

CAS SCIFINDERⁿ

使用技巧手册

2022 年 1 月



CAS SciFinderⁿ是美国化学文摘社（CAS）出品的新一代的权威科学的研究工具，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 SciFinderⁿ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 SciFinderⁿ 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 SciFinderⁿ 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 SciFinderⁿ 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 SciFinderⁿ 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 SciFinderⁿ 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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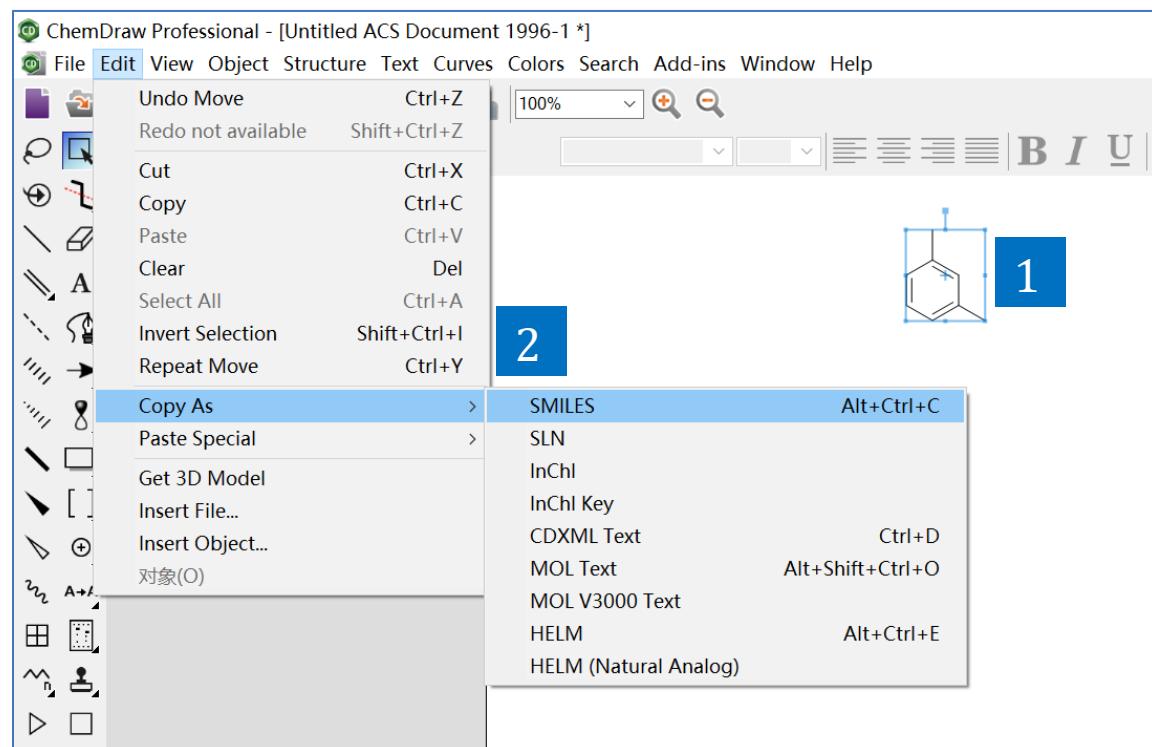
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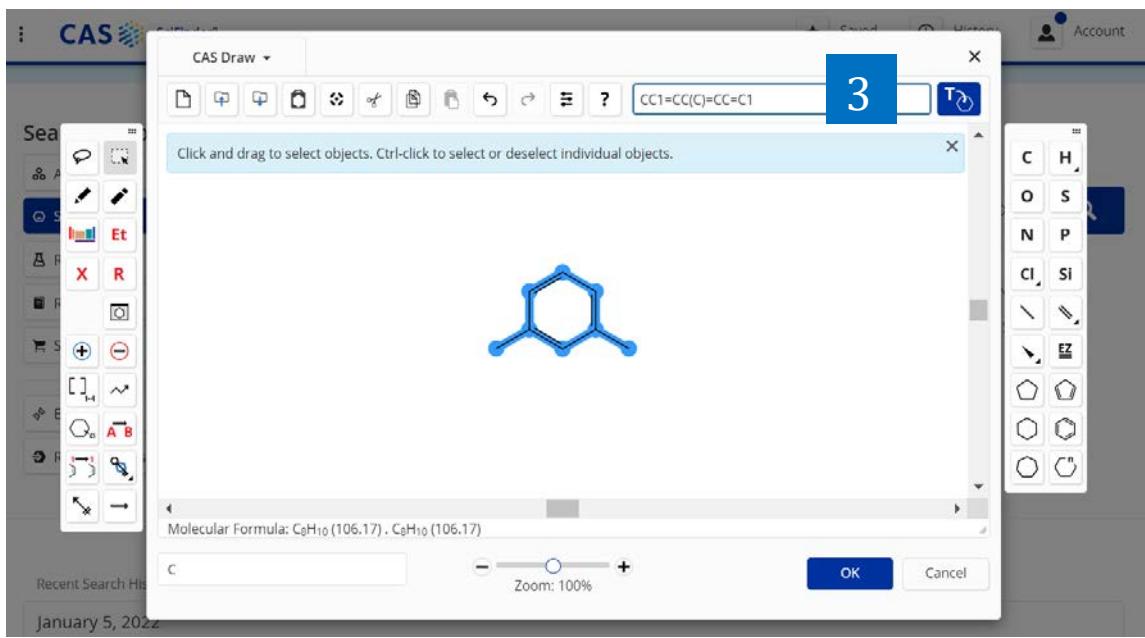
物质检索

与 ChemDraw 联用

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

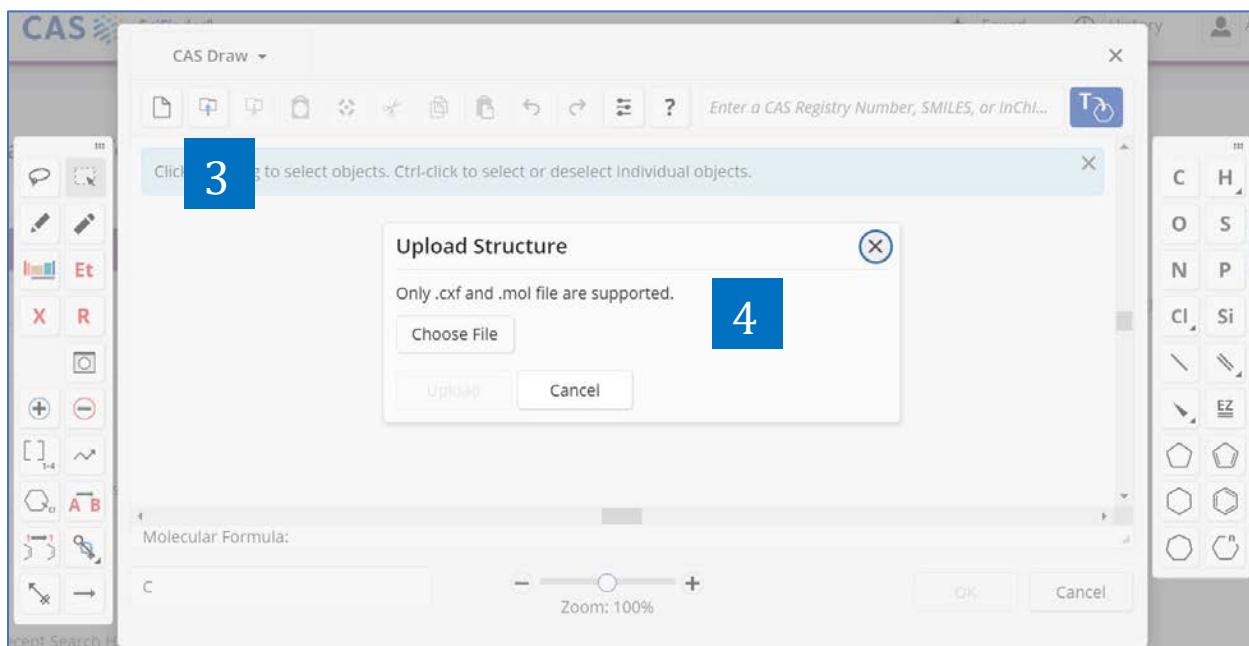
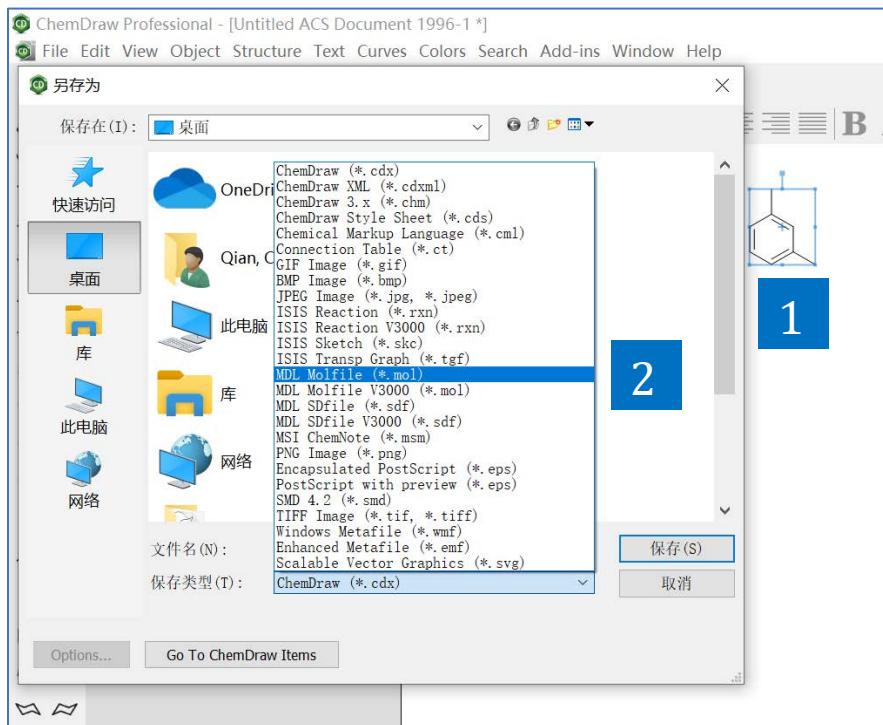
一. 利用在 ChemDraw 中获得的物质 SMILES、InChI，将结构导入到 CAS SciFinderⁿ 的结构编辑器中：





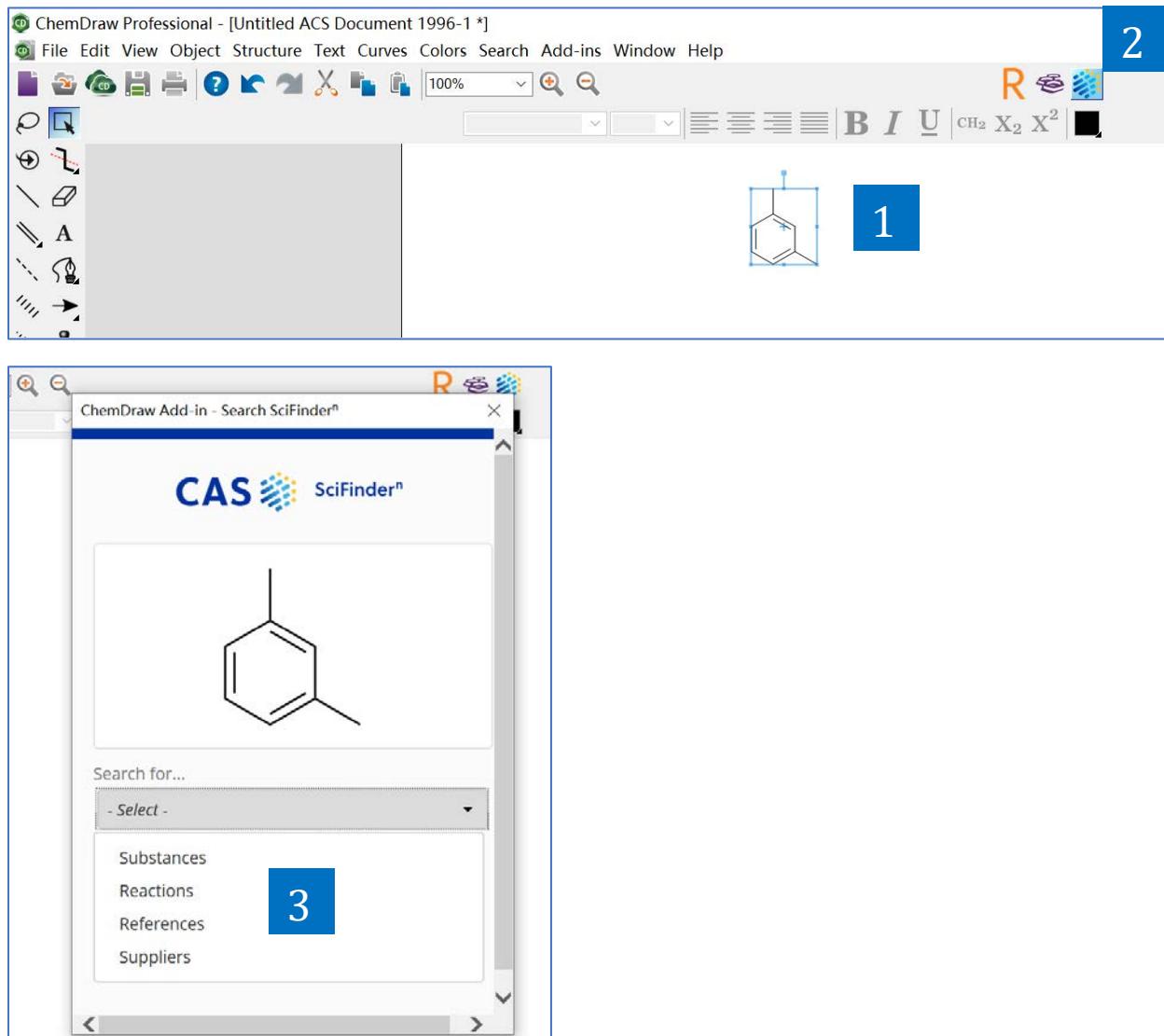
1. 在 ChemDraw 中绘制好结构，并选中。
2. 点击上方菜单 Edit，选择 Copy As，然后再选择 SMILES 或 InChI。
3. 在此粘贴在 ChemDraw 中获得的 SMILES 或 InChI，将结构导入到 CAS SciFinderⁿ 的结构编辑器中。

- 二. 将 ChemDraw 中绘制的结构保存为.mol 格式文件，然后再导入到 CAS SciFinderⁿ 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。

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

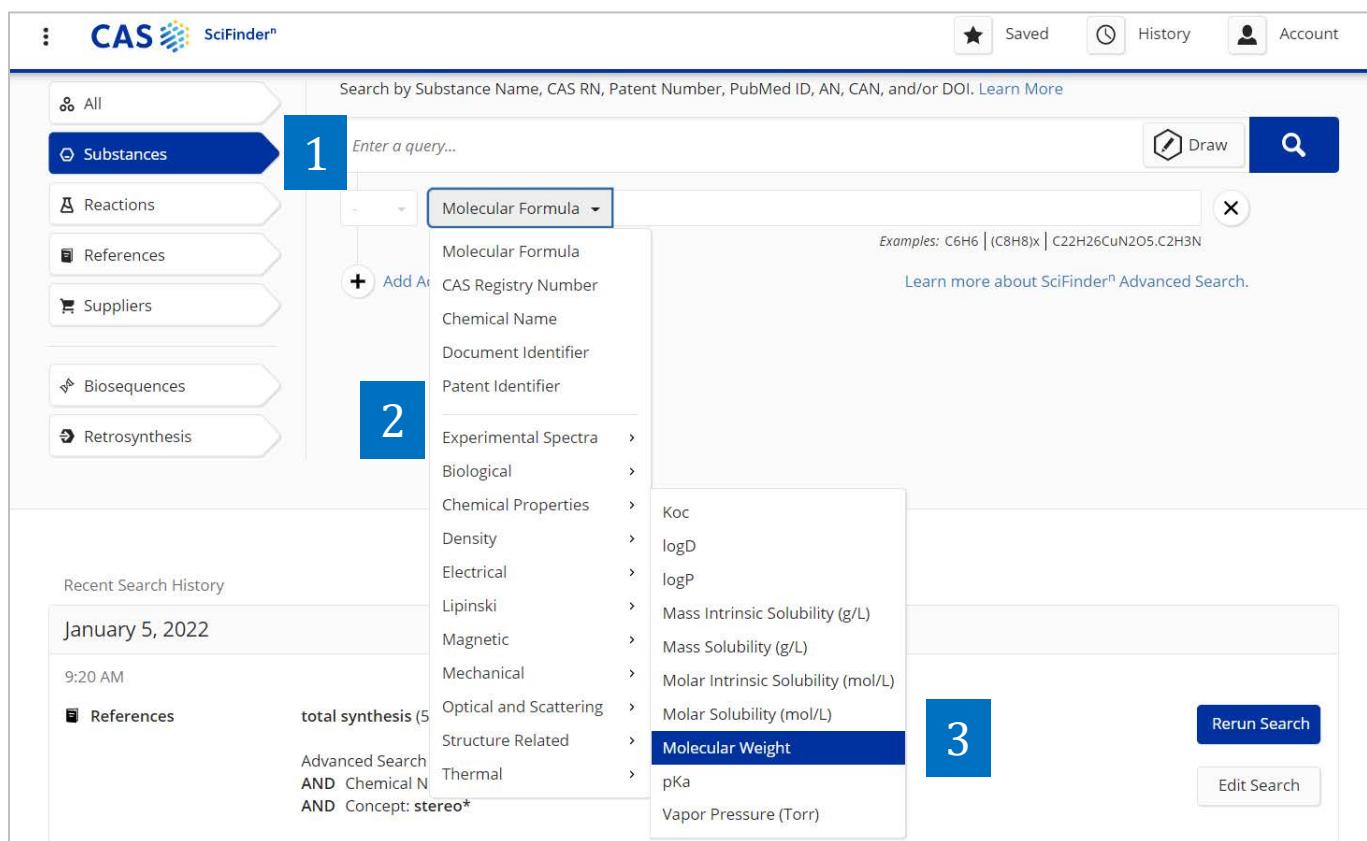


1. 绘制结构并选中。

2. 点击 

3. 选择检索类型，在 CAS SciFinderⁿ 中检索 Chemdraw 中绘制的结构。

通过质谱-核磁图联用助力物质结构解析



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 7

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... 4

Molecular Weight ▾ 272.38

Predicted values only.

AND ▾ 5 Carbon-13 NMR ▾ 155.02, 127 to 129

Allowance of ± 2 ppm.

Draw

Search

Examples: 46.07 | 125 to 350 | >300

6 Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187

Add Advanced Search Field

Learn more about SciFinderⁿ Advanced Search.

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

CAS SciFinderⁿ

Substances ▾ Edit Search Enter a query... 8

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)

Stereochemistry

Number of Components

Substance Class

Substances (6)

Sort: Relevance ▾ View: Partial ▾

1 221255-16-9 9 Double bond geometry shown C₁₈H₂₄O₂ (2Z,4E,6E,8E)-8-[(2E)-2-Ethylidene)cyclohexylidene]-3,7-dimethyl-2,4,6-octatrieno... Reference 147K Reactions 955 Suppliers 132

2 50-28-2 Absolute stereochemistry shown C₁₈H₂₄O₂ Estradiol 147K References 955 Reactions 132 Suppliers

3 221315-96-4 Double bond geometry shown C₁₈H₂₄O₂ (2E,4E,6E,8E)-8-[(2E)-2-Ethylidene)cyclohexylidene]-3,7-dimethyl-2,4,6-octatrieno... Reference 1 Reactions 0 Suppliers

4 57-91-0 Absolute stereochemistry shown C₁₈H₂₄O₂ Double bond geometry shown Reference 147K Reactions 955 Suppliers 132

5 221255-12-5 Double bond geometry shown C₁₈H₂₄O₂ Reference 147K Reactions 955 Suppliers 132

6 221315-95-3 Double bond geometry shown C₁₈H₂₄O₂ Reference 147K Reactions 955 Suppliers 132

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

The screenshot shows the CAS SciFinder Substance Detail page for substance 221255-16-9. The chemical structure is displayed, showing a cyclohexene ring substituted with a long chain containing multiple double bonds and methyl groups. The structure is labeled with '(E)' and '(Z)' indicating double bond geometry. Below the structure, it says 'Double bond geometry shown'. The key physical properties table includes:

Key Physical Properties	Value	Condition
Molecular Weight	10	-
Boiling Point (Predicted)	272.38	Press: 760 Torr
Density (Predicted)	457.2±14.0 °C	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	1.098±0.06 g/cm³	Most Acidic Temp: 25 °C
Spectra		

10. 查看物质分子量

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

▼ 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

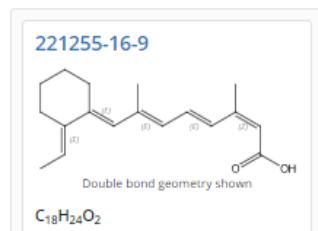
12. 点击超链接，查看核磁谱图

13. 谱图信息的文献来源

14. 缩放谱图

Carbon-13 NMR Spectrum Detail (1 of 1)

15



CAS Name
(2Z,4E,6E,8E)-8-[(2E)-2-Ethylidenecyclohexylidene]-3,7-dimethyl-2,4,6-octatrienoic acid

Conditions

Working Frequency
100 MHz

Solvent
[Chloroform-d \(865-49-6\)](#)

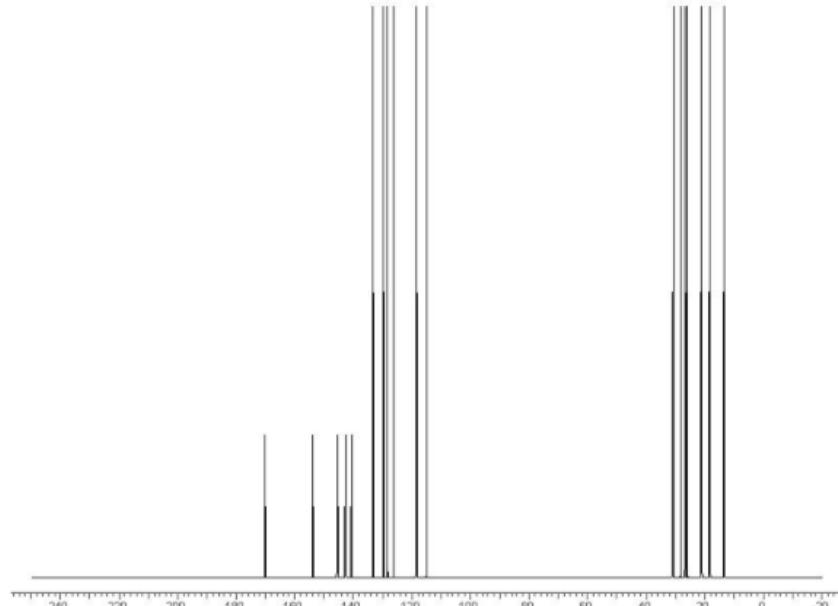
Temperature
27 °C

Spectrum Summary

Spectrum ID
12DIF_J_108.C

Peak Data
170.21, 153.87, 145.46, 142.61,
140.54, 133.27, 129.74, 128.36,
126.34, 118.5, 115.05, 30.81, 28.23,
26.69, 25.98, 21.21, 18.32, 13.33
ppm

Source
Spectral data were obtained from
Advanced Chemistry Development,
Inc.



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

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

Substance Detail (4 of 13)

CAS Registry Number
1186600-57-6

Chemical Structure:

Absolute stereochemistry shown

Key Physical Properties

Property	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

Hormone antagonists
Antiprogesterins (1)
Reproductive control agents
Contraceptives (1)

Target Indicators

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

The screenshot shows the CAS SciFinder search interface. Step 1 highlights the 'Substances' button in the sidebar. Step 2 highlights the search input field. Step 3 highlights the 'Draw' button. Step 4 highlights the 'Add Advanced Search' button. Step 5 highlights the search results area.

1 Substances

2 Enter a query... **3**

4 Add Advanced Search **5**

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

1 CAS SciFinder® Substances Enter a query... Edit

← 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 3 Filter Behavior Filter by Exclude ▾ Commercial Availability

Substances (16) Sort: Number of References: Descending View: Partial 4 5 6 7

1 610798-31-7 8 C₂₂H₂₁N₃O₄ Icotinib 573 References 133 Reactions 40 Suppliers

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.... 61 References 13 Reactions 39 Suppliers

3 1567366-94-2 C₂₂H₁₆D₅N₃O₄ N-[3-(Ethyne-2-d)phenyl]-7,8,10,11,13,14-hexahydro-10,11-d₂[1,4,7,10]tetraoxacy... 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.

9 1567366-93-1 C₂₂H₈D₁₃N₃O₄ N-[3-(Ethyne-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-(Ethyne-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-(Ethyne-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 C₂₂H₂₁N₃O₄ Icotinib 2 References 19 Reactions 0 Suppliers

8 1567366-82-8 C₂₂H₂₁N₃O₄ Icotinib 2 References 19 Reactions 0 Suppliers

9 1567366-75-9 C₂₂H₂₁N₃O₄ Icotinib 2 References 2 Reactions 0 Suppliers

- 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)

1

2

3

CAS Registry Number
610798-31-7

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

Download Email Save

O=Cc1ccc(cc1)Nc2nc3cc(OCCO)c(OCCO)c3n2

Feedback



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



Key Physical Properties	Value	Condition	4
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

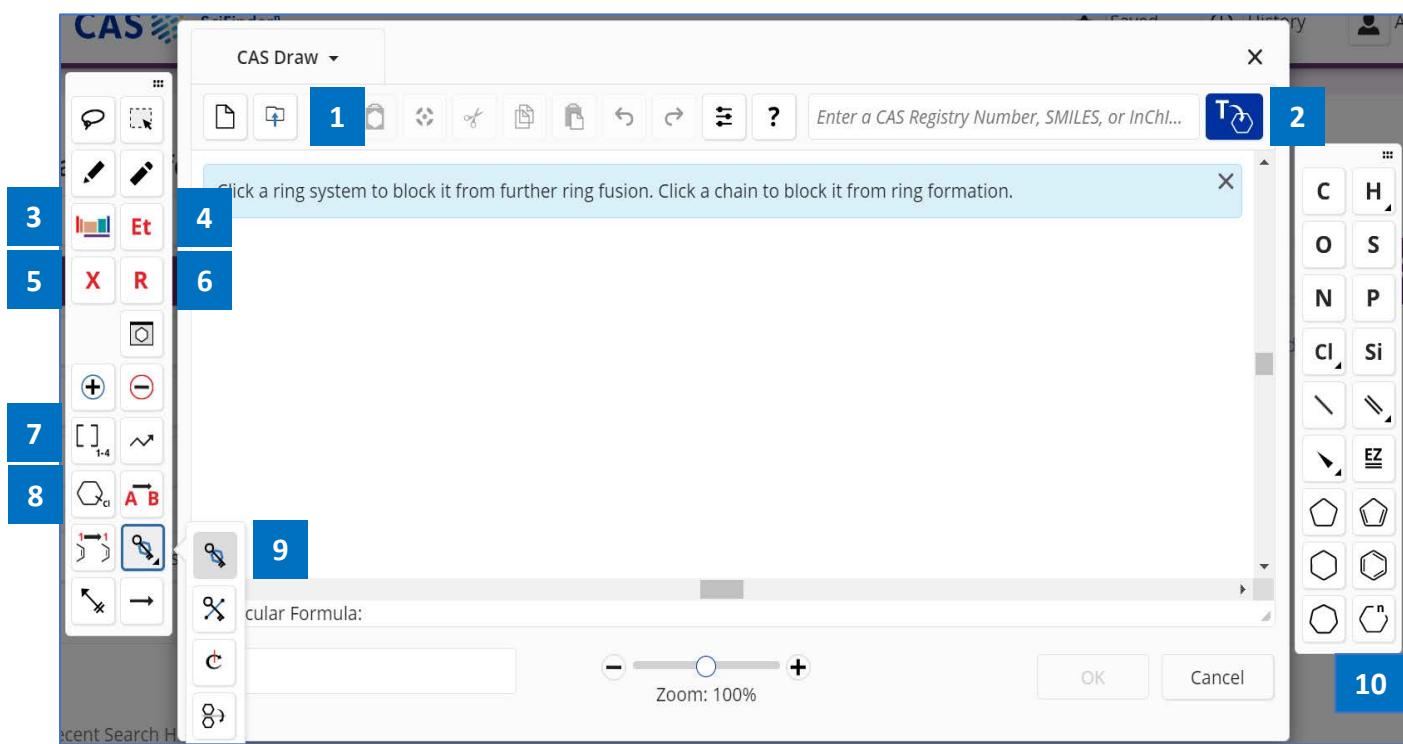
5



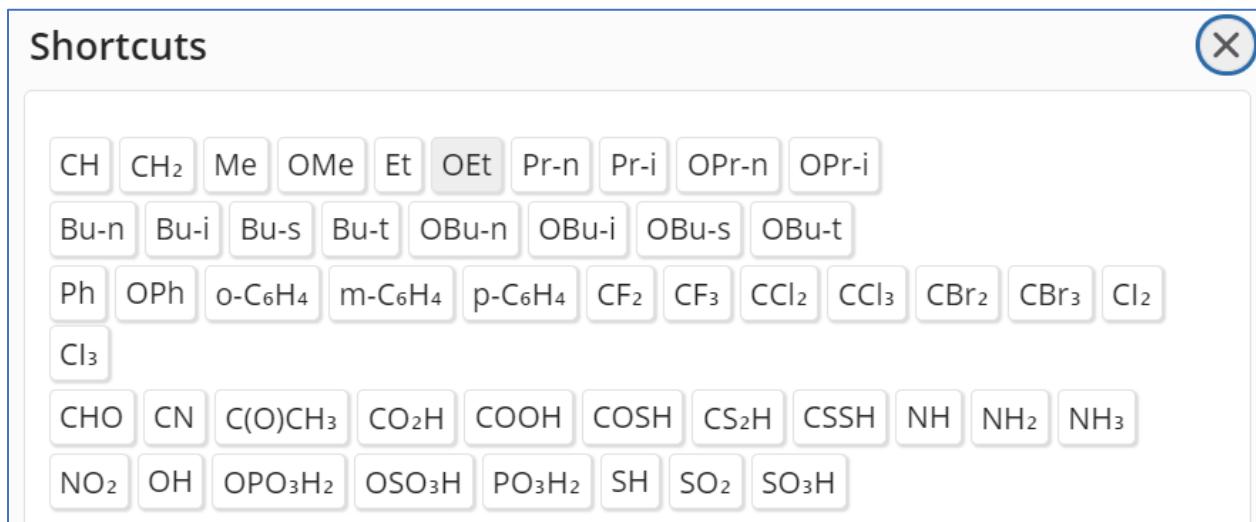
Feedback

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。

Variables X

- 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。

R-Group Definitions X

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10 R11 R12 >

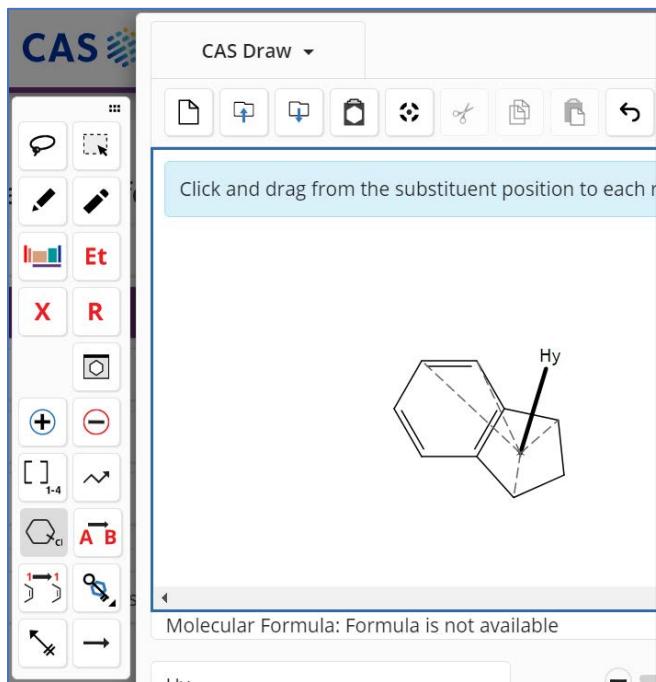
R1:

> Atoms

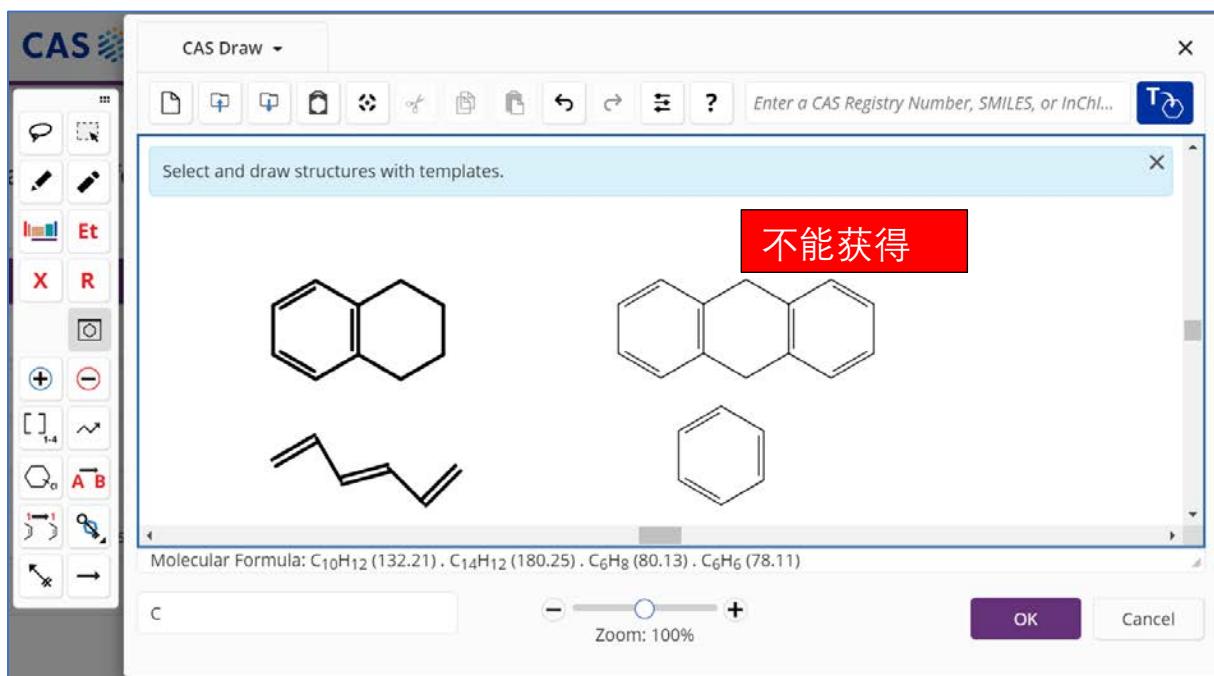
> Variables

> Shortcuts

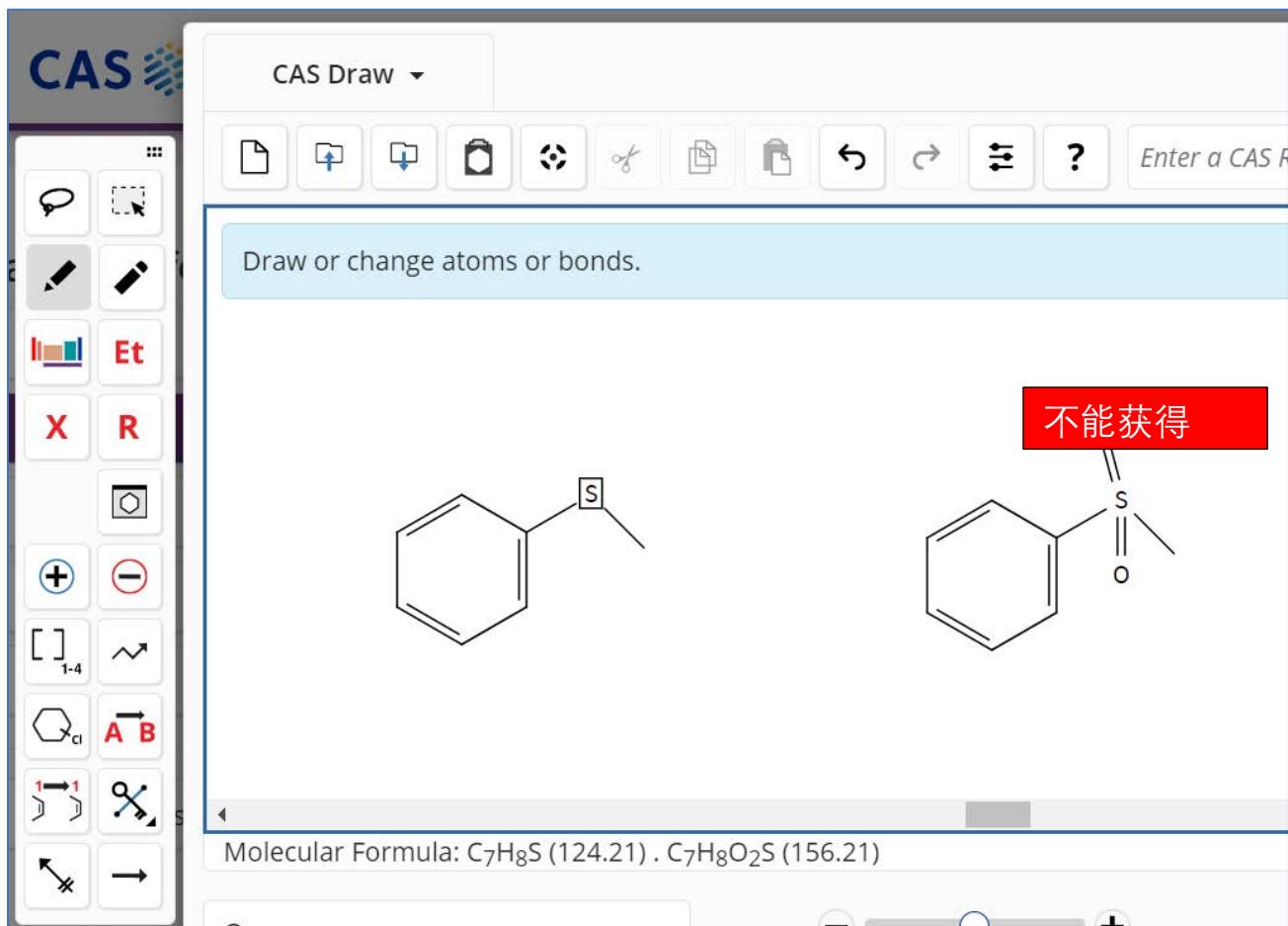
7. 重复原子或者基团。
8. 环上的取代位点不固定。

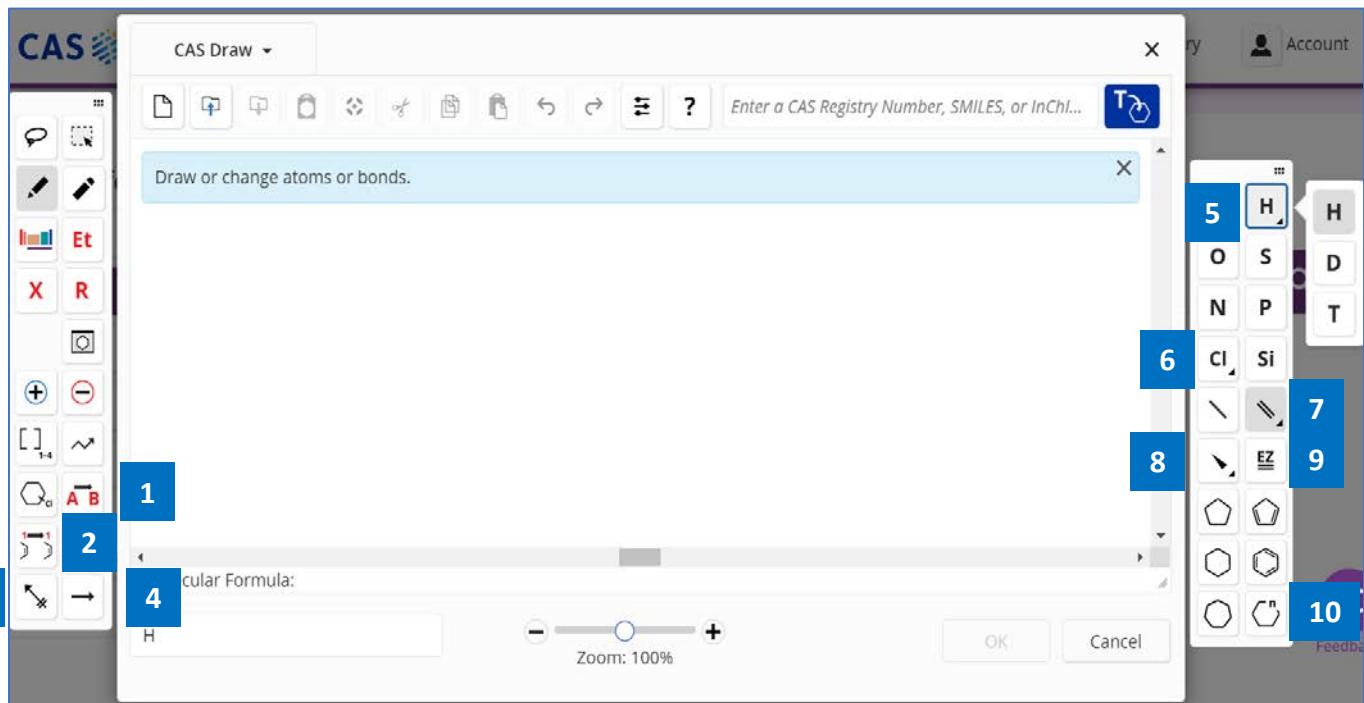


9. 环锁定。当用该功能锁定某个环（系），表示该环（系）不能成为更大环系的一部分；如果用该功能锁定某个链，则表示该链不能成为某个环（系）的一部分。例：

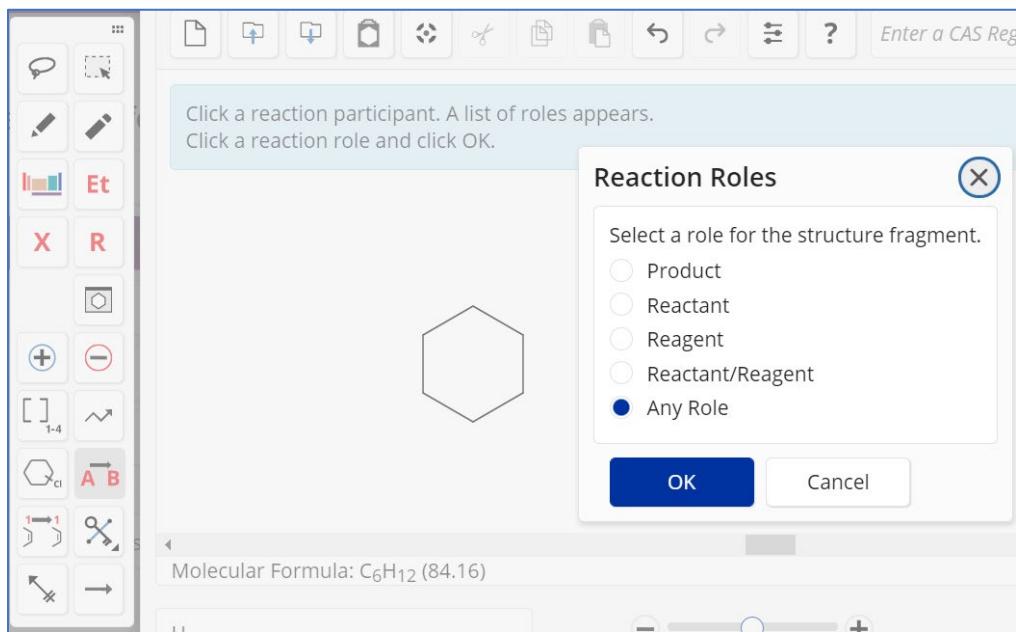


10. 锁定原子。若某原子被锁定，则表明该原子只能连接氢原子。例：





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 shows the CAS SciFinder search interface for substances. The left sidebar lists recent search history and navigation links for All, Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main search area has a query input field 'Enter a query...', a dropdown for 'Molecular Formula', and a 'Select' dropdown currently set to 'AND'. A 'Draw' button is available for drawing structures. The search results panel on the right displays a chemical structure of pyridine.

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 SciFinder search interface. On the left, there's a sidebar with categories: All (highlighted), Substances (selected, highlighted in blue), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main search area has a title 'Substances' and a subtitle 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More'. It includes a search bar 'Enter a query...', a molecular weight filter 'Molecular Weight 125 to 349' (with a dropdown menu 'Predicted values only.'), a carbon-13 NMR filter 'Carbon-13 NMR 115,141' (with a dropdown menu 'Allowance of ± 2 ppm.'), and an 'Add Advanced Search Field' button. To the right, there's a chemical structure of pyridine (highlighted with a blue box labeled 7) with options to 'Edit Drawing' or 'Remove'. A search button '8' is located at the top right. Other buttons include 'Edit', 'Feedback', and 'Search Patent Markush'.

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 SciFindern 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 SciFinderⁿ 帮助，请联系 china@acs-i.org, 010-63508026/7

CAS SciFinder® Substances Edit Search poly*

Return to Home

Filter Behavior

Filter by Exclude

Sort: Relevance View: Partial

Commercial Availability

Available (98) Not Available (10)

Reaction Role

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

Reference Role

Preparation (108)

Substances (108)

References Reactions Suppliers

1 25248-42-4 1

$(C_6H_{10}O_2)_n$

Polycaprolactone

38K References 3,262 Reactions 6 Suppliers

2 9003-39-8

$(C_6H_9NO)_x$

Poly(vinylpyrrolidone)

152K References 5,885 Reactions 192 Suppliers

3 25322-68-3

$(C_2H_4O)_nH_2O$

Poly(ethylene glycol)

398K References 54K Reactions 565 Suppliers

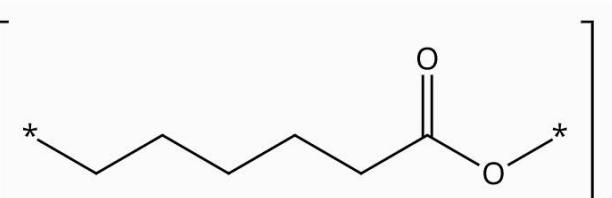
Feedback

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)

CAS Registry Number
25248-42-4



$(C_6H_{10}O_2)_n$

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

Polymer Class Terms
Polyester

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

2 Experimental Properties

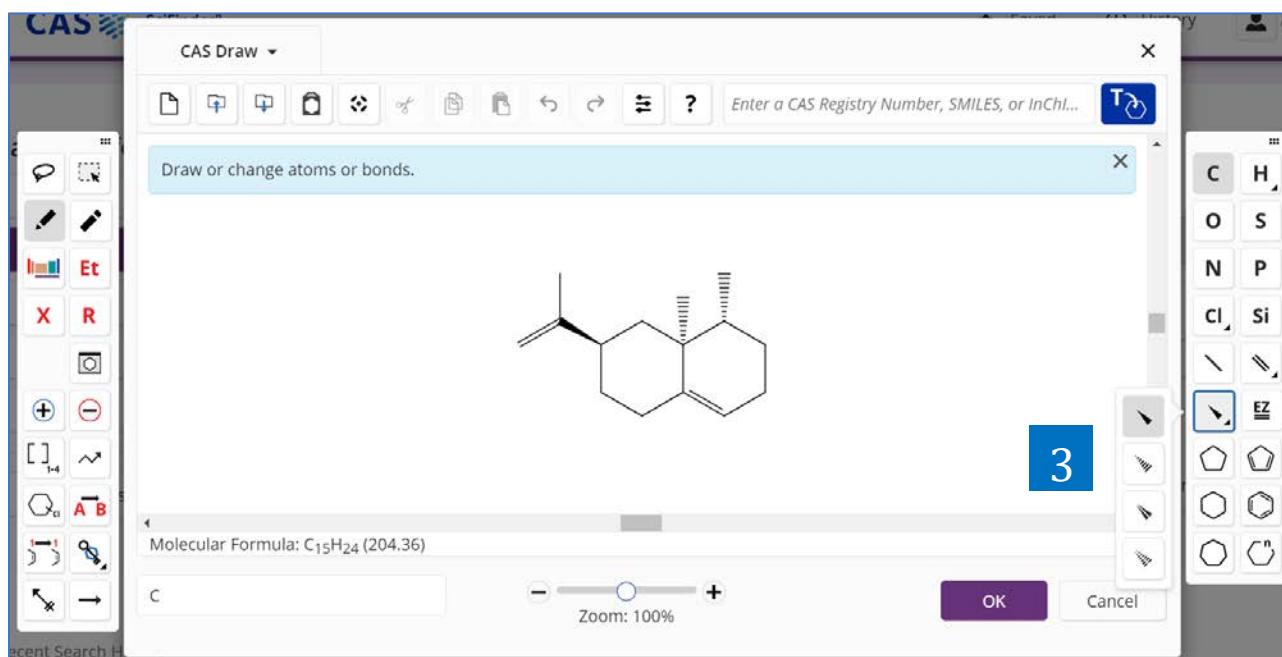
Biological	Chemical	Density	Electrical	Flow and Diffusion	Interface	Mechanical	Optical and Scattering	Structure Related	Thermal
3									
Property					Value		Condition	Source	
Glass Transition Temperature					63.6 °C		-	(1) CAS	
Glass Transition Temperature					62.8 °C		-	(1) CAS	
Glass Transition Temperature					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/cm^3 。
 3. 该聚合物的玻璃体转化温度。

手性化合物的检索

The screenshot shows the SciFinder interface. At the top, there is a navigation bar with the CAS logo, 'SciFinder®', and links for 'Saved', 'History', and 'Account'. Below the navigation bar, a banner for 'CAS Analytical Methods®' is displayed, followed by a search bar labeled 'Substances' and a search button. To the left of the search bar is a sidebar with various search categories: 'All', 'Substances' (which is highlighted with a blue arrow and the number '1'), 'Reactions', 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'. To the right of the search bar is a 'Draw' button and a magnifying glass icon. A large blue box labeled '2' is overlaid on the search bar area.

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。



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 shows the CAS SciFinder interface with the following details:

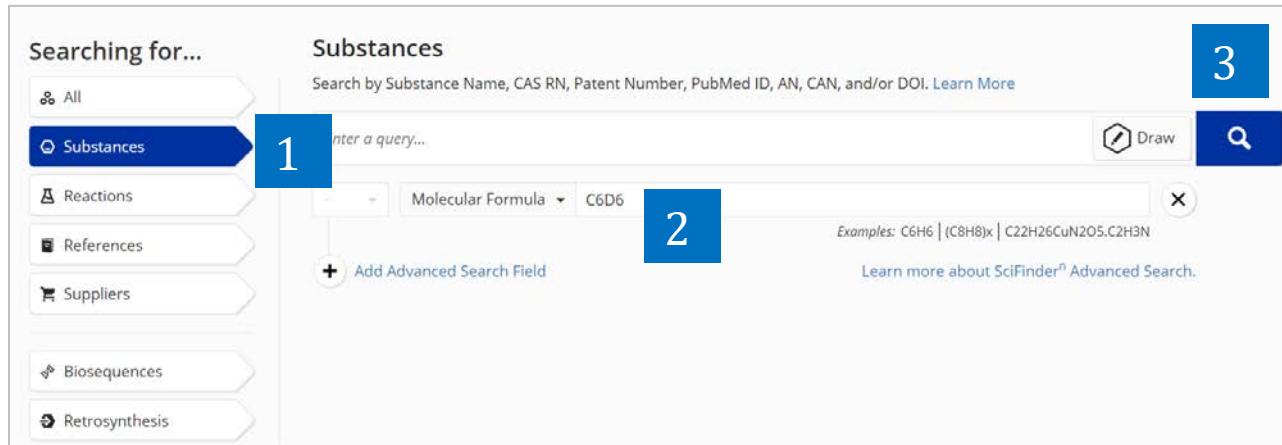
- Left Sidebar:**
 - Structure Match:**
 - As Drawn (22)** (highlighted in blue)
 - Substructure (5,432)
 - Similarity (22K)
 - Analyze Structure Precision
 - Chemscape Analysis:**
 - Visually explore structure similarity with a powerful new tool.
 - Learn more about Chemscape.
 - Create Chemscape Analysis**
 - Filter Behavior:**
 - Absolute Stereo Match (11)** (highlighted with a blue checkmark)
 - Absolute Stereo Mirror Image (1)
 - Relative Stereo Match (1)
 - Stereo that Doesn't Match Query (8)
 - No Stereo in Answer Structure (1)
- Top Bar:** Substances, Enter a query..., Edit, Search, Favorites, Help.
- Results Area:**
 - Substances (11)**
 - Filtering: Stereochemistry: Absolute Stereo Match
 - Relevance View: Partial
 - Buttons: Edit Drawing, Remove, Save And Alerts, Clear All Filters.
 - Search Patent Markush
 - Results:
 - 4630-07-3**: Valencene, C₁₅H₂₄, Absolute stereochemistry shown, Rotation (+).
 - 1174496-34-4**: (1*R*,7*R*,8*aS*)-1,2,3,5,6,7,8,8*a*-Octahydro-1,8*a*-dimethyl-7-[1-(methyl-*d*₃)ethenyl]-2,2...
 - 2279054-76-9**: (C₁₅H₂₄-C₃H₃N)_x, Components: 2
 - 225114-69-2**: (1*R*,7*R*,8*aS*)-1,2,3,5,6,7,8,8*a*-Octahydro-1,8*a*-dimethyl-7-[1-(methyl-*d*₃)ethenyl]-2,2...
 - 2374919-94-3**: 9012-76-4, Image Not Available.
 - 2279054-69-0**: (1*R*,7*R*,8*aS*)-1,2,3,5,6,7,8,8*a*-Octahydro-1,8*a*-dimethyl-7-[1-(methyl-*d*₃)ethenyl]-2,2...

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）。

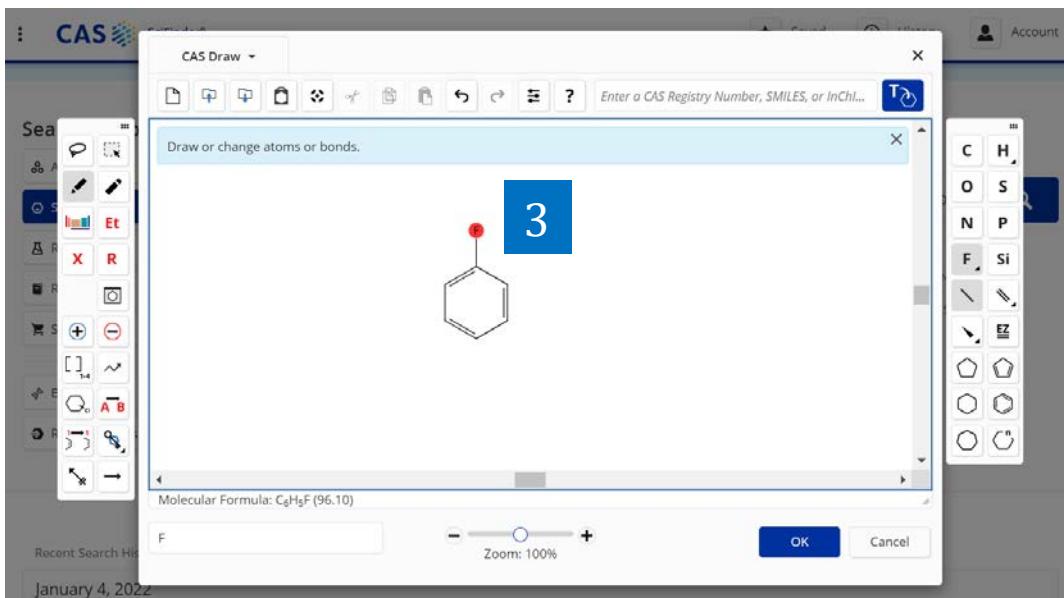


1. 点击 Substances
2. 点击 Add Advanced Search Field, 选择 Molecular Formula, 然后输入分子式（如可直接输入 H 的同位素 D 或 T）。
3. 开始检索

The screenshot shows the CAS SciFinder interface with the search bar set to "Substances". The left sidebar is expanded to show the "Isotopes" filter selected under "Filter Behavior". The main area displays a grid of substance cards. Each card includes a checkbox, the substance's name, its structure, and its CAS Registry Number. Below each name is a blue box indicating its isotope type, such as "C₆D₆". Each card also shows the number of references, reactions, and suppliers available.

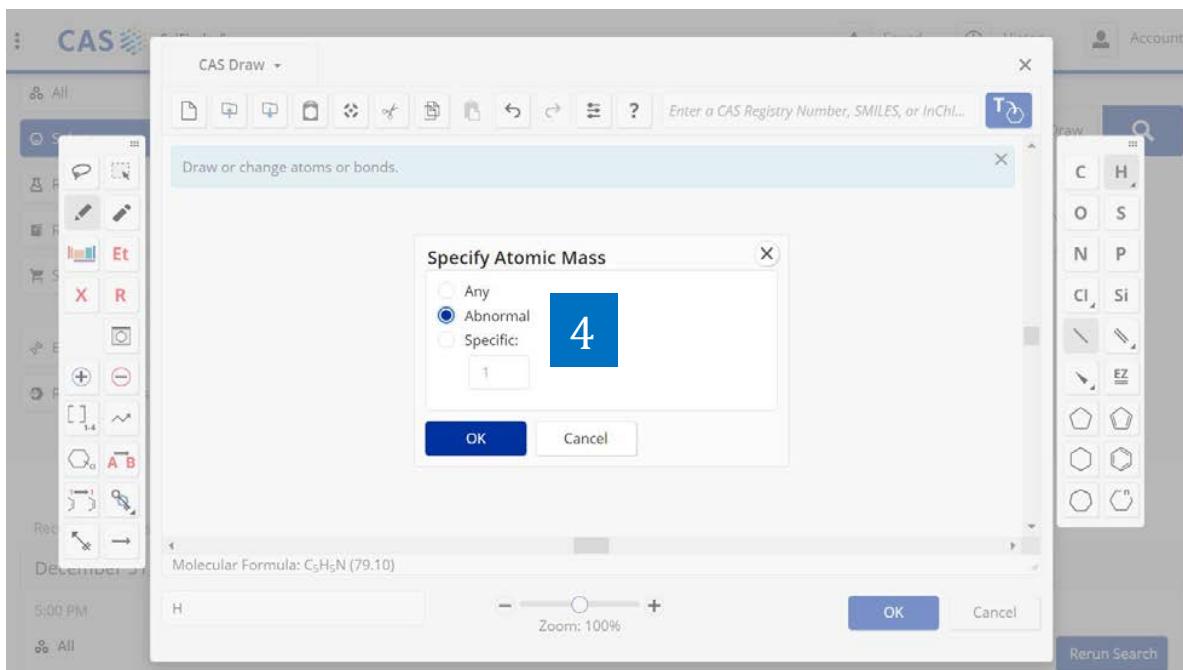
Card Number	Substance Name	Isotope Type	References	Reactions	Suppliers
1	1076-43-3	C ₆ D ₆	3,043	33K	127
2	38091-14-4	C ₆ D ₆	45	0	0
3	32602-97-4	C ₆ D ₆	9	0	5
4	34525-57-0	C ₆ D ₆			
5	73113-25-4	C ₆ D ₆			
6	55153-53-2	C ₆ D ₆			

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）。

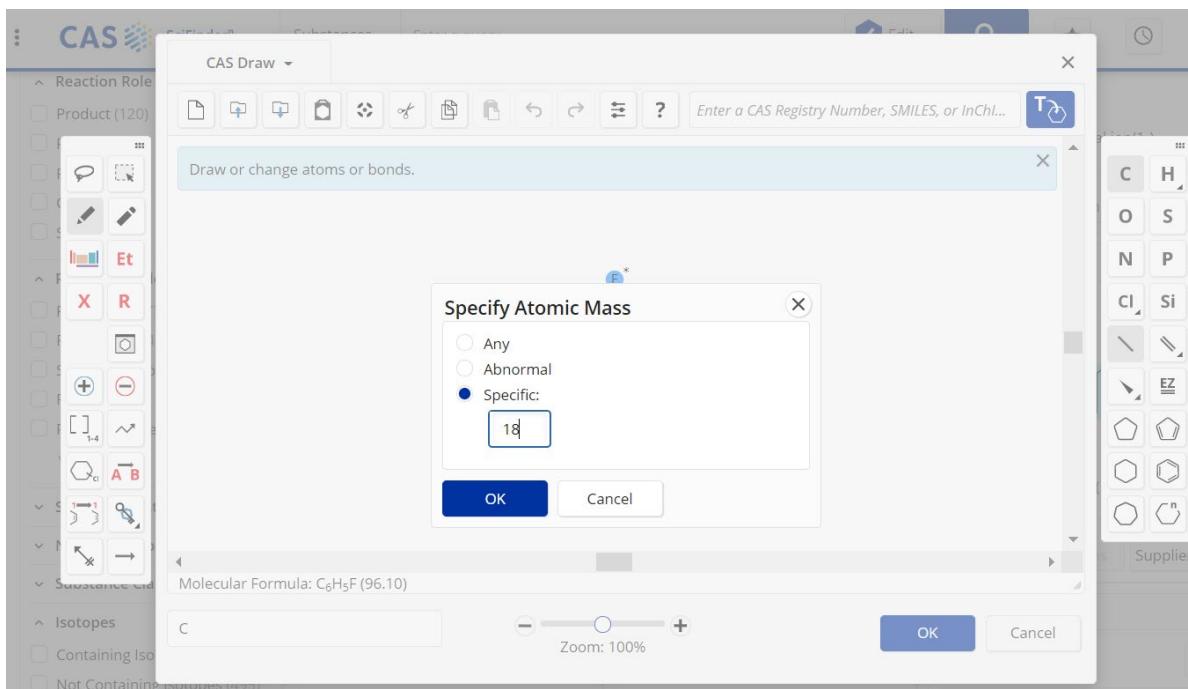


3. 鼠标悬在绘制结构中的原子上（例如 F），点击鼠标右键。

如需更多 CAS SciFinderⁿ 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... Edit ▾

AND Molecular Formula

Examples: C6H6 | (C8H8)x | C...

Learn more about Sci

Edit Drawing Remove

Search Patent Markush

5

5. 开始检索，获取感兴趣的结果。

CAS SciFinderⁿ Substances Edit ▾

[← 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

C₆H₅F
Fluoro-¹⁸Fbenzene

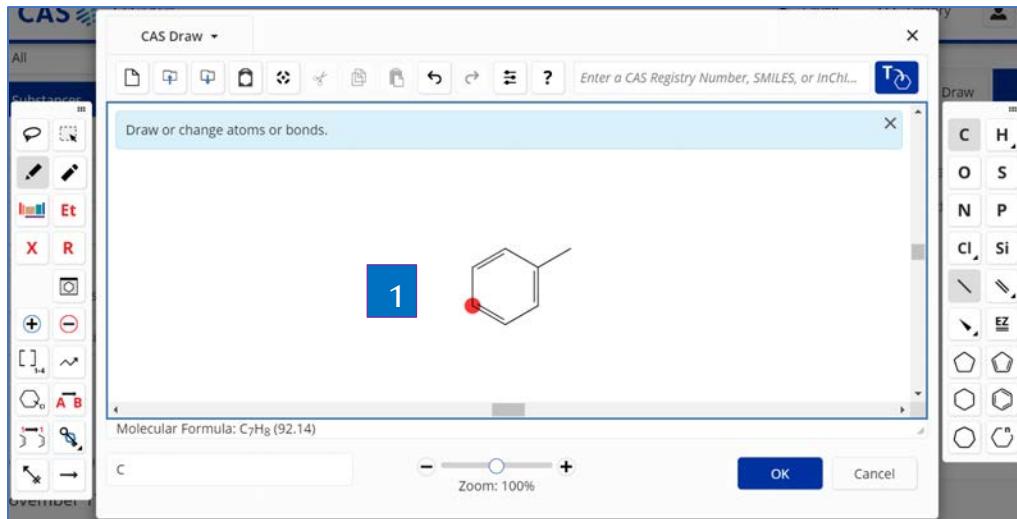
68 References 190 Reactions 1 Supplier

View: Partial Edit Drawing Remove Save And Alerts

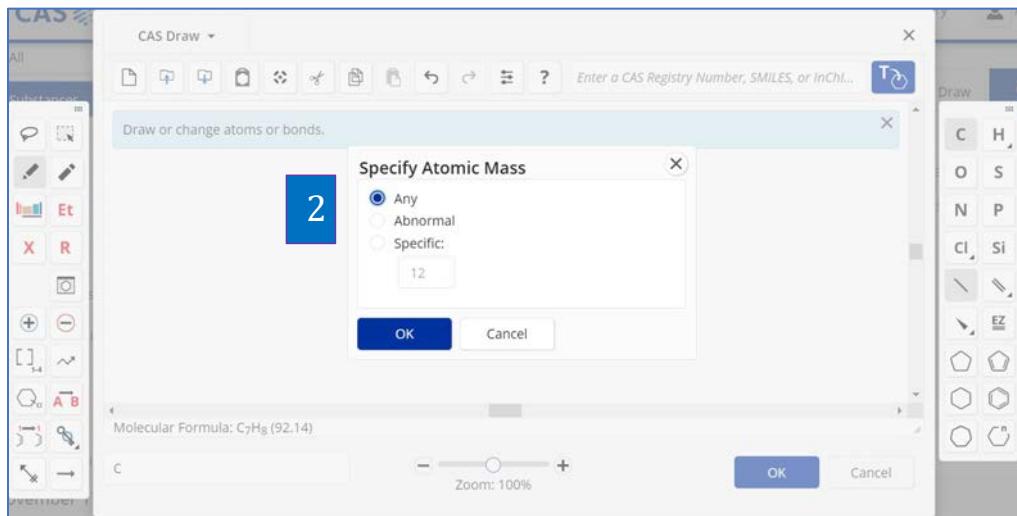
Search Patent Markush

绘制结构式时，如何绘制同位素

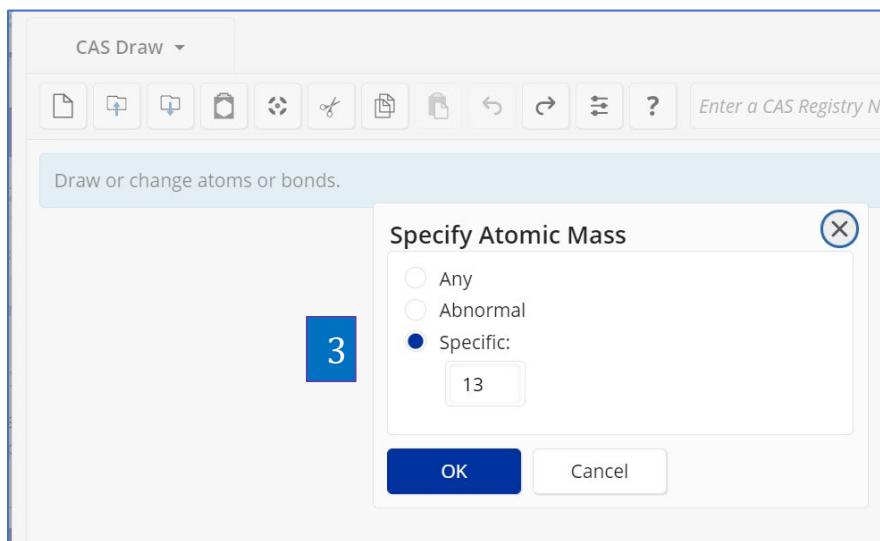
绘制结构时，可绘制特定原子的同位素，以获取其同位素标记的物质、同位素标记的物质参与的反应、研究同位素标记的物质的文献等信息。



1. 绘制结构，选中需要标记同位素的原子，点击鼠标右键。



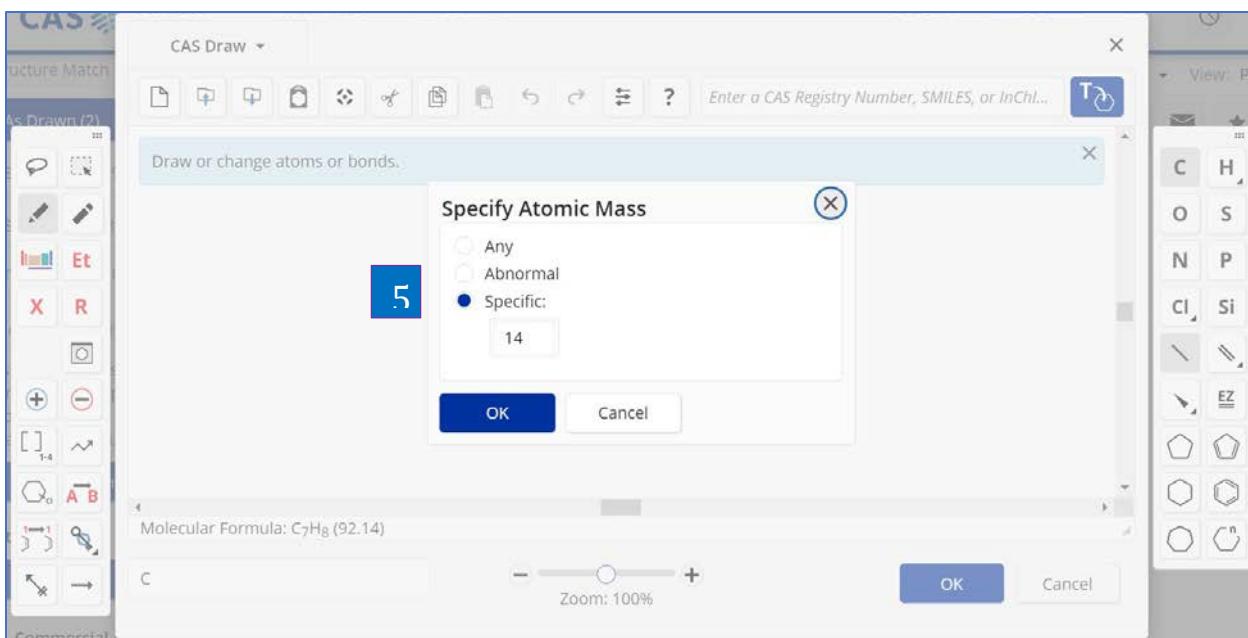
2. 在弹出窗口中，选择原子量为 Any（默认值，任意元素）、Abnormal（任意同位素）或 Specific（特定同位素）。



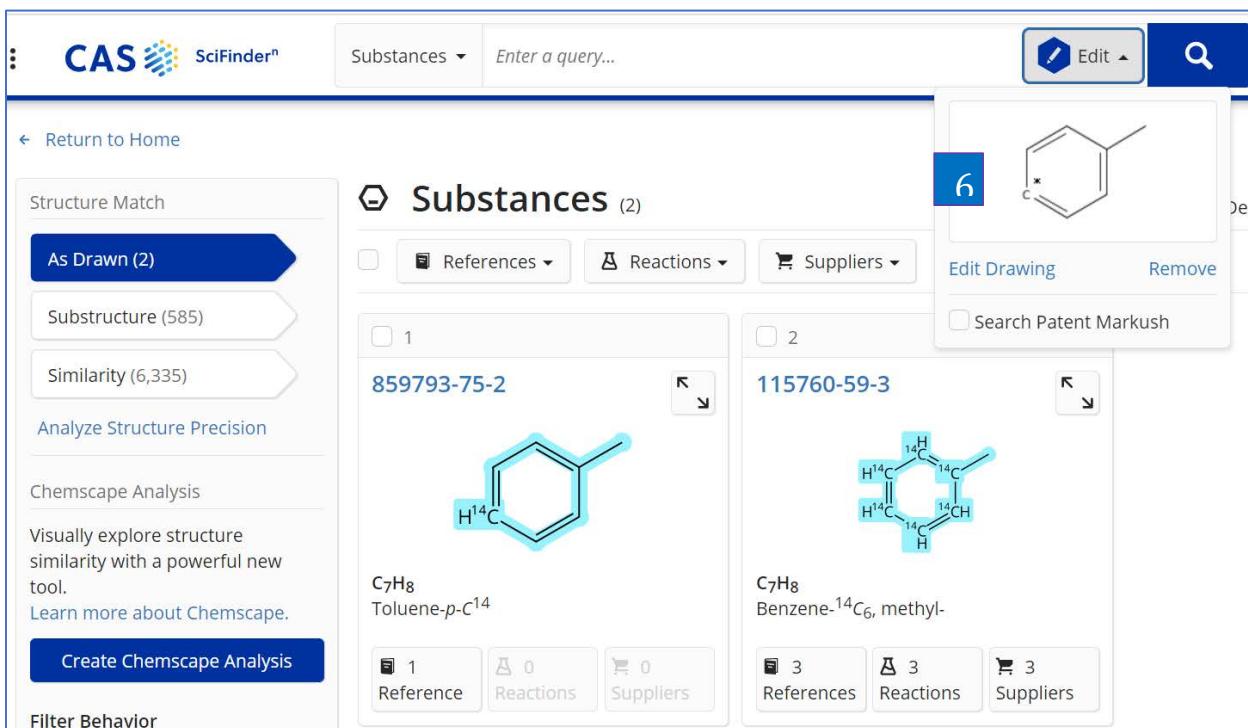
3. 选择 Specific，并输入数值 13，表面此处的碳原子为 ^{13}C 。

Result	Chemical Structure	Identifiers	Properties
1		287399-36-4	C ₇ H ₈ Benzene- ¹³ C, methyl-
2		287399-35-3	C ₇ H ₈ Benzene- ¹³ C, methyl-
3		78218-02-7	C ₇ H ₈ Benzene- ¹³ C, 4-methyl-

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¹⁴C，则输入值14

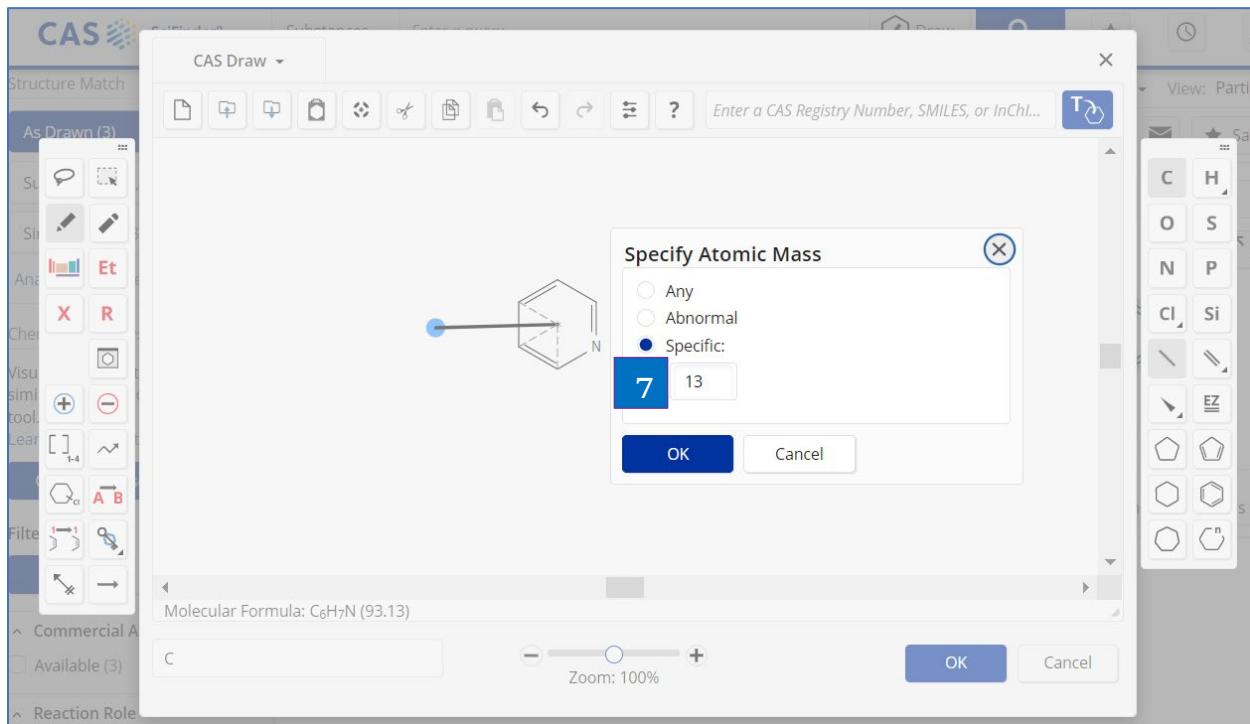


6. 获得指定原子为¹⁴C的物质。

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 ^{13}C 。



7. 将甲基碳的原子量设置为 13

Substances Edit

[← Return to Home](#)

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

8

Substances (4)

<input type="checkbox"/> 1	1630788-91-8	
C ₆ H ₅ N 4-Pyridinylmethylene- ¹³ C		<input type="checkbox"/> 1 Reference <input type="checkbox"/> 8 Reactions <input type="checkbox"/> 0 Suppliers
<input type="checkbox"/> 2	1529772-81-3	
C ₆ H ₄ D ₃ N 4-(Methyl- ¹³ C-d ₃)pyridine		<input type="checkbox"/> 1 Reference <input type="checkbox"/> 1 Reaction <input type="checkbox"/> 0 Suppliers
<input type="checkbox"/> 3	1404120-05-3	
C ₆ H ₇ N 4-(Methyl- ¹³ C)pyridine		<input type="checkbox"/> 3 References <input type="checkbox"/> 4 Reactions <input type="checkbox"/> 0 Suppliers
<input type="checkbox"/> 4	813432-91-6	

Edit Drawing Remove Search Patent Markush

Descending View: Partial

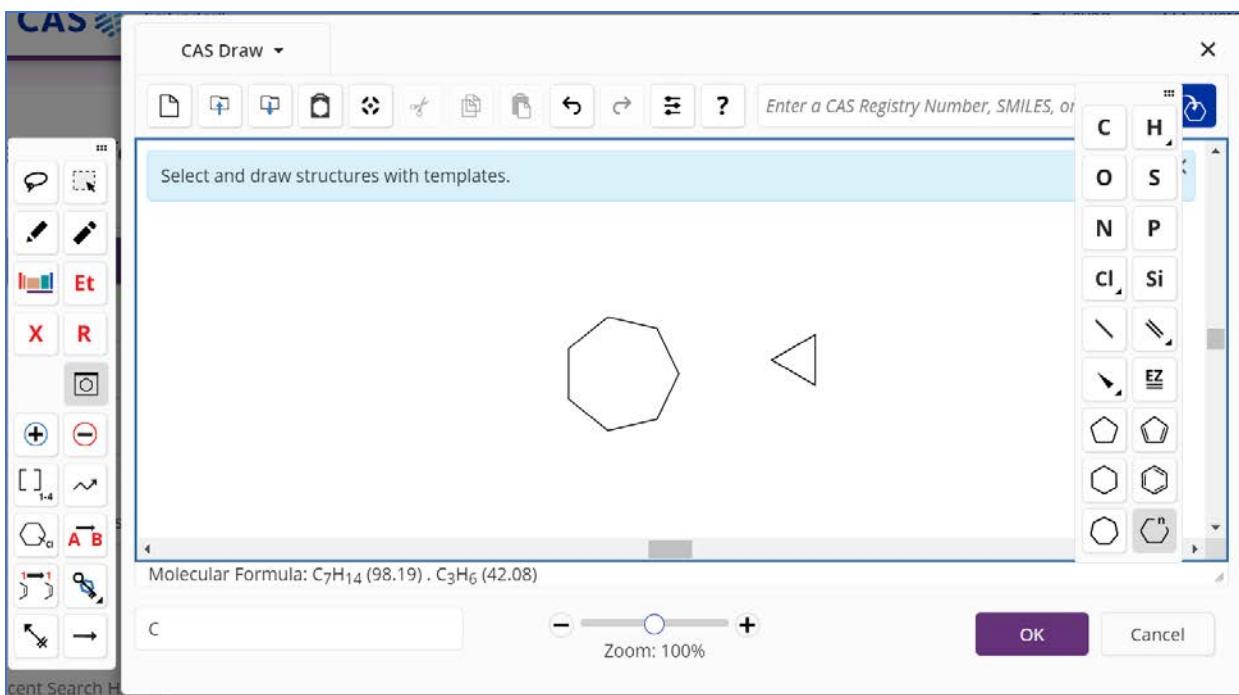
8. 获得满足要求的物质。

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 SciFinderⁿ 中用片段结构检索来实现。

The screenshot shows the CAS SciFinder search interface. On the left, there's a sidebar with options like 'All', 'Substances' (which is highlighted), 'Reactions', 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'. In the center, there's a search bar labeled '1 Enter a query...' and a link to 'Add Advanced Search Field'. To the right of the search bar are three numbered boxes: '2 Draw' (with a drawing icon) and '3' (with a magnifying glass icon). At the top right, there are links for 'Saved', 'History', and 'Account'.

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。



Substances Enter a query...

7 1821719-88-3 6
C₁₀H₁₉N Cycloheptanamine, 2-cyclopropyl-, (1R,2S)-

8 1488617-56-6
C₁₁H₂₁N α-Cyclopropylcycloheptanemethanamine

9 1344060-41-8
C₁₁H₁₉N 2-Cyclopropylcycloheptanamine

10 1340186-29-9
C₁₀H₁₉N 3-Cyclopropylcycloheptanamine

11 2350332-22-6
C₁₁H₂₀O Cycloheptanemethanol, α-cyclopropyl-, (αS)-

12 2350054-45-2
C₁₁H₂₀O Cycloheptanemethanol, α-cyclopropyl-, (αR)-

Reference Role
Stereochemistry
Number of Components
1 (71K)
2 (3,334)
3 (99)
4 (20)
5 or more (12)

Substance Class
Organic/Inorganic Small Molecule (71K)
Salt and Compound With (2,332)
Mixture (869)
Ring Parent (555)
Coordination Compound (457)

View All

Isotopes
Metals
Molecular Weight
Experimental Property
Experimental Spectrum

4 5

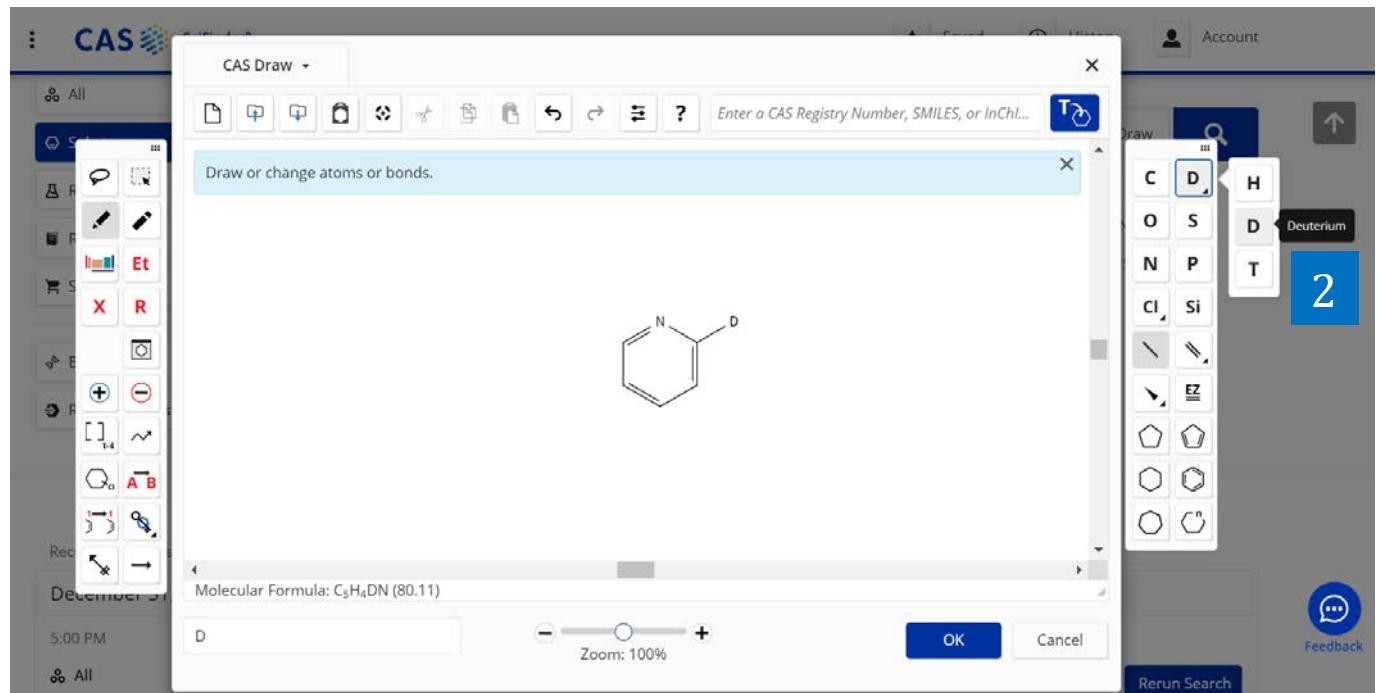
4. 在结果集页面左侧 Number of Components 下勾选相应选项，限定被检索的片段在同一个组分或多个不同组分中（如：选择 1，表示被检索片段在同一个组分中；选择 2，表示被检索片段分别在 2 个不同组分中等；以此类推）。
5. 可继续通过 Substance Class，筛选物质类型。
6. 点击 CAS 登记号，查看物质详情。

直接在结构中绘制氢的同位素 D 和 T

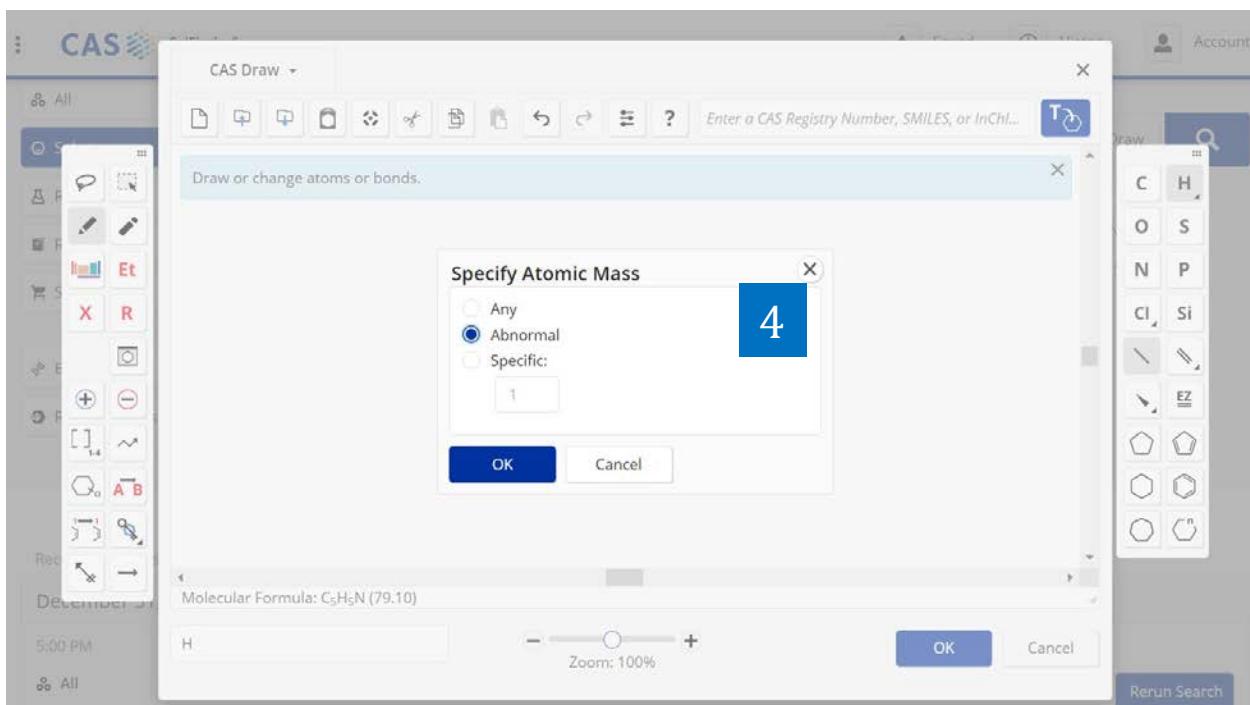
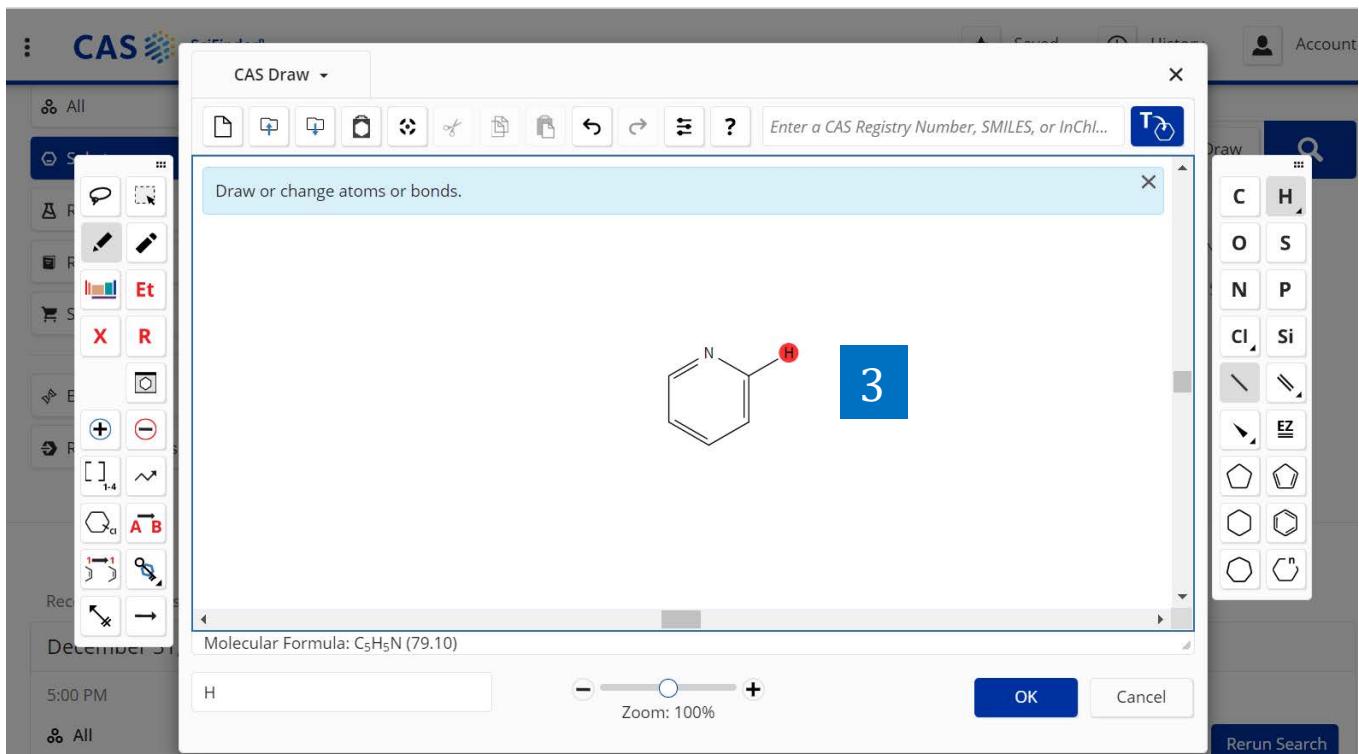
在 CAS SciFinderⁿ 的结构编辑器中，可以直接在结构中绘制氢的同位素原子 D 和 T，获取含有氘或氚同位素标记的物质。

The screenshot shows the CAS SciFinder interface. At the top, there is a navigation bar with the CAS logo, 'SciFinderⁿ', 'Saved' (with a star icon), 'History' (with a clock icon), and 'Account' (with a user icon). Below the navigation bar is a search bar labeled 'Searching for...' with a dropdown menu showing 'All', 'Substances' (which is highlighted in blue), 'Reactions', 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'. To the right of the search bar is a 'Substances' section containing a search input field 'Enter a query...', a 'Molecular Formula' dropdown, and a 'Draw' button. A blue box labeled '1' is placed over the 'Draw' button.

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。



- 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。

5

The screenshot shows the SciFinder search interface. On the left, there's a sidebar with arrows pointing to various categories: All, Substances (which is highlighted in blue), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main search area has a title 'Substances' and a search bar with placeholder text 'Enter a query...'. Below the search bar are dropdown menus for 'AND' and 'Molecular Formula', and a button to 'Add Advanced Search Field'. To the right of the search bar, there's a note about examples like C6H6 or (C8H8)x, and a link to learn more about substances. A chemical structure of pyridine with a deuterium atom (D) is displayed, along with options to 'Edit Drawing', 'Remove', and 'Search Patent Markush'. There's also a checkbox for 'Search Patent Markush'.

- 开始检索，获取感兴趣的结果。

The screenshot shows the SciFinder search results page for substances containing deuterium (D). At the top, there's a header with the CAS logo, 'SciFinder', and a search bar. The main content area is titled 'Substances (114)' and shows three results. Each result includes a chemical structure, the substance name, and its isotope form. For example, the first result is '7291-22-7' with the structure C5D5N (Pyridine-d₅). The second result is '1807-97-2' with the structure C5H4DN (Pyridine-2-d). The third result is '17265-96-2' with the structure C5H3D2N (Pyridine-2,6-d₂). Each result card also provides links to 'References', 'Reactions', and 'Suppliers'.

马库什结构检索

The screenshot shows the CAS SciFinder search interface. On the left, there is a sidebar with a dropdown menu labeled "Searching for..." containing options like "All", "Substances" (which is highlighted with a blue arrow and labeled "1"), "Reactions", "References", "Suppliers", "Biosequences", and "Retrosynthesis". The main search area is titled "Substances" and contains a search bar with placeholder text "Enter a query...". To the right of the search bar are two large blue buttons labeled "2" and "4", which likely correspond to "Edit" and "Search" functions. Below the search bar is an "Advanced Search Field" button. On the far right, there is a "Learn more about Sci" section with a chemical structure diagram, and below it are buttons for "Edit Drawing" (labeled "5"), "Search Patent Markush" (with a checked checkbox), and "Remove" (labeled "6").

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 Patent Markush Match

8 Patent Markush (16)

9 Broad-spectrum herbicide compositions containing cyclic amides with low herbicide injury, manufacture of the compositions, and weed control method

10 Patent claim 1

11 JP2008189578

12 PatentPak

13 Full Text

14 Isoxazolines as plant disease control agents

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

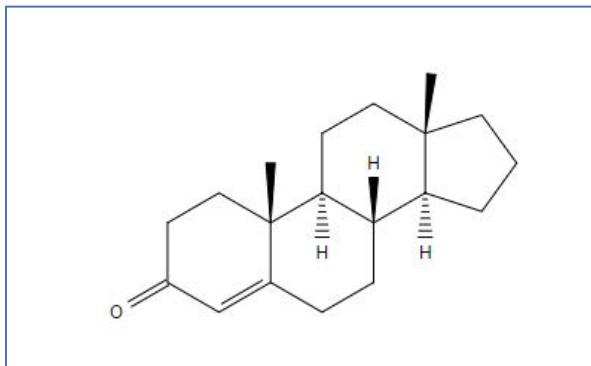
The screenshot shows the CAS SciFinder interface with a search query for "Patent Markush". The results page displays a chemical structure of a heteroaryl compound with numbered atoms (G21, 37, 379, 381, 382, 384). To the right of the structure, the patent information is presented:

- 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, Kaapjo; 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** (highlighted in a blue box)
- 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？



Screenshot of the SciFinder interface showing search results for steroid compounds.

Filter Behavior:

- Filter by:** Selected "Natural Product Occurrence" (225).
- Exclude:** None selected.

Substances: Enter a query... (empty)

Search Results:

Rank	Chemical Name	Structure	Absolute Stereochemistry Shown	References	Reactions	Suppliers
1	Androstanone 17 α -Methyldihydro-4,20-dien-3-one, (17 α)-		Absolute stereochemistry shown	18K References	1,127 Reactions	60 Suppliers
2	Testosterone C ₁₉ H ₂₈ O ₂		Absolute stereochemistry shown	122K References	1,266 Reactions	80 Suppliers
3	Epitestosterone C ₁₉ H ₂₈ O ₂		Absolute stereochemistry shown	1,472 References	58 Reactions	23 Suppliers
4	21317-81-7		Absolute stereochemistry shown	4 References	5 Reactions	0 Suppliers
5	571-25-5		Absolute stereochemistry shown	5 References	14 Reactions	7 Suppliers
6	2243-06-3		Absolute stereochemistry shown	6 References	26 Reactions	26 Suppliers

- 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。

Filter Behavior

Commercial Availability

Reaction Role

Product (91) **Exclude**

Number of Components

Substance Class

Isotopes

Absolute stereochemistry shown

C₁₉H₂₈O₃
6-Hydroxytestosterone

C₂₁H₃₀O₂
Pregna-4-ene-3,16-dione

C₁₉H₂₆O₄
Androst-4-ene-3,17-dione, 6,12-dihydroxy-, (6 β ,17 β)-

C₂₁H₂₆O₄
Pregna-4,20-dien-3-one, 15-hydroxy-, (15 β)-

Feedback

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... Edit Save And Alerts

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)

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

Excluding: Reaction Role: Product

3

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

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

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

4

5

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)

Absolute stereochemistry shown

Edit Structure Reset + Download

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。

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.](#)

Break Bond Protect Bond Clear All Bond Selections

CC(C)C[C@H](CCCC[C@H]1[C@@H]2[C@@]1(CC[C@H]2O)C(=O)C=C2)C

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 SciFinderⁿ 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。

The screenshot shows the CAS SciFinder search interface. On the left, there is a sidebar with arrows pointing right, containing links: All, Substances, Reactions, References, Suppliers (which is highlighted with a blue arrow and the number 1), Biosequences, and Retrosynthesis. The main search area has a header "Searching for..." and a sub-header "Suppliers". Below the sub-header is a search bar with the placeholder "Search by Substance Name and/or CAS RN. Learn More". The search bar contains the text "sudan red" and a blue button labeled "2". To the right of the search bar are icons for "X", "Draw", and a magnifying glass. A list of search results follows, including: Sudan, Sudan 3, Sudan III, Sudan P III, Sudan Red III, Sudan Violet, Sudan (IV) dye, and Sudan 4. On the far right of the search results area is a "Feedback" icon.

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

The screenshot shows the CAS SciFinder interface with the search term 'sudan red' entered in the search bar. The left sidebar contains a 'Filter Behavior' section with a 'Supplier' filter selected, indicated by a blue box labeled '3'. The main results table is titled 'Suppliers (62)' and includes columns for Supplier, Substance, Purity, Purchasing Details, and Availability. The first result, 'AK Scientific', is highlighted with a blue box labeled '4'. It shows details for Sudan II (3118-97-6) with purchase options from 1g to 25g. The second result, 'TCI', is also shown with its details. At the bottom, two additional entries for 'BIOSYNTH Carbosynth' are listed, each with a blue box labeled '5' over the supplier logo.

Supplier	Substance	Purity	Purchasing Details	Availability
AK Scientific AK Scientific Product Catalog United States	3118-97-6 Sudan II		Order From Supplier 1g, USD 14 5g, USD 27 25g, USD 54 Bulk Screening	Maintained in stock Ships within 1 week
TCI	3118-97-6 Sudan II [<chem>I=1-(2,4-Xylylidazo)-2-</chem>]	95-98%	Order From Supplier 25 g, USD 25.00	Maintained in stock

<input type="checkbox"/> 19 BIOSYNTH® Carbosynth Biosynth Carbosynth Product List United Kingdom	<input type="checkbox"/> 85-83-6 Solvent Red 24	<input type="checkbox"/> Product Information ↗
<input type="checkbox"/> 20 BIOSYNTH® Carbosynth Biosynth Carbosynth Product List United Kingdom	<input type="checkbox"/> 85-83-6 Solvent red 24	<input type="checkbox"/> Order From Supplier ↗ 250 g, USD 40 500 g, USD 75 1 Kg, USD 140

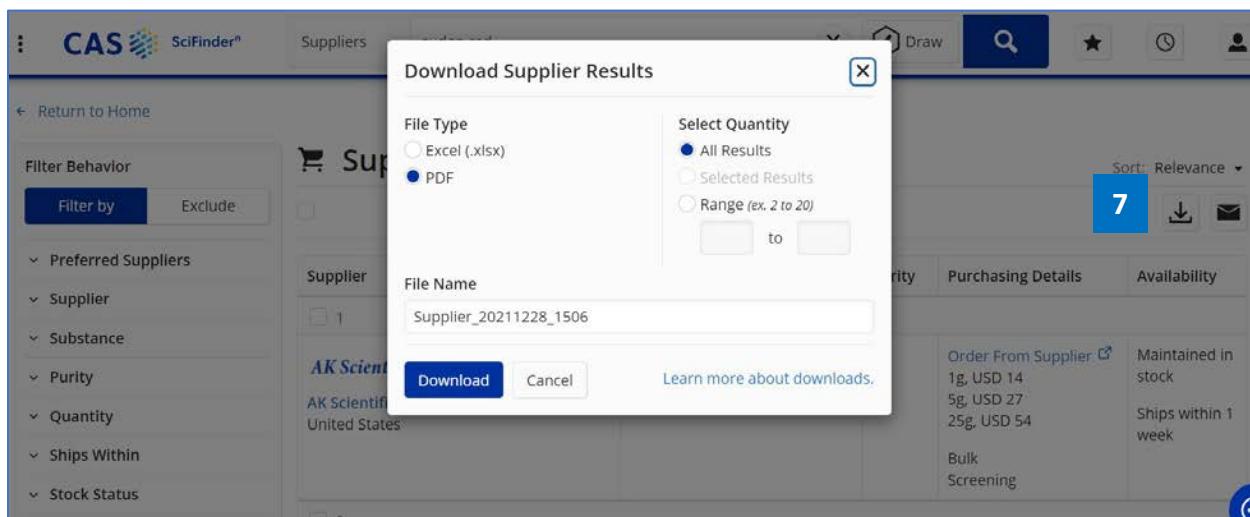
3. 供应商筛选选项，可以根据：优选供应商、供应商名称、产品纯度、产品量级、运送时间、储存状态、是否有直达订购链接、国家等对供应商结果进行筛选。
4. 可以按照供应商名称的字母排列顺序、运送时间或产品纯度对供应商进行重新排序。
5. 点击 order from suppliers，直接访问产品订购页面。
6. 点击 product information，访问该供应商对此产品的描述信息。

点击 order from suppliers 所获界面：

The screenshot shows the AKSci website interface. At the top, there's a search bar with placeholder text "Search by Catalog Number, CAS, MFCD, Keyword ...". Below it is a navigation menu with links to Home, Products, Services, Resources, Partners, Contact Us, and Help. A shopping cart icon indicates 0 items. The main content area displays a product card for "T805 Solvent Red 24, 95% (HPLC)". The product has several别名: Sudan IV, Biebrich scarlet R fat soluble, Oil Red IV, Scarlet Red Scharlach, and Sudan R. It features a chemical structure diagram. The "IDENTITY" section includes CAS Number (85-83-6), MDL Number (MFCD00003893), MF (C24H20N4O), and MW (380.45). The "SPECIFICATIONS & PROPERTIES" section lists Min. Purity Spec (95% (HPLC)), Spectra (NMR, LCMS, HPLC), Physical Form (Dark red to brown powder), Melting Point (175-178°C), and Storage instructions (Long-Term Store at room temperature). A note states it's sold as technical grade, not an analytical standard. The "Availability" table shows stock levels for 5g (\$14), 25g (\$21), and 100g (\$54). Buttons for "Request Quote" and "+ Add to Cart" are present. The page footer includes links to "Inhibitors, Bioactives, Reference Compounds", "Building Blocks, Intermediates, Reagents", and "Bulk Bio & Specialty Chemicals". A "My Account" dropdown and a "Logout" button are also visible.

点击 Product Information 所获界面：

The screenshot shows the BIOSYNTH CarboSynth website interface. The header includes a search bar, a structure search button, and a document search button. The main navigation menu has links to Products, Services, and Support. The breadcrumb navigation shows the path: Home / Fine Chemicals / Other Fine Chemicals / Solvent Red 24. The product page for FS03568 Solvent Red 24 features a large chemical structure diagram. A red "RESEARCH & DEVELOPMENT" button is located in the top right corner. The "TECHNICAL DATA" section contains tables for CoA SEARCH and TAGS, along with a "Chemical Formula:" field. The overall design is clean and professional, typical of a scientific or pharmaceutical supplier's website.



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。

Substance ID	Chemical Structure	Details
3118-97-6		C ₁₈ H ₁₆ N ₂ O Sudan Red 1,259 References, 69 Reactions, 61 Suppliers
1014689-15-6		C ₁₈ H ₁₀ D ₆ N ₂ O 1-[2-(4,6-Dimethylphenyl)diazenyl]-2-naphthalen-3,4,5,6,7,8-d ₆ -ol 2 References, 1 Reaction, 9 Suppliers
94378-04-8		C ₁₉ H ₁₈ N ₂ O 1-[2-(2,4,6-Trimethylphenyl)diazenyl]-2-naphthalenol 15 References, 8 Reactions, 2 Suppliers
15690-52-5		Product (6)
94378-05-9		Product (6)
150151-21-6		Product (6)

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。

The screenshot shows the SciFinder interface for reaction 3118-97-6. The left sidebar has a 'Suppliers' section with a checked checkbox for 'All Starting Materials (19)'. The main area displays a reaction scheme (Scheme 2) with two starting materials and one product. Below each material is a 'Suppliers' button. The product also has a 'Suppliers' button. The reaction summary indicates 1 step, 93% yield, and a reference to a one-pot synthesis of azo compounds.

1. Solvent
2. Commercial Availability
3. Products (7)
4. All Starting Materials (19)
5. Reaction Notes
6. Search Within Results
7. Source Reference
8. Document Type
9. Language
10. Publication Year
11. Publication Name
12. CA Section
13. Filter Content Report

Reactions 3118-97-6

1. Reagents: [Sodium Red](#), [Ozone](#)
Solvents: [2-Methoxyethanol](#)

By: Dussault, Patrick H.; et al
Journal of Organic Chemistry (2000), 65(25), 8407-8414

View Reaction Detail | Experimental Protocols | Full Text

Scheme 2 (2 Reactions)

Steps: 1 Yield: 93%

1. Reagents: [tert-Butyl nitrite](#)
Solvents: [Dichloromethane](#); 24 h, rt

Reaction Summary: Steps: 1 Yield: 93% One-pot synthesis of azo compounds in the absence of acidic or alkaline additives
By: Liu, Ting-Ting; et al

Suppliers (97) | Suppliers (78) | Suppliers (61)

Feedback

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 web interface. At the top, the search bar contains 'La*chol' and the number '1' is displayed in a blue box. The main search results page is titled 'Substances (3)'. On the left, there is a 'Filter Behavior' sidebar with sections for Commercial Availability, Reaction Role, Reference Role, and more. The results are listed in three columns:

- Result 1:** CAS Registry Number 8038-34-4. Notes: Waxy esters and alcs. from lanolin. Unspecified Lanochol.
- Result 2:** CAS Registry Number 8006-54-0. Notes: Fat-like substance derived from sheep wool. Contains a complex combination of esters and polyesters, consisting chiefly of cholestryl and isoocholesteryl esters of the higher fatty acids. Unspecified Lanichol.
- Result 3:** CAS Registry Number 84-79-7. Notes: C₁₅H₁₄O₃. Lapachol. It includes a chemical structure diagram.

Each result row has buttons for 'Reference', 'Reactions', and 'Suppliers'.

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

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) View All

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Experimental Property

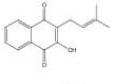
Experimental Spectrum

Regulatory Data by Country

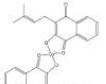
1 2100329-07-3 Image Not Available Notes: An herbal tea made from the inner bark of the Pau d'arco tree (*Handroanthus impetiginosus*) purported to have anti-inflammatory and anticarcinogenic activities Unspecified **Lapachorinde**

2 855637-05-7  C₃₀H₂₆O₆ **Lapachol, peroxide**

3 332083-20-2  C₁₅H₁₄O₃.K Components: 2 Component RN: 84-79-7 **Lapachol potassium salt**

4 184359-68-0  C₁₅H₁₄O₃.Ag Components: 2 Component RN: 84-79-7 **Lapachol silver salt**

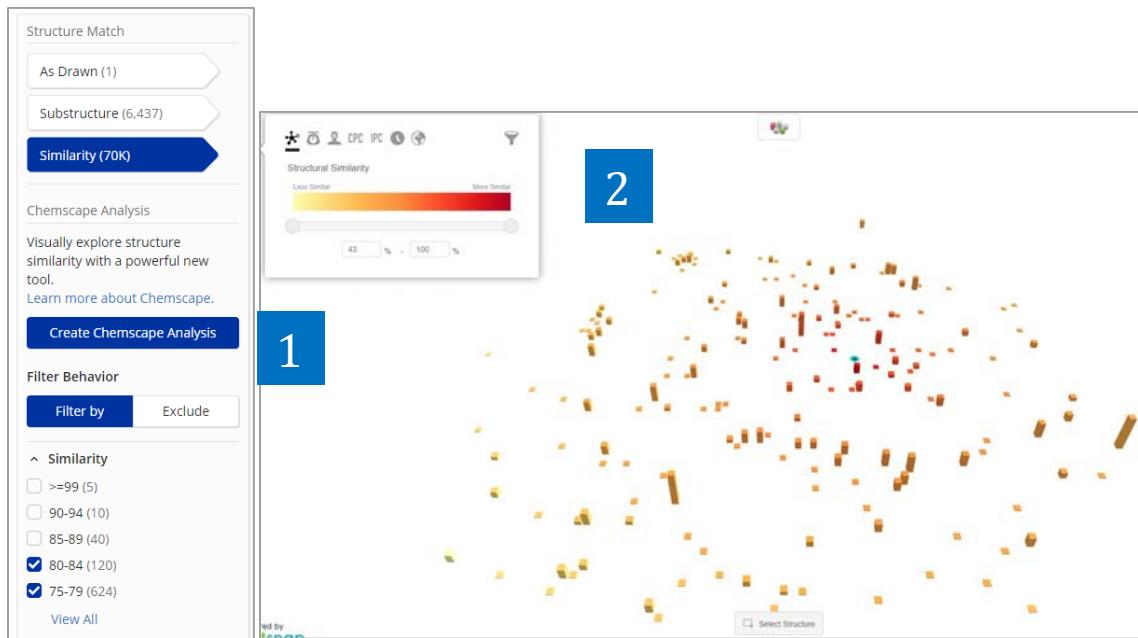
5 128528-86-9  C₃₀H₂₆BeO₆ **Lapachol, Be deriv.**

6 128271-49-8  C₃₀H₂₆CoO₆ **Lapachol, Co deriv.**

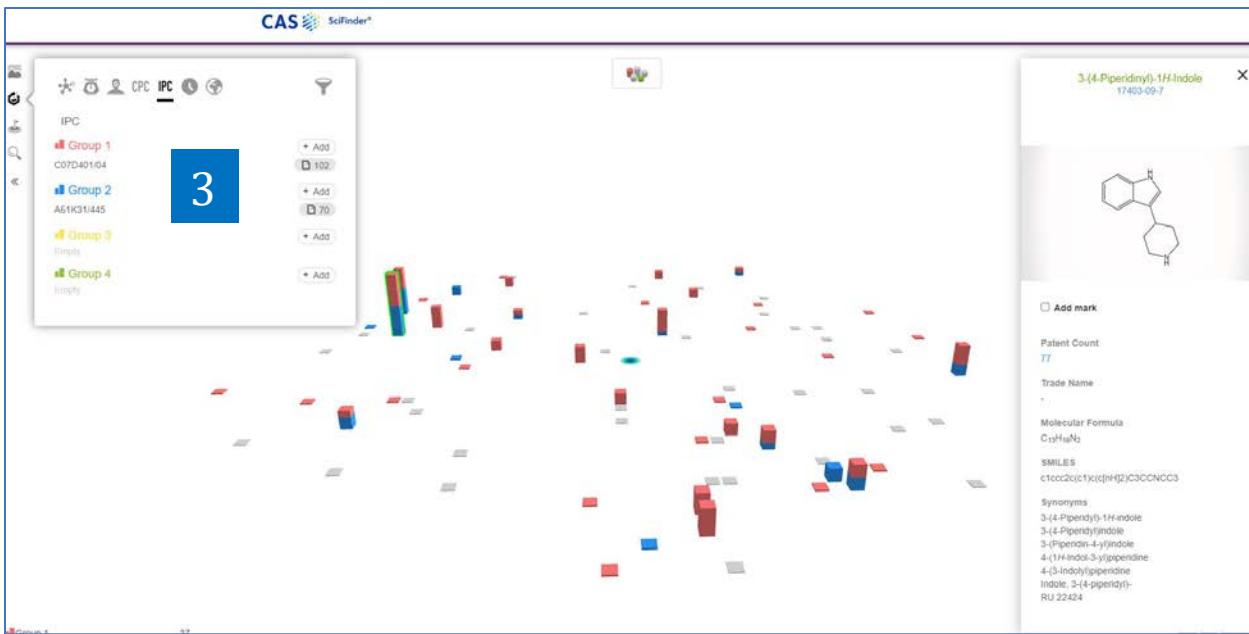
2. 此处输入 Lapacho*, 可以检索到 Lapachorinde, lapachol peroxide, lapachol potassium salt 等。

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。

1

Searching for... **Retrosynthesis**

Draw or import a structure to perform a retrosynthetic analysis. Learn more about Retrosynthesis searching.

Draw or change atoms or bonds.

Molecular Formula: C₁₉H₁₉BrN₄O₅ (463.29)

2

Start Retrosynthetic Analysis

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 SciFinderⁿ 账号的邮箱发送通知。

8. 创建路线。

Estimated Yield: 15%
Overall Price: \$427.41
(USD per 100 grams)

Commercially Available:
B, C, D, F, G, H, I

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$1,000.00/mol
Edit Plan Options

Scoring Profiles

Complexity Reduction:

Convergence:

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Feedback

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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。

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

A \Rightarrow B + C + D
Average Yield: 36%
Evidence (1,183)
Alternative Steps (86)

B \Rightarrow E
Maximum Yield: 80%
Evidence (182,661)
Alternative Steps (20)

C \Rightarrow F + G
Maximum Yield: -
Evidence (1)
Alternative Steps (17)

E \Rightarrow H + I
Maximum Yield: 51%
Evidence (400,236)
Alternative Steps (25)

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Feedback

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。

Alternative Steps (86)

Filter by

- Alternative Step Type
- Predicted (69)
- Stereochemistry
- Non-Selective (69)

14

5 of 86

A → B + C + D

Average Yield: 36%
Evidence (1,183)
Alternative Steps (86)

B → E

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

C → F + G

Maximum Yield: -
Evidence (-)
Alternative Steps (17)

D → H + I

Maximum Yield: 51%
Evidence (400,236)
Alternative Steps (25)

Select Predicted Step Evidence (983,581) Average Yield: 64%

6 of 86

Evidence (6,187) Average Yield: 63%

7 of 86

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14. 选择感兴趣的反应步骤，整个逆合成路线发生改变。

Retrosynthesis

Estimated Yield: 26%
Overall Price: \$138.22
(USD per 100 grams)

Commercially Available:
B, E, F, G, H

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit:
\$1,000.00/mol
Edit Plan Options

Scoring Profiles

Complexity Reduction
Convergence

15

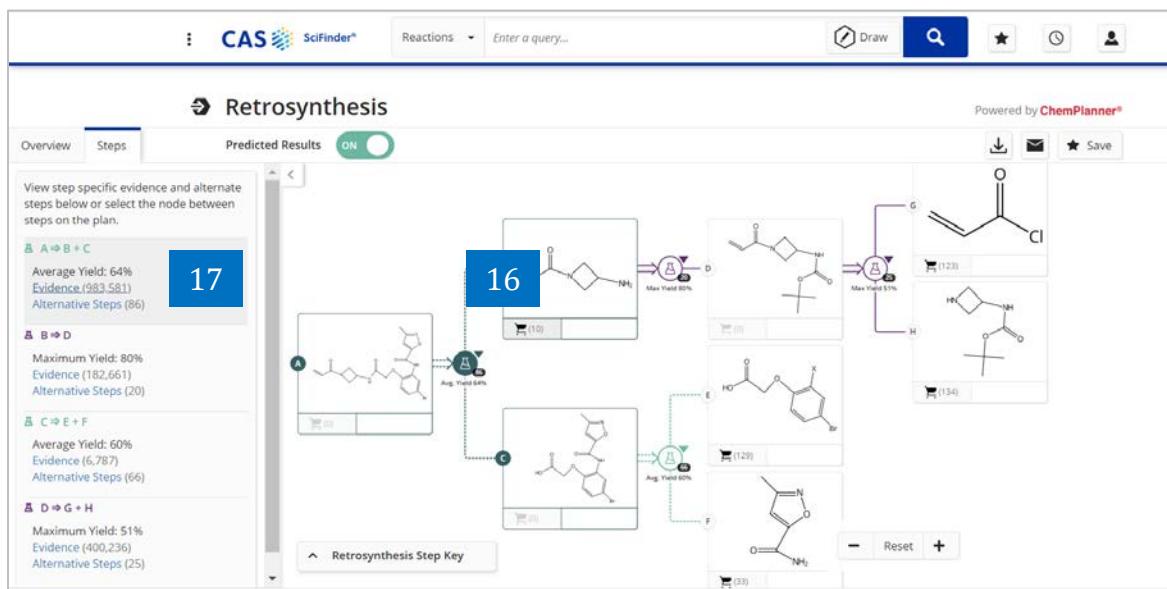
Predicted Results ON

Powered by ChemPlanner®

Retrosynthesis Step Key

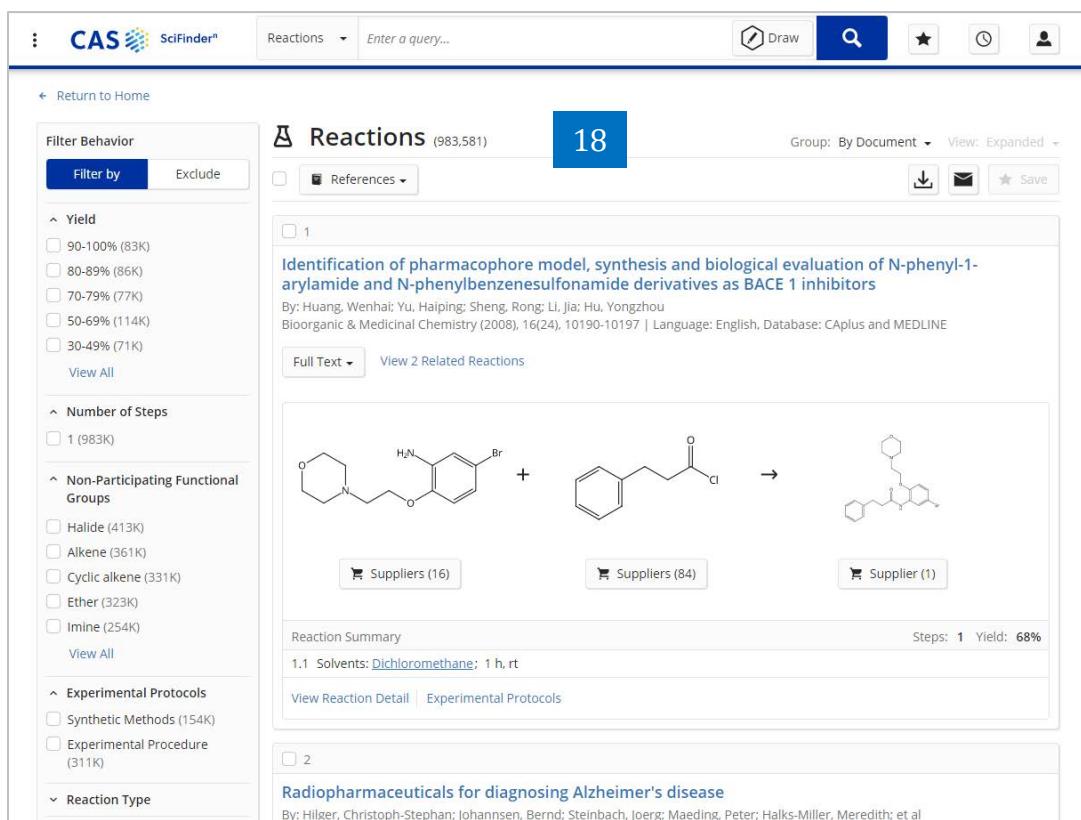
Reset

15. 整个实验路线发生改变，其中绿色路线为预测路线。



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。



18. 支持该步骤的反应结果集。

20
21
22

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。

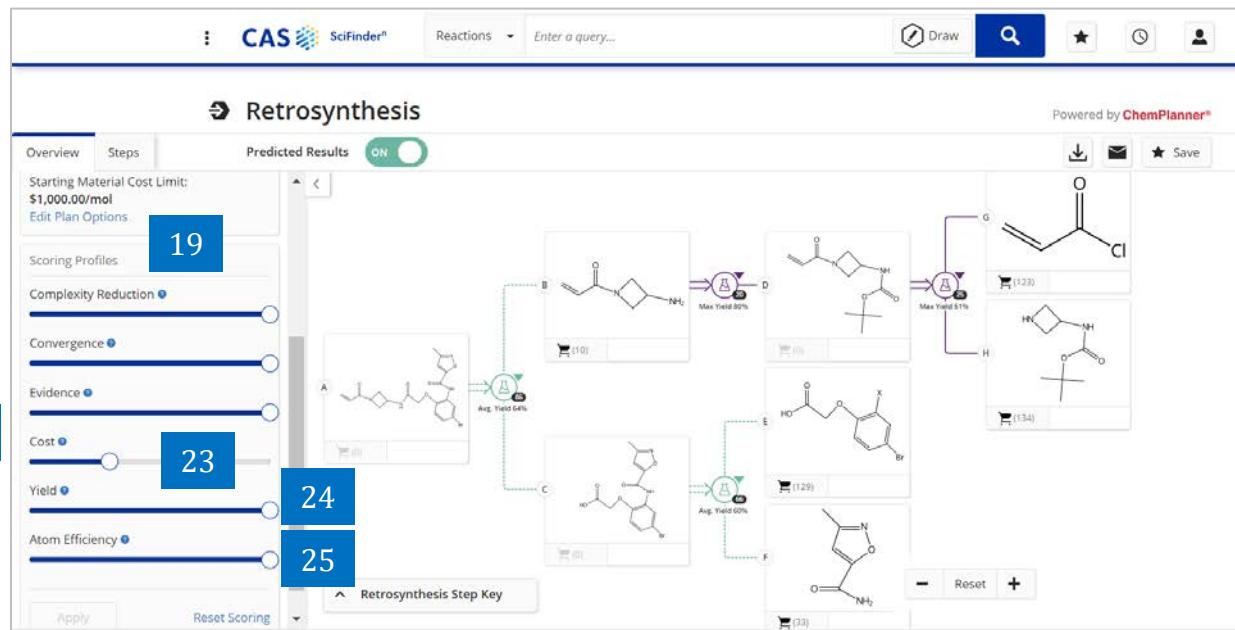
21. 汇聚：调高 Convergence 会提高路线的汇聚（减少反应路线的线性长度）。

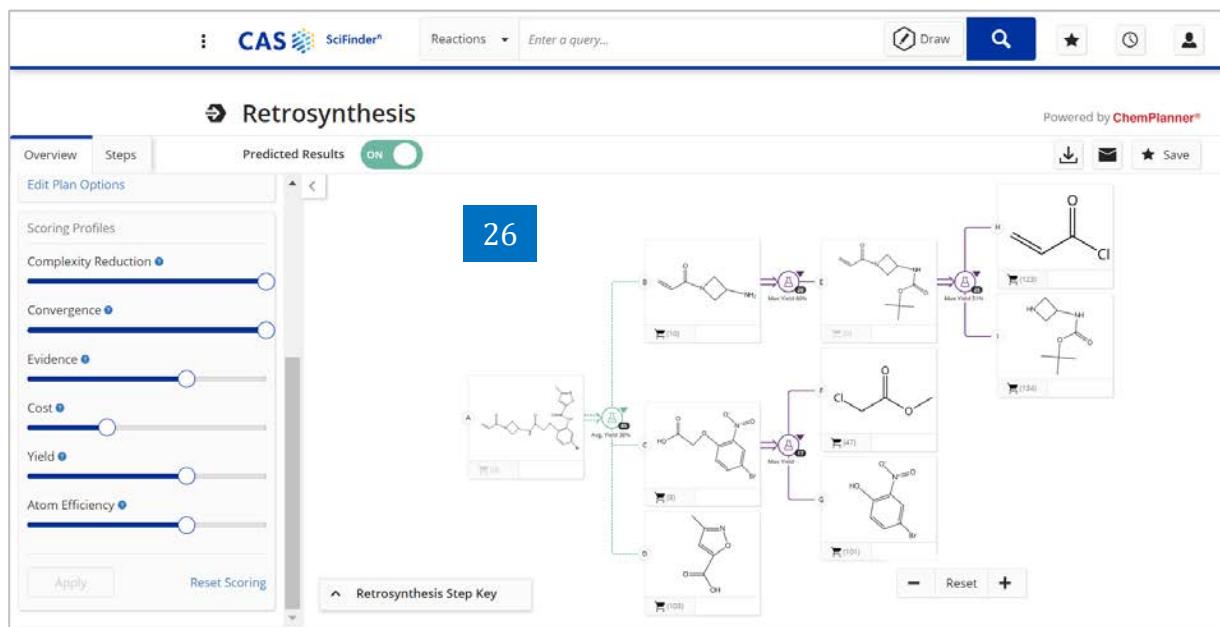
22. 依据：根据支持特定反应类型的证据例子的数量多少来排列计划步骤/备选方案。

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

Retrosynthesis

Powered by ChemPlanner®

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

A $\xrightarrow{\Delta}$ B
Maximum Yield: 88%
Evidence (1)
Alternative Steps (75)

B $\xrightarrow{\Delta}$ C
Maximum Yield: 99%
Evidence (3)
Alternative Steps (67)

C $\xrightarrow{\Delta}$ D Stereoselective
Average Yield: 71%
Evidence (118,730)
Alternative Steps (36)

D $\xrightarrow{\Delta}$ Final Product
Aug. Yield 71%
Evidence (8)

1

Retrosynthesis Step Key

Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.

Experimental Steps (purple arrow)

Predicted Steps (green dashed arrow)

Reset

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。

Alternative Steps (36)

Filter by

Alternative Step Type

Experimental (1)

Predicted (34)

Stereochemistry

Selective (1)

Non-Selective (34)

1 of 36

1 of 36

2 of 36 Stereoselective

Selected

Experimental Step

Evidence (2)

Maximum Yield: 96%

2 of 36 Stereoselective

Selected

Predicted Step

Evidence (118,730)

Average Yield: 71%

3

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 shows the Retrosynthesis module of the CAS SciFinder interface. On the left, there's a sidebar with 'Plan Options' and 'Scoring Profiles'. The 'Scoring Profiles' section contains five sliders labeled 'Complexity Reduction', 'Convergence', 'Evidence', 'Cost', and 'Yield'. Each slider has four levels: off, low, medium, and high. A large blue callout box with the number '1' points to the 'Overview' tab in the top navigation bar. Another blue callout box with the number '2' points to the 'Scoring Profiles' section. A third blue callout box with the number '3' points to the 'Apply' button at the bottom of the sidebar. The main area displays a retrosynthetic tree with various reaction steps and their yields.

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。

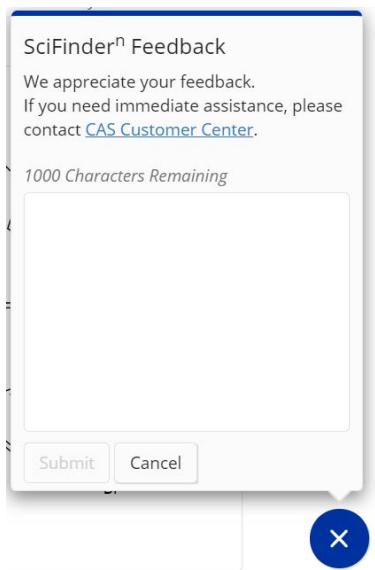
利用 Retrosynthesis 的产品反馈功能

The screenshot shows the Retrosynthesis feature in SciFinder. On the left, there's a sidebar with 'Plan Information' (Estimated Yield: 15%, Overall Price: \$427.41), 'Plan Options' (Synthetic Depth: 3, Predicted Rules: Common, Break & Protect Bonds: No), and 'Scoring Profiles'. The main area displays a retrosynthetic tree with nine steps (A-I). Step A is highlighted with a green box. Step B is highlighted with a red box. Step C is highlighted with a blue box. Step D is highlighted with a yellow box. Step E is highlighted with a purple box. Step F is highlighted with a pink box. Step G is highlighted with a grey box. Step H is highlighted with a light blue box. Step I is highlighted with a light green box. A large blue box labeled '1' is overlaid on the right side of the interface.

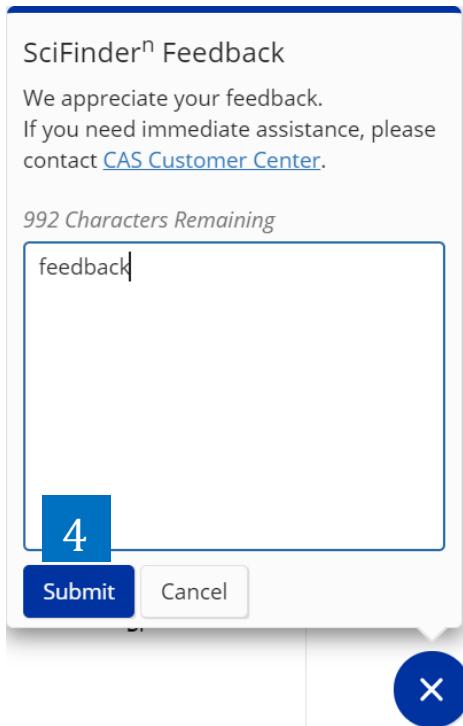
1. 在 Retrosynthesis 的结果页面，点击 Feedback 图标，进行使用反馈。

The screenshot shows the 'Retrosynthesis Plan Options' page in SciFinder. It includes sections for 'Select Synthetic Depth' (radio buttons for 1, 2, 3, 4, with 3 selected), 'Set Rules Supporting Predicted Reactions' (radio buttons for Common, Uncommon (includes Common Rules), and Rare (includes Common and Uncommon Rules), with Common selected), 'Set Starting Materials Cost Limit' (\$1000, USD/mol), and a 'Create Retrosynthesis Plan' button. A large blue box labeled '2' is overlaid on the right side 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 SciFinder interface with the following details:

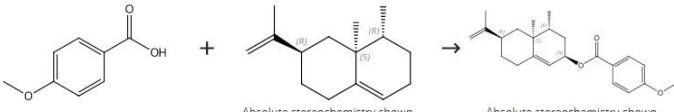
- Top Bar:** CAS SciFinder, Reactions (dropdown), 2014:365937, Draw, Search, Favorites, Recent, User.
- Left Sidebar (Filter Behavior):**
 - Filter by:** Yield (90-100% 13, 80-89% 5, 70-79% 1, 50-69% 10, 30-49% 6, 10-29% 1).
 - Number of Steps:** Non-Participating Functional Groups.
 - Experimental Protocols:** Synthetic Methods (36) is checked (highlighted with a blue box).
 - Reaction Type:** Stereochemistry.
 - Reagent:**
- Center Content:**
 - Reactions:** (36) - Grouped By Scheme, View: Expanded.
 - Filtering:** Experimental Protocols: Synthetic Methods.
 - Scheme 1 (1 Reaction):** Shows a reaction between a substituted benzyl alcohol and a substituted cyclohexene derivative. The product is a substituted cyclohexene with a ketone group. Labels indicate "Absolute stereochemistry shown, Rotation (+)".
 - Suppliers:** (95) and (35) for the reactants and product respectively.
 - Reaction Summary:** Steps: 1, Yield: 100%.
 - 1.1 Catalysts: Aluminum copper oxide, Solvents: Acetonitrile; 10 min, rt
 - 1.2 Reagents: tert-Butyl hydroperoxide, Solvents: Water; 24 h, 82 °C
 - Details:** Allylic Oxidation of Alkenes Catalyzed by a Copper-Aluminum Mixed Oxide. By: Garcia-Cabeza, Ana Leticia; et al. Organic Letters (2014), 16(6), 1598-1601.
 - Buttons:** View Reaction Detail, Experimental Protocols, Full Text (highlighted with a blue box), Collapse Scheme.

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。

Return to Results

Reaction Detail (Scheme 1, Reaction 1 of 1)

3 **4** **5**



Suppliers (95) Suppliers (35)

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	Aluminum copper oxide	Acetonitrile	10 min, rt
2	tert-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 <i>R</i> ,4 <i>R</i> ,4 <i>a</i> <i>S</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, Yield: 100%
Reactants	4-Methoxybenzoic acid Valencene
Reagents	tert-Butyl hydroperoxide
Catalysts	Aluminum copper oxide
Solvents	Acetonitrile Water
Procedure	<ol style="list-style-type: none"> 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 Na₂SO₄ 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 Química Orgánica, Facultad de Ciencias Universidad de Cádiz
Cádiz 11510
Spain

Transformation	Acyloxylation Reaction	7
Scale	milligram	8
Characterization Data	9	
\wedge (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>Proton NMR Spectrum 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).</p> <p>Carbon-13 NMR 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.</p> <p>IR Absorption Spectrum Film v_{max}: 2932, 1707, 1607, 1510, 1272, 1256, 1167, 1032, 847, 772 cm⁻¹.</p> <p>Optical Rotatory Power [α]_D²⁰ = +130.06 (<i>c</i> 1.70, CHCl₃).</p> <p>HRMS ESI: calcd. for C₂₃H₃₁O₃ [M+H]⁺ 355.2273; found 355.2271.</p>		
CAS Method Number 3-209-CAS-8900882		

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 Reactions search results for the query "sofosbuvir". The left sidebar contains various filters, with "Reaction Type" (1) and "Reaction Notes" (2) highlighted. The main content area shows a reaction scheme with two chemical structures and a "Suppliers (67)" button. Below the scheme are three reaction summaries, each with reagents, solvents, steps, yield, and a patent reference.

Reaction Summary	Steps: 1 Yield: 100%	Preparation and crystal structure of nucleoside phosphor amides as antiviral agents
1.1 Reagents: Sodium sulfite Solvents: Tetrahydrofuran, Water; 4 h, rt		By: Ross, Bruce S.; et al World Intellectual Property Organization, WO2011123645 A2 2011-10-06
View Reaction Detail Experimental Protocols	PatentPak Full Text	
Reaction Summary	Steps: 1 Yield: 100%	Preparation and crystal structure of nucleoside phosphor amides as antiviral agents
1.1 Reagents: Sodium sulfite Solvents: Tetrahydrofuran, Water; 4 h, rt		By: Ross, Bruce; et al United States, US8642756 B2 2014-02-04
View Reaction Detail	PatentPak Full Text	
Reaction Summary	Steps: 1 Yield: 100%	A process for the preparation of N-[[P(S),2'R]-2'-deoxy-2'-fluoro-2'-methyl-P-phenyl-5'-uridyl]L-alanine 1-methyl ethyl ester
1.1 Reagents: Sodium sulfite Solvents: Tetrahydrofuran, Water; 4 h, rt		By: Ross, Bruce S.; et al

- 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。
- 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。

Reactions sofosbuvir

Source Reference

Document Type: Journal (63), Patent (659)

Language: English

Publication Year: All

Publication Name: World Intellectual Property Organization (266), China (167), Canada (80), United States (73), India (49)

View All

CA Section: All

Filter Content Report: Download filter data from this result set.

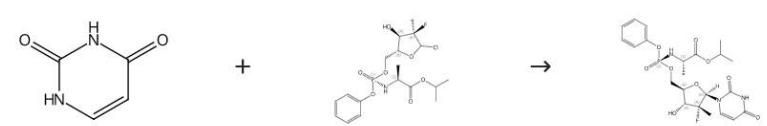
Solvents: tetrahydrofuran, water, 4 h, rt

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

View Reaction Detail | PatentPak | Full Text

Collapse Scheme

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



Absolute stereochemistry shown

Reaction Summary Steps: 1 Yield: 93% Preparation of medicine for inhibiting HCV

1.1 Reagents: *N,O*-Bis(trimethylsilyl)acetamide
Solvants: Chlorobenzene; 30 min, reflux; reflux → rt
1.2 Reagents: Tin tetrachloride; rt; rt → reflux

View Reaction Detail | PatentPak | Full Text

Collapse Scheme

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 shows the CAS SciFinder interface. On the left, there's a sidebar with a list of categories: All, Substances, Reactions (which is highlighted), References, Suppliers, Biosequences, and Retrosynthesis. In the center, there's a search bar with the placeholder "Enter a query...". Above the search bar, there's a message about using BLAST search for protein and nucleotide mining. To the right of the search bar, there are three numbered steps: 1 (highlighting the 'Reactions' category), 2 (highlighting the reaction scheme area), and 3 (highlighting the search button).

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。

1

2

Structure Match

- As Drawn (200)
- Substructure (1.7M)
- Similarity (18K)

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 Save And Alerts

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

PatentPak Full Text

Suppliers (67) Suppliers (85) Suppliers (4)

Reaction Summary

Steps: 1 Yield: 100%

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

[View Reaction Detail](#)

4. 根据 Structure Match, 选择 Similarity 的反应结果。
5. 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

The screenshot shows the CAS SciFinder search interface. On the left, a sidebar lists search categories: All, Substances, Reactions (which is highlighted with a blue arrow and the number 1), References, Suppliers, Biosequences, and Retrosynthesis. In the center, the 'Reactions' search page is displayed. It features a search bar with the placeholder 'Enter a query...' and a structure editor window containing a reaction scheme. To the right of the search bar are two blue boxes labeled '2' and '3'. Box 2 contains a 'Edit' button with a pencil icon. Box 3 contains a magnifying glass icon. Below the structure editor are 'Edit Drawing' and 'Remove' buttons.

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。

Reactions Edit

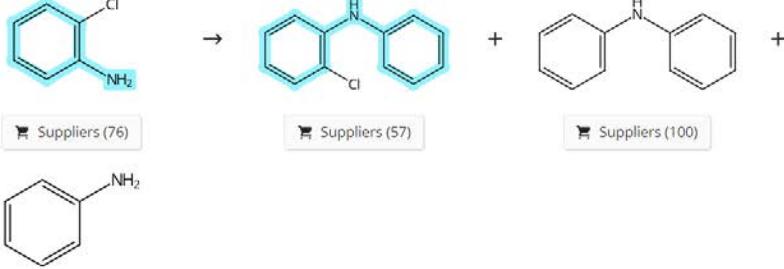
Structure Match
As Drawn (1,002)
Substructure (86K)
Similarity (3,037)

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

Reactions (1,554) Group: By Scheme View: Expanded
References Save And Alerts Clear All Filters

Scheme 1 (1 Reaction) Steps: 1 Yield: 37%


Clc1ccccc1N → c1ccc(Cl)c2c1Nc3ccccc32 + c1ccccc1Nc2ccccc2 + c1ccccc1Nc2ccccc2

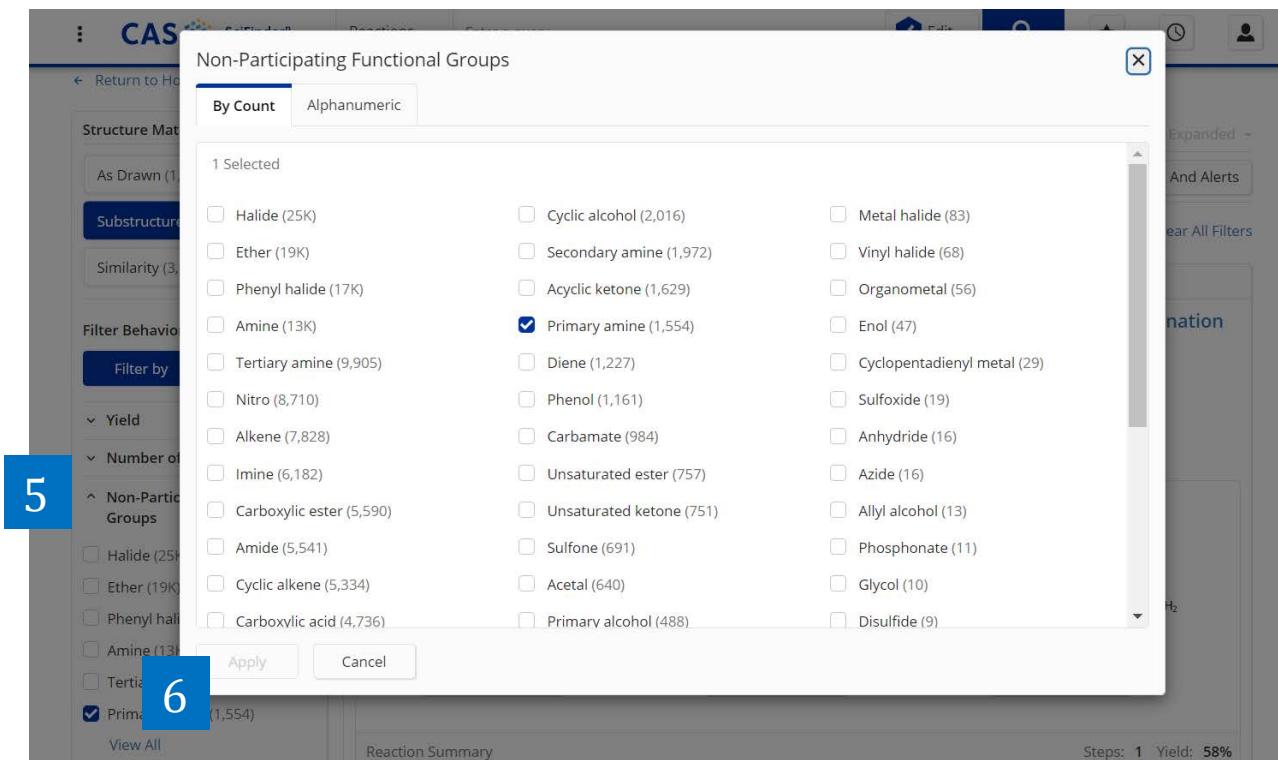
Suppliers (76) Suppliers (57) Suppliers (100)

Suppliers (95)

Reaction Summary Steps: 1 Yield: 37% The Surprisingly Facile Thermal Dehalogenation of Chlorinated Aromatics by a Hydroaromatic Donor Solvent. Tautomerization of Chlorinated Phenols and Anilines

1.1 Reagents: [9,10-Dihydroanthracene](#); 180 min, 630 K

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。

7

Reactions (1,554)

Filtering: Non-Participating Functional Groups: Primary amine

Start Retrosynthetic Analysis

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

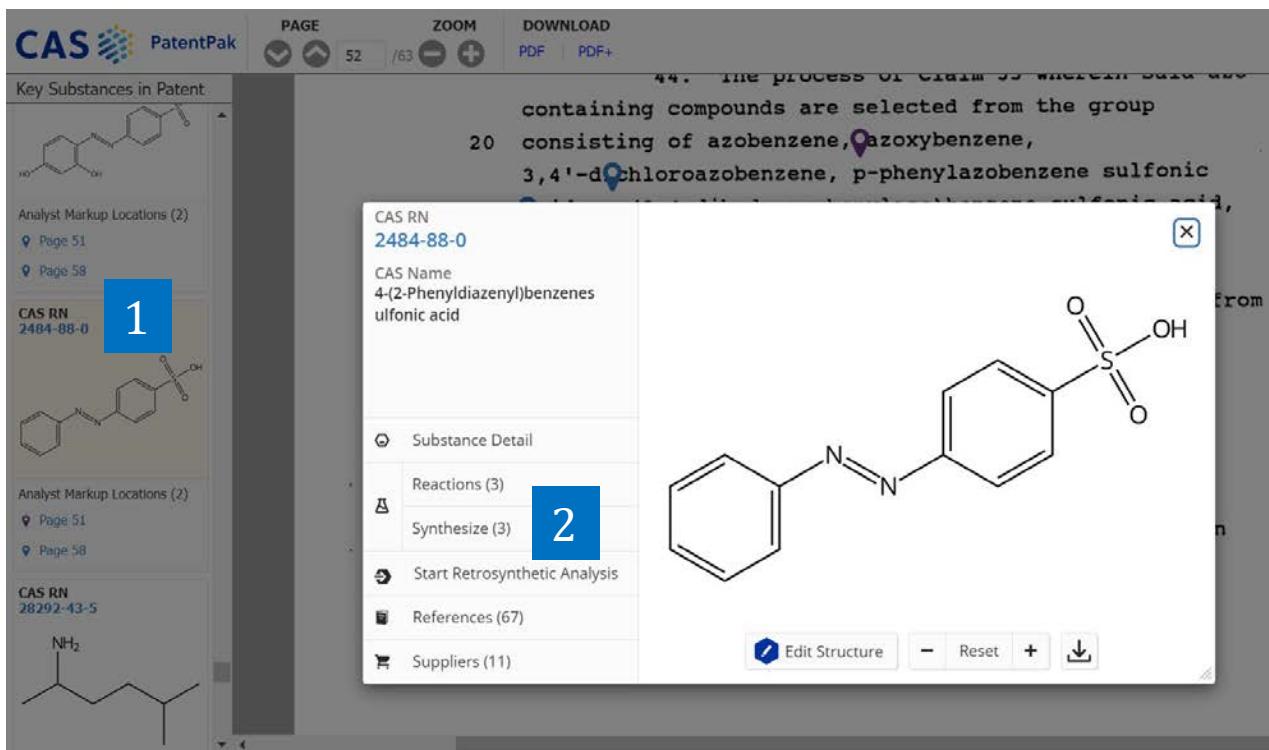
Full Text ▾

Reaction Summary

Steps: 1 Yield: 58%

7. 浏览目标结果。

在 PatentPak Viewer 中使用 Retrosynthesis



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。

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。

Filter Behavior

Filter by Exclude

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

- Cyclic ketone (66)
- Ketone (66)

Reactions (305)

Group: By Document View: Expanded

References

1

Microbial 11 α -hydroxylation of steroids
By: Wiersma, Marten; Van Der Meijden, Pieter
World Intellectual Property Organization, WO9721830 A1 1997-06-19 | Language: English, Database: CPlus

PatentPak Full Text View 2 Related Reactions **2**

Absolute stereochemistry shown

Suppliers (36) **Suppliers (11)**

Reaction Summary Steps: 1 Yield: 98%

1.1 Reagents: Glucose

[View Reaction Detail](#)

3. 选择 Group: By Document 对反应检索结果进行排序。
4. 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

Reactions (305)

3 Group: By Scheme View: Expanded

References ▾

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

Absolute stereochemistry shown

Absolute stereochemistry shown

Suppliers (36) Suppliers (11)

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

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

[Collapse Scheme](#)

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

Suppliers (68) Suppliers (29)

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

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

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

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

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

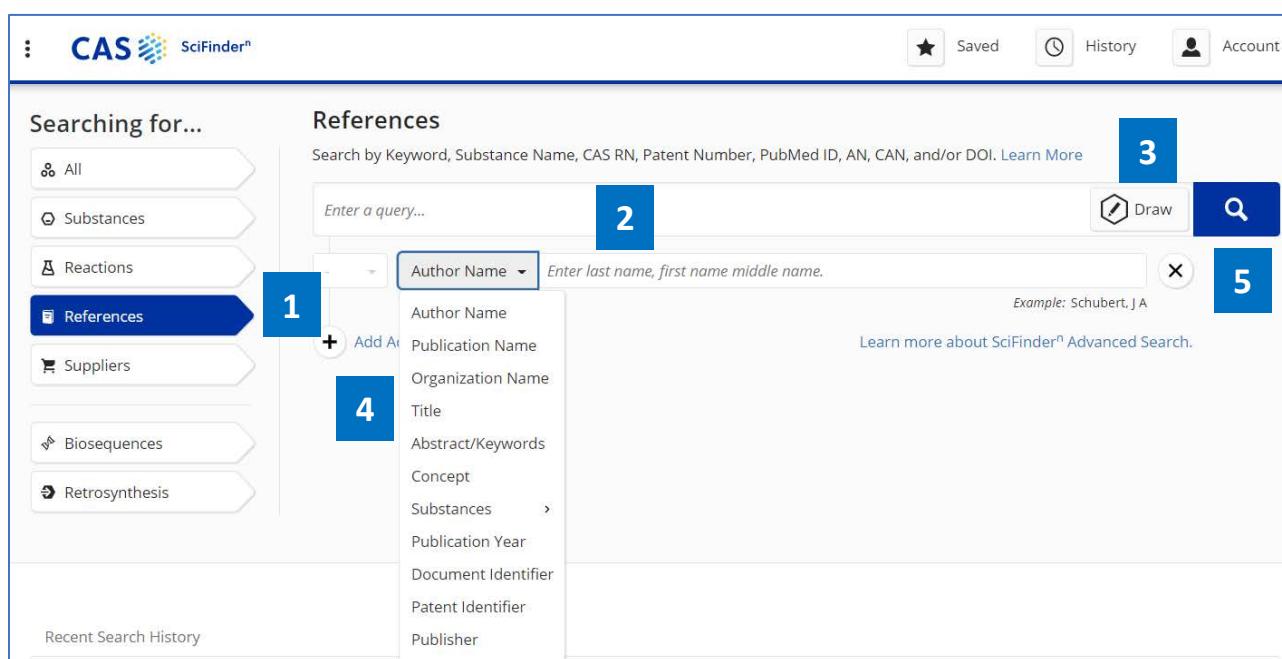
No Data Available

5. 选择 Group: By Scheme 对反应检索结果进行排序。

6. 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



1. 在 CAS SciFinderⁿ 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。

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

References (60,871)

Sort: Relevance View: Partial Abstract

Substances Reactions Citing

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

Pharmacological inhibitors of cyclin-dependent kinases

By: Knockaert, Marie; Greengard, Paul; Meijer, Laurent
Trends in Pharmacological Sciences (2002), 23(9), 417-425 | Language: English, Database: Cplus and MEDLINE

A review. **Cyclin-dependent kinases (CDKs)** regulate the cell division cycle, apoptosis, transcription and differentiation in addition to functions in the nervous system. Deregulation of **CDKs** in various diseases has stimulated an intensive search for selective pharmacol. **inhibitors** of these kinases. More than 50 **inhibitors** have been identified, among which >20 have been co-crystallized with CDK2. These **inhibitors** all target the ATP-binding pocket of the catalytic site of the kinase. The actual selectivity of most known **CDK inhibitors** and thus the underlying mechanism of action is still under investigation.

Inhibitors of mammalian G₁ cyclin-dependent kinases

By: Sherr, Charles J.; Roberts, James M.
Genes & Development (1995), 9(10), 1149-63 | Language: English, Database: Cplus and MEDLINE

A review with over 100 references. Biol. machines need brakes, and the nature and fidelity of their operation cannot be unraveled without some prior understanding of how accelerators work. The discovery of mammalian G₁ cyclins just 4 yr ago and the identification of their associated **cyclin-dependent kinases (cdks)** provided key insights soon thereafter as to how progression through the first gap phase (G₁) of the mammalian cell cycle might be regulated pos. Within the past 18 mo. we have begun to learn something about the neg. regulators-**cdk inhibitors**-that constrain their action.

Full Text Substances (1) Reactions (0) Citing (486) Citation Map

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

PATENT 1

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 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 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 [R^6 = halo, $NHNH_2$, amino, etc.; R^2 = halo, $NHNH_2$, alkyl, etc.; R^9 = 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 ($POCl_3$, lutidine, 120°, 3 h), treated with benzylamine ($n-BuOH$) followed by 3-aminopropanol to give II. II has $IC_{50} = 54.6 \mu M$ 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.

Chemical Structures:

Structure I: 2,6-dihydroxy-9-isopropyl-8-azapurine. SMILES: CN1C=NC2=C1C(=O)N(C)C(=N2O)C3=CC=C(C=C3)C4=CC=C(C=C4)N5C=CC=C5

Structure II: Compound II. SMILES: CC(C)N1C=NC2=C1C(OCCCCN3C=CC=C3)C(=N2O)C4=CC=C(C=C4)N5C=CC=C5

Keywords: azapurine cyclin dependent kinase inhibitor preparation

PatentPak PDF Get Prior Art Analysis Full Text ▾

Patent Family 4

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

Expand All | Collapse All

IPC Data **6**

Patent	Class	Patent Family Classification Codes
WO2004018473	IPCI	C07D 0487/00 A
AU2003260919	IPCI	C07D 0487/00 A
WO2004018473	IPCI	C07D 0487/00 A
EP1539760	IPCI	C07D 0487/00 A
JP2006511458	IPCI	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	IPCI	A61K 0031/519; C07D 0487/02
US7816350	IPCI	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 SciFinder search interface. On the left, there is a sidebar with various search categories: All, Substances, Reactions, References (which is highlighted with a blue arrow and the number 1), Suppliers, Biosequences, and Retrosynthesis. Below this is a 'Recent Search History' section. The main area is titled 'References' and contains a search bar with placeholder text 'Enter a query...'. To the right of the search bar is a dropdown menu set to 'Author Name' (highlighted with a blue arrow and the number 2). A list of search fields is displayed under this dropdown, including Author Name, Publication Name, Organization Name, Title, Abstract/Keywords, Concept, Substances, Publication Year, Document Identifier, Patent Identifier, and Publisher. The 'Concept' field is highlighted with a blue arrow and the number 3. At the top right of the interface are links for 'Saved', 'History', and 'Account'.

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。

The screenshot shows the SciFinder search interface. On the left, there is a sidebar with various search categories: All, Substances, Reactions, References (which is selected and highlighted in blue), Suppliers, Biosequences, and Retrosynthesis. The main search area has a search bar with the text "total synthesis" and a count of "4". Below the search bar are two dropdown menus: "AND" and "Chemical Name" with "taxol" selected. Another dropdown menu below it shows "AND" and "Concept" with "stereo*" selected. There is also a link to "Add Advanced Search Field". A blue box labeled "4" is placed over the search bar, and another blue box labeled "5" is placed over the "stereo*" dropdown.

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。

The screenshot shows the SciFinder search results page for the query "total synthesis". The results are titled "References (58)". The left sidebar contains a "Filter Behavior" section with "Filter by" selected, followed by filters for Document Type (Journal, Patent, Review, Conference, Dissertation), Substance Role (Preparation, Biological Study, Reactant or Reagent, Uses, Properties), Language (English, Japanese), and Publication Year. A blue box labeled "7" is placed over the "Properties" filter. The main results area shows two entries. The first entry is for "Total Synthesis of Microtubule-Stabilizing Agent (-)-Laulimalide" by Ghosh, Arun K.; Wang, Yong; Kim, Joseph T. from the Journal of Organic Chemistry (2001). The second entry is for "Total Synthesis of the Microtubule-Stabilizing Agent (-)-Laulimalide" by Paterson, Ian; De Savi, Chris; Tudge, Matthew from the Organic Letters (2001). Both entries include abstracts and links to full text, substances, reactions, citations, and citation maps.

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）。

Reference Detail (1 of 58)

← Prev Next →

Substances (105)

Reactions (1,887)

Citing (130)



Citation Map



Save

8

Total Synthesis of Microtubule-Stabilizing Agent (-)-Laulimalide**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/jo010854h](https://doi.org/10.1021/jo010854h)

CODEN: JOCEAH

ISSN: 0022-3263

ISSN-L: 0022-3263

Database Information

AN: 2001869107

CAN: 136:151030

PubMed ID: 11749630

CAplus and MEDLINE

Company/Organization

Department of Chemistry

University of Illinois at Chicago

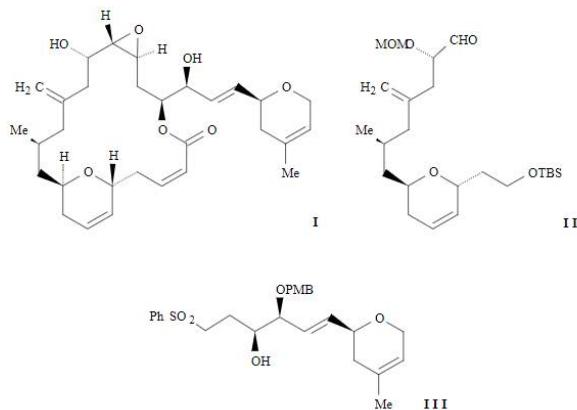
Chicago, Illinois 60607

United States

Emailarunghos@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 ramosa*. **I** represents a new class of antitumor agents with significant clin. potential. The **synthesis** is convergent and involved the assembly of C₉-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 alkyne acid followed by hydrogenation of the resulting alkynyl lactone over Lindlar's catalyst. Initial attempts of intramol. Still's variant of Horner-Evmonds olefination between the C₁₉-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**.



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**

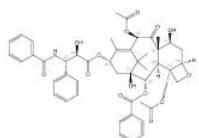
Full Text ▾

Expand All | Collapse All

- ▼ Concepts
- ▼ MEDLINE® Medical Subject Headings
- ▼ Supplementary Concepts
- ▲ Substances

Substances (105)

33069-62-4

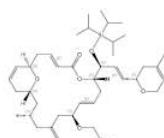


Absolute stereochemistry shown, Rotation (-)

 $C_{47}H_{51}NO_{14}$ **Taxol**

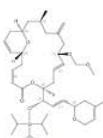
Role: Unspecified

725242-41-1

Absolute stereochemistry shown
Double bond geometry shown $C_{41}H_{66}O_7Si$

(1R,3E,9E,15S,17R)-7-[(1S,2E)-3-[(2S)-3,6-Dihydro-4-methyl-2H-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

725242-39-7

Absolute stereochemistry shown
Double bond geometry shown $C_{41}H_{66}O_7Si$

(1R,3Z,7S,9E,11S,15S,17R)-7-[(1S,2E)-3-[(2S)-3,6-Dihydro-4-methyl-2H-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

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。

The screenshot shows the SciFinder search interface. On the left, a sidebar titled "Searching for..." lists categories: All, Substances, Reactions, References (which is selected and highlighted in blue), Suppliers, Biosequences, and Retrosynthesis. A large blue box labeled "1" is positioned over the sidebar. In the center, the "References" search area is shown. It includes a search bar with "Organocatalysis", a dropdown menu set to "AND" and "Publisher", and a dropdown menu currently set to "American Chemical Society". Below the search bar is a button labeled "Add Advanced Search Field" with a plus sign. A blue box labeled "2" is positioned over this button. To the right, there is a link to "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，再在菜单中选中“publisher”，最后在输入框中输入出版社名称。

The screenshot shows the SciFinder search results page for the query "Organocatalysis". The top navigation bar includes the CAS logo, "SciFinder", "References", "Edit Search", and the search term "Organocatalysis". The main search results are displayed under the heading "References (869)". The results are sorted by "Times Cited" and viewed as "Full Abstract". The first result is a review titled "Organocatalysis by N-Heterocyclic Carbenes" by Enders, Dieter; Niemeier, Oliver; Henseler, Alexander, published in Chemical Reviews (Washington, DC, United States) (2007), 107(12), 5606-5655. The second result is a review titled "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, published in Accounts of Chemical Research (2004), 37(8), 580-591. Both results include links for "Full Text", "Substances (2)", "Reactions (0)", "Citing (2,258)", and "Citation Map". On the left, a filter sidebar titled "Filter Behavior" includes sections for "Document Type" (with "Journal" selected), "Language", "Publication Year" (with a histogram from 2000 to 2021), and "Available at My Institution". A blue box labeled "3" is positioned over the "Document Type" section.

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。

The screenshot shows the search results for 'Organocatalytic Reactions'. On the left, there is a sidebar with navigation links: 'Organization', 'Publication Name', 'Concept', and 'CA Section'. The 'Publication Name' section is expanded, showing a list of journals with counts: Organic Letters (108), Journal of the American Chemical Society (98), Journal of Organic Chemistry (90), ACS Catalysis (48), Accounts of Chemical Research (34). Below this is a 'View All' link. The main search results area displays the title 'Organocatalytic Reactions' by Flanigan, Darrin M.; Ro, Chemical Reviews (Washington, DC, United States) (1998). It includes a chemical reaction scheme with labels: 'Oxidation', 'Acylation', 'X', 'EWG', 'Y', 'Umpolung', 'Catalysis', and 'Annulation'. A 'Full Text' button is at the bottom of this panel.

Publication Name

Top Count Alphanumeric Search

0 Selected

- Organic Letters (108)
- Journal of the American Chemical Society (98)
- Journal of Organic Chemistry (90)
- ACS Catalysis (48)
- Accounts of Chemical Research (34)

View All

Full Text ▾

0 Selected

- Abstracts of Papers, 256th ACS National Meeting & Exposition, Boston, MA, United States, August 19-23, 2018 (7)
- Abstracts of Papers, 235th ACS National Meeting, New Orleans, LA, United States, April 6-10, 2008 (6)
- Abstracts of Papers, 236th ACS National Meeting, Philadelphia, PA, United States, August 17-21, 2008 (6)
- Abstracts of Papers, 242nd ACS National Meeting & Exposition, Denver, CO, United States, August 28-September (20)
- Chemical Reviews (Washington, DC, United States) (1998)
- Abstracts, 37th Northeast Regional Meeting of the American Chemical Society, Potsdam, NY, United States, June 2-5 (1)
- Abstracts, 38th Middle Atlantic Regional Meeting of the American Chemical Society, Hershey, PA, United States, June 4-7 (1)
- Abstracts, 40th Middle Atlantic Regional Meeting of the American Chemical Society, Queens, NY, United States, May 17-21 (1)
- Abstracts, 40th Northeast Regional Meeting of the American Chemical Society, Potsdam, NY, United States, June 2-5 (1)

Apply 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 SciFinderⁿ 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 shows the CAS SciFinder interface with the following details:

- Header:** CAS SciFinderⁿ, References dropdown, search bar containing "drying and pharmaceutical tablets", a blue search button with the number "1", and various navigation icons.
- Left Sidebar (Filter Behavior):**
 - Document Type: Journal (6,520), Patent (22K), Review (645), Biography (1), Book (9).
Buttons: Load More Results, Filter by, Exclude.
 - Language: Chinese (17K), English (8,710), Japanese (837), Korean (610), German (571).
Buttons: View All.
- Search Results:**
 - References (29,354):** Sort: Relevance, View: Partial Abstract.
Buttons: Substances (6), Reactions (0), Citing (76), Citation Map.
 - Result 1:** Formulation of a lyophilized dry emulsion tablet for the delivery of poorly soluble drugs
By: Corveley, S.; Remon, J. P.
International Journal of Pharmaceutics (1998), 166(1), 65-74 | Language: English, Database: Cplus
The objective was to develop a dry emulsion tablet for the flash delivery of poorly water soluble drugs using a lyophilization technique. The influence of formulation parameters on the characteristics of the lyophilized dry emulsion (LDE) tablets was investigated. Oil-in-water emulsions were made using a medium chain triglyceride as the oil phase and a maltodextrin solution (5-20%) as the water phase. In addition different emulsifier-tablet binder combinations were evaluated. The emulsions were filled into PVC blisters and freeze-dried. The resulting tablets were analyzed for strength, disintegrate, and dissolution.
 - Result 2:** Development of directly compressible powders via co-spray drying
By: Gonnissen, Y.; Remon, J. P.; Vervaet, C.
European Journal of Pharmaceutics and Biopharmaceutics (2007), 67(1), 220-226 | Language: English, Database: Cplus and MEDLINE
Continuous production of directly compressible powders was achieved by coprocessing acetaminophen and carbohydrates via spray drying. Binary and ternary powder mixtures containing drug substance and carbohydrates were prepared by co-spray drying.

2

In vitro and in vivo evaluation of a fast-disintegrating lyophilized dry emulsion tablet containing griseofulvin
By: Ahmed, Iman Saad; Aboul-Einien, Mona Hassan
European Journal of Pharmaceutical Sciences (2007), 32(1), 58-68 | Language: English, Database: Cplus and MEDLINE
Development of a fast-disintegrating lyophilized dry emulsion (LDE) tablet that enhanced the in vitro dissolution and in vivo absorption of griseofulvin (GF) is presented. The LDE tablets were prepared by freeze-drying o/w emulsions of GF, a drug for which bioavailability is known to be enhanced by fat co-administration. Oil-in-water emulsions were prepared using a gelatin solution (2%, w/v) as the water phase and medium chain triglycerides (Miglyol) or sesame oil as the oil phase. In addition, different emulsifiers were evaluated. The influence of formulation parameters on the disintegration

3

Evaluation of spray-drying as a method to prepare microparticles for controlled drug release
By: Palmieri, Giovanni Filippo; Wehrle, Pascal; Stamm, Andre
Drug Development and Industrial Pharmacy (1994), 20(18), 2859-79 | Language: English, Database: Cplus
The possibility to obtain microcapsules or microspheres for controlled release by spray-drying was evaluated. Drugs of different solubilities like theophylline and sodium sulfamethoxazole with Eudragit® EC as coating polymer were chosen. The polymers were either

4

5

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 displays the CAS SciFinder Reference Detail page for a specific publication. The top navigation bar includes the CAS SciFinder logo, search input ('drying and pharmaceutical tablets'), and various search and save icons. The main content area is titled 'Reference Detail' (3 of 1,078). On the left, a sidebar provides detailed journal information: Source (Journal of Pharmaceutical Investigation, Volume 46, Issue 6, 2016, DOI: 10.1007/s40005-016-0277-5), Database Information (AN: 2016:1510884, CAN: 170:250733, CAplus), Company/Organization (College of Pharmacy, Yeungnam University, Gyeongsan 38541, Korea, Republic of), Publisher (Springer), and Language (English). The central text area contains the abstract: 'Employing an optimized spray-drying process to produce ezetimibe tablets with an improved dissolution profile'. It is authored by Kim, Sungyub; Gupta, Bikram; Moon, Cheol; Oh, Euichaul; Jeong, Jee-Heon; Yong, Chul Soon; Kim, Jong Oh. The abstract discusses the low aqueous solubility of ezetimibe and how an optimized spray-drying process improves its dissolution profile. Below the abstract are keywords: ezetimibe, tablets, spray drying, process dissolution. A navigation sidebar on the right includes 'Full Text', 'Concepts', 'Substances', 'Formulations' (highlighted with a blue box and the number 9), and 'Cited Documents'. There is also an 'Expand All | Collapse All' link.

9. 点击 Formulations 查看制剂（配方）信息。

Ezetimibe Tablet: Drug Delivery Systems

[View CAS Formulus® Detail](#)

Location: Article Page 3, 8, Table 2

Purpose: Drug delivery systems

Target: solubility, bioavailability

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

Additional Components Reported in Full Text

Ezetimibe Tablet: Drug Delivery Systems

[View CAS Formulus® Detail](#)

Location: Article Page 2, 3, 8, 9, Table 2, 5

Purpose: Drug delivery systems

Target: solubility, bioavailability

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 interface. At the top, there is a navigation bar with the CAS SciFinder logo, a search input field containing "9040-27-1", and various icons for search, draw, and user profile. A large blue box labeled "1" highlights the search input field.

The main content area displays the search results for "Substances (1)". On the left, there is a filter sidebar with sections for Commercial Availability, Reaction Role, and Reference Role. A blue box labeled "2" highlights the "Reference Role" section, which includes filters for Adverse Effect and Agricultural Use.

The results list shows one entry: "9040-27-1" (Arabinoxylan). Below the entry, it says "Image Not Available". The entry is described as "Unspecified" and "Arabinoxylan". To the right of the entry, there are buttons for "3,667 References", "27 Reactions", and "7 Suppliers".

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。

The screenshot shows the SciFinder interface with the following details:

- Header:** CAS SciFinder, References, Enter a query..., Draw, Search, and user icons.
- Left Sidebar (Filter Behavior):** Document Type, Substance Role, Language, Publication Year, Author, Organization, Publication Name, Concept, CA Section, CAS Solutions, Formulation Purpose (selected), Food (25), Drug delivery systems (19), Dietary supplements (17), Antidiabetic agents (10), Antiobesity agents (9), View All.
- Top Right:** Sort: Relevance, View: Partial Abstract, download, email, save and alerts.
- Section 1 (Result 1):** Title: Cereal arabinoxylans: advances in structure and physiochemical 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→4) linked xylan backbone to which α -L-arabinofuranose units are attached as side residues via α (1→3) and/or α (1→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 Ara/Fuca_n substitution pattern. View More.
- Section 2 (Result 2):** Title: 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
- Bottom Center:** Full Text, 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 SciFinderⁿ 中检索药物的重利用信息：

The screenshot shows the CAS SciFinder interface. At the top, the search bar contains the CAS number '1166-34-3'. Below the search bar, the results are displayed under the heading 'Substances (1)'. The first result is highlighted with a blue box and labeled '1'. It shows the CAS number '1166-34-3', the chemical structure of Cinanserin, its chemical formula 'C₂₀H₂₄N₂OS', and its name 'Cinanserin'. Below the structure, there are buttons for '444 References' (which is also highlighted with a blue box) and '23 Suppliers'. On the far right of the result card is a 'Feedback' button.

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。

References (294)

Sort: Relevance ▾ View: Partial Abstract ▾

Filtering: Publication Year: No Min - 2000 X 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. X

1

Selective in vitro and in vivo binding of $[^{125}\text{I}]$ ADAM to serotonin transporters in rat brain
By: Choi, Seok-Rye; Hou, Catherine; Oya, Shunichi; Mu, Mu; Kung, Mei-Ping; Siciliano, Michael; Acton, Paul D.; Kung, Hank F.
Synapse (New York) (2000), 38(4), 403-412 | Language: English, Database: Cplus and MEDLINE

An improved iodinated tracer, ADAM (2-(2-((dimethylamino)methyl)-phenyl)thio)-5-iodophenylamine) for imaging serotonin transporters (SERT) with single photon emission computerized tomog. (SPECT), was prepared and characterized. Scatchard anal. of saturation binding of $[^{125}\text{I}]$ ADAM to rat frontal cortical membrane homogenates gave a K_d value of 0.15 ± 0.03 nM and a B_{\max} value of 194 ± 65 fmol/mg protein. Biodistribution of $[^{125}\text{I}]$ ADAM in rat brain after an iv injection showed a high specific binding in the regions of *lumohypothalamus, cortex, striatum, and hippocampus*, where SERT are concentrated and the.

View More ▾

Full Text ▾ Substances (2) Reactions (0) Citing (70) Citation Map

2

2-((2-((dimethylamino)methyl)phenyl)thio)-5-iodophenylamine (ADAM): an improved serotonin transporter ligand

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。

Concept

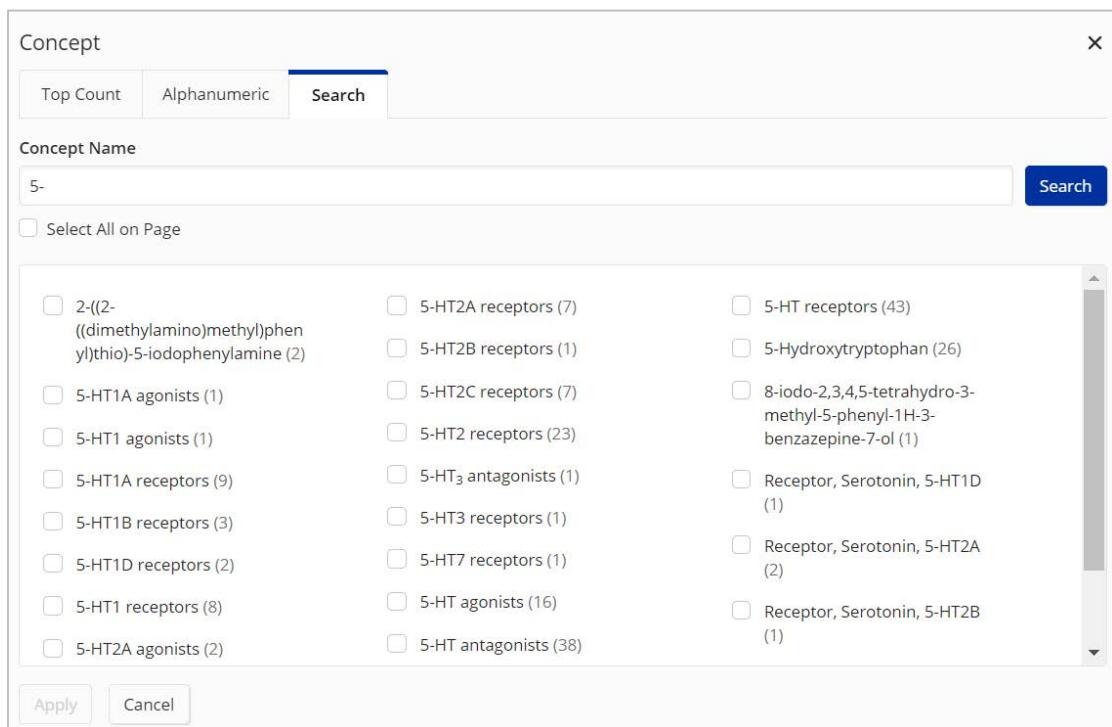
Top Count Alphanumeric Search

0 Selected 5

<input type="checkbox"/> Animals (249)	<input type="checkbox"/> Metergoline (18)	<input type="checkbox"/> Radioligand Assay (11)
<input type="checkbox"/> Male (158)	<input type="checkbox"/> 5-HT agonists (16)	<input type="checkbox"/> Receptors, Adrenergic, alpha (11)
<input type="checkbox"/> Cinanserin (141)	<input type="checkbox"/> Cerebral cortex (16)	<input type="checkbox"/> Swine (11)
<input type="checkbox"/> Rats (139)	<input type="checkbox"/> Quipazine (16)	<input type="checkbox"/> Tetrahydronaphthalenes (11)
<input type="checkbox"/> Serotonin (120)	<input type="checkbox"/> Receptors (16)	<input type="checkbox"/> 5-HT2A antagonists (10)
<input type="checkbox"/> Serotonin Antagonists (90)	<input type="checkbox"/> Behavior, Animal (15)	<input type="checkbox"/> Body temperature (10)
<input type="checkbox"/> Receptors, Serotonin (83)	<input type="checkbox"/> Frontal cerebral cortex (15)	<input type="checkbox"/> Brain corpus striatum (10)
<input type="checkbox"/> Female (61)	<input type="checkbox"/> Haloperidol (15)	<input type="checkbox"/> Immunosuppressive Agents (10)
<input type="checkbox"/> Rats, Inbred Strains (60)	<input type="checkbox"/> Motor activity (15)	<input type="checkbox"/> Mianserin (10)
<input type="checkbox"/> Brain (58)	<input type="checkbox"/> Rabbits (15)	<input type="checkbox"/> Naloxone (10)
<input type="checkbox"/> In Vitro Techniques (51)	<input type="checkbox"/> Blood pressure (14)	<input type="checkbox"/> Neurons (10)
<input type="checkbox"/> Methylsergide (44)	<input type="checkbox"/> Dogs (14)	

Apply Cancel

4. 点击 View All，查看所有 Concept。



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。可以继续在 Concept 搜索特定的核心研究点。

References (155)

Sort: Relevance View: Partial Abstract

Filtering: Publication Year: 2000 - No Max

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.](#)

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.
Journal of Nuclear Medicine (2001), 42(10), 1556-1562 | Language: English, Database: CAplus and MEDLINE
We reported recently a highly selective radioligand, 2-[{2-[(dimethylamino)methyl]phenyl]thio]-5-[¹²³I]iodophenylamine (ADAM), for SPECT imaging of serotonin transporters (SERT). In this article we describe the kinetic modeling of [¹²³I]ADAM and its ability to quantitatively measure the concentrations of SERT in the nonhuman primate brain. We also investigate simplified models of tracer behavior that do not require invasive arterial blood sampling. Methods: Three female baboons each underwent 3 [¹²³I]ADAM SPECT studies. The studies consisted of a dynamic sequence of counts/two 5-min View More

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

6. 将肉桂硫胺文献结果集的发表年限定为 2000 年之后。

Concept

Top Count Alphanumeric Search

7

<input type="checkbox"/> Radiopharmaceuticals (38)	<input type="checkbox"/> 5-HT7 receptors (9)	<input type="checkbox"/> Pharmacokinetics (7)
<input type="checkbox"/> Iodine Radioisotopes (28)	<input type="checkbox"/> Antidepressants (9)	<input type="checkbox"/> Psychosis (7)
<input type="checkbox"/> Serotonin (25)	<input type="checkbox"/> Brain hippocampus (9)	<input type="checkbox"/> 5-HT1B receptors (6)
<input type="checkbox"/> Single-photon-emission computed tomography (25)	<input type="checkbox"/> Cerebellum (9)	<input type="checkbox"/> 5-HT1 receptors (6)
<input type="checkbox"/> Midbrain (22)	<input type="checkbox"/> Major depression (9)	<input type="checkbox"/> 5-HT2A antagonists (6)
<input checked="" type="checkbox"/> Antiviral agents (20)	<input type="checkbox"/> Mental and behavioral disorders (9)	<input type="checkbox"/> 5-HT receptors (6)
<input type="checkbox"/> Middle Aged (19)	<input type="checkbox"/> Mice (9)	<input type="checkbox"/> Aging, animal (6)
<input type="checkbox"/> Serotonin Antagonists (19)	<input type="checkbox"/> Molecular docking (9)	<input type="checkbox"/> Animal gene (6)
<input type="checkbox"/> Tissue Distribution (19)	<input type="checkbox"/> Reproducibility of Results (9)	<input type="checkbox"/> Anxiety (6)
<input type="checkbox"/> Protein Binding (18)	<input type="checkbox"/> Serotonergic neurotransmission (9)	<input type="checkbox"/> Bipolar disorder (6)
<input type="checkbox"/> Rats (18)	<input type="checkbox"/> Tropones (9)	<input type="checkbox"/> Cell line (6)
<input type="checkbox"/> Mesencephalon (16)	<input type="checkbox"/> 5-HT3 receptors (8)	<input type="checkbox"/> Cognitive disorders (6)

8

9

Synapse (New York) (2000), 38(4), 403-412 | Language: English, Database: CAplus and MEDLINE
An improved iodinated tracer, ADAM (2-[{2-[(dimethylamino)methyl]phenyl}thio]-5-iodophenylamine) for imaging serotonin

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 shows the CAS SciFinder interface with the following details:

- Header:** CAS SciFinderⁿ, References, Enter a query..., Draw, Search, Favorites, Help.
- Left Sidebar (Filter Behavior):**
 - Document Type:** Biological Study (18), Uses (16), Properties (4), Preparation (3), Reactant or Reagent (1). A blue box highlights "View All".
 - Language:** Publication Year (10). A blue box highlights "10". A histogram shows publication years from 1998 to 2021. A blue box highlights "2000 to No Max Apply". Buttons for Reset and View Larger are visible.
 - Author and Organization filters are also present.**
- Search Bar:** Sort: Publication Date: Oldest, View: Partial Abstract.
- Search Results:**
 - References (20):** A blue box highlights "11".
 - Filtering:** Publication Year: 2000 - No Max, Concept: Antiviral agents.
 - Message:** CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinderⁿ users. Use the [CAS Solutions: Formulus filter](#) to view available content. [Learn more about Formulus.](#)
 - Result 1:** screening of anti-SARS coronavirus agents targeting protease 3CL. By: Shen, Jianhua; Jiang, Hualiang; Shen, Xu; Zuo, Jianping; Luo, Xiaomin; Bai, Donglu; Shen, Jingkang; Chen, Kaixian; Gui, Chunshan; Chen, Lili. China, CN1472336 A 2004-02-04 | Language: Chinese, Database: CAplus. The current invention uses protease 3CL of SARS coronavirus (CoV) as target for screening anti-CoV agents. The three-dimensional structure model of the protease 3CL was applied to search for the existing drug database via mol. docking-virtual screening method. Candidate compound that shows strong bonding activity to protease 3CL were selected and tested for the protective effects in SARS CoV infected cells. Cinanserin was synthesized. [View More](#)
 - Result 2:** Cinanserin is an inhibitor of the 3C-like proteinase of severe acute respiratory syndrome coronavirus and strongly reduces virus replication in vitro. By: Chen, Lili; Gui, Chunshan; Liu, Xiaomin; Yang, Qineang; Guenther, Stephan; Scandella, Elke; Drost, Christian; Bai, Donglu; He.
- Bottom Buttons:** PatentPak (blue box highlights "12"), Full Text, Substances (9), Reactions (0), Citing (1), Citation Map.

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 SciFinderⁿ 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。

[22] 申请日 2003.6.4 [21] 申请号 03129071.X
 [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
 共同申请人 上海先导药业有限公司
 [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

[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

权利要求书 2 页 说明书 13 页 附图 3 页

[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

[57] 摘要

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

13

S N 1 0 0 8 - 4 2 7 4

13. 在 CAS SciFinderⁿ 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 SciFinderⁿ 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 SciFindern 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, there is a sidebar with various search categories: All, Substances, Reactions, References (which is highlighted with a blue arrow labeled '1'), Suppliers, Biosequences, and Retrosynthesis. The main search area has a search bar containing 'Pesticide and ecotoxicity' (highlighted with a blue box labeled '2'). Below the search bar are dropdown menus for 'AND' and 'Author Name', and a text input field for 'Enter last name, first name middle name.' To the right of the search bar are buttons for 'Draw' and a magnifying glass icon. At the bottom right of the search area, there is a link 'Learn more about SciFinderⁿ Advanced Search.' The top right of the interface includes links for 'Saved', 'History', and 'Account'.

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。

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 (1,985)

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.](#)

Document Type

- Journal (1,882)
- Patent (10)
- Review (368)
- Book (2)
- Clinical Trial (2)

[View All](#)

Language

- English (1,834)
- German (63)
- Chinese (47)
- Japanese (10)

Assessing the Ecotoxicity of Pesticide Transformation Products
By: Sinclair, Chris J.; Boxall, Alistair B. A.
Environmental Science and Technology (2003), 37(20), 4617-4625 | Language: English, Database: CPlus and MEDLINE
Once released to the environment, pesticides may be degraded by abiotic and biotic processes. While parent compounds are assessed in detail in many regulatory schemes, the requirements for the assessment of transformation products are less well developed. This study was therefore performed to explore the relationships between the toxicity of transformation products and their parent compounds and to develop a pragmatic approach for use in the risk assessment of transformation products. Data were obtained on the properties and ecotoxicity of transformation products arising from a wide range of [redacted]
[View More](#)

Full Text Substances (117) Reactions (0) Citing (158) Citation Map

Wildlife Ecotoxicology of Pesticides: Can We Track Effects to the Population Level and Beyond?
By: Koehler, Heinz-R.; Triebskorn, Rita
Science (Washington, DC, United States) (2013), 341(6147), 759-765 | Language: English, Database: CPlus and MEDLINE

3. 所得结果集。

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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](#)

Pesticide or ecotoxicity

4

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

+ Add Advanced Search Field

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. At the top, there is a navigation bar with the CAS SciFinder logo, a search input field containing 'Pesticide or ecotoxicity', and various search and filter icons. A large blue number '5' is overlaid on the top right. Below the navigation bar, the main content area is titled 'References (272,371)'. It includes a sidebar for 'Filter Behavior' with sections for 'Document Type' (Journal, Patent, Review, Biography, Book), 'Language' (English, Chinese, German, Japanese, Russian), and 'Publication Year'. The main search results display two entries:

- Assessing the Ecotoxicity of Pesticide Transformation Products**
By: Sinclair, Chris J.; Boxall, Alistair B. A.
Environmental Science and Technology (2003), 37(20), 4617-4625 | Language: English, Database: CPlus and MEDLINE
Once released to the environment, pesticides may be degraded by abiotic and biotic processes. While parent compounds are assessed in detail in many regulatory schemes, the requirements for the assessment of transformation products are less well developed. This study was therefore performed to explore the relationships between the toxicity of transformation products and their parent compounds and to develop a pragmatic approach for use in the risk assessment of transformation products. Data were obtained on the properties and ecotoxicity of transformation products arising from a wide range of [View More](#)
- Wildlife Ecotoxicology of Pesticides: Can We Track Effects to the Population Level and Beyond?**
By: Koehler, Heinz-R.; Triebskorn, Rita
Science (Washington, DC, United States) (2013), 341(6147), 759-765 | Language: English, Database: CPlus and MEDLINE

At the bottom of the results, there are buttons for 'Full Text', 'Substances (117)', 'Reactions (0)', 'Citing (158)', and 'Citation Map'.

5. 所得结果集。

The screenshot shows the CAS SciFinder search interface. On the left, there is a sidebar with arrows pointing to different search categories: All, Substances, Reactions, References (which is highlighted in blue), Suppliers, Biosequences, and Retrosynthesis. The main search area is titled 'References' and contains a search bar with the query 'Pesticide not ecotoxicity'. A large blue number '6' is overlaid on the search bar. Below the search bar, there are dropdown menus for 'AND' and 'Author Name', and a text input field for 'Enter last name, first name middle name.' with an example 'Schubert, J A'. There is also a link 'Learn more about SciFinderⁿ Advanced Search.'

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。

如需更多 CAS SciFinderⁿ 帮助，请联系 china@acs-i.org, 010-63508026/7

CAS SciFinder

References ▾ Pesticide not ecotoxicity 7 X Draw Search Save Print User

[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 Download Email Save And Alerts

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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 nervous system.
[View More](#)

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

2 **Emission of pesticides into the air**
By: Van Den Berg, F.; Kublik, 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

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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 X Draw Search

AND Author Name X

[Example: Schubert, J A](#)

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

Add Advanced Search Field

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。

The screenshot shows the CAS SciFinder interface with the following details:

- Search Bar:** high efficiency and low toxicity and (pesticide or herbicide)
- Results Summary:** References (2,054)
- Sort and View Options:** Sort: Relevance, View: Partial Abstract
- Filter Options:** Substances (23), Reactions (0), Citing (0), Citation Map
- Result 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: CAplus
 - Description: 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 flumidorac-pentyl EC, 12-15 parts of fomesafen, 8-15 parts of clorsulfuron-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 triacontanol, 2-4 parts of urea, 10-20 parts of carb.
 - [View More](#)
- Result 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: CAplus
 - Description: 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®

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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 10

AND Author Name En name middle name.

[Example: Schubert, J A](#)

[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](#)

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; Gaddamangu, 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](#)

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.; Couladouros, 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 SciFinderⁿ 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。

The screenshot shows the CAS SciFinder interface with a search bar containing 'synth*'. The results page displays 13,004,948 references. The first result is titled 'Triblock copolymer syntheses of mesoporous silica with periodic 50 to 300 angstrom pores' by Zhao, Dongyuan; Feng, Jianglin; Huo, Qisheng; Melosh, Nicholas; Frederickson, Glenn H.; Chmelka, Bradley F.; Stucky, Galen D. from Science (Washington, D. C.) (1998), 279(5350), 548-552. The second result is 'Nitric oxide synthases: structure, function and inhibition' by Alderton, Wendy K.; Cooper, Chris E.; Knowles, Richard G. from Biochemical Journal (2001), 357(3), 593-615.

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

The screenshot shows the SciFinder interface with the search term 'alumin?um' entered in the search bar. The results page displays two entries:

- Entry 51:** A compilation of corrosion potentials reported for intermetallic phases in aluminum alloys. It is a review from the Journal of the Electrochemical Society (1995), 142(11), 3994-6. The abstract mentions a range of corrosion potentials for dilute aluminum binary alloys and their galvanic relations.
- Entry 52:** Grain refinement of aluminium and its alloys by heterogeneous nucleation and alloying. It is a review from International Materials Reviews (2002), 47(1), 3-29. The abstract discusses grain refinement methods and mechanisms.

On the left sidebar, there are filters for Document Type, Substance Role, and Language, each with several options listed.

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

注：

- 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；
- 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；
- 一个检索式中不可超过 5 个通配符，否则会出错。

The screenshot shows the SciFinder interface with a search query containing multiple wildcard characters. A red box highlights an error message: "The query cannot contain more than 5 valid wildcard search terms. Learn more about wildcard searching."

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&rhllterm= wildcard&hsyns=%20](https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-)

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。

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

4

Micro biological conversion of steroids. 4. Part Pregnenolone oxidation by Rhizopus nigricans VNICHFI-7
By: Kogan, L. M.; Elin, E. A.; v, A. S. Barman 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。

Concept X

Top Count Alphanumeric **Search** **2**

Concept Name
steroid* **3** **Search**

11 Selected

<input checked="" type="checkbox"/> Anabolic steroids (2)	<input checked="" type="checkbox"/> Steroid esters (1)	<input checked="" type="checkbox"/> Steroids, Chlorinated (1)
<input checked="" type="checkbox"/> Saponins, steroidal (1)	<input checked="" type="checkbox"/> Steroid Hydroxylases (1)	<input checked="" type="checkbox"/> Steroids, Fluorinated (1)
<input checked="" type="checkbox"/> Steroidal alkaloids (1)	<input checked="" type="checkbox"/> Steroids (42)	<input checked="" type="checkbox"/> Steroids, saponins (1)
<input checked="" type="checkbox"/> Steroidal hormones (1)	<input checked="" type="checkbox"/> Steroids, Brominated (1)	

4 **Apply** **Cancel**

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 SciFinder search results for "steroids and fermentation and \"rhizopus stolonifer\"". The left sidebar has a section titled "Concept" which is currently expanded, displaying a list of concepts:

- Rhizopus stolonifer (76)
- Fermentation (52)
- Steroids (42)
- Hydroxylation (33)
- Biotransformation (15)

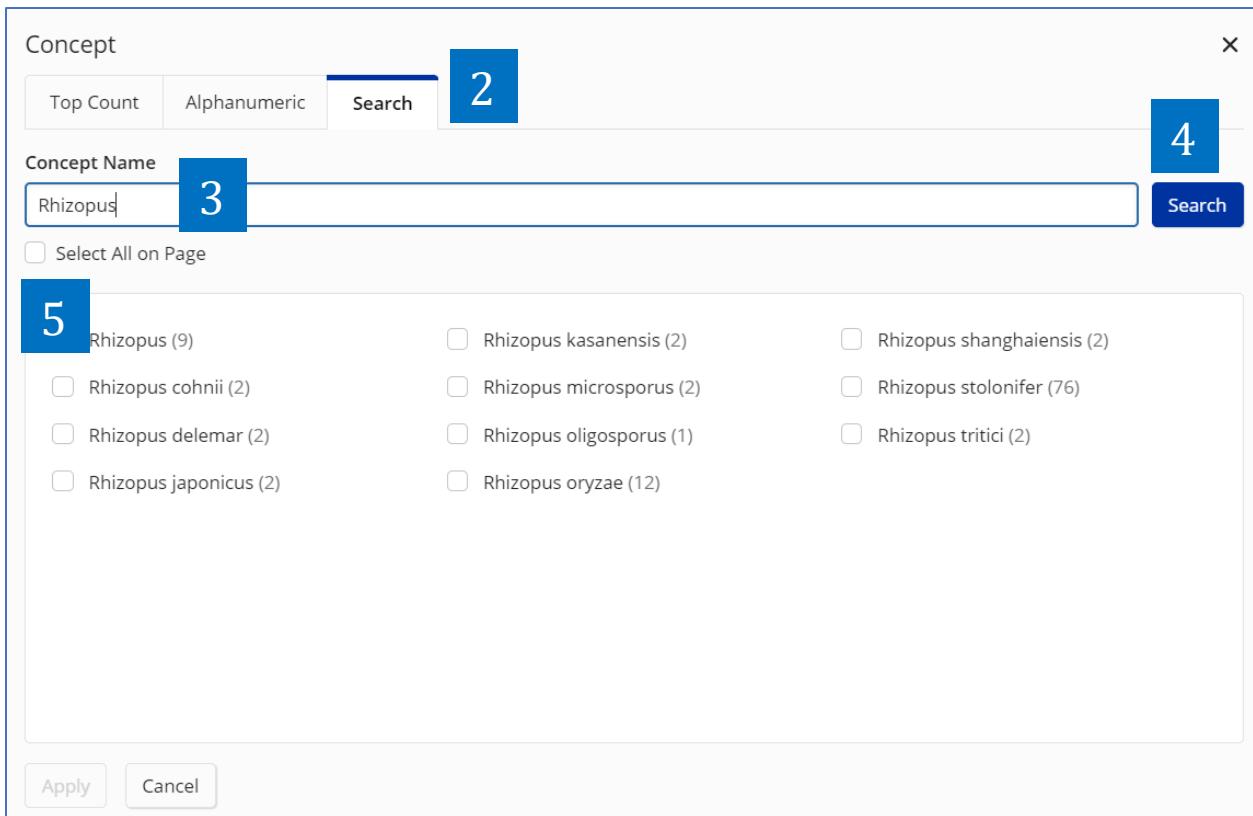
Below this list are buttons for "View All" and "CA Section". A large blue box highlights the number "1" next to the "View All" button.

The main search results area shows two entries:

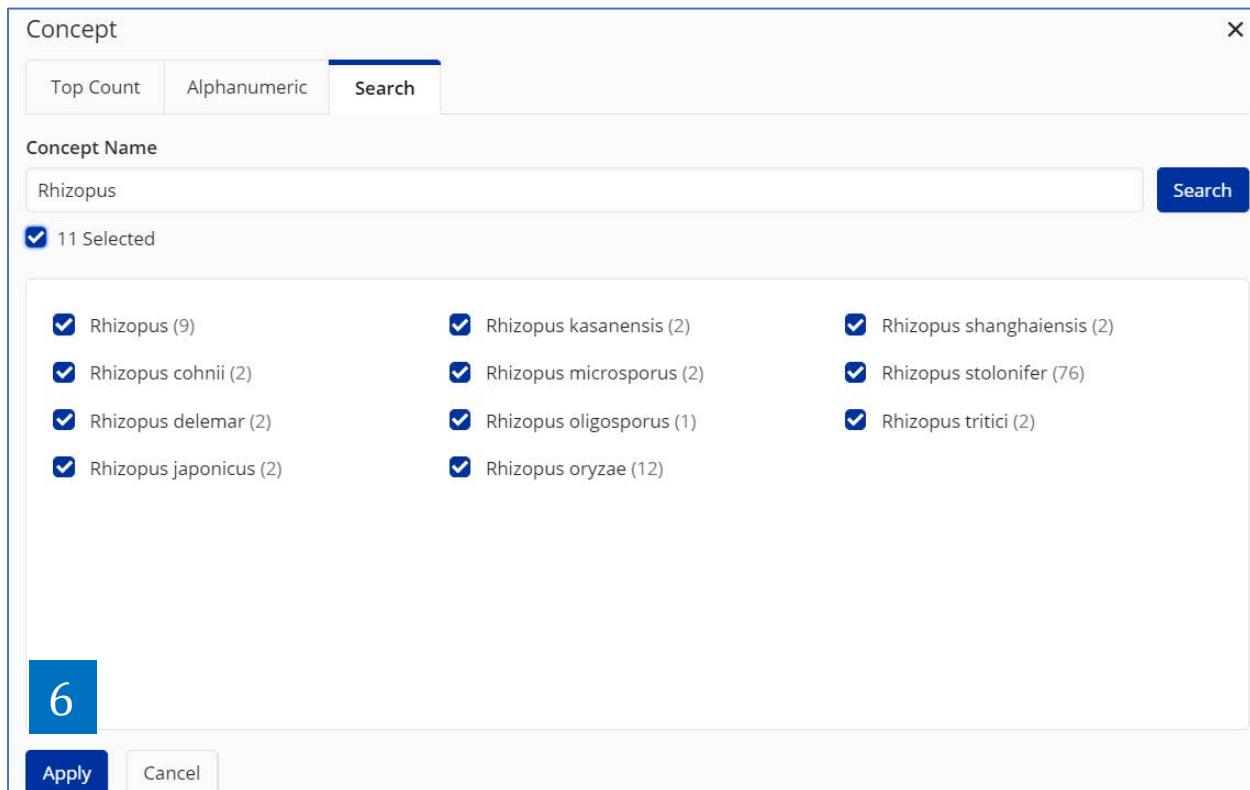
- Microbial oxidation of anabolic steroids**
By: Choudhary, M. Iqbal; Adnan, S.; Shah, A.; Atta-Ur-Rahman
Natural Product Research (2008), 22(15), 1289-1296 | Language: English, Database: CAPLUS and MEDLINE
Microbial transformation of two anabolic **steroids**, ethylestrenol (1) and nandrolone (2), were 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).
- 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
Machine Translated: In the **fermentation** of pregnenolone with Rh. nigricans VNICHFI-7 are d5-pregnene triol 3 β .7 α .11 α -on- (20) and d5-gene diol 3 β .11 α -dien- (7.20) formed

Below the first entry are buttons for "Full Text", "Substances (7)", "Reactions (2)", "Citing (13)", and "Citation Map".

1. 点击 View All，展开所有的子项。

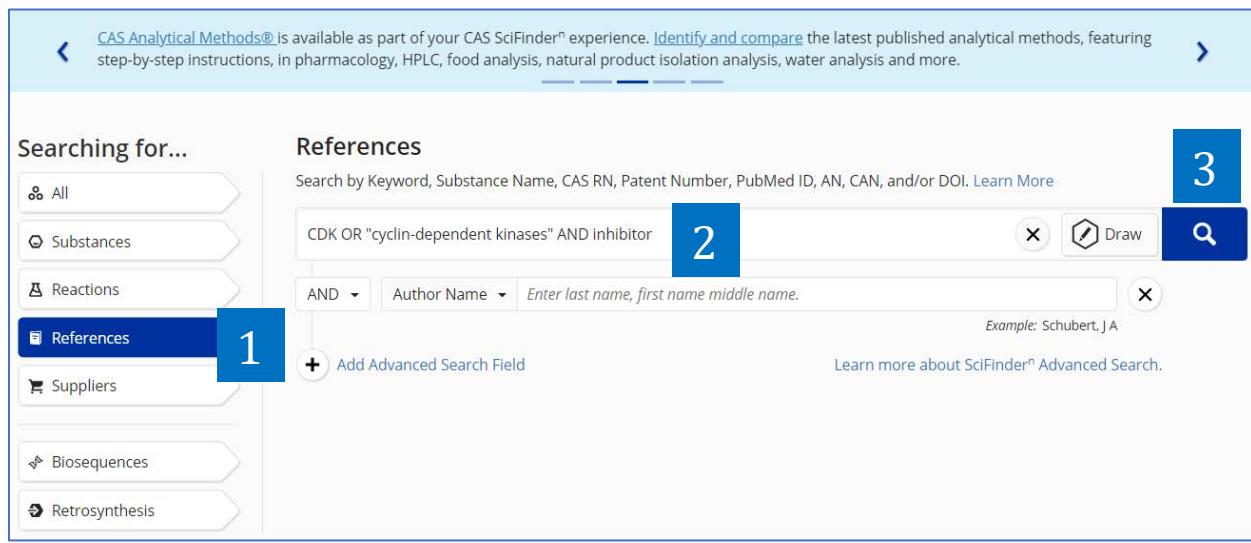


2. 点击 Search，在展开所有子项中进行检索。
3. 输入检索词。
4. 点击 Search 开始检索。
5. 勾选 Select All on Page，可以全部选中检索得到的子项。



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



1. 选择 References
2. 输入检索式
3. 开始检索

CAS SciFinderⁿ References CDK OR "cyclin-dependent kinases" AND inhibitor Draw

▼ Concept
▼ CA Section
▼ CAS Solutions
▼ Formulation Purpose
▼ Database
▼ Search Within Results

Filter Content Report
Download filter data from this result set.

A review with 93 references **Cyclin-dependent kinases** trigger and coordinate transitions between different phases the cell division cycle (CDK1, 2, 3, 4, 6, 7). They also play a role in apoptosis (CDK2), in neuronal cells (CDK5) and in the control of transcription (CDK7, 8, 9). Intensive screening has lead to the recent identification of a series of chem. **inhibitors** of **CDKs**: olomoucine, roscovitine, purvalanol, CVT-313, flavopiridol, γ -butyrolactone, indirubins, paullones and staurosporine. Some of these compounds display remarkable selectivities and efficiencies ($IC_{50} < 25 \text{ nM}$). Many have b.

[View More](#)

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

□ 5 **4**

Cyclin dependent kinase (CDK) inhibitors as anticancer drugs
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: CPlus 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 relationship.

[View More](#)

Full Text Substances (3) Reactions (0) Citing (118) 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: Cplus 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)

Substances (3) Reactions (0) Citing (118) Citation Map

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 ▾

Concepts

Antitumor agents	Homo sapiens
Cyclin-dependent kinase inhibitors	Human
	Neoplasm

Expand All | Collapse All

5

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

7

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
---	--	---

8

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 SciFinderⁿ 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 Prev Next 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
Cplus

Language: English

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinderⁿ 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](#)

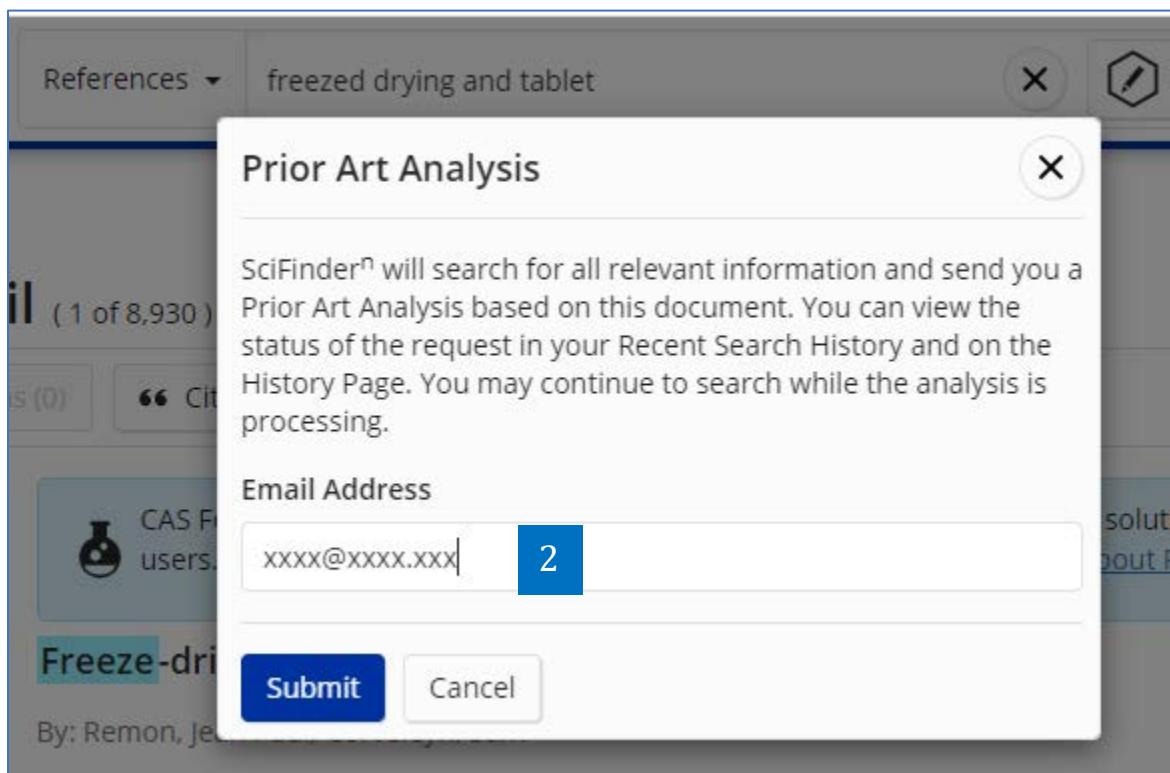
▼ IPC Data

▼ |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 SciFinderⁿ.

[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, Shellie; Pathak, Yashwant V.
Powder Technology (1993) | English

[Rapidly disintegrating tablets containing gums and carbohydrates](#)

By: Pebbley, 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: Ntawukulilyayo, J. D.; Vervaet, 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

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 SciFinderⁿ 浏览现有技术相关文献。

The screenshot shows the CAS SciFinder® interface with the following details:

- Header:** CAS SciFinder® logo, References dropdown, search bar "Enter a query...", and various navigation icons (Draw, Search, Star, Clock, User).
- Left Sidebar (Filter Behavior):**
 - Filter by:** Substances (87), Reactions (89), Clinical Trial (2), Letter (1).
 - Document Type:** Journal (87), Patent (89), Clinical Trial (2), Letter (1).
 - Language:** English (150), French (8), German (8), Japanese (5), Chinese (1). Includes a "View All" link.
 - Publication Year:** A histogram showing the distribution of publications from 1972 to 1999. It includes "No Min" and "No Max" buttons and an "Apply" button. A "View Larger" link is also present.
- Main Content:**

References (176)

5

Sort: Relevance | View: Full Abstract

1

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

By: Corveley, Sam; Remon, Jean Paul
International Journal of Pharmaceutics (1997), 152(2), 215-225 | Language: English, Database: CAplus

The influence of different formulation and process parameters on the characteristics of lyophilized oral dosage forms was investigated. Maltodextrins, gelatins, xanthan gum and hydroxyethyl cellulose were evaluated as excipients in the formulation of freeze-dried tablets. The resulting tablets were analyzed for mech. strength, porosity, disintegration time and residual moisture. Scanning electron micrographs of the fracture plane of the tablets were taken. Addnl. dissolution tests were performed on lyophilized tablets containing hydrochlorothiazide as a model drug. The concentration of the maltodextrins, used as the matrix forming agent, influenced the integrity and strength of the tablets. Increasing the maltodextrin concentrations resulted in stronger tablets. The concentration of the maltodextrins had also an influence on the pore size of the freeze-dried product. There was no influence of the DE value of the maltodextrin on the characteristics of the tablets. The disintegration time of the tablets was also affected by the maltodextrin concentration. The strength of the tablets depended on the xanthan gum concentration and the tablet dimensions. Compared to the formulations using xanthan gum as a binder in the same concentration, the disintegration time of the tablets containing hydroxyethyl cellulose (HEC) was much shorter: 55 s for the xanthan gum formulations and 7 s for the HEC formulations. The *in vivo* disintegration time was significantly higher at 0.5% (w/v) HEC compared to 0.25% (w/v)(P < 0.01). The *in vivo* disintegration time of the tables containing hydrolyzed gelatin Solugel LB as a binder was below 23 s for the *in vivo* tests. Unlike the xanthan gum formulations, no gel-like structure was formed upon contact with the saliva. The strength of the tablets was enhanced by using higher maltodextrin concentrations. The incorporation of hydrochlorothiazide in the formulations induced a decrease in strength of the tablets. The percentage of HCT released within 10 min was 64.55% and 77.84% for the reference tablets and the lyophilized table formulation, resp. the addition of PEG 6000 (1% w/v) resulted in an increase of drug release as 93.3% was released from the lyophilized tablets within 10 min. However, the incorporation of PEG 6000 in the formulation resulted in a decrease in the strength of the tablets.
- Bottom Navigation:** Full Text, Substances (4), Reactions (0), Citing (174), 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 SciFinder interface with the following details:

- Header:** CAS SciFinder®
- Search Bar:** References ▾ PCSK9 inhibitor
- Toolbar:** Draw, Search, Favorites, Help, User Profile
- Left Sidebar (Filter Behavior):**
 - Document Type:** Patent (21K) is selected (highlighted with a blue box). Other options include Journal (183K), Review (34K), Biography (8), and Book (129).
 - Substance Role:** Biological Study (798), Uses (214), Analytical Study (139), Properties (103), Preparation (50).
- Results Area:**
 - References:** 21,613 (Sort: Relevance, View: Partial Abstract)
 - Filtering:** Document Type: Patent
 - Message:** 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.](#)
 - Result 1:** **PCSK9 inhibitors and methods of use thereof**
By: Abou-Gharios, 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).
 - PatentPak Options:** Full Text, Reactions (0), Citing (2), Citation Map
 - Patent Details:** WO2016040305, English, A1, PDF, PDF+, Viewer; US20170290806, English, A1, PDF
 - Text Overlay:** in 9 (PCSK9) inhibitors for treating lipid disorders 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 browser interface. On the left, there is a vertical sidebar with four sections, each containing a chemical structure and its CAS Registry Number (RN). The sections are labeled 1, 2, 3, and 4 from top to bottom.
 - Section 1: CAS RN 743450-46-6, Analyst Markup Locations (1) Page 56.
 - Section 2: CAS RN 1006086-05-0, Analyst Markup Locations (1) Page 68.
 - Section 3: CAS RN 943-45-3D, Analyst Markup Locations (1) Page 56.
 - Section 4: CAS RN 678229-07-3, Analyst Markup Locations (1) Page 68.
 The main content area displays a patent claim with numbered steps. Step 2 is highlighted with a blue box and contains a chemical structure of a molecule with a phenyl ring, an oxygen atom, and a hydroxyl group. Step 4 is also highlighted with a blue box and contains another chemical structure.
 The claim text is as follows:

2. A method for disrupting the protein-protein interaction between PCSK9 and low-density lipoprotein receptor (LDLR), comprising:
administering a therapeutically effective amount of the composition of any one of claims 1-10 to a subject.

13. A method for treating a lipid disorder in a subject, comprising:
administering a therapeutically effective amount of the composition of any one of claims 1-10 to a subject.

14. The method of claim 13, wherein the lipid disorder is hypercholesterolemia.

15. The method of claim 13 or claim 14, wherein the composition further comprises an additional therapeutic agent selected from the group consisting of an HMGCoA reductase inhibitor, a nicotinic acid, a fibrate, and a bile acid-binding resin.

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

1 All Answer Types

2

3

4

All Answer Types

Top two answers by relevance from each answer type.

Substances (18)

1 24424-99-5

CC(C)(C)OC(=O)OC(=O)OC(C)(C)C

C₁₀H₁₈O₅
Di-tert-butyl dicarbonate

56K References 160K Reactions 138 Suppliers

2 75-31-0

CC(C)N

C₃H₉N
Isopropylamine

22K References 28K Reactions 62 Suppliers

View All Substances

Reactions (35)

Scheme 1 (1 Reaction)

Steps: 1 Yield: 99%

CC(C)(C)OC(=O)N1C=C(O)C(=O)c2ccccc2Cl>=>CC(C)(C)OC(=O)N1C=C(O)[C@H](C(=O)O)c2ccccc2Cl

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。

5. 选择 References，获得该专利及其同族信息。

CAS SciFinder® Substances WO2013173779 6 Draw

[Return to Home](#)

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

References Reactions Suppliers

<input type="checkbox"/> 1 1489004-67-2 Double bond geometry shown <chem>C19H26ClNO4</chem> Ethyl (oZ)-4-chloro-a-[[[(1,1-dimethylethoxy)carbonyl](1-methylethyl)amino]methylene]benzeneacetic acid 2 References 2 Reactions 0 Suppliers	<input type="checkbox"/> 2 1489004-64-9 <chem>C12H14ClNO2</chem> 4-Chloro-a-[[[(1-methylethyl)amino]methylene]benzeneacetic acid 2 References 2 Reactions 0 Suppliers	<input type="checkbox"/> 3 1489004-59-2 <chem>C19H24ClNO6</chem> a-[[Bis[(1,1-dimethylethoxy)carbonyl]amino)methylene]-4-chlorobenzeneacetic acid 2 References 6 Reactions 0 Suppliers
<input type="checkbox"/> 4 1489004-54-7 <chem></chem>	<input type="checkbox"/> 5 1489004-53-6 <chem></chem>	<input type="checkbox"/> 6 1489004-41-2 <chem></chem>

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

6. 选择 Substances，获得该专利披露的物质信息。

The screenshot shows the CAS SciFinder web interface. At the top, there is a navigation bar with the CAS SciFinder logo, a dropdown menu for 'Reactions', the document ID 'WO2013173779', a search bar containing the number '7', and various user icons. On the left, there is a sidebar titled 'Filter Behavior' with sections for 'Yield' (checkboxes for 90-100%, 70-79%, 50-69%, 30-49%, and 'No Yield Available'), 'Number of Steps' (checkboxes for 1, 2, 3, 4, 5), and 'Non-Participating Functional Groups' (checkboxes for Halide, Phenyl halide, Acyclic alkene, Alkene, and Carbamate). The main content area is titled 'Reactions (35)' and shows a specific reaction entry for 'Process for making amino acid compounds using enantioselective hydrogenation reactions'. It includes the author 'By: Remarchuk, Travis', the patent number 'WO2013173779', the date 'A1 2013-11-21', the language 'English', and the database 'Cplus'. Below this, there are buttons for 'PatentPak', 'Full Text', and 'View 23 Related Reactions'. The reaction itself is shown with two chemical structures connected by an arrow, labeled 'Absolute stereochemistry shown'. At the bottom of the reaction card, it says 'Steps: 1 Yield: 99%' and provides links to 'View Reaction Detail' and 'Experimental Protocols'.

7. 选择 Reactions，获得该专利披露的反应信息。

The screenshot shows the CAS SciFinder search interface. At the top, there is a search bar with the text 'Searching for...', a dropdown menu with 'All' selected, and various search categories: 'Substances', 'Reactions', 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'. To the right of the search bar, there are buttons for 'Saved', 'History', 'Account', and a search icon. The search results for 'CA2013-2873658' are displayed, showing the search term in the search bar and a search icon.

[Return to Home](#)[Show only](#)[Substances \(18\)](#)[Reactions \(35\)](#)[References \(2\)](#)[Suppliers \(0\)](#)

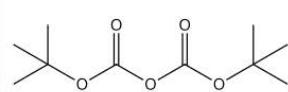
>All Answer Types

Top two answers by relevance from each answer type.

Substances (18)

1

24424-99-5



C₁₀H₁₈O₅
Di-tert-butyl dicarbonate

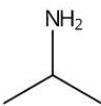
56K
References

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

生物序列检索

通过生物序列检索结果获取研究文献

Biosequences (10)

Sort: Alignment Identity ▾ View: Expanded ▾

Query Details MSGRHRKPTTSNVSVAKIAFTCAVLGGGGIAMAAQATAATDGEWDQVARCESGGNWSINTGNGYLGGLQFTQSTWAHHGGFAPSALAS... [View More](#)

1 Alignment Identity: 99.75%
Matches: 406 Mismatches: 1

2 Subject 1 737

3 References

Tuberculosis Compositions And Methods Of Treating Or Preventing Tuberculosis
Assignee: INTERNATIONAL AIDS VACCINE INITIATIVE, INC.
US20170362284 A1 | Seq ID No: 69

Tuberculosis compositions and methods of treating or preventing tuberculosis
Assignee: AERAS
WO2017218867 A1 | Seq ID No: 69

Recombinant cytomegalovirus vectors as vaccines for tuberculosis
Assignees: AERAS; OREGON HEALTH AND SCIENCE UNIVERSITY
WO2017223146 A1 | Seq ID No: 24

1. 获取 Biosequences 检索结果集中所有生物序列的研究文献。
2. 在 CAS SciFinderⁿ 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 shows the SciFinder Biosequences search interface. On the left, there's a sidebar with links: All, Substances, Reactions, References, Suppliers, Biosequences (which is highlighted), and Retrosynthesis. The main area has tabs for BLAST, CDR, and Motif, with 'Biosequences' selected. A search bar says 'Enter a protein or nucleotide string, or upload a .txt or .fasta file.' Below it, a sequence is pasted. To the right, there are buttons for 'Upload Sequence' and 'Clear Search'. On the far right, there are buttons for 'Sequence Type' (Nucleotide is selected), 'Search Within' (Nucleotides is selected), 'Include NCBI Sequences' (checked), 'Limit Total Sequence Results to' (set to 20000), and a large blue 'Start Biosequence Search' button.

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?	Gap Costs 2
<input type="text" value="50"/>	<input type="radio"/> Yes <input checked="" type="radio"/> No	<input type="text" value="2"/>
Query Coverage % 3	Word Size 4	Reward for Match 5 Penalty for Mismatch ?
<input type="text" value="50"/>	<input type="text" value="11"/>	<input type="text" value="2, -3"/>
BLAST Algorithm 6	E-Value 7	Exclude Low Complexity Regions 8
<input type="button" value="BLASTn"/>	<input type="text" value="10"/>	<input type="radio"/> Yes <input checked="" type="radio"/> 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 AAATAAAAAAAATAAAAAAT，多个 A 会导致比对分数偏高，序列中有 LCR 时可考虑排除。

BLAST Search Details

- Sequence Type: Nucleotide
- Search Within: Nucleotides
- BLAST Algorithm: BLASTn
- NCBI Included: Yes
- Alignment Identity: 50%
- Query Coverage: 50%
- E-Value: 10
- Match with Gaps?: No
- Gap Costs: Existence 5
- Extension 2
- Word Size: 11

Bioscape Analysis

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Filter by

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

Biosequences (919)

Query Details: ATGCAGATCCCACAGGCGCCCTGGCCAGTCGTCTGGCGGTGCTACAACACTGGCTGGCGGCCAGGATGGTCTTAGACTCCCCA... [View More](#)

1 Alignment Identity: 100%
Query (1) [864] Subject (1) [867]
Matches: 864 Mismatches: 0

View Less

4 Alignment References

Alignment Data
BLAST Score: 1728
E-Value: 0

Q 1 ATGCAGATCC CACAGGCGCC CTGGCCAGTC GTCTGGCGG TGCTACAACCTGGCTGGCGGCCAGGATGGTCTTAGACTCCCCA...
S 1 ATGCAGATCC CACAGGCGCC CTGGCCAGTC GTCTGGCGG TGCTACAACCTGGCTGGCGGCCAGGATGGTCTTAGACTCCCCA...
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 GAGAGCTTG TGCTAAACTG GTACCGCATG 210
S 141 GGACAACGCC ACCTTCACCT GCAGCTTCTC CAACACATCG GAGAGCTTG TGCTAAACTG GTACCGCATG 210

2 Alignment Identity: 100%
Query (1) [864] Subject (1) [867]
Matches: 864

- 序列结果排序标准。
- 可视化分析序列结果。
- 结果筛选。
- 序列对比详情。

Query Sequence QQLLKVVEEGG
 Subject Sequence QQLLKVVEEIGS

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 Subject 1 References

CAS Registry Numbers: 2306097-89-0, 503752-44-1
 NCBI Identifier: KJ865859.1, AY238517.1
 Length: 867 nt

Sequence

3

```

1 ATGCAGATCC CACAGGGCGC  AGTC TCTGGCGG TGCTACAAC TGGCTGGCGG CCAGGTGGT TCTTAGACTC
81 CCCAGACAGG CCTCTGAACCC CCCCCACCTT CTCCCCAGCC CTGCTCTGG TGACCGAAGG GGACAACGCC ACCTTCACCT
161 GCAGCTTCTC CAACACATCG GAGAGCTCG TGCTAAACTG GTACCGCATG AGCCCCAGCA ACCAGACGGA CAAGCTGGCC
241 GCCTTCCCG AGGACCGAG CCAGCCCCG CAGGACTGCG CCTTCCGTG TGACTTCCA CCTAACGGGC GTGACTTCCA
321 CATGAGCGTG GTCAGGGCCC GGCGCAATGA CAGCGGCACC TACCTCTGTG GGCCATCTC CCTGGCCCC AAGGGCGAGA
401 TCAAAGAGAG CCTGCGGCCA GAGCTCAGGG TGACAGAGAG AAGGGCAGAA GTGCCACAG CCCACCCAG CCCCTCACCC
481 AGGCCAGCG GCCAGTTCCA AACCTGGTG TTGGTGTG TGCGGCCCT GCTGGCAGC CTGGTGTG TAGTCTGGGT
561 CCTGGCCGTC ATCTGCTCCG GGGCCGACG AGGGACAATA GGAGCCAGGC GCACCGGCCA GCCCCGTGAAG GAGGACCCCT
641 CAGGGCGTGCC TGTGTCTCT TTGGACTATG GGGAGCTGGA TTTCAGTG CGAGAGAAGA CCCCCGGAGCC CCCCGTGCCCC
721 TGTGTCCCTG AGCAGACGGA GTATGCCACC ATTGTCTTC CTAGCGGAAT GGCGACCTCA TCCCCGGGCC GCAGGGGCTC
  
```

4

→ C ncbi.nlm.nih.gov/nuccore/KJ865859.1

GenBank ▾ Send

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., Hoetzenegger,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。

Alignment Subject References 1

使用PD-1轴拮抗剂和HPK1拮抗剂用于治疗癌症的方法和组合物

Assignee: 豪夫迈·罗氏有限公司
CN107206088 A | Seq ID No: 1

Novel pd1 isoforms, and uses thereof for potentiating immune responses

Assignee: VERSITECH LIMITED
US20140302070 A1 | Seq ID No: 24

Compositions and methods for identification, assessment, prevention, and treatment of melanoma using pd-l1 isoforms

Assignee: DANA-FARBER CANCER INSTITUTE, INC.
CA2935804 A1 | Seq ID No: 1

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

Bioscape Analysis

Visually explore sequence similarity with a new tool.

Learn more about Bioscape.

Create Bioscape Analysis

1

2

3

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。

The screenshot shows the CAS SciFinder search interface. On the left, there is a sidebar with arrows pointing to various categories: All, Substances, Reactions, References, Suppliers, Biosequences (which is highlighted in blue), and Retrosynthesis. The main search area is titled "Biosequences" and contains a search bar with placeholder text "Enter a protein or nucleotide string, or upload a .txt or .fasta file. Learn more about Biosequence Search.". Below the search bar are tabs for BLAST, CDR, Motif, Upload Sequence, and Clear Search. To the right of the search bar are buttons for "Saved", "History", and "Account". Further down, there are sections for "Sequence Type" (set to "Nucleotide"), "Search Within" (set to "Proteins" and has a checked checkbox for "Include NCBI Sequences"), and a dropdown for "Limit Total Sequence Results to" (set to 1000). At the bottom right is a large blue button labeled "Start Biosequence Search" with a speech bubble icon and a "Feedback" link.

- 输入序列信息后，勾选 Include NCBI Sequences。

The screenshot shows the search results page for a biosequence search. The top navigation bar includes "Substances" and a search bar. On the left, there are filters for "Word Size: 3", "Bioscape Analysis" (with a "Create Bioscape Analysis" button), and "Filter by E-Value" (set to 0 to 10⁶). Below these are sliders for "Query Coverage %" (0 to 100) and "Subject Coverage %" (0 to 100). The main results area shows a sequence alignment. A green bar at the top indicates "Matches: 407" and "Mismatches: 0". The alignment itself has a "Subject" section (labeled 2) and a "Query" section (labeled 3). The subject sequence starts with "MSGRHRKPTTNSVAKIAFTGAVLGGGGIAMAQATAATGGEWQVARCESGGNWSINTGNGLGGLQFTQSTWAHGGGEFAPSQ". The query sequence starts with "MSG...". Below the alignment, the "References" tab is selected, showing a list of NCBI identifiers: CCC63477.1, KAN93036.1, ALA77280.1, CAL70905.1, AET18174.1, ALV10075.1, AGE66835.1, A0A758HJL9, A0A7U4BSU5, A0A0H3M8Z9, AKO23866.1, WP_011799137.1, AMO09483.1. The sequence itself is labeled "Length: 407 aa". The bottom right corner features a "Feedback" button.

- 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。

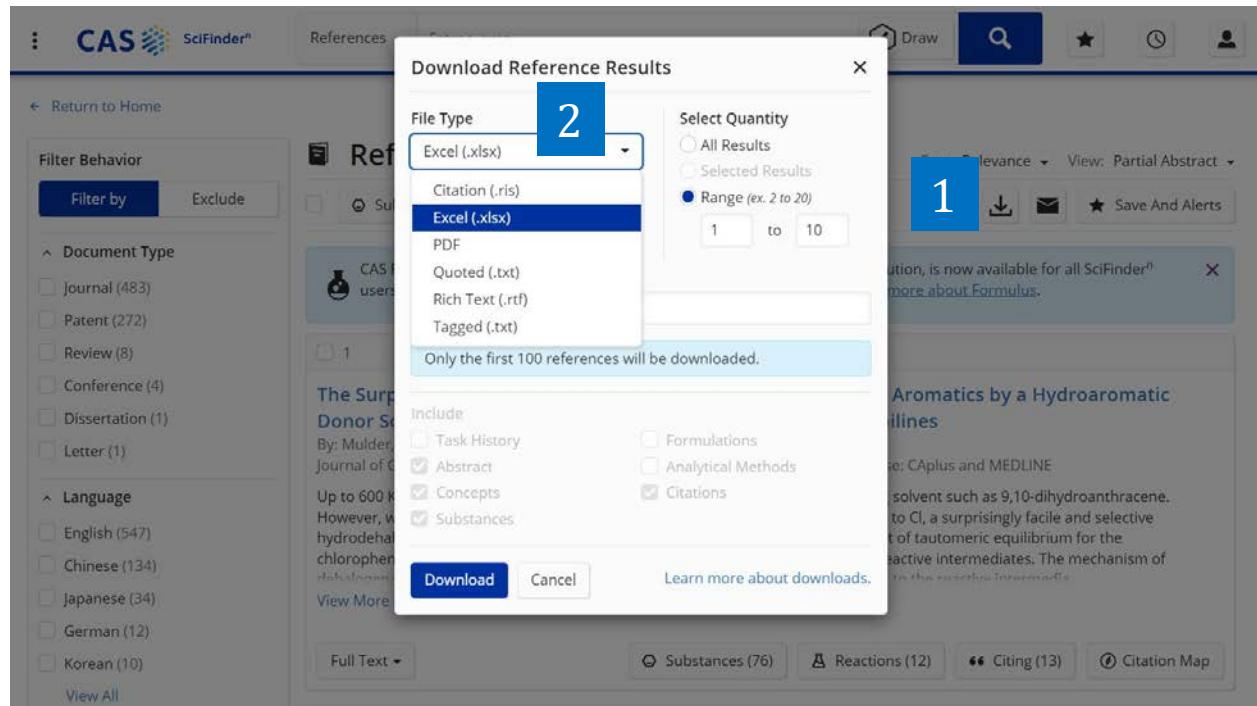
3. 点击 NCBI Identifier 超链接，则可直接打开 NCBI 中该序列信息页。

The screenshot shows the NCBI protein details page for A0ATU4BSU5. The main content area displays the protein's name, possible resuscitation-promoting factor rpfa [Mycobacterium tuberculosis variant bovis BCG str. Moreau RDJ], and its GenBank accession number, CCC63477. The page includes tabs for GenPept, FASTA, and Graphics. It displays detailed information about the protein's source (Mycobacterium tuberculosis variant bovis BCG str. Moreau RDJ), reference (Genome sequence of Mycobacterium bovis BCG Moreau, the Brazilian var. strain against tuberculosis), and features (Transglycosylase domain). The right sidebar provides links to BLAST, conserved domains, and related structures.

4. NCBI 中的目标序列详情。

检索结果后处理

使用 Excel 文件导出文献详情

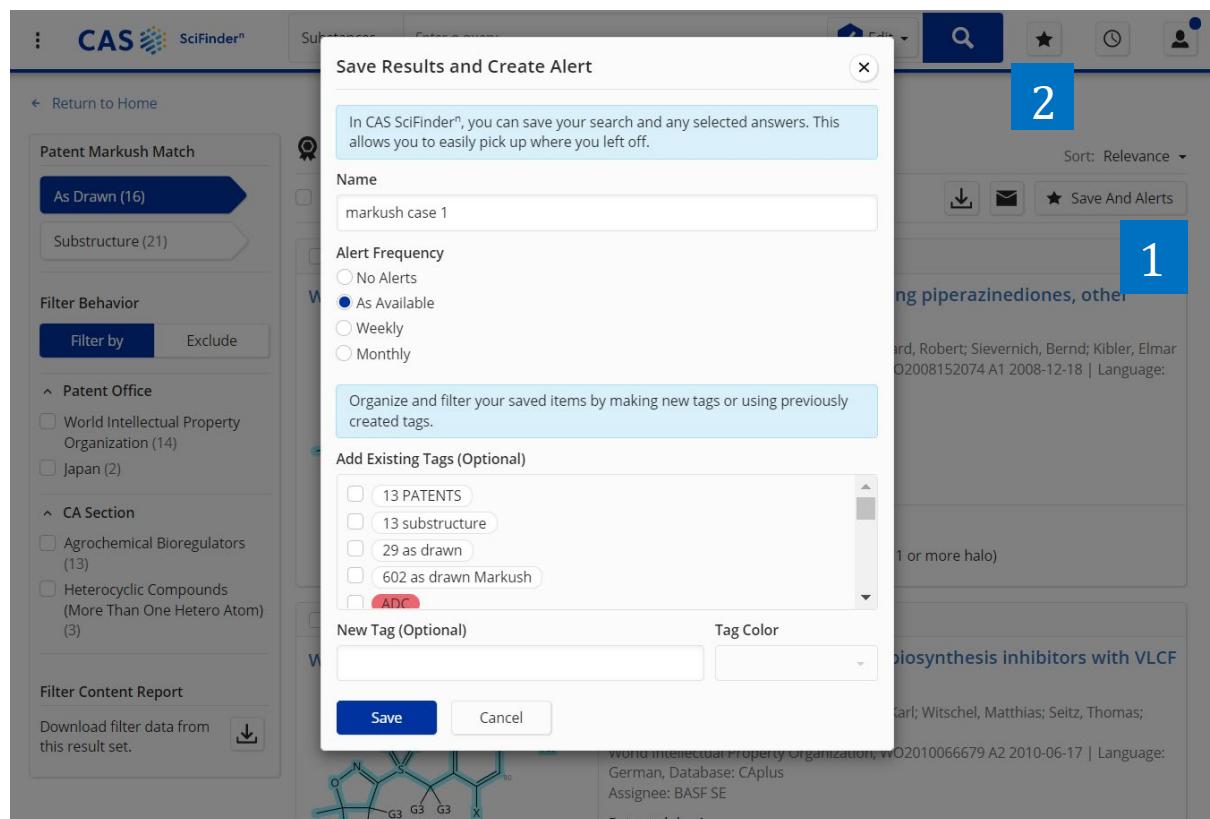


1. 在文献结果集页面，点击下载图标
2. 在弹出窗口中的 File Type 下选择 Excel(.xlsx)，即可使用 Excel 文件格式下载文献详情。

3. Excel 文件格式下载的文献详情。

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。

Substances Enter a query... Edit ★ Q ✉ ✖

Filter by

- Result Type
 - Patent Markush (17)
 - Reactions (76)
 - References (192)
 - Retrosynthesis (11)
 - Substances (104)
- Alerts
 - Unviewed (78)
 - Alerts Set (108)
 - No Alerts (292)
- Tags
 - 13 PATENTS (3)
 - ADC (2)
 - patent, Chinese, EOC (2)
 - 13 substructure (1)
 - 29 as drawn (1)

View All

Combine Saved Results 3

markush case 1 edit

January 5, 2022, 12:28 PM

Patent Markush As Drawn

Rerun Search

steroids and fermentation and "rhizopus stolonifer" edit

December 31, 2021, 3:08 PM

References steroids and fermentation and "rhizopus stolonifer"

Rerun Search

INDOLE edit

3. 点击 Combine, 进行多个结果集的逻辑处理。

Combine Saved Results 1 2 3

Select a Result Type:

- Substances Select
- Patent Markush 4 Select
- Reactions Select
- References Select

Learn More About Combine

steroids and fermentation and "rhizopus stolonifer" edit

December 31, 2021, 3:08 PM

References steroids and fermentation and "rhizopus stolonifer"

Rerun Search

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

Combine Saved Patent Markush Results

Select a Combine Option:

- Add**
- Intersect
- Subtract

Learn More About Combine

steroids and fermentation and "rhizopus stolonifer" ✓

December 31, 2021, 3:08 PM

References steroids and fermentation and "rhizopus stolonifer"

Rerun Search

5. 选择需要进行的逻辑操作。

Combine Saved Patent Markush Results: Add

Select Up to 5 Saved Items:

<input checked="" type="checkbox"/> markush case 1	Query	January 5, 2022
<input type="checkbox"/> TEST	Query	December 22, 2021
<input checked="" type="checkbox"/> MARKUSH CASE	Query	November 18, 2021
<input type="checkbox"/> markush WO2010124385	Query	June 11, 2021
<input type="checkbox"/> markush-1	Query	April 16, 2021
<input type="checkbox"/> markush case 4.9.2021	Query	April 9, 2021
<input type="checkbox"/> test-1	Query	April 1, 2020
<input type="checkbox"/> markush structure ...e.g.1	Query	March 26, 2020
<input type="checkbox"/> CASE 1 -MARKUSH	Query	February 20, 2020
<input type="checkbox"/> X-O, S, Se; Ar-Cy	Query	February 20, 2020

View Results Cancel

Return to Combine Option

Rerun Search

6. 选择需要 combine 的结果集。

7. 点击 View Results, 获得 combine 后的结果集。

SUBSTANCES Enter a query... Draw Search

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 Save And Alerts

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: Cplus
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 VLCF 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: Cplus
Assignee: BASF SE

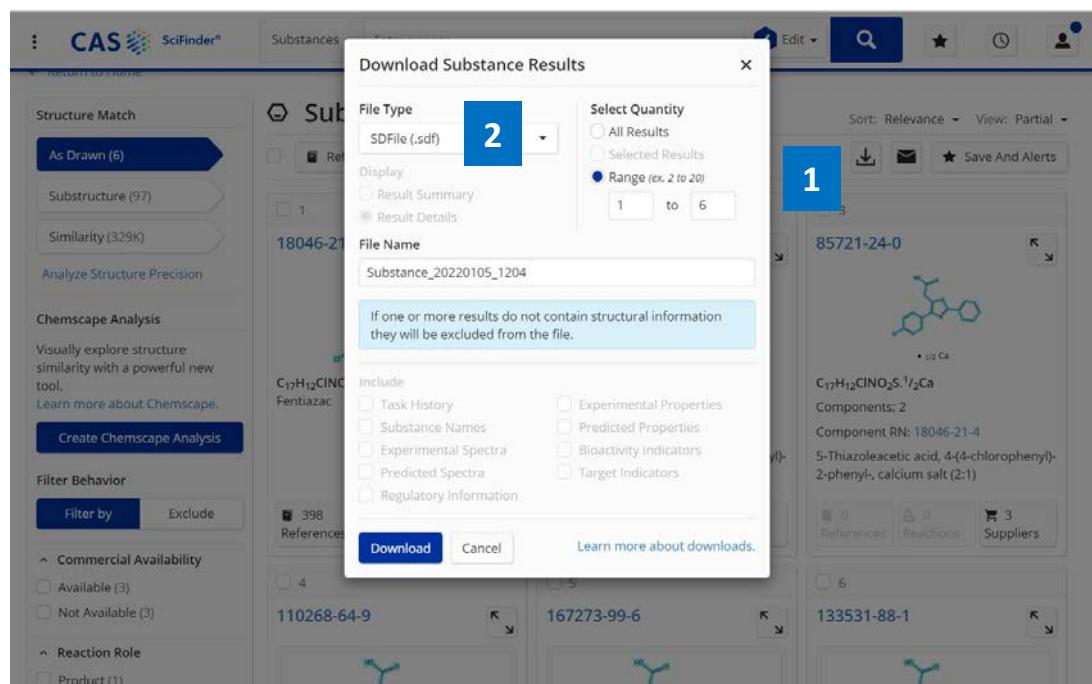
The screenshot shows the SciFinder interface with a search query for "Patent Markush". The results page displays two patent documents. Patent WO2008152074 is titled "Hericidal compositions containing piperazinediones, other active substances, and safeners". Patent WO2010066679 is titled "Hericidal mixtures of cellulose biosynthesis inhibitors with VLCF A Inhibitors". Both patents include their respective chemical structures, abstracts, and citation details.

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。

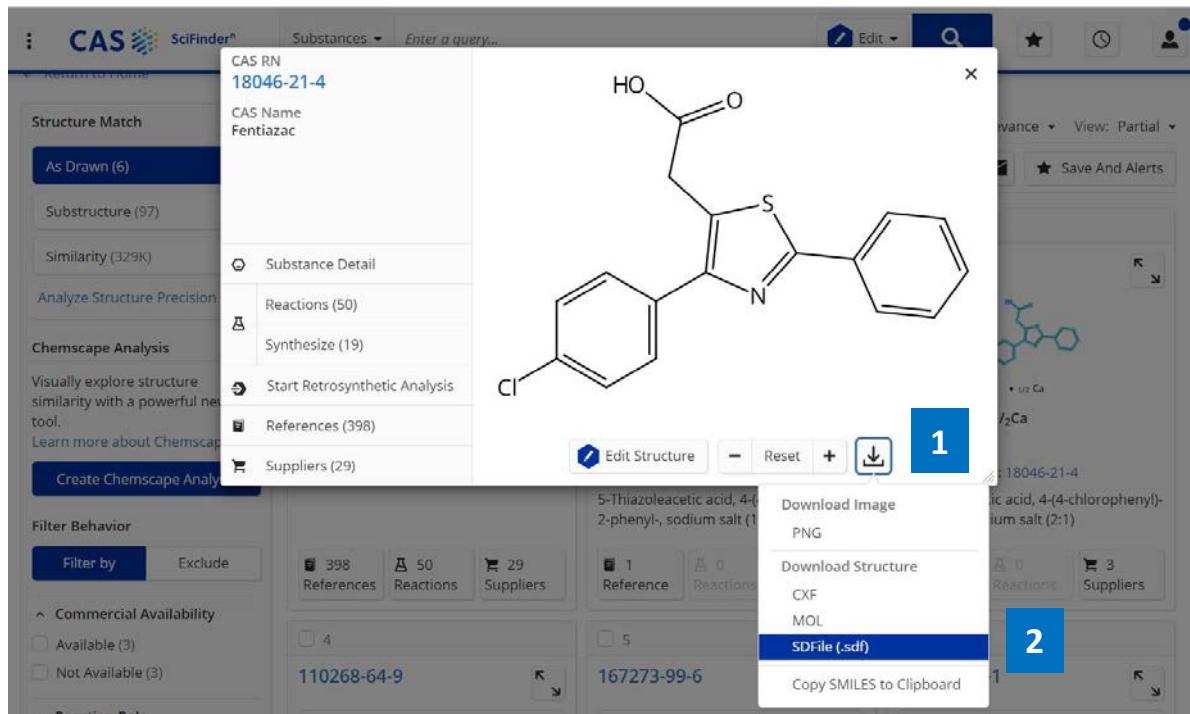
方法一：直接在物质结果集页面点击 ，选择 SDFFile，可以批量导出可编辑的结构数据文件。



1. 点击  按钮

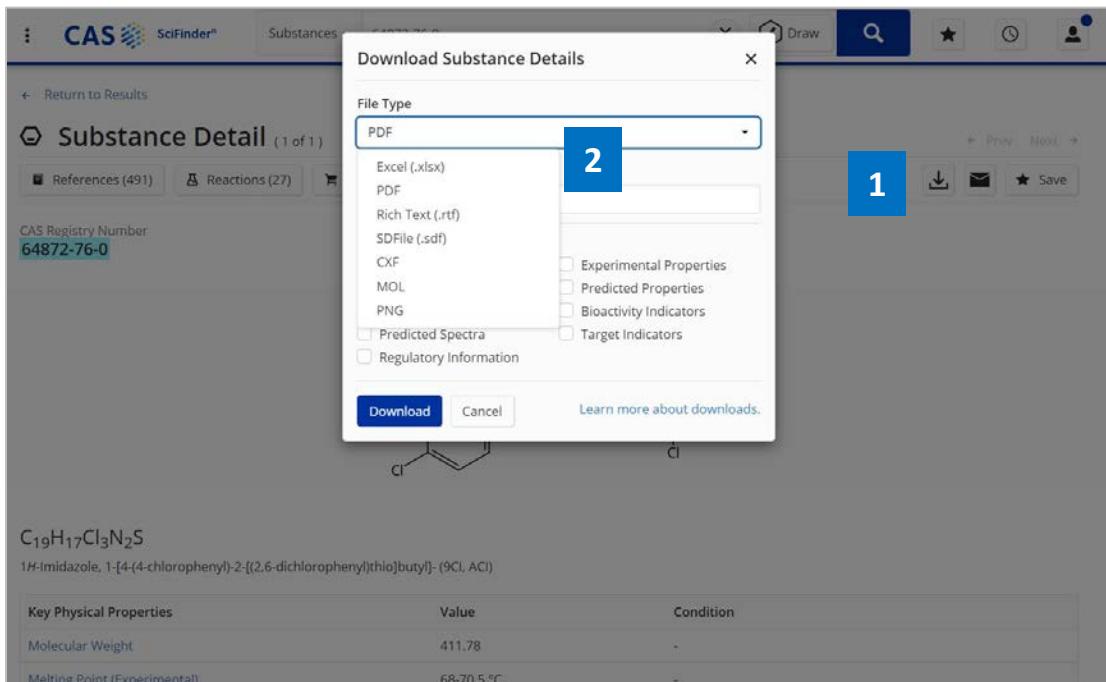
2. 选择 SDFFile

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）。



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
Vincaleukoblastine
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>
Vincaleukoblastine
> <molecular.formula>
C46H58N4O9
> <molecular.weight>
810.97
> <melting.point.experimental>
211-216 °C
> <density.predicted>
1.37±0.1 g/cm ³ 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：

The screenshot shows a Microsoft Excel spreadsheet titled "Substance_20220105_1216.xlsx". The table contains the following data:

Type	Category	Property	Value and Units	Temperature	Pressure	pH
Experimental	Thermal	Melting Point	48-70.5 °C			
Predicted	Biological	Bioconcentration Factor	126	25 °C		pH 1
Predicted	Biological	Bioconcentration Factor	135	25 °C		pH 2
Predicted	Biological	Bioconcentration Factor	195	25 °C		pH 3
Predicted	Biological	Bioconcentration Factor	269	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	37600	25 °C		pH 7
Predicted	Biological	Bioconcentration Factor	55200	25 °C		pH 8
Predicted	Biological	Bioconcentration Factor	57900	25 °C		pH 9

设置 Alert

在 CAS SciFinderⁿ 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 shows the CAS SciFinder interface. A 'Save Results and Create Alert' dialog box is open in the center. The dialog has the following fields:

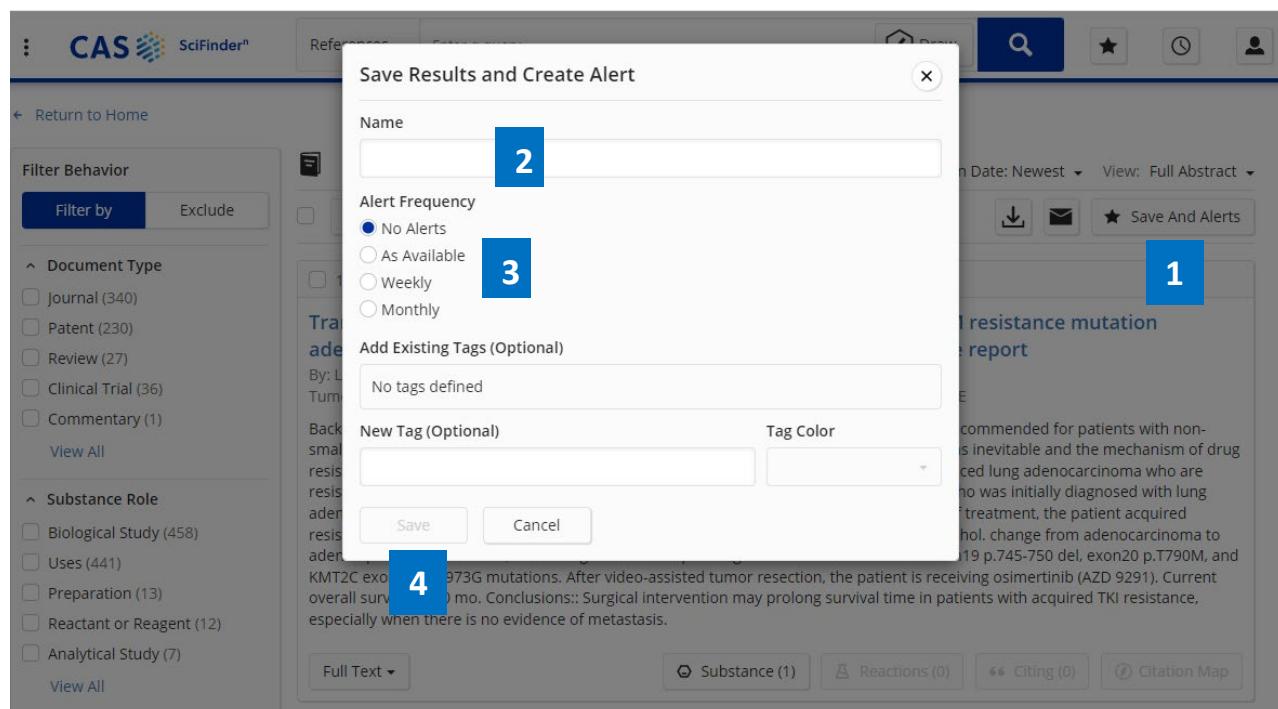
- Name:** icotinib Markush (highlighted with a blue box labeled 2)
- Alert Frequency:** No Alerts (radio button selected) (highlighted with a blue box labeled 3)
- Add Existing Tags (Optional):** No tags defined
- New Tag (Optional):** (empty input field)
- Tag Color:** (dropdown menu)
- Buttons:** Save (blue button labeled 4) and Cancel

In the background, the patent search results for CN106188072 are visible. The patent title is "Deuterated 4-[(3-ethynyl phenyl) amino]-6,7-benzene-12-crown-4-quinazoline derivative useful in treatment of cancer and its preparation". The patent is by Liu, Wenpei; Wu, Changxing; Feng, Dezhe, China, CN106188072 A 2016-12-07 | Language: Chinese, Database: Cplus. The patent claim 1 is shown, along with a chemical structure diagram and download options.

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。

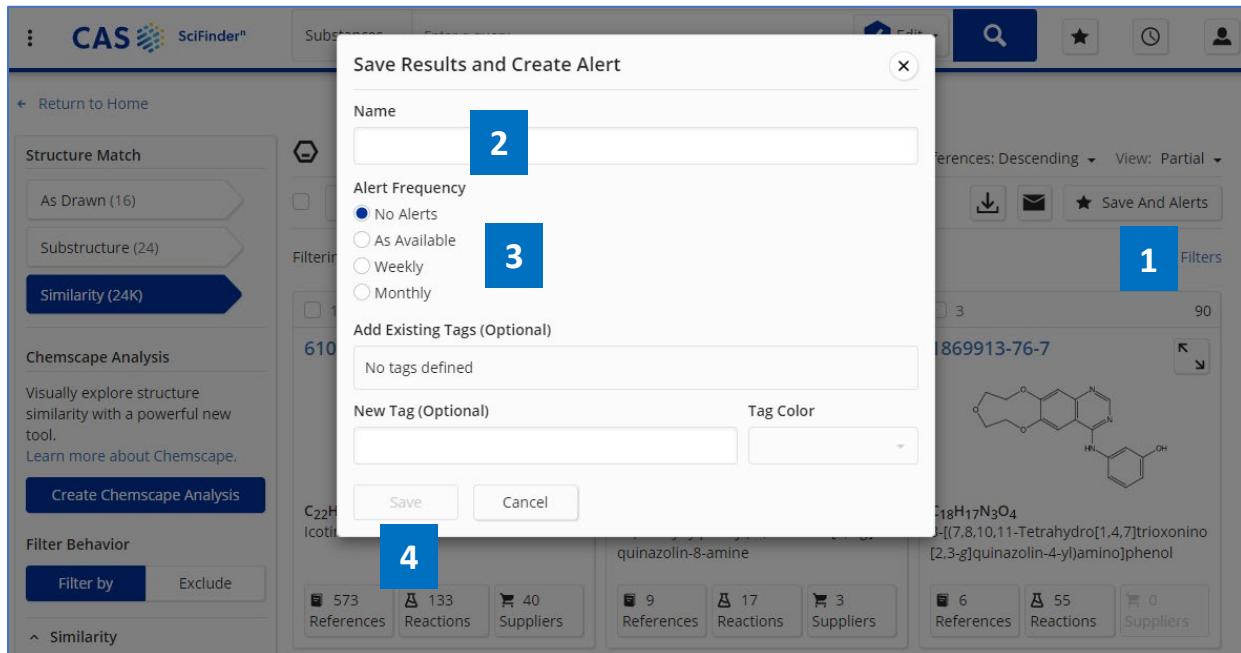
3. 选择 No Alerts 表示不设置提醒；选择 As Available、 Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

二. 文献检索后，设置 Alert



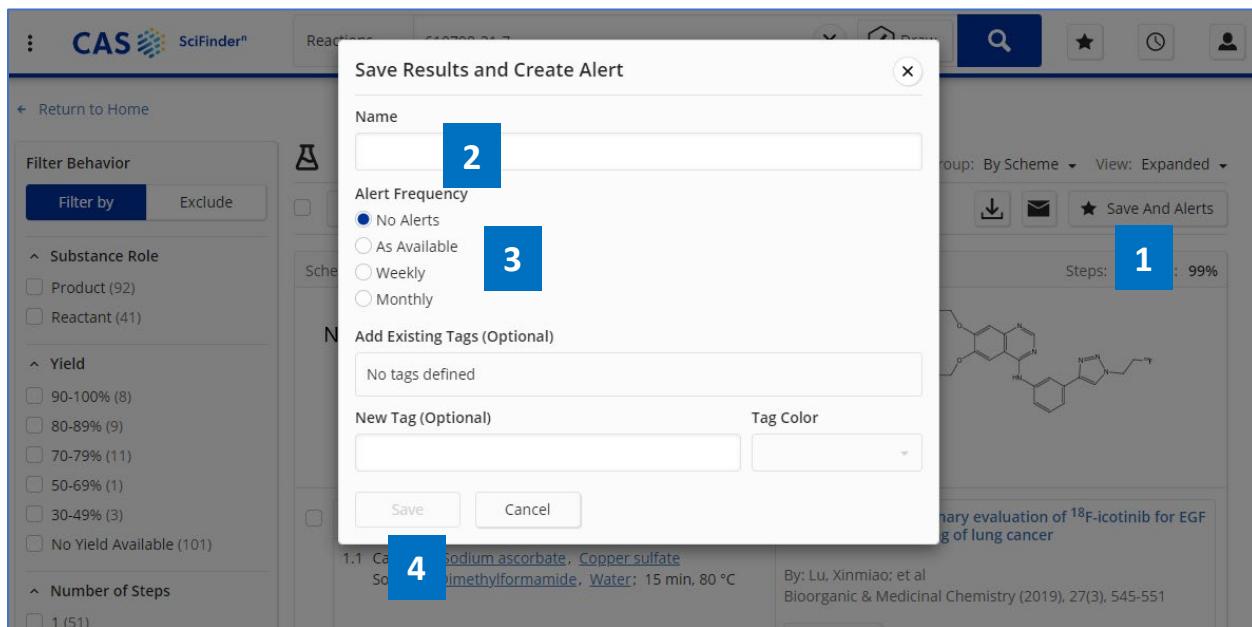
1. 在文献结果集页面点击 Save And Alerts。
2. 输入保存文件的名称。
3. 选择 No Alerts 表示不设置提醒；选择 As Available、 Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

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。

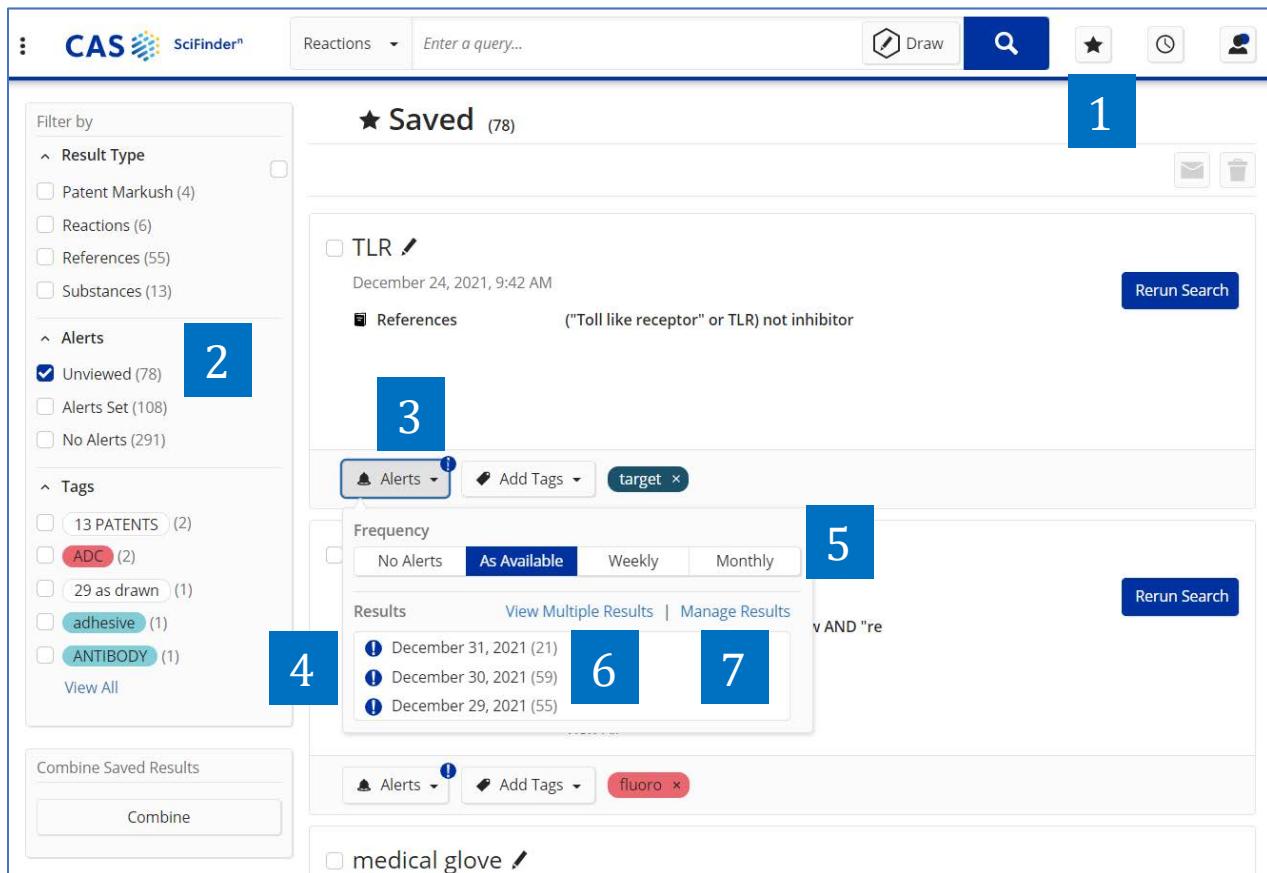
如果在保存结果集（Markush 结构，文献，物质或者反应）的过程中未设置 Alert，则可以通过以下方法进行：

The screenshot shows the SciFinder interface with the following elements:

- Top Bar:** CAS SciFinder, Reactions dropdown (set to 610798-31-7), Draw tool, Search icon, Favorites icon, Refresh icon, and User profile icon.
- Left Sidebar:** Filter by Result Type (Patent Markush, Reactions, References, Retrosynthesis, Substances) and Alerts (Unviewed, Alerts Set, No Alerts).
- Main Area:**
 - Section 1:** ★ Saved (43). A list item for "具体化合物专利" (Patent for Specific Compound) is shown, dated December 10, 2021, 2:58 PM. It includes a References link and a Rerun Search button.
 - Section 2:** Alerts dropdown menu (highlighted with a blue box) and Add Tags button.
 - Section 3:** Frequency dropdown (highlighted with a blue box) showing options: No Alerts (selected), As Available, Weekly, Monthly. It also includes a References link and a Rerun Search button.
- Bottom Sidebar:** Combine Saved Results (Combine button) and Migrate Alerts & Saved Results (Migrate button).

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

Alerts 分类选项



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

The screenshot shows the SciFinder search results for the query "steroids and fermentation and \"rhizopus stolonifer\"". The results are sorted by relevance and viewed in partial abstract. A blue box labeled '1' highlights the 'Save And Alerts' button in the top right corner of the main search area.

- 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。

The screenshot shows the 'Save Results and Create Alert' dialog box. It includes fields for 'Name' (set to 'steroids and fermentation and "rhizopus stolonifer"'), 'Alert Frequency' (set to 'As Available'), and an 'Add Existing Tags (Optional)' section. A new tag 'fermentation' is added with a 'Light Blue' color. A blue box labeled '2' is over the 'Name' field, '3' is over the 'Alert Frequency' section, and '4' is over the 'New Tag (Optional)' input field.

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

The screenshot shows the CAS SciFinder interface with the following elements:

- Top Bar:** Includes the CAS SciFinder logo, a search bar containing "steroids and fermentation and "rhizopus stolonifer"" with a clear button, a "Draw" button, a star icon, a magnifying glass icon, and a user profile icon.
- Left Sidebar:** Contains sections for "Filter by", "Result Type" (with options like Patent, Reactions, References, Retrosynthesis, Substances), "Alerts" (with Unviewed, Alerts Set, No Alerts), and "Tags" (with 13 PATENTS, ADC, patent, Chinese, EOC, 13 substructure, 29 as drawn).
- Saved Section:** Titled "★ Saved (399)". It shows a search result for "steroids and fermentation and "rhizopus stolonifer"" from December 31, 2021, at 3:08 PM. It includes a "References" section and a "Rerun Search" button.
- Search Result 6:** Titled "INDOLE". It shows a search result for "INDOLE" from December 24, 2021, at 4:11 PM. It includes a "Reactions" section and a "Substructure" section with a chemical reaction diagram.
- Alerts Section:** Indicated by a blue box labeled "7". It shows the "Alerts" section with a count of 7 unviewed alerts.

5. 点击保存的文件夹，查看设置提醒的保存项。
6. 当 Alerts 右上角出现感叹号图标，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

The screenshot shows the CAS SciFinder interface. At the top, there is a navigation bar with the CAS SciFinder logo, a dropdown menu for 'Substances', a search bar with placeholder text 'Enter a query...', and several icons for edit, search, save, and user profile. Below the navigation bar, a link to 'Return to Home' is visible. On the left, there's a sidebar with 'Structure Match' options: 'As Drawn (0)' (highlighted with a blue arrow), 'Substructure (0)', and 'Similarity (78K)'. Under 'Filter Content Report', there is a link to 'Download filter data from this result set'. The main content area is titled 'Substances (0)' and contains a message: 'We couldn't find any results. Please update your search query and try again.' It also includes links to 'Download Task History for this search' and 'Save your Search to be informed when new content is published'. A large blue box labeled '1' is overlaid on the bottom right of the main content area.

1. 当在 CAS SciFinderⁿ 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。

The screenshot shows the 'Save Results and Create Alert' dialog box. It has fields for 'Name' (with a blue box labeled '2'), 'Alert Frequency' (with a blue box labeled '3' over the 'No Alerts' option), and sections for 'Add Existing Tags (Optional)' and 'New Tag (Optional)'. At the bottom are 'Save' and 'Cancel' buttons. The background shows the same CAS SciFinder interface as the previous screenshot, with the 'Save And Alerts' button highlighted.

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
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		

3

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 SciFinderⁿ 链接至其他 CAS 解决方案

The screenshot shows the CAS SciFinder interface. At the top left, there is a blue vertical bar with the number '1'. In the top right corner, there are three icons: a star for 'Saved', a clock for 'History', and a person for 'Account'. Below these are two horizontal buttons: one with a blue background and white text, and another with a light blue background and dark blue text.

Searching for...

- All
- Substances** (highlighted)
- 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

Molecular Formula Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N

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

SCIFINDER DISCOVERY PLATFORM

- CAS SciFinderⁿ
- CAS Analytical Methods
- CAS Formulus** (highlighted)
- STN IP PROTECTION SUITE
- STNext
- CAS Scientific Patent Explorer
- REGULATORY
- CAS Chemical Compliance Index
- ACCOUNT MANAGEMENT
- CAS Profile

2

The second screenshot is identical to the first one, showing the CAS SciFinder interface with the 'Substances' search page visible. The blue vertical bar with the number '2' is present on the left side. The 'CAS Formulus' option in the sidebar is highlighted.

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 SciFinderⁿ 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，可以通过 CAS Profile 进行账号管理等。