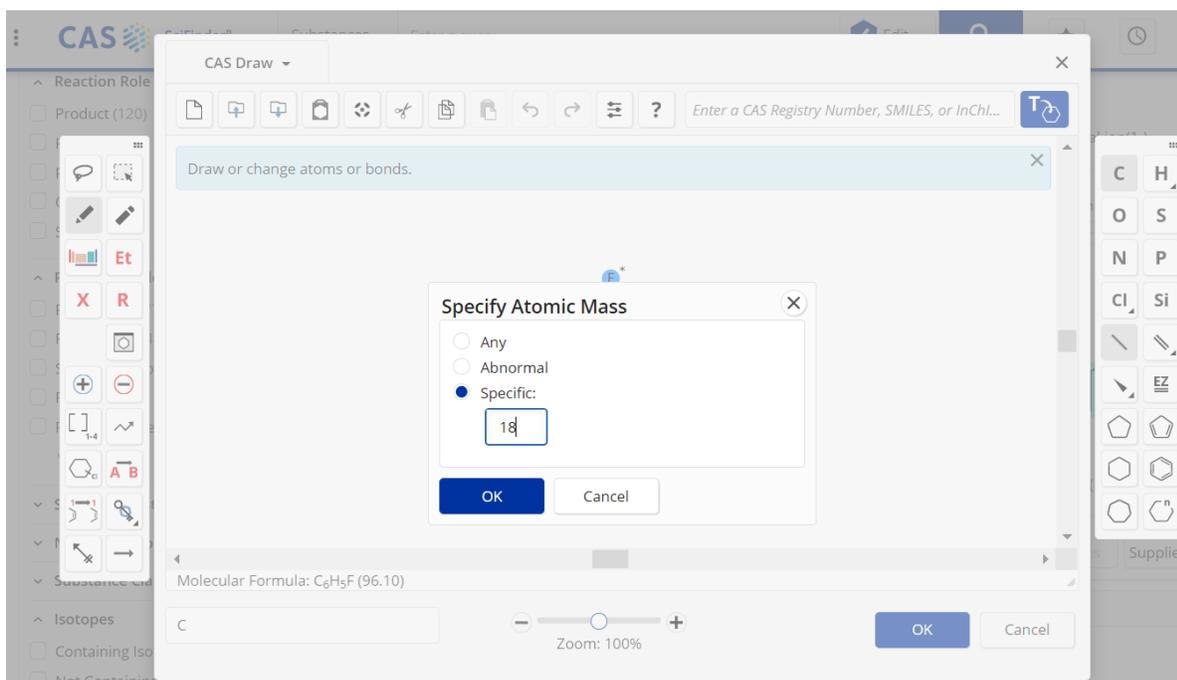
方法二：通过结构式检索同位素标记的物质（适用于所有元素的同位素标记分子）。

3. 鼠标悬在绘制结构中的原子上（例如 F），点击鼠标右键。

如需更多 CAS SciFinder[®] 帮助，请联系 china@acs-i.org, 010-63508026/7



4. 在弹出窗口中点击 Abnormal，可获取所有 F 原子的同位素标记物；点 Specific 可输入特定的氟同位素相对原子质量，例如输入 18，点击 OK。



Searching for...

All

Substances

Reactions

References

Suppliers

Biosequences

Retrosynthesis

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

AND Molecular Formula

Examples: C₆H₆ | (C₈H₈)_x | C₆H₅NO₂

+ Add Advanced Search Field

Learn more about SciFinder

5

Edit

Search

Chemical structure: Fluoro-¹⁸Fbenzene

Edit Drawing Remove

Search Patent Markush

5. 开始检索，获取感兴趣的结果。

CAS SciFinder[®]

Substances Enter a query...

Edit Search

Return to Home

Structure Match

As Drawn (1)

Substructure (3,282)

Similarity (2,398)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. [Learn more about Chemscape.](#)

Create Chemscape Analysis

Substances (1)

References Reactions Suppliers

1

3857-04-3

Chemical structure: Fluoro-¹⁸Fbenzene

C₆H₅F
Fluoro-¹⁸Fbenzene

68 References 190 Reactions 1 Supplier

Edit Drawing Remove

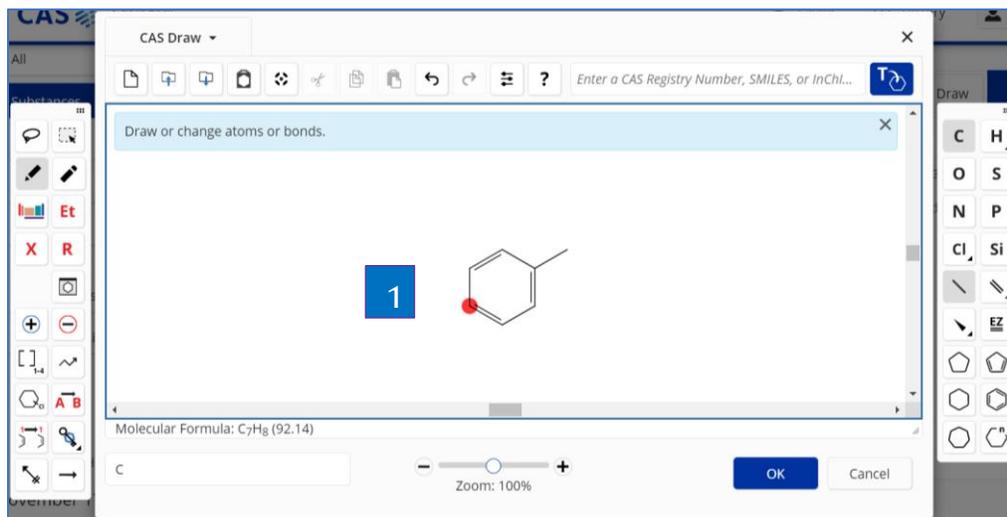
Search Patent Markush

View: Partial

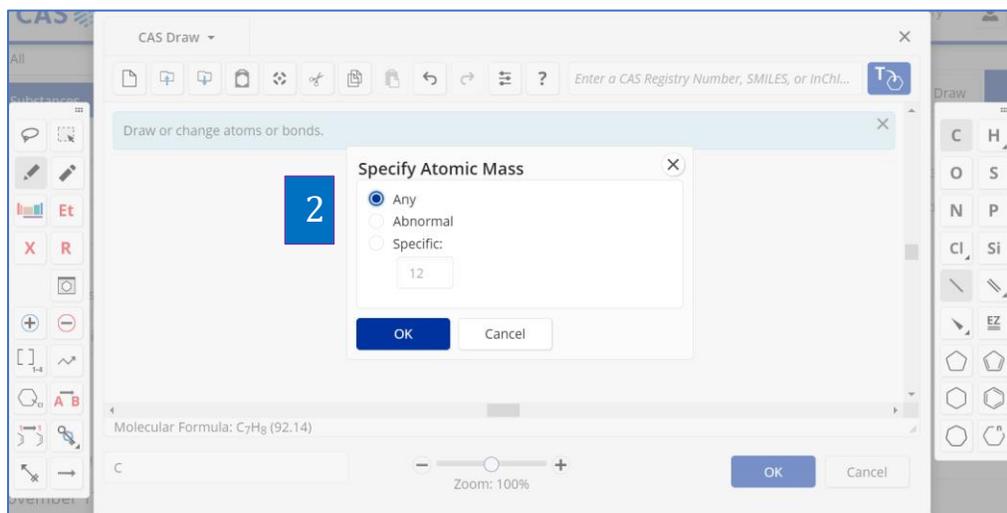
Save And Alerts

绘制结构式时，如何绘制同位素

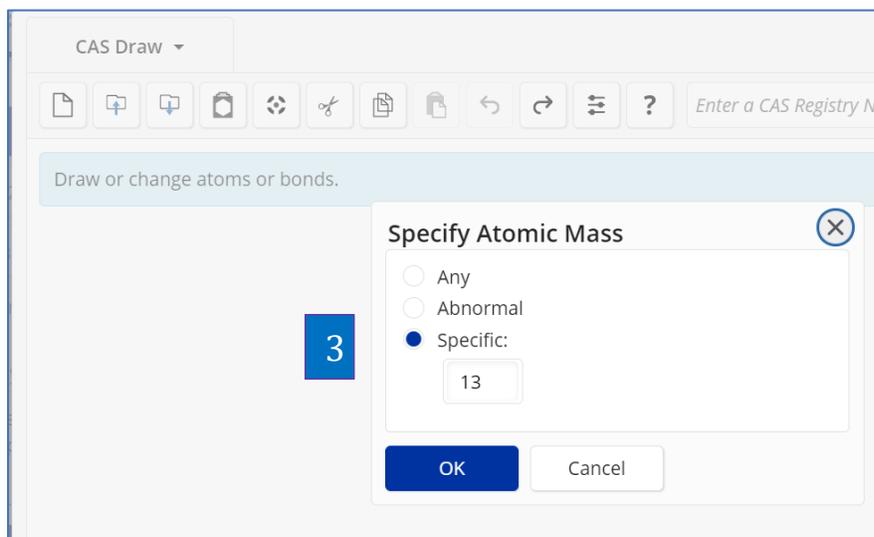
绘制结构时，可绘制特定原子的同位素，以获取其同位素标记的物质、同位素标记的物质参与的反应、研究同位素标记的物质的文献等信息。



1. 绘制结构，选中需要标记同位素的原子，点击鼠标右键。

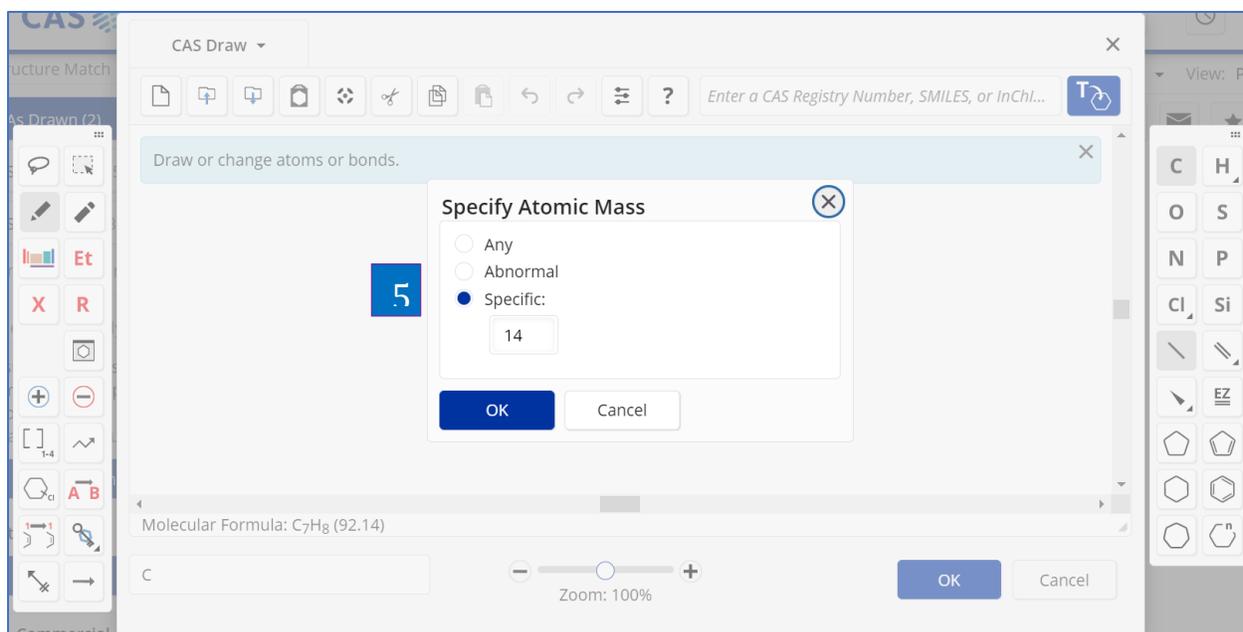


2. 在弹出窗口中，选择原子量为 Any（默认值，任意元素）、Abnormal（任意同位素）或 Specific（特定同位素）。



3. 选择 Specific，并输入数值 13，表面此处的碳原子为 ^{13}C 。

4. 所得结果均为满足设定需要：甲基对位的碳为 ^{13}C 。



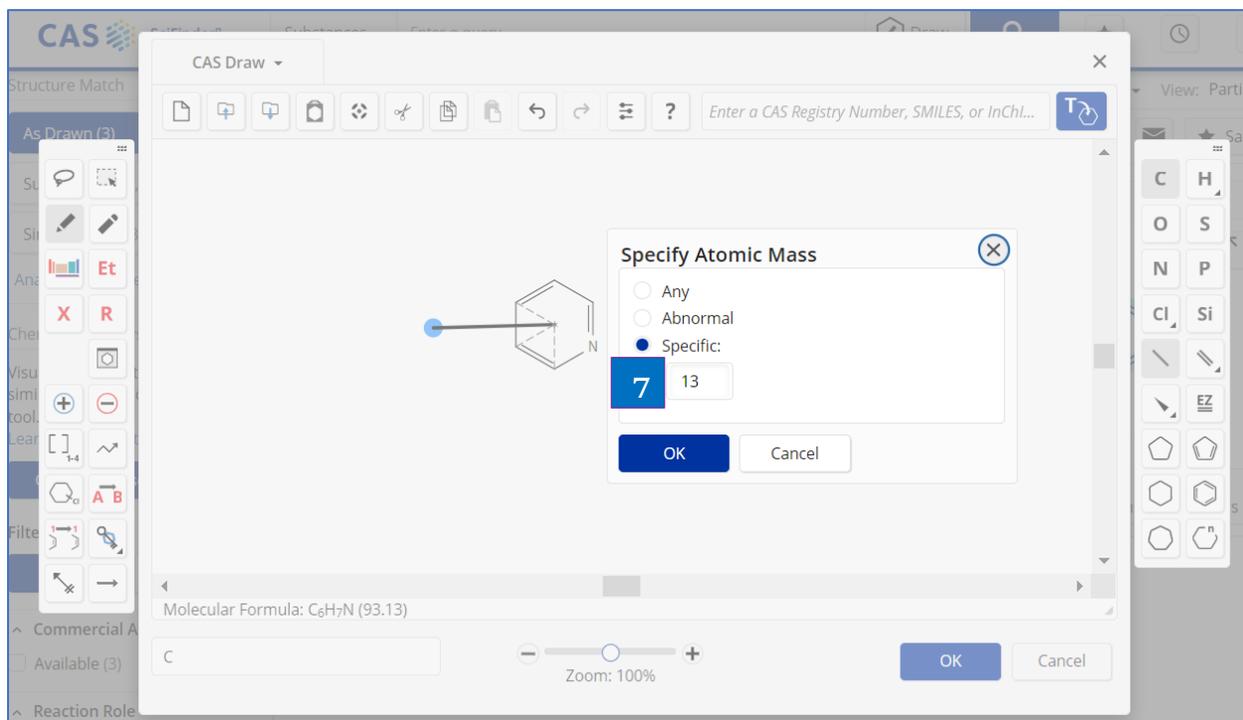
5. 若希望甲基对位的碳原子为 ^{14}C ，则输入值 14

6. 获得指定原子为 ^{14}C 的物质。

案例

获取具如下结构特征的物质：

吡啶环中 N 原子的邻位、间位或者对位至少连接一个甲基，且甲基碳为 ¹³C。



7. 将甲基碳的原子量设置为 13

CAS SciFinder® Substances

8

Substances (4)

Structure Match

As Drawn (4)

Substructure (292)

Similarity (3,128)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Not Available (4)

Reaction Role

References Reactions Suppliers

1630788-91-8

Cc1cccnc1

C_6H_5N
4-Pyridinylmethylene- ^{13}C

1 Reference 8 Reactions 0 Suppliers

1529772-81-3

C1=CC=C(C=C1)C2=CC=CC=N2

$C_6H_4D_3N$
4-(Methyl- ^{13}C - d_3)pyridine

1 Reference 1 Reaction 0 Suppliers

1404120-05-3

Cc1cccnc1

C_6H_7N
4-(Methyl- ^{13}C)pyridine

3 References 4 Reactions 0 Suppliers

813432-91-6

Cc1ccccn1

4

Descending View: Partial

Edit Drawing Remove

Search Patent Markush

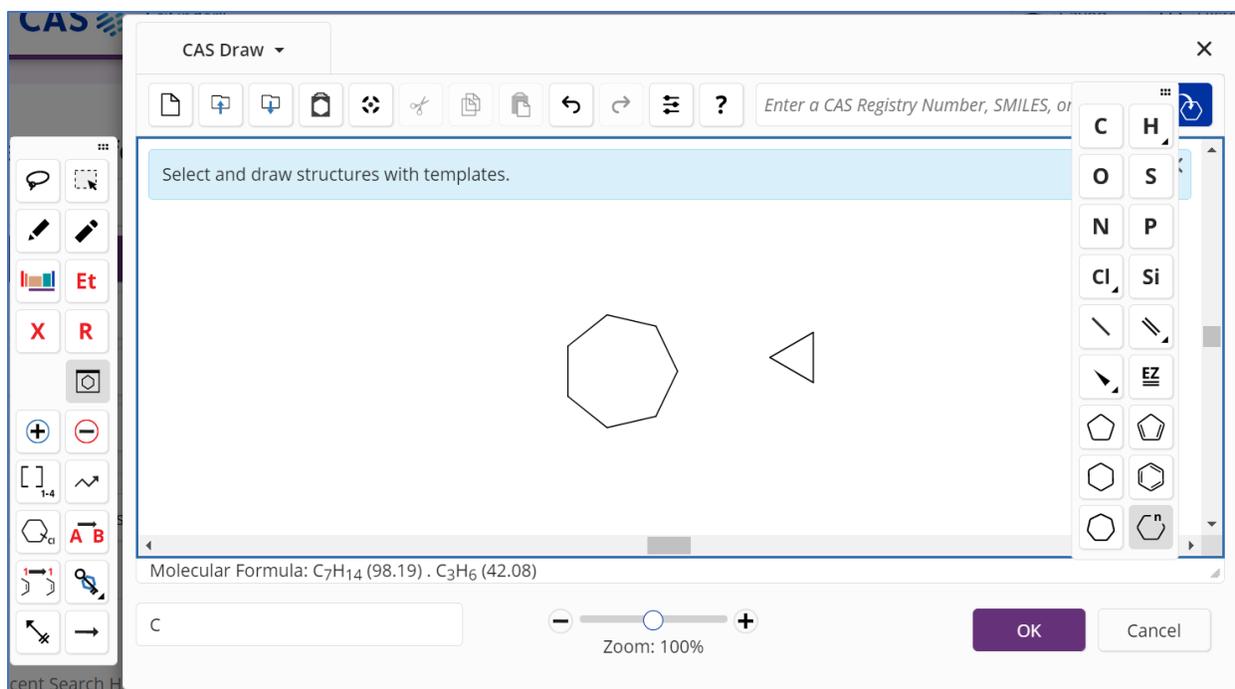
8. 获得满足要求的物质。

片段结构的物质检索

如果希望某些重要的结构片段一定要出现在物质中，且对这些片段相互之间的连接方式和位置不明确要求的话，则可以在 CAS SciFinder[®] 中用片段结构检索来实现。

The screenshot shows the CAS SciFinder search interface. On the left, under 'Searching for...', the 'Substances' option is selected. In the center, the 'Substances' search bar is highlighted with a blue box and the number '1'. To the right, the 'Draw' button is highlighted with a blue box and the number '2', and the search button is highlighted with a blue box and the number '3'. The interface includes a navigation menu on the left, a top navigation bar with 'Saved', 'History', and 'Account' options, and a banner at the top about BLAST search.

1. 选择 Substances，进行物质检索。
2. 点击 Draw，打开结构编辑器并绘制结构。
3. 开始检索。



CAS SciFinder®

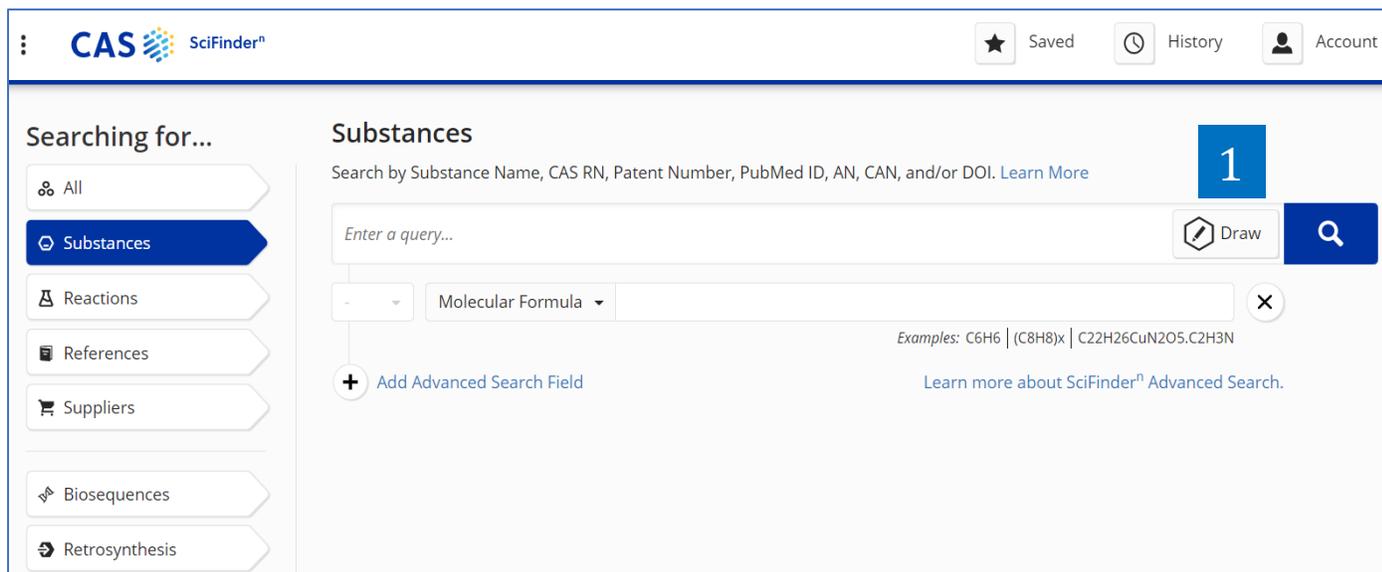
Substances Enter a query... Edit

Reference	Reactions	Suppliers
<p>7</p> <p>1821719-88-3</p> <p>Absolute stereochemistry shown</p> <p>$C_{10}H_{19}N$ Cycloheptanamine, 2-cyclopropyl-, (1R,2S)-</p> <p>0 References 0 Reactions 1 Supplier</p>	<p>8</p> <p>1488617-56-6</p> <p>$C_{11}H_{21}N$ α-Cyclopropylcycloheptanemethanamine</p> <p>0 References 0 Reactions 6 Suppliers</p>	<p>9</p> <p>1344060-41-8</p> <p>$C_{10}H_{19}N$ 2-Cyclopropylcycloheptanamine</p> <p>0 References 0 Reactions 3 Suppliers</p>
<p>10</p> <p>1340186-29-9</p> <p>$C_{10}H_{19}N$ 3-Cyclopropylcycloheptanamine</p>	<p>11</p> <p>2350332-22-6</p> <p>Absolute stereochemistry shown</p> <p>$C_{11}H_{20}O$ Cycloheptanemethanol, α-cyclopropyl-, (αS)-</p>	<p>12</p> <p>2350054-45-2</p> <p>Absolute stereochemistry shown</p> <p>$C_{11}H_{20}O$ Cycloheptanemethanol, α-cyclopropyl-, (αR)-</p>

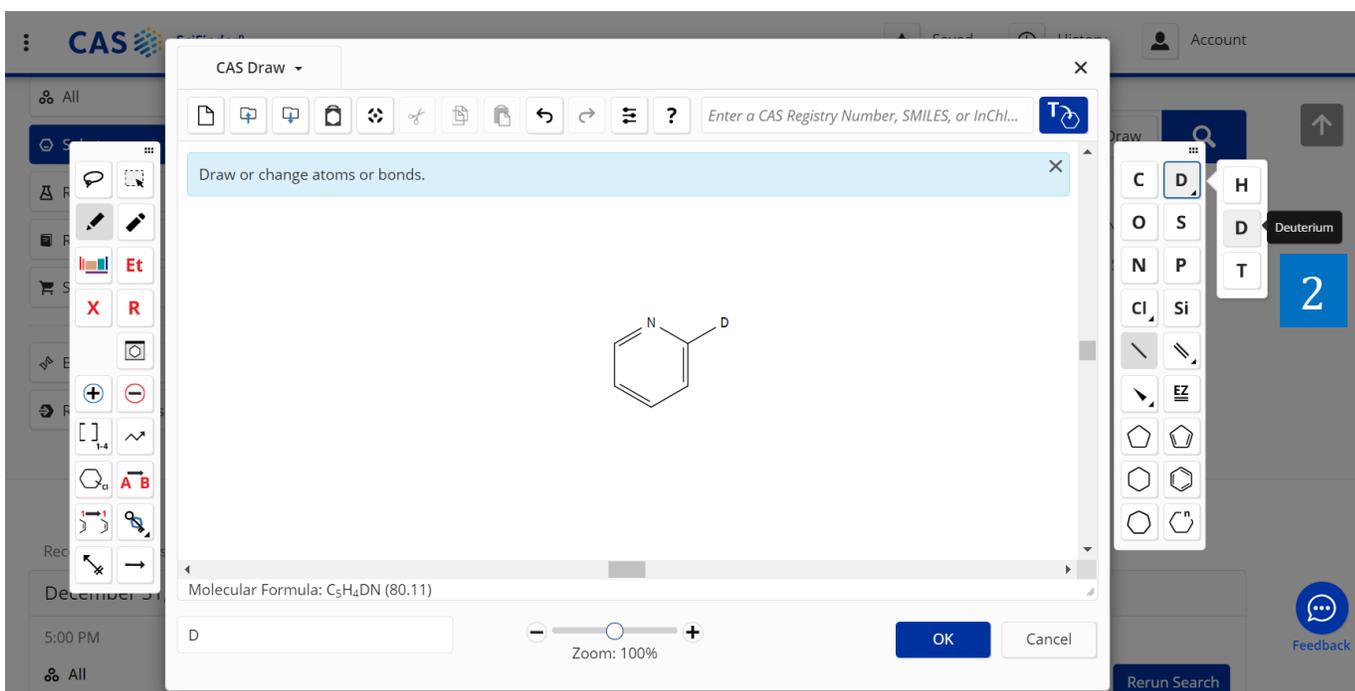
4. 在结果集页面左侧 Number of Components 下勾选相应选项，限定被检索的片段在同一个组分或多个不同组分中（如：选择 1，表示被检索片段在同一个组分中；选择 2，表示被检索片段分别在 2 个不同组分中等；以此类推）。
5. 可继续通过 Substance Class，筛选物质类型。
6. 点击 CAS 登记号，查看物质详情。

直接在结构中绘制氢的同位素 D 和 T

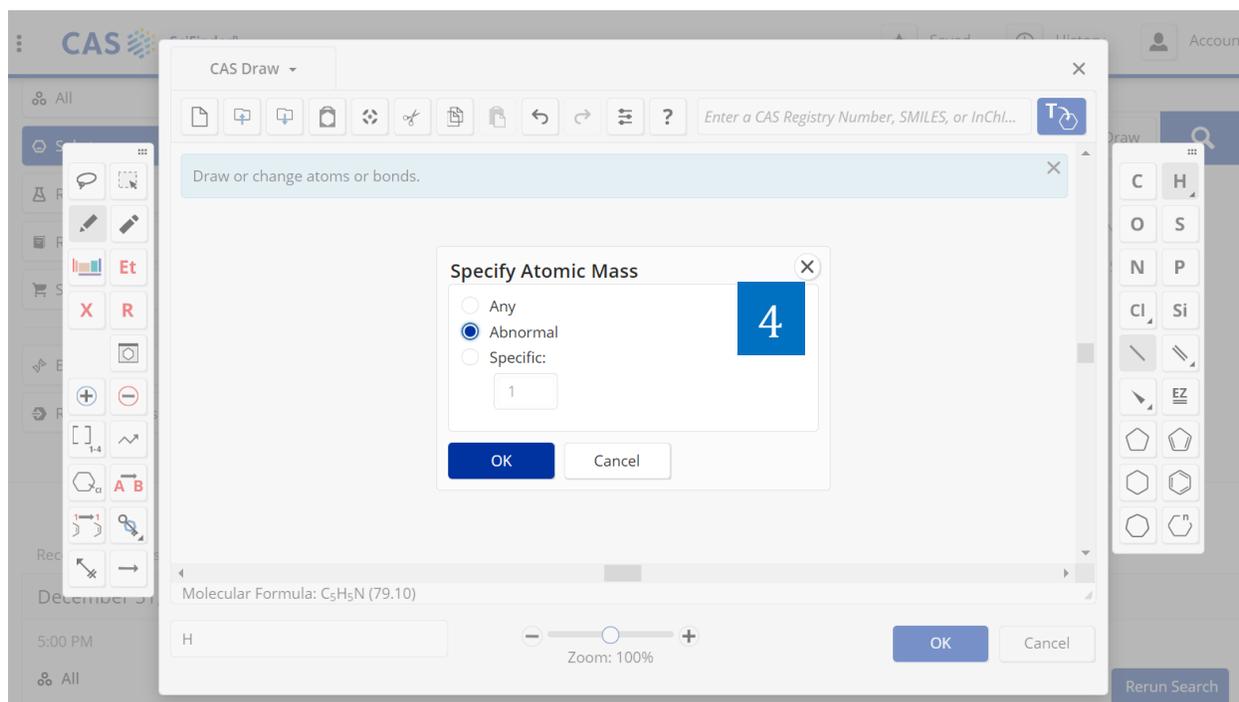
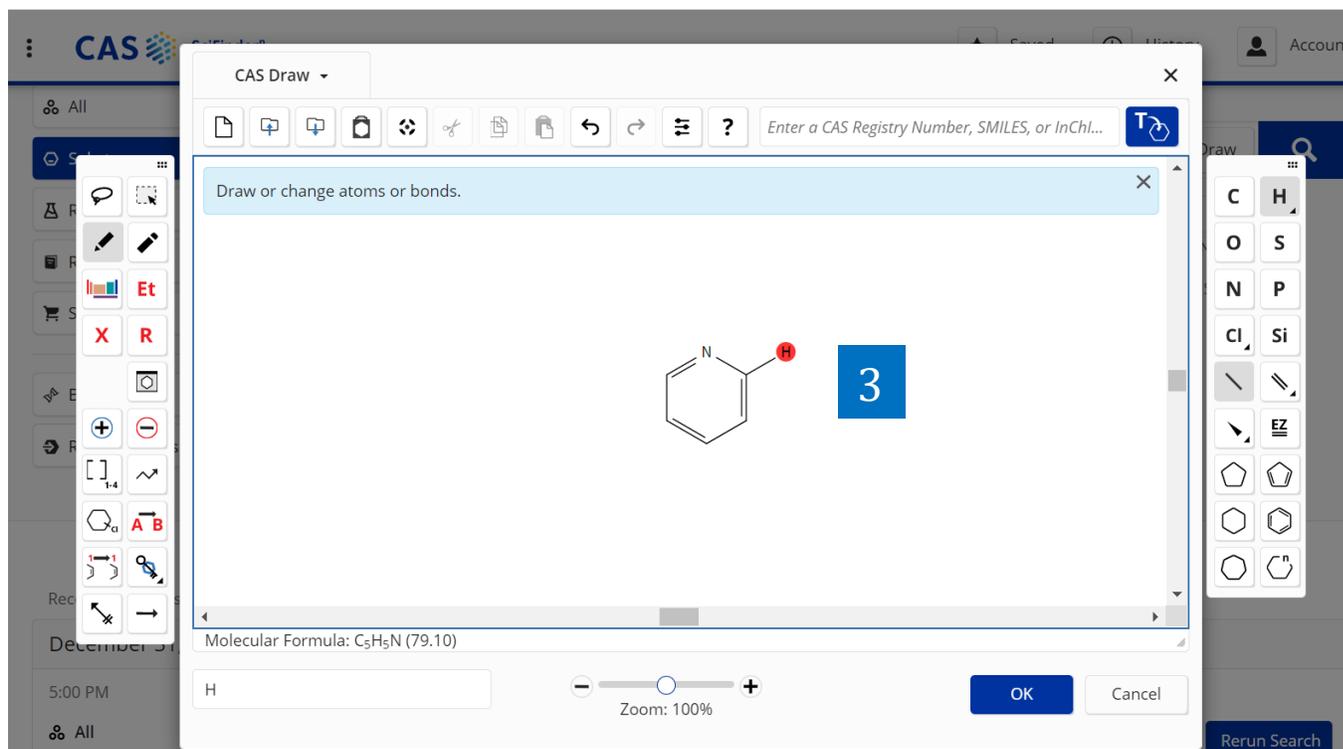
在 CAS SciFinder[®] 的结构编辑器中，可以直接在结构中绘制氢的同位素原子 D 和 T，获取含有氘或氚同位素标记的物质。



1. 点击 Draw，打开结构编辑器。



2. 点击 H 原子按键，选择 D 或者 T 绘制。



如需更多 CAS SciFinder[®] 帮助，请联系 china@acs-i.org, 010-63508026/7

- 或者，鼠标置于 H 上，然后点击鼠标邮件，进行氢原子的同位素设置。
- 在弹出窗口中点击 Abnormal，可获取所有氢同位素标记物质；点 Specific 可输入特定的氢同位素相对原子质量，例如输入 2 或 3 可分别检索 D 或 T。

Searching for...

- All
- Substances**
- Reactions
- References
- Suppliers
- Biosequences
- Retrosynthesis

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

AND Molecular Formula

Examples: C₆H₆ | (C₈H₈)_x | C

+ Add Advanced Search Field

Learn more about Sci

5

Edit Drawing Remove

Search Patent Markush

- 开始检索，获取感兴趣的结果。

CAS SciFinder®

Substances Enter a query...

Return to Home

Structure Match

- As Drawn (114)**
- Substructure (7,271)
- Similarity (7,956)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

[Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Substances (114)

References Reactions Suppliers

1 7291-22-7

C5D5N
Pyridine-*d*₅

731 References 953 Reactions 122 Suppliers

2 1807-97-2

C5H4DN
Pyridine-2-*d*

53 References 29 Reactions 8 Suppliers

3 17265-96-2

C5H3D2N
Pyridine-2,6-*d*₂

38 References 13 Reactions 9 Suppliers

Relevance View: Partial

Edit Drawing Remove

Search Patent Markush

Save And Alerts

马库什结构检索

The screenshot shows the CAS SciFinder search interface. At the top, there is a navigation bar with the CAS SciFinder logo, a 'Saved' button, a 'History' button, and an 'Account' button. Below the navigation bar, there is a banner with a left arrow, text: 'You can now use [BLAST search](#) to mine our newly enhanced collection of more than 500M proteins and nucleotides from 60+ patent authorities dating back to 1957. Plus [visually review sequence similarity and frequency](#) across your patent search results.', and a right arrow. The main content area is divided into two sections: 'Searching for...' and 'Substances'. The 'Searching for...' section has a list of search categories: All, Substances (highlighted with a blue bar and a '1' callout), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The 'Substances' section has a search bar with the text 'Enter a query...' and a '2' callout. Below the search bar is an 'Add Advanced Search Field' button. To the right of the search bar is an 'Edit' button with a dropdown arrow and a search button with a magnifying glass icon and a '4' callout. Below the search bar is a chemical structure drawing tool with a '5' callout. The drawing tool has an 'Edit Drawing' button and a 'Remove' button with a '6' callout. Below the drawing tool is a checkbox labeled 'Search Patent Markush' with a '3' callout.

1. 选择 Substances
2. 点击 Draw，打开结构编辑器绘制检索结构
3. 上传结构后，勾选 Search Patent Markush
4. 开始检索
5. 点击 Edit Drawing，可重新编辑结构
6. 点击 Remove，去除已上传的结构

7. Markush 结构检索结果的匹配方式: As Drawn, Substructure
8. 点击专利号, 获取专利文献详情
9. 专利的著录信息
10. 该马库什结构在专利中出现的位置
11. PatentPak: 获取专利 (同族) 全文、定位专利中的重要物质
12. 专利的全文链接, 链接至相应专利局网站
13. 马库什结构详情

马库什结构检索结果页直接呈现专利著录信息

Return to Home

Patent Markush Match

As Drawn (1)

Substructure (1)

Filter Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (1)

CA Section

Heterocyclic Compounds (More Than One Hetero Atom) (1)

Filter Content Report

Download filter data from this result set.

Patent Markush (1)

References

1

WO2018062978

Preparation of heteroaryl compounds as antiviral agents

By: Min, Ji Young; Chang, So Young; Lee, Ji Hye; Kang, Sun Hee; Kong, Sun Ju; Jo, Su Yeon; Park, Kaapjoo; Kim, Young Mi; Choi, Junghwan
World Intellectual Property Organization, WO2018062978 A1 2018-04-05 | Language: Korean, Database: CPlus
Assignee: Institut Pasteur Korea

Patent claim 1

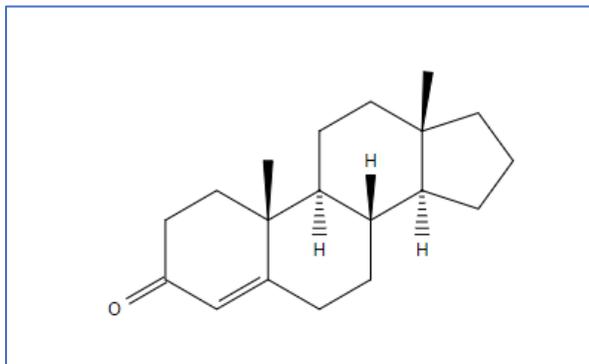
PATENTPAK Full Text

378,379,381,382,384: opt. substd. by G16

1. 马库什结构检索结果页除展示马库什结构、专利号外，同时展示专利标题、发明人、专利局、专利原始撰写语种、申请人等信息。

如何检索一个天然产物是否被合成

包含如下结构的天然产物，哪些还没有被合成出来？



CAS SciFinder

Substances

Filter Behavior

Filter by Exclude

Commercial Availability

Reaction Role

Reference Role

Preparation (22K)

Synthetic Preparation (15K)

Biological Study (7,001)

Reactant (6,091)

Reactant or Reagent (6,091)

Natural Product Occurrence (225)

[View All](#)

Stereochemistry

Substance	References	Reactions	Suppliers
Androstenedione (C ₁₉ H ₂₆ O ₂)	18K	1,127	60
Testosterone (C ₁₉ H ₂₈ O ₂)	122K	1,266	80
Epitestosterone (C ₁₉ H ₂₈ O ₂)	1,472	58	23

1. 在物质结果集页面左侧，勾选 Reference Role 选项下的 Natural Product Occurrence，将物质限定为天然产物。

The screenshot shows the CAS SciFinder search results page. On the left, the 'Filter Behavior' panel is visible, with 'Exclude' selected under 'Filter by' and 'Product' checked under 'Reaction Role'. A blue box with the number '2' highlights the 'Product' checkbox. The main search results area displays three results:

- Result 1:** C₁₉H₂₈O₃, 6-Hydroxytestosterone. 25 References, 1 Reaction, 0 Suppliers. CAS number: 2645439-96-7.
- Result 2:** C₂₁H₃₀O₂, Pregn-4-ene-3,16-dione. 5 References, 0 Reactions, 1 Supplier. CAS number: 2101914-12-7.
- Result 3:** C₁₉H₂₆O₄, Androst-4-ene-3,16-dione, 6,17-dihydroxy-, (6 β ,17 β)-. 1 Reference, 0 Reactions, 0 Suppliers. CAS number: 2230170-01-9.

2. 选择 Filter Behavior Exclude，再勾选 Reaction Role 选项下的 Product，排除已有合成反应的天然产物。

CAS SciFinder® Substances Enter a query...

As Drawn (16) Substructure (30K) Similarity (170K) Analyze Structure Precision

Chemscape Analysis Visually explore structure similarity with a powerful new tool. Learn more about Chemscape. Create Chemscape Analysis

Filter Behavior Filter by Exclude Commercial Availability Reaction Role Reactant (2)

References Reactions Suppliers Save And Alerts

Filtering: Reference Role: Natural Product Occurrenc... Stereochemistry: 3 Selected Clear All Filters

Excluding: Reaction Role: Product

1 34442-08-5 6-Hydroxytestosterone C₁₉H₂₈O₃ 25 References 1 Reaction 0 Suppliers

2 84924-96-9 (24S)-Stigmast-4-en-3-one C₂₉H₄₈O 15 References 0 Reactions 1 Supplier

3 39025-25-7 (16β,22R)-16,20,22-Trihydroxycholest-4-en-3-one C₂₇H₄₄O₄ 13 References 0 Reactions 1 Supplier

CAS RN 84924-96-9 CAS Name (24S)-Stigmast-4-en-3-one

Substance Detail Reactions (0) Synthesize (0) Start Retrosynthetic Analysis References (15) Suppliers (1)

84924-96-9 (24S)-Stigmast-4-en-3-one C₂₉H₄₈O Absolute stereochemistry shown

Edit Structure Reset

3. 获得没有合成反应的天然产物。
4. 点击目标天然产物的结构。
5. 在弹出窗口中点击 Start Retrosynthetic Analysis，开始逆合成路线分析。

CAS SciFinder[®] Reactions Enter a query... Draw

Retrosynthesis Plan Options

Powered by ChemPlanner[®]

Select Synthetic Depth [Learn more.](#)

1
 2
 3
 4

Set Rules Supporting Predicted Reactions [Learn more.](#)

Common
 Uncommon (includes Common Rules)
 Rare (includes Common and Uncommon Rules)

Set Starting Materials Cost Limit [Learn more.](#)

1000 USD/mol

Email me when my plan is complete

[Create Retrosynthesis Plan](#) 6

Break and Protect Bonds [Learn more.](#)

[Clear All Bond Selections](#)

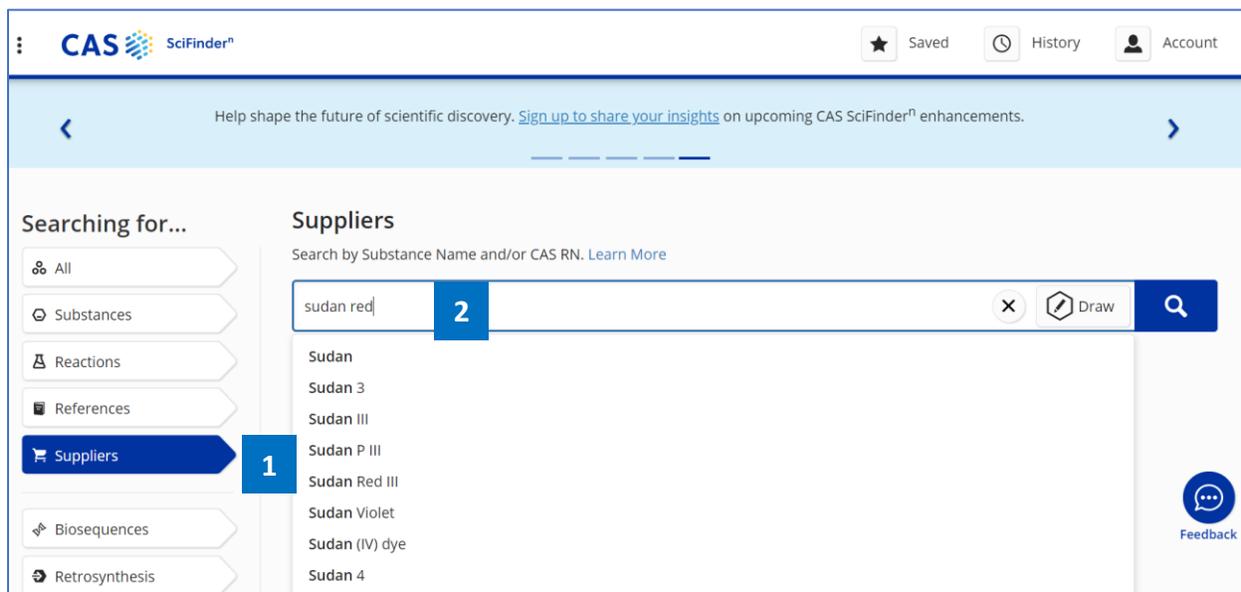
6. 点击 Create Retrosynthesis Plan，获取该物质的预测逆合成路线。

获取化学品供应商信息

在 CAS SciFinder[®]中可通过以下三种方式获取化学品供应商的信息：

- 1、直接在 Suppliers 检索框中输入所需化学品的物质名称（包括商品名、俗名等）或者 CAS 登记号进行检索。
- 2、在物质结果集页面，点击相应的 suppliers 获得供应商信息。
- 3、在反应结果集中页面点击相应的 Suppliers 获取供应商信息。

方法 1、直接在 Suppliers 检索框中输入所需化学品的物质名称（包括商品名、俗名等）或者 CAS 登记号进行检索。



1. 点击 Suppliers
2. 输入所需化学品的物质名称（包括商品名，俗名等），或者 CAS 登记号

Return to Home

Filter Behavior

Filter by Exclude

Preferred Suppliers

Supplier **3**

Substance

Purity

Quantity

Ships Within

Stock Status

Order From Supplier

Country

Suppliers (62) **4** Sort: Relevance

Supplier	Substance	Purity	Purchasing Details	Availability
<input type="checkbox"/> 1				
AK Scientific AK Scientific Product Catalog United States	3118-97-6 Sudan II		Order From Supplier 5 1g, USD 14 5g, USD 27 25g, USD 54 Bulk Screening	Maintained in stock Ships within 1 week
<input type="checkbox"/> 2				
TGI	3118-97-6 Sudan II [=1-(2,4-Xylidylazo)-2-	95-98%	Order From Supplier 5 25 g, USD 25.00	Maintained in stock
<input type="checkbox"/> 19				
BIOSYNTH[®] Carbosynth Biosynth Carbosynth Product List United Kingdom	85-83-6 Solvent Red 24		Product Information 6	
<input type="checkbox"/> 20				
BIOSYNTH[®] Carbosynth Biosynth Carbosynth Product List United Kingdom	85-83-6 Solvent red 24		Order From Supplier 5 250 g, USD 40 500 g, USD 75 1 Kg, USD 140	

3. 供应商筛选选项，可以根据：优选供应商、供应商名称、产品纯度、产品量级、运送时间、储存状态、是否有直达订购链接、国家等对供应商结果进行筛选。
4. 可以按照供应商名称的字母排列顺序、运送时间或产品纯度对供应商进行重新排序。
5. 点击 order from suppliers，直接访问产品订购页面。
6. 点击 product information，访问该供应商对此产品的描述信息。

点击 order from suppliers 所获界面:

AKSci Fine & Specialty Chemicals
in Catalog & Bulk
AK Scientific, Inc.

Inhibitors, Bioactives, Reference Compounds
Building Blocks, Intermediates, Reagents
Bulk Bio & Specialty Chemicals

Search by Catalog Number, CAS, MFCD, Keyword ...

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Home Products Services Resources Partners Contact Us Help

T805 **Solvent Red 24, 95% (HPLC)** [Add to Favorites](#)

Sudan IV
Bleibrich scarlet R fat soluble
Oil Red IV
Scarlet Red Scharlach
Sudan R

Size	Price	Availability	Qty
5g	\$14	IN STOCK	<input type="text"/>
25g	\$21	IN STOCK	<input type="text"/>
100g	\$54	IN STOCK	<input type="text"/>

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Current as of November 9, 2021

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IDENTITY
CAS Number: 85-83-6
MDL Number: MFCD0003893
MF: C24H20N4O
MW: 380.45

SPECIFICATIONS & PROPERTIES
Min. Purity Spec: 95% (HPLC)
Spectra: NMR, LCMS, HPLC
Physical Form: Dark red to brown powder
Melting Point: 175-178°C
Long-Term Storage: Store at room temperature
Note: Sold as technical grade. Not an analytical standard. No purity specification available.

CATEGORIES
[Specialty Chemicals > Dyes and Pigments](#)

[PubChem](#)

点击 Product Information 所获界面:

BIOSYNTH
Carbosynth

Search by Product No, Name, CAS No, Keyword or Tag(s)...

Search by structure Document Search

Products Services Support

Home / Fine Chemicals / Other Fine Chemicals / Solvent Red 24

FS03568 **Solvent Red 24** RESEARCH & DEVELOPMENT

TECHNICAL DATA

CoA SEARCH

TAGS

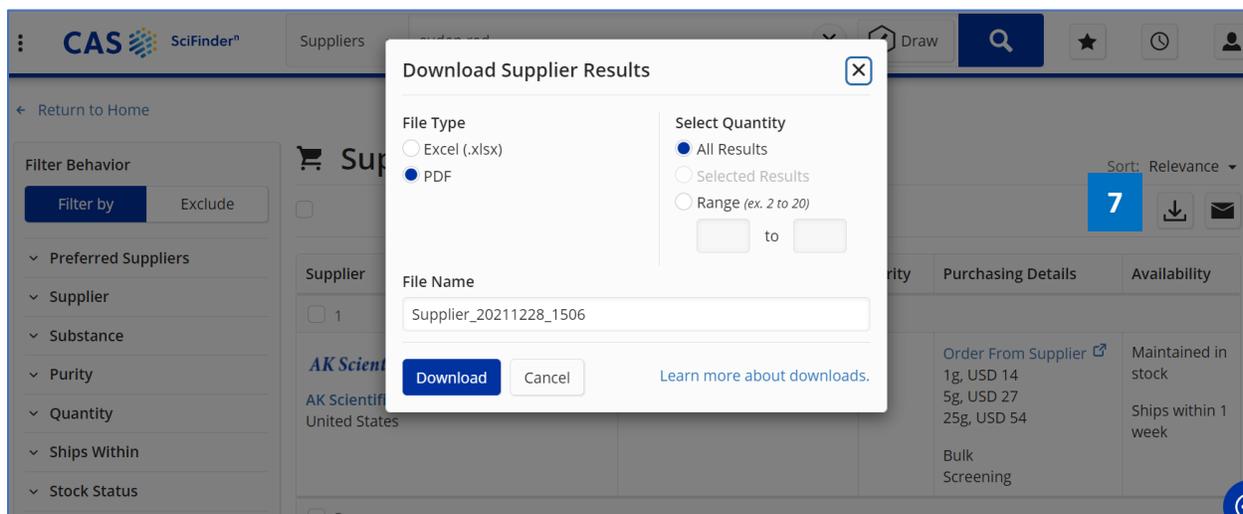
TECHNICAL DATA

CAS No: 85-83-6

Product Code: FS03568

MDL No: MFCD0003893

Chemical Formula:



7. 供应商结果集可以导出为 Excel 或者 PDF 格式文件。

方法二、在物质结果集页面，点击相应的 suppliers 获得供应商信息。

1. 在物质结果集页面，筛选有供应商信息的物质。
2. 点击 Suppliers 按钮，查看供应商信息。

方法三、在反应结果集页面点击相应的 Suppliers 获取供应商信息。

1

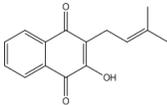
2

1. 在反应结果集页面，筛选起始物或者产物有供应商信息的反应。
2. 点击 Suppliers 按钮，查看供应商信息。

用物质名检索时可使用通配符 “*”

注：通配符 “*” 代表 0 或多个字符；可用于词中或者词尾。

The screenshot shows the CAS SciFinder search results for the query "La*chol". The search bar at the top contains "La*chol" and a blue box with the number "1". The results are displayed in a grid format, sorted by CAS RN: Descending. The results are as follows:

CAS RN	Chemical Name	Chemical Structure	Molecular Formula	References	Reactions	Suppliers
8038-34-4	Unspecified Lanochol	Image Not Available		1	0	0
8006-54-0	Unspecified Lanichol	Image Not Available		432	0	24
84-79-7	Lapachol		C ₁₅ H ₁₄ O ₃	996	430	58

1. 此处输入 La*chol，可以检索到 Lapachol, Lanochol 和 Lanichol 等。

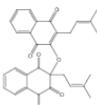
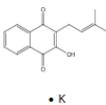
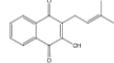
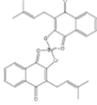
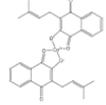
CAS SciFinder[®] Substances Lapacho* 2

Substances (14) Sort: CAS RN: Descending View: Partial

Filter Behavior
 Filter by Exclude

- Commercial Availability
 - Available (5)
 - Not Available (9)
- Reaction Role
 - Product (5)
 - Reactant (3)
- Reference Role
 - Preparation (8)
 - Synthetic Preparation (8)
 - Biological Study (7)
 - Properties (7)
 - Uses (7)
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Data by Country

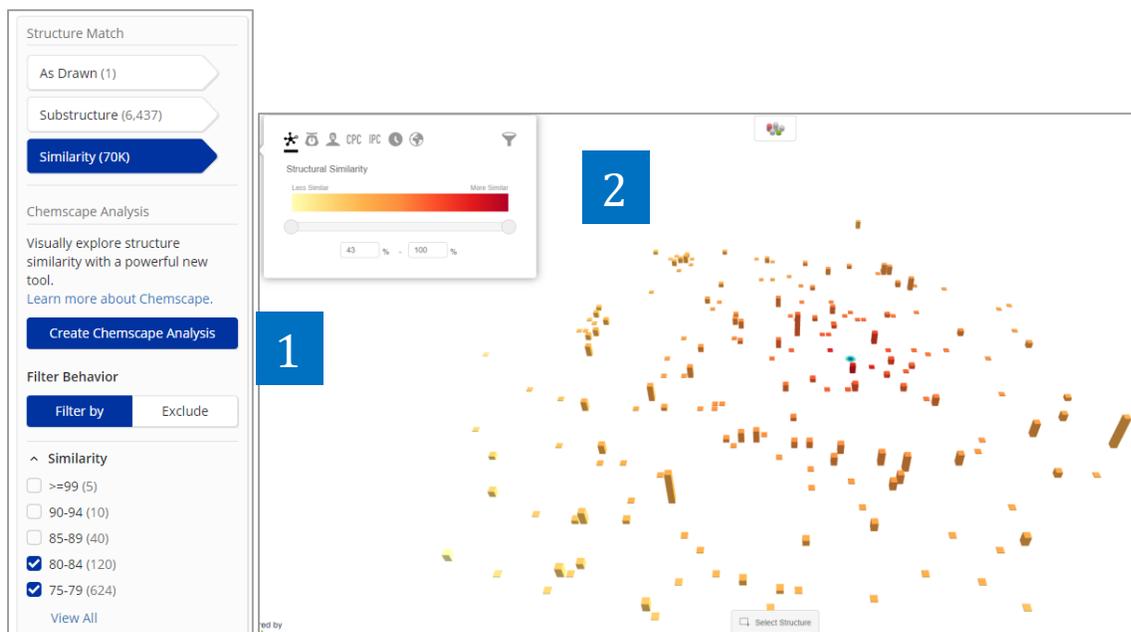
References Reactions Suppliers Save And Alerts

1	2	3	4	5	6
<p>2100329-07-3</p> <p>Image Not Available</p> <p>Notes: An herbal tea made from the inner bark of the Pau d'arco tree (<i>Handroanthus impetiginosus</i>) purported to have anti-inflammatory and anticarcinogenic activities</p> <p>Unspecified Lapachorinde</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>855637-05-7</p>  <p>$C_{30}H_{26}O_6$ Lapachol, peroxide</p> <p>3 References 3 Reactions 1 Supplier</p>	<p>332083-20-2</p>  <p>$C_{15}H_{14}O_3 \cdot K$ Components: 2 Component RN: 84-79-7 Lapachol potassium salt</p> <p>5 References 0 Reactions 1 Supplier</p>	<p>184359-68-0</p>  <p>$C_{15}H_{14}O_3 \cdot Ag(I)$ Components: 2 Component RN: 84-79-7 Lapachol silver salt</p> <p>1 Reference 1 Reactions 0 Suppliers</p>	<p>128528-86-9</p>  <p>$C_{30}H_{26}BeO_6$ Lapachol, Be deriv.</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>128271-49-8</p>  <p>$C_{30}H_{26}CoO_6$ Lapachol, Co deriv.</p> <p>1 Reference 0 Reactions 0 Suppliers</p>

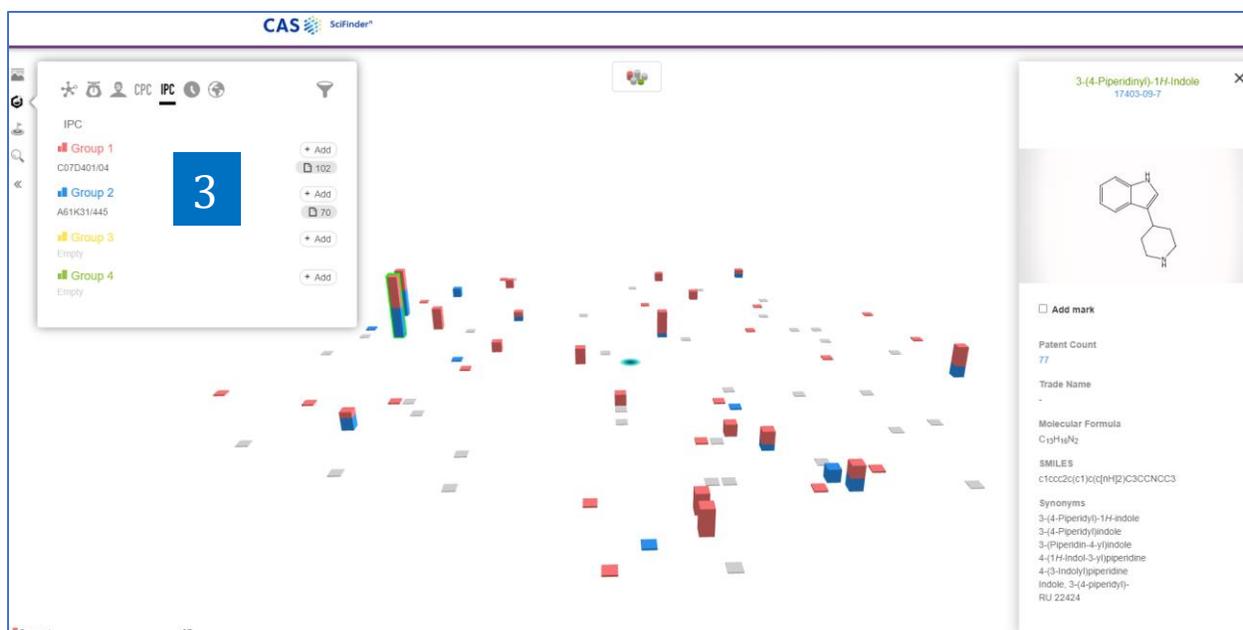
2. 此处输入 Lapacho*，可以检索到 Lapachorinde, lapachol peroxide, lapachol potassium salt 等。

可视化分析结构检索结果（Chemscape 分析）

利用 Chemscape 可视化一组物质结果集的结构相似性和专利全景。结构检索后的物质结果集页面会出现 Create Chemscape Analysis 选项。



1. 点击 Create Chemscape Analysis 进行可视化分析。
2. 视图中物质所处位置与其和被检索物质结构的相似度相关，每个柱子代表一个物质，柱子高度与该物质被披露的专利数量相关。



3. 根据申请人、CPC、IPC、公布年和专利受理机构等对物质进行分组。

反应检索

逆合成路线设计工具 (Retrosynthesis)

逆合成路线设计工具可用于未知化合物和已知化合物，设计预测的或者已经报道的逆合成路线。

The screenshot displays the CAS SciFinder Retrosynthesis tool interface. On the left, a sidebar titled "Searching for..." lists various search categories, with "Retrosynthesis" highlighted in blue and marked with a blue box containing the number "1". The main workspace is titled "Retrosynthesis" and contains a chemical structure of a complex molecule. Below the structure, the molecular formula is given as $C_{19}H_{19}BrN_4O_5$ (463.29). A toolbar at the top of the workspace includes icons for drawing and editing, and a text input field for "Enter a CAS Registry Numbers, SMILES...". A "Start Retrosynthetic Analysis" button is located at the bottom right of the workspace, marked with a blue box containing the number "2". The zoom level is set to 90%.

1. 点击 Retrosynthesis, 打开结构编辑器。
2. 结构绘制完成后, 点击 Start Retrosynthetic Analysis 打开 Retrosynthesis Plan Options 窗口。
3. 合成深度通过为最长路径设置最多四个步骤来限制逆合成计划中允许的合成步骤数。
4. 选择支持预测反应的规则:

通用规则 (Common rules) 包括实验室中经常使用的反应类型, 有大量的文献实例支持的规则;

不常见 (Uncommon rules) 或稀有 (Rare rules) 规则则是由较少实例支持的规则, 但有可能揭示更多新颖的合成方法。

5. 设置起始物成本 (单位为: 美元/摩尔或美元/克)。
6. 设置断开键 (break bond) 和保护键 (protect bond): 断开键的含义为整个路线最后一步合成的键, 一个路线只能设置一根断开键; 保护键的含义为整个路线都不会发生变化的键, 一条路线可以同时设置几根保护键。
7. 化合物的预测逆合成路线可能需要数分钟完成 (约 10 分钟左右), 可以点击 Email me when my plan is completed。即路线预测完毕后向注册 CAS SciFinder[®] 账号的邮箱发送通知。

8. 创建路线。

9. 结果呈现：Overview 显示完整逆合成路线，预估产率和成本。

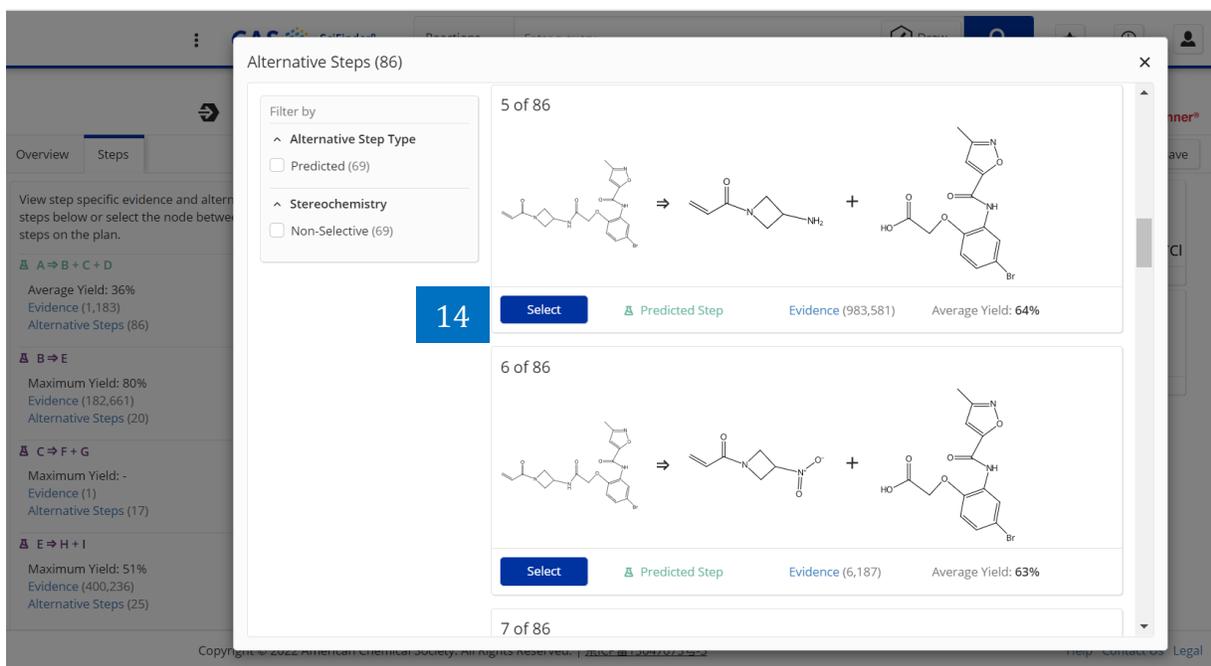
10. 紫色代表来源于已经报道的反应；绿色代表预测的反应路线。

11. 点击 Steps，显示合成路线中具体步骤信息，产率及可替代步骤。

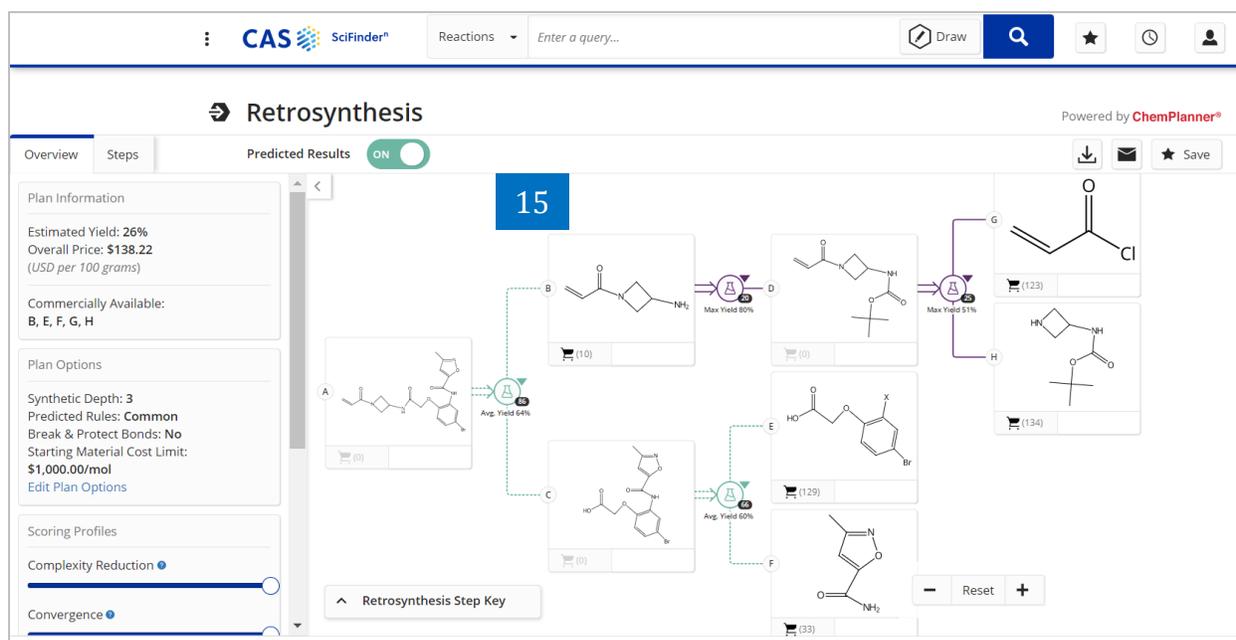
12. Evidence 表示支持此反应步骤的反应和文献信息，点击即获得反应信息结果集。

13. Alternative Steps 可替代反应步骤。

如需更多 CAS SciFinder[®] 帮助，请联系 china@acs-i.org, 010-63508026/7



14. 选择感兴趣的反应步骤，整个逆合成路线发生改变。



15. 整个实验路线发生改变，其中绿色路线为预测路线。

Retrosynthesis Powered by ChemPlanner[®]

Overview Steps Predicted Results ON

View step specific evidence and alternate steps below or select the node between steps on the plan.

17

A ⇒ B + C
 Average Yield: 64%
 Evidence (983,581)
 Alternative Steps (86)

B ⇒ D
 Maximum Yield: 80%
 Evidence (182,661)
 Alternative Steps (20)

C ⇒ E + F
 Average Yield: 60%
 Evidence (6,787)
 Alternative Steps (66)

D ⇒ G + H
 Maximum Yield: 51%
 Evidence (400,236)
 Alternative Steps (25)

Retrosynthesis Step Key

16. 当鼠标移到某一步骤时，右侧路线图中该路线的底物 / 产物标识转为高亮。

17. 点击 Evidence，查看支持此反应步骤的反应和文献信息。

Reactions (983,581) **18**

Group: By Document View: Expanded

Filter Behavior: Filter by Exclude

Yield: 90-100% (83K), 80-89% (86K), 70-79% (77K), 50-69% (114K), 30-49% (71K), View All

Number of Steps: 1 (983K)

Non-Participating Functional Groups: Halide (413K), Alkene (361K), Cyclic alkene (331K), Ether (323K), Imine (254K), View All

Experimental Protocols: Synthetic Methods (154K), Experimental Procedure (311K)

Reaction Type

References

1

Identification of pharmacophore model, synthesis and biological evaluation of N-phenyl-1-arylamide and N-phenylbenzenesulfonamide derivatives as BACE 1 inhibitors
 By: Huang, Wenhai; Yu, Haiping; Sheng, Rong; Li, Jia; Hu, Yongzhou
 Bioorganic & Medicinal Chemistry (2008), 16(24), 10190-10197 | Language: English, Database: C&plus and MEDLINE

Full Text View 2 Related Reactions

Suppliers (16) Suppliers (84) Supplier (1)

Reaction Summary Steps: 1 Yield: 68%

1.1 Solvents: Dichloromethane; 1 h, rt

View Reaction Detail Experimental Protocols

2

Radiopharmaceuticals for diagnosing Alzheimer's disease
 By: Hilger, Christoph-Stephan; Johannsen, Bernd; Steinbach, Joerg; Maeding, Peter; Halks-Miller, Meredith; et al

18. 支持该步骤的反应结果集。

The screenshot displays the CAS SciFinder Retrosynthesis interface. On the left, a 'Scoring Profiles' panel is visible, featuring sliders for various optimization criteria: Complexity Reduction (19), Convergence (21), Evidence (22), Cost (23), Yield (24), and Atom Efficiency (25). The main workspace shows a retrosynthetic plan for a target molecule, with steps labeled A through H. The plan includes chemical structures and associated data such as 'Max Yield 80%' and 'Avg. Yield 61%'. The interface also shows a 'Starting Material Cost Limit: \$1,000.00/mol' and a 'Predicted Results' section with a 'ON' toggle. The top navigation bar includes 'CAS SciFinder', 'Reactions', and a search bar. The bottom right has a 'Reset' button.

19. Scoring Profile 评分配置，可以设置为 Off(极左)、Low、Medium 或 High(极右); 每个评分配置的默认设置是 “Medium” 。将滑块一直移动到左边会将该设置的评分 “关闭” 。

20. 降低复杂性：降低步骤起始物相对于该步产物的复杂性。

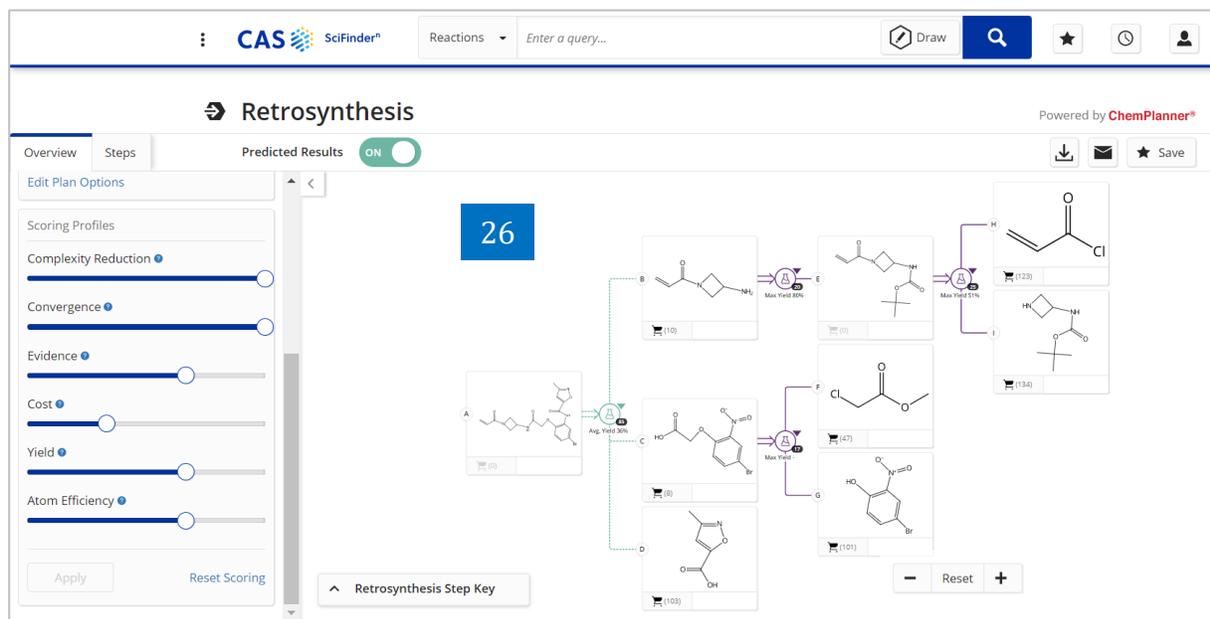
21. 汇聚：调高 Convergence 会提高路线的汇聚（减少反应路线的线性长度）。

22. 依据：根据支持特定反应类型的证据例子的数量多少来排列计划步骤/备选方案。

23. 成本：根据起始物的成本价格（由低到高）来排列计划步骤/备选方案。

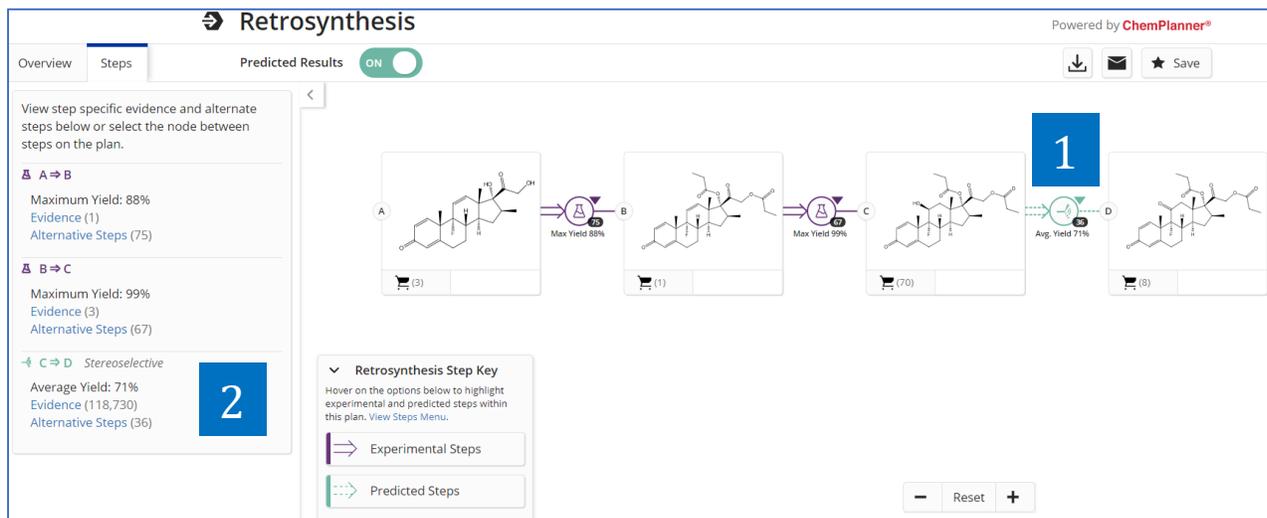
24. 产率：增加路线计划中每一步的产率，这有助于提高目标分子的产率。

25. 原子经济性：减少未被包含在产物中的反应物的原子数。提高原子经济性，就是提高反应物中的原子转化为产物中原子的比例。

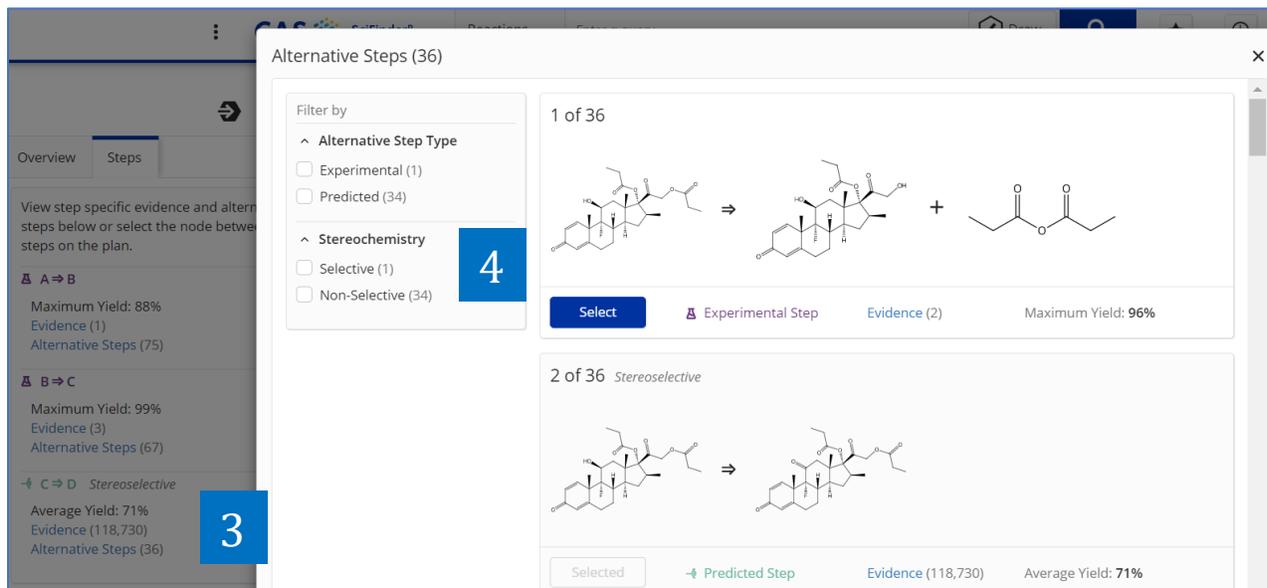


26. 更改评分配置之后的路线。

逆合成路线之立体选择性反应



1. 此符号表示该步反应为立体选择性反应。
2. 在左侧对应的 Steps 也会以 Stereoselective 标记立体选择性反应。



3. 点击 Alternative Steps 查看替代步骤。
4. 在替代步骤结果集页面，可通过 Stereochemistry 选择立体选择性反应。

逆合成路线之自定义分值 (Scoring) 功能

The screenshot displays the 'Retrosynthesis' interface. On the left, the 'Plan Options' panel is visible, with the 'Scoring Profiles' section highlighted. This section contains six sliders: Complexity Reduction, Convergence, Evidence, Cost, Yield, and Atom Efficiency. A '3' is placed over the 'Apply' button. The main workspace shows a retrosynthetic plan starting from a target molecule (A) and branching into precursors B, C, D, E, F, G, H, and I. Each step is labeled with its maximum yield (e.g., Max Yield 80% for step B to E) and a shopping cart icon with a cost value (e.g., (10) for B, (121) for H). A 'Retrosynthesis Step Key' is located at the bottom left of the workspace.

1. 在逆合成路线结果中，点击左侧 Overview。
2. 一共有 5 项，每项有 4 个设置 (off, low, medium, high)。用鼠标拖动滚动条，即可调整设置级别。

Complexity Reduction: 降低每步反应物相对于产物的复杂度；

Convergence: 调整逆合成路收敛性；

Evidence: 每步反应的支持文献数量；

Yield: 每一步反应的产率，对目标分子的产率有影响；

Atom Efficiency: 反应物的原子转化经济性。

以上五项选择的更详细信息，可在 CAS SciFinderⁿ help 中获得：

https://scifinder-n.cas.org/help/#t=Working_with_Search_Results%2FRetrosynthesis%2FRetrosynthesis_Page_-_Options_Tab.htm&rhsearch=scoring%20profile&rhhlterm=scoring%20profile&rhsyns=%20

3. 点击 Apply，完成设置。

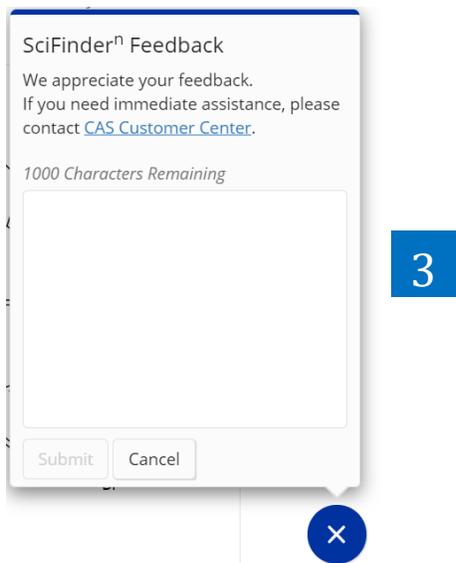
利用 Retrosynthesis 的产品反馈功能

The screenshot shows the CAS SciFinder Retrosynthesis interface. The main area displays a predicted retrosynthetic plan with various chemical structures and reaction steps labeled A through H. On the left, there is a 'Plan Information' sidebar with details like 'Estimated Yield: 15%', 'Overall Price: \$427.41', and 'Synthetic Depth: 3'. A 'Feedback' icon is visible in the bottom right corner of the interface.

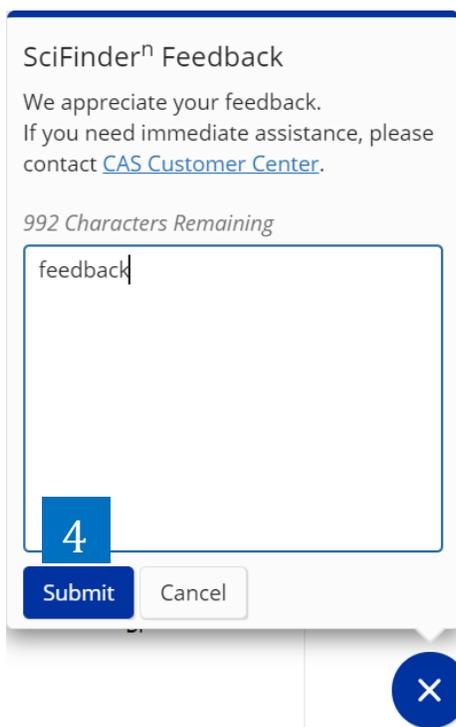
1. 在 Retrosynthesis 的结果页面，点击 Feedback 图标，进行使用反馈。

The screenshot shows the CAS SciFinder Retrosynthesis Plan Options interface. The main area shows settings for 'Select Synthetic Depth' (set to 3), 'Set Rules Supporting Predicted Reactions' (set to Common), and 'Set Starting Materials Cost Limit' (set to 1000 USD/mol). There are also options for 'Break and Protect Bonds'. A 'Feedback' icon is visible in the bottom right corner of the interface.

2. 也可以在 Retrosynthesis 的 Plan option 页面点击 Feedback 图标，进行使用反馈。



3. 点击 Feedback 后，弹出此窗口，请在此输入反馈内容。



4. 点击 Submit，提交反馈信息。

合成实验详情的获取

The screenshot shows the CAS SciFinder interface for a reaction search. The search results are filtered by 'Experimental Protocols: Synthetic Methods'. The reaction scheme shows the allylic oxidation of an alkene catalyzed by a Copper-Aluminum Mixed Oxide. The reaction summary provides details on catalysts, solvents, and reagents. Two blue boxes with numbers 1 and 2 highlight the 'Synthetic Methods' filter and the 'Experimental Protocols' link, respectively.

1. 在反应结果集页面左侧选择 Experimental Protocols 项下的 Synthetic Methods。
2. 点击 Experimental Protocols 获取 CAS 科学家增值标引的实验详情。

CAS SciFinder[®] Reactions 2014:365937

Return to Results

Reaction Detail (Scheme 1, Reaction 1 of 1)

3 4 5

↓ ↓ ↓ Save

Suppliers (95)

Absolute stereochemistry shown, Rotation (+)
[Stage 2]

Suppliers (35)

Absolute stereochemistry shown, Rotation (+)
100%

Steps: 1
Yield: 100%

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	Aluminum copper oxide	Acetonitrile	10 min, rt
2	<i>tert</i> -Butyl hydroperoxide	-	Water	24 h, 82 °C

CAS Reaction Number: 31-209-CAS-8900882

JOURNAL

Allylic Oxidation of Alkenes Catalyzed by a Copper-Aluminum Mixed Oxide

By: Garcia-Cabeza, Ana Leticia; et al
View All

Organic Letters (2014), 16(6), 1598-1601

Full Text

Notes

regioselective

6

Experimental Protocols

Synthetic Methods Experimental Procedure

Products (2*R*,4*R*,4*a*S,6*R*)-2,3,4,4*a*,5,6,7,8-Octahydro-4,4*a*-dimethyl-6-(1-methylethenyl)-2-naphthalenyl 4-methoxybenzoate, Yield: 100%

Reactants 4-Methoxybenzoic acid
Valencene

Reagents *tert*-Butyl hydroperoxide

Catalysts Aluminum copper oxide

Solvents Acetonitrile
Water

Procedure

- Suspend 60 mg of Cu-Al Ox in 4 mL of acetonitrile in a tube under open atmosphere.
- Add 1.0 mmol of acid derivative to the system.
- Stir the mixture for 10 minutes.
- Add (+)-valencene (1.0 mmol or 4.0 mmol) and *tert*-butylhydroperoxide (1.5 equivalents or 3.0 equivalents of 70% aqueous solution) to the mixture.
- Stir the reaction mixture at 82°C.
- After 24 hours, add saturated aqueous Na₂SO₃ solution (10 mL) to the mixture.
- Extract the solution with ethyl acetate (3 x 10 mL).
- Wash the solution with a saturated aqueous EDTA solution (10 mL).
- Dry the solution over anhydrous Na₂SO₄.
- Filter the reaction mixture through a Al₂O₃/K₂CO₃/Celite pad.
- Rinse the reaction mixture abundantly with ethyl acetate.
- Remove the solvent under vacuum.

Company/Organization
Departamento de Quimica Organica, Facultad de Ciencias Universidad de Cadiz Cadiz 11510 Spain

Transformation	Acyloxylation Reaction	7										
Scale	milligram	8										
Characterization Data		9										
<p>^ (2<i>R</i>,4<i>R</i>,4<i>aS</i>,6<i>R</i>)-2,3,4,4<i>a</i>,5,6,7,8-Octahydro-4,4<i>a</i>-dimethyl-6-(1-methylethenyl)-2-naphthalenyl 4-methoxybenzoate</p> <table border="1"> <tr> <td>Proton NMR Spectrum</td> <td>400 MHz, CDCl₃; δ = 8.00 (d, <i>J</i> = 9.0 Hz, 2H), 6.90 (d, <i>J</i> = 9.0 Hz, 2H), 5.56 (br d, <i>J</i> = 5.0 Hz, 1H), 5.33 (ddd, <i>J</i> = 6.9, 3.9, 2.0 Hz, 1H), 4.70 (br s, 2H), 3.84 (s, 3H), 2.36 (m, 1H), 2.28 (tt, <i>J</i> = 12.5, 3.0 Hz, 1H), 2.18 (ddd, <i>J</i> = 14.3, 4.1, 2.6, 1H), 1.92 (dt, <i>J</i> = 12.9, 2.7 Hz, 1H), 1.79 (m, 2H), 1.72 (br s, 3H), 1.28 (m, 4H), 0.94 (s, 3H), 0.91 (d, <i>J</i> = 6.6 Hz, 3H).</td> </tr> <tr> <td>Carbon-13 NMR</td> <td>100 MHz, CDCl₃; δ = 166.1, 163.1, 150.7, 150.1, 131.6, 123.5, 117.9, 113.4, 108.6, 68.1, 55.4, 51.8, 44.4, 40.6, 38.2, 35.8, 33.1, 32.4, 20.8, 16.9, 15.1.</td> </tr> <tr> <td>IR Absorption Spectrum</td> <td>Film ν_{max}: 2932, 1707, 1607, 1510, 1272, 1256, 1167, 1032, 847, 772 cm⁻¹.</td> </tr> <tr> <td>Optical Rotatory Power</td> <td>[α]_D²⁰ = +130.06 (c 1.70, CHCl₃).</td> </tr> <tr> <td>HRMS</td> <td>ESI: calcd. for C₂₃H₃₁O₃ [M+H]⁺ 355.2273; found 355.2271.</td> </tr> </table> <p>CAS Method Number 3-209-CAS-8900882</p>			Proton NMR Spectrum	400 MHz, CDCl ₃ ; δ = 8.00 (d, <i>J</i> = 9.0 Hz, 2H), 6.90 (d, <i>J</i> = 9.0 Hz, 2H), 5.56 (br d, <i>J</i> = 5.0 Hz, 1H), 5.33 (ddd, <i>J</i> = 6.9, 3.9, 2.0 Hz, 1H), 4.70 (br s, 2H), 3.84 (s, 3H), 2.36 (m, 1H), 2.28 (tt, <i>J</i> = 12.5, 3.0 Hz, 1H), 2.18 (ddd, <i>J</i> = 14.3, 4.1, 2.6, 1H), 1.92 (dt, <i>J</i> = 12.9, 2.7 Hz, 1H), 1.79 (m, 2H), 1.72 (br s, 3H), 1.28 (m, 4H), 0.94 (s, 3H), 0.91 (d, <i>J</i> = 6.6 Hz, 3H).	Carbon-13 NMR	100 MHz, CDCl ₃ ; δ = 166.1, 163.1, 150.7, 150.1, 131.6, 123.5, 117.9, 113.4, 108.6, 68.1, 55.4, 51.8, 44.4, 40.6, 38.2, 35.8, 33.1, 32.4, 20.8, 16.9, 15.1.	IR Absorption Spectrum	Film ν _{max} : 2932, 1707, 1607, 1510, 1272, 1256, 1167, 1032, 847, 772 cm ⁻¹ .	Optical Rotatory Power	[α] _D ²⁰ = +130.06 (c 1.70, CHCl ₃).	HRMS	ESI: calcd. for C ₂₃ H ₃₁ O ₃ [M+H] ⁺ 355.2273; found 355.2271.
Proton NMR Spectrum	400 MHz, CDCl ₃ ; δ = 8.00 (d, <i>J</i> = 9.0 Hz, 2H), 6.90 (d, <i>J</i> = 9.0 Hz, 2H), 5.56 (br d, <i>J</i> = 5.0 Hz, 1H), 5.33 (ddd, <i>J</i> = 6.9, 3.9, 2.0 Hz, 1H), 4.70 (br s, 2H), 3.84 (s, 3H), 2.36 (m, 1H), 2.28 (tt, <i>J</i> = 12.5, 3.0 Hz, 1H), 2.18 (ddd, <i>J</i> = 14.3, 4.1, 2.6, 1H), 1.92 (dt, <i>J</i> = 12.9, 2.7 Hz, 1H), 1.79 (m, 2H), 1.72 (br s, 3H), 1.28 (m, 4H), 0.94 (s, 3H), 0.91 (d, <i>J</i> = 6.6 Hz, 3H).											
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IR Absorption Spectrum	Film ν _{max} : 2932, 1707, 1607, 1510, 1272, 1256, 1167, 1032, 847, 772 cm ⁻¹ .											
Optical Rotatory Power	[α] _D ²⁰ = +130.06 (c 1.70, CHCl ₃).											
HRMS	ESI: calcd. for C ₂₃ H ₃₁ O ₃ [M+H] ⁺ 355.2273; found 355.2271.											

3. 下载、分享或保存实验详情
4. 报道反应的文献
5. 实验中涉及的所有物质及其在反应中的角色
6. 实验中涉及的所有实验步骤
7. 反应转化类型
8. 反应量级
9. 产物的谱图表征信息及属性特征

获取特定反应类型及其文献来源

The screenshot shows the CAS SciFinder interface for searching reactions. The search term is 'sofosbuvir'. The left sidebar contains a 'Filter Behavior' section with 'Filter by' selected. Under 'Reaction Type', 'Full (683)' is selected, highlighted with a blue box containing the number '1'. Under 'Reaction Notes', 'Stereoselective (156)' is selected, highlighted with a blue box containing the number '2'. The main area displays 'Reactions (720)' with a 'Scheme 1 (6 Reactions)' section showing a chemical reaction scheme. Below the scheme are three reaction summary entries, each with reagents (Sodium sulfite), solvents (Tetrahydrofuran, Water), and conditions (4 h, rt). The right side of each entry provides the title of the associated patent and the author information.

1. 在反应结果集页面，通过左侧 Reaction Type，查看反应类型为完整反应或仅有产物的反应。
2. 在反应结果集页面，通过左侧 Reaction Notes，浏览或获取反应涉及的安全信息等。

CAS SciFinder[®] Reactions sofosbuvir

Sovents: [Tetrahydrofuran](#), [water](#), 4 h, rt

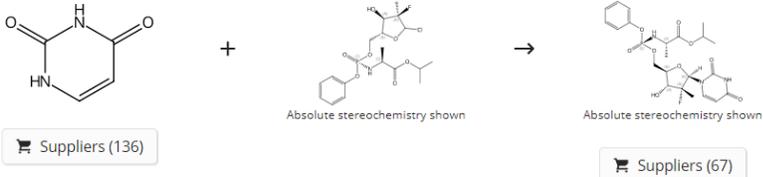
By: Ross, Bruce S.; et al
Canada, CA2988217 C 2020-06-23

[View Reaction Detail](#) [PatentPak](#) [Full Text](#)

[View All Reaction Summaries](#)

[Collapse Scheme](#)

Scheme 2 (1 Reaction) Steps: 1 Yield: 93%



[Suppliers \(136\)](#) [Suppliers \(67\)](#)

Reaction Summary Steps: 1 Yield: 93% [Preparation of medicine for inhibiting HCV](#)

1.1 Reagents: [N,O-Bis\(trimethylsilyl\)acetamide](#)
Solvents: [Chlorobenzene](#); 30 min, reflux; reflux → rt

1.2 Reagents: [Tin tetrachloride](#); rt; rt → reflux

By: Shi, Liping; et al
China, CN112940053 A 2021-06-11

[View Reaction Detail](#) [PatentPak](#) [Full Text](#)

[Collapse Scheme](#)

Search Within Results

Source Reference

Document Type

Journal (63)

Patent (659)

Language

Publication Year

Publication Name

World Intellectual Property Organization (266)

China (167)

Canada (80)

United States (73)

India (49)

[View All](#)

CA Section

Filter Content Report

Download filter data from this result set. [Download](#)

3. 在反应结果集页面，通过左侧的 Publication Name，可以选择自己感兴趣的反应文献来源。

相似反应检索

The screenshot displays the CAS SciFinder web interface. At the top, there is a navigation bar with the CAS SciFinder logo, a 'Saved' button, a 'History' button, and an 'Account' button. Below this is a light blue banner with a message about using BLAST search. The main content area is titled 'Reactions' and includes a search bar with the placeholder text 'Enter a query...'. To the left of the search bar is a vertical menu with options: 'All', 'Substances', 'Reactions' (highlighted with a blue bar and a blue '1'), 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'. To the right of the search bar are two blue buttons: 'Edit' (with a blue '2') and a search button (with a blue '3'). Below the search bar, a chemical reaction drawing is shown, with 'Edit Drawing' and 'Remove' buttons underneath it.

1. 选择 Reactions，进行反应检索。
2. 点击结构编辑器，绘制反应原料和产物。
3. 点击开始反应检索。

CAS SciFinder® Reactions Edit

Return to Home

Structure Match

As Drawn (200)

Substructure (1.7M)

1 Similarity (18K)

2 Similarity

Broad (18K) Medium (11K) Narrow (4,916)

Filter Behavior

Filter by Exclude

Yield

90-100% (3,001)

80-89% (2,079)

70-79% (1,616)

50-69% (2,116)

30-49% (1,285)

[View All](#)

Number of Steps

1 (18K)

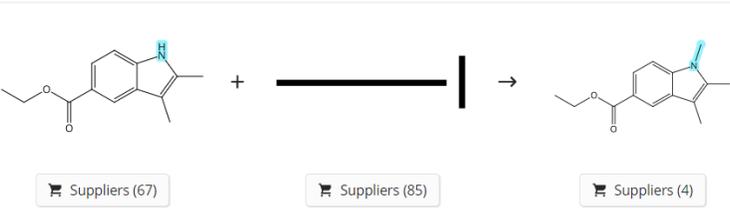
Reactions (18,368) Group: By Document View: Expanded

References

1

Indole compounds for the treatment of neurodegenerative diseases

By: Galyan, Simon Marius; Judd, Duncan Bruce
World Intellectual Property Organization, WO2021173593 A1 2021-09-02 | Language: English, Database: CAPlus



Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: [Sodium hydride](#)
Solvents: [Dimethylformamide](#); 0 °C; 2 h, 25 °C

[View Reaction Detail](#)

- 根据 Structure Match，选择 Similarity 的反应结果。
- 通过 Similarity 相似度，拉动显示条，自由选择查看相似度 Broad, Medium 或 Narrow 的结果。

筛选不参与反应的官能团

1. 点击 Reactions 进行反应检索。

2. 点击结构编辑器输入反应式。

3. 开始检索。

CAS SciFinder[®] Reactions (1,554) Group: By Scheme View: Expanded

Structure Match: As Drawn (1,002) Substructure (86K) Similarity (3,037)

Filter Behavior: Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

- Halide (25K)
- Ether (19K)
- Phenyl halide (17K)
- Amine (13K)
- Tertiary amine (9,905)
- Primary amine (1,554)

View All

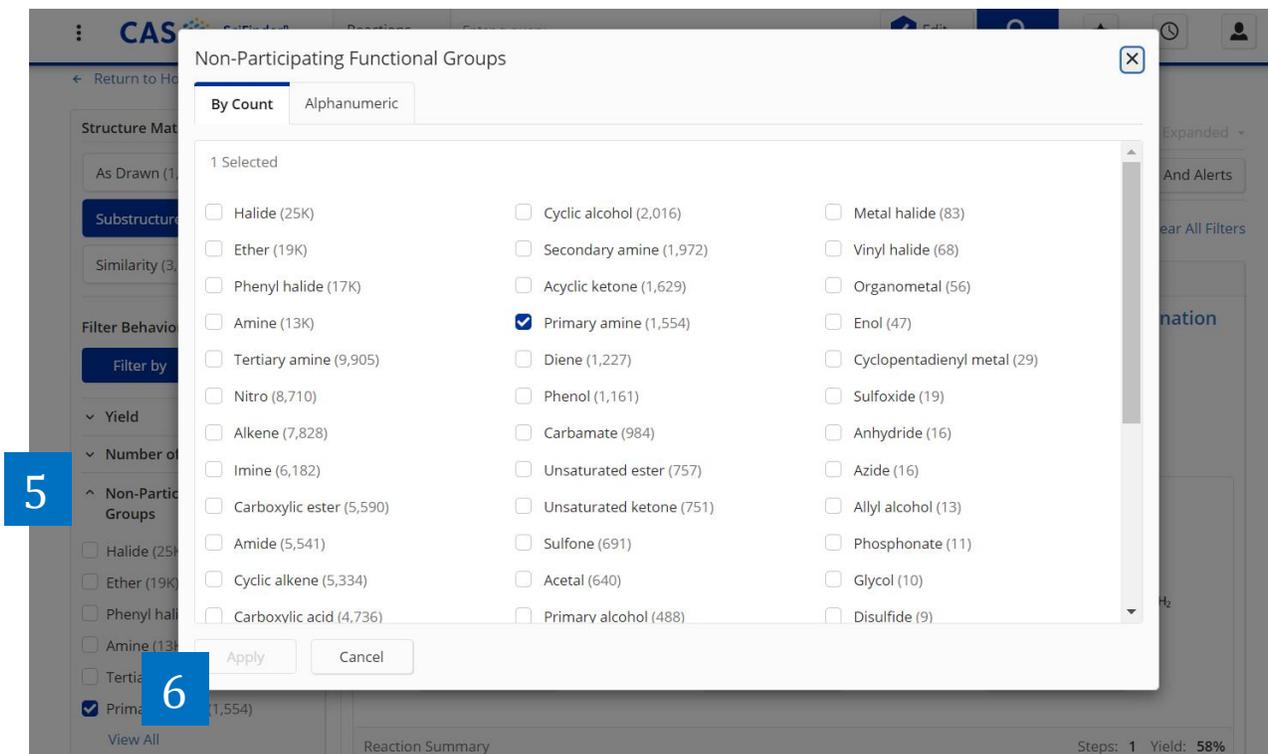
4

Reaction Summary Steps: 1 Yield: 37%

1.1 Reagents: 9,10-Dihydroanthracene; 180 min, 630 K
1.2 Reagents: 2-Methoxynaphthalene, Nitric acid

The Surprisingly Facile Thermal Dehalogenation of Chlorinated Aromatics by a Hydroaromatic Donor Solvent. Tautomerization of Chlorinated Phenols and Anilines

4. 反应结果集页面左侧 Non-Participating Functional Groups 筛选项下列出了不参与反应的官能团（按照反应结果数量排序），如果要查看所有不参与反应的官能团，则可点击 View All 获得完整的官能团列表。



5. 根据结果数量或官能团名称字母顺序排列不参与反应的官能团。
6. 勾选目标官能团后，点击 Apply 获取该官能团不参与反应的结果。

CAS SciFinder[®] Reactions 7 Edit Search Star Clock User

[Return to Home](#)

Structure Match

As Drawn (1,002)

Substructure (86K)

Similarity (3,037)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

- Halide (25K)
- Ether (19K)
- Phenyl halide (17K)
- Amine (13K)
- Tertiary amine (9,905)
- Primary amine (1,554)

[View All](#)

Reactions (1,554)

References

Filtering: Non-Participating Functional Groups: **Primary amine**

41

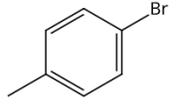
Discovery of N-(Naphthalen-1-yl)-N'-alkyl Oxalamide Ligands Enables Cu-Catalyzed Aryl Amination with High Turnovers

By: Gao, Jie; Bhunia, Subhajit; Wang, Kailiang; Gan, Lu; Xia, Shanghua; et al
Organic Letters (2017), 19(11), 2809-2812 | Language: English, Database: CPlus and MEDLINE

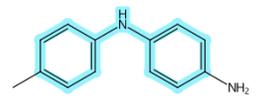
Full Text



Suppliers (85)



Suppliers (65)



Suppliers (16)

Reaction Summary Steps: 1 Yield: 58%

7. 浏览目标结果。

在 PatentPak Viewer 中使用 Retrosynthesis

The screenshot shows the PatentPak Viewer interface. On the left sidebar, under 'Key Substances in Patent', the first entry is highlighted with a red box labeled '1'. This entry is for CAS RN 2484-88-0, 4-(2-Phenyldiazenyl)benzenesulfonic acid. A pop-up window is open over this entry, showing its details. In this window, the 'Start Retrosynthetic Analysis' button is highlighted with a red box labeled '2'. The main window displays the chemical structure of 4-(2-Phenyldiazenyl)benzenesulfonic acid.

1. 在 PatentPak Viewer 中，点击物质结构。
2. 在弹出窗口中点击 Start Retrosynthetic Analysis，对此物质进行逆合成反应路线分析。

按相似性分组 Retrosynthesis 替代路线及互动选项

- 对替代反应路线 (Alternative Steps) 按相似性进行分组：可以就某一步反应展开所有的相似反应，也可以隐藏这些相似反应。
- 每一步路线节点处添加互动项：可直接在逆合成反应路线中，显示就某一步反应查看替代反应路线、支持的文献，也可以删除不感兴趣的反应路线或者物质，且被删除的内容可以被恢复。

具体操作如下：

B => E Alternative Steps (13)

Filter by

- Alternative Step Type
 - Experimental (1)
 - Predicted (12)
- Stereochemistry
 - Selective (1)
 - Non-Selective (12)

5 of 6 Predicted Step

CC(N)C1=CC=C(Cl)N=N1 >> CC(N)C1=CC=C(Cl)N=C1=O

Select View 3 similar Alternatives View Evidence (1,411) Average Yield: 74%

6 of 6 Predicted Step

CC(N)C1=CC=C(Cl)N=N1 >> CC(N)C1=CC=C(N)N=C1

Select View Evidence (9,454) Average Yield: 61%

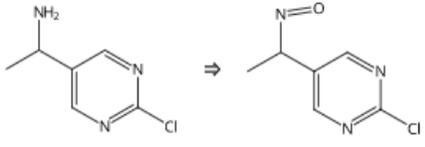
1. 点击 “View 3 similar Alternatives” ，查看替代 alternative 路线的相似反应路线。

B ⇒ E Alternative Steps (13)

Filter by

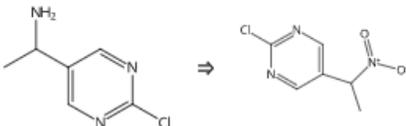
- Alternative Step Type
 - Experimental (1)
 - Predicted (12)
- Stereochemistry
 - Selective (1)
 - Non-Selective (12)

5 of 6 Predicted Step



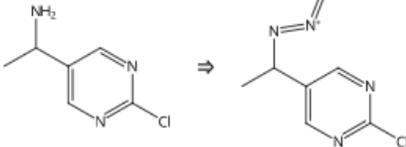
[Select](#) [Hide 3 similar Alternatives](#) [View Evidence \(1,411\)](#) Average Yield: 74%

5.1 Predicted Step



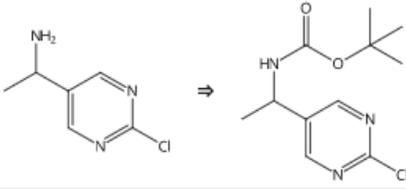
[Select](#) [View Evidence \(188,791\)](#) Average Yield: 79%

5.2 Predicted Step



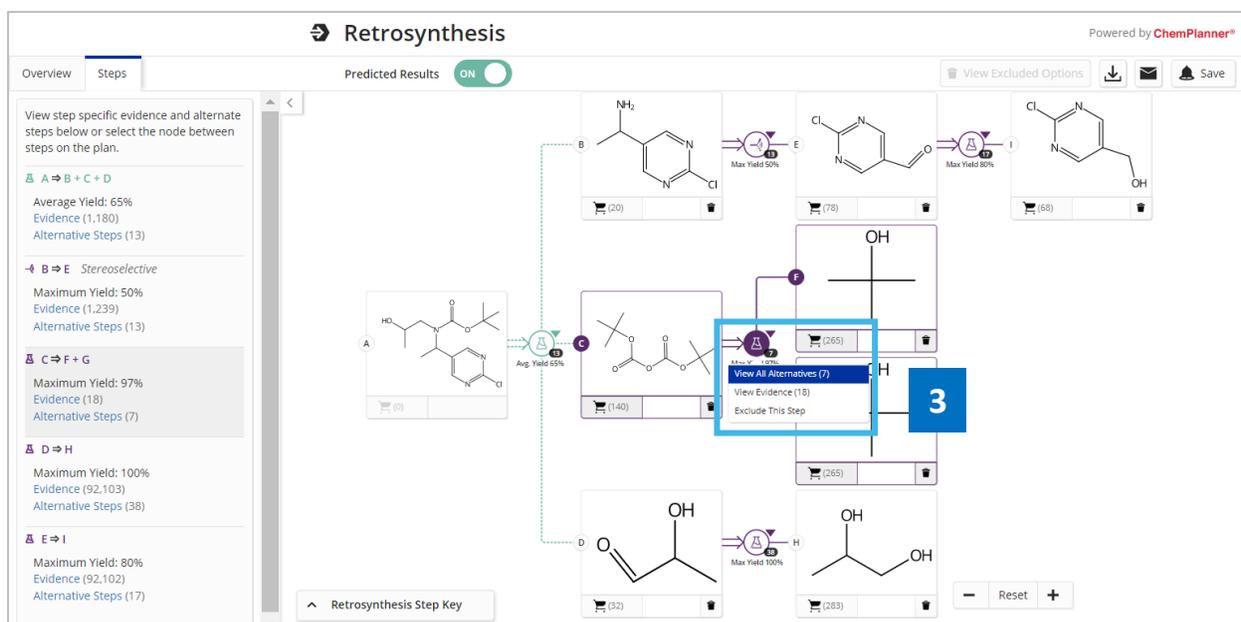
[Select](#) [View Evidence \(26,726\)](#) Average Yield: 78%

5.3 Predicted Step



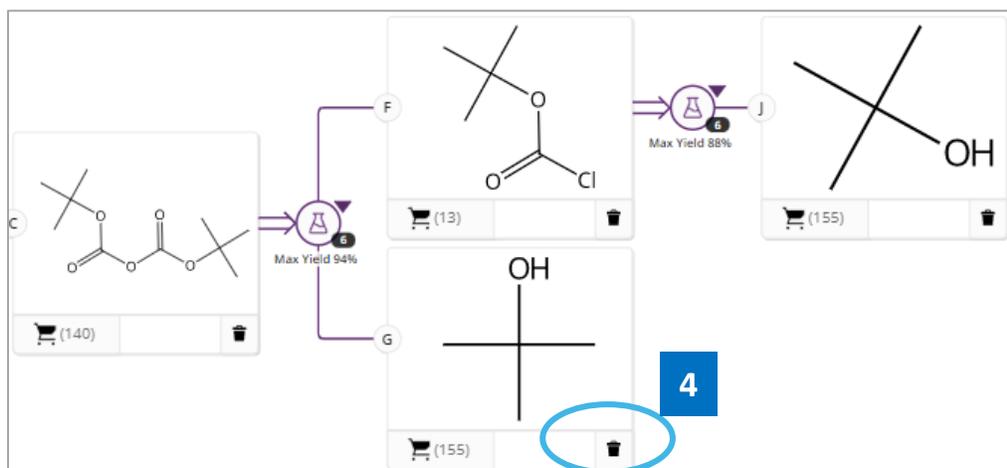
[Select](#) [View Evidence \(185,629\)](#) Average Yield: 80%

2. 相似的替代路线也可被隐藏 (hide)。

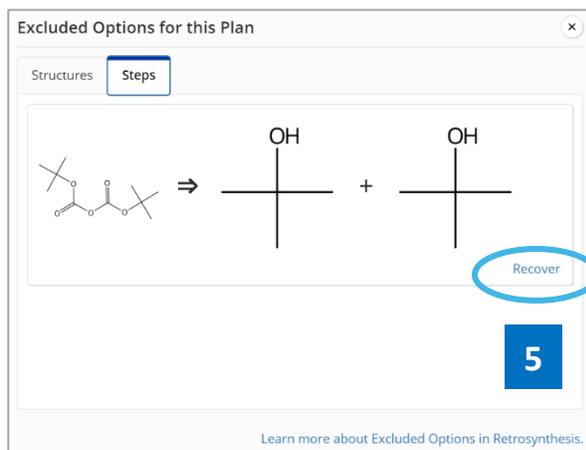
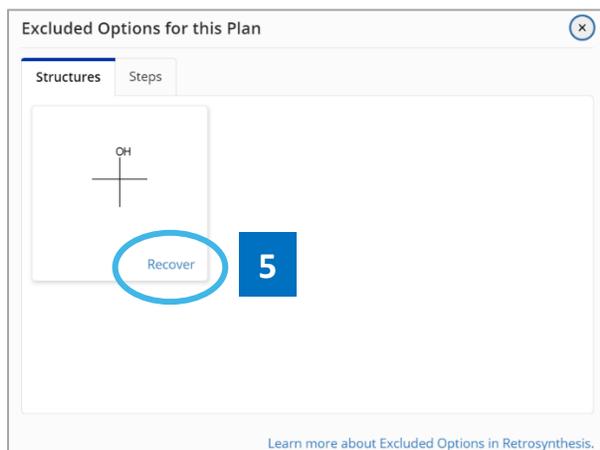
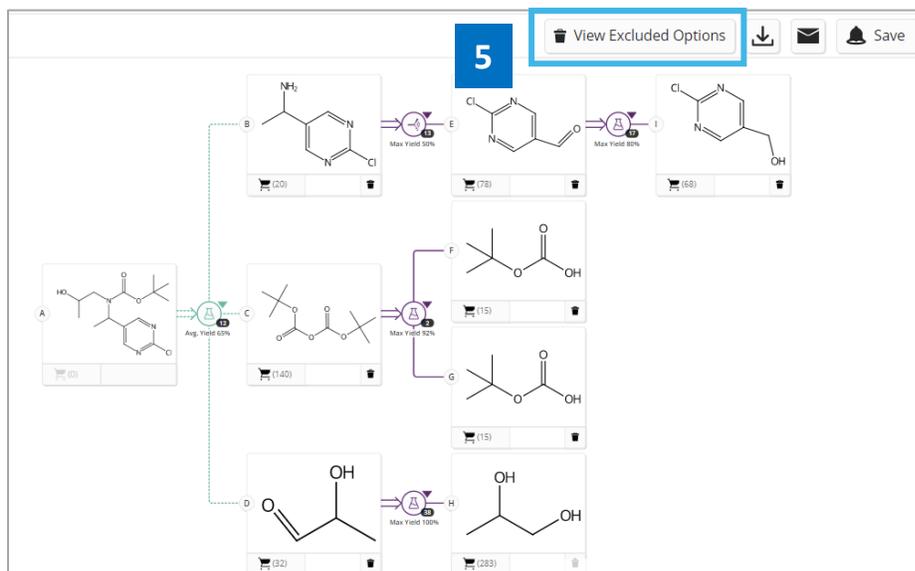


3. 点击逆合成路线节点中的下拉箭头，可显示互动项：View All alternatives, View Evidence, Exclude This step。

点击“View All alternatives”查看该步的替代反应路线、点击“View Evidence”查看支持反应的文献、点击“Exclude This step”可删除不感兴趣的反应路线；



4. 点击路线中某物质右侧垃圾桶标志，可从整个路线中删除这个物质，物质被删除后，系统会自动再补上另一个物质。



5. 所有被删除的反应路线或物质可通过“View Excluded Options”来查看，也可被恢复 (recover)。

反应结果集的排序

在 CAS SciFindern 反应结果集页面，提供两种结果排列方式：

- 1- By Scheme, 将来自不同文献，底物和产物相同的多条记录仅展示为一条记录。
- 2- By Document, 当一篇文献报道了多条反应时，仅展示其中与被检索反应式最相关的一条反应。

The screenshot shows the CAS SciFindern interface for reaction results. On the left, there is a 'Filter Behavior' sidebar with options to 'Filter by' or 'Exclude'. Under 'Yield', there are radio buttons for ranges like 90-100% (3), 80-89% (2), etc. Under 'Number of Steps', there are radio buttons for 1 (82), 2 (45), etc. Under 'Non-Participating Functional Groups', there are radio buttons for 'Cyclic ketone (66)' and 'Ketone (66)'. The main area is titled 'Reactions (305)' and shows 'Group: By Document' and 'View: Expanded'. A 'References' dropdown is highlighted with a blue box containing the number '1'. Below it, the reaction title 'Microbial 11 α -hydroxylation of steroids' is shown, along with author information and a 'View 2 Related Reactions' button, which is highlighted with a blue box containing the number '2'. The reaction scheme shows a steroid molecule being converted to its 11 α -hydroxylated form. Below the scheme are 'Suppliers (36)' and 'Suppliers (11)' buttons. At the bottom, a 'Reaction Summary' box indicates 'Steps: 1 Yield: 98%' and lists reagents: '1.1 Reagents: Glucose'. A 'View Reaction Detail' link is also present.

6. 选择 Group: By Document 对反应检索结果进行排序。
7. 当选择按照 By Document 时，点击 View 2 Related Reactions 查看该文献报道的所有反应。

Filter Behavior

Yield

90-100% (3)

80-89% (2)

70-79% (1)

50-69% (4)

30-49% (2)

[View All](#)

Number of Steps

1 (82)

2 (45)

3 (36)

4 (32)

5 (27)

6-10 (37)

Non-Participating Functional Groups

Reactions (305) Group: By Scheme View: Expanded

Scheme 1 (1 Reaction) Steps: 1 Yield: 98%



Absolute stereochemistry shown

Reaction Summary Steps: 1 Yield: 98% **Microbial 11 α -hydroxylation of steroids**

1.1 Reagents: [Glucose](#)

By: Wiersma, Marten; et al
World Intellectual Property Organization, WO9721830 A1
1997-06-19

Cyclic ketone (66)

Ketone (66)

Alkene (65)

Cyclic alkene (65)

Unsaturated ketone (53)

[View All](#)

Experimental Protocols

Synthetic Methods (7)

Experimental Procedure (187)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Document Type

Language

Scheme 2 (4 Reactions) Steps: 1 Yield: 93%



Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown

Reaction Summary Steps: 1 Yield: 93% **Process for extraction of 11 α -hydroxycanrenone from fermentation broth and purification using a micro-emulsion system**

1.1 Reagents: [Glucose](#), [Monopotassium phosphate](#)
Solvents: [Water](#); 240 h, pH 5 - 6, 28 °C

By: Gaikawai, Raghavendra P.; et al
India, IN2011MU00884 A 2014-03-28

Reaction Summary Steps: 1 **Microbial 11 α -hydroxylation of steroids**

1.1 Reagents: [Glucose](#)

By: Wiersma, Marten; et al
World Intellectual Property Organization, WO9721830 A1
1997-06-19

Reaction Summary Steps: 1 **Preparation of 7 α -carboxyl-9,11-epoxy steroids and intermediates useful therein and a general process for the epoxidation of olefinic double bonds**

No Data Available

8. 选择 Group: By Scheme 对反应检索结果进行排序。

9. 当选择按照 By Scheme 时, 反应结果会呈现底物和产物相同的文献。

文献检索

文献信息的获取

The screenshot shows the CAS SciFinder® interface. On the left, under 'Searching for...', the 'References' category is selected (1). The main area is titled 'References' and contains a search bar (2) with the placeholder 'Enter a query...'. Below the search bar is a dropdown menu (4) with 'Author Name' selected. To the right of the search bar is a 'Draw' button (3) and a search button (5). The search bar also contains the text 'Enter last name, first name middle name.' and an example 'Example: Schubert, J A'. The interface also shows 'Saved', 'History', and 'Account' options at the top right.

1. 在 CAS SciFinder[®] 主页选择 References，进行文献检索。
2. 输入检索信息：关键词、物质名称、CAS 号、专利号或者文献 ID 号等。
3. 点击 Draw，绘制结构，可以通过结构式（反应式）直接检索文献；也可以同时在 2 所示的文本框中输入相应文本，联合检索文本与结构获取相关文献，所得文献结果既匹配输入的文本，还匹配绘制的物质（反应）结构。
4. 点击 Add Advanced Search Field，可输入更多检索条件进行检索。
5. 开始检索。

The screenshot displays the CAS SciFinder interface with the following elements highlighted by numbered callouts:

- 1:** Sort dropdown menu (Relevance).
- 2:** View dropdown menu (Partial Abstract).
- 3:** Filter Behavior section (Filter by/Exclude).
- 4:** Download options (PDF, rtf, etc.).
- 5:** Save And Alerts button.
- 6:** Save And Alerts button.
- 7:** Title of the first reference: "Pharmacological inhibitors of cyclin-dependent kinases".
- 8:** Full Text button.
- 9:** Substance button.
- 10:** Reactions button.
- 11:** Citing button.
- 12:** Citation Map button.

1. 点击文献结果集页面 Sort 右侧小箭头，对结果按照引用次数、相关性、公开日期等进行排序
2. 点击 View 右侧小箭头，选择结果展示的详略
3. 全面的文献结果筛选或者排除选项
4. 通过 PDF, rtf, ris, txt, xlsx 等格式下载检索结果
5. 通过电子邮件分享检索结果
6. 保存检索结果, 并可同时设置信息更新提醒
7. 点击题目, 查看文献详情
8. 获取文献中的物质
9. 获取文献中的反应

10. 获取引用本文章的文献

11. 引文地图, 获取前向及后向引用

12. 获取全文链接

Reference Detail (48 of 728)

Substances (723) Reactions (1,943) Citing (11) Citation Map **2** **3** Prev Next

Download Save

1

PATENT

Patent Number
WO2004018473

Publication Date
2004-03-04

Application Number
WO2003-IB4188

Application Date
2003-08-22

Kind Code
A2

Assignee
Institute of Experimental Botany
ASCR, Czech Republic

Source
World Intellectual Property
Organization
CODEN: PIXXD2

Database Information
AN: 2004:182882
CAN: 140:217666
Cplus

Language
English

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. [View content from CAS Formulus®](#) in this document. [Learn more about Formulus®](#).

Preparation of di- and tri-substituted 8-azapurine derivatives as cyclin-dependent kinase inhibitors

By: Fuksova, Kveta; Havlicek, Libor; Krystof, Vladimir; Lenobel, Rene; Strnad, Miroslav

Title compounds I [R⁶ = halo, NHH₂, amino, etc.; R² = halo, NHH₂, alkyl, etc.; R⁹ = alkyl, cycloalkyl, etc.] are prepared. For instance, 4-amino-5-carboxamido-1-isopropyl-1,2,3-triazole (preparation given) is converted to 2,6-dihydroxy-9-isopropyl-8-azapurine (EtOH, NaOEt, (EtO)₂CO, 90°, 4 h). The dihydroxy derivative is converted to the corresponding dichloride (POCl₃, lutidine, 120°, 3 h), treated with benzylamine (n-BuOH) followed by 3-aminopropanol to give II. II has IC₅₀ = 54.6 μM for CDK2-cyclin E. The present invention relates to a compound of formula (I), or a pharmaceutically acceptable acid salt thereof. I are useful in the treatment of hyperproliferative skin disorders, viral infections, cancer, etc. The invention also relates to the use of 2,6,9-trisubstituted-8-azapurines in maintaining mammalian oocytes at the germinal vesicle stage.

Keywords: azapurine cyclin dependent kinase inhibitor preparation

PatentPak PDF Get Prior Art Analysis Full Text

4

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2004018473	English	A2	PDF	2004-03-04	WO2003-IB4188	2003-08-22
					GB2002-19746	2002-08-23
AU2003260919	English	A1		2004-03-11	AU2003-260919	2003-08-22
WO2004018473	English	A3		2004-05-21	WO2003-IB4188	2003-08-22
EP1539760	Undetermined	A2		2005-06-15	EP2003-792601	2003-08-22
JP2006511458	Japanese	T		2006-04-06	JP2004-530478	2003-08-22
US20060035909	English	A1		2006-02-16	US2005-1151059	2005-02-04
US7816350	English	B2		2010-10-19	US2005-1151059	2005-02-04

5

Expand All | Collapse All

IPC Data **6**

Patent	Class	Patent Family Classification Codes
WO2004018473	IPC	C07D 0487/00 A
AU2003260919	IPC	C07D 0487/00 A
WO2004018473	IPC	C07D 0487/00 A
EP1539760	IPC	C07D 0487/00 A
JP2006511458	IPC	C07D 0487/04; A61K 0031/519; A61K 0031/136; A61K 0033/24; A61K 0031/337; A61K 0031/704; A61P 0025/00; A61P 0009/00; A61P 0013/12; A61P 0037/06; A61P 0017/06; A61P 0031/00; A61P 0025/28; A61P 0043/00; A61P 0011/06; A61P 0029/00; A61P 0035/00; A61P 0003/10; A61P 0027/02; A61P 0017/00; A61P 0031/12; A61P 0031/20; A61P 0035/02; A61P 0011/00; A61P 0031/18; A61P 0017/14; C12Q 0001/48; C12N 0009/99; G01N 0033/50; G01N 0033/15; A01N 0043/90; A61P 0033/00
US20060035909	IPC	A61K 0031/519; C07D 0487/02
US7816350	IPC	C07D 0487/04; A61K 0031/519; A61P 0035/00; A61P 0025/28; A61P 0017/06; A61P 0003/10; A61P 0013/12; A61P 0037/02; A61P 0031/20; A61P 0031/22

Concepts **7**
 Substances **8**
 Formulations **9**
 Cited Documents **10**

1. 文献书目信息
2. 文献相关信息：物质、反应、引文、引文地图
3. 点击左右箭头，查看上一篇或下一篇文献的详情
4. 获取专利相关的现有技术
5. 专利族成员信息
6. 专利分类号
7. CAS 科学家标引的文章中重要技术术语
8. 文献中报道的物质及其在文献中的研究角色
9. 文献中的制剂配方信息
10. 文献的参考文献

高级文献检索

使用高级文献检索，可以快速获得更相关的结果。

The screenshot shows the CAS SciFinder Advanced Search interface. On the left, under 'Searching for...', the 'References' option is selected with a blue arrow and a '1' in a blue box. In the center, a dropdown menu is open, listing search fields: Author Name, Publication Name, Organization Name, Title, Abstract/Keywords, Concept, Substances, Publication Year, Document Identifier, Patent Identifier, and Publisher. A '2' in a blue box is next to the dropdown. The 'Author Name' field is highlighted with a blue box and a '3' in a blue box. The search bar contains the text 'Enter a query...' and 'Enter last name, first name middle name.' with an example 'Schubert, J A'.

1. 在主页面，选择 References。
2. 选择逻辑运算符 and, or ,not，连接不同的检索字段。
3. 根据需要，选择相应的检索字段。

例：紫杉醇全合成，并包含“stereo”这一 concept。

4. 在相应的字段输入检索词。
5. 可以使用通配符“*”，通配符*代表 1 或者多个字符，可用于词中或者词尾。

6. 获得文献结果集
7. 通过 substance role 限定物质的具体研究信息，如：制备（preparation）。

CAS SciFinder® References Edit Search total synthesis Draw

Reference Detail (1 of 58)

Substances (105) Reactions (1,887) Citing (130) Citation Map Save

Total Synthesis of Microtubule-Stabilizing Agent (-)-Laulimalide 8

By: Ghosh, Arun K.; Wang, Yong; Kim, Joseph T.

JOURNAL
Source
 Journal of Organic Chemistry
 Volume: 66
 Issue: 26
 Pages: 8973-8982
 Journal: Article; Research Support, U.S. Gov't, P.H.S.
 2001
 DOI: [10.1021/jo0110854h](https://doi.org/10.1021/jo0110854h)
 CODEN: JOCEAH
 ISSN: 0022-3263
 ISSN-L: 0022-3263

Database Information
 AN: 2001:869107
 CAN: 136:151030
 PubMed ID: 11749630
 Cplus and MEDLINE

Company/Organization
 Department of Chemistry
 University of Illinois at Chicago
 Chicago, Illinois 60607
 United States

Email
arunghos@uic.edu

Publisher
 American Chemical Society

An enantioselective first **total synthesis** of laulimalide (I) is described. I, a remarkably potent antitumor macrolide, has been isolated from the Indonesian sponge Hyattella sp. and the Okinawan sponge Fasciospongia rimosa. I represents a new class of antitumor agents with significant clin. potential. The **synthesis** is convergent and involved the assembly of C₃-C₁₆ segment II and C₁₇-C₂₈ segment III by Julia olefination. The sensitive C₂-C₃ cis-olefin functionality was installed by Yamaguchi macrolactonization of a hydroxy alkynic acid followed by hydrogenation of the resulting alkyonic lactone over Lindlar's catalyst. Initial attempts of intramol. Still's variant of Horner-Emmons olefination between the C₁₅-phosphonocetate and C₃-aldehyde provided a 1:2 mixture of cis- and trans-macrolactones. The trans-isomer was photoisomerized to a mixture of cis- and trans-isomers. The other key steps involved ring-closing olefin metathesis to construct both dihydropyran units, stereoselective anomeric alkylation to functionalize the dihydropyran ring, stereoselective reduction of the resulting alkynyl ketone to set the C₂₀-hydroxyl stereochem., and a novel Julia olefination protocol for the installation of the C₁₃-exo-methylene unit. The sensitive epoxide at C₁₆-C₁₇ was introduced in a highly stereoselective manner by Sharpless epoxidation at the final stage of the **synthesis**.

The image displays three chemical structures labeled I, II, and III. Structure I is the complex macrolide laulimalide, featuring a large ring with multiple stereocenters, including a cis-olefin, a dihydropyran ring, and a sensitive epoxide at the C₁₆-C₁₇ position. Structure II is a key intermediate containing a dihydropyran ring, a methyl group, a MOM-protected aldehyde, and a terminal alkyne. Structure III is another intermediate, showing a dihydropyran ring, a methyl group, a hydroxyl group, and a phosphonate group.

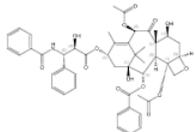
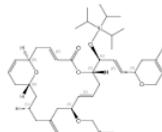
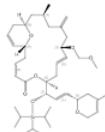
Keywords: laulimalide **total synthesis** asym macrolactonization Yamaguchi; metathesis olefin ring closing photoisomerization laulimalide **preparation**; olefination Julia Horner Emmons laulimalide **preparation**; Sharpless epoxidation stereoselective reduction laulimalide **preparation**; alkylation stereoselective anomeric hydrogenation laulimalide **preparation**

Full Text ▾

[Expand All](#) | [Collapse All](#)

- ▾ Concepts
- ▾ MEDLINE[®] Medical Subject Headings
- ▾ Supplementary Concepts
- ▾ Substances

🔍 Substances (105)

<p>33069-62-4</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p>C₄₇H₅₁NO₁₄ Taxol</p> <p>Role: Unspecified</p>	<p>725242-41-1</p>  <p>Absolute stereochemistry shown Double bond geometry shown</p> <p>C₄₁H₆₆O₇Si (1<i>R</i>,3<i>E</i>,9<i>E</i>,15<i>S</i>,17<i>R</i>)-7-[[1<i>S</i>,2<i>E</i>]-3-[(2<i>S</i>)-3,6-Dihydro-4-methyl-2<i>H</i>-pyran-2-yl]-1-[[[tris(1-methylethyl)silyl]oxy]-2-propen-1-yl]-11-(methoxymethoxy)-15-methyl-13-methylene-6,21-dioxabicyclo[15.3.1]heneicosa-3,9,19-trien-5-one</p>	<p>725242-39-7</p>  <p>Absolute stereochemistry shown Double bond geometry shown</p> <p>C₄₁H₆₆O₇Si (1<i>R</i>,3<i>Z</i>,7<i>S</i>,9<i>E</i>,11<i>S</i>,15<i>S</i>,17<i>R</i>)-7-[[1<i>S</i>,2<i>E</i>]-3-[(2<i>S</i>)-3,6-Dihydro-4-methyl-2<i>H</i>-pyran-2-yl]-1-[[[tris(1-methylethyl)silyl]oxy]-2-propen-1-yl]-11-(methoxymethoxy)-15-methyl-13-methylene-6,21-dioxabicyclo[15.3.1]heneicosa-3,9,19-trien-5-one</p>
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8. 未限定检索字段的词语，则可能出现在标题、摘要、Keywords、Concept、MEDLINE Medical Subject Headings、Supplementary Concepts 和 Substances 中；并以湖蓝色标亮显示。

出版社检索

在进行文献检索时，可选择 Add Advanced Search Field，输入出版社名称，将检索结果限定为某出版社旗下出版刊物中的文献。

Searching for...

- All
- Substances
- Reactions
- References**
- Suppliers
- Biosequences
- Retrosynthesis

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Organocatalysis

AND Publisher American Chemical Society

+ Add Advanced Search Field

[Learn more about SciFinder[®] Advanced Search.](#)

1. 选择 References，在检索框中输入主题词。
2. 点击 Add Advanced Search Field，然后点击 Select 下拉菜单，再在菜单中选择“publisher”，最后在输入框中输入出版社名称。

CAS SciFinder[®] References Edit Search Organocatalysis

Return to Home

Filter Behavior

Filter by Exclude

Document Type

- Journal (494)
- Review (84)
- Conference (368)
- Editorial (1)
- Preprint (16)

Language

Publication Year

2000 to 2021

No Min to No Max Apply

View Larger

Available at My Institution

References (869)

Sort: Times Cited View: Full Abstract

Substances Reactions Citing

1

Organocatalysis by N-Heterocyclic Carbenes

By: Enders, Dieter; Niemeier, Oliver; Henseler, Alexander

Chemical Reviews (Washington, DC, United States) (2007), 107(12), 5606-5655 | Language: English, Database: CAPlus and MEDLINE

A review. This review highlights the extensive applications and reaction pathways of thiazol-, triazol-, imidazol-, and imidazolin-2-ylidenes as versatile synthetic methods.

Full Text Substances (2) Reactions (0) Citing (2,258) Citation Map

2

Enamine-Based Organocatalysis with Proline and Diamines: The Development of Direct Catalytic Asymmetric Aldol, Mannich, Michael, and Diels-Alder Reactions

By: Notz, Wolfgang; Tanaka, Fujie; Barbas, Carlos F. III

Accounts of Chemical Research (2004), 37(8), 580-591 | Language: English, Database: CAPlus and MEDLINE

A review. Enamines and imines have long been recognized as key intermediates in enzyme catalysis, particularly within a class of enzymes organic chemists would very much like to emulate, the aldolases. Here we summarize the contributions of this laboratory to converting enzymic enamines, and in some cases imines, into a versatile catalytic asym. strategy powered by small organic mols.

Feedback

3. 在结果集页面，可通过 Document Type 分析/筛选该出版社旗下各类型文献。

4

The screenshot displays the CAS SciFinder interface. On the left, a sidebar contains filters for Organization, Publication Name, Concept, and CA Section. The Publication Name filter is expanded, showing a list of journals and their respective document counts: Organic Letters (108), Journal of the American Chemical Society (98), Journal of Organic Chemistry (90), ACS Catalysis (48), and Accounts of Chemical Research (34). A 'View All' link is provided below the list. In the center, a preview of a document titled 'Organocatalytic Reaction' is shown, featuring a chemical reaction scheme with labels for 'Oxidation Acylation', 'Base Catalysis', 'Annulation', and 'Umpolung Catalysis'. On the right, a 'Publication Name' window is open, displaying a list of publications with checkboxes for selection. The list includes various ACS National Meetings and regional meetings, along with their dates and locations. The window has tabs for 'Top Count', 'Alphanumeric', and 'Search', and buttons for 'Apply' and 'Cancel'.

4. 也可通过 Publication Name 筛选出该出版社旗下某期刊发表的文献。

获取制剂（配方）信息

在 CAS SciFinder[®] 中，可通过以下两种方式获取制剂（配方）信息：

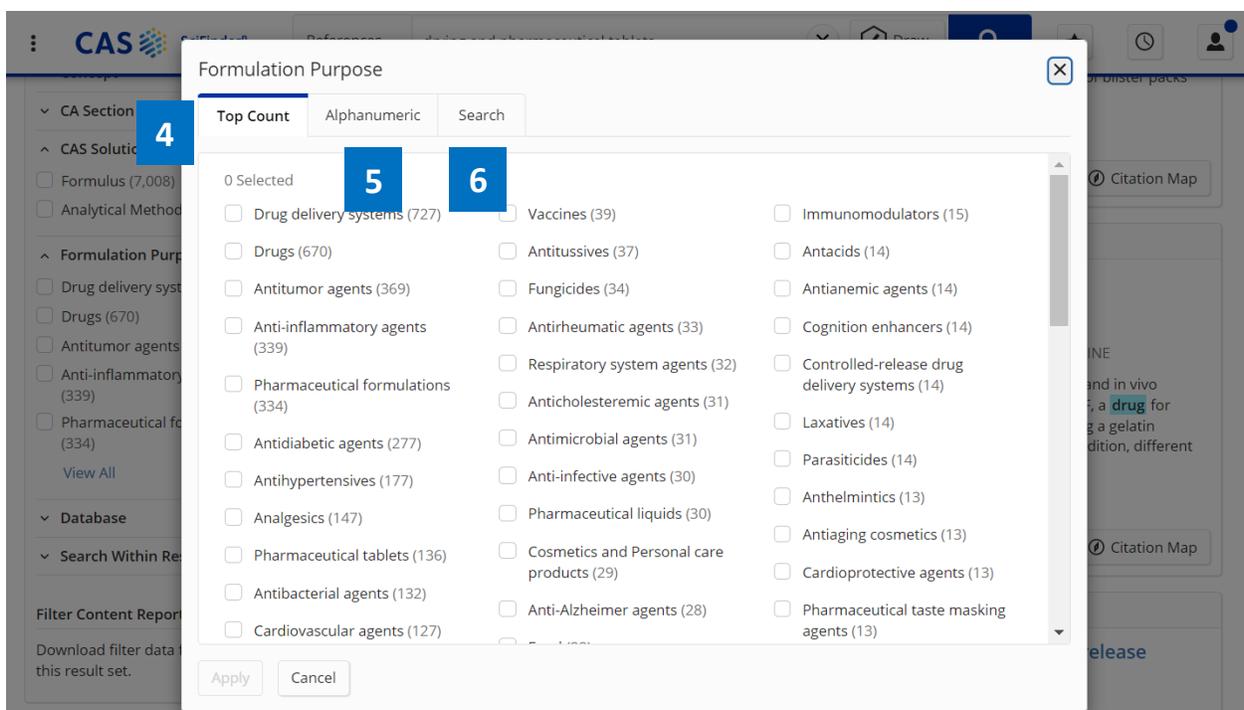
- 一. 直接在 References 检索框中输入检索式，在得到的文献结果页面左侧选择 Formulation Purpose, 获得感兴趣的制剂（配方）信息。
- 二. 从物质检索开始，通过物质获取文献，然后在文献结果页面左侧选择 Formulation Purpose, 获得感兴趣的制剂（配方）信息。

方法一： 直接在 References 检索框中输入检索式，在得到的文献结果页面左侧选择 Formulation Purpose, 获得感兴趣的制剂（配方）信息：

The screenshot displays the CAS SciFinder interface for a search on 'drying and pharmaceutical tablets'. The search results are sorted by relevance and shown as partial abstracts. The first result is 'Formulation of a lyophilized dry emulsion tablet for the delivery of poorly soluble drugs' by Corveleyn, S.; Remon, J. P. (1998). The abstract describes the development of a dry emulsion tablet for poorly water-soluble drugs using lyophilization. The second result is 'Development of directly compressible powders via co-spray drying' by Gonnissen, Y.; Remon, J. P.; Vervaet, C. (2007), which describes the continuous production of directly compressible powders via co-processing of acetaminophen and carbohydrates.

The screenshot shows the CAS SciFinder search results page for the query "drying and pharmaceutical tablets". The interface includes a search bar at the top with the query entered. On the left, there is a sidebar with various filters. Two blue boxes with numbers 2 and 3 highlight specific filter options: "Formulus (7,008)" under "CAS Solutions" and "Drug delivery systems (727)" under "Formulation Purpose". The main content area displays search results, including a list of articles with titles, authors, and abstracts. The first article is titled "In vitro and in vivo evaluation of a fast-disintegrating lyophilized dry emulsion tablet containing griseofulvin". The second article is titled "Evaluation of spray-drying as a method to prepare microparticles for controlled drug release".

1. 选择 References，输入检索式
2. 在文献结果集页面左侧，勾选 CAS Solutions 下的 Formulus，可以获得制剂（配方）的更多信息。
3. 在文献结果集页面左侧，勾选 Formulation Purpose 下的相应选项，获取针对某适应症的制剂信息，点击 View All 可查看全部选项列表。



4. 根据文献数量对选项进行排序。
5. 根据选项字母顺序排序。
6. 直接输入感兴趣的 formulation purpose, 快速获取目标信息。

7. 可以选择一个或者几个选项。
8. 点击题目查看文献信息详情。

The screenshot shows the CAS SciFinder interface. At the top, there is a search bar with the query "drying and pharmaceutical tablets". Below the search bar, the page title is "Reference Detail (3 of 1,078)". On the left side, there is a sidebar with "JOURNAL" information, including the source "Journal of Pharmaceutical Investigation", volume, issue, and pages. The main content area displays the title "Employing an optimized spray-drying process to produce ezetimibe tablets with an improved dissolution profile" and the authors "By: Kim, Sungyub; Gupta, Biki; Moon, Cheol; Oh, Euichaul; Jeong, Jee-Heon; Yong, Chul Soon; Kim, Jong Oh". Below the title, there is a "Keywords" section with "ezetimibe tablets spray drying process dissolution". At the bottom, there is a navigation menu with options: "Concepts", "Substances", "Formulations" (highlighted with a blue box and the number "9"), and "Cited Documents".

9. 点击 Formulations 查看制剂（配方）信息。

The screenshot shows the CAS SciFinder interface. At the top, there is a search bar with the text 'drying and pharmaceutical tablets'. Below the search bar, there are navigation tabs for 'Substances' and 'Formulations'. The 'Formulations' tab is selected, and the search results are displayed. The first result is 'Ezetimibe Tablet: Drug Delivery Systems'. Below the title, there is a link to 'View CAS Formulus® Detail'. The 'Location' is 'Article Page 3, 8, Table 2', the 'Purpose' is 'Drug delivery systems', and the 'Target' is 'solubility, bioavailability'. A table lists the components of the formulation:

Component	Function	Amount Reported
Ezetimibe	cholesterol inhibiting agent	10 mg/tablet
(+)-Lactose	diluents	100 mg/tablet
Cellulose	diluents	50 mg/tablet
Silica	lubricants	12.5 mg/tablet

Below the table, there is a link to 'View CAS Formulus® Detail' and another search result for 'Ezetimibe Tablet: Drug Delivery Systems' with similar details.

10. 点击 View Formulus Detail，将进入 CAS 另一个解决方案 Formulus (关于 Formulus 的更多信息，请咨询美国化学摘社北京代表处：china@acs-i.org)

11. 该制剂（配方）在原文中出现的位置。

12. 制剂（配方）用途。

13. 制剂（配方）中的成分。

14. 各成分所起的作用。

15. 成分含量。

16. 点击蓝色超链接的物质名，可以获取其物质信息详情。

方法二：从物质检索开始，通过物质获取文献，然后在文献结果页面左侧选择 Formulation Purpose，获得感兴趣的制剂（配方）信息（以获取阿拉伯木聚糖制剂信息为例）：

The screenshot shows the CAS SciFinder web interface. At the top, there is a search bar with the text 'Substances 9040-27-1'. Below the search bar, there is a 'Filter Behavior' section with a 'Filter by' button and an 'Exclude' button. The main content area displays 'Substances (1)' with a 'View: Partial' dropdown. Below this, there are buttons for 'References', 'Reactions', and 'Suppliers'. A results list shows one entry for '9040-27-1' with the name 'Unspecified Arabinoxylan'. Below the name, there are statistics: '3,667 References', '27 Reactions', and '7 Suppliers'. A blue box with the number '1' is positioned over the search bar, and another blue box with the number '2' is positioned over the 'References' button.

1. 进行物质检索，获得物质检索结果集。
2. 由物质获得文献结果集。

CAS SciFinder®

References (3,667)

Sort: Relevance View: Partial Abstract

Substances Reactions Citing

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder[®] users. Use the [CAS Solutions: Formulus filter](#) to view available content. [Learn more about Formulus.](#)

1

Cereal arabinoxylans: advances in structure and physicochemical properties
 By: Izydorczyk, Marta S.; Biliaderis, Costas G.
 Carbohydrate Polymers (1995), 28(1), 33-48 | Language: English, Database: CPlus

A review with 89 references They consist of a linear β -(1 \rightarrow 4) linked xylan backbone to which α -L-arabinofuranose units are attached as side residues via α -(1 \rightarrow 3) and/or α -(1 \rightarrow 2) linkages. Several structural models have been put forward based on enzymic degradation studies and structure elucidation of oligosaccharides by NMR, methylation, and periodate oxidation techniques. These tentative models present different substitution patterns of arabinoses along the xylan chain. Cereal arabinoxylans exhibit a great deal of structural heterogeneity with respect to ratio of Araf/Yxp substitution pattern ...

View More

2

Arabinoxylans and Endoxylanases in Wheat Flour Bread-making
 By: Courtin, C. M.; Delcour, J. A.
 Journal of Cereal Science (2002), 35(3), 225-243 | Language: English, Database: CPlus

A review. For the past 50 yr the function of arabinoxylans in bread-making was the subject of much debate and controversy. In the

3

Food (25)
 Drug delivery systems (19)
 Dietary supplements (17)
 Antidiabetic agents (10)
 Antiobesity agents (9)

View All

Substance (1) Reactions (0) Citing (607) Citation Map

3. 在 Formulation Purpose 中勾选所需目标制剂信息。其余内容同方法一，在此不再赘述。

药物重定位 (Repositioning)

药物重定位指对现有药物进行研究以用于新的治疗目的。这种模式已经取得了许多成功，相比于新药研发，其可大大缩减研发成本和时间。因此药物重定位逐渐成为很多科研机构、医药企业看重的策略之一。

此处以肉桂硫胺为例，介绍如何在 CAS SciFinder[®] 中检索药物的重利用信息：

The screenshot displays the CAS SciFinder search results for the substance Cinanserin. The search bar at the top shows the CAS number 1166-34-3. The left sidebar contains filter options under 'Filter Behavior', including 'Commercial Availability', 'Reaction Role', and 'Reference Role'. The main content area shows the chemical structure of Cinanserin, its name, molecular formula (C₂₀H₂₄N₂OS), and the number of references (444) and suppliers (23). A blue box highlights the number '2' in the 'References' section, indicating the number of references selected for viewing.

1. 通过肉桂硫胺的 CAS 登记号、化学名称或者结构式等方式检索得到肉桂硫胺的物质信息。
2. 获取报道肉桂硫胺的文献。

3. 在文献页面，通过左侧的 Publication Year 限定文献结果，如：筛选 2000 年以前发表的文献。

4. 点击 View All, 查看所有 Concept.

Concept

Top Count Alphanumeric Search

Concept Name

5- Search

Select All on Page

<input type="checkbox"/> 2-((2-(dimethylamino)methyl)phenyl)thio-5-iodophenylamine (2)	<input type="checkbox"/> 5-HT _{2A} receptors (7)	<input type="checkbox"/> 5-HT receptors (43)
<input type="checkbox"/> 5-HT _{1A} agonists (1)	<input type="checkbox"/> 5-HT _{2B} receptors (1)	<input type="checkbox"/> 5-Hydroxytryptophan (26)
<input type="checkbox"/> 5-HT ₁ agonists (1)	<input type="checkbox"/> 5-HT _{2C} receptors (7)	<input type="checkbox"/> 8-iodo-2,3,4,5-tetrahydro-3-methyl-5-phenyl-1H-3-benzazepine-7-ol (1)
<input type="checkbox"/> 5-HT _{1A} receptors (9)	<input type="checkbox"/> 5-HT ₂ receptors (23)	<input type="checkbox"/> Receptor, Serotonin, 5-HT _{1D} (1)
<input type="checkbox"/> 5-HT _{1B} receptors (3)	<input type="checkbox"/> 5-HT ₃ antagonists (1)	<input type="checkbox"/> Receptor, Serotonin, 5-HT _{2A} (2)
<input type="checkbox"/> 5-HT _{1D} receptors (2)	<input type="checkbox"/> 5-HT ₃ receptors (1)	<input type="checkbox"/> Receptor, Serotonin, 5-HT _{2B} (1)
<input type="checkbox"/> 5-HT ₁ receptors (8)	<input type="checkbox"/> 5-HT ₇ receptors (1)	
<input type="checkbox"/> 5-HT _{2A} agonists (2)	<input type="checkbox"/> 5-HT agonists (16)	
	<input type="checkbox"/> 5-HT antagonists (38)	

Apply Cancel

5. 浏览 2000 年之前文献中的 Concept，发现肉桂硫胺作为一种 5-HT 系列受体拮抗剂，早期一直用作抗精神疾病药物。因此早期文献中以 5-HT，Brain, Antidepressants 等 concept 为主。可以继续 Concept 搜索特定的核心研究点。

The screenshot shows the CAS SciFinder interface. The top navigation bar includes the CAS logo, a search bar with the text "Enter a query...", and icons for "Draw", "Search", "Star", "Clock", and "User". The main content area is titled "References (155)" and includes a "Filtering:" section with a dropdown menu set to "Publication Year: 2000 - No Max". A notification banner at the top right states: "CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. Use the CAS Solutions: Formulus filter to view available content. Learn more about Formulus." Below this, two search results are listed. The first result is "Quantification of serotonin transporters in nonhuman primates using [¹²³I]ADAM and SPECT" by Acton, Paul D.; Choi, Seok-Rye; Hou, Catherine; Plessl, Karl; Kung, Hank F. The second result is "¹²³I-ADAM binding to serotonin transporters in patients with major depression and healthy controls: a preliminary study" by Newberg, Andrew B.; Amsterdam, Jay D.; Wintering, Nancy; Ploessl, Karl; Swanson, Randel L.; Shults, Justine; Alavi, Abass. The left sidebar shows "Filter Behavior" with "Filter by" and "Exclude" buttons. Under "Document Type", "Substance Role" is set to 6. Under "Language", "Publication Year" is set to 2000 to No Max. Under "Author" and "Organization", there are expandable sections.

6. 将肉桂硫胺文献结果集的发表年限定为 2000 年之后。

The screenshot shows the CAS SciFinder interface with a "Concept" dialog box open. The dialog box has a "Top Count" tab selected and a search bar. A list of concepts is displayed, with "Antiviral agents (20)" selected and a blue box with the number 8 next to it. Other concepts include Radiopharmaceuticals (38), Iodine Radioisotopes (28), Serotonin (25), Single-photon-emission computed tomography (25), Midbrain (22), Middle Aged (19), Serotonin Antagonists (19), Tissue Distribution (19), Protein Binding (18), Rats (18), Mesencephalon (16), 5-HT7 receptors (9), Antidepressants (9), Brain hippocampus (9), Cerebellum (9), Major depression (9), Mental and behavioral disorders (9), Mice (9), Molecular docking (9), Reproducibility of Results (9), Serotonergic neurotransmission (9), Tropanes (9), 5-HT3 receptors (8), Pharmacokinetics (7), Psychosis (7), 5-HT1B receptors (6), 5-HT1 receptors (6), 5-HT2A antagonists (6), 5-HT receptors (6), Aging, animal (6), Animal gene (6), Anxiety (6), Bipolar disorder (6), Cell line (6), Cognitive disorders (6), and Cysteine Endopeptidases (6). The background shows the search results page with the number 9 highlighted.

7. 浏览 2000 年后文献中涉及的 Concept（也可以点击 Search, 输入关注的适应症）。

8. 发现 Antiviral agents 的研究结果较多，勾选此词条，进一步获取相关研究信息。
9. 点击 Apply，得到肉桂硫胺用于抗病毒研究方面的文献。

The screenshot displays the CAS SciFinder[®] search results page. At the top, there is a search bar with the text 'Enter a query...' and a 'Draw' button. The main content area is titled 'References (20)' and shows a list of search results. On the left side, there is a 'Filter Behavior' panel with options for 'Filter by' and 'Exclude'. Below this, there are sections for 'Document Type', 'Substance Role', 'Language', and 'Publication Year'. The 'Publication Year' section features a bar chart showing the number of results per year from 1998 to 2021, with a significant increase in 2021. The 'Publication Year' filter is set to '2000 to No Max' and 'Apply' is highlighted. The first reference is titled 'screening of anti-SARS coronavirus agents targeting protease 3CL' and is highlighted with a blue box labeled '11'. Below the title, the authors and abstract are visible. The second reference is partially visible and highlighted with a blue box labeled '12'.

10. 通过 Publication Year 可以发现，有关 Antiviral agents 的文献多发表于 2000 年以后（灰色条表示在 1998 也包含 Antiviral agents 的 Concept 结果，这也是 CAS SciFinder[®] 中有关肉桂硫胺抗病毒方面的第一篇报道）。
11. Sort 中选择：Publication Date: Oldest，将文献结果集按照发表日期的新旧重新排序。
12. 点击 PatentPak，获取专利全文。

[43] 公开日 2004 年 2 月 4 日	[11] 公开号 CN 1472336A
<p>[22] 申请日 2003.6.4 [21] 申请号 03129071.X</p> <p>[71] 申请人 中国科学院上海药物研究所 地址 201203 上海市浦东张江高科技园区祖冲之路 555 号</p> <p>共同申请人 上海先导药业有限公司</p> <p>[72] 发明人 沈建华 蒋华良 沈旭 左建平 罗小民 白东鲁 沈竞康 陈凯先 贵春山 陈莉莉 陈静 杨以阜 庄贤韩 杨一鸣 何煦昌 柳红 熊斌 罗海彬 孙涛 叶飞</p>	<p>[74] 专利代理机构 隆天国际知识产权代理有限公司 代理人 楼仙英</p>
权利要求书 2 页 说明书 13 页 附图 3 页	
<p>[54] 发明名称 SARS 冠状病毒 3CL 蛋白酶三维结构模型与抗 SARS 药物</p>	
<p>[57] 摘要</p> <p>通过分子模拟获得 SARS - CoV 病毒 3CL 蛋白酶的三维结构；以此为药物靶标，筛选了现有药物数据库 CMC (Comprehensive Medicinal Chemistry, MDLInformation System, Inc.)，发现一系列具有 SARS - CoV 病毒 3CL 蛋白酶抑制活性的化合物；对其中的肉桂硫胺进行分子和病毒水平测试，发现其具有较好的抑制 SARS - CoV 病毒 3CL 蛋白酶和抗 SARS - CoV 病毒活性；合成了肉桂硫胺类似物，进行了分子和病毒水平测试，发现这类化合物均有抑制 SARS - CoV 病毒 3CL 蛋白酶和抗 SARS - CoV 病毒活性，可用于治疗和/或预防 SARS - CoV 病毒的</p>	

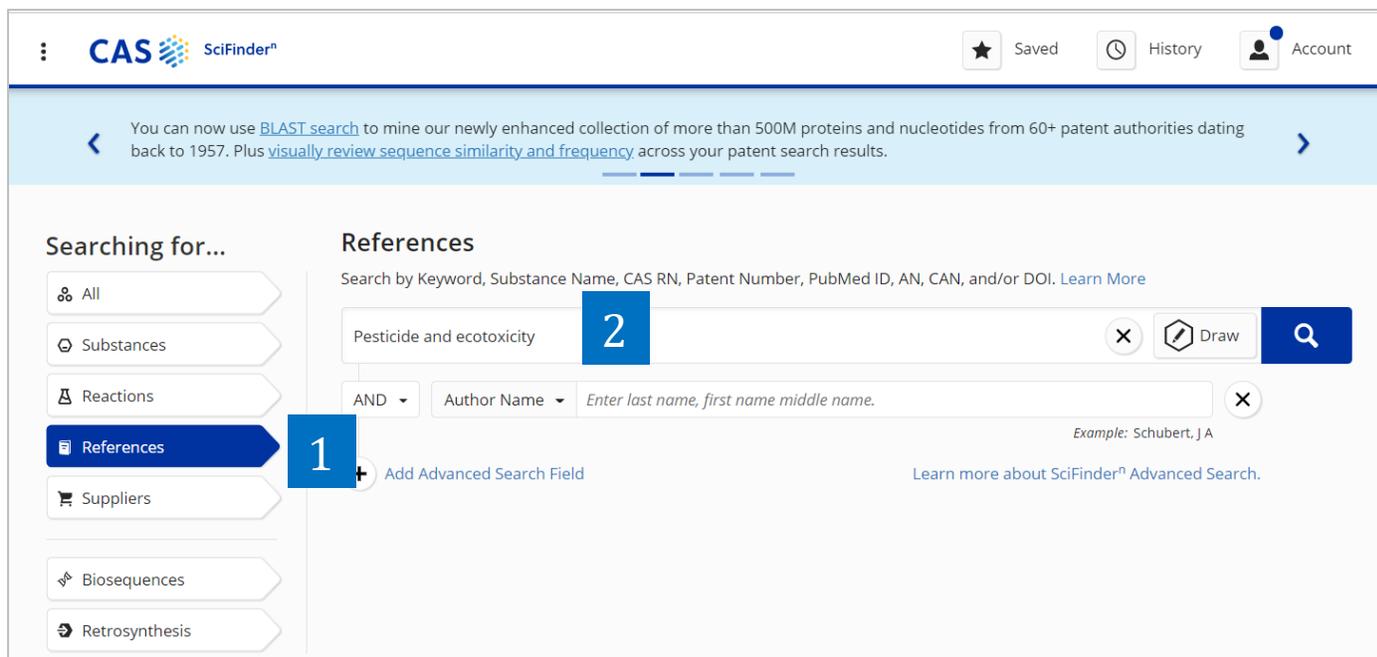
13. 在 CAS SciFinder[®]中通过 PatentPak 直接下载的专利原文。

布尔逻辑运算符在文献检索中的应用

在 CAS SciFinder[®] 中用文本词语检索文献时，可使用以下布尔逻辑运算符：

1. AND：表示两个（多个）被检索的词语同时出现在同一篇文献中；
2. OR：表示在检索结果中出现任意一个被检索词即可；
3. NOT：排除某个被检索词出现在检索结果中；
4. “ ”：表示被检索的是一个确定的词语或词组；
5. ()：在检索式中有多个布尔逻辑运算符时，可用括号指定不同布尔逻辑运算符间的运行顺序。

注：CAS SciFinder[®] 中布尔逻辑运算符默认的运算顺序是 OR > AND > NOT



The screenshot shows the CAS SciFinder search interface. On the left, under 'Searching for...', the 'References' option is selected and highlighted with a blue bar and a red '1'. The main search area is titled 'References' and contains a search box with the text 'Pesticide and ecotoxicity' and a red '2' next to it. Below the search box, the operator 'AND' is selected from a dropdown menu. The interface also includes a search button, a 'Draw' button, and a 'Saved' button. A banner at the top of the search area provides information about the BLAST search feature.

1. 点击 References。
2. 使用 AND 连接两个检索词，如 Pesticide and ecotoxicity，表示在检索结果中 Pesticide 和 ecotoxicity 同时出现。

The screenshot shows the CAS SciFinder interface. At the top, the search bar contains 'Pesticide and ecotoxicity' and a blue box with the number '3'. Below the search bar, there are navigation options like 'Return to Home' and a 'References' section with 1,985 results. The results are sorted by 'Relevance' and shown as 'Partial Abstract'. A filter sidebar on the left allows filtering by 'Document Type' (Journal, Patent, Review, Book, Clinical Trial) and 'Language' (English, German, Chinese, Japanese). The first result is 'Assessing the Ecotoxicity of Pesticide Transformation Products' by Sinclair, Chris J.; Boxall, Alistair B. A. The second result is 'Wildlife Ecotoxicology of Pesticides: Can We Track Effects to the Population Level and Beyond?' by Koehler, Heinz-R.; Triebkorn, Rita.

3. 所得结果集。

The screenshot shows the CAS SciFinder search interface. On the left, there is a 'Searching for...' sidebar with options: All, Substances, Reactions, References (highlighted), Suppliers, Biosequences, and Retrosynthesis. The main search area has a search bar with 'Pesticide or ecotoxicity' and a blue box with the number '4'. Below the search bar, there are search filters: 'AND', 'Author Name', and a text input field 'Enter last name, first name middle name.' with an example 'Schubert, J A'. There is also an 'Add Advanced Search Field' button and a link to 'Learn more about SciFinder Advanced Search'.

4. 使用 OR 连接两个检索词，如 Pesticide and ecotoxicity，表示 Pesticide 和 ecotoxicity 任意一个出现即可。

The screenshot shows the CAS SciFinder interface with a search for "Pesticide or ecotoxicity". The results page displays a list of references. The first reference is titled "Assessing the Ecotoxicity of Pesticide Transformation Products" by Sinclair, Chris J.; Boxall, Alistair B. A. The second reference is titled "Wildlife Ecotoxicology of Pesticides: Can We Track Effects to the Population Level and Beyond?" by Koehler, Heinz-R.; Triebkorn, Rita. The interface includes a filter sidebar on the left with options for Document Type, Language, and Publication Year. A notification banner at the top mentions CAS Formulus[®].

5. 所得结果集。

The screenshot shows the CAS SciFinder search interface. The search criteria are "Pesticide not ecotoxicity". The interface includes a search bar with a search button, a filter sidebar on the left, and a search results section. The search criteria are displayed in a search bar with a search button. The search criteria are "Pesticide not ecotoxicity". The search criteria are displayed in a search bar with a search button. The search criteria are "Pesticide not ecotoxicity".

6. 使用 NOT 连接两个单词或词组，如 Pesticide not ecotoxicity，则得到只包含 Pesticide 而去除 ecotoxicity 的结果。

CAS SciFinder[®] | References | Pesticide not ecotoxicity | 7

Return to Home

Filter Behavior

Filter by | Exclude

Document Type

- Journal (152K)
- Patent (87K)
- Review (23K)
- Biography (29)
- Book (879)
- [View All](#)

Language

- English (141K)
- Chinese (69K)
- German (11K)
- Japanese (9,926)
- Russian (6,089)
- [View All](#)

Publication Year

References (252,986) | Sort: Relevance | View: Partial Abstract

Substances | Reactions | Citing | Save And Alerts

CAS Formulus[®], the comprehensive formulations database and workflow solution, is now available for all SciFinder[®] users. Use the [CAS Solutions: Formulus filter](#) to view available content. [Learn more about Formulus.](#)

1

Immunotoxicity of Organophosphorous Pesticides

By: Galloway, Tamara; Handy, Richard
Ecotoxicology (2003), 12(1,2,3,4), 345-363 | Language: English, Database: CAplus

A review of the toxic effects of organophosphate (OP) **pesticides** on the immune systems and immune functions of invertebrates, fish, and higher vertebrate wildlife. The fundamental features and mechanisms of OP-induced immunotoxicity are illustrated with reference to parathion, chlorpyrifos, malathion, and diazinon. Immunotoxicity may be direct via inhibition of serine hydrolases or esterases in components of the immune system, through oxidative damage to immune organs, or by modulation of signal transduction pathways controlling immune functions. Indirect effects include modulation by the nerv...

[View More](#)

Full Text | Substances (4) | Reactions (0) | Citing (320) | Citation Map

2

Emission of pesticides into the air

By: Van Den Berg, F.; Kubiak, R.; Benjey, W. G.; Majewski, M. S.; Yates, S. R.; Reeves, G. L.; Smelt, J. H.; Van Der Linden, A. M. A.
Water, Air, and Soil Pollution (1999), 115(1-4), 195-218 | Language: English, Database: CAplus

A review with 106 references concerning **pesticide** emissions to the atm. following agricultural application is given. Topics discussed

7. 所得结果集。

CAS SciFinder[®] | Saved | History | Account

You can now use [BLAST search](#) to mine our newly enhanced collection of more than 500M proteins and nucleotides from 60+ patent authorities dating back to 1957. Plus [visually review sequence similarity and frequency](#) across your patent search results.

Searching for...

- All
- Substances
- Reactions
- References**
- Suppliers
- Biosequences
- Retrosynthesis

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

high efficiency and low toxicity and (pesticide or herbicide) | 8

AND | Author Name | Enter last name, first name middle name. | Example: Schubert, J A

+ Add Advanced Search Field | [Learn more about SciFinder[®] Advanced Search.](#)

8. 当使用多个布尔逻辑运算符时，可使用括号()，指定逻辑运算符的运算顺序。如 high efficiency and low toxicity and (pesticide or herbicide)，此时表示优先运算 pesticide or herbicide。

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#) [Load More Results](#)

References (2,054) Sort: Relevance View: Partial Abstract

Substances Reactions Citing Save And Alerts

CAS Formulus[®], the comprehensive formulations database and workflow solution, is now available for all SciFinder[®] users. Use the [CAS Solutions: Formulus filter](#) to view available content. [Learn more about Formulus.](#)

1

High efficiency and low toxic herbicide for garden
By: Shi, Yuelong; Zeng, Songjun; Wu, Yingliang; Liu, Wenbin; Wu, Kunlin; Tang, Jing
China, CN107568220 A 2018-01-12 | Language: Chinese, Database: CPlus

A **high efficiency** and **low toxic** garden **herbicide**, comprises the following raw materials in weight parts: 1-2 parts of oxyfluorfen EC, 14-28 parts of butachlor, 10-12 parts of acetochlor, 15-40 parts of triethanolamine, 4-8 parts of amicarbazone and 5-10 parts of clodinafop-propargyl, 10-20 parts of flumiclorac-pentyl EC, 12-15 parts of fomesafen, 8-15 parts of cloransulam-Me, 5-10 parts of organosilicon, 20-35 parts of fenoxaprop-p-Et, 5-10 parts of glyphosate, 0.3-0.5 parts of gibberellin, 0.1-0.2 parts of indole acetic acid, 10-12 parts of triacetonol, 2-4 parts of urea, 10-20 parts of carb...

[View More](#)

PatentPak Full Text Substances (23) Reactions (0) Citing (0) Citation Map

2

Herbicide containing tralkoxydim with high efficiency and low toxicity, and its preparation method
By: Zhang, Xiaowen; Yang, Jie; Shi, Zhongjun; Liu, Rui
China, CN109287630 A 2019-02-01 | Language: Chinese, Database: CPlus

The title **herbicide** comprises (by weight parts): tralkoxydim 10-20, 2-amino-3-chlorobenzoic acid Me ester 15-30, bensulfuron-Me 5-

9. 所得结果集。

CAS SciFinder®

Retrosynthesis plans now have a new rule-set trained on our full collection of single-step reactions, offering greater coverage of synthetic methods and added novelty. [Learn more about Retrosynthesis searching in CAS SciFinder®.](#)

Searching for...

- All
- Substances
- Reactions
- References
- Suppliers
- Biosequences
- Retrosynthesis

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

"total synthesis" and taxol

AND Author Name Enter name middle name. Example: Schubert, J A

+ Add Advanced Search Field [Learn more about SciFinder® Advanced Search.](#)

10. 引号“ ”，表示被检索的词（词组）为确定的，不能出现不同拼写或词组被拆分的情况，如 "total synthesis" and taxol。此时指 total synthesis 是一个固定词组。

CAS SciFinder®

References "total synthesis" and taxol

Return to Home

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#)

Load More Results

Filter Behavior

Filter by Exclude

Document Type

- Journal (169)
- Patent (9)
- Review (64)
- Commentary (1)
- Conference (34)
- View All

Language

- English (203)
- Japanese (13)
- Chinese (11)
- German (2)
- Danish (1)

References (236)

Sort: Relevance View: Partial Abstract

Substances Reactions

1

Two-Phase Synthesis of Taxol

By: Kanda, Yuzuru; Nakamura, Hugh; Umemiya, Shigenobu; Puthukanoori, Ravi Kumar; Murthy Appala, Venkata Ramana; Gaddamanugu, Gopi Krishna; Paraselli, Bheema Rao; Baran, Phil S.
Journal of the American Chemical Society (2020), 142(23), 10526-10533 | Language: English, Database: CAplus and MEDLINE

Taxol is widely regarded as amongst the most famed natural isolates ever discovered, and has been the subject of innumerable studies in both basic and applied science. Its documented success as an anticancer agent, coupled with early concerns over supply, stimulated a furious worldwide effort from chemists to provide a solution for its preparation through total synthesis. Those pioneering studies proved the feasibility of retrosynthetically-guided access to synthetic **Taxol**, albeit in minute quantities and with enormous effort. In practice, all medicinal chem. efforts and eventual commercializa.

View More

Full Text

Substances (50) Reactions (1,307) Citing (41) Citation Map

2

Total synthesis of taxol

By: Nicolaou, K. C.; Yang, Z.; Liu, J. J.; Ueno, H.; Nantermet, P. G.; Guy, R. K.; Claiborne, C. F.; Renaud, J.; Coulaudouros, E. A.
Nature (London, United Kingdom) (1994), 367(6464), 630-4 | Language: English, Database: CAplus and MEDLINE

The total synthesis of taxol (I) from the benzofuranone II by a convergent strategy, which opens a chem. pathway for the production of both I and a variety of designed taxoids is reported.

View More

11. 所得结果集。

通配符的使用

在 CAS SciFinder[®] 中进行文献检索时，支持使用通配符进行更广泛的检索。可使用的通配符有*和?：

*代表 0 或多个字符；? 代表 0 或一个字符。

通配符可位于词中间或词尾，不可位于词首。

使用通配符检索时，匹配到的词语可能位于文献的标题、摘要、关键词、CAplus Concept、Medline MeSH 或 Substances 中。

1. 输入 synth*，会匹配到 synthesis, syntheses, synthetic 和 synthesizing 等词。

CAS SciFinder[®] search results for "alumin?um". The search bar displays "alumin?um" and a blue box with the number "2". The results list two entries:

- 51: **A compilation of corrosion potentials reported for intermetallic phases in aluminum alloys**. By: Buchheit, R. G. Journal of the Electrochemical Society (1995), 142(11), 3994-6 | Language: English, Database: CPlus
- 52: **Grain refinement of aluminum and its alloys by heterogeneous nucleation and alloying**. By: Murty, B. S.; Kori, S. A.; Chakraborty, M. International Materials Reviews (2002), 47(1), 3-29 | Language: English, Database: CPlus

The left sidebar shows filters for Document Type (Journal, Patent, Review, Biography, Book), Substance Role (Uses, Properties, Process, Preparation, Reactant or Reagent), and Language (English, Chinese, Japanese, Russian, German).

2. 输入 alumin?um, 会匹配到 aluminum 和 aluminium 等词。

注:

- I. 一个检索词中至少含有 3 个非通配符字符, 否则会检索到任何词语;
- II. 一个检索词中最好只用一个通配符, 否则 CAS SciFindern 会忽略通配符, 如输入 (R*,S*,R*,S*)-2,3,6,7-Tetrachlorooctane, 则得到的检索结果则为(R*,S*,R*,S*)-2,3,6,7-Tetrachlorooctane;
- III. 一个检索式中不可超过 5 个通配符, 否则会出错。

CAS SciFinder[®] search bar showing an error message: "The query cannot contain more than 5 valid wildcard search terms." The search bar contains the query "tot* synth* nat* prod* terpen* last*" and a blue box with the number "3".

更详细说明可参考: https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FReferences_Search%2FReference_Wildcard_Searching_Rules.htm&rhsearch=wildcard&rhhlterm=wildcard&hsyns=%20

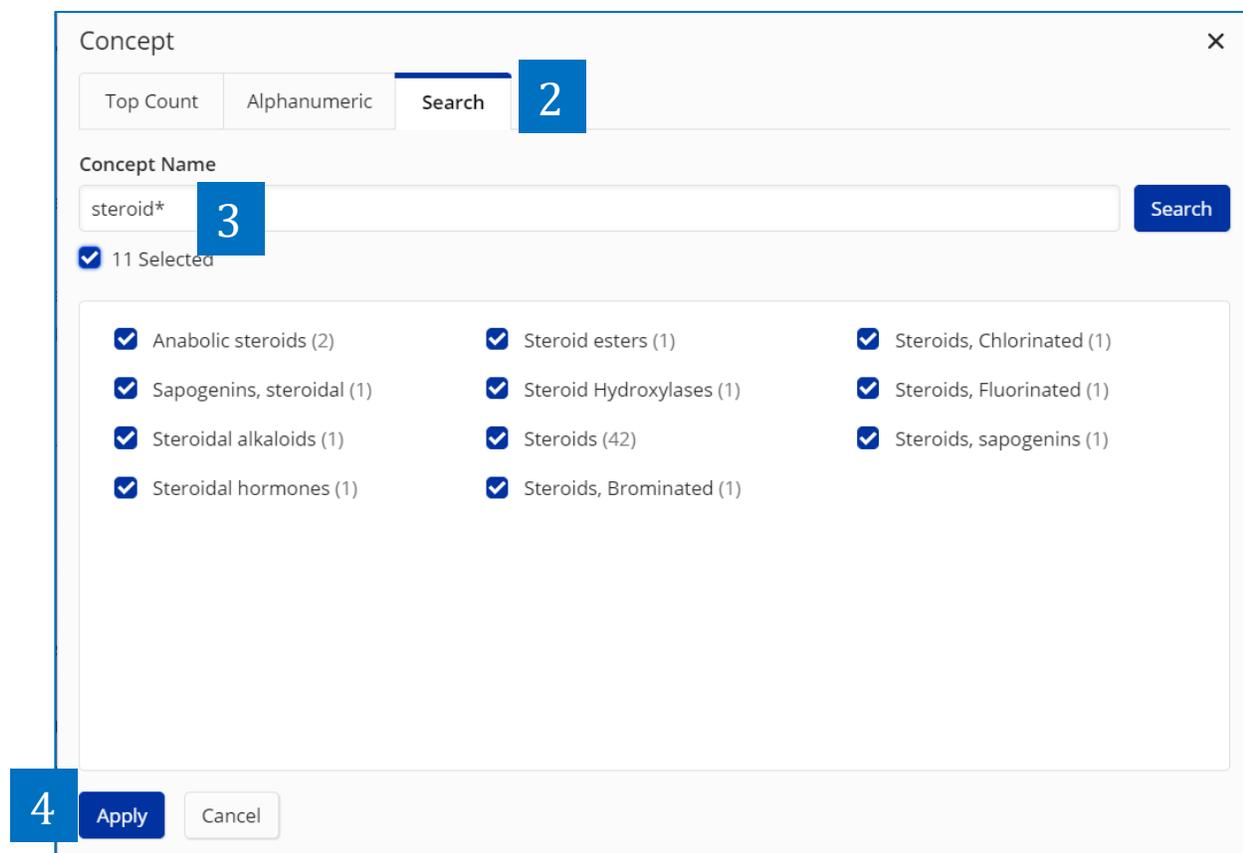
Concept 筛选项中支持使用通配符 “*” 进行检索

注：通配符 “*” 代表 0 或多个字符；且可用于词中或者词尾。

The screenshot shows the CAS SciFinder search results page. The search query is "steroids and fermentation and rhizopus stolonifer". The left sidebar shows the "Concept" filter selected, with a "View All" button and a badge showing "1". The main content area displays the following results:

- Microbial oxidation of anabolic steroids**
By: Choudhary, M. Iqbal; Adnan, S.; Shah, A.; Atta-Ur-Rahman
Natural Product Research (2008), 22(15), 1289-1296 | Language: English, Database: CPlus and MEDLINE
Microbial transformation of two anabolic steroids, ethylestrenol (1) and nandrolone (2), were carried out. Ethylestrenol (1), when incubated with *Rhizopus stolonifer* (TSY 0471), yielded two oxidative metabolites named 17 α -ethyl-3 β ,17 β -dihydroxy-19-norandrost-4-ene (3) and 17 α -ethyl-17 β -hydroxy-19-norandrost-4-en-3-one (4), while incubation of compound 2 with the same fungus yielded two oxidative metabolites, 19-norandrost-4-en-3,17-dione (5) and 6 α ,17 β -dihydroxy-19-norandrost-1,4-dien-3-one (6).
Full Text ▾ | Substances (7) | Reactions (2) | Citing (13) | Citation Map
- Micro biological conversion of steroids. 4. Part Pregnenolone oxidation by *Rhizopus nigricans* VNICHFI-7**
By: Kogan, L. M.; Elin, E. A.; v, A. S. Barmen o; Torgov, I. V.
Chemisches Zentralblatt (1967), 138(51/52), 162-162 | Language: German, Database: CHEMZENT

1. 在文献结果集页面左侧，点击 Concept 选项下的 View All, 展开 Concept 列表。

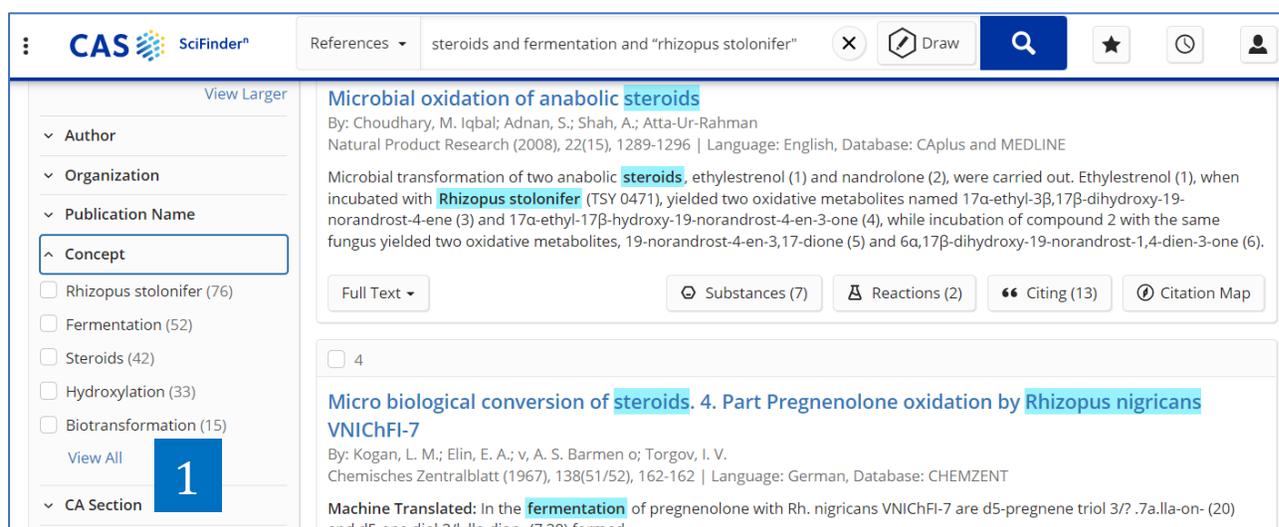


2. 点击 Search。
3. 输入检索词。可以添加星号 (*) 进行扩词，比如 steroid*，可以检索到 steroid, steroids, steroidal 等概念词，点击 Select All on Page。
4. 点击 Apply，获得含有此页面概念词的所有文献。

文献结果集的聚类筛选项中的全选功能

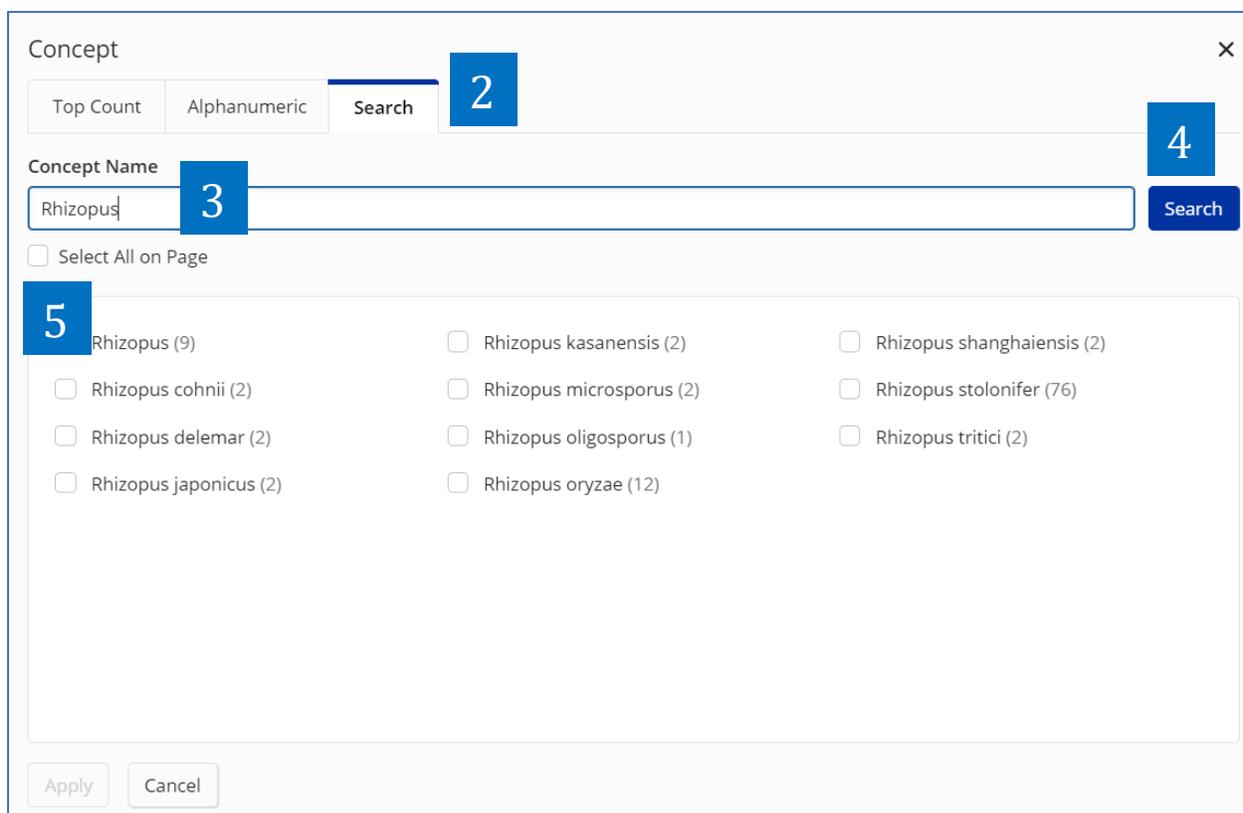
在文献检索结果集左侧的聚类筛选项里，点击 View All 展开所有的子项后，可以通过点击 Search 在所有子项中进行检索，同时可以通过 Select All on Page 全部选中检索到的子项。在 Concept, CA Section, Organization, Publication Name, Author 等分析项中都提供子项全选功能。

如下所示的是在 Concept 中对检索得到的子项进行全选的操作。

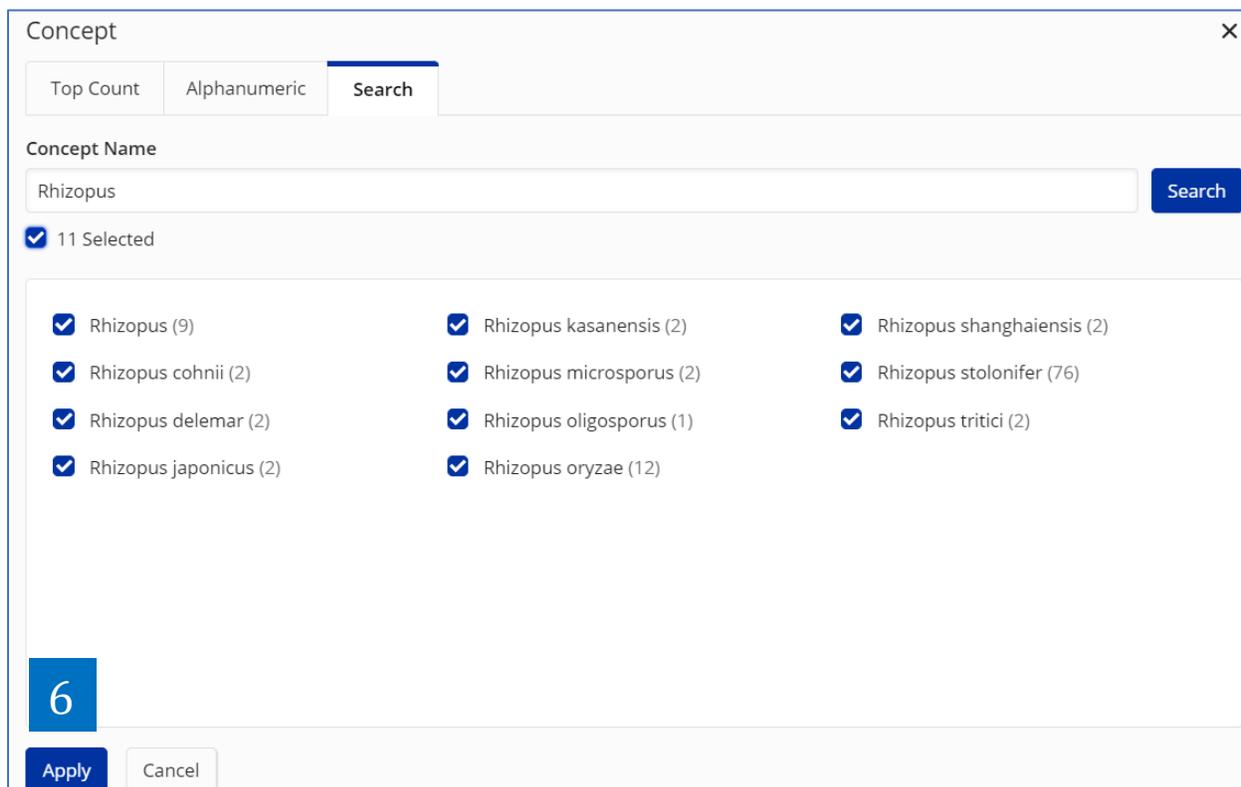


The screenshot shows the CAS SciFinder interface. On the left, the 'Concept' filter is expanded, showing a list of sub-items: Rhizopus stolonifer (76), Fermentation (52), Steroids (42), Hydroxylation (33), and Biotransformation (15). The 'View All' button is highlighted with a red box and the number 1. The main content area displays search results for 'steroids and fermentation and "rhizopus stolonifer"'. The first result is 'Microbial oxidation of anabolic steroids' by Choudhary, M. Iqbal; Adnan, S.; Shah, A.; Atta-Ur-Rahman. The second result is 'Micro biological conversion of steroids. 4. Part Pregnenolone oxidation by Rhizopus nigricans VNICHFI-7' by Kogan, L. M.; Elin, E. A.; v, A. S. Barmen o; Torgov, I. V. The interface includes a search bar, navigation icons, and a list of filters.

1. 点击 View All，展开所有的子项。



2. 点击 Search，在展开所有子项中进行检索。
3. 输入检索词。
4. 点击 Search 开始检索。
5. 勾选 Select All on Page，可以全部选中检索得到的子项。



6. 选中全部子项后，点击 Apply 获得筛选后的结果集。

查看文献中的关键词

The screenshot displays the CAS SciFinder search interface. At the top, a banner reads: "CAS Analytical Methods® is available as part of your CAS SciFinder® experience. [Identify and compare](#) the latest published analytical methods, featuring step-by-step instructions, in pharmacology, HPLC, food analysis, natural product isolation analysis, water analysis and more." Below this, the "Searching for..." section on the left lists various search categories: All, Substances, Reactions, References (highlighted with a blue bar and a white "1" in a blue box), Suppliers, Biosequences, and Retrosynthesis. The "References" section on the right is titled "References" and includes the instruction "Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)". A search input field contains the query "CDK OR 'cyclin-dependent kinases' AND inhibitor" (with a white "2" in a blue box) and a "Draw" button. Below the input field, there is a dropdown menu set to "AND", another dropdown set to "Author Name", and a text input field with the placeholder "Enter last name, first name middle name." and a "Draw" button. An example "Example: Schubert, J A" is shown below. A white "3" in a blue box is positioned above the search input field. At the bottom of the search area, there is a "+ Add Advanced Search Field" button and a link "Learn more about SciFinder® Advanced Search."

1. 选择 References
2. 输入检索式
3. 开始检索

CAS SciFinder[®] Search Results: CDK OR "cyclin-dependent kinases" AND inhibitor

5

Cyclin dependent kinase (CDK) inhibitors as anticancer drugs 4

By: Sanchez-Martinez, Concepcion; Gelbert, Lawrence M.; Lallena, Maria Jose; de Dios, Alfonso
 Bioorganic & Medicinal Chemistry Letters (2015), 25(17), 3420-3435 | Language: English, Database: CAplus and MEDLINE

A review. Sustained proliferative capacity is a hallmark of cancer. In mammalian cells proliferation is controlled by the cell cycle, where **cyclin-dependent kinases (CDKs)** regulate critical checkpoints. CDK4 and CDK6 are considered highly validated anticancer drug targets due to their essential role regulating cell cycle progression at the G1 restriction point. This review provides an overview of recent advances on **cyclin dependent kinase inhibitors** in general with special emphasis on CDK4 and CDK6 **inhibitors** and compounds under clin. evaluation. Chem. structures, structure activity relationsh...

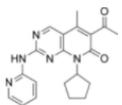
View More ▾

Full Text ▾ Substances (11) Reactions (0) Citing (292) Citation Map

6

Discovery of a Potent and Selective Inhibitor of Cyclin-Dependent Kinase 4/6

By: Toogood, Peter L.; Harvey, Patricia J.; Repine, Joseph T.; Sheehan, Derek J.; VanderWel, Scott N.; Zhou, Hairong; Keller, Paul R.; McNamara, Dennis J.; Sherry, Debra; Zhu, Tong; et al
 Journal of Medicinal Chemistry (2005), 48(7), 2388-2406 | Language: English, Database: CAplus and MEDLINE

 A pharmacol. approach to inhibition of **cyclin-dependent kinases** 4 and 6 (Cdk4/6) using highly selective small mol. **inhibitors** has the potential to provide novel cancer therapies for clin. use. Achieving high levels of selectivity for Cdk4/6, vs. other ATP-dependent kinases, presents a significant challenge. The pyrido[2,3-d]pyrimidin-7-one template provides an effective platform for the inhibition of a broad cross-section of kinases, including **Cdks**. It is now demonstrated that the modification of pyrido[2,3-d]pyrimidin-7-ones to include a 2-aminopyridine side chain

4. 点击文献题名，查看文献详情

Reference Detail (5 of 60,871) ← Prev Next →

Substances (3) Reactions (0) Citing (118) Citation Map Download Email Save

JOURNAL

Source
 Bioorganic & Medicinal Chemistry Letters
 Volume: 25
 Issue: 17
 Pages: 3420-3435
 Journal: General Review: Art Review
 2015
 DOI:
[10.1016/j.bmcl.2015.05.100](https://doi.org/10.1016/j.bmcl.2015.05.100)

CODEN: BMCLE8
E-ISSN: 1464-3405
ISSN-L: 0960-894X

Database Information
 AN: 2015:1031191
 CAN: 163:214062
 PubMed ID: 26115571
 CPlus and MEDLINE

Company/Organization
 Discovery Chemistry Research and

Cyclin dependent kinase (CDK) inhibitors as anticancer drugs

By: Sanchez-Martinez, Concepcion; Gelbert, Lawrence M.; Lallena, Maria Jose; de Dios, Alfonso

A review. Sustained proliferative capacity is a hallmark of cancer. In mammalian cells proliferation is controlled by the cell cycle, where **cyclin-dependent kinases (CDKs)** regulate critical checkpoints. CDK4 and CDK6 are considered highly validated anticancer drug targets due to their essential role regulating cell cycle progression at the G1 restriction point. This review provides an overview of recent advances on **cyclin dependent kinase inhibitors** in general with special emphasis on CDK4 and CDK6 **inhibitors** and compounds under clin. evaluation. Chem. structures, structure activity relationships, and relevant preclin. properties will be described.

Keywords: review **cyclin dependent kinase inhibitor** antitumor cancer; **CDK inhibitors**; Cell cycle

Full Text ▾ Expand All | Collapse All

Concepts

Antitumor agents	Homo sapiens
Cyclin-dependent kinase inhibitors	Human
	Neoplasm

Company/Organization
 Discovery Chemistry Research and Technologies
 Eli Lilly and Company
 Alcobendas (Madrid) 28108
 Spain

Email
sanchez-martinez_concepcion@lilly.com

Publisher
 Elsevier B.V.

Language
 English

MEDLINE® Medical Subject Headings

Antineoplastic Agents Qualifier: pharmacology; therapeutic use	Cyclin-Dependent Kinase Inhibitor Proteins Qualifier: metabolism
Cell Cycle	Humans
	Neoplasms Qualifier: drug therapy

Substances

Substances (3)

150428-23-2 Image Not Available Unspecified CDK Role: Biological Study, Unclassified, Biological Study	303014-92-8 Image Not Available Unspecified CDK6 Role: Biological Study, Unclassified, Biological Study	147014-97-9 Image Not Available Unspecified Cyclin-dependent kinase 4 Role: Biological Study, Unclassified, Biological Study
--	---	--

Cited Documents

5. Keywords 即为该文献的关键词

6. Concepts 为 CAS 词库中的受控词，是 CAS 科学家人工解读后得出的信息

7. 如果该文献同时被 Medline 数据库收录，文献信息详情中也将展示医学主题词表 (MeSH) 中的词语

现有技术分析

在 CAS SciFinder[®] 中获取目标专利后，可点击 Get Prior Art Analysis 基于本专利的 Concept、Substances、IPC 等进行现有技术分析。

Reference Detail (1 of 8,930)

Substances (15) Reactions (0) Citing (112) Citation Map Save

PATENT

Patent Number: US6010719
Publication Date: 2000-01-04
Application Number: US1997-931257
Application Date: 1997-09-16
Kind Code: A
Assignee: Universiteit Gent, Belgium
Source: United States, CODEN: USXXAM
Database Information: AN: 2000:10527, CAN: 132:69330, CAplus
Language: English

CAS Formulus[®], the comprehensive formulations database and workflow solution, is now available for all SciFinder[®] users. [View content from CAS Formulus[®]](#) in this document. [Learn more about Formulus[®]](#).

Freeze-dried disintegrating tablets

By: Remon, Jean Paul; Corveleyn, Sam

Freeze-dried disintegrating tablets contain at least a therapeutic agent, a matrix forming agent and a binding agent, in which the tablets contain more than 20% by weight of a matrix forming agent selected from the group consisting of maltodextrins having a dextrose equivalent value between 12 and 40, isomalt and mixtures thereof, the weight ratio between said matrix forming agent and the binding agent being comprised between 2:1 and 50:1. A son. containing hydrochlorothiazide, xanthan gum and maltodextrin was lyophilized to give tablets.

Keywords: tablet freeze dried disintegrating

PATENTPAK Viewer Get Prior Art Analysis Full Text

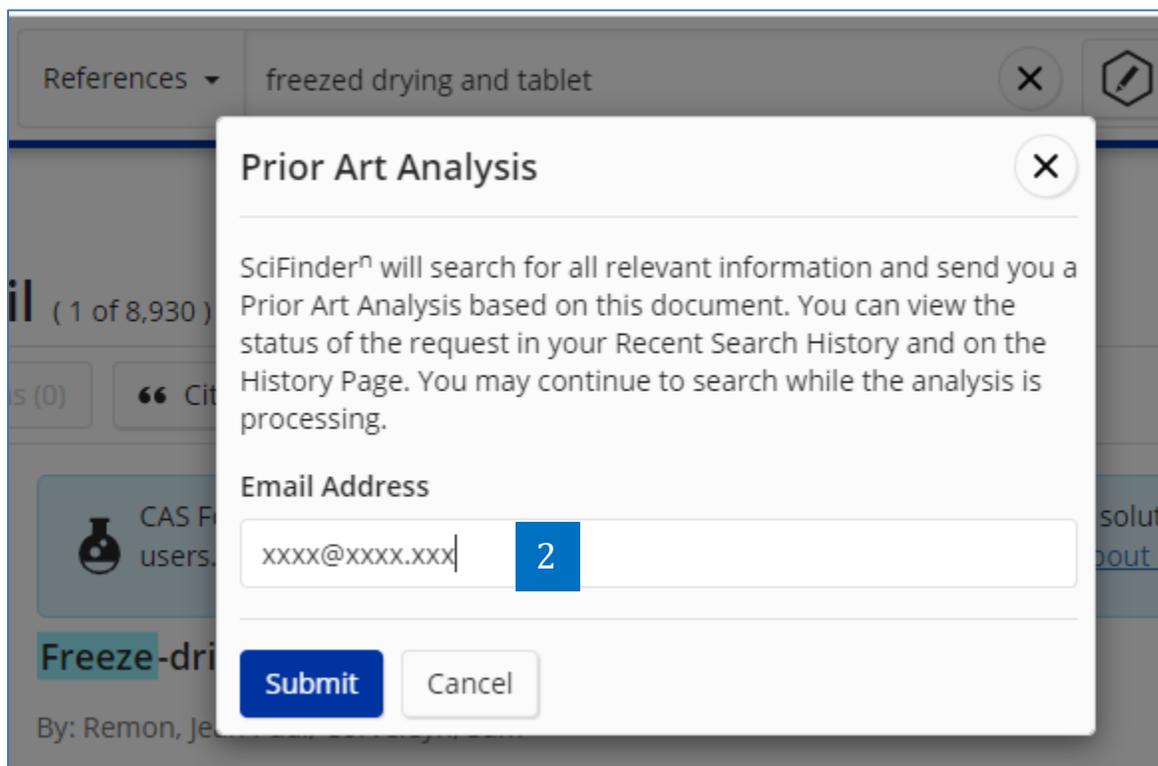
Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
US6010719	English	A	PDF PDF+ Viewer	2000-01-04	US1997-931257	1997-09-16

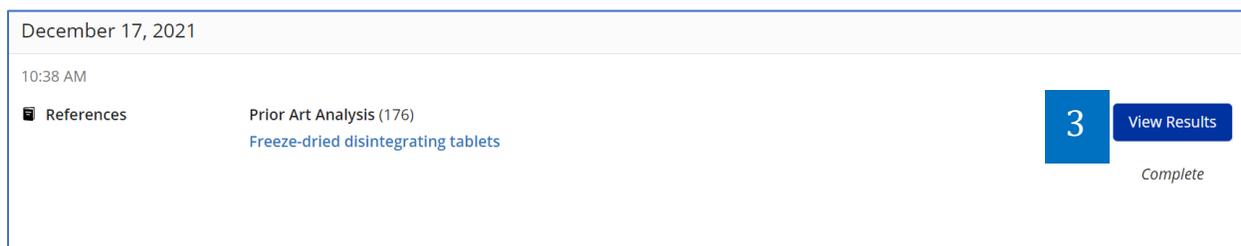
Expand All | Collapse All

- IPC Data
- Concepts
- Substances
- Formulations

1. 点击专利文献标题，进入 Reference Detail 页面，点击“Get Prior Art Analysis”。



2. 在此处输入正确的邮箱，然后点击 Submit。



3. 提交现有技术分析后，可以在检索历史中查看。

Your Prior Art Analysis is Complete

This analysis is based on the reference:

Freeze-dried disintegrating tablets

By: Remon, Jean Paul; Corveleyn, Sam
United States | English | US6010719

Here are the top similar documents based on your request. You can view all references in SciFinder[®].

Formulation and production of rapidly disintegrating tablets by lyophilization using hydrochlorothiazide as a model drug

By: Corveleyn, Sam; Remon, Jean-Paul
International Journal of Pharmaceutics (1997) | English

Maltodextrins as lyoprotectants in the lyophilization of a model protein, LDH

By: Corveleyn, Sam; Remon, Jean-Paul
Pharmaceutical Research (1996) | English

Evaluation of maltodextrins as tablet excipients. I. Micromeritic and compressional characterization

By: Nath, Shelli; Pathak, Yashwant V.
Powder Technology (1993) | English

Rapidly disintegrating tablets containing gums and carbohydrates

By: Pebley, Walter S.; Jager, Norman E.; Thompson, Sally J.
United States | English | US5298261

In vitro and in vivo evaluation of a xanthan gum-n-octenylsuccinate starch matrix tablet containing ibuprofen as a model drug

By: Ntawukuliyayo, J. D.; Vervaeet, C.; Remon, J. P.; Goertz, J. P.; Berlo, J. A.
International Journal of Pharmaceutics (1996) | English

Showing the Top Documents

View all results in

4

- 同时您填写的邮件中将收到现有技术分析完成的邮件。在邮件中点击 View all results in，将跳转到 CAS SciFinder[®] 浏览现有技术相关文献。

The screenshot displays the CAS SciFinder[®] search results page. At the top, there is a search bar with the text 'Enter a query...' and a 'References' dropdown menu. The main content area is titled 'References (176)' with a blue box containing the number '5'. Below the title, there are filters for 'Substances', 'Reactions', and 'Citing'. The first result is a paper titled 'Formulation and production of rapidly disintegrating tablets by lyophilization using hydrochlorothiazide as a model drug' by Corveleyn, Sam; Remon, Jean Paul, published in the International Journal of Pharmaceutics (1997), 152(2), 215-225. The abstract text is visible, discussing the influence of different formulation and process parameters on the characteristics of lyophilized oral dosage forms. On the left side, there is a 'Filter Behavior' section with options to 'Filter by' or 'Exclude'. Below this, there are sections for 'Document Type' (Journal, Patent, Clinical Trial, Letter), 'Language' (English, French, German, Japanese, Chinese), and 'Publication Year' (1972 to 1999). At the bottom of the interface, there are buttons for 'Full Text', 'Substances (4)', 'Reactions (0)', 'Citing (174)', and 'Citation Map'.

5. 获得现有技术相关文献集。

专利信息的获取——PatentPak 的使用

The screenshot shows the CAS SciFinder interface for a search on 'PCSK9 inhibitor'. The search results are displayed in a list format. The first result is highlighted with a blue box. The interface includes a search bar, navigation tabs, and a list of results. A specific result is highlighted with a blue box, and five numbered callouts (1-5) point to key features: 1. Document Type filter (Patent), 2. PatentPak button, 3. PDF link, 4. PDF+ link, and 5. Viewer link.

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)
[Load More Results](#)

References (21,613) Sort: Relevance View: Partial Abstract

Substances Reactions Citing

Filtering: Document Type: Patent Clear All Filters

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder[®] users. Use the [CAS Solutions: Formulus filter](#) to view available content. [Learn more about Formulus.](#)

1

PCSK9 inhibitors and methods of use thereof
By: Abou-Gharbia, Magid; Childers, Wayne E.
World Intellectual Property Organization, WO2016040305 A1 2016-03-17 | Language: English, Database: CAplus

The present invention relates to compositions and methods for treating lipid disorders in a subject. In one embodiment, the compositions of the present invention can be used to inhibit protease proprotein convertase subtilisin-like kexin type 9 (PCSK9). In another embodiment, the compositions of the present invention can be used to disrupt the protein-protein interaction between PCSK9 and low-d. lipoprotein receptor (LDLR).

2

PatentPak Full Text Reactions (0) Citing (2) Citation Map

Patent	Language	Kind C	PDF	PDF+	Viewer
WO2016040305	English	A1	PDF	PDF+	Viewer
US20170290806	English	A1	PDF		

in 9 (PCSK9) inhibitors for treating conditions associated therewith

1. 在文献结果集中选择文献类型为 Patent
2. 点击 PatentPak 旁的小箭头，查看专利族列表
3. PDF: 获取专利 PDF 全文
4. PDF+: 获取附有物质标记信息的专利 PDF 全文
5. Viewer: PatentPak 浏览器，在线快速阅读专利全文

PatentPak 浏览器:

The screenshot shows the PatentPak interface. On the left, a sidebar lists 'Key Substances in Patent' with three entries, each showing a chemical structure, a CAS RN, and 'Analyst Markup Locations (1)'. Callout 3 points to the CAS RN of the first entry. Callout 1 points to the 'Analyst Markup Locations' link. The main area displays a patent claim (claim 2) with callout 4 pointing to the 'PDF+' download button. Callout 2 points to the text of the claim. Callout 1 also points to a location marker on the claim text.

1. 物质位置信息：点击页码定位符号，右侧 PDF 全文快速跳转至该物质出现的页码处，同时对应物质的位置符号由蓝色变为紫色。
2. PDF 全文中对应的物质位置符号。
3. 点击 CAS 登记号，获取物质详情。
4. 下载专利全文：PDF: 获取专利 PDF 全文；PDF+: 获取附有物质标记信息的专利 PDF 全文。

利用专利公开号或者申请号进行检索

当用专利公开号或者申请号进行检索时，可以选择 All 或分别选择 Substances、Reactions 或 References 进行检索。

注：国家代码与数字间不能出现空格，如 WO2013173779

The screenshot displays the CAS SciFinder interface. At the top, the search bar contains 'All' and the patent number 'WO2013173779'. A search button is visible to the right. On the left, a sidebar menu allows filtering by 'Substances (18)', 'Reactions (35)', 'References (2)', and 'Suppliers (0)'. The main content area is titled 'All Answer Types' and shows 'Top two answers by relevance from each answer type.' Under the 'Substances (18)' section, two results are shown: 1) Di-tert-butyl dicarbonate (C₁₀H₁₈O₅) with 56K references, 160K reactions, and 138 suppliers; 2) Isopropylamine (C₃H₉N) with 22K references, 28K reactions, and 62 suppliers. Below this, the 'Reactions (35)' section shows a reaction scheme (Scheme 1) with a 99% yield.

1. 选择 All，同时获取该专利中披露的反应、物质、专利中披露的物质的供应商及本专利的文献信息。
2. 输入专利号。
3. 开始检索。
4. 本专利披露的物质、反应、专利中披露的物质的供应商及本专利的文献信息。

The screenshot displays the CAS SciFinder interface. At the top, the search bar contains 'References' and 'WO2013173779'. A large blue box with the number '5' is overlaid on the search bar. The main content area shows two search results under the heading 'References (2)'. The first result is titled 'Process for making amino acid compounds' and the second is 'Process for making amino acid compounds using enantioselective hydrogenation reactions'. Both results include a brief description and a chemical structure. The interface also features a 'Filter Behavior' sidebar on the left with options for Document Type, Language, and Publication Year. At the bottom of the sidebar, there is a 'Filter Content Report' link.

5. 选择 References, 获得该专利及其同族信息。

CAS SciFinder® Substances WO2013173779 6

← Return to Home

Substances (18) Sort: CAS RN: Descending View: Partial

Filter Behavior: Filter by Exclude

Commercial Availability:

- Available (11)
- Not Available (7)

Reaction Role:

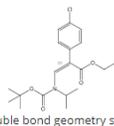
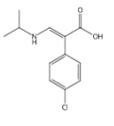
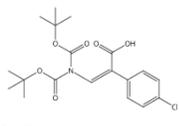
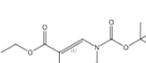
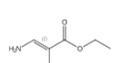
- Product (18)
- Reactant (14)
- Reagent (3)
- Catalyst (4)
- Solvent (3)

Reference Role:

- Preparation (18)
- Synthetic Preparation (18)
- Reactant (17)
- Reactant or Reagent (17)
- Industrial Manufacture (16)
- View All

Stereochemistry

References Reactions Suppliers Save And Alerts

<p>1</p> <p>1489004-67-2</p>  <p>Double bond geometry shown</p> <p>C₁₉H₂₆ClNO₄ Ethyl (αZ)-4-chloro-α-[[[(1,1-dimethylethoxy)carbonyl]](1-methylethyl)amino]methyl...</p> <p>2 References 2 Reactions 0 Suppliers</p>	<p>2</p> <p>1489004-64-9</p>  <p>C₁₂H₁₄ClNO₂ 4-Chloro-α-[[[(1-methylethyl)amino]methylene]benzeneacetic acid</p> <p>2 References 2 Reactions 0 Suppliers</p>	<p>3</p> <p>1489004-59-2</p>  <p>C₁₉H₂₄ClNO₆ α-[[Bis[[1,1-dimethylethoxy]carbonyl]amino]methylene]-4-chlorobenzeneacetic acid</p> <p>2 References 6 Reactions 0 Suppliers</p>
<p>4</p> <p>1489004-54-7</p> 	<p>5</p> <p>1489004-53-6</p> 	<p>6</p> <p>1489004-41-2</p> 

6. 选择 Substances, 获得该专利披露的物质信息。

The screenshot shows the CAS SciFinder interface. At the top, there is a search bar with the text 'WO2013173779' and a search icon. Below the search bar, the page is titled 'Reactions (35)'. On the left side, there is a 'Filter Behavior' section with options to 'Filter by' or 'Exclude'. Under 'Filter by', there are several categories: 'Yield' (with options like 90-100%, 70-79%, etc.), 'Number of Steps' (with options like 1, 2, 3, etc.), and 'Non-Participating Functional Groups' (with options like Halide, Phenyl halide, etc.). The main content area shows a list of reactions, with the first one selected. The selected reaction is titled 'Process for making amino acid compounds using enantioselective hydrogenation reactions' by Remarchuk, Travis. It is a patent document (WO2013173779) from 2013. Below the title, there is a chemical reaction scheme showing the hydrogenation of an enamine derivative to a chiral amino acid derivative. The reaction summary indicates 1 step and 99% yield. The reagents are Hydrogen and Lithium tetrafluoroborate. The catalyst is Ruthenium(1+), (η⁶-benzene)[1.1'-(1S)-[1.1'-binaphthalene]-2,2'-diylbis(1,1-diph...)]. The solvent is Ethanol, and the conditions are 24 h, 50 psi, rt. There are links for 'View Reaction Detail' and 'Experimental Protocols'.

7. 选择 Reactions，获得该专利披露的反应信息。

使用专利申请号获得同样的结果，在此不一一赘述。

The screenshot shows the CAS SciFinder interface. At the top, there is a search bar with the text 'CA2013-2873658'. Below the search bar, the page is titled 'Searching for...'. On the left side, there is a list of search categories: 'All', 'Substances', 'Reactions', 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'. The 'Reactions' category is selected. The main content area shows the search results for 'CA2013-2873658'. There are links for 'Saved', 'History', and 'Account' at the top right. The search bar has a 'Draw' icon and a search icon.

CAS SciFinder[®] All CA2013-2873658 Draw

← Return to Home

Show only

- Substances (18)
- Reactions (35)
- References (2)
- Suppliers (0)

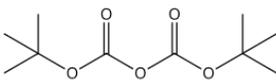
All Answer Types

Top two answers by relevance from each answer type.

Substances (18)

1

24424-99-5

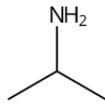


C₁₀H₁₈O₅
Di-tert-butyl dicarbonate

56K References 160K Reactions 138 Suppliers

2

75-31-0



C₃H₉N
Isopropylamine

22K References 28K Reactions 62 Suppliers

[View All Substances](#)

Reactions (35)

Scheme 1 (1 Reaction) Steps: 1 Yield: 99%



Absolute stereochemistry shown

专利优先权申请信息

在专利文献详情页面可获取专利优先权申请信息，包括优先权申请号和申请日。

← Return to Results
← Prev Next →

Reference Detail (1 of 1)

↓ ✉ 💾 Save

PATENT

Patent Number
[WO2016141092](#)

Publication Date
2016-09-09

Application Number
WO2016-US20499

Application Date
2016-03-02

Kind Code
A1

Assignee
Gilead Sciences, Inc., United States

Source
World Intellectual Property
Organization
CODEN: PIXXD2

Database Information
AN: 2016:1475937
CAN: 165:406001
CAplus

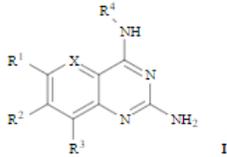
Language
English

CAS Formulus[®], the comprehensive formulations database and workflow solution, is now available for all SciFinder[®] users. [View content from CAS Formulus[®]](#) in this document. [Learn more about Formulus[®]](#).

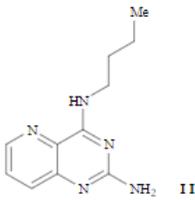
Preparation of toll-like receptor modulating 4,6-diamino-pyrido[3,2-d]pyrimidines and use in mono- and combination therapy

By: Aktoudianakis, Evangelos; Chin, Gregory; Mackman, Richard L.; Metobo, Samuel E.; Mish, Michael R.; Pyun, Hyung-Jung; Zablocki, Jeff

The invention relates to preparation of aminopyridopyrimidines of formula I wherein all the variables are as defined in the disclosure, as toll like receptor modulators, and pharmaceutical compositions containing the same. The example compound II was prepared according the disclosed procedure and was tested for modulatory activity of toll-like receptors (data shown). Compounds I can modulate toll-like receptors (e.g. TLR-8), and can be used in treatment and prevention of various diseases in mono and combination therapy.



I



II

Keywords: aminopyridopyrimidine preparation toll like receptor modulator disease treatment prevention

PatentPak Viewer
Get Prior Art Analysis
Full Text ▾

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2016141092	English	A1	PDF PDF+ Viewer	2016-09-09	WO2016-US20499	2016-03-02
CA2978188	English	A1	PDF	2016-09-09	CA2016-2978188	2016-03-02
AU2016216673	English	A1	PDF	2016-09-22	AU2016-216673	2016-03-02
KR2016113243	Korean	A	PDF	2016-09-28	KR2016-7023289	2016-03-02
US20160289229	English	A1	PDF	2016-10-06	US2016-1515059070	2016-03-02
EP3097102	English	A1		2016-11-30	EP2016-711723	2016-03-02
AU2016216673	English	B2		2017-02-02	AU2016-216673	2016-03-02
JP2017509667	Japanese	T	PDF	2017-04-06	JP2016-560343	2016-03-02
US9670205	English	B2	PDF	2017-06-06	US2016-1515059070	2016-03-02
KR1756050	Korean	B1	PDF	2017-07-07	KR2016-7023289	2016-03-02
JP6182278	Japanese	B2	PDF	2017-08-16	JP2016-560343	2016-03-02
CN107108615	Chinese	A	PDF	2017-08-29	CN2016-80004812	2016-03-02
KR2017114273	Korean	A	PDF	2017-10-13	KR2017-7018099	2016-03-02
EP3097102	English	B1	PDF	2017-10-18	EP2016-711723	2016-03-02
IL254164	English	A		2017-10-31	IL2016-254164	2016-03-02
CR2017000395	Spanish	A		2017-11-07	CR2017-395	2016-03-02
ES2656225	Spanish	T3	PDF	2018-02-26	ES2016-711723	2016-03-02
MD2017000081	Romanian	A2	PDF	2018-03-31	MD2017-81	2016-03-02
EP3321265	English	A1	PDF	2018-05-16	EP2017-196596	2016-03-02
SG10201904440	English	A1		2019-06-27	SG2019-10201904440	2016-03-02

[View All](#) ▾

Priority Application

Priority Application Number	Application Date
US2015-62128397	2015-03-04
US2015-62250403	2015-11-03

[Expand All](#) | [Collapse All](#)

- ▼ IPC Data
- ▼ Concepts
- ▼ Substances
- ▼ Formulations
- ▼ Cited Documents

生物序列检索

通过生物序列检索结果获取研究文献

The screenshot displays the CAS SciFinder Biosequences interface. The top navigation bar includes the CAS SciFinder logo, a search bar, and utility icons. The main content area is divided into a left sidebar and a central panel. The sidebar contains 'BLAST Search Details' and 'Bioscape Analysis' sections. The central panel shows a search result for 'Biosequences (10)' with a 'References' tab highlighted by a blue box with the number '1'. Below this, a 'Query Details' section shows a sequence: `MSGRHRKPTTSNVSVAKIAFTGAVLGGGIAMAAQATAATDGEWDQVARGESGQNSINTGNGYLGGLQFTQSTWAAHGGGEFAPSAQLAS...`. A sequence alignment is shown below, with 'Query' (length 407) and 'Subject' (length 737) sequences. The alignment identity is 99.75%, with 406 matches and 1 mismatch. A 'References' tab in the alignment view is highlighted by a blue box with the number '2'. Below the alignment, a list of references is shown, with the first reference 'Tuberculosis Compositions And Methods Of Treating Or Preventing Tuberculosis' highlighted by a blue box with the number '3'.

1. 获取 Biosequences 检索结果集中所有生物序列的研究文献。
2. 在 CAS SciFinder[®] 中获取此序列的研究文献。
3. 在 Biosequences 中，浏览此序列的研究文献。

生物序列检索 (BLAST)

The screenshot displays the Biosequences search page in CAS SciFinder. On the left, a sidebar lists search categories: All, Substances, Reactions, References, Suppliers, Biosequences (selected), and Retrosynthesis. The main area is titled 'Biosequences' and contains a search input field with a sequence, tabs for 'BLAST', 'CDR', and 'Motif', and buttons for 'Upload Sequence' and 'Clear Search'. Below the input field is a large text area containing a DNA sequence. To the right of the sequence, there are options for 'Sequence Type' (Nucleotide selected, Protein), 'Search Within' (Nucleotides selected, Proteins), and a checked checkbox for 'Include NCBI Sequences'. At the bottom right, there is a 'Limit Total Sequence Results to' dropdown set to 20000 and a 'Start Biosequence Search' button. Numbered callouts 1, 2, 3, and 4 are overlaid on the image to highlight specific features.

1. 选择 Biosequences 后及进入序列检索页面。此时，可以选择在检索框中手动输入或粘贴序列，也可以通过点击 Upload Sequence 上传文本或 FASTA 格式文件。如果以 FASTA 格式输入，则最多可以同时检索 100 条序列。可选择被检索序列的类型、要检索的域(核苷酸或蛋白质)，以及期望展示的检索结果数量。
2. 选择检索类型和检索域。
3. 选择是否包含 NCBI 中的序列。
4. 选择展示结果数量。

Advanced Biosequence Search ^ Adjust Parameters for Short Sequences | Reset All

Alignment Identity % [?] **1** Match with Gaps? Yes No

50

Gap Costs [?] **2**

Existence 5 Extension 2 ▾

Query Coverage % [?] **3** Word Size [?] **4**

50 11 ▾

Reward for Match **5**
Penalty for Mismatch [?]

2, -3 ▾

BLAST Algorithm **6** E-Value [?] **7**

BLASTn ▾ 10 ▾

Exclude Low Complexity Regions [?] **8**

Yes No

1. 值越高，目标序列与查询序列的一致性越高。
2. 较高的 Gap Costs 导致与含有较少空位的序列匹配。
3. 值越高，检索序列比对上的比例越高。
4. 起始相似性检索的最低匹配长度 word size 越大，匹配越严格。
5. 匹配奖励，错配罚分。
6. MegaBLAST 查找非常相似的序列；BLASTn 支持相似度较低的序列的查找；BLASTn-short 允许更短序列的比对（比如短到 7 个碱基的序列）。
7. E 值越小，匹配越严格。
8. LCR 如 AAATAAAAAAATAAAAAAT，多个 A 会导致比对分数偏高，序列中有 LCR 时可考虑排除。

1 Sort: Alignment Identity View: Expanded

2 Create Bioscope Analysis

3 Filter by

- E-Value: 0 to 10^6
- Query Coverage %: 0 to 100
- Subject Coverage %: 0 to 100
- Alignment Identity %: 0 to 100

4 Alignment Data

BLAST Score: 1728
E-Value: 0

Q	1	ATGCAGATCC CACAGGCGCC CTGGCCAGTC GTCTGGGCGG TGCTACAAC TGGCTGGCGG CCAAGGATGGT	70
S	1	ATGCAGATCC CACAGGCGCC CTGGCCAGTC GTCTGGGCGG TGCTACAAC TGGCTGGCGG CCAAGGATGGT	70
Q	71	TCTTAGACTC CCCAGACAGG CCCTGGAACC CCCCCACCTT CTCCCCAGCC CTGCTCGTGG TGACCGAAGG	140
S	71	TCTTAGACTC CCCAGACAGG CCCTGGAACC CCCCCACCTT CTCCCCAGCC CTGCTCGTGG TGACCGAAGG	140
Q	141	GGACAACGCC ACCTTCACCT GCAGCTTCTC CAACACATCG GAGAGCTTCG TGCTAAACTG GTACCGCATG	210
S	141	GGACAACGCC ACCTTCACCT GCAGCTTCTC CAACACATCG GAGAGCTTCG TGCTAAACTG GTACCGCATG	210

1. 序列结果排序标准。
2. 可视化分析序列结果。
3. 结果筛选。
4. 序列对比详情。

Query Sequence

QQLLVVEEGG

Subject Sequence

QQLLVVEEIGS

Alignment

$$\text{Query Coverage (100\%)} = \frac{\text{Alignment Length}}{\text{Query Length}} = \frac{10}{10}$$

$$\text{Subject Coverage (91\%)} = \frac{\text{Alignment Length}}{\text{Subject Length}} = \frac{10}{11}$$

$$\text{Sequence Identity (90\%)} = \frac{\text{Number of Matches}}{\text{Alignment Length}} = \frac{9}{10}$$

Alignment **1** Subject **ces** References

CAS Registry Numbers: 2306097-89-0, 503752-44-1 **2**

NCBI Identifier: [KJ865859.1](#), [AY238517.1](#)

Length: 867 nt

Sequence **3**

```

1  ATGCAGATCC CACAGGCGCC AGTC GTCTGGGCGG TGCTACAAC TGGCTGGCGG CCAGGATGGT TCTTAGACTC
81  CCCAGACAGG CCCTGGAAC CCCCCACCTT CTCCCCAGCC CTGCTCGTGG TGACCGAAGG GGACAACGCC ACCTTCACTT
161 GCAGCTTCTC CAACACATCG GAGAGCTTCG TGCTAAACTG GTACCGCATG AGCCCCAGCA ACCAGACGGA CAAGCTGGCC
241 CCTTCCCGG AGGACCGCAG CCAGCCGCGC CAGGACTGCC GCTTCCGTGT CACACAATG CCCAACGGGC GTGACTTCCA
321 CATGAGCGTG GTCAGGGCCC GGCACAATGA CAGCGGCACC TACCTCTGTG GGGCCATCTC CCTGGCCCCC AAGGCGCAGA
401 TCAAAGAGAG CCTGCGGGA GAGCTCAGGG TGACAGAGAG AAGGGCAGAA GTGCCACAG CCCACCCAG CCCCTCACCC
481 AGGCCAGCCG GCCAGTTCCA AACCTGGTG GTTGGTGTG TGGGCGGCCT GCTGGGCAGC CTGGTGTGTC TAGTCTGGGT
561 CCTGGCCGTC ATCTGCTCCC GGGCCGACG AGGGACAATA GGAGCCAGGC GCACCGGCCA GCCCTGAAG GAGGACCCCT
641 CAGCCGTGCC TGTGTTCTCT GTGGACTATG GGGAGCTGGA TTTCCAGTGG CGAGAGAAGA CCCCGGAGCC CCCCGTGCCC
721 TGTGTCCTG AGCAGACGGA GTATGCCACC ATTGTCTTTC CTAGCGGAAT GGGCACCTCA TCCCCGCCCC GCAGGGGCTC

```

ncbi.nlm.nih.gov/nuccore/KJ865859.1 **4** Send

GenBank

Homo sapiens cell-line A375 programmed cell death 1 protein (PDCD1) mRNA, complete cds

GenBank: KJ865859.1

[FASTA](#) [Graphics](#) [PopSet](#)

Go to:

LOCUS KJ865859 867 bp mRNA linear PRI 22-SEP-2015

DEFINITION Homo sapiens cell-line A375 programmed cell death 1 protein (PDCD1) mRNA, complete cds.

ACCESSION KJ865859

VERSION KJ865859.1

KEYWORDS .

SOURCE Homo sapiens (human)

ORGANISM [Homo sapiens](#)
Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini; Catarrhini; Hominidae; Homo.

REFERENCE 1 (bases 1 to 867)

AUTHORS Kleffel,S., Posch,C., Barthel,S.R., Mueller,H., Schlapbach,C., Guenova,E., Elco,C.P., Lee,N., Juneja,V.R., Zhan,Q., Lian,C.G., Thomi,R., Hoetzenecker,W., Cozzio,A., Dummer,R., Mihm,M.C. Jr., Flaherty,K.T., Frank,M.H., Murphy,G.F., Sharpe,A.H., Kupper,T.S. and Schatton,T.

TITLE Melanoma Cell-Intrinsic PD-1 Receptor Functions Promote Tumor Growth

JOURNAL Cell 162 (6), 1242-1256 (2015)

1. 目标序列信息。
2. 目标序列 CAS 登记号。
3. 目标序列的 NCBI 编号，点击 NCBI 编号，即可链接至 NCBI 页面。
4. NCBI 页面展示的目标序列详情。



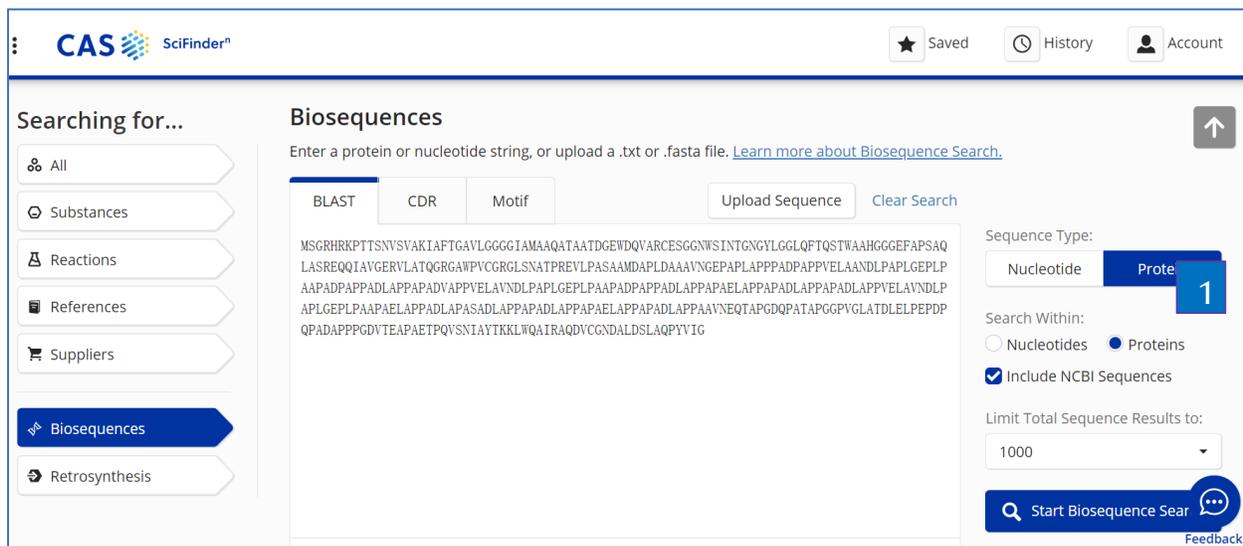
1. Biosequences 中目标序列的相关专利。
2. 在 CAS SciFinder[®] 中获取目标序列的专利和非专利文献。



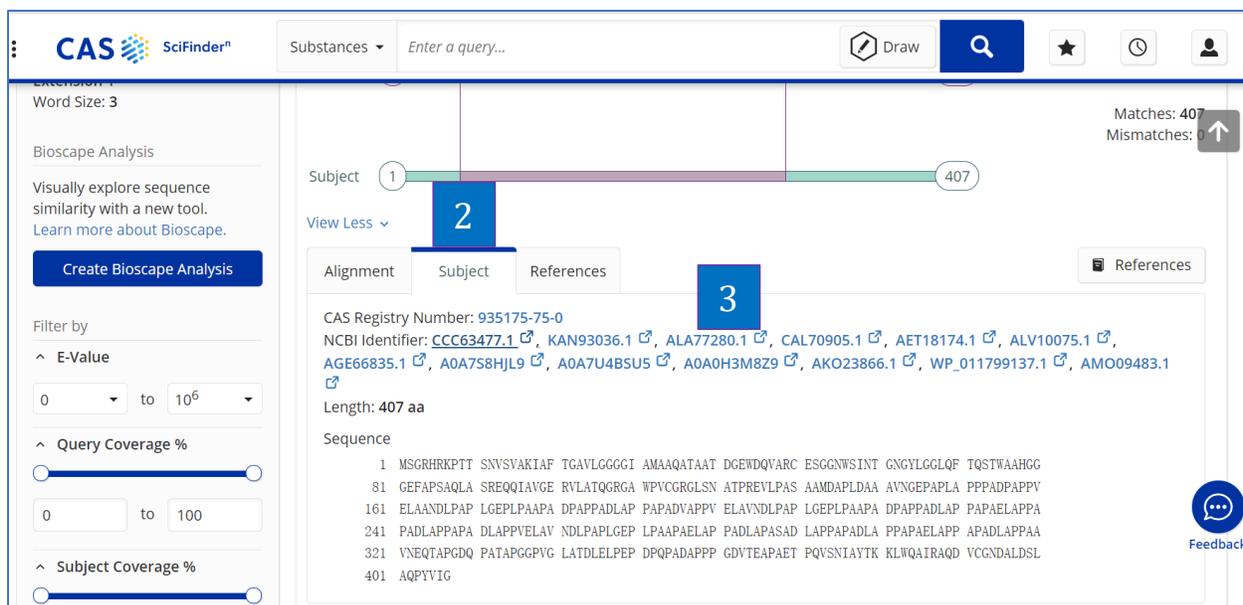
3. 点击 Create Bioscape Analysis 后，获得序列可视化分析页面。
4. 选中某序列。
5. 被选中序列的信息及其相关专利。

在 Biosequences 中检索时选择包含来自 NCBI 的序列

在选择 Biosequences 进行检索时，可勾选 Include NCBI Sequences, 以获取来自 NCBI 的序列。



1. 输入序列信息后，勾选 Include NCBI Sequences。



2. 在结果集页面，点击 Subject，查看目标序列。如果该序列同时被 NCBI 收录，则将展示其 NCBI Identifier。

3. 点击 NCBI Identifier 超链接，则可直接打开 NCBI 中该序列信息页。

COVID-19 Information
Public health information (CDC) | Research information (NIH) | SARS-CoV-2 data (NCBI) | Prevention and treatment information (HHS) | Esoalot

4

GenPept → Send to → Change region shown → Customize view →

possible resuscitation-promoting factor rpfA [Mycobacterium tuberculosis variant bovis BCG str. Moreau RDJ]

GenBank: [CCCG3477.1](#)

Identical Proteins FASTA Graphics

LOCUS CCCG3477 407 aa linear BCT 03-NOV-2016

DEFINITION possible resuscitation-promoting factor rpfA [Mycobacterium tuberculosis variant bovis BCG str. Moreau RDJ].

ACCESSION CCCG3477

VERSION CCCG3477.1

DELINE BioProject: [PRJNA70288](#)
BioSample: [SAMN04338327](#)
embl accession: [AM12029_2](#)

RESOURCE

KEYWORDS

SOURCE Mycobacterium tuberculosis variant bovis BCG str. Moreau RDJ

ORGANISM Mycobacterium tuberculosis variant bovis BCG str. Moreau RDJ
Bacteria; Actinobacteria; Corynebacteriales; Mycobacteriaceae; Mycobacterium; Mycobacterium tuberculosis complex.

REFERENCE 1
AUTHORS Gomes, L. R., Otto, T. D., Vasconcelos, E. A., Ferraz, P. M., Maia, R. M., Moreira, R. S., Ferreira, M. A., Castello-Branco, L. R., Degrave, W. M. and Mendonca-Lima, L.

TITLE Genome sequence of Mycobacterium bovis BCG Moreau, the Brazilian vaccine strain against tuberculosis

JOURNAL J. Bacteriol. 193 (19): 3600-3600. (2011)

PUMED [21914892](#)

REFERENCE 2 (residues 1 to 407)
AUTHORS Mendonca-Lima, L.

TITLE Direct Submission

JOURNAL Submitted (22-NOV-2006) Mendonca-Lima L., Biochemistry and Molecular Biology, Instituto Oswaldo Cruz - Fiocruz, Av. Brasil, 4305, 21040-900 Rio de Janeiro - RJ, BRAZIL

FEATURES

source 1..407
/organism="Mycobacterium tuberculosis variant bovis BCG str. Moreau RDJ"
/strain="Moreau RDJ"
/isolate="SI21 FAP RJ Passage BSG vaccine culture"
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/note="Translysoylase-like domain: pfam0073"
/db_xref="CCD:332604"

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/note="In Mycobacterium bovis, a 240 bp deletion leads to a shorter product compared to its homolog in Mycobacterium tuberculosis strain H37Rv and Mycobacterium bovis BCG strains Pasteur and Moreau (327 aa versus 407 aa). Differs from Rv0867c by 1aa E235D"
/transl_table=11
/db_xref="EnsemblGenomes-Om:BCGM_0884c"
/db_xref="EnsemblGenomes-Tr:CCCG3477"

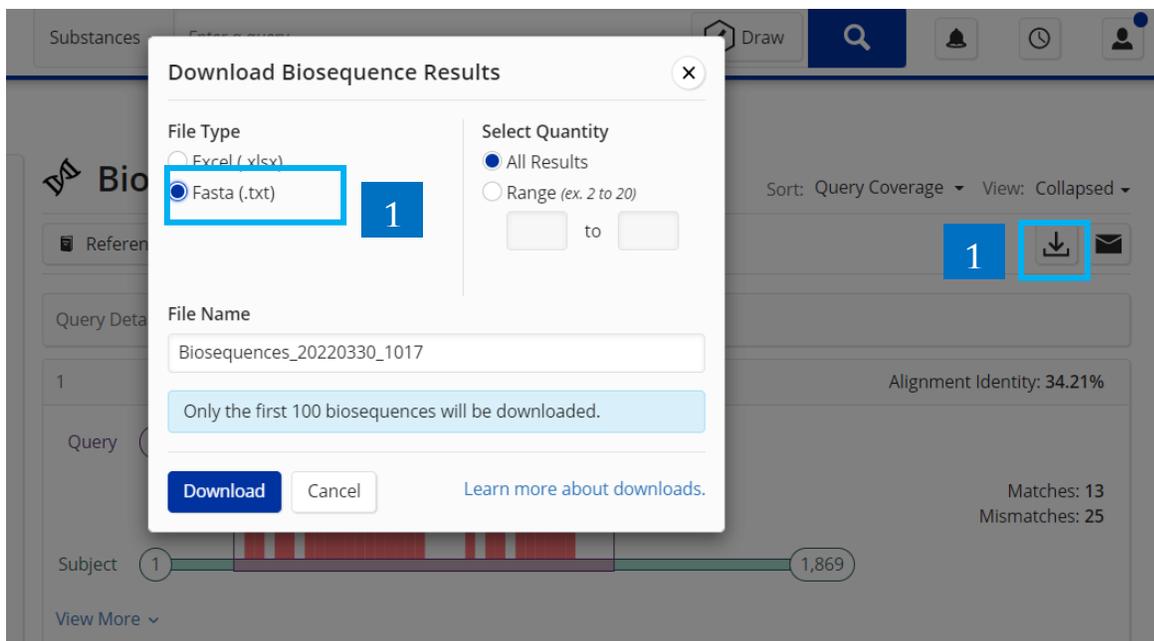
ORIGIN
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61 gnr/rltlof turtwahnq gdfapnala sreqiavve rvlatsgza vpvcrerln
121 stpvevlpaa hantp/lea avpavpalia pppadpdpv vlsandlipo lqep/pana
181 dpapadlap pppadpdpv vlsandlipo lqep/pana dpapadlap ppsalappa
241 pdlappapa dlppvrlav ndlpaplpo lpsapaelp pdlappadp lappadala
301 pppaelapp apadlappa vneatpdpq patappspve lardlelpep dpapadapp
361 sdvrtpepae psvvnlarkv klvqatraq vmdalqal sduvvis

Recent activity [Turn Off](#) [Clear](#)
possible resuscitation-promoting factor rpfA [Mycobacterium tuberculosis variant... Protein
Q ADATU4BSU5 (0) Protein
[See more...](#)

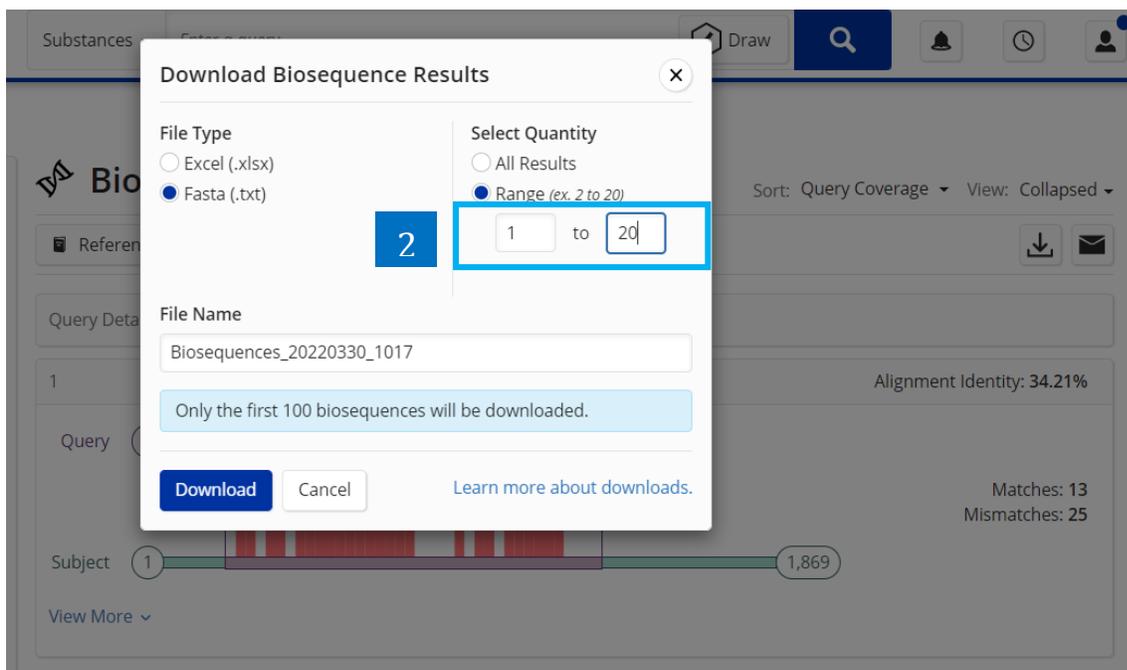
4. NCBI 中的目标序列详情。

使用 FAST 格式下载生物序列检索结果

生物序列检索结果的下载功能增强：支持 FASTA 格式下载。



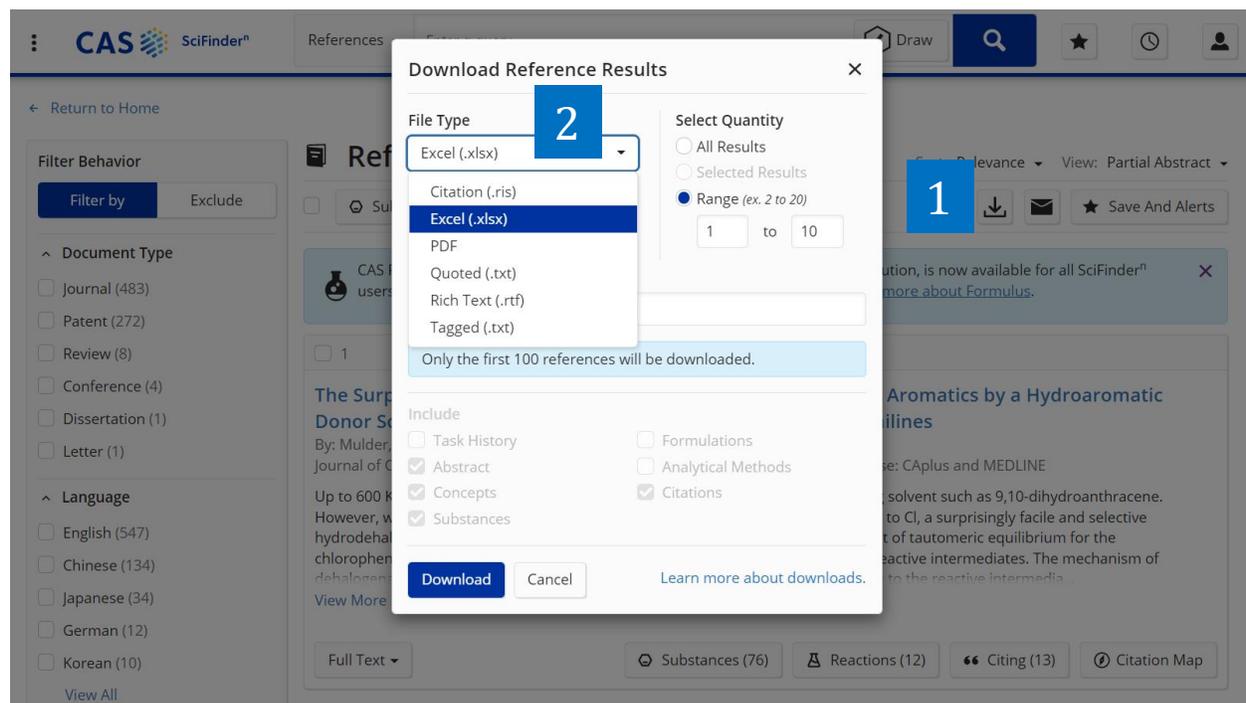
1. 点击下载，选择 File Type: Fasta (.txt)。可下载序列检索结果的前 100 条。



2. 可通过 Select Quantity: Range，输入下载范围。

检索结果后处理

使用 Excel 文件导出文献详情



1. 在文献结果集页面，点击下载图标
2. 在弹出窗口中的 File Type 下选择 Excel(.xlsx)，即可使用 Excel 文件格式下载文献详情。

AutoSave Off Reference_20220105_1413.xlsx Search Cheng, Xiaoyan Z

File Home Insert Page Layout Formulas Data Review View Help ChemOffice20 Acrobat

Clipboard Font Alignment Number Styles Cells Editing Ideas Sensitivity

A1

3

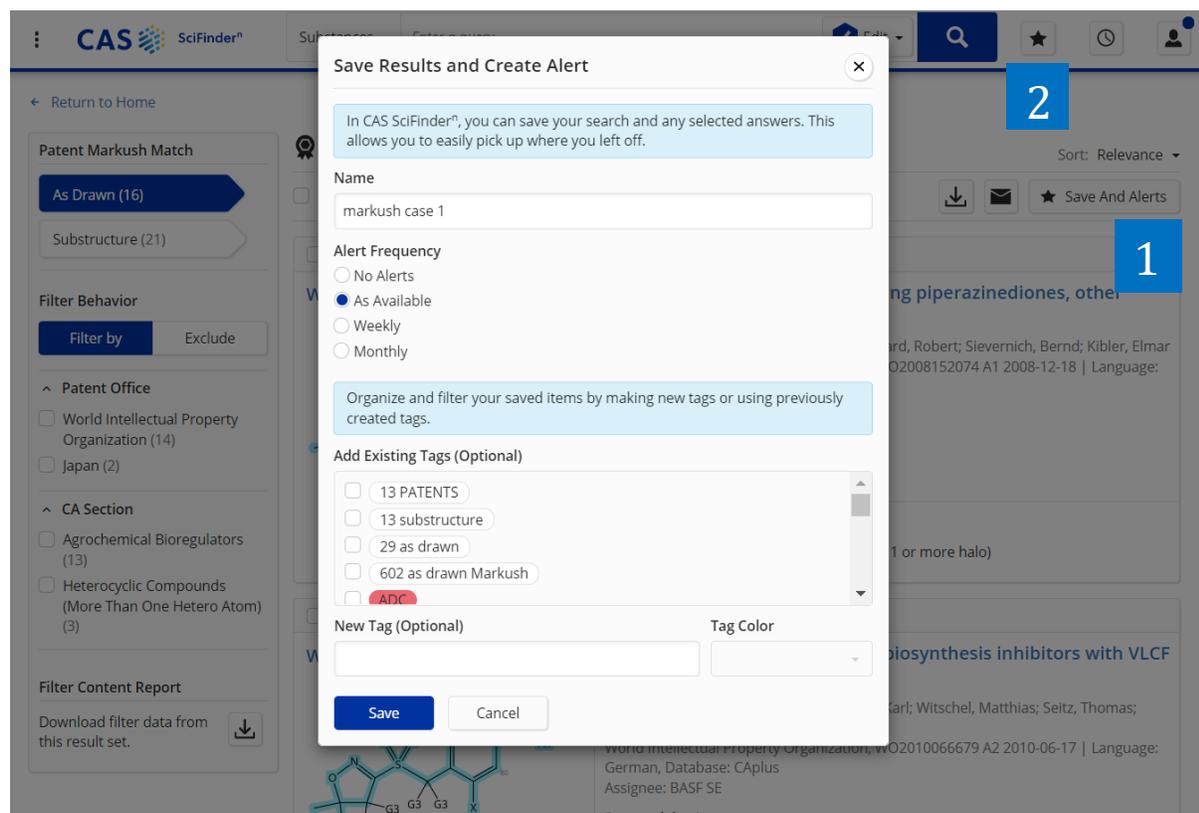
Patent Number	Title	Abstract	Database	Language	Volume	Issue	Page	Document Type	Publication Date	Concepts	CAS Registry Numbers
US6083279A	Preparation of substituted aromatic amines	The substituted aromatic amine (such as 1-(phenyl)-2-phenylethylamine) is prepared by (A) oxidizing an aromatic amine (such as aniline) in the presence of an oxidizing agent (such as oxygen or hydrogen peroxide) and a metal pentacyano ferrous complex (such as sodium pentacyanoferrous) to form an arylamino pentacyanoferrous complex, and (B) catalytically reducing the arylamino pentacyanoferrous complex with a reducing agent (such as hydrogen) in the presence of a catalyst having 2 metals selected from Group VIII elements (such as carbon supported platinum or ruthenium).	Capus	English			7 pages	Patent	2000-05-30	Aromatic amine; FCT (Reactant); FACT (Reagent or Reagent); Diamine; Fole; PF (Industrial Manufacture); PREP (Preparation); Catalytic; Group VIII element; Fole; CAT (Catalyst); LSES; Siles; Catalyst; Polymers; Iron; Indole; amine; Fole; PF (Industrial Manufacture); PREP (Preparation); Redox reaction; catalyst; Production	14025525; 1443492; 144700; 744053; 17542; 62533
US5552531A	Preparation of diphenylamines	The title process comprises reaction between an aromatic amine compound and an aromatic or aliphatic amine or amide in the presence of a base and a protonic material. Thus, PNMe ₂ Br ₂ is treated with an aryl amine PNMe ₂ containing NCO ₂ Me ₂ and Et ₃ COv ₂ to give 100% 4-PhNCO ₂ Me ₂ Ph ₂ N.	Capus	English			4 pages	Patent	1996-09-03		10751952; 3395470; 708660; 1306305; 291803; 702405; 5; 106430; 836470; 104949; 10332; 30038; 62533; 58270
WO9324450A1	Preparation of substituted aromatic amines from the reaction of aromatic amine compounds and nucleophilic compounds	Optionally substituted aromatic amines (e.g., 4-aminodiphenylamine) are prepared by reacting a nucleophilic compound (e.g., aniline, substituted aliphatic amine, etc.) with an amine-containing compound (e.g., acetonitrile, etc.) in the presence of a solvent and in the presence of a base (e.g., NaOH, Na ₂ CO ₃ , etc.) and an optional protonic material (e.g., H ₂ O), where the molar ratio of protonic material to base is 0-5:1. The substituted aromatic amines may be selectively alkylated to produce alkylated diamines or substituted derivatives.	Capus	English			62 pages	Patent	1993-12-09	Aldehyde; Fole; FCT (Reactant); FACT (Reagent or Reagent); Aromatic amine; Fole; SPN (Synthetic Preparation); PREP (Preparation); Aromatic compound; amine; Fole; SPN (Synthetic Preparation); PREP (Preparation); Amino compound; amine; Fole; SPN (Synthetic Preparation); PREP (Preparation); Ketone; Fole; FCT (Reactant); FACT (Reagent or Reagent); Quaternary ammonium compound; tertiary; hydroxide; Fole; SPN (Synthetic Preparation); PREP (Preparation); Reductive alkylation	15380972; 14044143; 14044; 7886070; 67203053; 691074; 12625425; 1745123; 135244; 698725; 5232783; 3424532; 1; 251653; 2484880; 2002412; 782456; 633983; 620944; 6198; 101165; 523695; 382837; 2376; 10133; 124826; 120630; 122396; 10063; 119344; 10794; 10121; 105503; 876450; 106476; 10434; 10715; 125844; 10542; 100418; 36407; 30040; 78950; 75318; 6; 62533; 60395; 60322; 57508; 5;

Patent Literature Non-Patent Literature

3. Excel 文件格式下载文献详情。

Combine 的应用

Combine 功能：可用于对多个检索结果集（包括文献、物质、Markush 和反应的检索结果集）进行逻辑处理（包括合并、取交集和排除）。



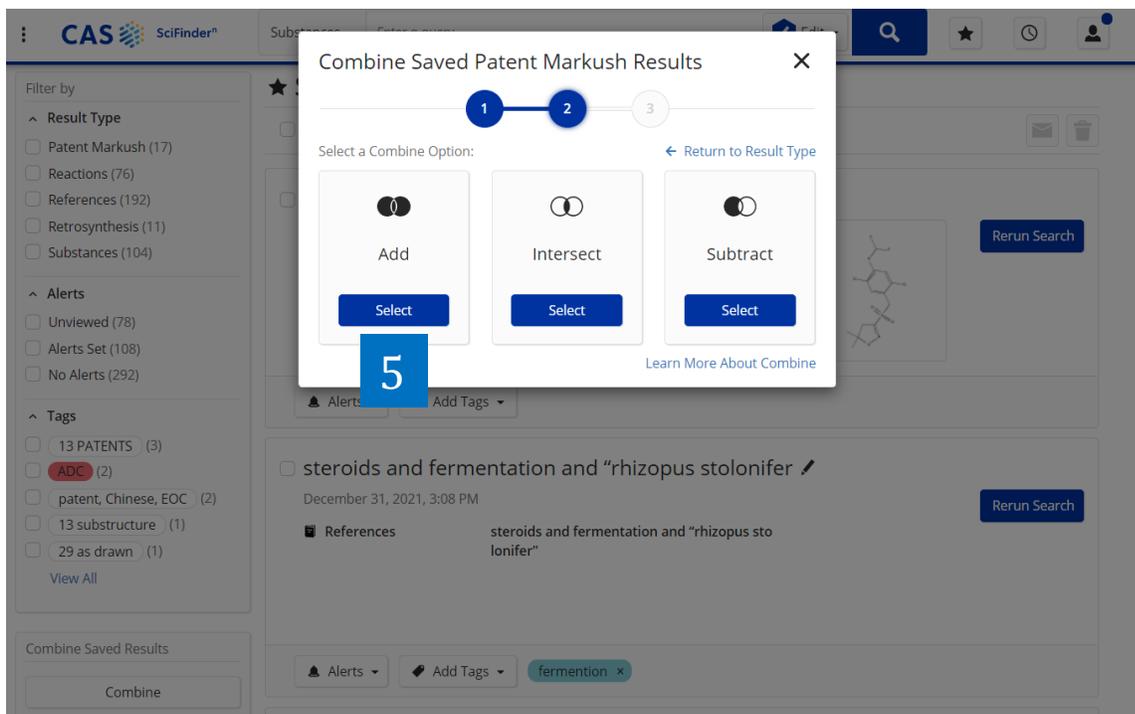
1. 点击 Save And Alerts，在弹出窗口中填写 Name，点击 Save，保存检索结果集。
2. 打开保存的检索结果集，进行 Combine 操作。

The screenshot shows the CAS SciFinder interface. On the left, there are filter options for Result Type (Patent Markush, Reactions, References, Retrosynthesis, Substances), Alerts (Unviewed, Alerts Set, No Alerts), and Tags (13 PATENTS, ADC, patent, Chinese, EOC, 13 substructure, 29 as drawn). The main area displays a list of saved searches. The first search is 'markush case 1' (January 5, 2022, 12:28 PM) with a 'Patent Markush' tag and a chemical structure. The second search is 'steroids and fermentation and "rhizopus stolonifer"' (December 31, 2021, 3:08 PM) with a 'References' tag. A blue box with the number '3' highlights the 'Combine Saved Results' button and the 'Combine' input field.

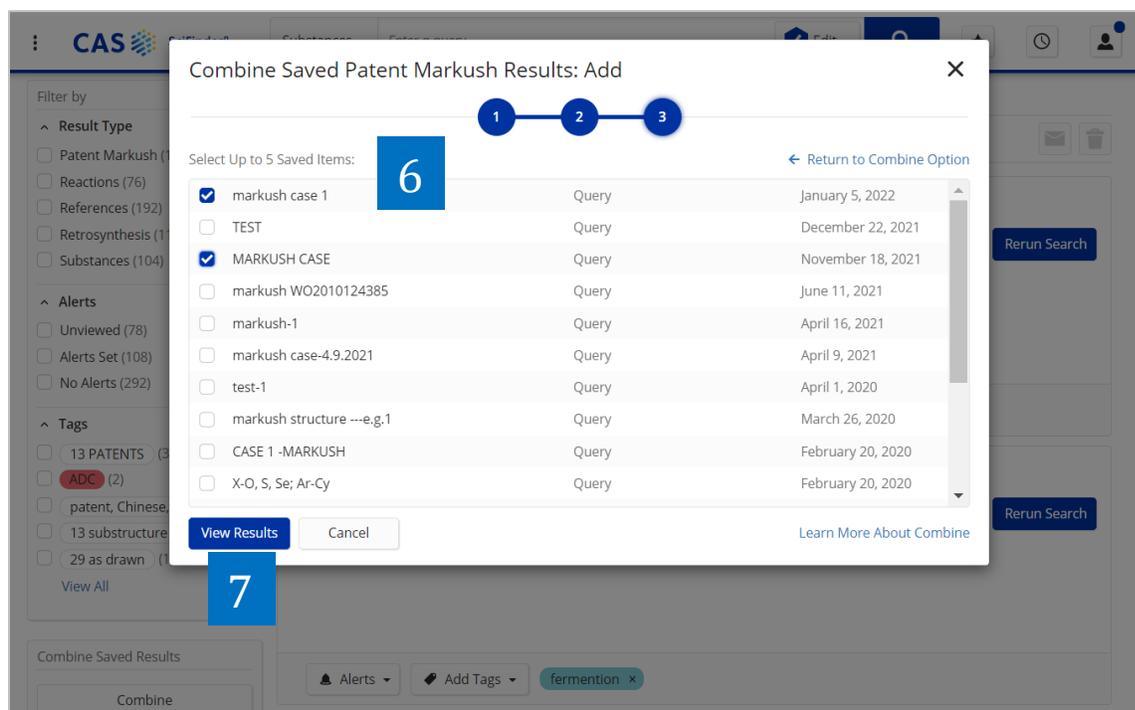
3. 点击 Combine, 进行多个结果集的逻辑处理。

The screenshot shows the 'Combine Saved Results' dialog box. It has a progress indicator with three steps, where step 1 is active. Below the progress indicator, there are four options: Substances, Patent Markush, Reactions, and References. Each option has a 'Select' button. The 'Patent Markush' option is highlighted with a blue box containing the number '4'. There is also a 'Learn More About Combine' link at the bottom right of the dialog.

4. 选择需要 combine 的检索结果集类型，例如 Patent Markush。



5. 选择需要进行的逻辑操作。



6. 选择需要 combine 的结果集。

7. 点击 View Results, 获得 combine 后的结果集。

CAS SciFinder® Substances Enter a query... Draw Search Star Clock User

Return to Home

Filter Behavior Filter by Exclude

Patent Office

- World Intellectual Property Organization (519)
- China (199)
- United States (105)
- Japan (69)
- Korea, Republic of (49)

View All

CA Section

- Heterocyclic Compounds (More Than One Hetero Atom) (374)
- Heterocyclic Compounds (One Hetero Atom) (225)
- Optical, Electron, and Mass Spectroscopy and Other Related Properties (104)
- Pharmacology (77)
- Benzene, Its Derivatives, and Condensed Benzenoid Compounds (47)

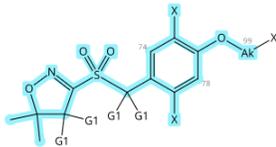
View All

Patent Markush (1,030) Sort: Patent Number: Descending

References

1

WO2008152074



Herbicidal compositions containing piperazinediones, other active substances, and safeners

By: Hupe, Eike; Moberg, William Karl; Reinhard, Robert; Sievernich, Bernd; Kibler, Elmar
World Intellectual Property Organization, WO2008152074 A1 2008-12-18 | Language: German, Database: Caplus
Assignee: Basf SE

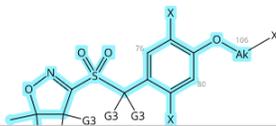
Patent claim 15

PatentPak Full Text

74,78: opt. substd. by (1-3) G3
99: alkyl <containing 1-4 C> (opt. substd. by 1 or more halo)

2

WO2010066679



Herbicidal mixtures of cellulose biosynthesis inhibitors with VLCC A inhibitors.

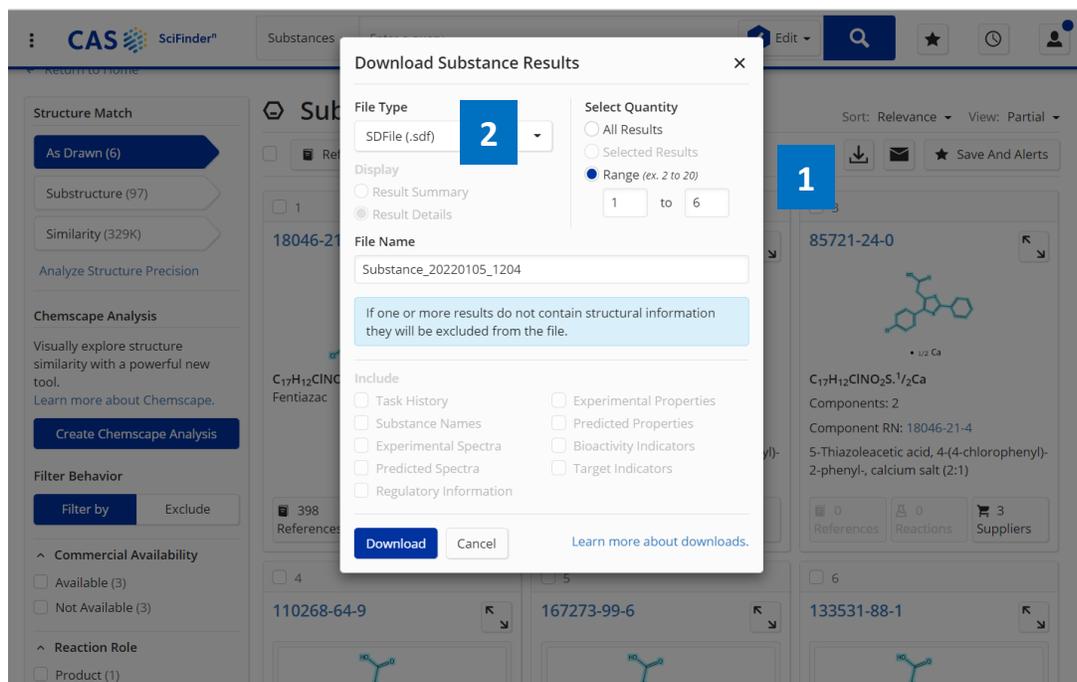
By: Parra Rapado, Liliana; Moberg, William Karl; Witschel, Matthias; Seitz, Thomas; Simon, Anja; Newton, Trevor William
World Intellectual Property Organization, WO2010066679 A2 2010-06-17 | Language: German, Database: Caplus
Assignee: BASF SE

将物质结果导出为可以编辑的结构数据文件

有以下三种方法可以将物质结果导出为可以编辑的结构数据文件：

- I. 直接在物质结果集页面点击 ，选择 SDFFile，可以批量导出可编辑的结构数据文件。
- II. 若需要导出某一选定物质的结构数据文件，则可以点击该物质的结构，在打开的新窗口中点击 ，选择所需下载的结构数据文件格式(CXF, MOL, SDF)
- III. 若需要导出某一选定物质的结构数据文件及其属性值，则可以在 substance detail 页面点击 ，同时下载结构数据文件(CXF, MOL, SDF)和属性值（EXCEL）文件。

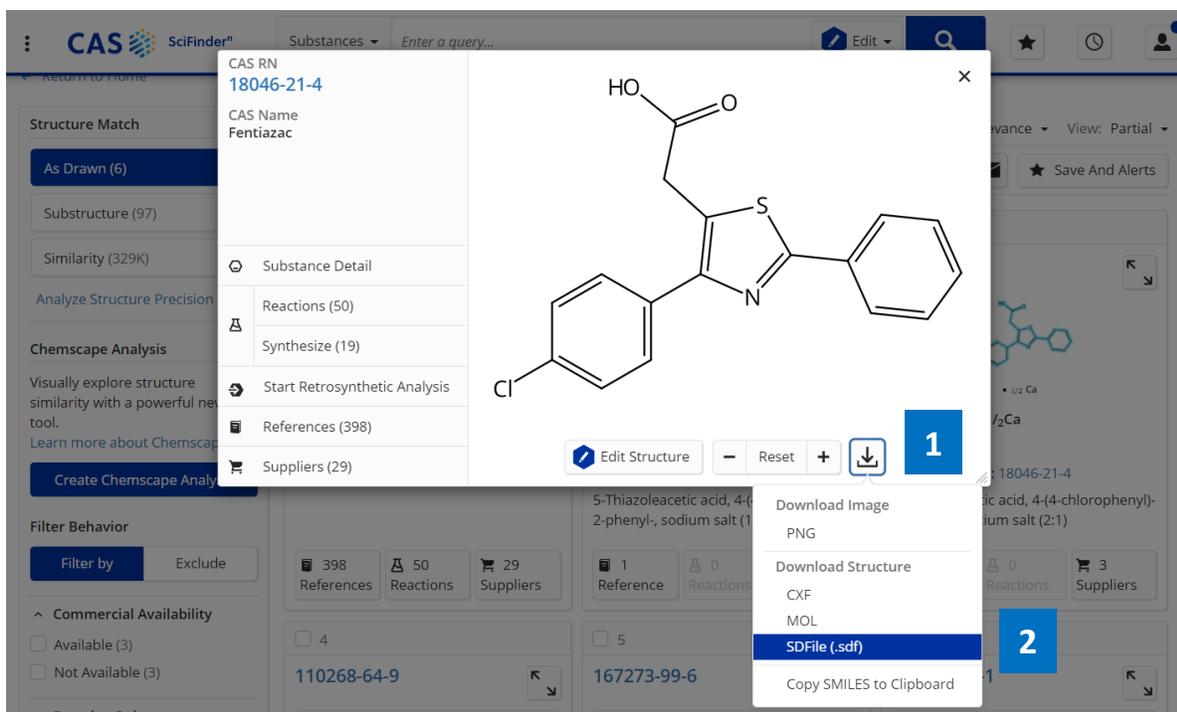
方法一：直接在物质结果集页面点击 ，选择 SDFFile，可以批量导出可编辑的结构数据文件。



1. 点击  按钮

2. 选择 SDFFile

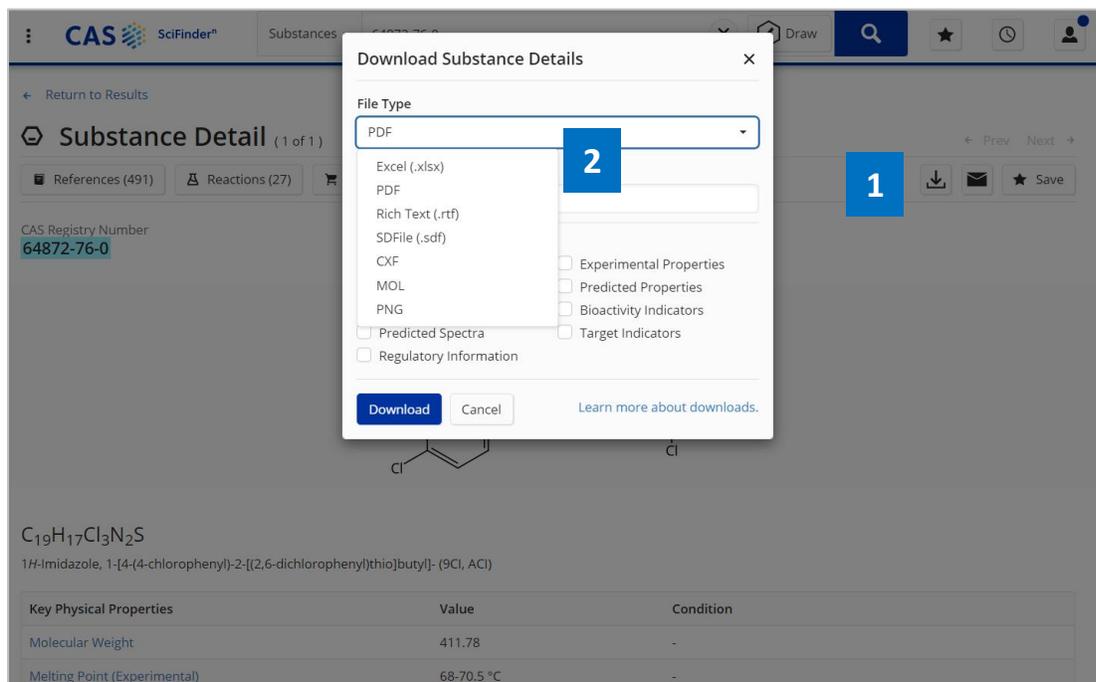
方法二：若需要导出某一选定物质的结构数据文件，则可以点击该物质的结构，在打开的新窗口中点击 ，选择所需下载的结构数据文件格式（CXF, MOL, SDF）。



The screenshot displays the CAS SciFinder interface. A chemical structure of 5-(4-chlorophenyl)-2-phenylthiazole-3-carboxylic acid is shown in a central window. The window has a title bar with 'CAS RN 18046-21-4' and 'CAS Name Fentiazac'. Below the structure, there are buttons for 'Edit Structure', 'Reset', and a download icon (labeled '1'). A dropdown menu is open from the download icon, showing options: 'Download Image (PNG)', 'Download Structure (CXF, MOL, SDFFile (.sdf), Copy SMILES to Clipboard)'. The 'SDFFile (.sdf)' option is highlighted (labeled '2'). The background shows the SciFinder search results page with various filters and search options.

1. 点击  按钮
2. 选择所需下载的结构数据文件格式(CXF, MOL, SDF)

方法三：若需要导出某一选定物质的结构数据文件及其属性值，则可以在 substance detail 页面点击 ，同时下载结构数据文件(CXF, MOL, SDF)和属性值（EXCEL）文件。



1. 点击  按钮
2. 选择所需下载的结构数据文件(CXF, MOL, SDF)和属性值文件 EXCEL

请注意：如果物质没有结构或无法建模，则将无法使用此下载选项。

结构数据 SDF 文件下载示例：

```

865-21-4 (1).sdf - Notepad
File Edit Format View Help
Vincalukoblastine
C46H58N4O9
865-21-4 Copyright (C) 2019 ACS
 62 70 0 0 1 0 0 0 0 0999 V2000
75193.548426691.5323 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
80891.129029975.8065 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63326.612912592.7419 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
69024.1935 9308.4677 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57629.0323 9308.4677 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
74721.774212592.7419 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
69024.193515895.1613 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50969.7581 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
75193.548419487.9032 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
84302.419424750.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
90000.000021465.7258 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
84302.419431336.6935 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26764.112919487.9032 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19306.451623788.3065 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20594.758136762.0968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14897.177440046.3710 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20594.758130175.4032 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 8637.096836435.4839 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
60895.161354090.7258 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
66592.741950806.4516 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59770.161346070.5645 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57157.258129975.8065 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
63326.612933586.6935 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
57157.258122772.1774 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
44800.403229975.8065 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50969.758133586.6935 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
69495.967729975.8065 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0
57 58 2 0 0 0 0 0
M END
> <cas.rn>
865-21-4

> <cas.index.name>
Vincalukoblastine

> <molecular.formula>
C46H58N4O9

> <molecular.weight>
810.97

> <melting.point.experimental>
211-216 °C

> <density.predicted>
1.37±0.1 g/cm3 Temp: 20 °C; Press: 760 Torr

> <pka.predicted>
11.36±0.60 Most Acidic Temp: 25 °C

$$$$

```

属性值 EXCEL 文件下载示例：

Substance Name: 64872-76-0

Type	Category	Property	Value and Units	Temperature	Pressure	pH
Experimental	Thermal	Melting Point	66-70.5 °C	25 °C		
Predicted	Biological	Bioconcentration Factor	184	25 °C		pH 1
Predicted	Biological	Bioconcentration Factor	185	25 °C		pH 2
Predicted	Biological	Bioconcentration Factor	195	25 °C		pH 3
Predicted	Biological	Bioconcentration Factor	289	25 °C		pH 4
Predicted	Biological	Bioconcentration Factor	1220	25 °C		pH 5
Predicted	Biological	Bioconcentration Factor	9110	25 °C		pH 6
Predicted	Biological	Bioconcentration Factor	97600	25 °C		pH 7
Predicted	Biological	Bioconcentration Factor	58200	25 °C		pH 8
Predicted	Biological	Bioconcentration Factor	57900	25 °C		pH 9

设置 Alert

在 CAS SciFinder[®] 中，可对以下 4 种检索方式设置 Alert：

- 马库什结构检索
- 文献检索
- 物质检索
- 反应检索

一. 马库什结构检索后，设置 Alert

The screenshot displays the CAS SciFinder interface. A modal dialog box titled "Save Results and Create Alert" is open. The dialog box contains the following fields and options:

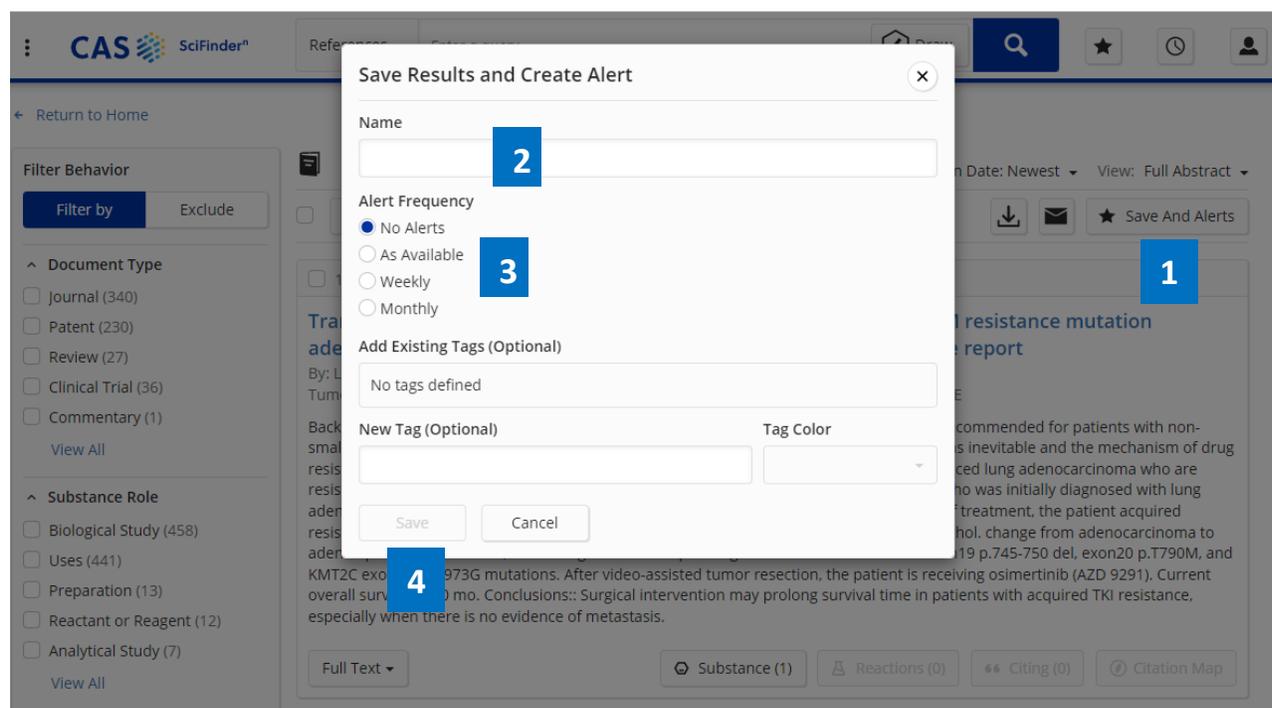
- Name:** A text input field containing "icotinib Markush".
- Alert Frequency:** Radio button options: No Alerts, As Available, Weekly, Monthly.
- Add Existing Tags (Optional):** A text input field containing "No tags defined".
- New Tag (Optional):** A text input field.
- Tag Color:** A dropdown menu.
- Buttons:** "Save" and "Cancel".

The background shows search filters on the left and a search result for "Deuterated 4-[(3-ethynyl phenyl) amino]-6,7-benzene-12-crown-4-quinazoline derivative useful in treatment of cancer and its preparation". The chemical structure is shown with G1 labels. The patent information includes: "By: Liu, Wenpei; Wu, Changxing; Feng, Dezhe; China, CN106188072 A 2016-12-07 | Language: Chinese, Database: CPlus".

1. 在马库什结构检索结果集页面点击 Save And Alerts。
2. 输入保存文件的名称。

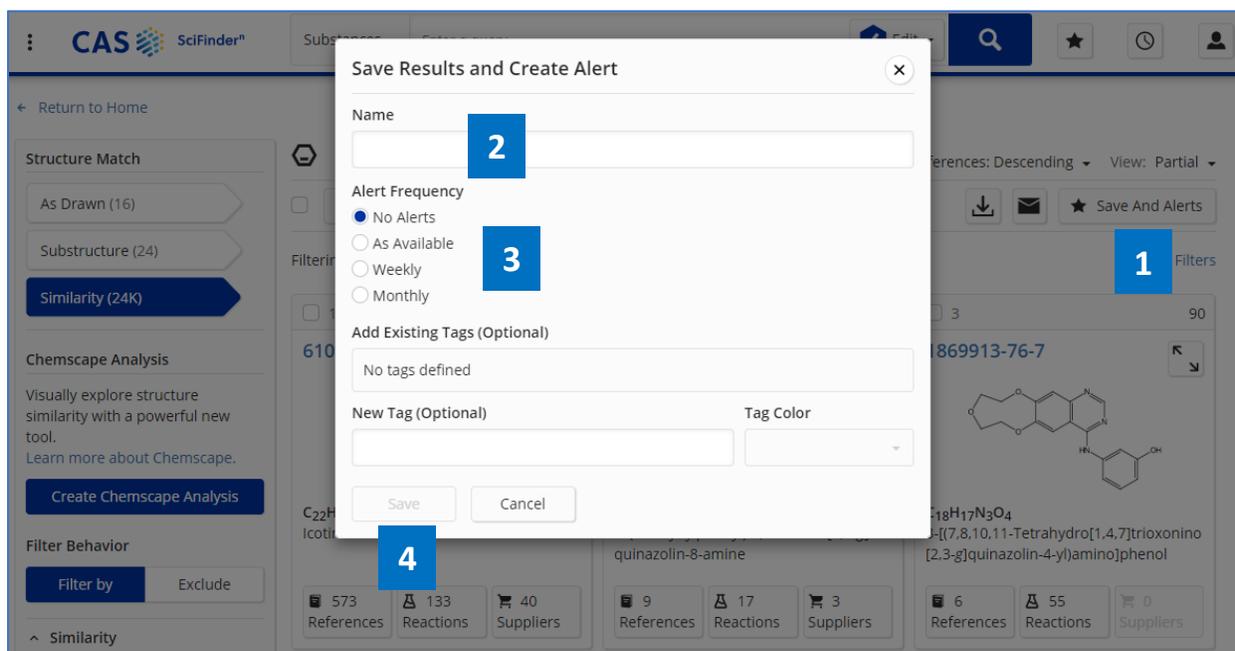
3. 选择 No Alerts 表示不设置提醒；选择 As Available、Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

二. 文献检索后，设置 Alert



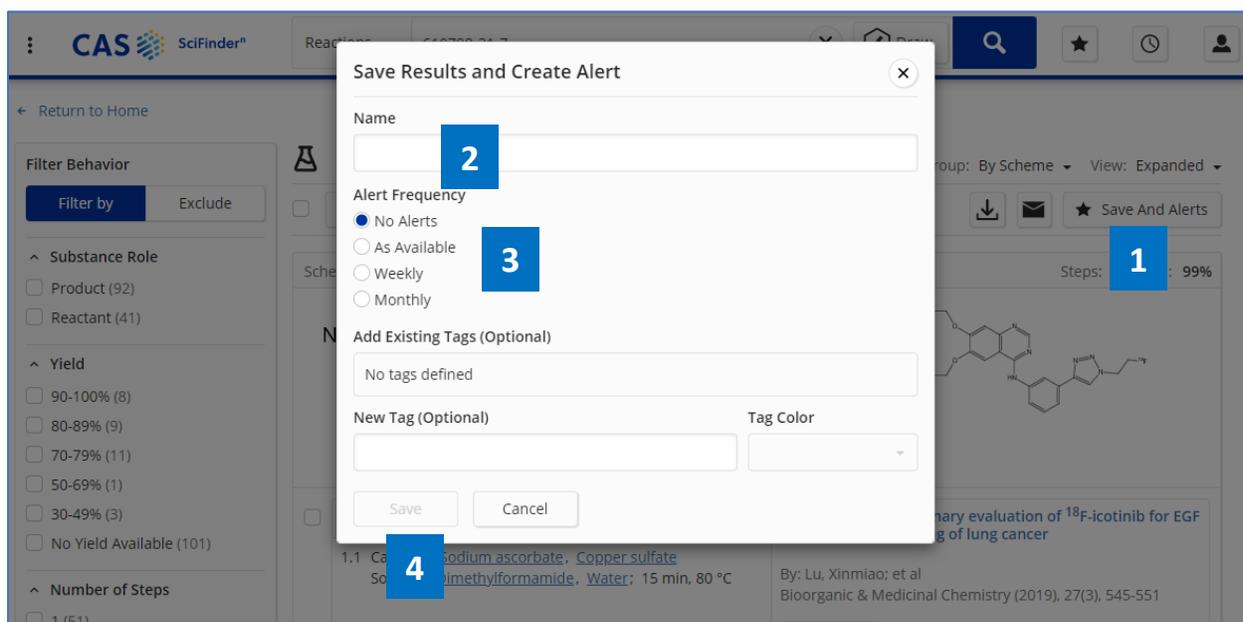
1. 在文献结果集页面点击 Save And Alerts。
2. 输入保存文件的名称。
3. 选择 No Alerts 表示不设置提醒；选择 As Available、Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

三. 物质检索后，设置 Alert



1. 在物质结果集页面点击 Save And Alerts。
2. 输入保存文件的名称。
3. 选择 No Alerts 表示不设置提醒；选择 As Available、Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

四. 反应检索后，设置 Alert



1. 在物质结果集页面点击 Save And Alerts。
2. 输入保存文件的名称。
3. 选择 No Alerts 表示不设置提醒；选择 As Available、Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

如果在保存结果集（Markush 结构，文献，物质或者反应）的过程中未设置 Alert,则可以通过以下方法进行：

The screenshot shows the CAS SciFinder interface. At the top, there is a search bar with 'Reactions' and '610798-31-7' selected. A star icon in the top right corner is highlighted with a blue box labeled '1'. Below the search bar, there is a 'Filter by' section with 'Result Type' and 'Alerts' categories. The 'Alerts' section has three options: 'Unviewed (2)', 'Alerts Set (2)', and 'No Alerts (41)'. A blue box labeled '2' highlights the 'Alerts' dropdown menu. Below the filter section, there are buttons for 'Combine Saved Results' and 'Migrate Alerts & Saved Results'. The main content area shows a '★ Saved (43)' section. The first entry is '具体化合物专利' with a date of 'December 10, 2021, 2:58 PM'. Below it, there is a 'References' section with 'Reference Results from Substances + Filters' and a 'Rerun Search' button. A blue box labeled '3' highlights the 'Frequency' settings, which include 'No Alerts', 'As Available', 'Weekly', and 'Monthly' options.

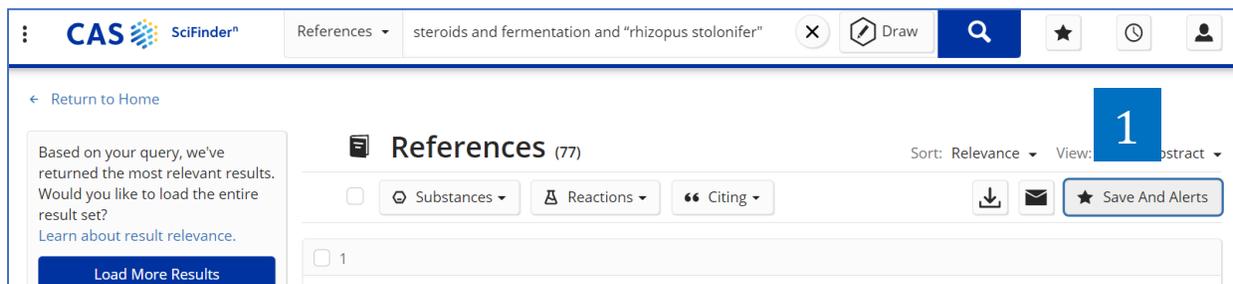
1. 点击 ，查看保存结果集。
2. 点击 ，进行设置。
3. 设置提醒频率。

Alerts 分类选项

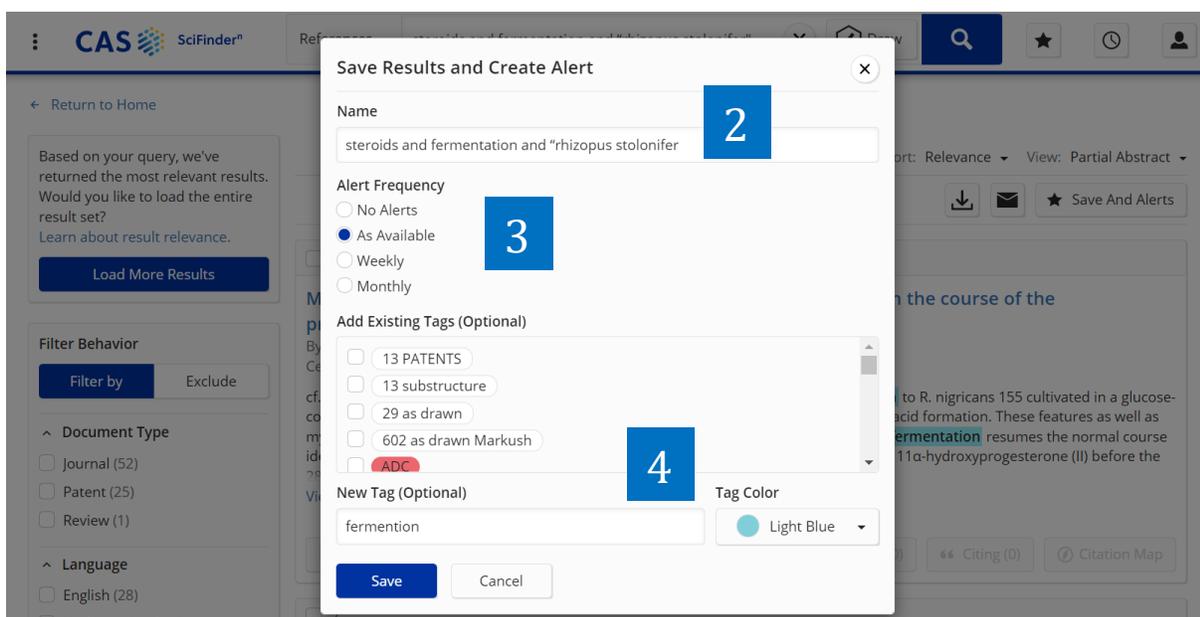
The screenshot shows the CAS SciFinder Alerts interface. The top navigation bar includes the CAS SciFinder logo, a search bar, and icons for Draw, Search, Star, Clock, and User. The main content area is titled '★ Saved (78)'. On the left, there is a 'Filter by' sidebar with sections for Result Type, Alerts, and Tags. The Alerts section is expanded, showing 'Unviewed (78)', 'Alerts Set (108)', and 'No Alerts (291)'. The Alerts section is also expanded, showing 'Alerts', 'Add Tags', and 'target'. The Alerts dropdown menu is open, showing 'Frequency' options: 'No Alerts', 'As Available', 'Weekly', and 'Monthly'. The Results section shows a list of alerts: 'December 31, 2021 (21)', 'December 30, 2021 (59)', and 'December 29, 2021 (55)'. The interface also includes a 'Combine Saved Results' section and a 'medical glove' search result.

1. 点击 ，查看保存的结果集。
2. Alerts 提供三个选项：Unviewed（未被阅读的新增信息），Alerts Set（已设置 Alert），No Alerts（未设置 Alert）。
3. 点击 Alerts 查看新增（更新）的信息。
4. 查看新增（更新）的信息。
5. 更改提醒设置。如：取消提醒(No Alerts)、即时提醒(As Available)、每周提醒(Weekly)或每月(Monthly)提醒。
6. 可以同时浏览多个提醒结果。
7. 可以对提醒结果设置已阅或删除提醒的结果。

最新信息提醒



1. 在检索结果（文献、物质、反应或 Markush）页面，点击右侧 Save And Alerts，保存结果并设置提醒。

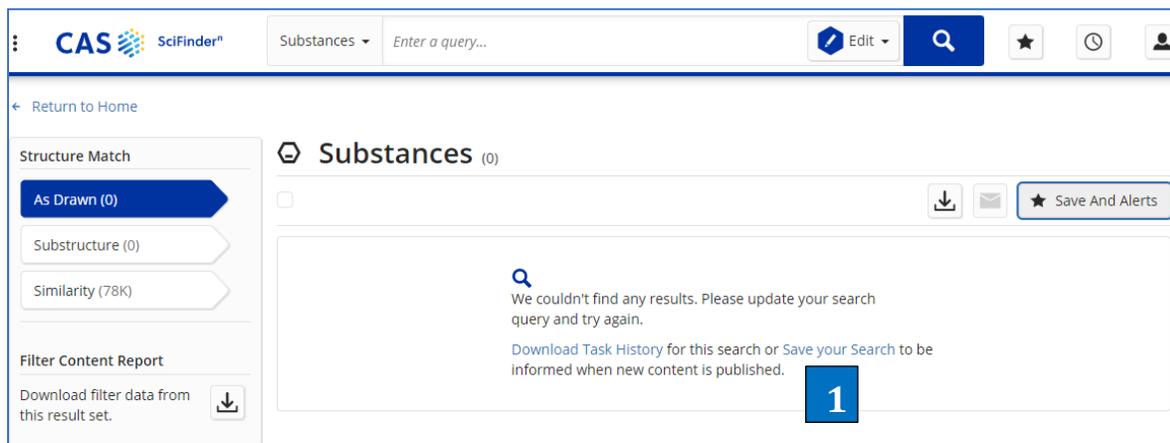


2. 输入本次保存&提醒的文件名。
3. 设置提醒频率：As Available 即时提醒、Weekly 每周提醒、Monthly 每月提醒。
4. 可根据需要标注标签(new tag)，并选择标签颜色(tag color)。

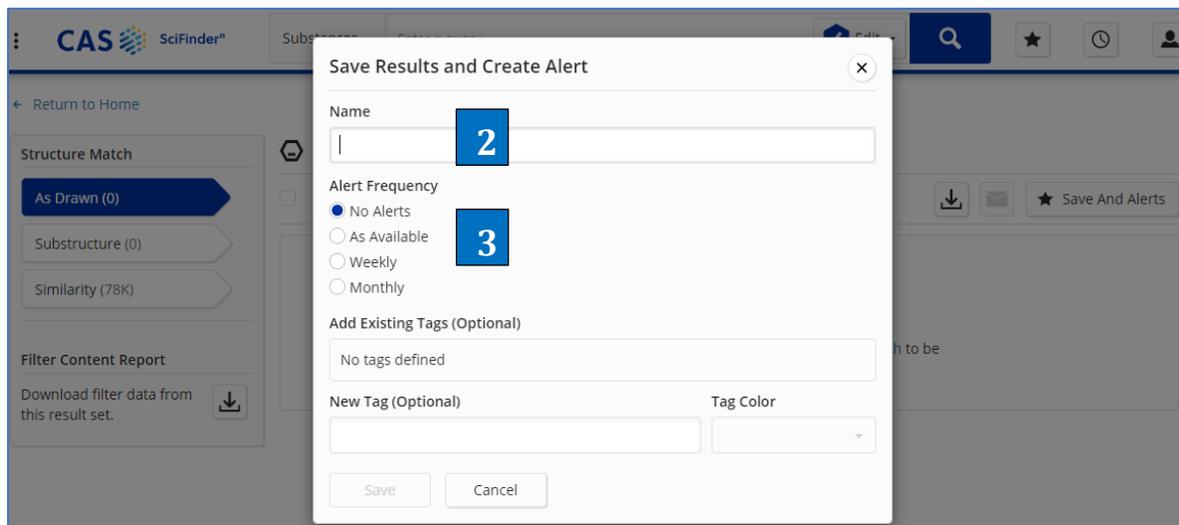
The screenshot displays the CAS SciFinder web interface. At the top, the search bar contains the query "steroids and fermentation and 'rhizopus stolonifer'". The interface is divided into a left sidebar and a main content area. The sidebar, titled "Filter by", includes sections for "Result Type" (Patent Markush, Reactions, References, Retrosynthesis, Substances), "Alerts" (Unviewed, Alerts Set, No Alerts), and "Tags" (13 PATENTS, ADC, patent, Chinese, EOC, 13 substructure, 29 as drawn). The main content area shows a "Saved" folder with 399 items. A search result for "steroids and fermentation and 'rhizopus stolonifer'" is highlighted, showing a timestamp of December 31, 2021, 3:08 PM, a "References" section, and a "fermentation" tag. Below it, a result for "INDOLE" is shown with a timestamp of December 24, 2021, 4:11 PM, a "Reactions" section, and a chemical structure diagram. Blue callout boxes with numbers 5, 6, and 7 are overlaid on the interface to indicate specific actions: 5 points to the search bar, 6 points to the Alerts icon, and 7 points to the Alerts: Unviewed link in the sidebar.

5. 点击保存的文件夹，查看设置提醒的保存项。
6. 当 Alerts 右上角出现叹号图标，表示已有更新的信息但还未被阅读。点击 Alerts，即可呈现更新信息列表，点击相应信息即可查看新信息。
7. 也可通过 Alerts: Unviewed 查看未阅读的提醒信息。

无检索结果时，如何设置 Alerts



1. 当在 CAS SciFinder[®]中检索结果为 0 时，页面将显示“Save your Search”，点击 Save your Search，在弹出页面设置 Alerts。



2. 自定义文件名。
3. 可选择 As Available（有更新即提醒）、Weekly（如有更新，一周提醒一次）或 Monthly（如有更新，一月提醒一次）设置提醒频率。

注：文献，物质，反应检索结果为 0 时，均可采用上述方法设置 Alerts。

在导出的文件中查看检索过程

SciFinder[®] Page 1

CAS SciFinder[®] Task History

Initiating Search 1 December 31, 2021, 3:32PM

References: steroids and fermentation and "rhizopus stolonifer"

Filtered By:

Publication Year: **2020**
Search Within Results: **intermediates**

Search Tasks 2

Task	Search Type	View
Returned Reference Results + Filters	References	View Results 3
Retrieved Related Substance Results + Filters	Substances	View Results
Filtered By:		
Reaction Role: Catalyst		
Reference Role: Occurrence		
Exported: Retrieved Related Reaction Results + Filters	Reactions	View Results
Filtered By:		
Substance Role: Catalyst		

1. Initiating Search 即检索式。
2. 检索过程。
3. 点击 View Results 打开该步操作的结果集页面。

其他

从 CAS SciFinder[®] 链接至其他 CAS 解决方案

The image displays two screenshots of the CAS SciFinder[®] interface. The top screenshot shows the main search page with a '1' in a blue box indicating the first step. The bottom screenshot shows the 'CAS App Switcher' menu with a '2' in a blue box indicating the second step.

Step 1: The main search page shows the 'Substances' search interface. A blue box with the number '1' is positioned over the top left corner of the page, near the CAS SciFinder[®] logo and navigation icons.

Step 2: The 'CAS App Switcher' menu is shown on the left side of the page. A blue box with the number '2' is positioned over the menu items. The menu includes the following options: CAS SciFinder[®], CAS Analytical Methods, CAS Formulus, STN IP PROTECTION SUITE, STNext, CAS Scientific Patent Explorer, REGULATORY, CAS Chemical Compliance Index, ACCOUNT MANAGEMENT, and CAS Profile.

1. 点击检索页面左上角三个点，打开 CAS App Switcher。
2. 授权用户选择任一选项，即可链接至相应平台：SciFinder Discovery Platform（除了 CAS SciFinder[®] 外，还包括 CAS Analytical Methods 和 CAS Formulus）、STN IP Suite（包括 STNext 和 CAS Scientific Patent Explorer）、CAS Chemical Compliance Index，并可以通过 CAS Profile 进行账号管理等。