

CAS SCIFINDERⁿ

使用技巧手册

2022 年 1 月



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

CAS SciFinder[®] 独特内容和特色：

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

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

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

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

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

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

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

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

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

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

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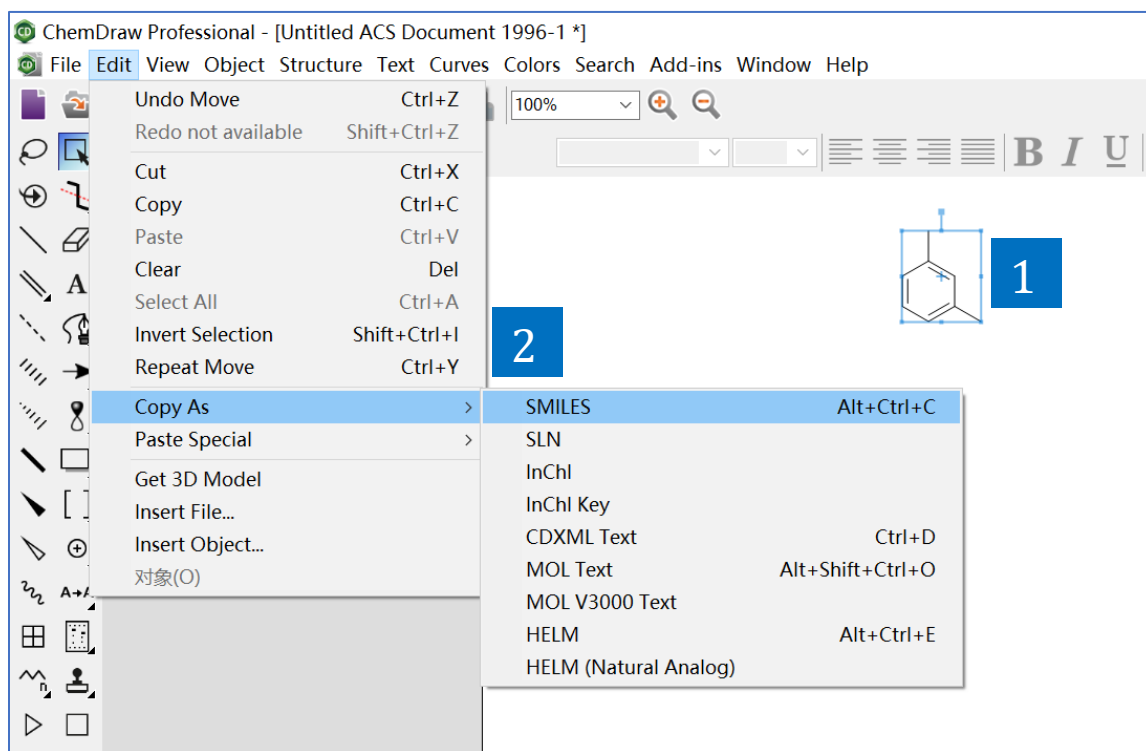
从 CAS SciFinder[®] 链接至其他 CAS 解决方案.....166

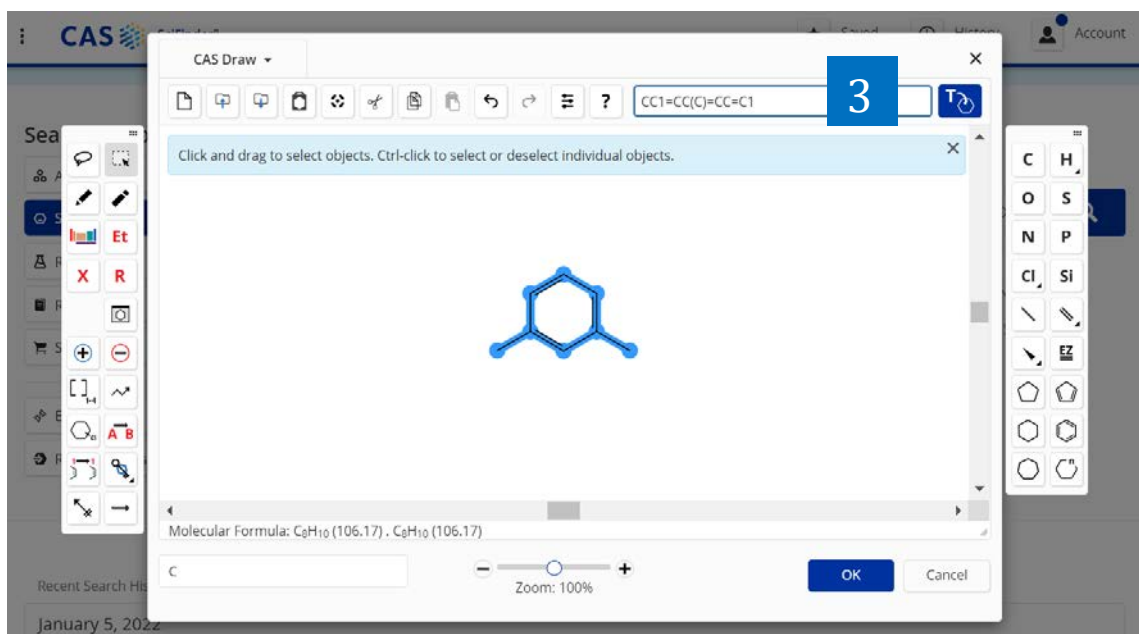
物质检索

与 ChemDraw 联用

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

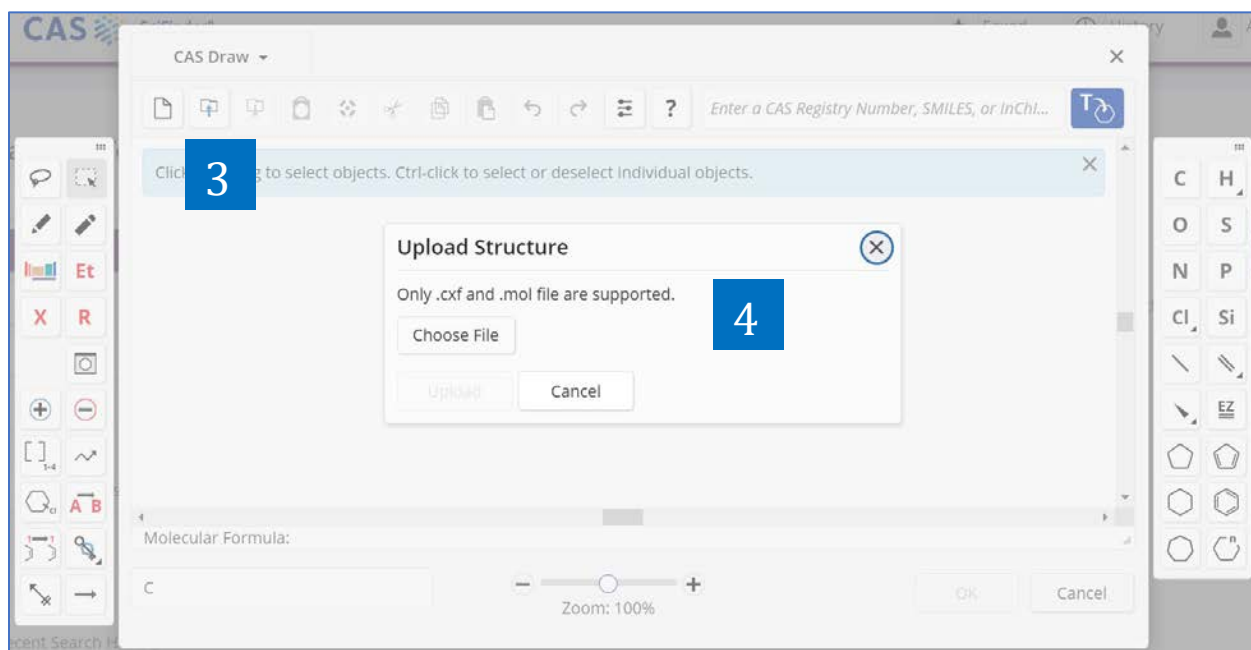
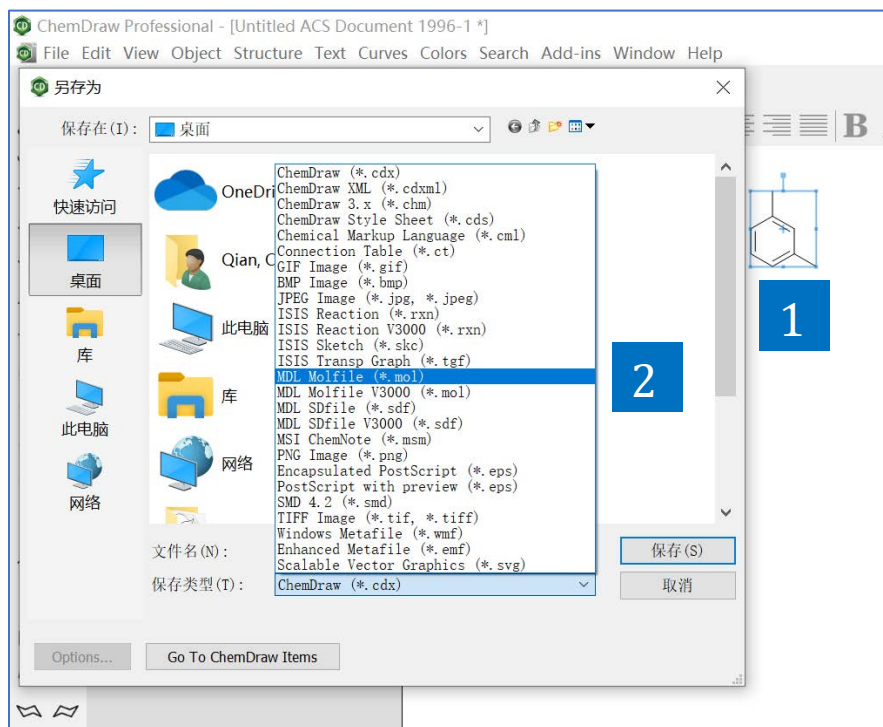
- 一. 利用在 ChemDraw 中获得的物质 SMILES、InChI，将结构导入到 CAS SciFinder[®] 的结构编辑器中：





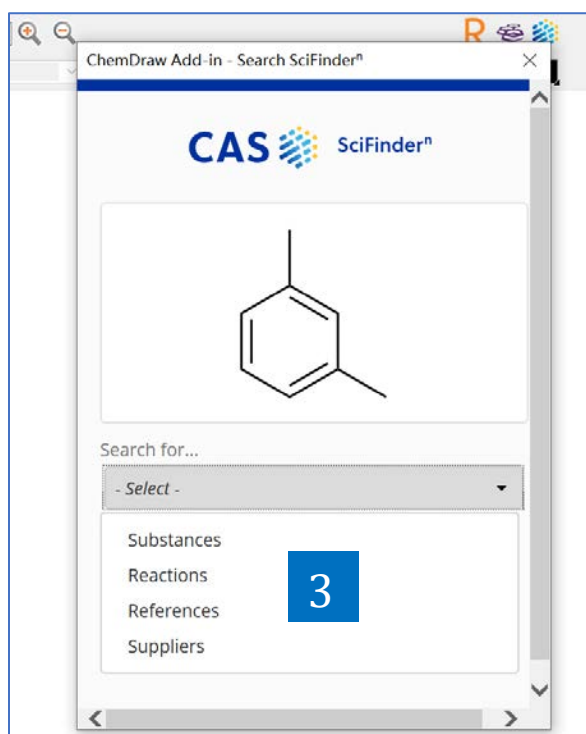
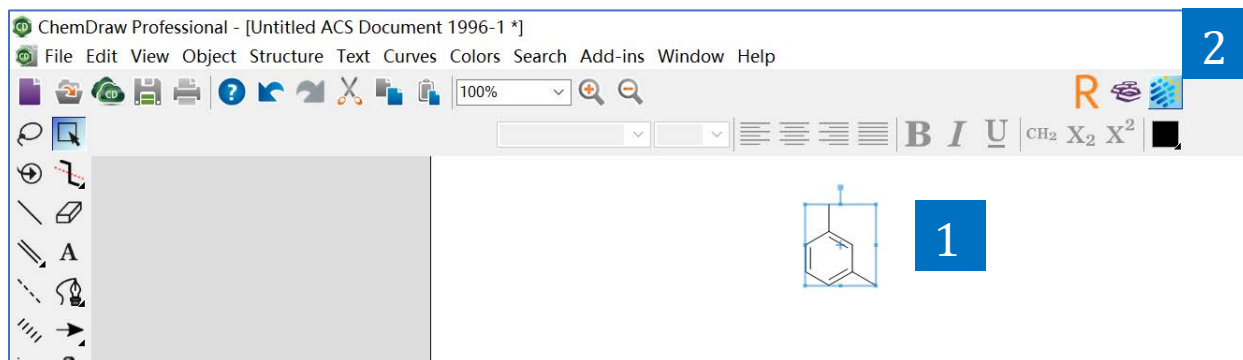
1. 在 ChemDraw 中绘制好结构，并选中。
2. 点击上方菜单 Edit，选择 Copy As, 然后再选择 SMILES 或 InChI。
3. 在此粘贴在 ChemDraw 中获得的 SMILES 或 InChI，将结构导入到 CAS SciFinder[®] 的结构编辑器中。

二. 将 ChemDraw 中绘制的结构保存为.mol 格式文件，然后再导入到 CAS SciFinder[®] 的结构编辑器中：



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

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-核磁谱图联用助力物质结构解析

The screenshot displays the CAS SciFinder[®] Advanced Search interface. The search bar at the top contains the text "Enter a query..." and a dropdown menu is open, showing various search criteria. The criteria listed are: Molecular Formula, CAS Registry Number, Chemical Name, Document Identifier, Patent Identifier, Experimental Spectra, Biological, Chemical Properties, Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, Thermal, Molecular Weight, pKa, and Vapor Pressure (Torr). The "Molecular Weight" option is highlighted. The search bar also includes a "Draw" button and a search button. The left sidebar shows navigation options like Substances, Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The bottom right has buttons for "Rerun Search" and "Edit Search".

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

Searching for...

Substances

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

Enter a query...

Molecular Weight 272.38

Predicted values only. Examples: 46.07 | 125 to 350 | >300

AND Carbon-13 NMR 155.02, 127 to 129

Allowance of ± 2 ppm. Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187

+ Add Advanced Search Field

Learn more about SciFinder[®] Advanced Search.

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 SciFinder[®]

Substances Edit Search Enter a query...

Substances (6)

Sort: Relevance View: Partial

Filter Behavior

Filter by Exclude

Commercial Availability

Available (2)

Not Available (4)

Reaction Role

Product (2)

Reactant (2)

Reagent (2)

Catalyst (1)

Reference Role

Properties (6)

Adverse Effect (2)

Agricultural Use (2)

Analyte (2)

Analytical Reagent Use (2)

View All

Stereochemistry

Number of Components

Substance Class

1 221255-16-9

Double bond geometry shown

$C_{18}H_{24}O_2$
(2Z,4E,6E,8E)-8-[(2E)-2-Ethylidenecyclohexylidene]-3,7-dimethyl-2,4,6-octatrieno...

1 Reference 0 Reactions 0 Suppliers

2 50-28-2

Absolute stereochemistry shown

$C_{18}H_{24}O_2$
Estradiol

147K References 955 Reactions 132 Suppliers

3 221315-96-4

Double bond geometry shown

$C_{18}H_{24}O_2$
(2E,4E,6E,8E)-8-[(2E)-2-Ethylidenecyclohexylidene]-3,7-dimethyl-2,4,6-octatrieno...

1 Reference 0 Reactions 0 Suppliers

4 57-91-0

Absolute stereochemistry shown

5 221255-12-5

Double bond geometry shown

6 221315-95-3

Double bond geometry shown

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

CAS SciFinder[®] Substances Edit Search Enter a query... Draw

Substance Detail (1 of 6)

Reference (1) Reactions (0) Suppliers (0)

CAS Registry Number
221255-16-9

Double bond geometry shown

C₁₈H₂₄O₂
2,4,6-Octatrienoic acid, 8-[(2E)-2-ethylidenecyclohexylidene]-3,7-dimethyl-, (2Z,4E,6E,8E)- (9CI, ACI)

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

Spectra

10. 查看物质分子量

Expand All | Collapse All

▼ Other Names and Identifiers

^ Experimental Spectra

¹³C NMR

11

	Source
View Carbon-13 NMR Spectrum	(1) ACD

12

13 Sources

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

▼ Predicted Properties

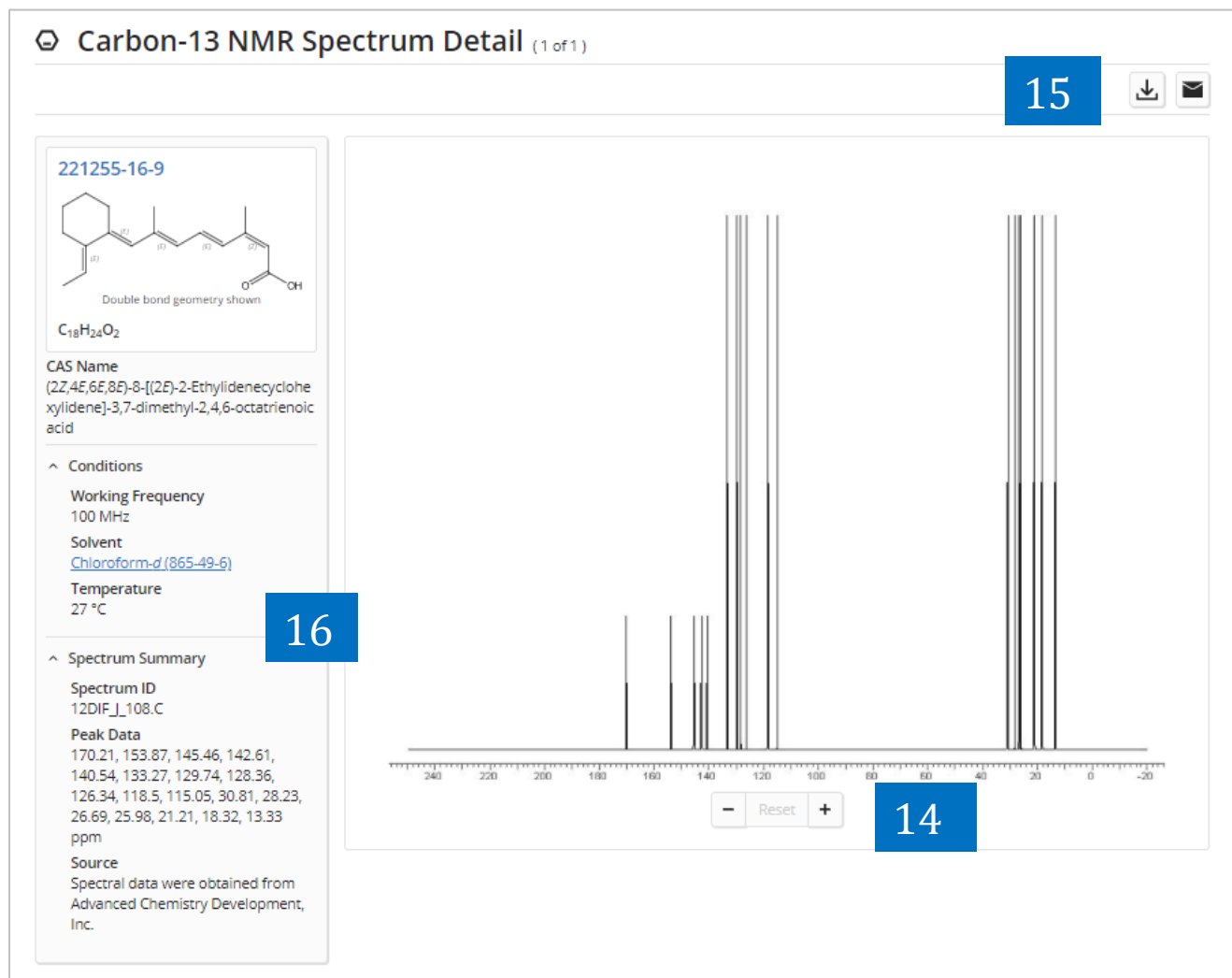
▼ Predicted Spectra

▼ Additional Details

11. 物质详情中的实验谱图

12. 点击超链接，查看核磁谱图

13. 谱图信息的文献来源



14. 缩放谱图

15. 下载谱图图片和谱图详情

16. 测试条件和谱图数据

通过生物活性、靶点筛选物质

CAS SciFinder®

Substances Enter a query...

Edit

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Bioactivity Indicator

Reproductive control agents (58)

Hormone antagonists (13)

Cardiovascular agents (12)

Receptor antagonists (11)

Nervous system agents (9)

View All

Target Indicator

Nuclear proteins (13)

Signaling proteins (13)

Transcription factors (13)

Cell cycle regulatory proteins (2)

Enzymes (2)

Membrane proteins (2)

Search Within Results

1186600-57-6

3

Absolute stereochemistry shown

$C_{26}H_{32}O_3$
(2''S,6'R,7'R,8'R,9'S,10'R,13'S,14'S,15'R,16'R)-1',3'',4'',6',7',8',9',10',11',1...

1 Reference 1 Reaction 0 Suppliers

1373991-22-0

Absolute stereochemistry shown

$C_{24}H_{32}O_3$
3'H-Cyclopropa[6,7]-18-norpregna-4,6-diene-21-carboxylic acid, 13-ethyl-6,7-dihy...

2 References 4 Reactions 0 Suppliers

1373991-21-9

Absolute stereochemistry shown

$C_{24}H_{32}O_3$
3'H-Cyclopropa[6,7]-18-norpregna-4,6-diene-21-carboxylic acid, 13-ethyl-6,7-dihy...

2 References 4 Reactions 0 Suppliers

1186600-56-5

7 94

Absolute stereochemistry shown

$C_{26}H_{32}O_3$
(2''R,6'S,7'S,8'R,9'S,10'R,13'S,14'S)-3'',4'',6',7',8',9',10',11',12',13',14',15...

1 Reference 1 Reaction 0 Suppliers

1186600-55-4

8 94

Absolute stereochemistry shown

$C_{25}H_{32}O_3$
(2''R,6'R,7'R,8'R,9'S,10'R,13'S,14'S)-3'',4'',6',7',8',9',10',11',12',13',14',15...

1 Reference 1 Reaction 0 Suppliers

1186600-54-3

9 90

Absolute stereochemistry shown

$C_{26}H_{32}O_3$
(1'S,2'R,2''S,8'R,9'S,10'S,13'S,14'R,15'S,16'S)-1',2',3'',4'',7',8',9',10',11',1...

2 References 2 Reactions 0 Suppliers

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

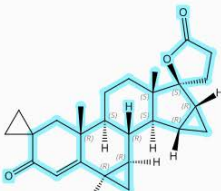
CAS SciFinder[®] Substances Enter a query...

Return to Results

Substance Detail (4 of 13) 4

Reference (1) Reaction (1) Suppliers (0)

CAS Registry Number
1186600-57-6



Absolute stereochemistry shown

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

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

Other Names and Identifiers

Predicted Properties

Predicted Spectra

Bioactivity Indicators 5

- Hormone antagonists
 - Antiprogestins (1)
- Reproductive control agents
 - Contraceptives (1)

Target Indicators 6

- Nuclear proteins
 - Androgen receptors (1)
 - Glucocorticoid receptors (1)
 - Mineralocorticoid receptors (1)
 - Progesterone receptors (1)
- Signaling proteins
 - Androgen receptors (1)
 - Glucocorticoid receptors (1)
 - Mineralocorticoid receptors (1)
 - Progesterone receptors (1)
- Transcription factors
 - Androgen receptors (1)
 - Glucocorticoid receptors (1)
 - Mineralocorticoid receptors (1)
 - Progesterone receptors (1)

Additional Details

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

获取物质信息

The screenshot displays the CAS SciFinder[®] web interface. On the left, a sidebar titled 'Searching for...' lists various search categories: All, Substances (highlighted), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main area is titled 'Substances' and includes a search bar with the placeholder 'Enter a query...'. A dropdown menu is open, showing search criteria: Molecular Formula, CAS Registry Number, Chemical Name, Document Identifier, Patent Identifier, Experimental Spectra, Biological, Chemical Properties, Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, and Thermal. The search bar contains the text 'Molecular Formula'. To the right of the search bar is a 'Draw' button. Below the search bar, there are examples of search queries: 'C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N'. A 'Recent Search History' section is visible at the bottom left, showing a search for 'Substances' on December 28, 2021, at 3:17 PM. The results section shows 'As Drawn (16)', 'Substructure (30K)', and 'Similarity (170K)'. A chemical structure is displayed in the bottom right corner. The interface also includes a 'Saved' button, a 'History' button, and an 'Account' button in the top right corner.

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

CAS SciFinder[®] Substances Enter a query...

Return to Home

Structure Match **1**

As Drawn (16)

Substructure (24)

Similarity (24K)

Analyze Structure Precision **2**

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior **3**

Filter by Exclude

Commercial Availability

Substances (16)

Sort: Number of References: Descending View: Partial

References Reactions Suppliers **4**

Save And Alerts

5 **6**

7

8

610798-31-7

C22H21N3O4

Icotinib

573 References 133 Reactions 40 Suppliers

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

1567366-94-2

C22H16D5N3O4

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

2 References 19 Reactions 0 Suppliers

1567366-92-0

C22H12D9N3O4

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

2 References 19 Reactions 0 Suppliers

1567366-91-9

C22H20DN3O4

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

2 References 2 Reactions 0 Suppliers

1567366-90-8

1567366-82-8

1567366-75-9

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

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

Substance Detail (1 of 16)

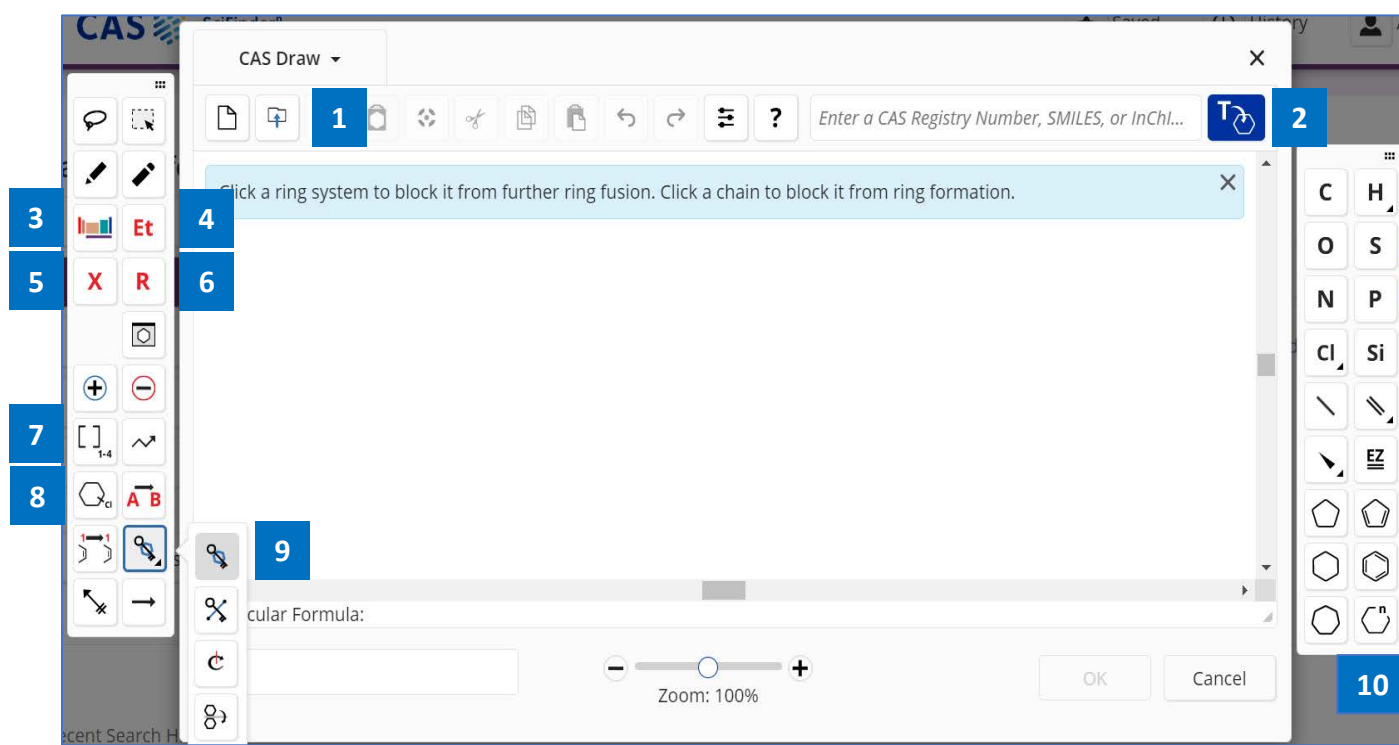
References (558) Reactions (133) Suppliers (39)

CAS Registry Number
610798-31-7

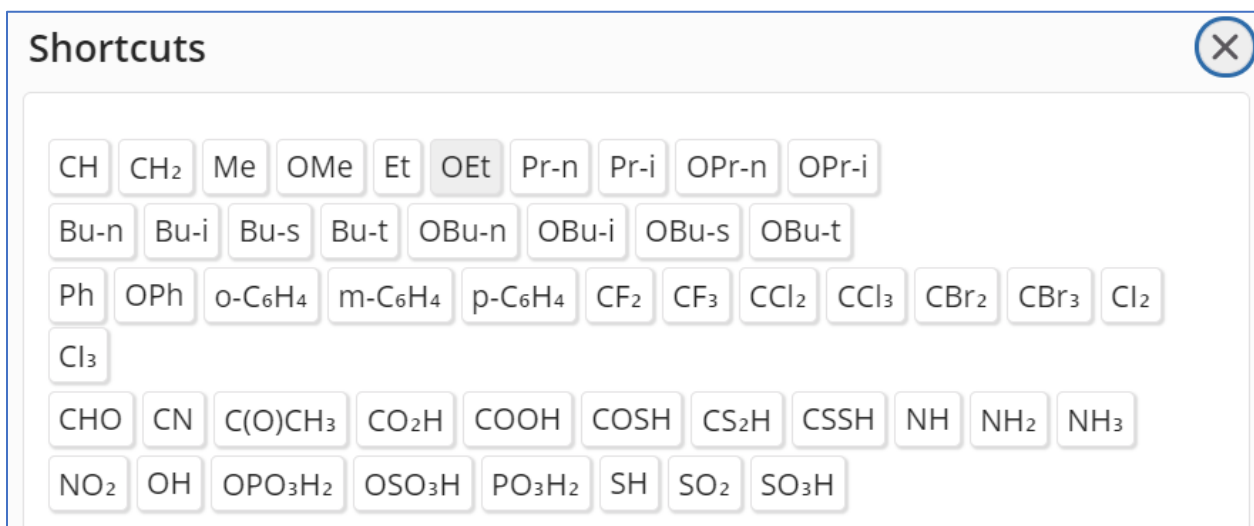
Chemical structure: C#Cc1ccc(Nc2nc3cc4c(cc3n2)OCCOCCO4)cc1

Feedback

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

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

R1

R2

R3

R4

R5

R6

R7

R8

R9

R10

R11

R12

>

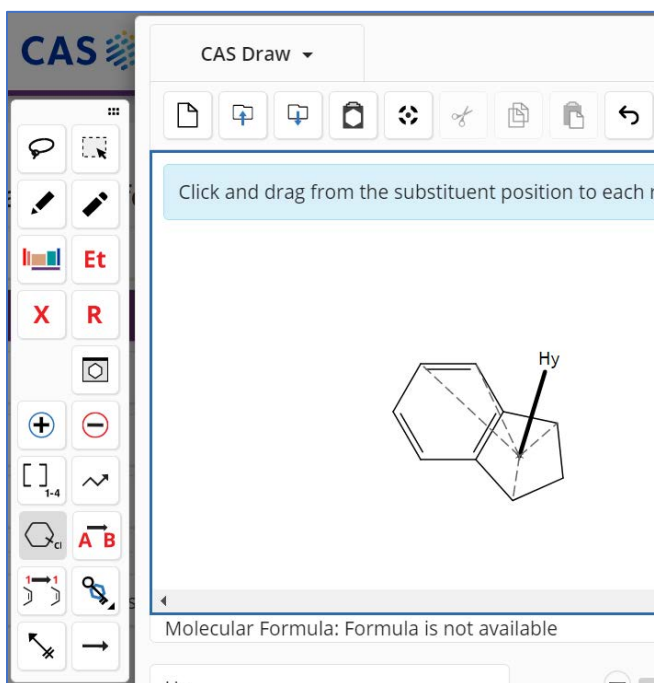
R1:

> Atoms

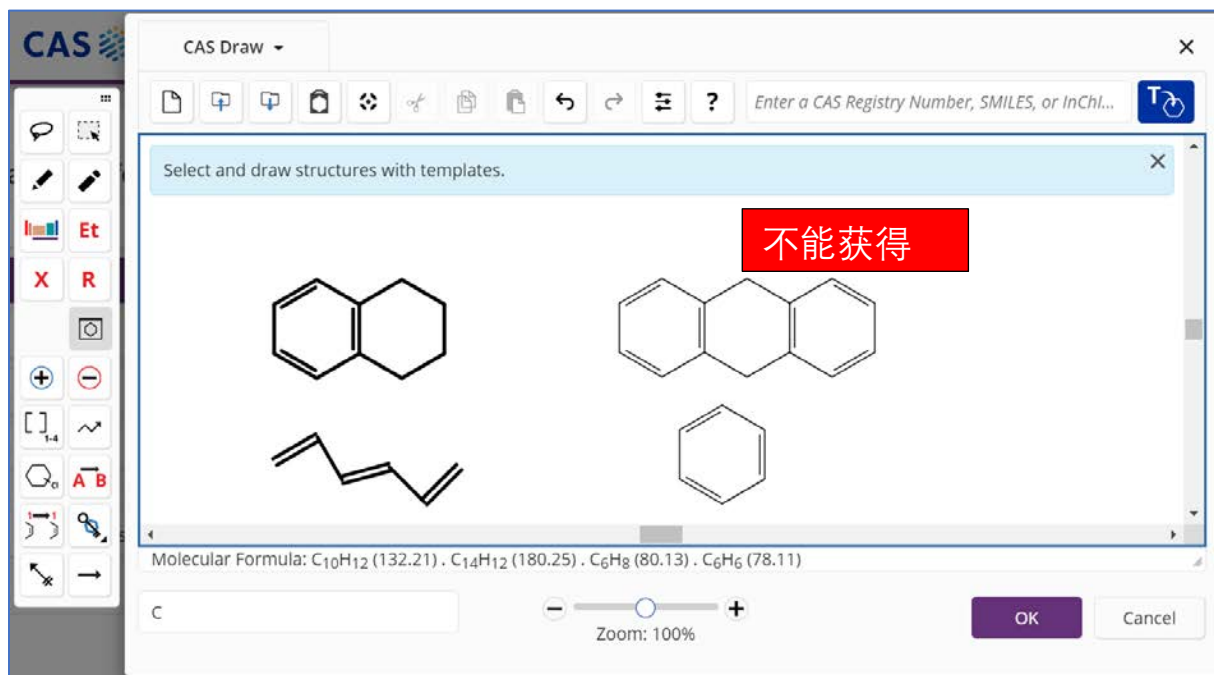
> Variables

> Shortcuts

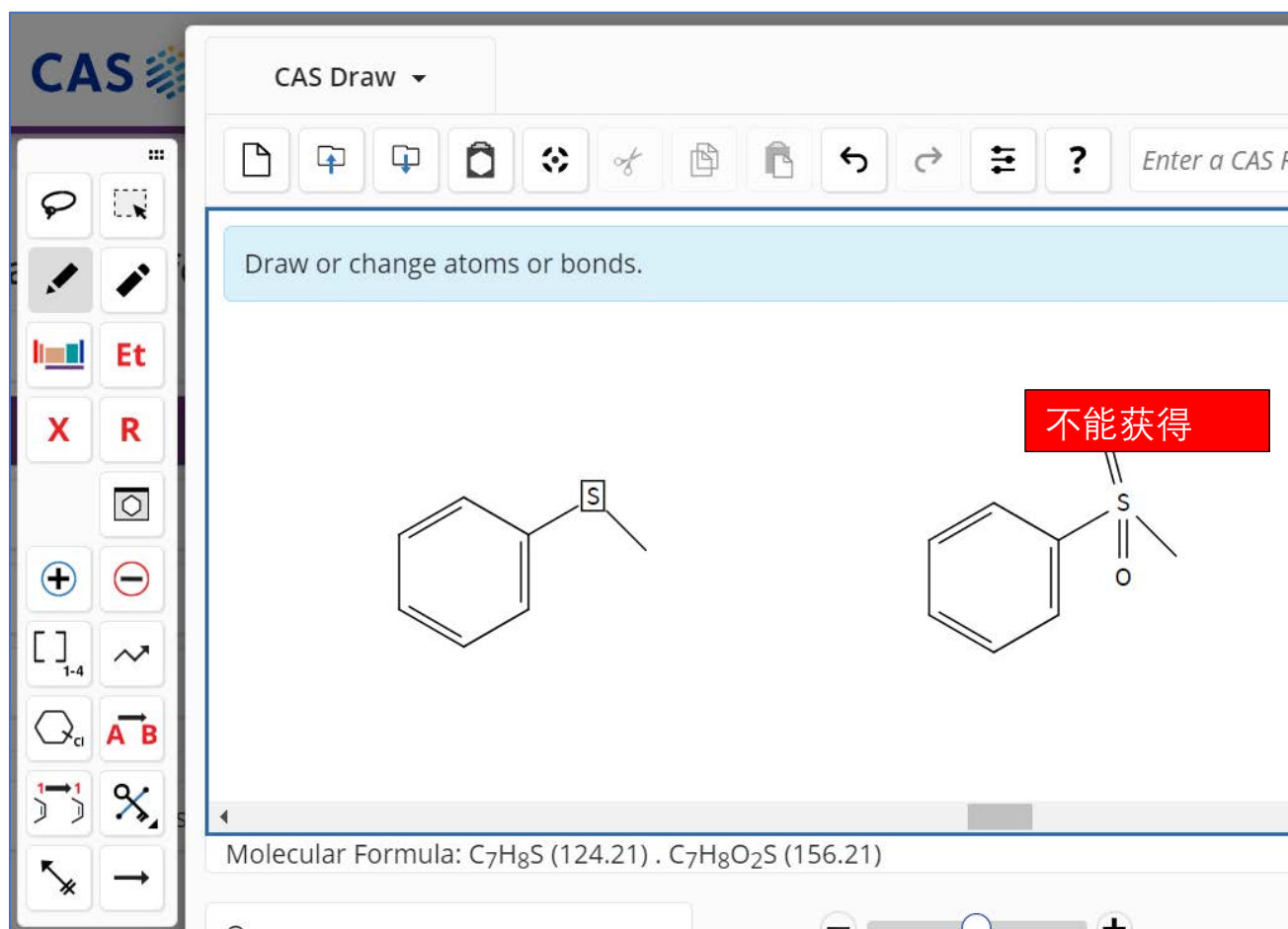
7. 重复原子或者基团。
8. 环上的取代位点不固定。

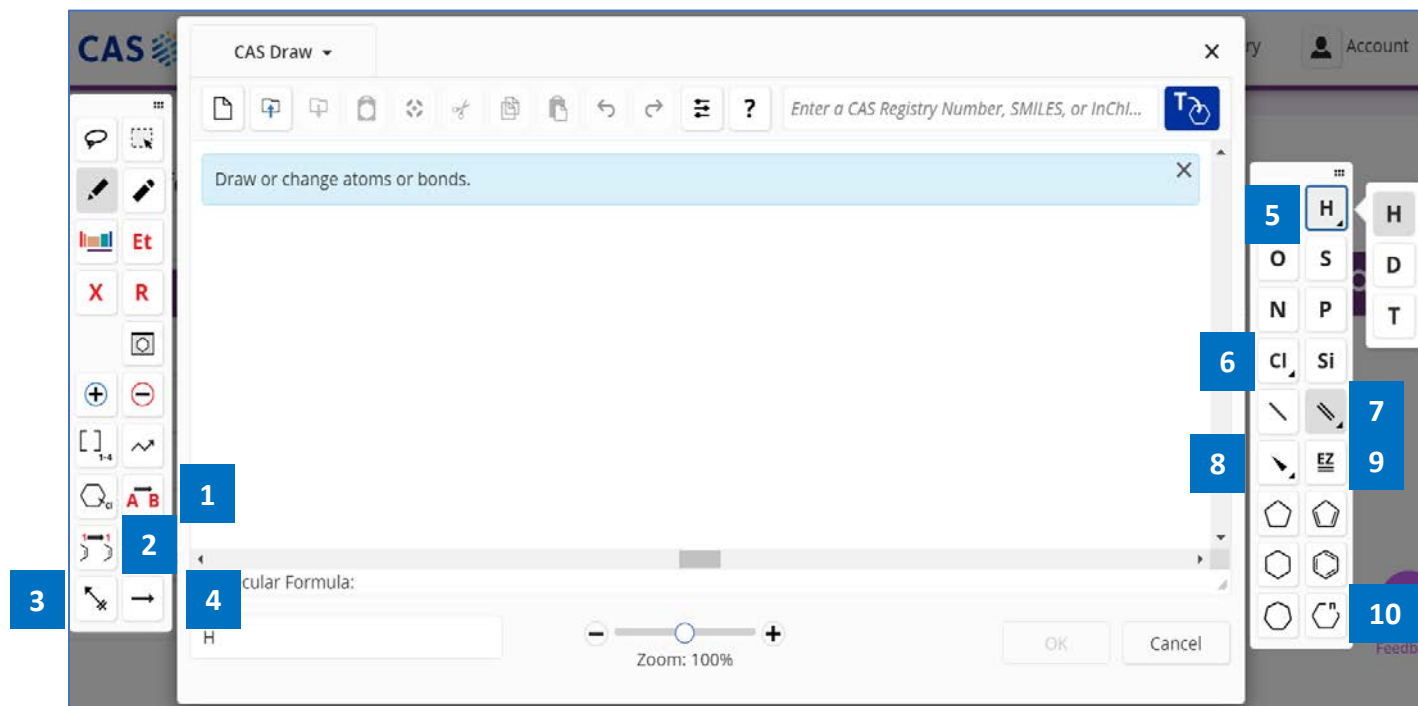


9. 环锁定。当用该功能锁定某个环（系），表示该环（系）不能成为更大环系的一部分；如果用该功能锁定某个链，则表示该链不能成为某个环（系）的一部分。例：

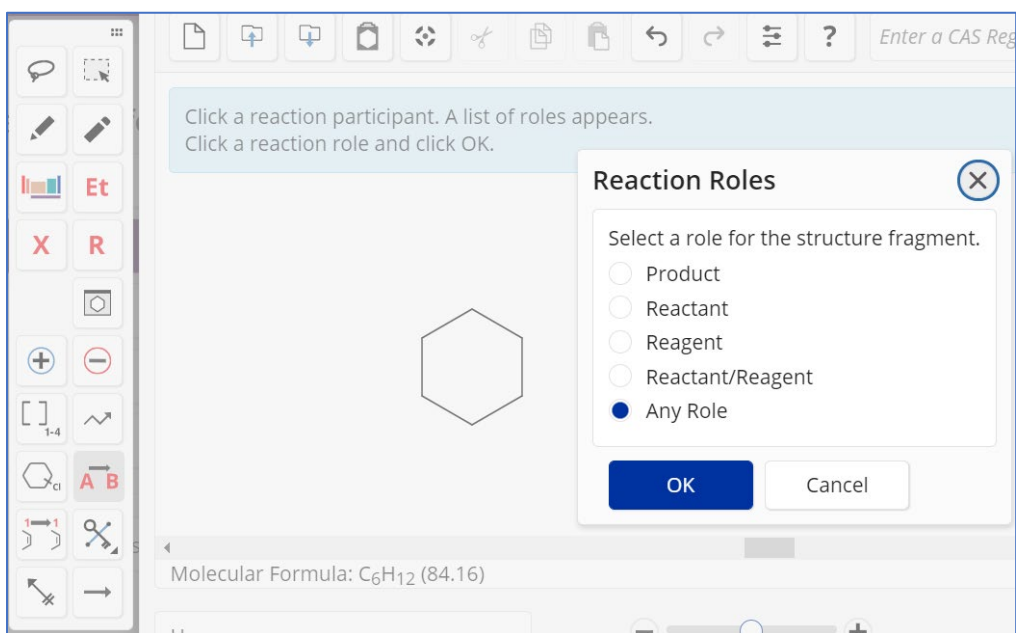


10. 锁定原子。若某原子被锁定，则表明该原子只能连接氢原子。例：





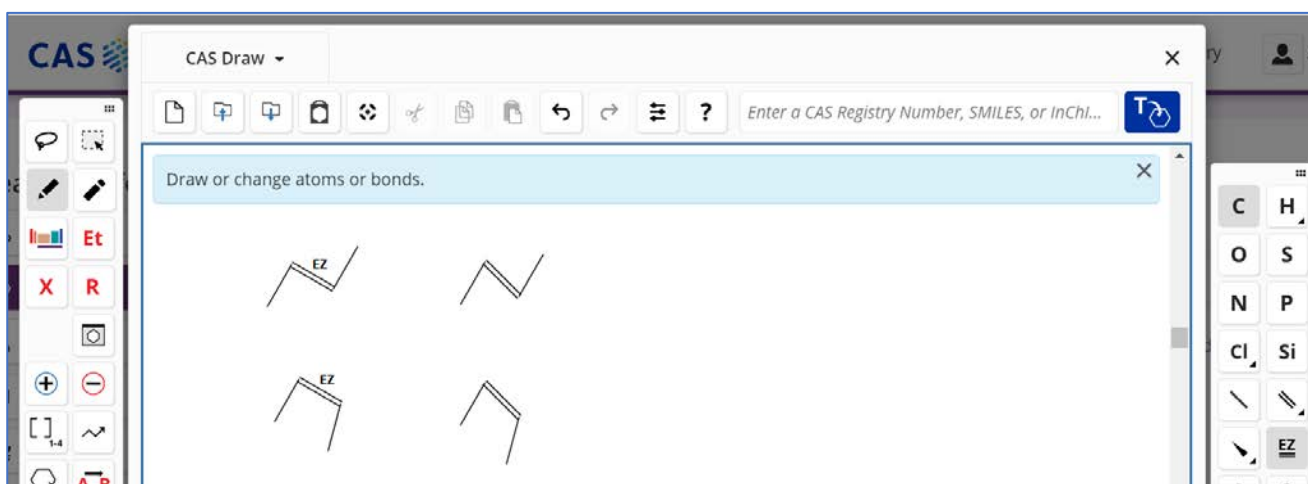
1. 反应角色定义工具，用于定义物质在反应中的角色。



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。



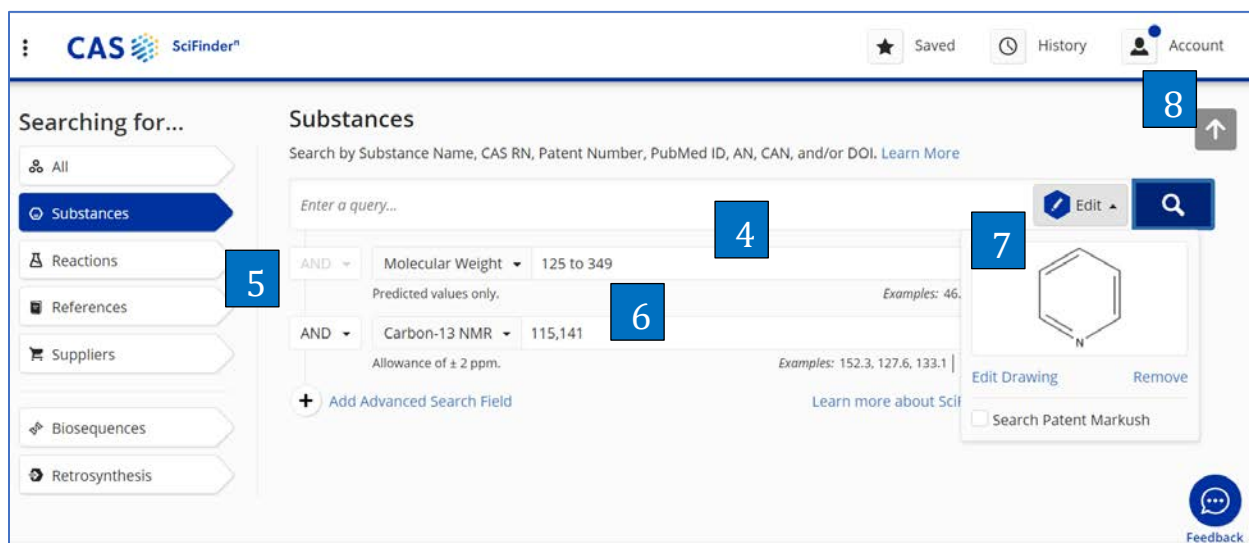
10. 绘制指定碳原子个数的碳环。

物质高级检索

The screenshot displays the CAS SciFinder[®] Advanced Search interface. On the left, a sidebar lists search categories: All, Substances (highlighted with a blue bar and a '1' marker), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The main search area is titled 'Substances' and includes a search bar with a 'Draw' button (marked with a '3'). A dropdown menu is open under the 'AND' operator (marked with a '2'), showing various search fields: Molecular Formula, CAS Registry Number, Chemical Name, Document Identifier, Patent Identifier, Experimental Spectra, Biological, Chemical Properties, Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, and Thermal. A chemical structure of pyridine is displayed on the right, with a 'Rerun Search' button and an 'Edit Search' button. The interface also shows a 'Recent Search History' section with a date of December 28, 2021, and a time of 5:19 PM. The search results section shows 'Substances' with 'Advanced Search' and 'AND Molecular V' and 'AND Carbon-13' filters. The 'View All' button is visible.

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



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

The screenshot displays the CAS SciFinder interface for a search of chemical substances. On the left, there are navigation options like 'Structure Match' (As Drawn, Substructure, Similarity) and 'Chemscape Analysis'. The main area shows three results, each with a chemical structure, its CAS number, and name. Below each result are statistics for references, reactions, and suppliers. The top bar includes a search bar and navigation icons.

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

The screenshot shows the 'Advanced Search' section of the CAS SciFinder interface. The search criteria are defined in a list: 'poly*' (labeled 1), 'Glass Transition Temperature (°C) 50 to 100' (labeled 2), and 'Density (g/cm3) <1.5' (labeled 3). The search button is highlighted with a blue box and the number 4. The interface also includes a 'Saved' button, a 'History' button, and an 'Account' button.

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

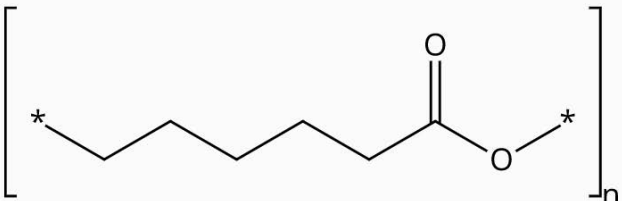
获得符合检索需求的结果

可在物质信息详情中查看完整信息。

Substance Detail (1 of 107) ← Prev Next →

References (37K) Reactions (3,067) Suppliers (8) Download Email Save

CAS Registry Number
25248-42-4



$(C_6H_{10}O_2)_n$ **1**
Poly[oxy(1-oxo-1,6-hexanediyl)] (9CI, ACl)

Polymer Class Terms
Polyester

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

2

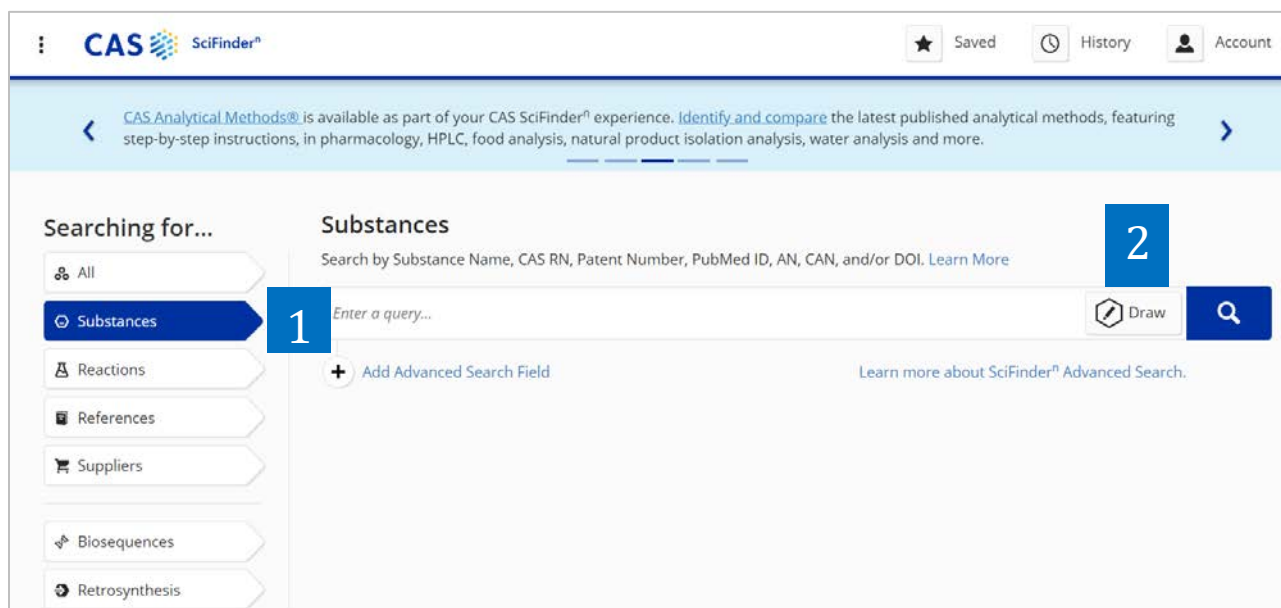
^ Experimental Properties

Biological	Chemical	Density	Electrical	Flow and Diffusion	Interface	Mechanical	Optical and Scattering	Structure Related	Thermal																								
<table border="1"> <thead> <tr> <th>Property</th> <th>Value</th> <th>Condition</th> <th>Source</th> </tr> </thead> <tbody> <tr> <td>Glass Transition Temperature</td> <td>63.6 °C</td> <td>-</td> <td>(1) CAS</td> </tr> <tr> <td>Glass Transition Temperature</td> <td>62.8 °C</td> <td>-</td> <td>(1) CAS</td> </tr> <tr> <td>Glass Transition Temperature</td> <td>62.0 °C</td> <td>-</td> <td>(1) CAS</td> </tr> <tr> <td>Glass Transition Temperature</td> <td>61.8 °C</td> <td>-</td> <td>(1) CAS</td> </tr> <tr> <td>Glass Transition Temperature</td> <td>60.4 °C</td> <td>-</td> <td>(1) CAS</td> </tr> </tbody> </table>										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
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																														

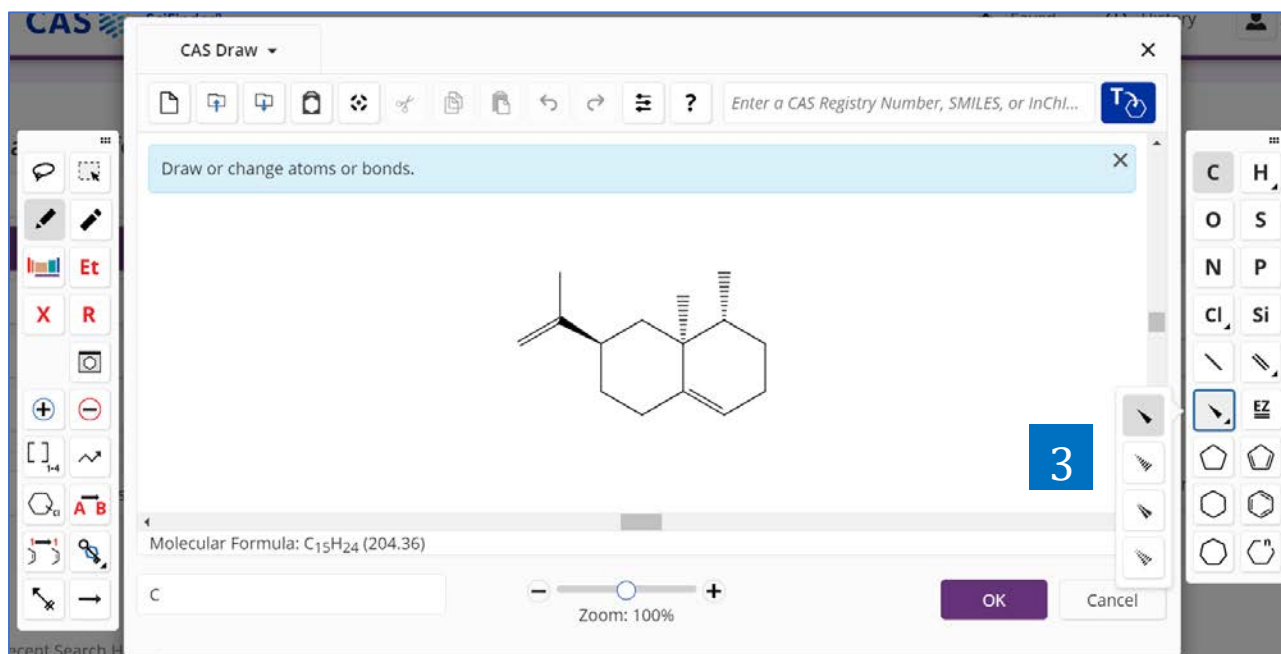
3

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

手性化合物的检索



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。



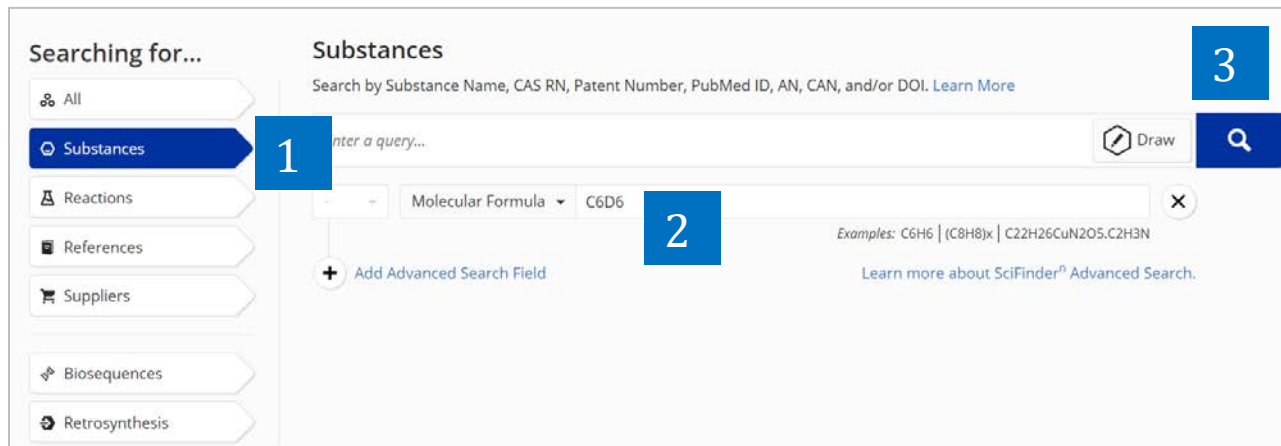
3. 绘制结构时，使用手性异构键标注结构中的手性特征。

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

Substances (19)

Sort: Relevance View: Partial

References Reactions Suppliers

Result #	Label	Chemical Structure	Formula	Description	References	Reactions	Suppliers
1	1076-43-3		C ₆ D ₆	Benzene-d ₆	3,043	33K	127
2	38091-14-4		C ₆ D ₆	Benzene-d ₆ , radical ion(1+)	45	0	0
3	32602-97-4		C ₆ D ₆	Benzene-1,2,3,4,5,6- ¹³ C ₆ -1,2,3,4,5,6-d ₆	9	0	5
4	34525-57-0		C ₆ D ₆	Benzene-d ₆ , radical ion(1-)			
5	73113-25-4		C ₆ D ₆	2,4-Hexadiyne-1,1,1,6,6,6-d ₆ , radical ion(1+)			
6	55153-53-2		C ₆ D ₆	Benzene- ¹³ C-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）。

CAS Draw

Draw or change atoms or bonds.

Molecular Formula: C₆H₅F (96.10)

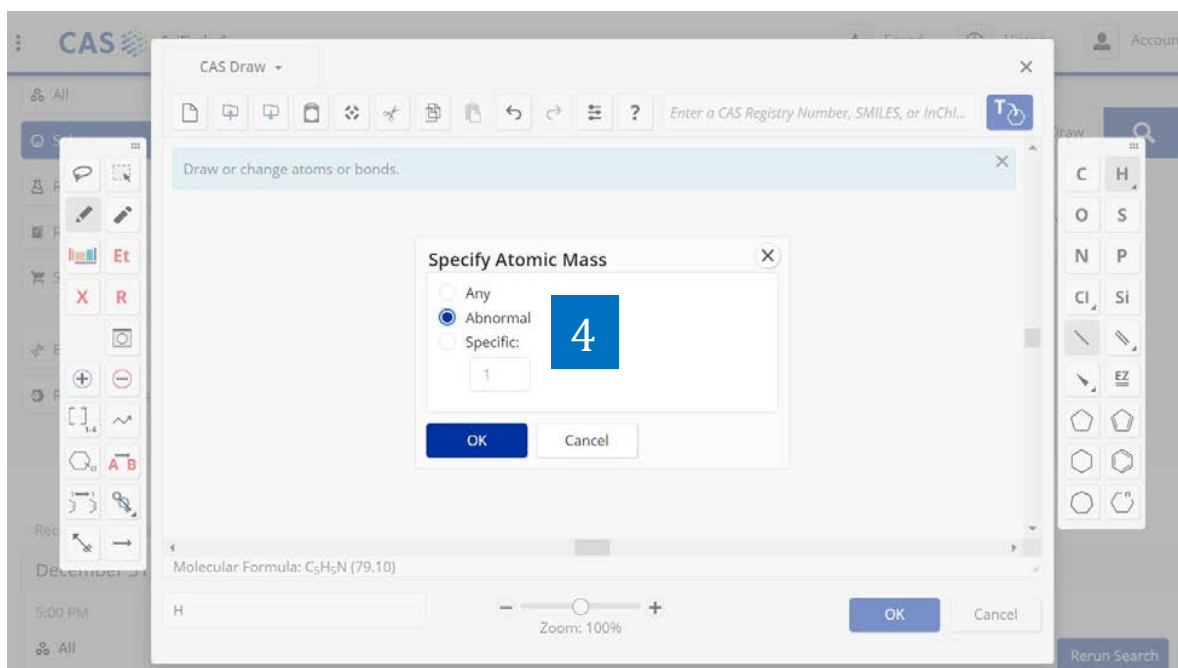
F

Zoom: 100%

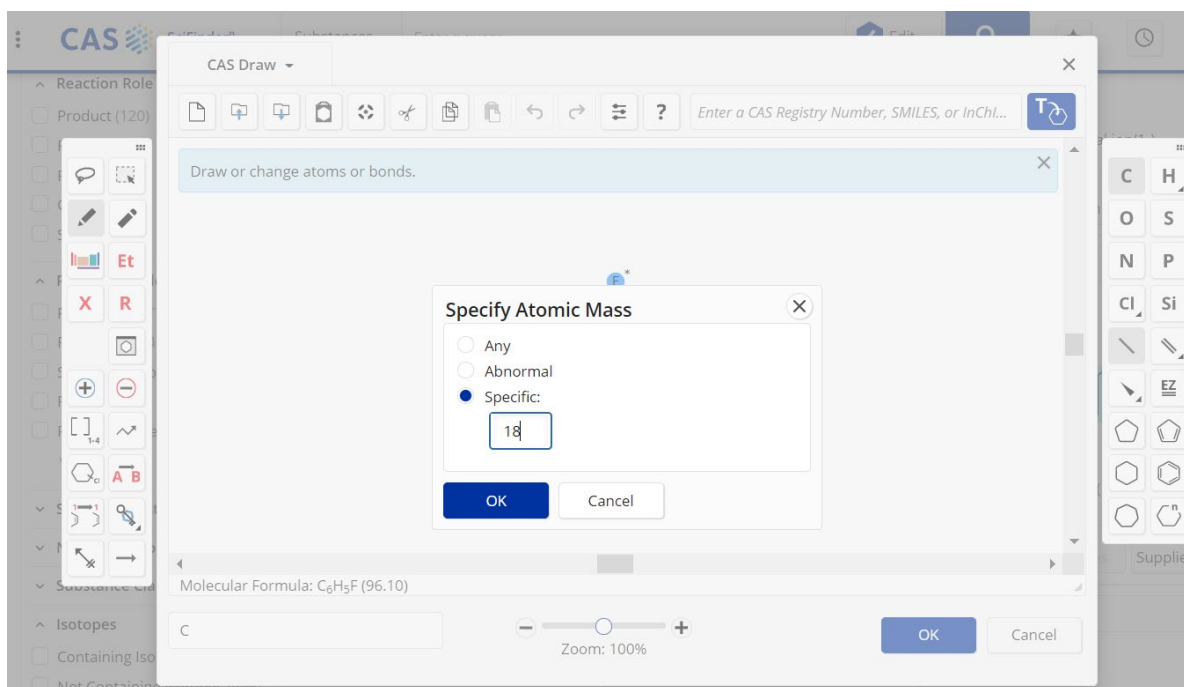
OK Cancel

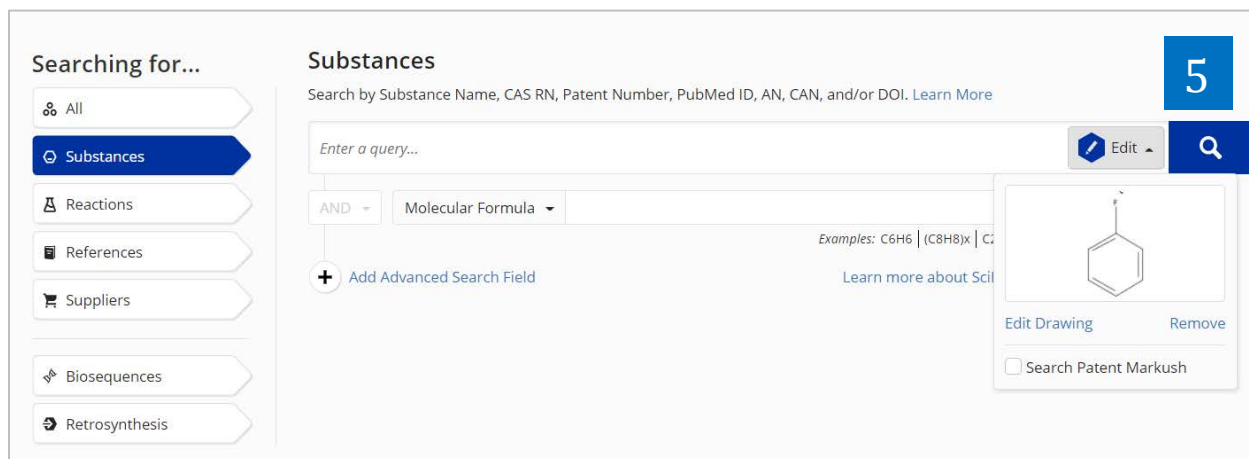
3. 鼠标悬在绘制结构中的原子上（例如 F），点击鼠标右键。

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

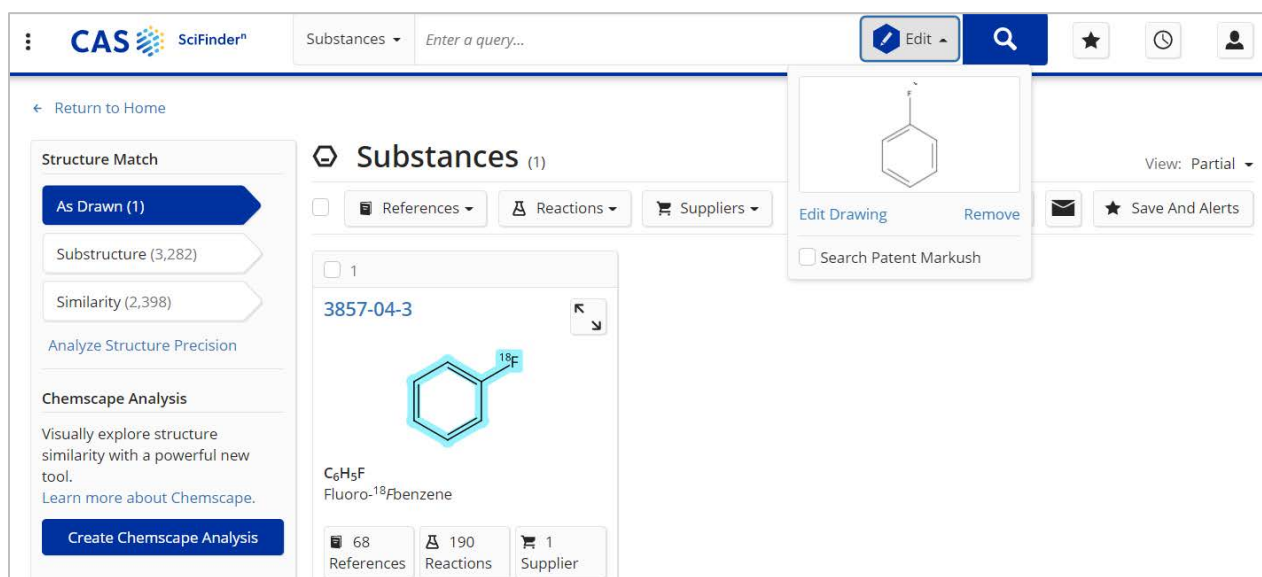


4. 在弹出窗口中点击 Abnormal，可获取所有 F 原子的同位素标记物；点 Specific 可输入特定的氟同位素相对原子质量，例如输入 18，点击 OK。



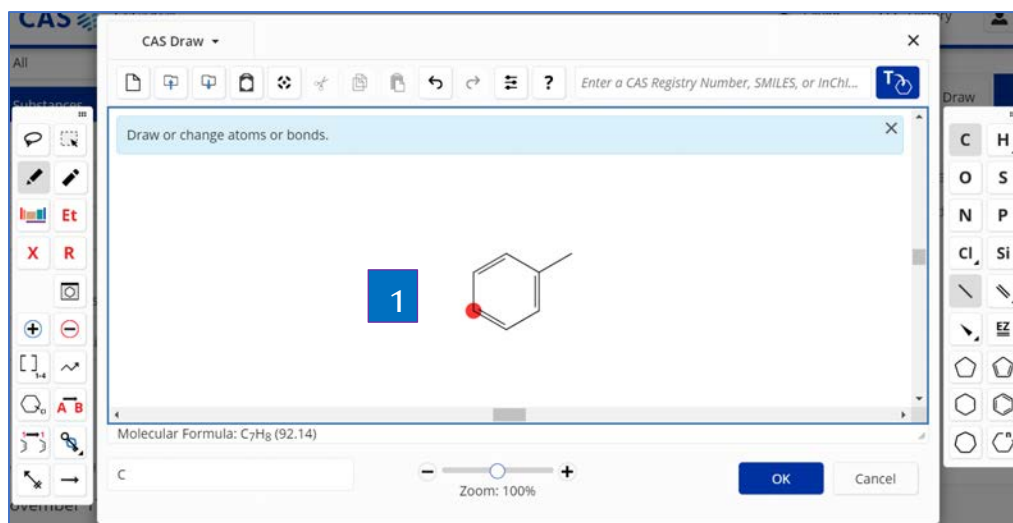


5. 开始检索，获取感兴趣的结果。

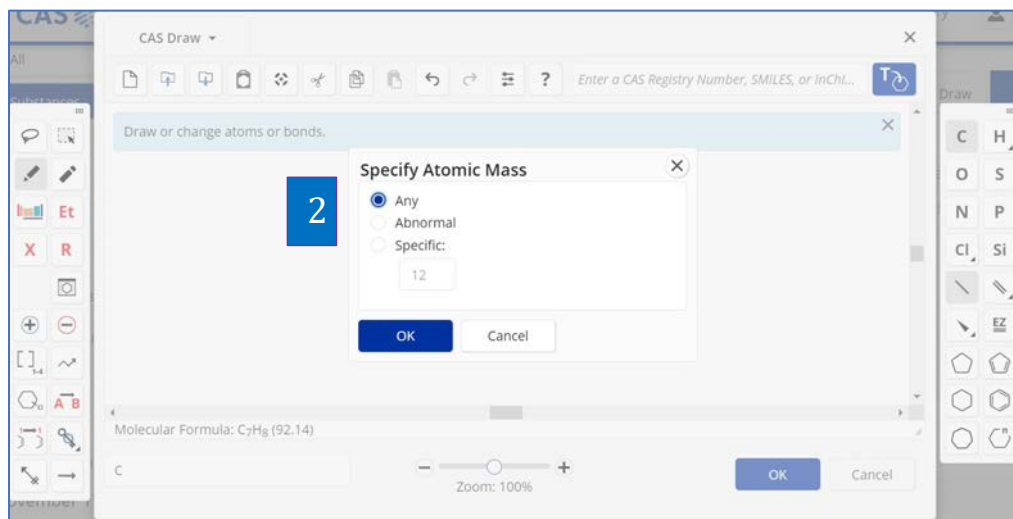


绘制结构式时，如何绘制同位素

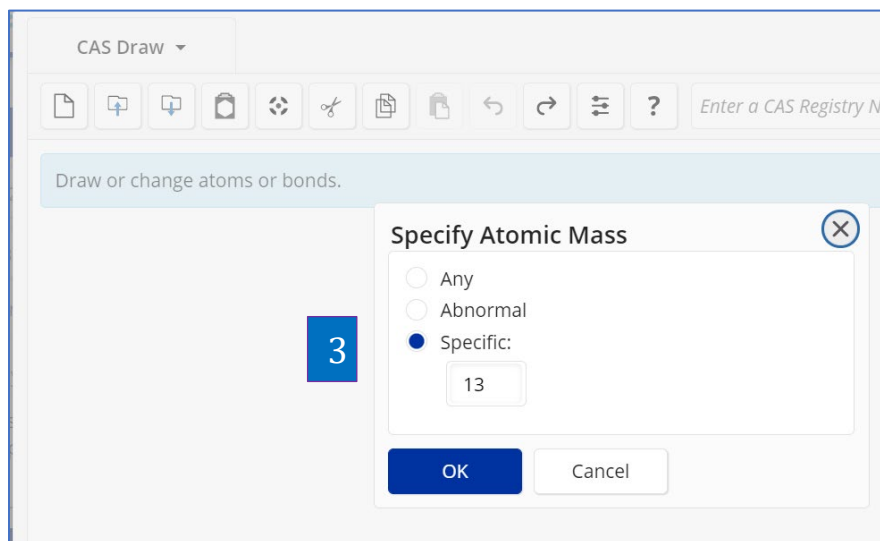
绘制结构时，可绘制特定原子的同位素，以获取其同位素标记的物质、同位素标记的物质参与的反应、研究同位素标记的物质的文献等信息。



1. 绘制结构，选中需要标记同位素的原子，点击鼠标右键。

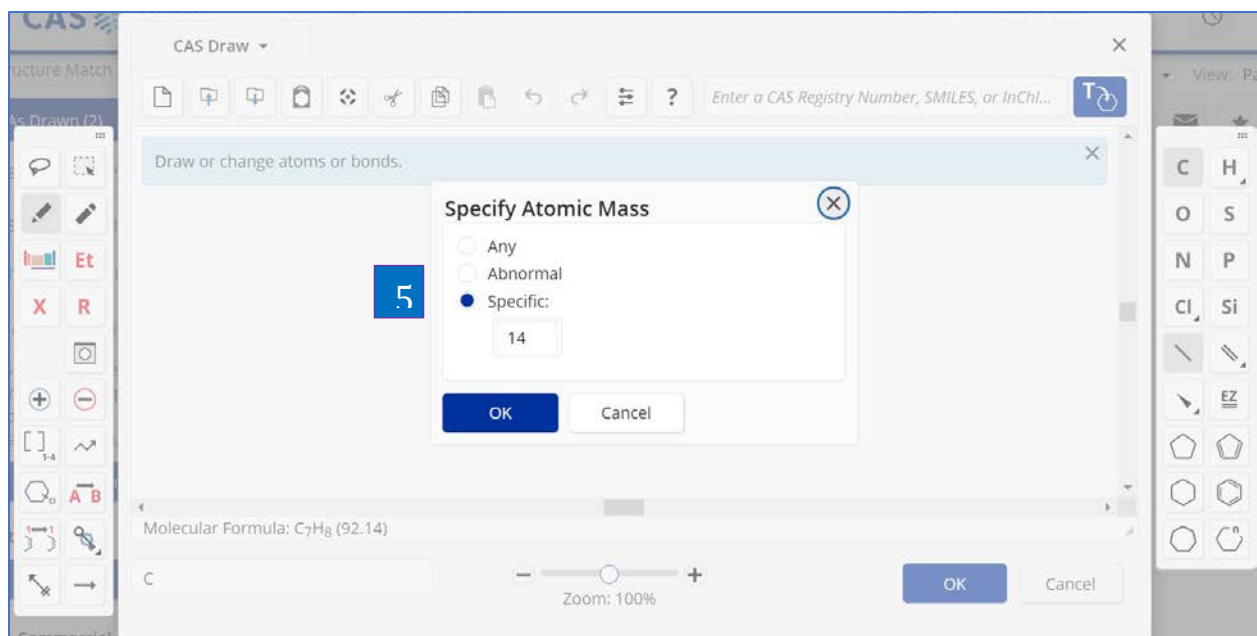


2. 在弹出窗口中，选择原子量为 Any（默认值，任意元素）、Abnormal（任意同位素）或 Specific（特定同位素）。



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

4. 所得结果均为满足设定需要：甲基对位的碳为 ^{13}C 。



5. 若希望甲基对位的碳原子为 ^{14}C ，则输入值 14

CAS SciFinder

Substances Enter a query...

Return to Home

Structure Match

As Drawn (2)

Substructure (585)

Similarity (6,335)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Substances (2)

References Reactions Suppliers

1 859793-75-2

C₇H₈
Toluene-*p*-C¹⁴

1 0 0
Reference Reactions Suppliers

2 115760-59-3

C₇H₈
Benzene-¹⁴C₆, methyl-

3 3 3
References Reactions Suppliers

6

Edit Drawing Remove

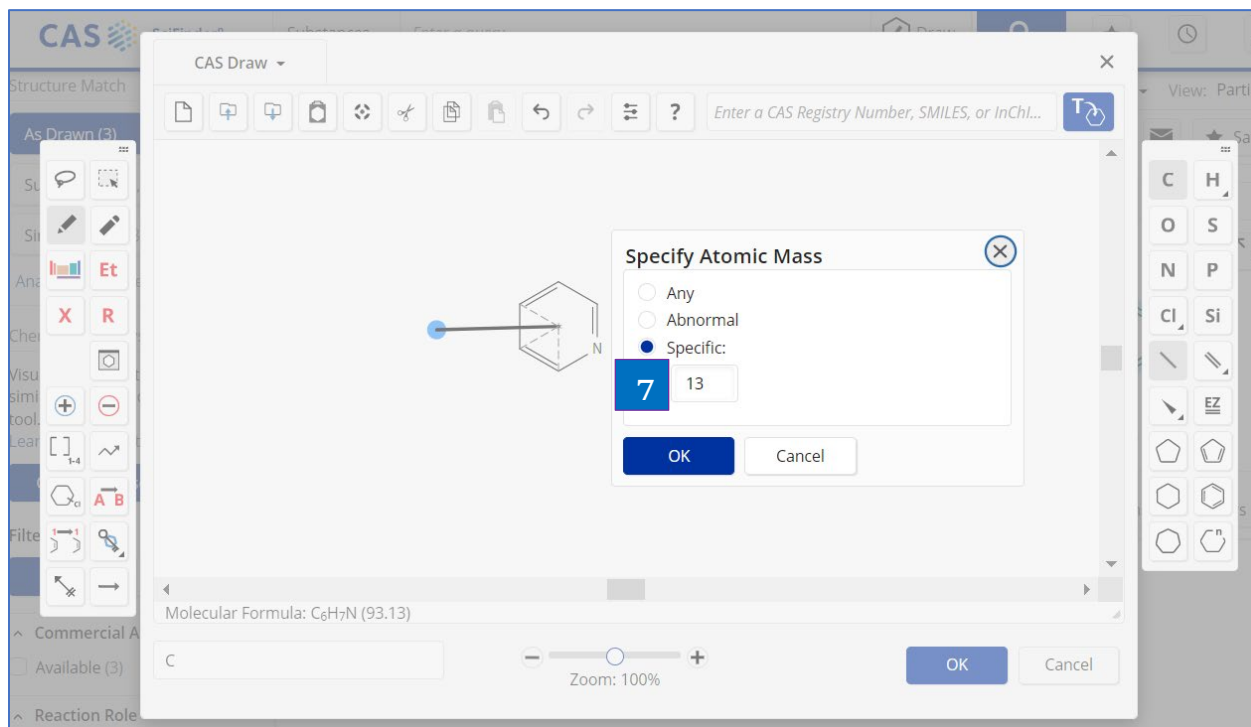
Search Patent Markush

6. 获得指定原子为 ^{14}C 的物质。

案例

获取具如下结构特征的物质：

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



7. 将甲基碳的原子量设置为 13

CAS SciFinder[®] Substances Enter a query...

8

Substances (4)

Structure Match

As Drawn (4)

Substructure (292)

Similarity (3,128)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Not Available (4)

Reaction Role

References Reactions Suppliers

1 8 0

Reference Reactions Suppliers

1 1 0

Reference Reaction Suppliers

3 4 0

References Reactions Suppliers

4

1630788-91-8

Cc1cccnc1

C_6H_5N
4-Pyridinylmethylene- ^{13}C

1529772-81-3

Cc1cccnc1

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

1404120-05-3

Cc1cccnc1

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

813432-91-6

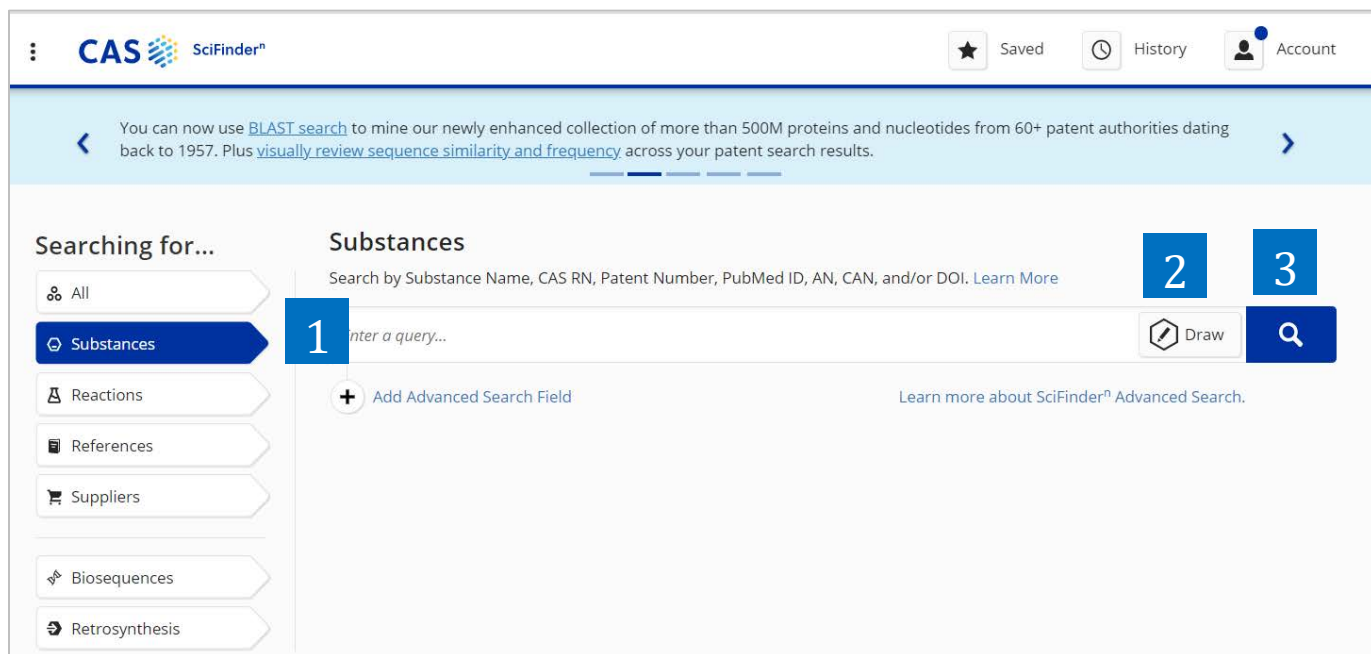
Cc1cccnc1

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

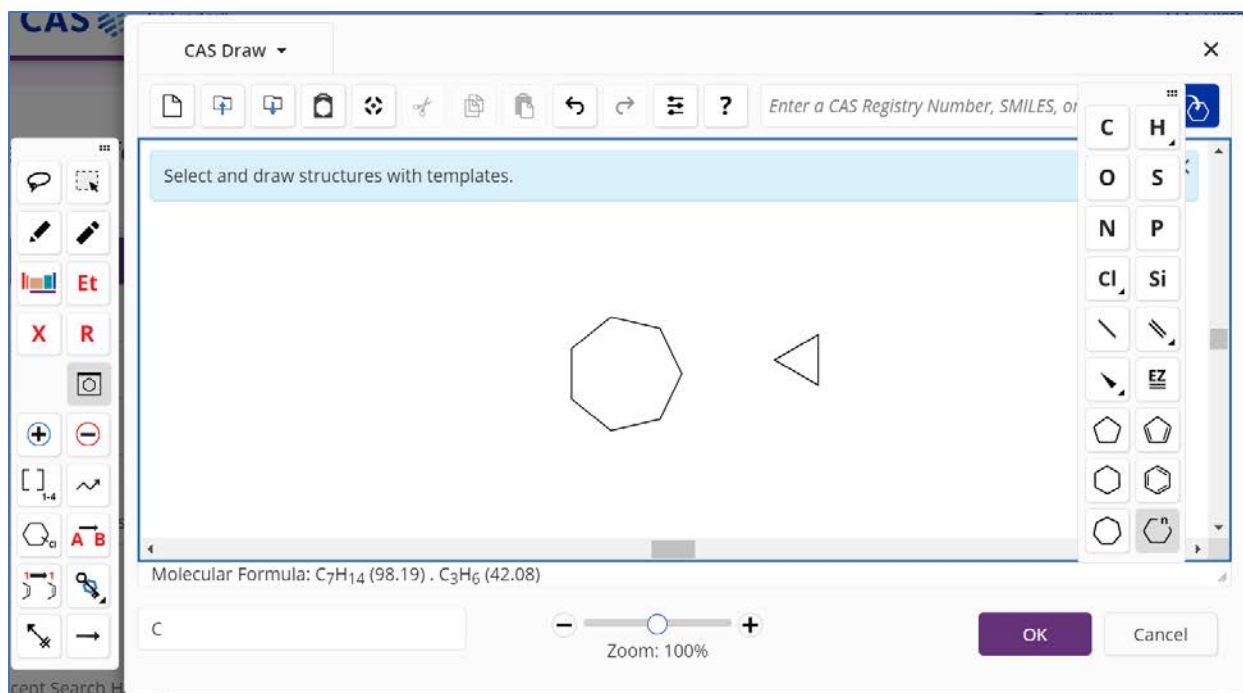
8. 获得满足要求的物质。

片段结构的物质检索

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



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



CAS SciFinder®

Substances Enter a query...

Reference Reactions Suppliers

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

1821719-88-3

C₁₀H₁₉N

Cycloheptanamine, 2-cyclopropyl-, (1R,2S)-

Absolute stereochemistry shown

References Reactions Supplier

1488617-56-6

C₁₁H₂₁N

α-Cyclopropylcycloheptanemethanamine

References Reactions Suppliers

1344060-41-8

C₁₀H₁₉N

2-Cyclopropylcycloheptanamine

References Reactions Suppliers

1340186-29-9

C₁₀H₁₉N

3-Cyclopropylcycloheptanamine

References Reactions Suppliers

2350332-22-6

C₁₁H₂₀O

Cycloheptanemethanol, α-cyclopropyl-, (αS)-

Absolute stereochemistry shown

References Reactions Suppliers

2350054-45-2

C₁₁H₂₀O

Cycloheptanemethanol, α-cyclopropyl-, (αR)-

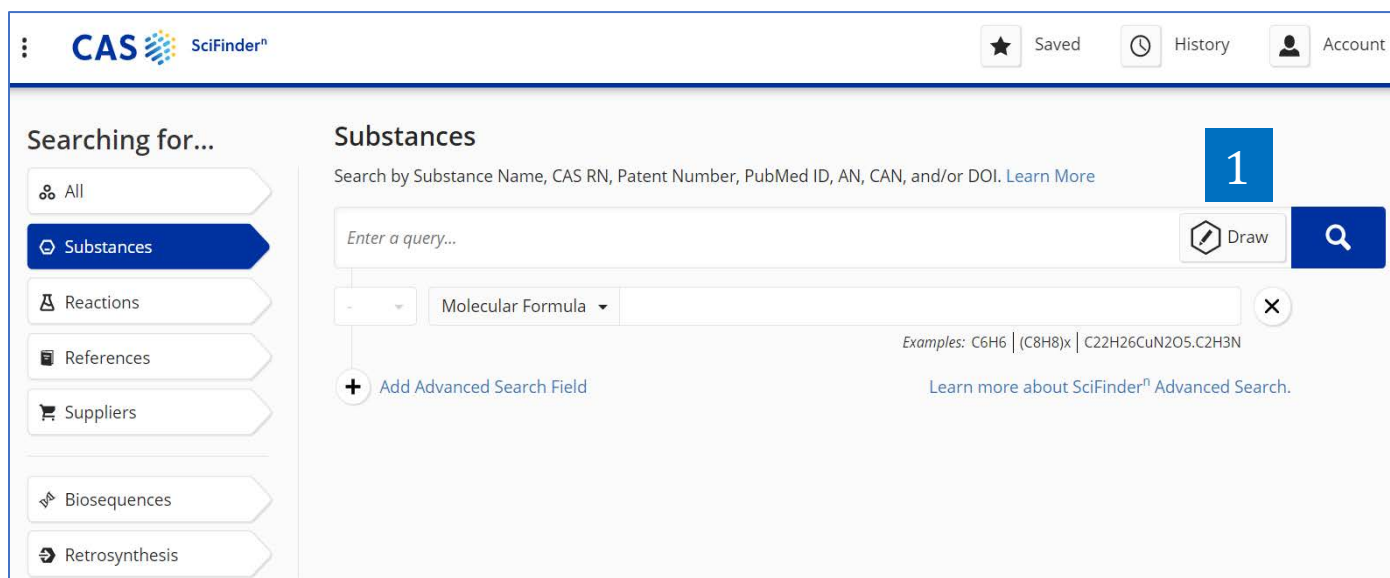
Absolute stereochemistry shown

References Reactions Suppliers

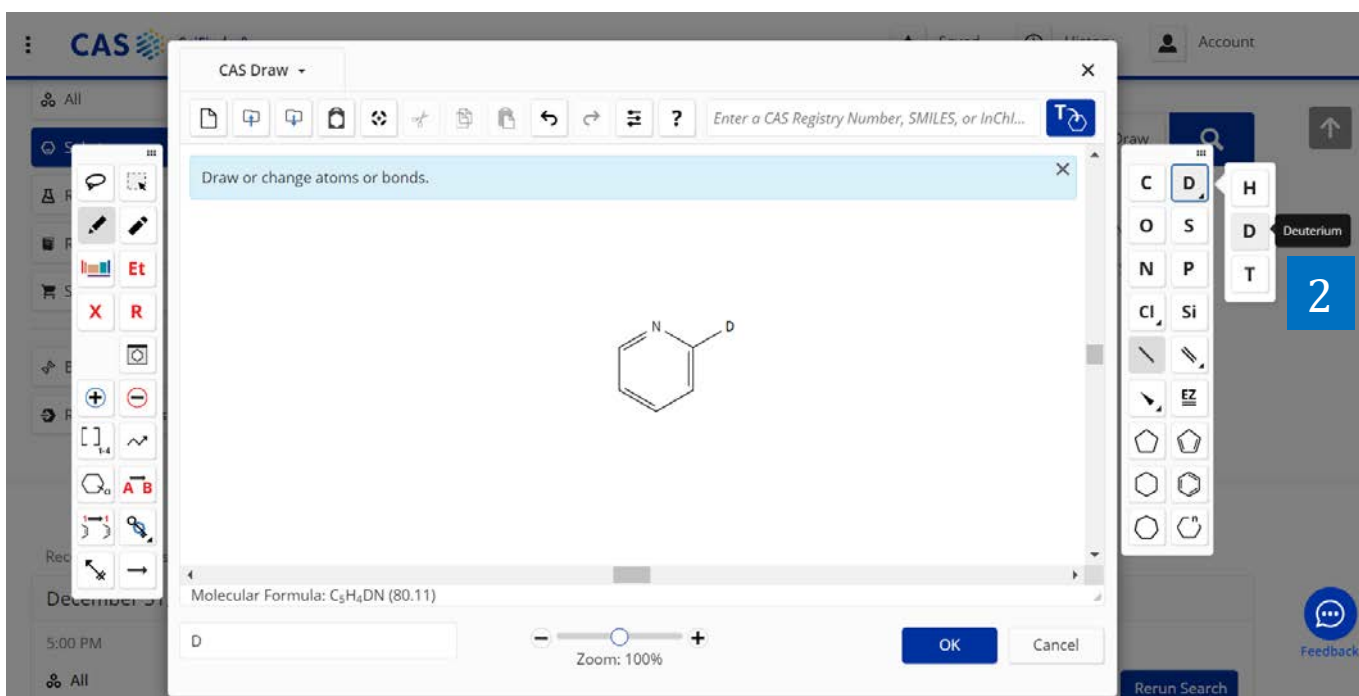
4. 在结果集页面左侧 Number of Components 下勾选相应选项，限定被检索的片段在同一个组分或多个不同组分中（如：选择 1，表示被检索片段在同一个组分中；选择 2，表示被检索片段分别在 2 个不同组分中等；以此类推）。
5. 可继续通过 Substance Class，筛选物质类型。
6. 点击 CAS 登记号，查看物质详情。

直接在结构中绘制氢的同位素 D 和 T

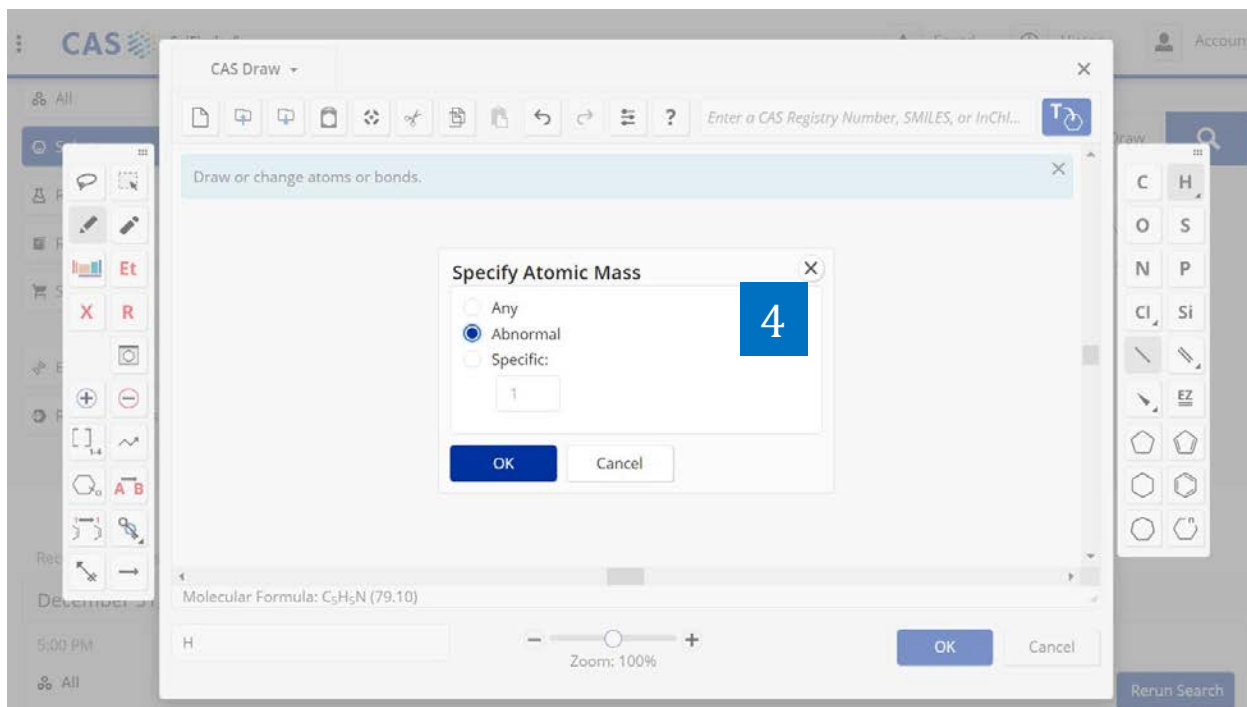
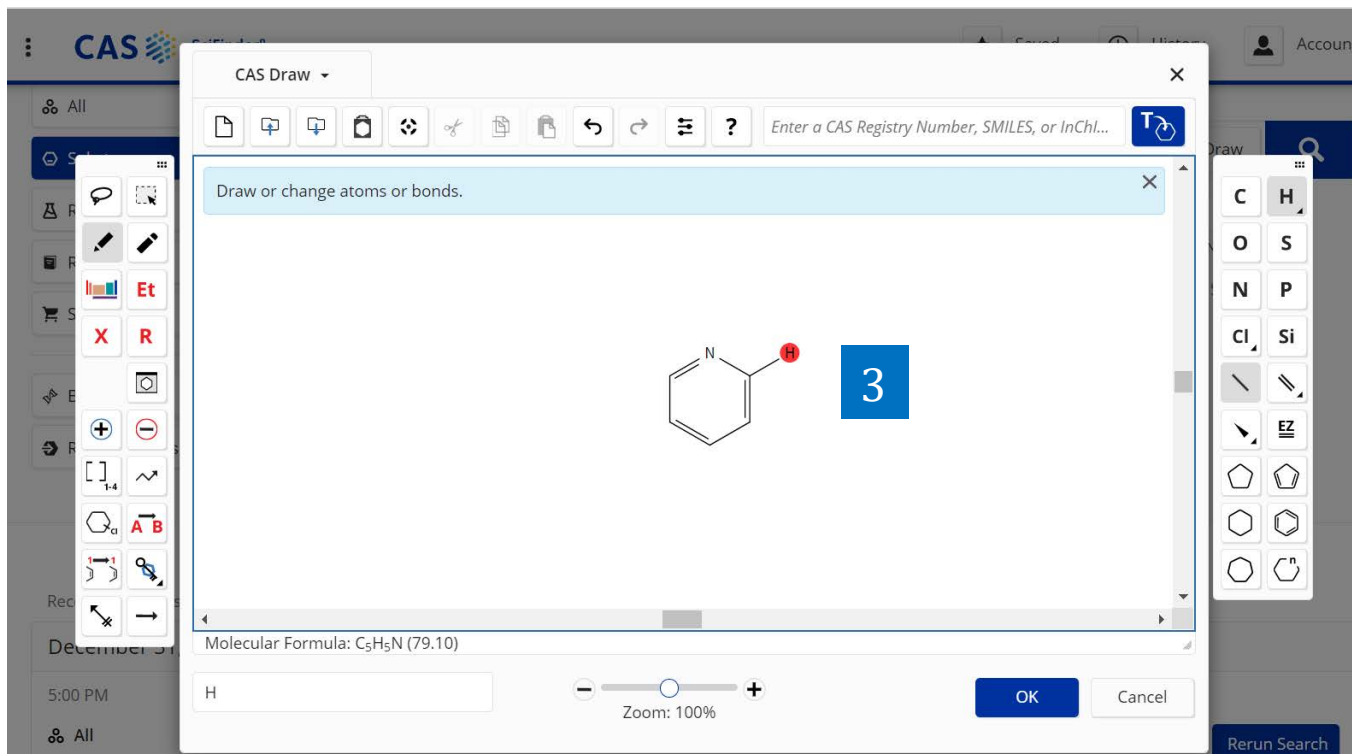
在 CAS SciFinder[®] 的结构编辑器中，可以直接在结构中绘制氢的同位素原子 D 和 T，获取含有氘或氚同位素标记的物质。



1. 点击 Draw，打开结构编辑器。



2. 点击 H 原子按键，选择 D 或者 T 绘制。



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

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

Searching for...

Substances

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

Enter a query...

AND Molecular Formula

Examples: C₆H₆ | (C₈H₈)_x | C

+ Add Advanced Search Field

Learn more about SciFinder

Edit Drawing Remove

☐ Search Patent Markush

5

- 开始检索，获取感兴趣的结果。

CAS SciFinder[®]

Substances Enter a query...

Edit

Return to Home

Structure Match

As Drawn (114)

Substructure (7,271)

Similarity (7,956)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

[Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Substances (114)

References Reactions Suppliers

1 7291-22-7

C₅D₅N
Pyridine-d₅

731 References 953 Reactions 122 Suppliers

2 1807-97-2

C₅H₄DN
Pyridine-2-d

53 References 29 Reactions 8 Suppliers

3 17265-96-2

C₅H₃D₂N
Pyridine-2,6-d₂

38 References 13 Reactions 9 Suppliers

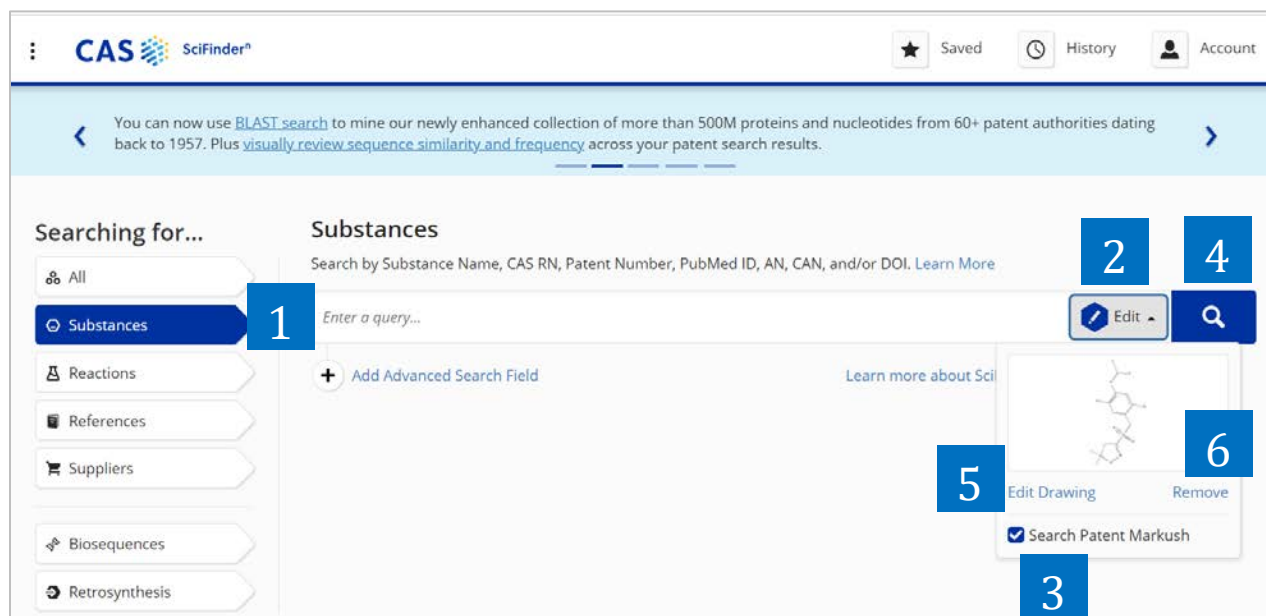
Relevance View: Partial

Edit Drawing Remove

☐ Search Patent Markush

5

马库什结构检索



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

The screenshot displays the CAS SciFinder Patent Markush Match interface. The top navigation bar includes the CAS SciFinder logo, a search bar, and user account options. The left sidebar contains filters for 'Patent Office' (World Intellectual Property Organization, Japan) and 'CA Section' (Agrochemical Bioregulators, Heterocyclic Compounds). The main content area shows two patent results. The first result, JP2008189578, is titled 'Broad-spectrum herbicide compositions containing cyclic amides with low herbicide injury, manufacture of the compositions, and weed control method'. It includes a chemical structure diagram with labels 11, 12, and 13. The second result, JP2009215221, is titled 'Isoxazolines as plant disease control agents'. The interface also includes a 'Patent Markush Match' section with 'As Drawn (16)' and 'Substructure (21)' options, and a 'Filter Behavior' section with 'Filter by' and 'Exclude' buttons. A 'Patent Pak' button is visible next to the first result.

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

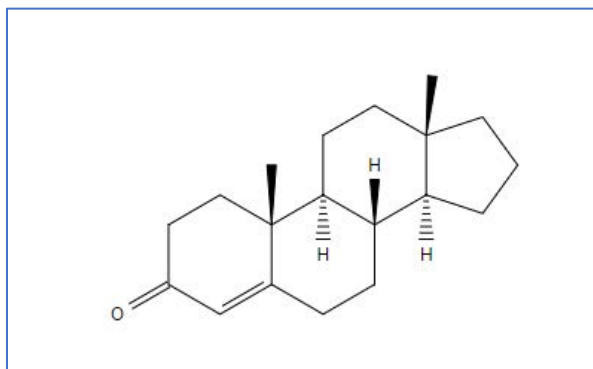
马库什结构检索结果页直接呈现专利著录信息

The screenshot shows the CAS SciFinder interface for a Patent Markush Match search. The main content area displays the chemical structure of a Markush compound, which is a substituted benzene ring with a pyridine ring attached. The structure is labeled with 'G21' and '378, 379, 381, 382, 384'. To the right of the structure, the patent information for WO2018062978 is shown, including the title 'Preparation of heteroaryl compounds as antiviral agents', the inventors (Min, Ji Young; Chang, So Young; Lee, Ji Hye; Kang, Sun Hee; Kong, Sun Ju; Jo, Su Yeon; Park, Kaapjoo; Kim, Young Mi; Choi, Junghwan), the World Intellectual Property Organization (WIPO) number, the date (2018-04-05), the language (Korean), the database (CAplus), and the assignee (Institut Pasteur Korea). The patent claim 1 is also displayed, stating '378,379,381,382,384: opt. substd. by G16'. The interface includes a search bar at the top, a 'Patent Markush Match' section on the left, and a 'Filter Behavior' section on the right.

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？



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

The screenshot shows the CAS SciFinder[®] interface. On the left, the 'Filter Behavior' panel is active, with 'Exclude' selected under 'Filter by'. Under 'Reaction Role', 'Product' is checked, and a blue box with the number '2' highlights this checkbox. The main search results area displays three steroid compounds, each with its chemical structure and a 'Feedback' button.

Compound Name	Chemical Formula	References	Reactions	Suppliers
6-Hydroxytestosterone	C ₁₉ H ₂₈ O ₃	25	1	0
Pregn-4-ene-3,16-dione	C ₂₁ H ₃₀ O ₂	5	0	1
Androst-4-ene-3,16-dione, 6,17-dihydroxy-, (6β,17β)-	C ₁₉ H ₂₆ O ₄	1	0	0

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

References Reactions Suppliers

Filtering: Reference Role: Natural Product Occurrenc... Stereochemistry: 3 Selected [Clear All Filters](#)

Excluding: Reaction Role: Product

As Drawn (16)

Substructure (30K)

Similarity (170K)

Analyze Structure Precision

Chemscapc Analysis

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

Create Chemscapc Analysis

Filter Behavior

Filter by Exclude

Commercial Availability

Reaction Role

Reactant (2)

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

4

3 39025-25-7

Absolute stereochemistry shown

C₂₇H₄₄O₄
(16β,22R)-16,20,22-Trihydroxycholest-4-en-3-one

13 References 0 Reactions 1 Supplier

CAS RN
[84924-96-9](#)

CAS Name
(24S)-Stigmast-4-en-3-one

Substance Detail

Reactions (0)

Synthesize (0)

Start Retrosynthetic Analysis

References (15)

Suppliers (1)

5

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。

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

Retrosynthesis Plan Options

Powered by ChemPlanner[®]

Select Synthetic Depth [Learn more.](#)

☐ 1
☐ 2
☒ 3
☐ 4

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

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

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

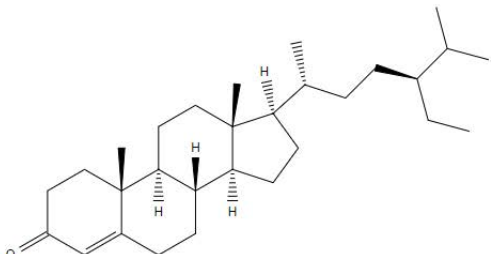
1000 USD/mol

☐ Email me when my plan is complete

[Create Retrosynthesis Plan](#)

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

[Clear All Bond Selections](#)



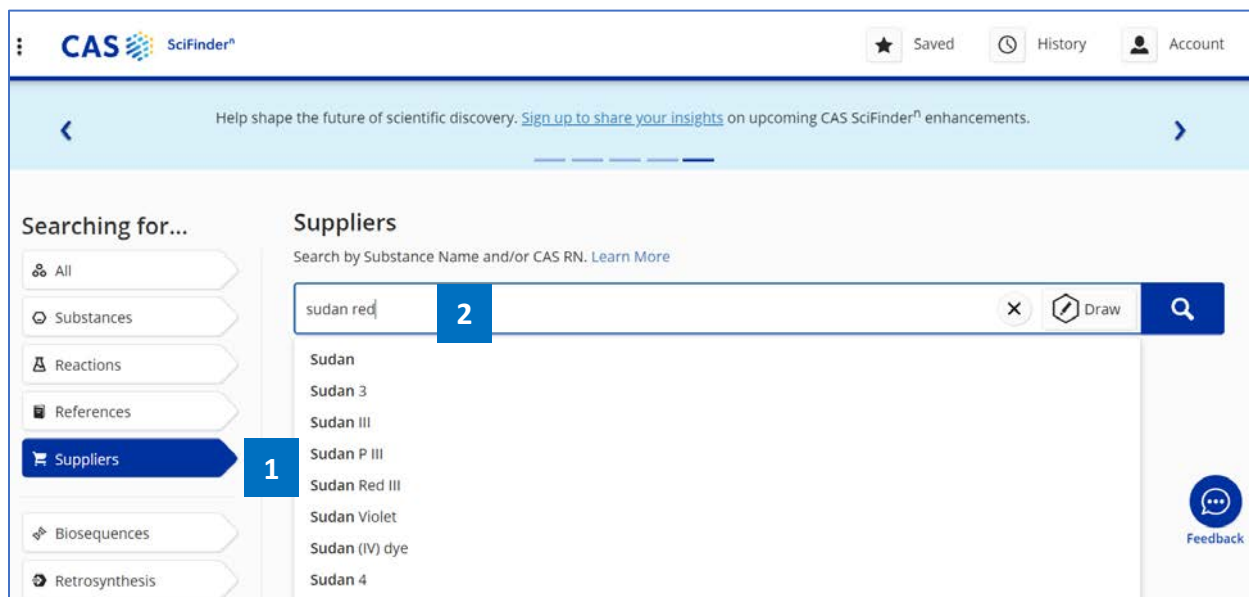
6. 点击 Create Retrosynthesis Plan，获取该物质的预测逆合成路线。

获取化学品供应商信息

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

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

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



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

Return to Home

Filter Behavior

Filter by Exclude

Preferred Suppliers

Supplier **3**

Substance

Purity

Quantity

Ships Within

Stock Status

Order From Supplier


Country

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

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



**Fine & Specialty Chemicals
in Catalog & Bulk**

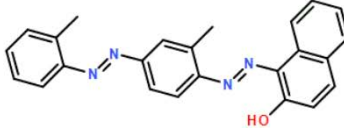
Inhibitors, Bioactives, Reference Compounds
Building Blocks, Intermediates, Reagents
Bulk Bio & Specialty Chemicals

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[Resources](#)
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[Help](#)

T805
Solvent Red 24, 95% (HPLC)

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



IDENTITY
CAS Number: 85-83-6
MDL Number: MFCD00003893
MF: C24H20N4O
MW: 380.45

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

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

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Current as of November 9, 2021


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

[PubChem](#)

点击 Product Information 所获界面：

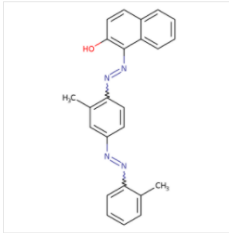


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FS03568

Solvent Red 24



TECHNICAL DATA

CoA SEARCH

TAGS

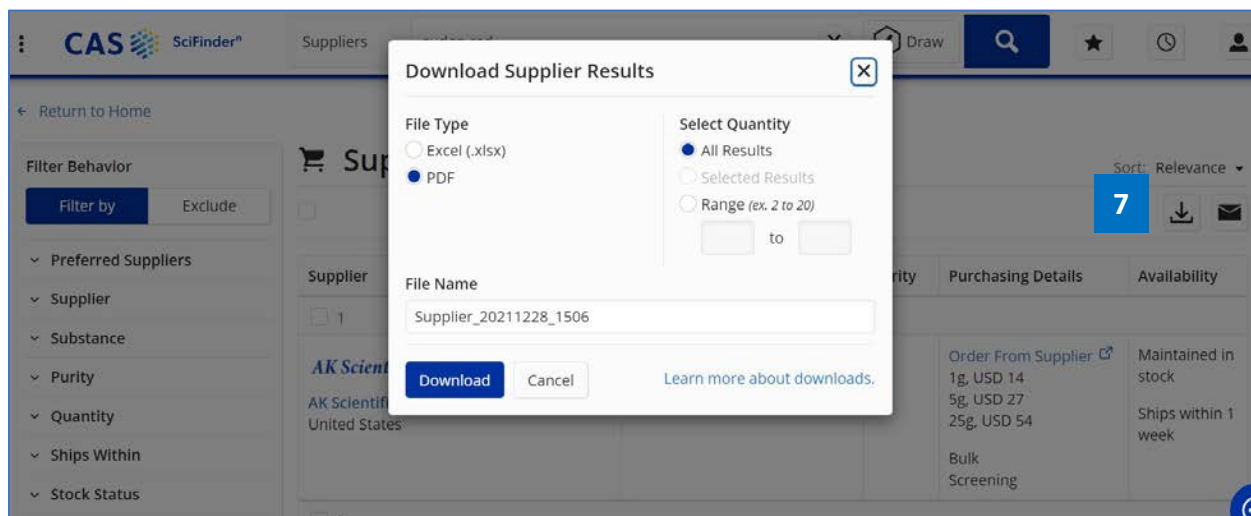
TECHNICAL DATA

CAS No: 85-83-6

Product Code: FS03568

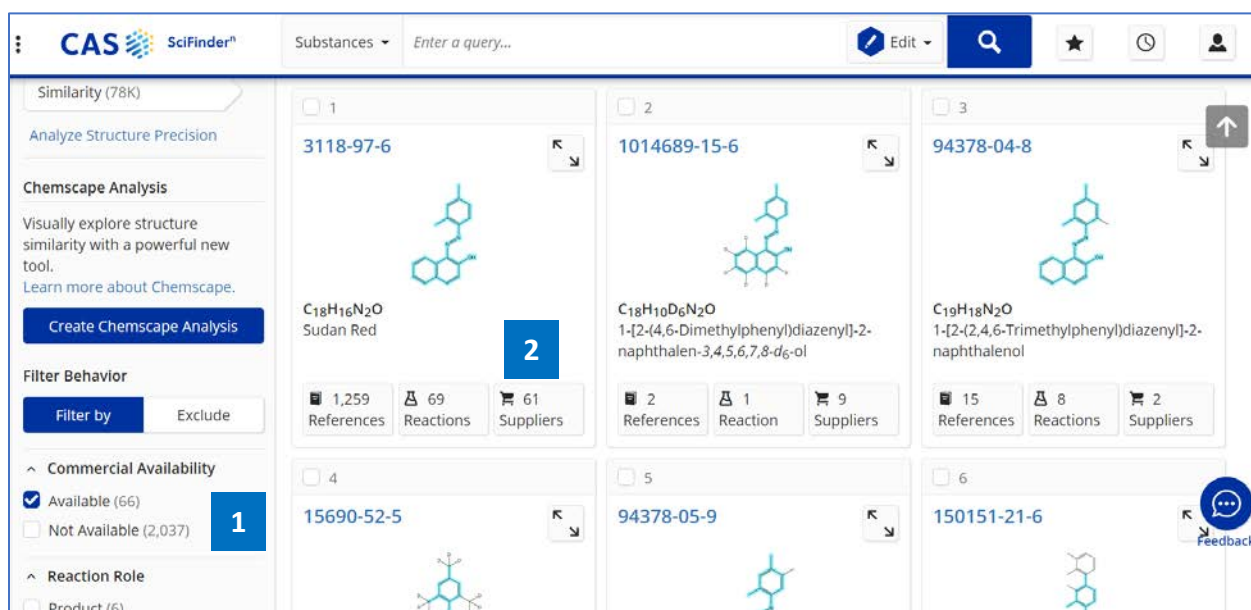
MDL No: MFCD00003893

Chemical Formula:



7. 供应商结果集可以导出为 Excel 或者 PDF 格式文件。

方法二、在物质结果集页面，点击相应的 suppliers 获得供应商信息。



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

方法三、在反应结果集页面点击相应的 Suppliers 获取供应商信息。

The screenshot displays the CAS SciFinder interface for a reaction search. The top navigation bar includes the CAS logo, search filters (Reactions, 3118-97-6), and icons for Draw, Search, Favorites, History, and User. A left sidebar contains various filters: Solvent, Commercial Availability (Products (7), All Starting Materials (19)), Reaction Notes, Search Within Results, Source Reference, Document Type, Language, Publication Year, Publication Name, and CA Section. The main content area shows a reaction scheme labeled 'Scheme 2 (2 Reactions)' with 'Steps: 1 Yield: 93%'. The reaction involves 2-naphthol and 2-aminotoluene reacting to form a product. Below the reactants are 'Suppliers (97)' and 'Suppliers (78)' buttons, respectively. The product has a 'Suppliers (61)' button. A blue box with the number '1' is placed over the 'All Starting Materials (19)' filter, and a blue box with the number '2' is placed over the 'Suppliers (61)' button. Below the reaction scheme, a 'Reaction Summary' section provides details: '1.1 Reagents: tert-Butyl nitrite', 'Solvents: Dichloromethane; 24 h, rt', and 'By: Liu, Ting-Ting; et al'. A 'Full Text' button is also visible. A 'Feedback' icon is in the bottom right corner.

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 interface. At the top, the search bar contains 'La*chol' with a blue box containing the number '1'. Below the search bar, the results are displayed under the 'Substances (3)' tab. The results are sorted by 'CAS RN: Descending'. Three results are shown:

- Result 1:** CAS RN 8038-34-4. Notes: Waxy esters and alcs. from lanolin. Unspecified Lanochol. 1 Reference.
- Result 2:** CAS RN 8006-54-0. Notes: Fat-like substance derived from sheep wool. Contains a complex combination of esters and polyesters, consisting chiefly of cholesteryl and ischolesteryl esters of the higher fatty acids. Unspecified Lanichol. 432 References, 24 Suppliers.
- Result 3:** CAS RN 84-79-7. Chemical structure of Lapachol (C₁₅H₁₄O₃). 996 References, 430 Reactions, 58 Suppliers.

A left sidebar contains filter options for Commercial Availability, Reaction Role, and Reference Role.

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

CAS SciFinder® Substances Lapacho* 2

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

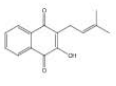
Substances (14)
 Sort: CAS RN: Descending View: Partial

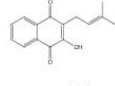
References Reactions Suppliers

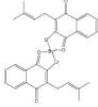
1 2 3 4 5 6

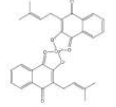
2100329-07-3
 Image Not Available
 Notes: An herbal tea made from the inner bark of the Pau d'arco tree (Handroanthus impetiginosus) purported to have anti-inflammatory and anticarcinogenic activities
 Unspecified
[Lapachorinde](#)
 1 Reference 0 Reactions 0 Suppliers

855637-05-7

 $C_{30}H_{26}O_6$
[Lapachol, peroxide](#)
 3 References 3 Reactions 1 Supplier

332083-20-2

 $C_{15}H_{14}O_3 \cdot K$
 Components: 2
 Component RN: 84-79-7
[Lapachol potassium salt](#)
 5 References 0 Reactions 1 Supplier

184359-68-0

 $C_{15}H_{14}O_3 \cdot Ag(I)$
 Components: 2
 Component RN: 84-79-7
[Lapachol silver salt](#)
 1 Reference 1 Reactions 0 Suppliers

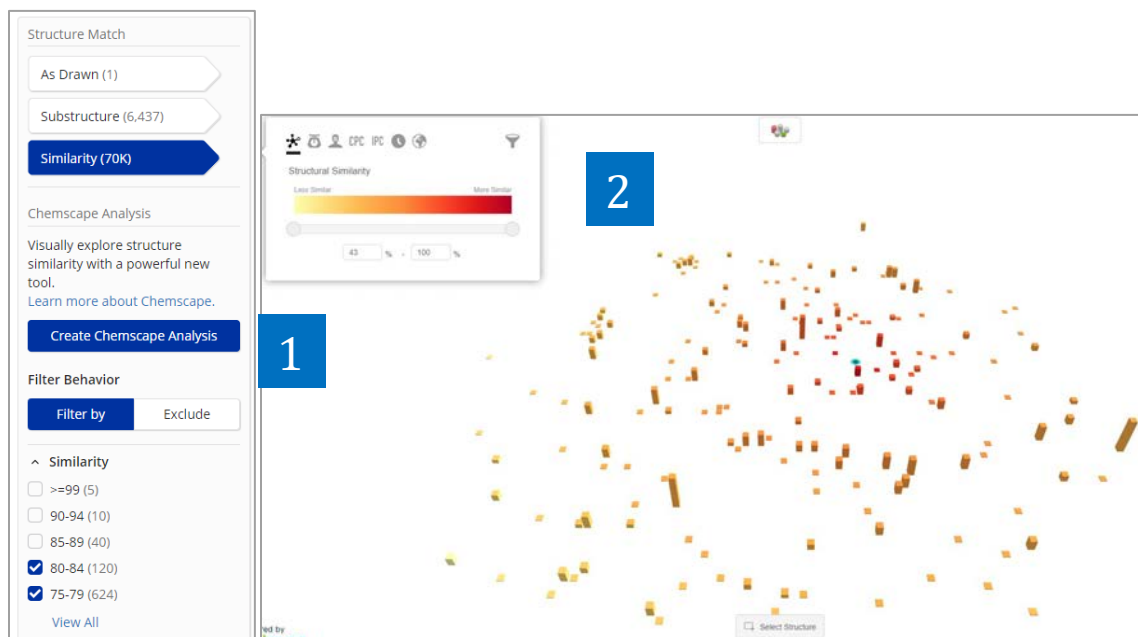
128528-86-9

 $C_{30}H_{26}BeO_6$
[Lapachol, Be deriv.](#)
 1 Reference 0 Reactions 0 Suppliers

128271-49-8

 $C_{30}H_{26}CoO_6$
[Lapachol, Co deriv.](#)
 1 Reference 0 Reactions 0 Suppliers

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

可视化分析结构检索结果（Chemscape 分析）

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



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



3. 根据申请人、CPC、IPC、公布年和专利受理机构等对物质进行分组。

反应检索

逆合成路线设计工具 (Retrosynthesis)

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

The screenshot displays the CAS SciFinder Retrosynthesis tool interface. On the left, a sidebar titled "Searching for..." lists various search categories: All, Substances, Reactions, References, Suppliers, Biosequences, and Retrosynthesis (highlighted with a blue bar and a blue box labeled "1"). The main workspace is titled "Retrosynthesis" and contains a drawing toolbar on the left and a central canvas for drawing chemical structures. The canvas shows a complex molecule with a brominated benzene ring, a pyrazole ring, and a cyclobutane ring. Below the canvas, the molecular formula is displayed as "Molecular Formula: C₁₉H₁₉BrN₄O₅ (463.29)". A zoom slider is set to 90%. A blue button labeled "Start Retrosynthetic Analysis" is located at the bottom right of the workspace, with a blue box labeled "2" next to it.

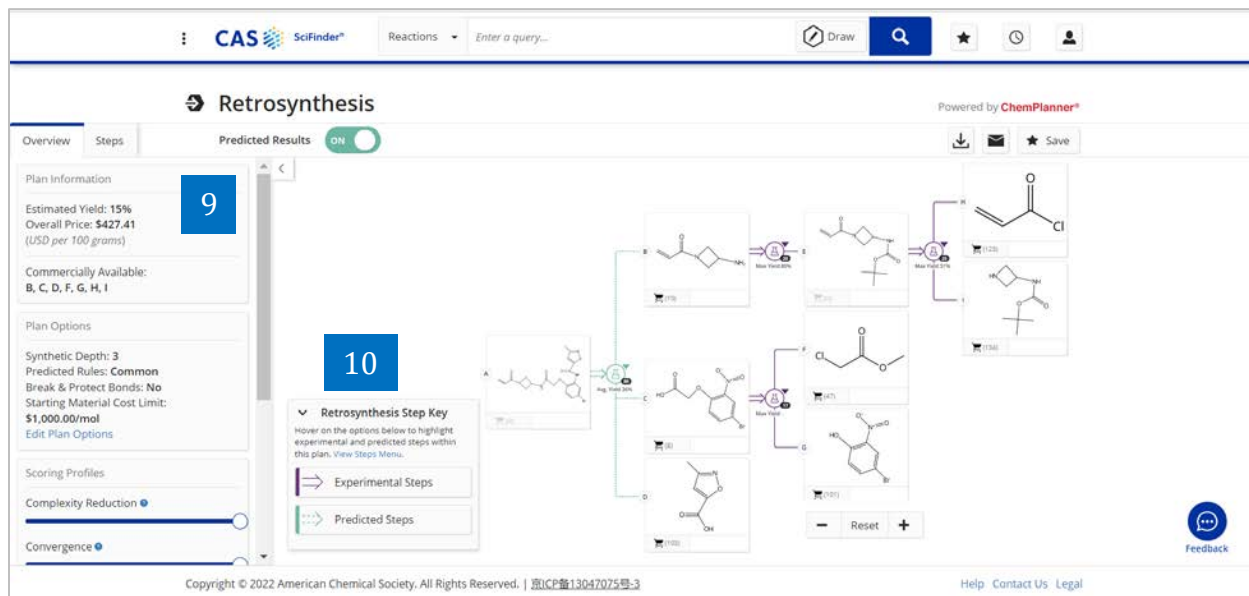
1. 点击 Retrosynthesis, 打开结构编辑器。
2. 结构绘制完成后, 点击 Start Retrosynthetic Analysis 打开 Retrosynthesis Plan Options 窗口。
3. 合成深度通过为最长路径设置最多四个步骤来限制逆合成计划中允许的合成步骤数。
4. 选择支持预测反应的规则:

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

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

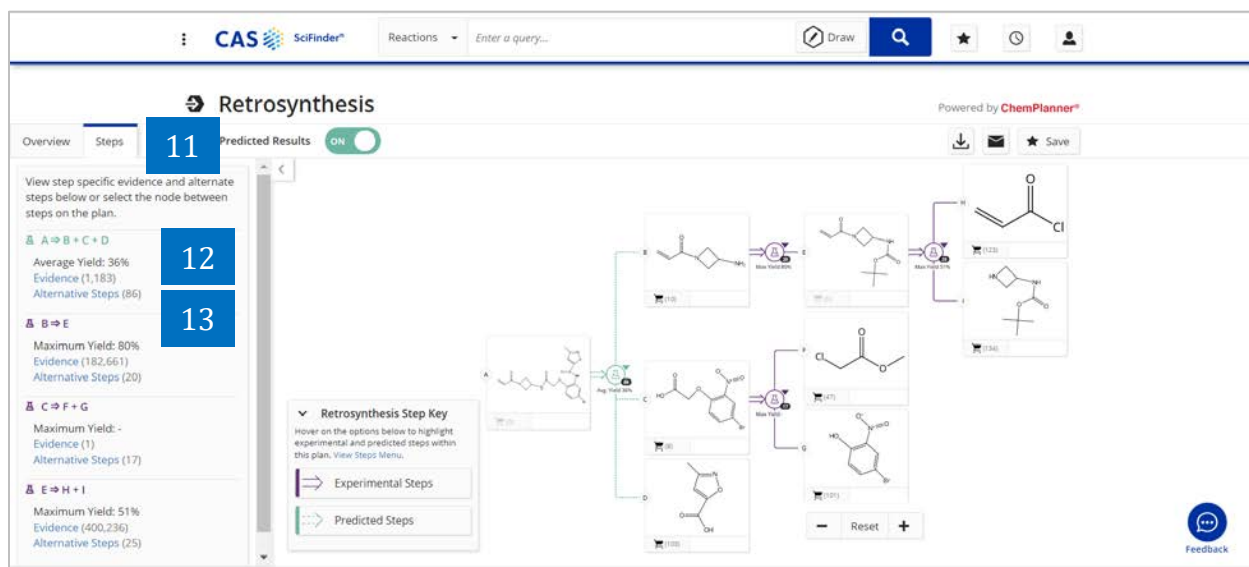
5. 设置起始物成本 (单位为: 美元/摩尔或美元/克)。
6. 设置断开键 (break bond) 和保护键 (protect bond): 断开键的含义为整个路线最后一步合成的键, 一个路线只能设置一根断开键; 保护键的含义为整个路线都不会发生变化的键, 一条路线可以同时设置几根保护键。
7. 化合物的预测逆合成路线可能需要数分钟完成 (约 10 分钟左右), 可以点击 Email me when my plan is completed。即路线预测完毕后向注册 CAS SciFinder[®] 账号的邮箱发送通知。

8. 创建路线。



9. 结果呈现：Overview 显示完整逆合成路线，预估产率和成本。

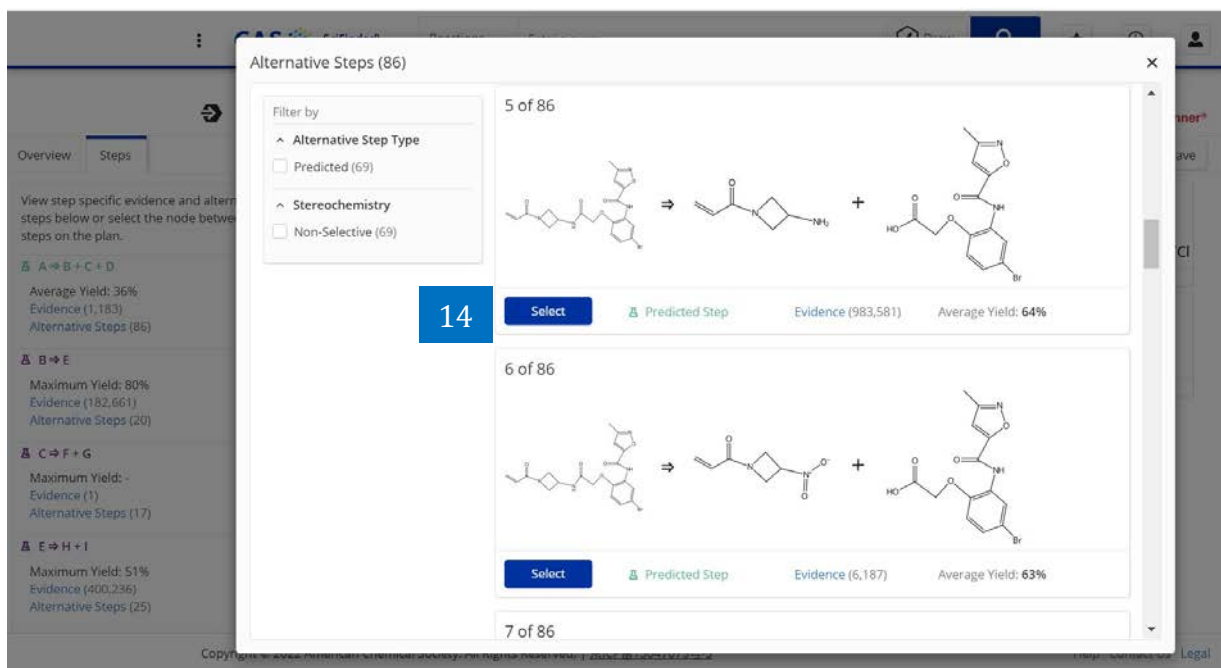
10. 紫色代表来源于已经报道的反应；绿色代表预测的反应路线。



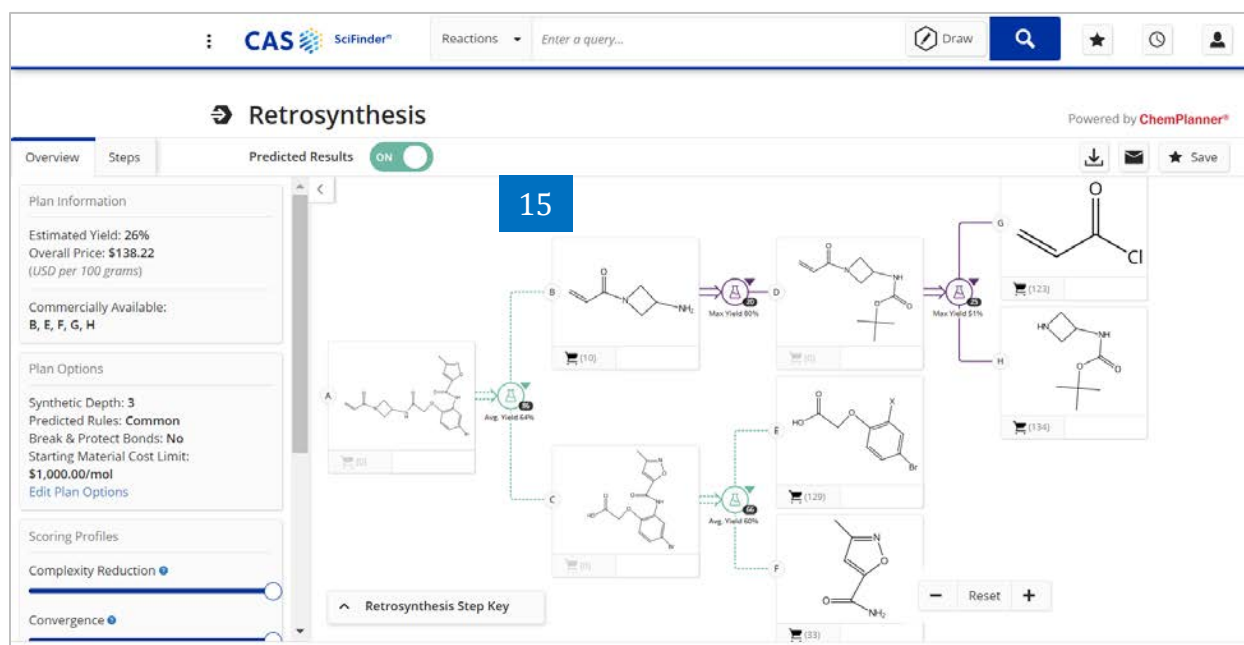
11. 点击 Steps，显示合成路线中具体步骤信息，产率及可替代步骤。

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

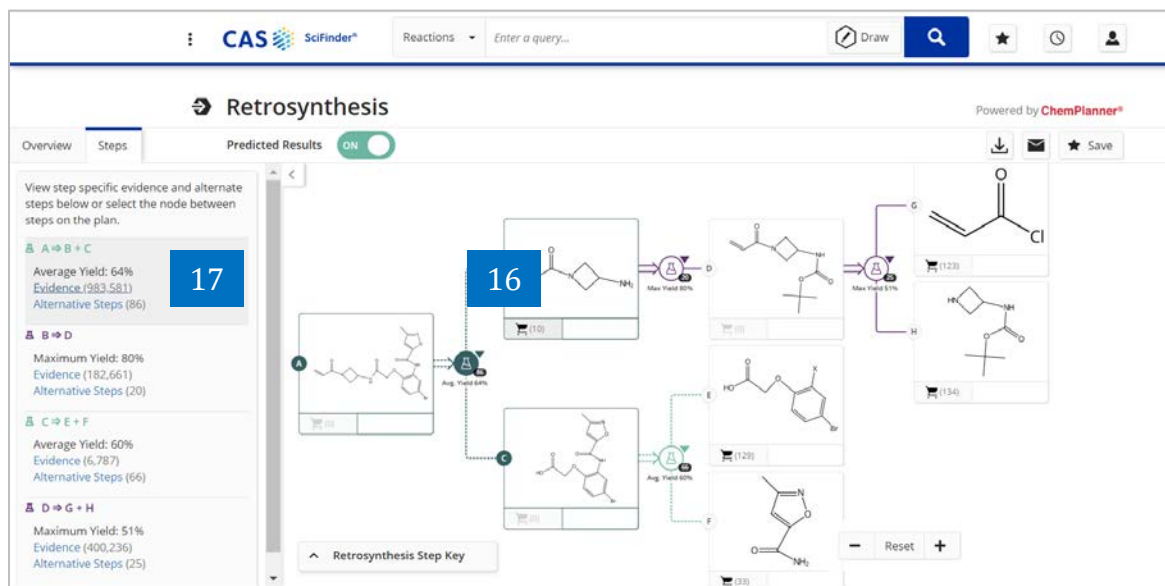
13. Alternative Steps 可替代反应步骤。



14. 选择感兴趣的反应步骤，整个逆合成路线发生改变。



15. 整个实验路线发生改变，其中绿色路线为预测路线。



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

17. 点击 Evidence，查看支持此反应步骤的反应和文献信息。

Reactions (983,581) **18**

Group: By Document View: Expanded

Filter Behavior
Filter by Exclude

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

Number of Steps
☐ 1 (983K)

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

Experimental Protocols
☐ Synthetic Methods (154K)
☐ Experimental Procedure (311K)

Reaction Type

References

1

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

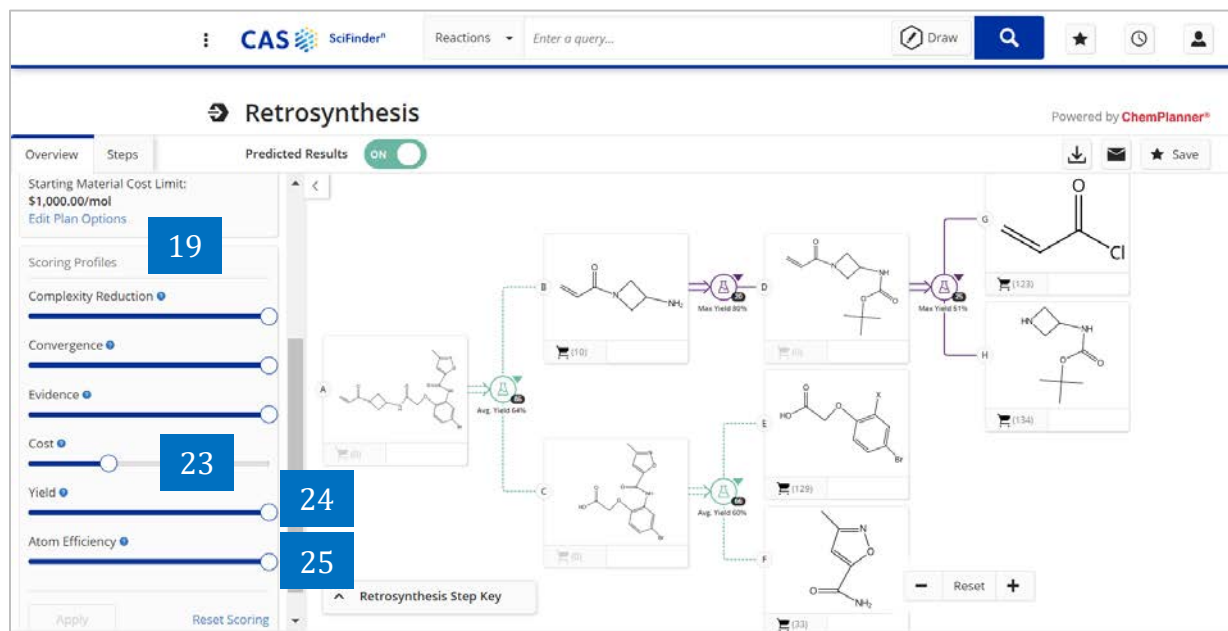
Full Text View 2 Related Reactions

Reaction Summary
1.1 Solvents: Dichloromethane; 1 h, rt
View Reaction Detail Experimental Protocols

2

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

18. 支持该步骤的反应结果集。



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

20. 降低复杂性：降低步骤起始物相对于该步产物的复杂性。

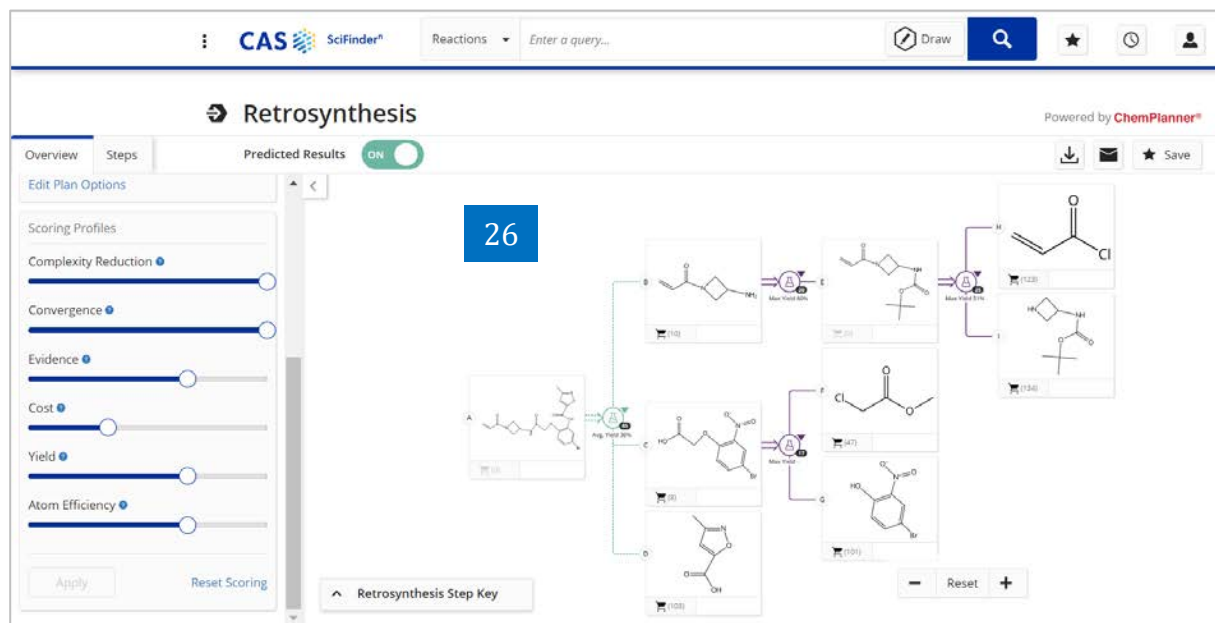
21. 汇聚：调高 Convergence 会提高路线的汇聚（减少反应路线的线性长度）。

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

23. 成本：根据起始物的成本价格（由低到高）来排列计划步骤/备选方案。

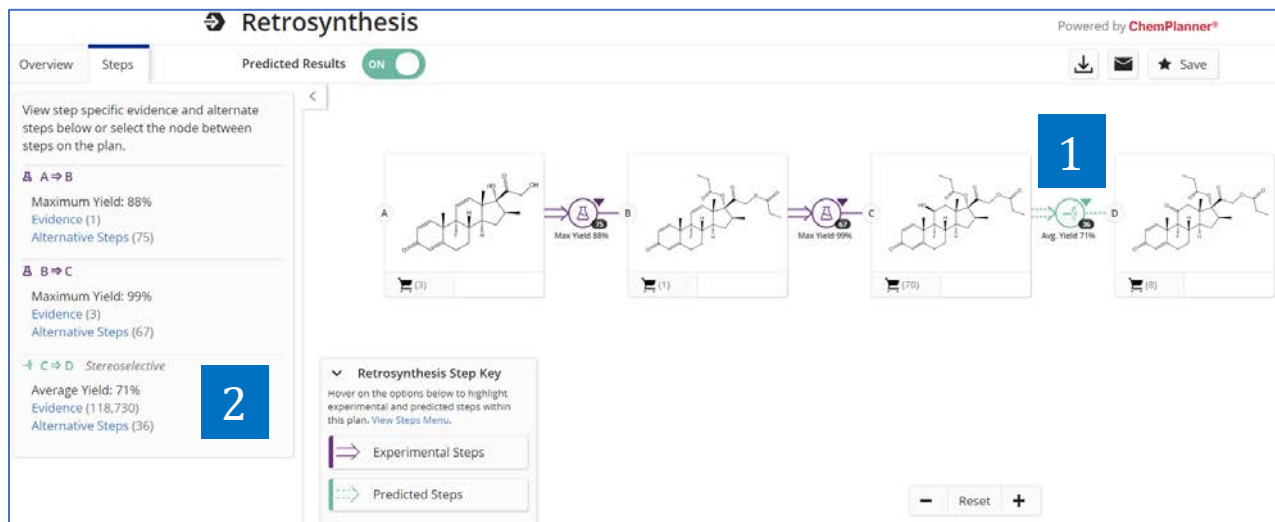
24. 产率：增加路线计划中每一步的产率，这有助于提高目标分子的产率。

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

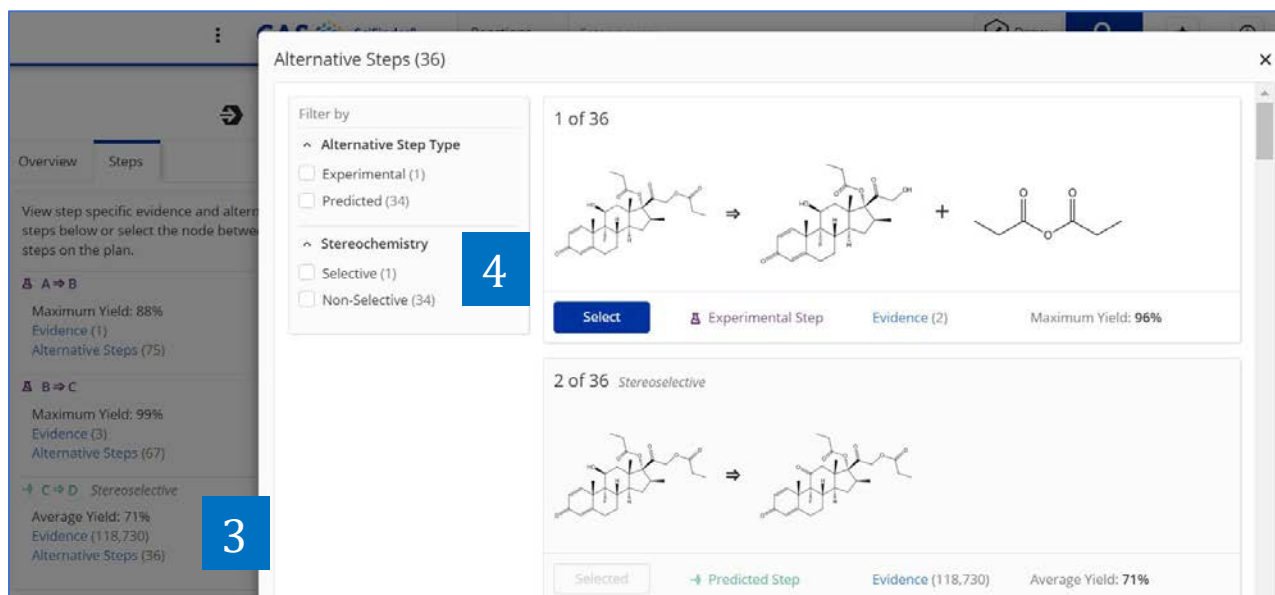


26. 更改评分配置之后的路线。

逆合成路线之立体选择性反应



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



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

逆合成路线之自定义分值 (Scoring) 功能

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

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

Convergence: 调整逆合成路收敛性；

Evidence: 每步反应的支持文献数量；

Yield: 每一步反应的产率，对目标分子的产率有影响；

Atom Efficiency: 反应物的原子转化经济性。

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

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

3. 点击 Apply，完成设置。

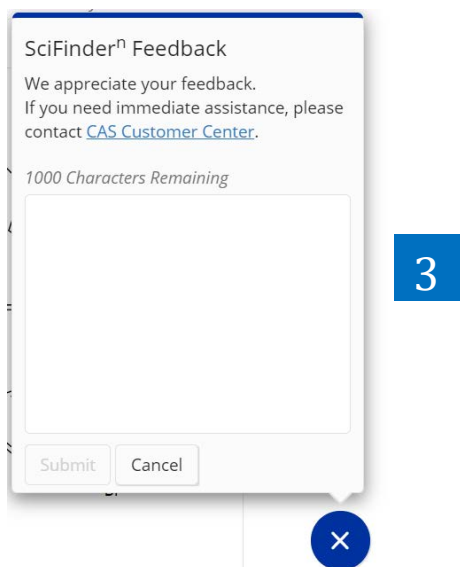
利用 Retrosynthesis 的产品反馈功能

The screenshot shows the CAS SciFinder Retrosynthesis interface. The 'Predicted Results' tab is selected, displaying a retrosynthetic plan for a target molecule. The plan includes a 'Retrosynthesis Step Key' and a 'Feedback' button in the bottom right corner. The interface also displays plan information such as estimated yield (15%), overall price (\$427.41), and commercial availability (B, C, D, F, G, H, I).

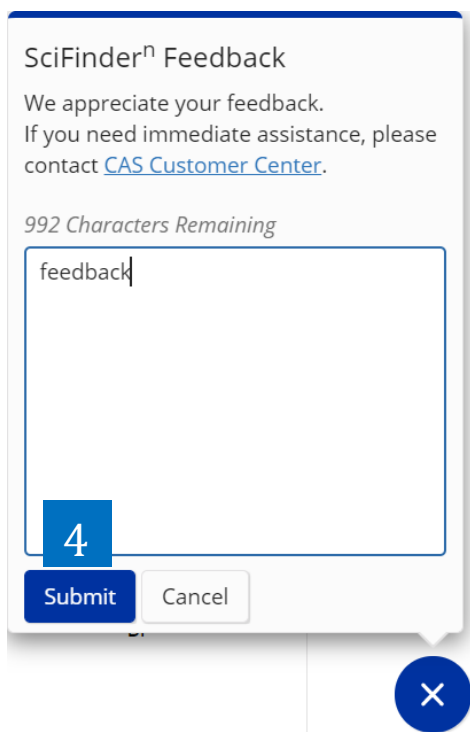
1. 在 Retrosynthesis 的结果页面，点击 Feedback 图标，进行使用反馈。

The screenshot shows the CAS SciFinder Retrosynthesis Plan Options interface. The 'Plan Options' tab is selected, displaying settings for synthetic depth (1, 2, 3, 4), rules supporting predicted reactions (Common, Uncommon, Rare), and starting materials cost limit (1000 USD/mol). A 'Feedback' button is visible in the bottom right corner.

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 displays the CAS SciFinder interface for a reaction search. The top navigation bar includes the CAS SciFinder logo, a search bar with the ID 2014:365937, and icons for drawing, search, and user profile. The main content area is titled "Reactions (36)" and shows a chemical reaction scheme (Scheme 1) involving the oxidation of an alkene to an allylic alcohol. The reaction is catalyzed by a copper-aluminum mixed oxide. The scheme includes absolute stereochemistry and rotation values. Below the scheme, a "Reaction Summary" section provides details on catalysts, solvents, and reagents. The left sidebar contains a "Filter Behavior" section with options for "Yield", "Number of Steps", "Non-Participating Functional Groups", "Experimental Protocols", "Reaction Type", "Stereochemistry", and "Reagent". The "Experimental Protocols" filter is selected, and the "Synthetic Methods" sub-filter is also selected. A blue box with the number "1" highlights the "Experimental Protocols" filter. Another blue box with the number "2" highlights the "Experimental Protocols" link in the "Reaction Summary" section.

1. 在反应结果集页面左侧选择 Experimental Protocols 项下的 Synthetic Methods。

2. 点击 Experimental Protocols 获取 CAS 科学家增值标引的实验详情。

CAS SciFinder[®] Reactions 2014:365937

Return to Results

Reaction Detail (Scheme 1, Reaction 1 of 1)

3 4 5

Download Email Save

Steps: 1
Yield: 100%

Suppliers (95) [Stage 2] Suppliers (35)

Absolute stereochemistry shown, Rotation (+) 100%

Step 1

Alternative Steps (0)

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

CAS Reaction Number: 31-209-CAS-8900882

JOURNAL

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

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

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

Full Text

Notes regioselective

6

Experimental Protocols

Synthetic Methods Experimental Procedure

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

Reactants 4-Methoxybenzoic acid
Valencene

Reagents *tert*-Butyl hydroperoxide

Catalysts Aluminum copper oxide

Solvents Acetonitrile
Water

Procedure

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

Company/Organization
Departamento de Química
Orgánica, Facultad de Ciencias
Universidad de Cádiz
Cádiz 11510
Spain

Transformation	Acyloxylation Reaction	7
Scale	milligram	8
Characterization Data	9	
^ (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		
Proton NMR Spectrum	400 MHz, CDCl ₃ : δ = 8.00 (d, <i>J</i> = 9.0 Hz, 2H), 6.90 (d, <i>J</i> = 9.0 Hz, 2H), 5.56 (br d, <i>J</i> = 5.0 Hz, 1H), 5.33 (ddd, <i>J</i> = 6.9, 3.9, 2.0 Hz, 1H), 4.70 (br s, 2H), 3.84 (s, 3H), 2.36 (m, 1H), 2.28 (tt, <i>J</i> = 12.5, 3.0 Hz, 1H), 2.18 (ddd, <i>J</i> = 14.3, 4.1, 2.6, 1H), 1.92 (dt, <i>J</i> = 12.9, 2.7 Hz, 1H), 1.79 (m, 2H), 1.72 (br s, 3H), 1.28 (m, 4H), 0.94 (s, 3H), 0.91 (d, <i>J</i> = 6.6 Hz, 3H).	
Carbon-13 NMR	100 MHz, CDCl ₃ : δ = 166.1, 163.1, 150.7, 150.1, 131.6, 123.5, 117.9, 113.4, 108.6, 68.1, 55.4, 51.8, 44.4, 40.6, 38.2, 35.8, 33.1, 32.4, 20.8, 16.9, 15.1.	
IR Absorption Spectrum	Film ν _{max} : 2932, 1707, 1607, 1510, 1272, 1256, 1167, 1032, 847, 772 cm ⁻¹ .	
Optical Rotatory Power	[α] _D ²⁰ = +130.06 (c 1.70, CHCl ₃).	
HRMS	ESI: calcd. for C ₂₃ H ₃₁ O ₃ [M+H] ⁺ 355.2273; found 355.2271.	
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 displays the CAS SciFinder interface for a search on 'sofosbuvir'. The main section, titled 'Reactions (720)', shows a chemical reaction scheme for the synthesis of sofosbuvir. The left sidebar contains a 'Filter Behavior' section with various filters. Two blue boxes with numbers 1 and 2 highlight specific filter categories: 'Reaction Type' (labeled 1) and 'Reaction Notes' (labeled 2). The right sidebar shows the 'Reaction Summary' for the selected reaction, including reagents, solvents, and literature references.

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

CAS SciFinder[®] Reactions sofosbuvir

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

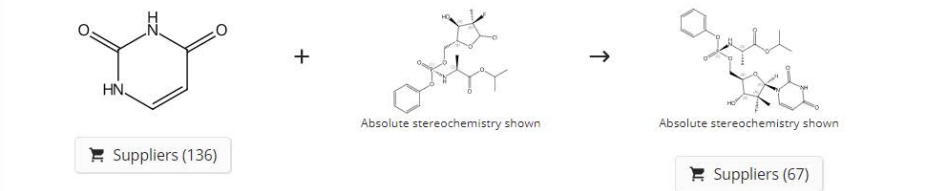
By: Ross, Bruce S.; et al
Canada, CA2988217 C 2020-06-23

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

[View All Reaction Summaries](#)

[Collapse Scheme](#)

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



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

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

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

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

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

[Collapse Scheme](#)

Search Within Results

Source Reference

Document Type

☐ Journal (63)

☐ Patent (659)

Language

Publication Year

Publication Name

☐ World Intellectual Property Organization (266)

☐ China (167)

☐ Canada (80)

☐ United States (73)

☐ India (49)

[View All](#)

CA Section

Filter Content Report

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

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

相似反应检索

Searching for...

Reactions

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

Enter a query...

2 3

Edit

Edit Drawing Remove

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

CAS SciFinder® Reactions Enter a query...

Return to Home

Structure Match

As Drawn (200)

Substructure (1.7M)

Similarity (18K)

1

2

Similarity

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

Filter Behavior

Filter by Exclude

Yield

90-100% (3,001)

80-89% (2,079)

70-79% (1,616)

50-69% (2,116)

30-49% (1,285)

View All

Number of Steps

1 (18K)

Reactions (18,368)

Group: By Document View: Expanded

References

1

Indole compounds for the treatment of neurodegenerative diseases

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

PatentPak Full Text

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

Reaction Summary

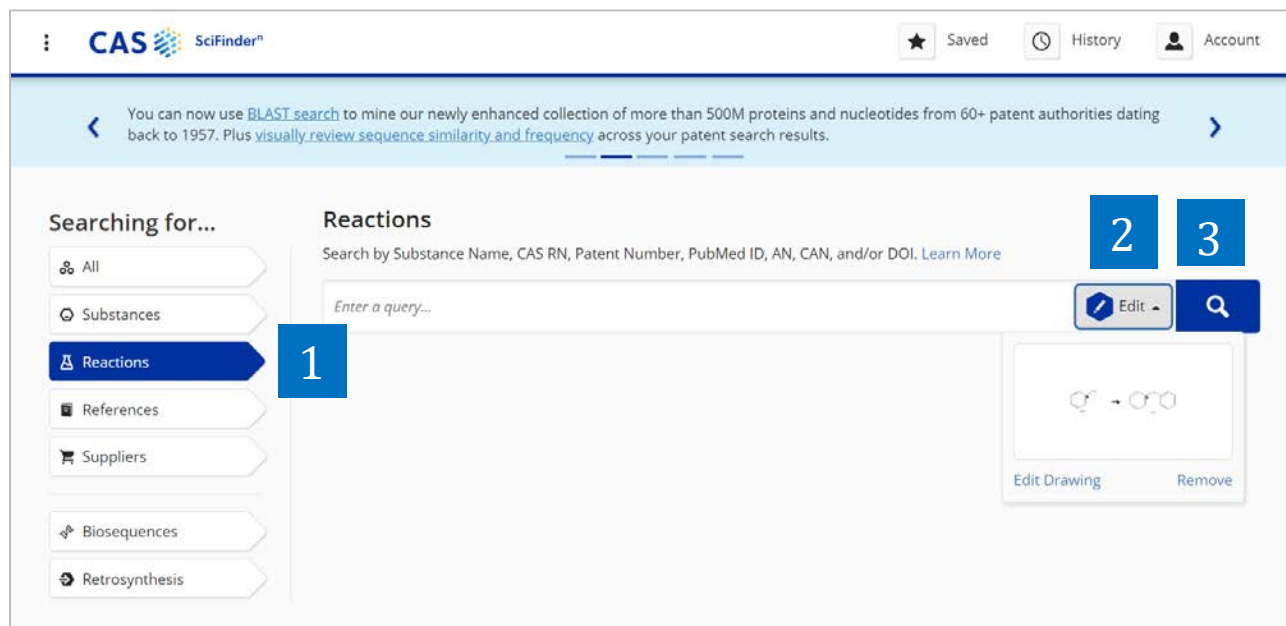
Steps: 1 Yield: 100%

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



1. 点击 Reactions 进行反应检索。
2. 点击结构编辑器输入反应式。
3. 开始检索。

CAS SciFinder® Reactions Enter a query...

Return to Home

Structure Match

- As Drawn (1,002)
- Substructure (86K)**
- Similarity (3,037)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

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

[View All](#)

Reactions (1,554)

Group: By Scheme View: Expanded

References

Filtering: Non-Participating Functional Groups: Primary amine X [Clear All Filters](#)

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

[Suppliers \(76\)](#)
[Suppliers \(57\)](#)
[Suppliers \(100\)](#)

[Suppliers \(95\)](#)

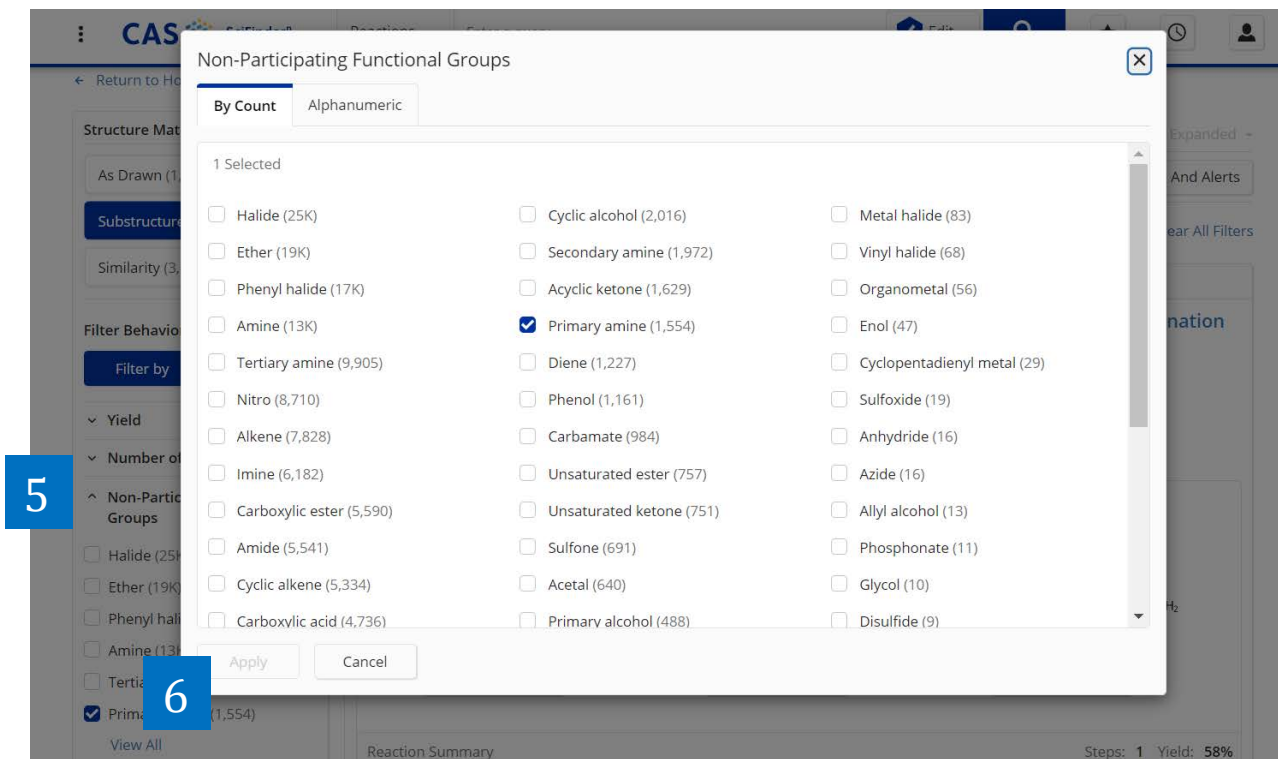
Reaction Summary Steps: 1 Yield: 37%

1.1 Reagents: 9,10-Dihydroanthracene; 180 min, 630 K

1.2 Reagents: 2-Methoxyphenol, Nitric acid

[The Surprisingly Facile Thermal Dehalogenation of Chlorinated Aromatics by a Hydroaromatic Donor Solvent. Tautomerization of Chlorinated Phenols and Anilines](#)

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



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

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

[Return to Home](#)

Structure Match

As Drawn (1,002)

Substructure (86K)

Similarity (3,037)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

☐ Halide (25K)

☐ Ether (19K)

☐ Phenyl halide (17K)

☐ Amine (13K)

☐ Tertiary amine (9,905)

☒ Primary amine (1,554)

[View All](#)

Reactions (1,554)


☐ References

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

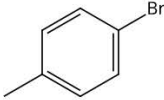
☐ 41

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

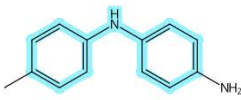
By: Gao, Jie; Bhunia, Subhajit; Wang, Kailiang; Gan, Lu; Xia, Shanghua; et al
Organic Letters (2017), 19(11), 2809-2812 | Language: English, Database: CAlus and MEDLINE



☐ Suppliers (85)




☐ Suppliers (65)



☐ Suppliers (16)

Reaction Summary Steps: 1 Yield: 58%



[Edit Drawing](#) [Remove](#)

[Start Retrosynthetic Analysis](#)

document View: Expanded

☐ ☒ Save And Alerts

[Clear All Filters](#)

7. 浏览目标结果。

在 PatentPak Viewer 中使用 Retrosynthesis

The screenshot illustrates the PatentPak Viewer interface. On the left, a sidebar titled 'Key Substances in Patent' lists several compounds. A blue box with the number '1' highlights the entry for CAS RN 2484-88-0. The main window displays a text snippet from a patent document, which includes the name of the compound. A pop-up window for CAS RN 2484-88-0 is open, showing the chemical structure of 4-(2-Phenyldiazenyl)benzenesulfonic acid. A blue box with the number '2' highlights the 'Start Retrosynthetic Analysis' button in the pop-up's left-hand menu.

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。

The screenshot displays the CAS SciFinder interface for reaction results. On the left, a 'Filter Behavior' sidebar allows filtering by 'Yield' (ranging from 30-49% to 90-100%) and 'Number of Steps' (ranging from 1 to 6-10). It also includes a section for 'Non-Participating Functional Groups' with options for 'Cyclic ketone' and 'Ketone'. The main area, titled 'Reactions (305)', shows results grouped by document. The first result, 'Microbial 11α-hydroxylation of steroids', is highlighted. It includes the authors 'Wiersma, Marten; Van Der Meijden, Pieter', the patent reference 'WO9721830 A1 1997-06-19', and the database 'CAplus'. The reaction scheme shows a steroid molecule being converted to a hydroxylated steroid. Below the scheme, there are buttons for 'Suppliers (36)' and 'Suppliers (11)'. The reaction summary indicates 'Steps: 1' and 'Yield: 98%'. The page also includes a 'View Reaction Detail' link.

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

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

Reactions (305)

Group: By Scheme View: Expanded

☐ **References**

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



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

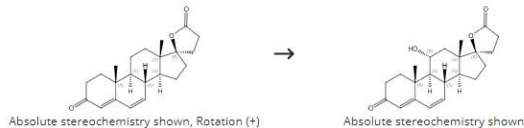
Reaction Notes

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: Gaikawari, 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**

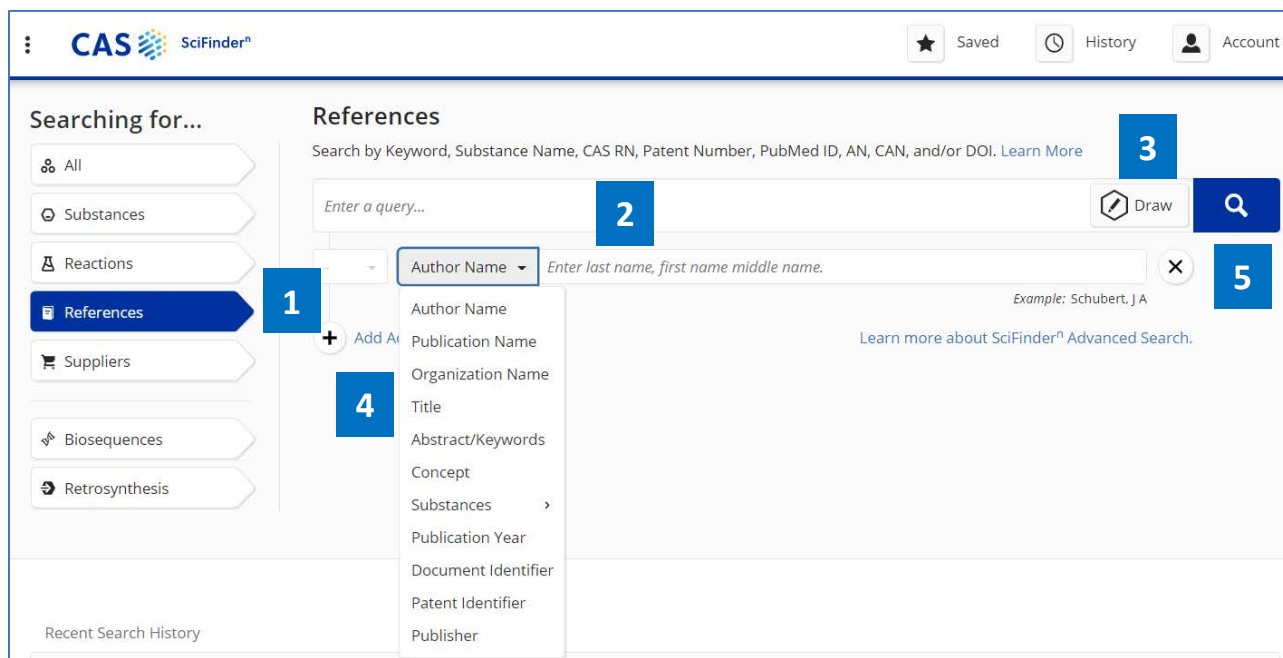
No Data Available

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

The screenshot shows the CAS SciFinder[®] interface with the search query "CDK OR 'cyclin-dependent kinases' AND inhibitor". The results are sorted by Relevance. The left sidebar shows filter options. The main content area displays two reference entries. Numbered callouts highlight specific UI elements: 1. Sort dropdown, 2. View dropdown, 3. Filter Behavior section, 4. Download icon, 5. Email icon, 6. Save And Alerts button, 7. Reference title, 8. Full Text button, 9. Substance count, 10. Reactions count, 11. Citing count, 12. Citation Map button.

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

10. 获取引用本文章的文献

11. 引文地图, 获取前向及后向引用

12. 获取全文链接

Reference Detail (48 of 728)

Substances (723) Reactions (1,943) Citing (11) Citation Map

1

2

3

4

5

PATENT

Patent Number
WO2004018473

Publication Date
2004-03-04

Application Number
WO2003-IB4188

Application Date
2003-08-22

Kind Code
A2

Assignee
Institute of Experimental Botany
ASCR, Czech Republic

Source
World Intellectual Property
Organization
CODEN: PIXXD2

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

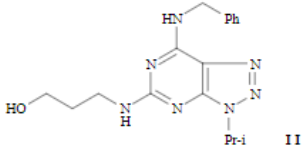
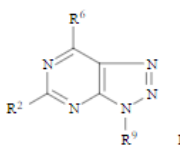
Language
English

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 [R⁶ = halo, NHHN₂, amino, etc.; R² = halo, NHHN₂, alkyl, etc.; R⁹ = alkyl, cycloalkyl, etc.] are prepared For instance, 4-amino-5-carboxamido-1-isopropyl-1,2,3-triazole (preparation given) is converted to 2,6-dihydroxy-9-isopropyl-8-azapurine (EtOH, NaOEt, (EtO)₂CO, 90°, 4 h). The dihydroxy derivative is converted to the corresponding dichloride (POCl₃, lutidine, 120°, 3 h), treated with benzylamine (n-BuOH) followed by 3-aminopropanol to give II. II has IC₅₀ = 54.6 μM for CDK2-cyclin E. The present invention relates to a compound of formula (I), or a pharmaceutically acceptable acid salt thereof. I are useful in the treatment of hyperproliferative skin disorders, viral infections, cancer, etc. The invention also relates to the use of 2,6,9-trisubstituted-8-azapurines in maintaining mammalian oocytes at the germinal vesicle stage.



Keywords: azapurine cyclin dependent kinase inhibitor preparation

PatentPak PDF Get Prior Art Analysis Full Text

Patent Family

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

Expand All | Collapse All

88

IPC Data

6

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

Concepts

7

Substances

8

Formulations

9

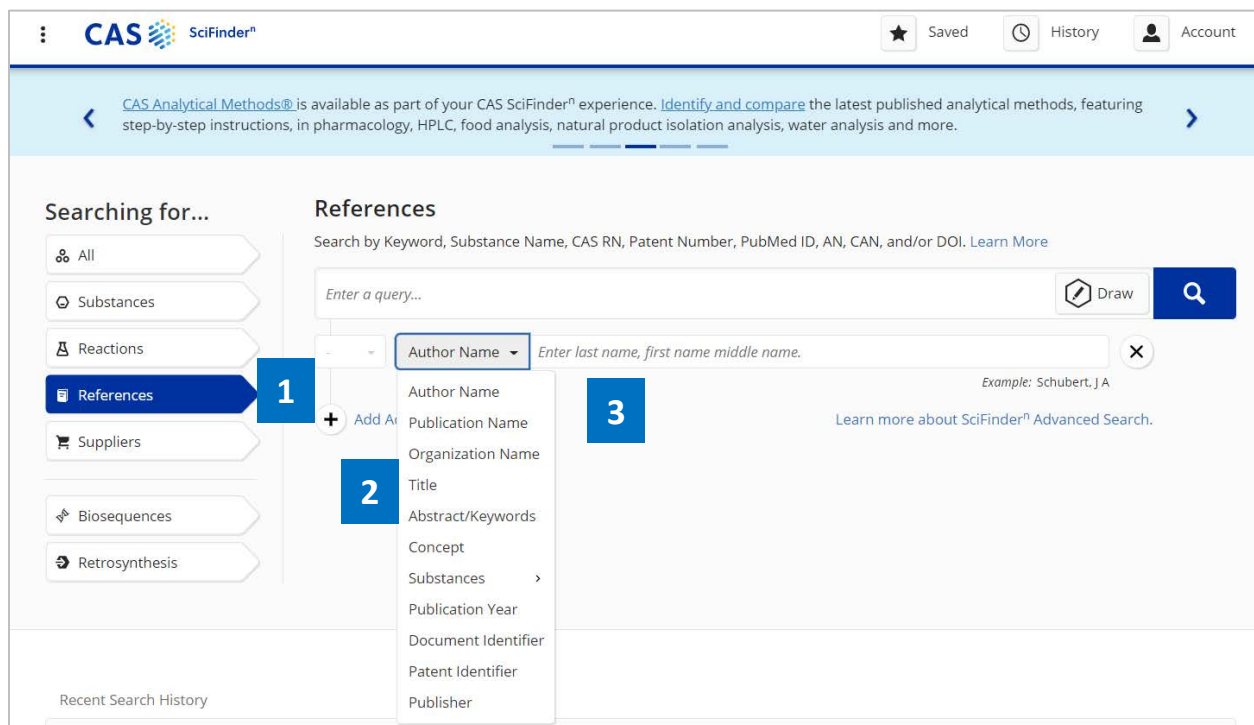
Cited Documents

10

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

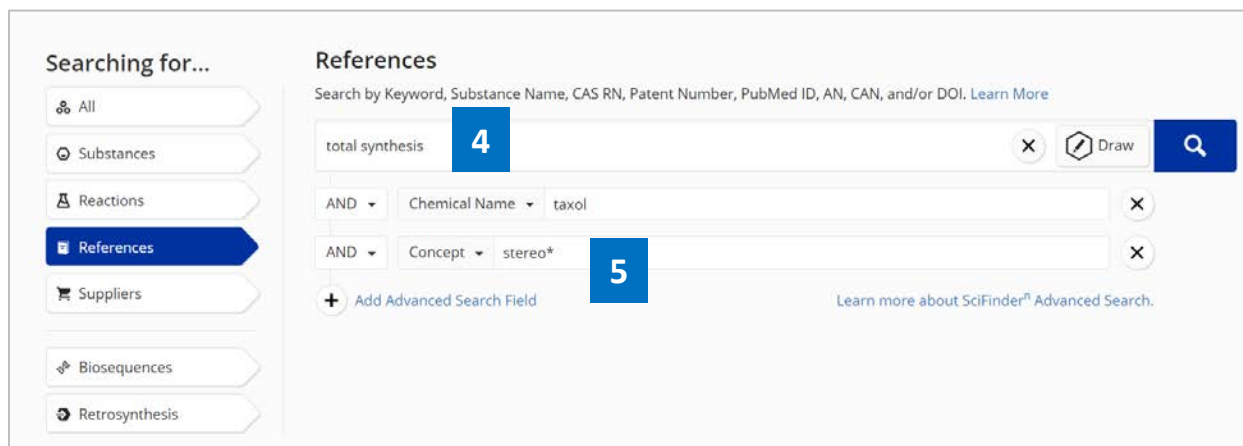
高级文献检索

使用高级文献检索，可以快速获得更相关的结果。

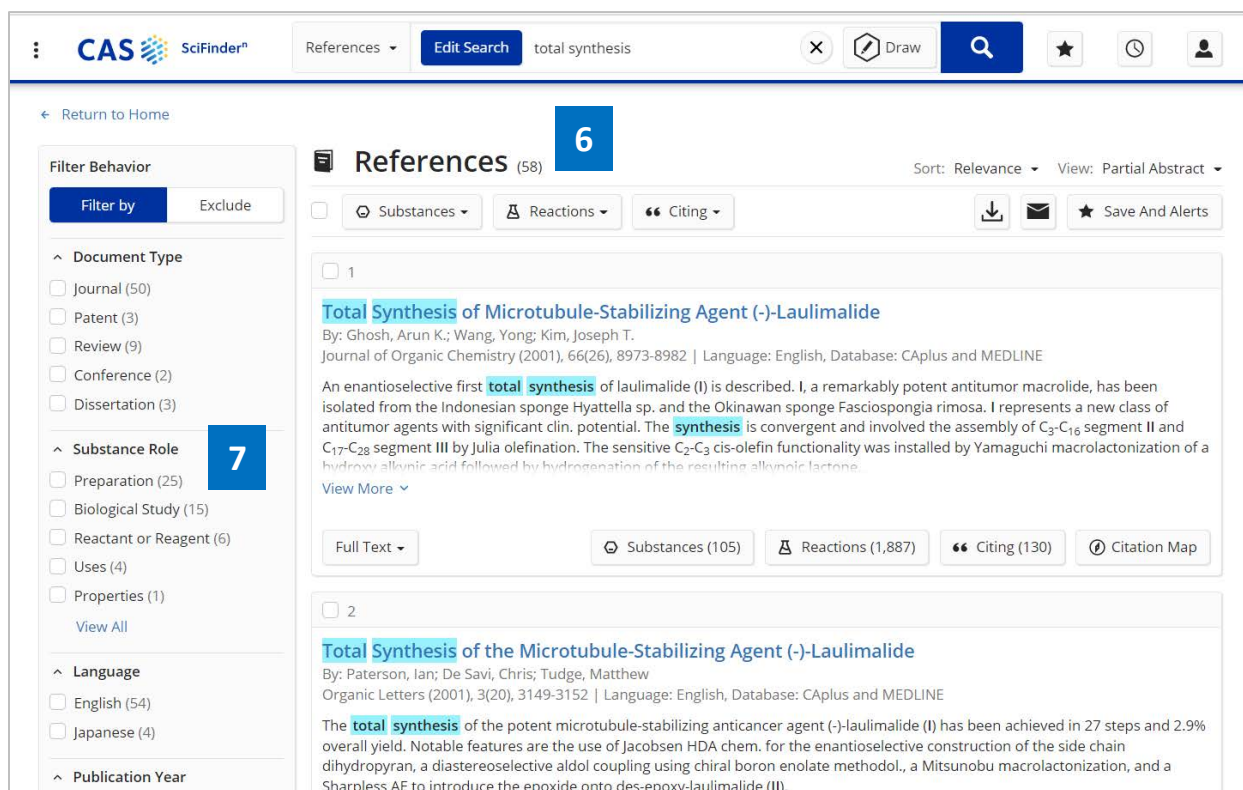


1. 在主页面，选择 References。
2. 选择逻辑运算符 and, or ,not，连接不同的检索字段。
3. 根据需要，选择相应的检索字段。

例：紫杉醇全合成，并包含 “stereo” 这一 concept。



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



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

CAS SciFinder® References Edit Search total synthesis

Reference Detail (1 of 58) Prev Next

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

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

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

8

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

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

Email
arunghos@uic.edu

Publisher
 American Chemical Society

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

The image displays three chemical structures labeled I, II, and III. Structure I is the target molecule, (-)-Laulimalide, a complex 28-membered macrolide with multiple stereocenters, including a cis-olefin at C2-C3, a dihydropyran ring, and a sensitive epoxide at C16-C17. Structure II is a key intermediate, a 16-membered macrolide containing a dihydropyran ring and a MOM-protected aldehyde at C1. Structure III is another intermediate, a 16-membered macrolide featuring a dihydropyran ring and a PMB-protected aldehyde at C1. The structures are drawn with stereochemical wedges and dashes to indicate their three-dimensional arrangement.

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

Full Text ▾

Expand All | Collapse All

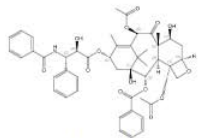
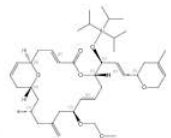
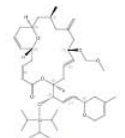
▼ Concepts

▼ MEDLINE® Medical Subject Headings

▼ Supplementary Concepts

▲ Substances

🔍 Substances (105)

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

出版社检索

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

The screenshot shows the SciFinder search interface. On the left, under 'Searching for...', the 'References' option is selected and highlighted with a blue bar and a blue box containing the number '1'. In the main search area, the search term 'Organocatalysis' is entered. Below the search bar, there is a dropdown menu for 'AND' and a 'Publisher' dropdown menu. The 'Publisher' dropdown is open, showing 'American Chemical Society' selected. A blue box with the number '2' highlights the '+ Add Advanced Search Field' button. A link 'Learn more about SciFinder[®] Advanced Search.' is also visible.

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

The screenshot shows the SciFinder search results page for 'Organocatalysis'. The top navigation bar includes the CAS logo, 'SciFinder[®]', and a 'References' dropdown menu. The search term 'Organocatalysis' is displayed in the top bar. The main content area is titled 'References (869)'. On the left, there is a 'Filter Behavior' section with a 'Filter by' button and an 'Exclude' button. Under 'Document Type', the 'Journal (494)' option is selected and highlighted with a blue box containing the number '3'. Other options include 'Review (84)', 'Conference (368)', 'Editorial (1)', and 'Preprint (16)'. Under 'Language', 'English' is selected. Under 'Publication Year', a bar chart shows the distribution of publications from 2000 to 2021. The main search results list shows two entries. The first entry is '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 entry is '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. The page also includes a 'Feedback' button in the bottom right corner.

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

4

The screenshot displays the CAS SciFinder interface. On the left, a sidebar contains filters for 'Organization', 'Publication Name', 'Concept', and 'CA Section'. The 'Publication Name' filter is expanded, showing a list of journals and their article counts: Organic Letters (108), Journal of the American Chemical Society (98), Journal of Organic Chemistry (90), ACS Catalysis (48), and Accounts of Chemical Research (34). A 'View All' link is also present. The main content area shows a search result for 'Organocatalytic Reaction' by Flanigan, Darrin M., et al. in Chemical Reviews. A chemical reaction scheme is displayed, showing the conversion of a starting material to a product via a catalytic cycle involving an organocatalyst. The reaction is labeled 'Oxidation Acylation' and 'Unpinning Catalysis'. The 'Full Text' button is visible. On the right, a 'Publication Name' panel is open, showing a list of publications with checkboxes for selection. The list includes various ACS journals and meeting abstracts, such as 'Abstracts of Papers, 256th ACS National Meeting & Exposition, Boston, MA, United States, August 19-23, 2018 (7)' and 'Abstracts of Papers, 235th ACS National Meeting, New Orleans, LA, United States, April 6-10, 2008 (6)'. The 'Top Count' tab is selected, and the 'Search' button is visible.

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

获取制剂（配方）信息

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

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

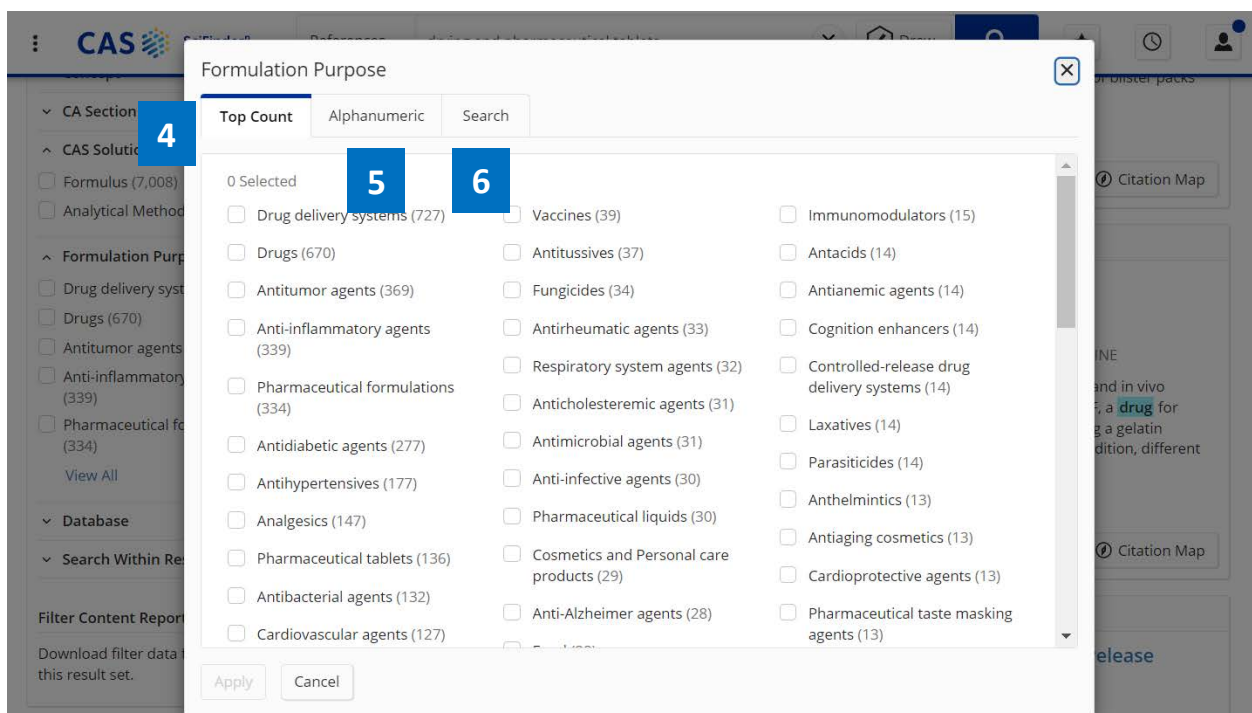
方法一： 直接在 References 检索框中输入检索式，在得到的文献结果页面左侧选择 Formulation Purpose, 获得感兴趣的制剂（配方）信息：

The screenshot displays the CAS SciFinder interface. At the top, the search bar contains the query "drying and pharmaceutical tablets" with a result count of 1. The left sidebar shows filter options for Document Type and Language. The main content area lists two references:

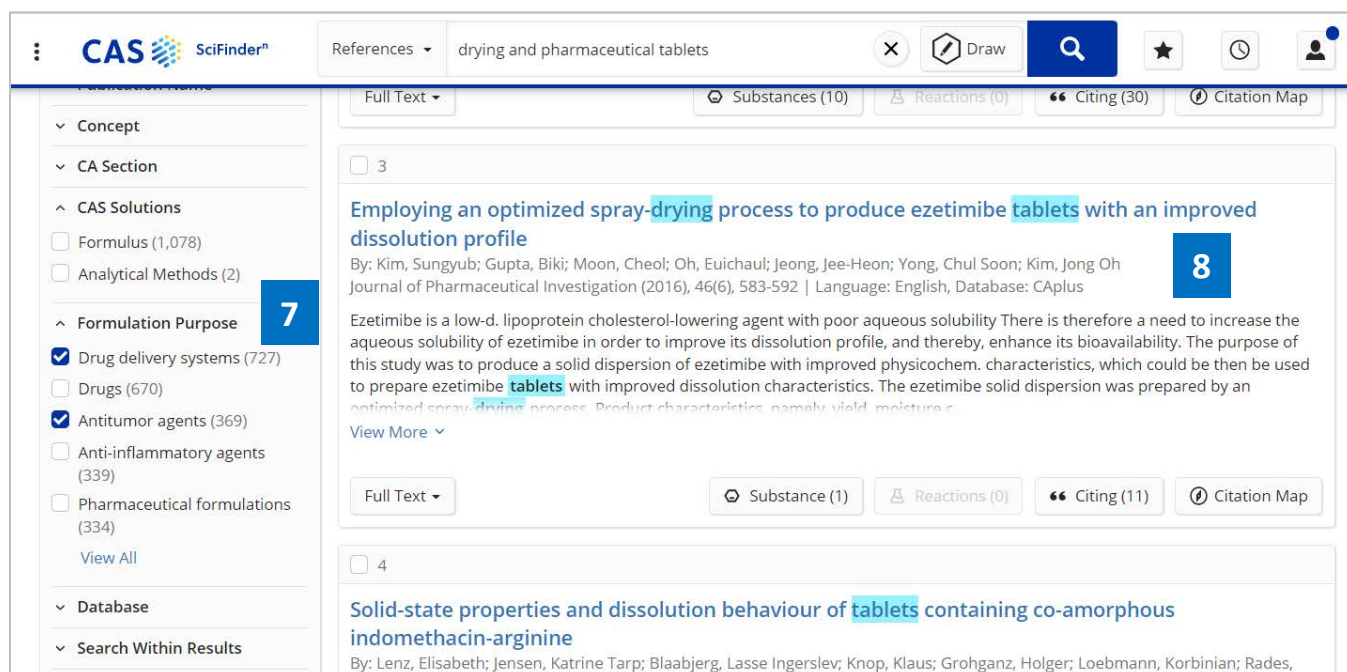
- Reference 1:** "Formulation of a lyophilized dry emulsion tablet for the delivery of poorly soluble drugs". By: Corveleyn, S.; Remon, J. P. International Journal of Pharmaceutics (1998), 166(1), 65-74. The abstract describes the development of a dry emulsion tablet for poorly water-soluble drugs using lyophilization.
- Reference 2:** "Development of directly compressible powders via co-spray drying". By: Gonnissen, Y.; Remon, J. P.; Vervaeke, C. European Journal of Pharmaceutics and Biopharmaceutics (2007), 67(1), 220-226. The abstract describes the continuous production of directly compressible powders via co-spray drying.

The screenshot displays the CAS SciFinder web interface. At the top, the search bar contains the query 'drying and pharmaceutical tablets'. The left sidebar features a 'Filter Content Report' section with two main categories: 'CAS Solutions' and 'Formulation Purpose'. Under 'CAS Solutions', the 'Formulus' option is selected, indicated by a blue box with the number '2'. Under 'Formulation Purpose', the 'Drug delivery systems' option is selected, indicated by a blue box with the number '3'. The main content area shows a list of search results. The first result is titled 'In vitro and in vivo evaluation of a fast-disintegrating lyophilized dry emulsion tablet containing griseofulvin' by Ahmed, Iman Saad; Aboul-Einien, Mona Hassan, published in the European Journal of Pharmaceutical Sciences (2007), 32(1), 58-68. The second result is titled 'Evaluation of spray-drying as a method to prepare microparticles for controlled drug release' by Palmieri, Giovanni Filippo; Wehrle, Pascal; Stamm, Andre, published in Drug Development and Industrial Pharmacy (1994), 20(18), 2859-79. Both results have buttons for 'Full Text', 'Substances', 'Reactions', 'Citing', and 'Citation Map'.

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



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



7. 可以选择一个或者几个选项。
8. 点击题目查看文献信息详情。

The screenshot shows the CAS SciFinder interface. At the top, the search bar contains "drying and pharmaceutical tablets". The main section is titled "Reference Detail (3 of 1,078)". Below this, there are tabs for "Substance (1)", "Reactions (0)", "Citing (11)", and "Citation Map". A sidebar on the left contains metadata for the journal "Journal of Pharmaceutical Investigation", including volume, issue, pages, and DOI. The main content area displays the title "Employing an optimized spray-drying process to produce ezetimibe tablets with an improved dissolution profile" and the authors "By: Kim, Sungyub; Gupta, Bikti; Moon, Cheol; Oh, Euichaul; Jeong, Jee-Heon; Yong, Chul Soon; Kim, Jong Oh". The abstract describes the optimization of the spray-drying process for ezetimibe tablets. A "Keywords" section lists "ezetimibe tablets", "spray drying", and "process dissolution". At the bottom, there is a "Full Text" button and a list of categories: "Concepts", "Substances", "Formulations", and "Cited Documents". The "Formulations" category is highlighted with a blue box containing the number "9".

9. 点击 Formulations 查看制剂（配方）信息。

10 View CAS Formulus® Detail

11 Location: Article Page 3, 8, Table 2
Purpose: Drug delivery systems
Target: solubility, bioavailability

12 **13**

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

14 **15**

16 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 web interface. At the top, there is a search bar with the text 'Substances' and '9040-27-1'. To the right of the search bar are icons for 'Draw', 'Search', 'Star', 'Clock', and 'User'. Below the search bar, there is a 'Filter Behavior' section with 'Filter by' and 'Exclude' buttons. The 'Filter Behavior' section has three expandable categories: 'Commercial Availability' (with 'Available (1)' checked), 'Reaction Role' (with 'Product (1)', 'Reactant (1)', and 'Catalyst (1)' listed), and 'Reference Role' (with 'Adverse Effect (1)' and 'Agricultural Use (1)' listed). To the right of the filters, there is a 'Substances (1)' section. It shows a list of substances with a checkbox, a document icon, and the text '9040-27-1'. Below the substance name, it says 'Image Not Available' and 'Unspecified Arabinosyran'. At the bottom of the substance list, there are three buttons: 'References' (with '3,667' next to it), 'Reactions' (with '27' next to it), and 'Suppliers' (with '7' next to it). A blue box with the number '1' is placed over the search bar, and a blue box with the number '2' is placed over the 'References' button.

1. 进行物质检索，获得物质检索结果集。
2. 由物质获得文献结果集。

CAS SciFinder®

References (3,667)

Sort: Relevance View: Partial Abstract

Filter Behavior

Filter by Exclude

Document Type

Substance Role

Language

Publication Year

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Formulation Purpose

Food (25)

Drug delivery systems (19)

Dietary supplements (17)

Antidiabetic agents (10)

Antiobesity agents (9)

View All

1

Cereal arabinoxylans: advances in structure and physiochemical properties

By: Izydorczyk, Marta S.; Billaderis, Costas G.
Carbohydrate Polymers (1995), 28(1), 33-48 | Language: English, Database: CPlus

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

View More

2

Arabinoxylans and Endoxylanases in Wheat Flour Bread-making

By: Courtin, C. M.; Delcour, J. A.
Journal of Cereal Science (2002), 35(3), 225-243 | Language: English, Database: CPlus

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

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

药物重定位 (Repositioning)

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

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

The screenshot shows the CAS SciFinder[®] interface. At the top, the search bar contains the CAS number 1166-34-3 and a blue button labeled '1'. Below the search bar, the 'Substances (1)' section displays the chemical structure of Cinanserin, its molecular formula C₂₀H₂₄N₂OS, and its name. To the left, a 'Filter Behavior' sidebar allows filtering by 'Commercial Availability', 'Reaction Role', and 'Reference Role'. At the bottom of the substance card, it shows '444 References' and '23 Suppliers'. A blue button labeled '2' is highlighted next to the 'References' count. The interface also includes a 'Return to Home' link, a 'View: Partial' dropdown, and 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。

CAS SciFinder®

References (294)

Sort: Relevance View: Partial Abstract

Filter Behavior

Filter by Exclude

Document Type

Substance Role

Biological Study (158)

Uses (12)

Process (10)

Properties (6)

Preparation (5)

Reactant or Reagent (1)

View All

Language

Publication Year

1963 2021

No Min to 2000 Apply

Reset View Larger

3

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.

1

Selective in vitro and in vivo binding of [¹²⁵I]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 [¹²⁵I]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 [¹²⁵I]ADAM in rat brain after an iv injection showed a high specific binding in the regions of hippocampus, 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。

CAS SciFinder®

View All

Language

Publication Year

1963 2021

No Min to 2000 Apply

Reset View Larger

Author

Organization

Publication Name

Concept

Animals (249)

Male (158)

Cinanserin (141)

Rats (139)

Serotonin (120)

Serotonin Antagonists (90)

Receptors, Serotonin (83)

Female (61)

Rats, Inbred Strains (60)

Brain (58)

In Vitro Techniques (51)

Methysergide (44)

Metergoline (18)

5-HT agonists (16)

Cerebral cortex (16)

Quipazine (16)

Receptors (16)

Behavior, Animal (15)

Frontal cerebral cortex (15)

Haloperidol (15)

Motor activity (15)

Rabbits (15)

Blood pressure (14)

Dogs (14)

Radioligand Assay (11)

Receptors, Adrenergic, alpha (11)

Swine (11)

Tetrahydronaphthalenes (11)

5-HT2A antagonists (10)

Body temperature (10)

Brain corpus striatum (10)

Immunosuppressive Agents (10)

Mianserin (10)

Naloxone (10)

Neurons (10)

0 Selected

5

4

Apply Cancel

4. 点击 View All，查看所有 Concept。

Concept

Top Count Alphanumeric **Search**

Concept Name

5- **Search**

☐ Select All on Page

<input type="checkbox"/> 2-((2- ((dimethylamino)methyl)phen yl)thio)-5-iodophenylamine (2)	<input type="checkbox"/> 5-HT2A receptors (7)	<input type="checkbox"/> 5-HT receptors (43)
<input type="checkbox"/> 5-HT1A agonists (1)	<input type="checkbox"/> 5-HT2B receptors (1)	<input type="checkbox"/> 5-Hydroxytryptophan (26)
<input type="checkbox"/> 5-HT1 agonists (1)	<input type="checkbox"/> 5-HT2C receptors (7)	<input type="checkbox"/> 8-iodo-2,3,4,5-tetrahydro-3- methyl-5-phenyl-1H-3- benzazepine-7-ol (1)
<input type="checkbox"/> 5-HT1A receptors (9)	<input type="checkbox"/> 5-HT2 receptors (23)	<input type="checkbox"/> Receptor, Serotonin, 5-HT1D (1)
<input type="checkbox"/> 5-HT1B receptors (3)	<input type="checkbox"/> 5-HT ₃ antagonists (1)	<input type="checkbox"/> Receptor, Serotonin, 5-HT2A (2)
<input type="checkbox"/> 5-HT1D receptors (2)	<input type="checkbox"/> 5-HT3 receptors (1)	<input type="checkbox"/> Receptor, Serotonin, 5-HT2B (1)
<input type="checkbox"/> 5-HT1 receptors (8)	<input type="checkbox"/> 5-HT7 receptors (1)	
<input type="checkbox"/> 5-HT2A agonists (2)	<input type="checkbox"/> 5-HT agonists (16)	
	<input type="checkbox"/> 5-HT antagonists (38)	

Apply Cancel

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

CAS SciFinder® References (155) Sort: Relevance View: Partial Abstract

Filtering: Publication Year: 2000 - No Max

Quantification of serotonin transporters in nonhuman primates using $[^{123}\text{I}]\text{ADAM}$ 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: CAsplus and MEDLINE

We reported recently a highly selective radioligand, 2-((2-((dimethylamino)methyl)phenyl)thio)-5- $[^{123}\text{I}]$ iodophenylamine (ADAM), for SPECT imaging of serotonin transporters (SERT). In this article we describe the kinetic modeling of $[^{123}\text{I}]\text{ADAM}$ and its ability to quant. and reproducibly 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 $[^{123}\text{I}]\text{ADAM}$ SPECT studies. The studies consisted of a dynamic sequence of seven 10-min...

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

<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"/> Tropanes (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)
		<input type="checkbox"/> Cysteine Endopeptidases (6)

Apply Cancel

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

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

The screenshot displays the CAS SciFinder[®] web interface. At the top, there is a search bar with the text 'Enter a query...' and a 'Draw' button. Below the search bar, the 'References' section is active, showing 20 results. The 'Filter Behavior' panel on the left includes options for 'Filter by' (selected) and 'Exclude'. Under 'Document Type', 'Substance Role' is expanded, showing 'Biological Study (18)', 'Uses (16)', 'Properties (4)', 'Preparation (3)', and 'Reactant or Reagent (1)'. The 'Language' filter is set to 'English'. The 'Publication Year' filter is set to '2000 to No Max', with a blue box labeled '10' next to it. The 'Apply' button is highlighted. The main results area shows a list of references. The first reference is titled 'screening of anti-SARS coronavirus agents targeting protease 3CL' and is highlighted with a blue box labeled '11'. The second reference is titled 'Cinanserin is an inhibitor of the 3C-like proteinase of severe acute respiratory syndrome coronavirus and strongly reduces virus replication in vitro' and is highlighted with a blue box labeled '12'. The interface also includes a 'PatentPak' button and a 'Full Text' button.

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

[43] 公开日 2004 年 2 月 4 日		[11] 公开号 CN 1472336A	
[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	
[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		权利要求书 2 页 说明书 13 页 附图 3 页	

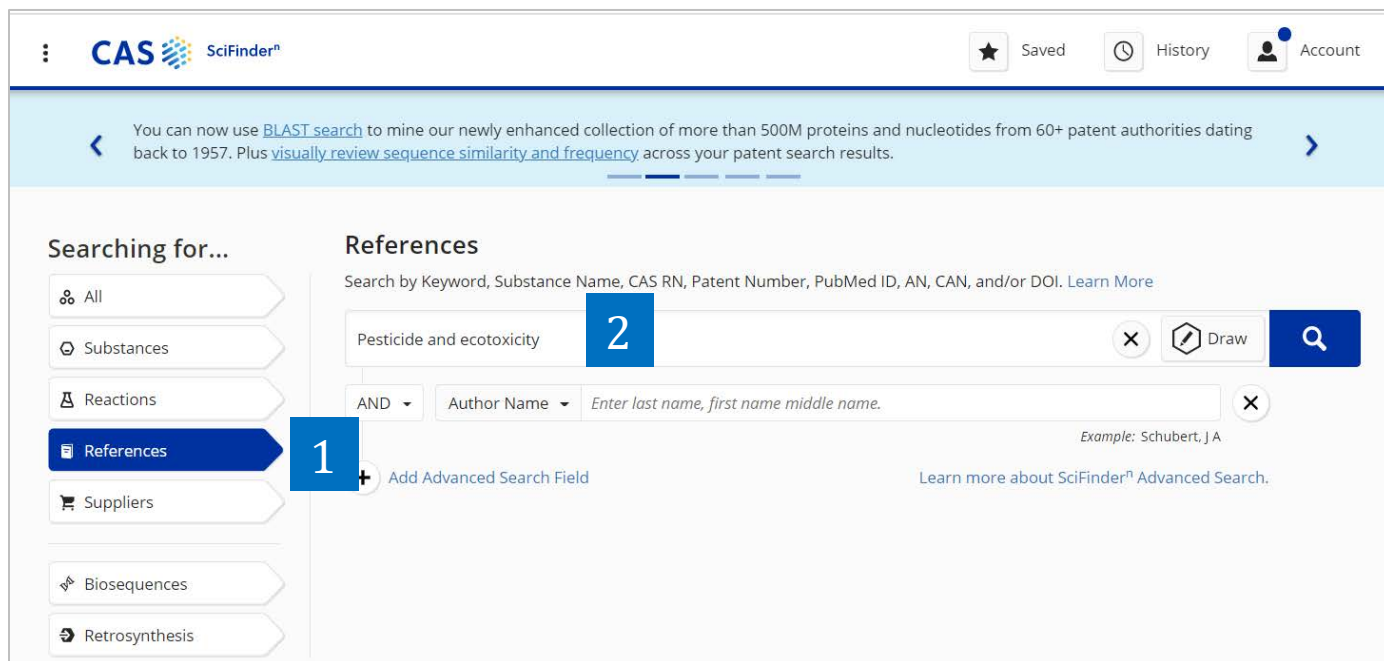
13. 在 CAS SciFinderⁿ中通过 PatentPak 直接下载的专利原文。

布尔逻辑运算符在文献检索中的应用

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

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

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



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。

CAS SciFinder[®] References Pesticide and ecotoxicity 3

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 (1,985) Sort: Relevance View: Partial Abstract

Substances Reactions Citing Save And Alerts

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

Filter Behavior

Filter by Exclude

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)

1

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: CAPLUS 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 **pesticides**.

[View More](#)

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

2

Wildlife Ecotoxicology of Pesticides: Can We Track Effects to the Population Level and Beyond?

By: Koehler, Heinz-R.; Triebkorn, Rita

Science (Washington, DC, United States) (2013), 341(6147), 759-765 | Language: English, Database: CAPLUS and MEDLINE

3. 所得结果集。

CAS SciFinder[®] Saved History Account

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

Searching for...

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

References

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

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。

5. 所得结果集。

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

CAS SciFinder[®] References Pesticide not ecotoxicity 7

Return to Home

Filter Behavior

Filter by Exclude

Document Type

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

Language

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

Publication Year

References (252,986)

Sort: Relevance View: Partial Abstract

Substances Reactions Citing

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

1

Immunotoxicity of Organophosphorous Pesticides

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

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

[View More](#)

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

2

Emission of pesticides into the air

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

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

7. 所得结果集。

CAS SciFinder[®] Saved History Account

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

Searching for...

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

References

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

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

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

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

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

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

[Load More Results](#)

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

☐ Substances ☐ Reactions ☐ Citing ☐ Save And Alerts

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Language

- ☐ English (1,302)
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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

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

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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

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。

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"total synthesis" and taxol ✕ 📐 Draw 🔍

AND ▼ Author Name ▼ Enter name middle name. ✕

Example: Schubert, J A

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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 ✕ 📐 Draw 🔍 ★ 🕒 👤

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- ☐ Review (64)
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Language

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- ☐ Japanese (13)
- ☐ Chinese (11)
- ☐ German (2)
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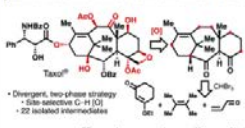
References (236) 11 Sort: Relevance View: Partial Abstract

☐ Substances ☐ Reactions ☐ Citing

☐ 1

Two-Phase Synthesis of Taxol

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

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

☐ 2

Total synthesis of taxol

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

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11. 所得结果集。

通配符的使用

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

*代表 0 或多个字符；？代表 0 或一个字符。

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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、CPlus Concept、Medline MeSH 或 Substances 中。

The screenshot displays the CAS SciFinder search results for the query 'synth*'. The search bar at the top shows 'synth*' with a magnifying glass icon. The results are listed under the 'References' tab, showing 13,004,948 results. The first result is 'Triblock copolymer syntheses of mesoporous silica with periodic 50 to 300 angstrom pores' by Zhao, Dongyuan; Feng, Jialin; Huo, Qisheng; Melosh, Nicholas; Frederickson, Glenn H.; Chmelka, Bradley F.; Stucky, Galen D. 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. Biochemical Journal (2001), 357(3), 593-615. The interface includes a search bar with 'synth*' and a magnifying glass icon, a 'References' tab, and a 'Filter Behavior' sidebar with options for Document Type, Substance Role, and Language.

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

CAS SciFinder[®] References alumin?um 2

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51

A compilation of corrosion potentials reported for intermetallic phases in aluminum alloys
 By: Buchheit, R. G.
 Journal of the Electrochemical Society (1995), 142(11), 3994-6 | Language: English, Database: CAplus

A review. A compilation of corrosion potentials reported for Al-based intermetallic compounds is presented. The range of corrosion potentials for dilute **aluminum** binary alloys is also given. This compilation is intended to serve as an aid in establishing galvanic relations among discrete microstructural elements in **aluminum** alloys. This compilation is based primarily on data reported in the corrosion literature with a focus on corrosion potentials for intermetallic compound particles found in com. alloys. A review with 26 references

Full Text ▾ Substances (2) Reactions (0) Citing (329) Citation Map

52

Grain refinement of aluminum and its alloys by heterogeneous nucleation and alloying
 By: Murty, B. S.; Kori, S. A.; Chakraborty, M.
 International Materials Reviews (2002), 47(1), 3-29 | Language: English, Database: CAplus

A review. Grain refinement of Al and its alloys is a common industrial practice. The field has been extensively investigated by many workers over the past 50 yr, not only to develop efficient grain refiners for different Al alloys, but also to achieve an understanding of the mechanism of grain refinement. The present review confines itself to the literature on grain refinement by heterogeneous nucleation and alloying. Initially, the fundamentals of grain refinement by inoculants are outlined. The types of grain refiner, Al-Ti-B master alloys in particular, and their methods of manufacture are

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

注:

- I. 一个检索词中至少含有 3 个非通配符字符, 否则会检索到任何词语;
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CAS SciFinder[®] References tot* synth* nat* prod* terpen* last* 3

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Concept 筛选项中支持使用通配符 “*” 进行检索

注：通配符 “*” 代表 0 或多个字符；且可用于词中或者词尾。

The screenshot shows the CAS SciFinder interface. The search bar at the top contains the query "steroids and fermentation and rhizopus stolonifer". The left sidebar shows the "Concept" filter selected, with a list of concepts including Rhizopus stolonifer (76), Fermentation (52), Steroids (42), Hydroxylation (33), and Biotransformation (15). A blue box with the number "1" highlights the "View All" link under the Concept section. The main content area displays the title "Microbial oxidation of anabolic steroids" and a list of related concepts, including "Micro biological conversion of steroids. 4. Part Pregnenolone oxidation by Rhizopus nigricans VNICHFI-7".

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。

The screenshot shows a 'Concept' search window. At the top, there are three tabs: 'Top Count', 'Alphanumeric', and 'Search' (highlighted with a blue box and the number 2). Below the tabs is a 'Concept Name' input field containing 'steroid*' (highlighted with a blue box and the number 3). To the right of the input field is a 'Search' button. Below the input field, it says '11 Selected' with a checkmark icon. A list of 11 concepts is displayed, each with a checked checkbox and a count in parentheses. At the bottom left, there is a blue box with the number 4, and to its right are 'Apply' and 'Cancel' buttons.

Concept Name	Count
<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"/> Sapogenins, 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, sapogenins	(1)
<input checked="" type="checkbox"/> Steroidal hormones	(1)
<input checked="" type="checkbox"/> Steroids, Brominated	(1)

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

文献结果集的聚类筛选项中的全选功能

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

如下所示的是在 Concept 中对检索得到的子项进行全选的操作。

The screenshot shows the CAS SciFinder search results page. On the left sidebar, under the 'Concept' filter, there is a list of sub-items: Rhizopus stolonifer (76), Fermentation (52), Steroids (42), Hydroxylation (33), and Biotransformation (15). A red box with the number '1' highlights the 'View All' button next to the 'Concept' header. The main content area displays two search results. The first result is titled 'Microbial oxidation of anabolic steroids' and the second is 'Micro biological conversion of steroids. 4. Part Pregnenolone oxidation by Rhizopus nigricans VNICHFI-7'. Both results show the authors, publication details, and a brief description of the study.

1. 点击 View All，展开所有的子项。

Concept ×

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

Concept Name **3** Rhizopus **4** Search

☐ Select All on Page

5

<input type="checkbox"/> Rhizopus (9)	<input type="checkbox"/> Rhizopus kasanensis (2)	<input type="checkbox"/> Rhizopus shanghaiensis (2)
<input type="checkbox"/> Rhizopus cohnii (2)	<input type="checkbox"/> Rhizopus microsporus (2)	<input type="checkbox"/> Rhizopus stolonifer (76)
<input type="checkbox"/> Rhizopus delemar (2)	<input type="checkbox"/> Rhizopus oligosporus (1)	<input type="checkbox"/> Rhizopus tritici (2)
<input type="checkbox"/> Rhizopus japonicus (2)	<input type="checkbox"/> Rhizopus oryzae (12)	

Apply Cancel

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。

Concept

Top Count Alphanumeric **Search**

Concept Name

Rhizopus **Search**

☒ 11 Selected

<input checked="" type="checkbox"/> Rhizopus (9)	<input checked="" type="checkbox"/> Rhizopus kasanensis (2)	<input checked="" type="checkbox"/> Rhizopus shanghaiensis (2)
<input checked="" type="checkbox"/> Rhizopus cohnii (2)	<input checked="" type="checkbox"/> Rhizopus microsporus (2)	<input checked="" type="checkbox"/> Rhizopus stolonifer (76)
<input checked="" type="checkbox"/> Rhizopus delemar (2)	<input checked="" type="checkbox"/> Rhizopus oligosporus (1)	<input checked="" type="checkbox"/> Rhizopus tritici (2)
<input checked="" type="checkbox"/> Rhizopus japonicus (2)	<input checked="" type="checkbox"/> Rhizopus oryzae (12)	

6

Apply Cancel

6. 选中全部子项后，点击 Apply 获得筛选后的结果集。

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CDK OR "cyclin-dependent kinases" AND inhibitor

AND Author Name Enter last name, first name middle name.

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Example: Schubert, J A

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1 2 3

1. 选择 References
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3. 开始检索

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

References ▾

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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 (**CDK** 7, 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 (IC₅₀ < 25 nM). Many have b...

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5

Cyclin dependent kinase (CDK) inhibitors as anticancer drugs 4

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

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

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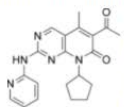
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6

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

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

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

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 Bioorganic & Medicinal Chemistry Letters
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 Journal: General Review; Art Review
 2015
 DOI:
[10.1016/j.bmcl.2015.05.100](https://doi.org/10.1016/j.bmcl.2015.05.100)

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

Database Information
 AN: 2015:1031191
 CAN: 163:214062
 PubMed ID: 26115571
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5

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

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6

Concepts

Antitumor agents	Homo sapiens
Cyclin-dependent kinase inhibitors	Human
	Neoplasm

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

Email
sanchez-martinez_concepcion@lilly.com

Publisher
 Elsevier B.V.

Language
 English

7

MEDLINE® Medical Subject Headings

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

Substances

Substances (3)

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

Patent Number: US6010719

Publication Date: 2000-01-04

Application Number: US1997-931257

Application Date: 1997-09-16

Kind Code: A

Assignee: Universiteit Gent, Belgium

Source: United States
CODEN: USXXAM

Database Information: AN: 2000:10527
CAN: 132:69330
CAplus

Language: English

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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

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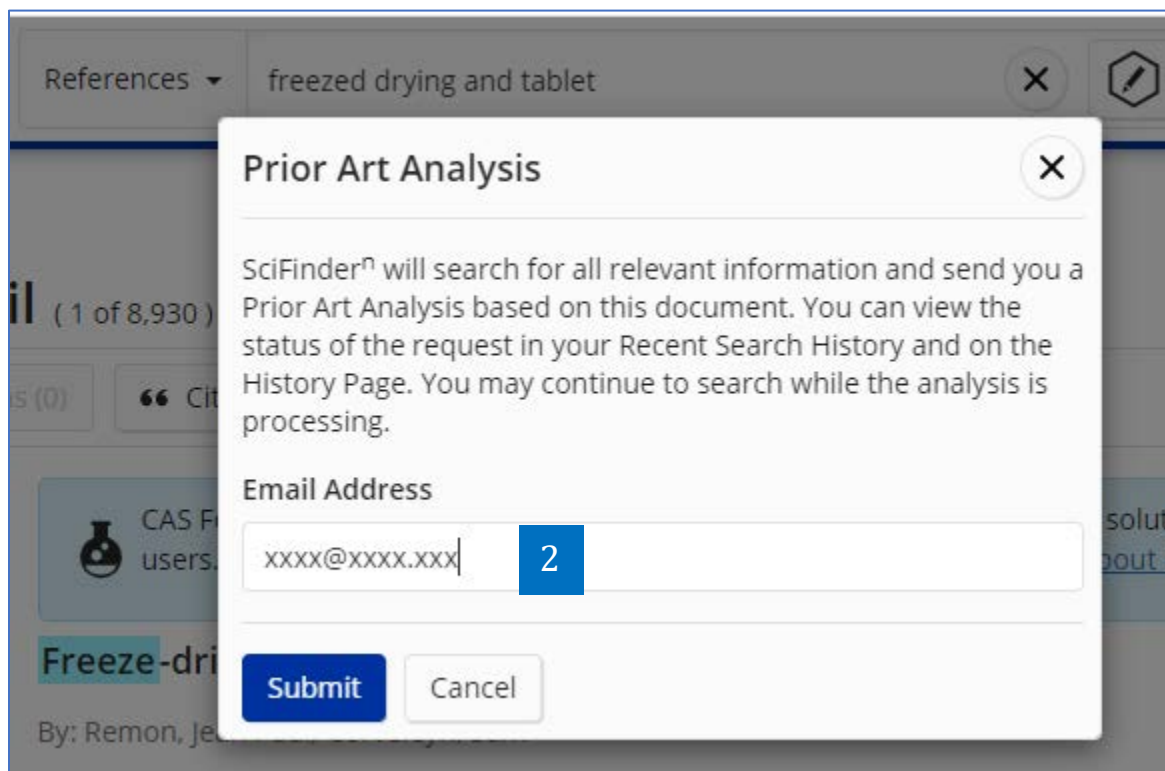
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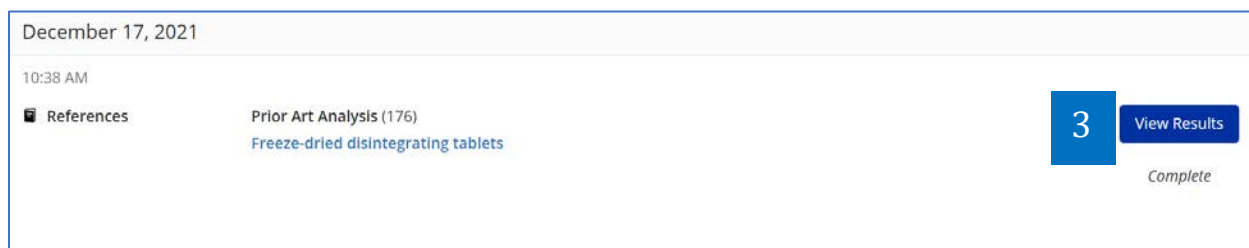
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By: Remon, Jean Paul; Corveleyn, Sam
United States | English | US6010719

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

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

By: Corveleyn, Sam; Remon, Jean-Paul
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Evaluation of maltodextrins as tablet excipients. I. Micromeritic and compressional characterization

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

Rapidly disintegrating tablets containing gums and carbohydrates

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

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

By: Ntawukulilyayo, J. D.; Vervaeke, C.; Remon, J. P.; Goertz, J. P.; Berlo, J. A.
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Substances Reactions Citing

1

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), 152(2), 215-225 | Language: English, Database: Capius

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 tablets 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.

Full Text

Substances (4) Reactions (0) Citing (174) Citation Map

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Document Type

- ☐ Journal (183K)
- ☒ Patent (21K) **1**
- ☐ Review (34K)
- ☐ Biography (8)
- ☐ Book (129)
- [View All](#)

Substance Role

- ☐ Biological Study (798)
- ☐ Uses (214)
- ☐ Analytical Study (139)
- ☐ Properties (103)
- ☐ Preparation (50)

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

☐ Substances ☐ Reactions ☐ Citing

Filtering: Document Type: Patent

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1

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

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

2

PatentPak **3** **4** **5**

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

in 9 (PCSK9) inhibitors for treating
tions 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
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PatentPak 浏览器:

The screenshot displays the CAS PatentPak interface. On the left, a sidebar lists 'Key Substances in Patent' with entries for CAS RN 943-45-30, 743450-46-6, 1886086-05-0, and 678229-07-3. Each entry includes a chemical structure and 'Analyst Markup Locations (1)'. On the right, the main area shows patent claims 2, 13, 14, and 15. The interface includes a top navigation bar with 'PAGE', 'ZOOM', and 'DOWNLOAD' (PDF, PDF+) options. Numbered callouts are placed over the interface: 1 points to a substance entry, 2 points to a patent claim, 3 points to the CAS RN, and 4 points to the download buttons.

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。
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利用专利公开号或者申请号进行检索

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

注：国家代码与数字间不能出现空格，如 WO2013173779

The screenshot displays the CAS SciFinder search results for the patent WO2013173779. The interface includes a search bar at the top with the patent number and a dropdown menu set to 'All'. On the left, a sidebar shows filters for Substances (18), Reactions (35), References (2), and Suppliers (0). The main content area is titled 'All Answer Types' and shows 'Top two answers by relevance from each answer type.' Under the 'Substances (18)' section, two results are listed: 1. 24424-99-5, Di-tert-butyl dicarbonate, with 56K references, 160K reactions, and 138 suppliers; 2. 75-31-0, Isopropylamine, with 22K references, 28K reactions, and 62 suppliers. Below this, the 'Reactions (35)' section shows 'Scheme 1 (1 Reaction)' with a chemical reaction scheme and a yield of 99%.

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。

CAS SciFinder[®] 5

References WO2013173779

Return to Home

Filter Behavior

Filter by Exclude

Document Type

Patent (2)

Language

English (2)

Publication Year

2009 2019

No Min to No Max Apply

View Larger

Author

Organization

Publication Name

Concept

CA Section

Database

Search Within Results

Filter Content Report

References (2)

Sort: Relevance View: Partial Abstract

Substances Reactions Citing

Save And Alerts

1

Process for making amino acid compounds

By: Remarchuk, Travis

United States, US9278917 B2 2016-03-08 | Language: English, Database: CAPLUS

The invention provides new processes for making and purifying amino acid compounds, which are useful in the preparation of AKT inhibitors used in the treatment of diseases such as cancer, including the compound (S)-2-(4-chlorophenyl)-1-(4-((5R,7R)-7-hydroxy-5-methyl-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-yl)piperazin-1-yl)-3-(isopropylamino)propan-1-one.

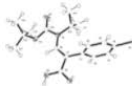
PatentPak Full Text Substances (17) Reactions (12) Citing (0) Citation Map

2

Process for making amino acid compounds using enantioselective hydrogenation reactions

By: Remarchuk, Travis

World Intellectual Property Organization, WO2013173779 A1 2013-11-21 | Language: English, Database: CAPLUS



The invention provides processes for making and purifying amino acid compounds of formula I (R¹ and R² are independently H, C₁₋₁₂ alkyl, and amino-protecting group) and their salts, which are useful in the preparation of AKT inhibitors, including the compound (S)-2-(4-chlorophenyl)-1-(4-((5R,7R)-7-hydroxy-5-methyl-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-yl)piperazin-1-yl)-3-(isopropylamino)propan-1-one. Compound I [R¹ = H; R² = Boc] was prepared by condensation of Et 4-chlorophenylacetate with Et formate and isopropylamine followed by Boc-protection; the resulting (E)-Et 3-((tert-butoxycarbonyl...

View More

PatentPak Full Text Substances (18) Reactions (23) Citing (1) Citation Map

5. 选择 References，获得该专利及其同族信息。

CAS SciFinder® Substances WO2013173779 6

Return to Home

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

Substances (18)

Sort: CAS RN: Descending View: Partial

References Reactions Suppliers

1 1489004-67-2

Double bond geometry shown

$C_{19}H_{26}ClNO_4$
Ethyl (αZ)-4-chloro-α-[[[(1,1-dimethylethoxy)carbonyl](1-methylethyl)amino]methyl]benzeneacetic acid

2 References 2 Reactions 0 Suppliers

2 1489004-64-9

$C_{12}H_{14}ClNO_2$
4-Chloro-α-[[[(1-methylethyl)amino]methylene]benzeneacetic acid

2 References 2 Reactions 0 Suppliers

3 1489004-59-2

$C_{19}H_{24}ClNO_6$
α-[[Bis[(1,1-dimethylethoxy)carbonyl]amino]methylene]-4-chlorobenzeneacetic acid

2 References 6 Reactions 0 Suppliers

4 1489004-54-7

5 1489004-53-6

6 1489004-41-2

6. 选择 Substances，获得该专利披露的物质信息。

Reactions (35) Group: By Document View: Expanded

Filter Behavior: Filter by Exclude

Yield: 90-100% (3), 70-79% (1), 50-69% (2), 30-49% (2), No Yield Available (27)

Number of Steps: 1 (8), 2 (6), 3 (4), 4 (2), 5 (1)

Non-Participating Functional Groups: Halide (8), Phenyl halide (8), Acyclic alkene (4), Alkene (4), Carbamate (4)

Process for making amino acid compounds using enantioselective hydrogenation reactions
By: Remarchuk, Travis
World Intellectual Property Organization, **WO2013173779** A1 2013-11-21 | Language: English, Database: CAplus

PatentPak Full Text View 23 Related Reactions

Reaction Summary Steps: 1 Yield: 99%

1.1 Reagents: [Hydrogen](#), [Lithium tetrafluoroborate](#)
Catalysts: [Ruthenium\(1+\)](#), [\(η⁶-benzene\)\[1.1'-\(1S\)-\[1.1'-binaphthalene\]-2,2'-diylbis\[1.1-diph...](#)
Solvents: [Ethanol](#); 24 h, 50 psi, rt

[View Reaction Detail](#) [Experimental Protocols](#)

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使用专利申请号获得同样的结果，在此不一一赘述。

Searching for... All

Substances Reactions References Suppliers Biosequences Retrosynthesis

All Answer Types

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CA2013-2873658

生物序列检索

通过生物序列检索结果获取研究文献

The screenshot displays the CAS SciFinder Biosequences interface. The top navigation bar includes the CAS SciFinder logo, a search bar with the text "Enter a query...", and icons for "Draw", "Search", "Star", "Clock", and "User". Below the navigation bar, the main content area is titled "Biosequences (10)". On the left, there is a sidebar with "BLAST Search Details" and "Bioscape Analysis" sections. The "BLAST Search Details" section lists parameters such as "Sequence Type: Protein", "Search Within: Proteins", "BLAST Algorithm: BLASTp", "NCBI Included: Yes", "Alignment Identity: -", "Query Coverage: 90%", "E-Value: 10", "Match with Gaps?: No", "Gap Costs: Existence 11", "Extension 1", and "Word Size: 3". The "Bioscape Analysis" section includes a button "Create Bioscape Analysis". The main content area shows a "Query Details" section with a sequence: "MSGRRHKPTTSNVSVAKIAFTGAVLGGGIIAMAAQATAATDGEWDQVARGESGQNWISINTGNGYLGLQFTQSTWAAHGGGEFAPSAQLAS...". Below this, there is a sequence alignment diagram showing a "Query" sequence (1 to 407) aligned with a "Subject" sequence (1 to 737). The alignment identity is 99.75%. To the right of the alignment, it states "Matches: 406" and "Mismatches: 1". Below the alignment, there is a "References" section with three entries: "Tuberculosis Compositions And Methods Of Treating Or Preventing Tuberculosis", "Tuberculosis compositions and methods of treating or preventing tuberculosis", and "Recombinant cytomegalovirus vectors as vaccines for tuberculosis". Each entry includes the assignee and sequence ID number.

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

生物序列检索 (BLAST)

The screenshot displays the CAS SciFinder Biosequences search page. On the left, a sidebar lists search categories: All, Substances, Reactions, References, Suppliers, Biosequences (highlighted), and Retrosynthesis. The main area is titled 'Biosequences' and includes a text input field for a protein or nucleotide string, an 'Upload Sequence' button, and a 'Clear Search' button. Below the input field is a text area containing a sample nucleotide sequence. To the right of the input field are tabs for 'BLAST', 'CDR', and 'Motif', with 'BLAST' selected. Further right is a 'Sequence Type' dropdown menu with 'Nucleotide' and 'Protein' options, 'Nucleotide' being selected. Below this is a 'Search Within:' section with radio buttons for 'Nucleotides' (selected) and 'Proteins', and a checked checkbox for 'Include NCBI Sequences'. At the bottom right is a 'Limit Total Sequence Results to:' dropdown menu set to '20000'. A 'Start Biosequence Search' button is located at the bottom right. Numbered callouts 1 through 4 are overlaid on the image: 1 points to the BLAST tab, 2 points to the Sequence Type dropdown, 3 points to the 'Include NCBI Sequences' checkbox, and 4 points to the 'Limit Total Sequence Results to' dropdown.

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

Alignment Subject 1 References

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

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

Length: 867 nt

Sequence 3

```

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

```

→ ↺ ↻ ncbi.nlm.nih.gov/nuccore/KJ865859.1

GenBank 4 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., Hoetzenecker,W., Cozzio,A., Dummer,R., Mihm,M.C. Jr., Flaherty,K.T., Frank,M.H., Murphy,G.F., Sharpe,A.H., Kupper,T.S. and Schatton,T.

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

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

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



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



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

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- Biosequences**
- Retrosynthesis

Biosequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about Biosequence Search.](#)

BLAST	CDR	Motif	Upload Sequence	Clear Search
MSGRRHKPTTSVSVAKIAFTGAVLGGGGIAMAQAATAATDGEWDQVARCESGGNWSINTGNVGLGGLQFTQTSTWAHGGGEFAPSAQ LASREQQIAGVERVLATQGRGAWPVCGRGLSNATPREVLPSAAMDAPLDAAVNGEPAPLAPPADPAPPVELANDLPAPLGEPL AAPADPAPPADLAPPAPADVAPPVELAVNDLPAPLGEPLAAPADPAPPADLAPPAPAEAPPADLAPPADLAPPVELAVNDLP APLGEPLAAPAEAPPADLAPASADLAPPADLAPPAPAEAPPAPADLAPPAVNEQTAPGDQPATAPCGPVGLATDLEPEPDP QPADAPPPGDVTEAPAETPQVSNIAITKKLQAIQAIRQDVCGNDALDSLAPQYIG				

Sequence Type:

Nucleotide Proteins **1**

Search Within:

☐ Nucleotides ☒ Proteins

☒ Include NCBI Sequences

Limit Total Sequence Results to:

1000

Start Biosequence Search

The screenshot displays the CAS Bioscope Analysis tool interface. The top navigation bar includes the CAS logo, a search bar with the text "Enter a query...", and icons for "Draw", "Search", "Star", "Clock", and "User". The left sidebar contains a "Filter by" section with three filters: "E-Value" (0 to 10⁶), "Query Coverage %" (0 to 100), and "Subject Coverage %" (0 to 100). The main content area shows a sequence alignment of 407 amino acids. The sequence is displayed in a table with columns for "Subject" and "References". The sequence is: 1 MSGRHRKPTT SNVSYAKIAF TGAVLGGGGI AMAAQATAAT DGEWDQVARC ESGGNWSINT GNGYLGGLQF TQSTWAAHGG 81 GEFAPSAQLA SREQIIVAGE RVLATQGRGA WPCVGRGLSN ATPREVLPAS AAMDAPLDA AVNGEPAPLA PPPADPAPPV 161 ELAANDLPAP LGEPLPAAPA DPAPPADLAP PAPADVAPPV ELAVNDLPAP LGEPLPAAPA DPAPPADLAP PAPAELAPPA 241 PADLAPPAPA DLAPPVELAV NDLPAPLGEP LPAAPAEAP PADLAPASAD LAPPAPADLA PPAPAEALAPP APADLAPPAA 321 VNEGTPAGDQ PATAPGGPYG LATDLELPEP DPQPADAPPV GDVTEAPAE PQVSNIAATK KLWQAIRAQD VCGNDALDSL 401 AQPVTIVG. The sequence is highlighted in green, indicating a match. The interface also shows "Matches: 407" and "Mismatches: 0".

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

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

COVID-19 Information

Public health information (CDC) | Research information (NIH) | SARS-CoV-2 data (NCBI) | Prevention and treatment information (HHS) | Esolol

4

GenPept

Send to

Change region shown

Customize view

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

GenBank: CCG63477.1

Identical Proteins

FASTA

Graphics

LOCUS

CCG63477

407 aa

linear

BCG 03-NOV-2016

DEFINITION

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

ACCESSION

CCG63477

VERSION

CCG63477.1

DELIN

BioProject: PRJNA70268

BioSample: SAMN04332321

embl accession: AB12029.2

RESOURCE

KEYWORDS

SOURCE

ORGANISM

REFERENCE

1

AUTHORS

TITLE

JOURNAL

PUBMED

21914899

REFERENCE

2

AUTHORS

TITLE

JOURNAL

FEATURES

source

Protein

Region

CDS

ORIGIN

Analyze this sequence

Run BLAST

Identify Conserved Domains

Highlight Sequence Features

Find in this Sequence

Related information

BioProject

Nucleotide

PubMed

Taxonomy

CDD Search Results

Conserved Domains (Concise)

Conserved Domains (Full)

Related Structures (List)

Related Structures (Summary)

Recent activity

Turn Off

Clear

possible resuscitation-promoting factor rpfa [Mycobacterium tuberculosis variant... Protein

ADATU4BSU5 (0)

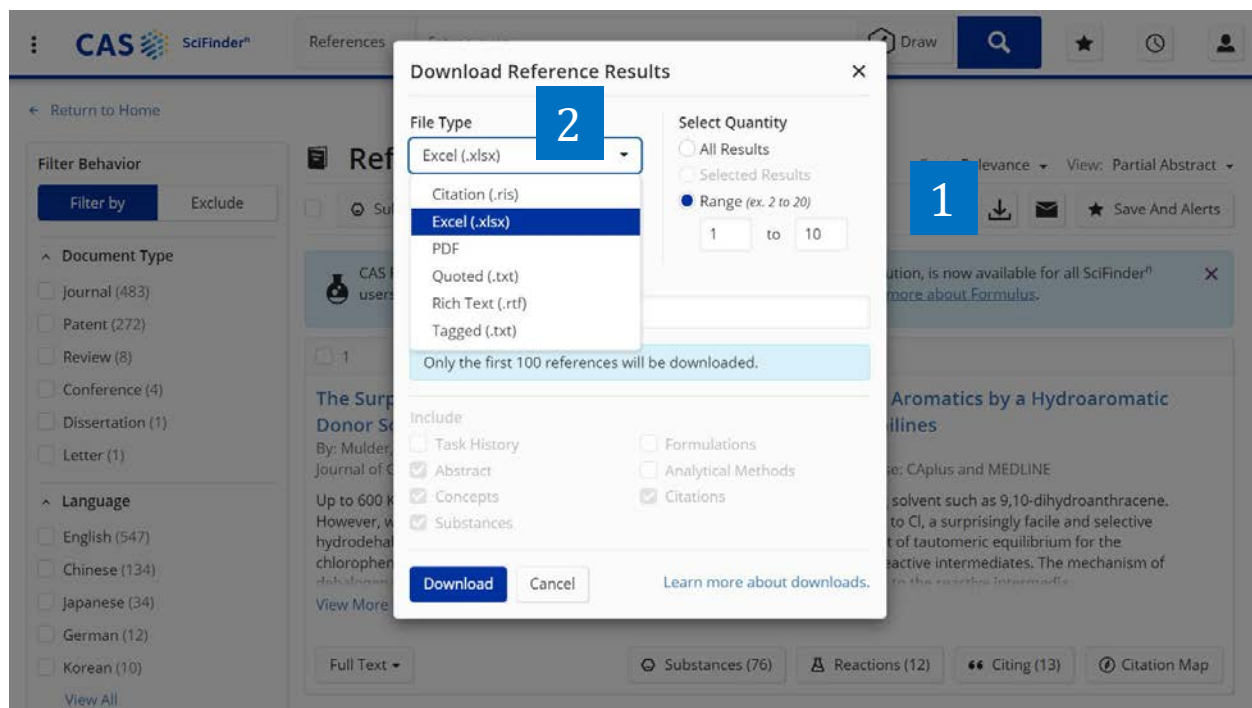
Protein

See more...

4. NCBI 中的目标序列详情。

检索结果后处理

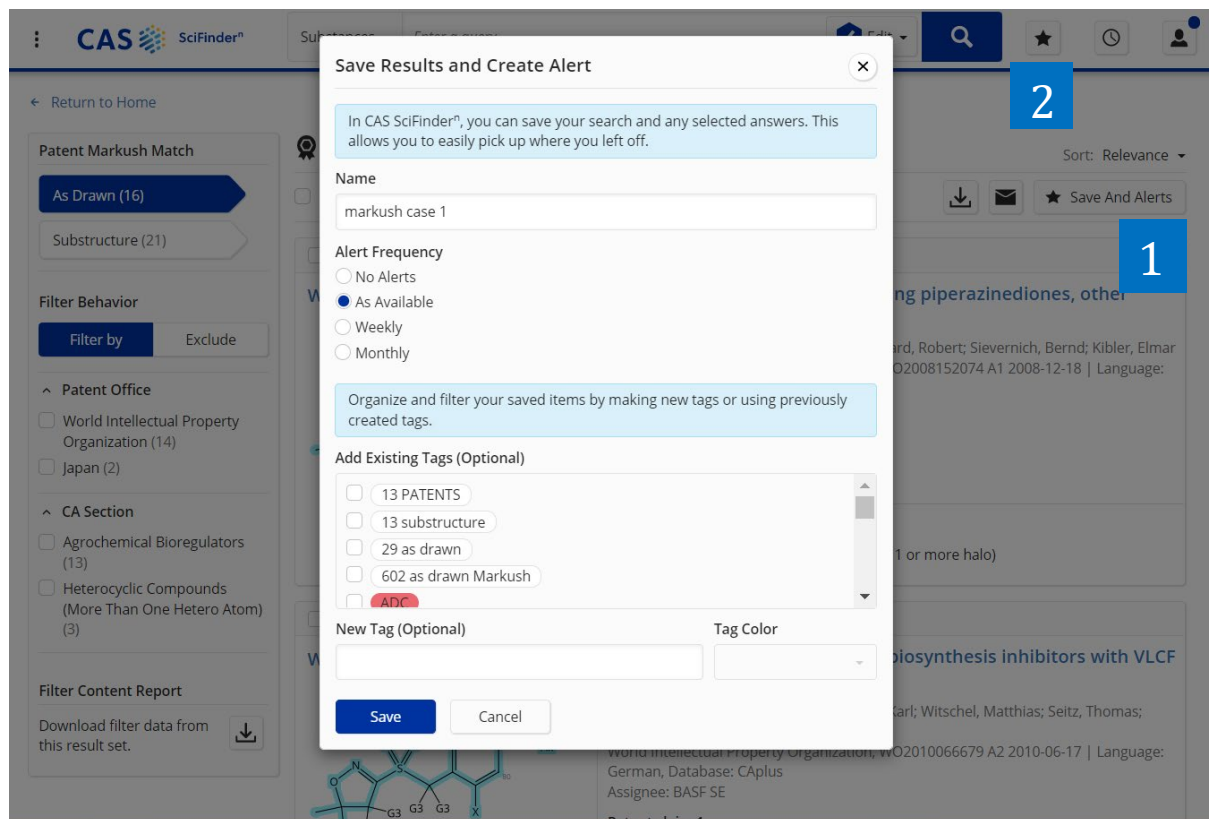
使用 Excel 文件导出文献详情



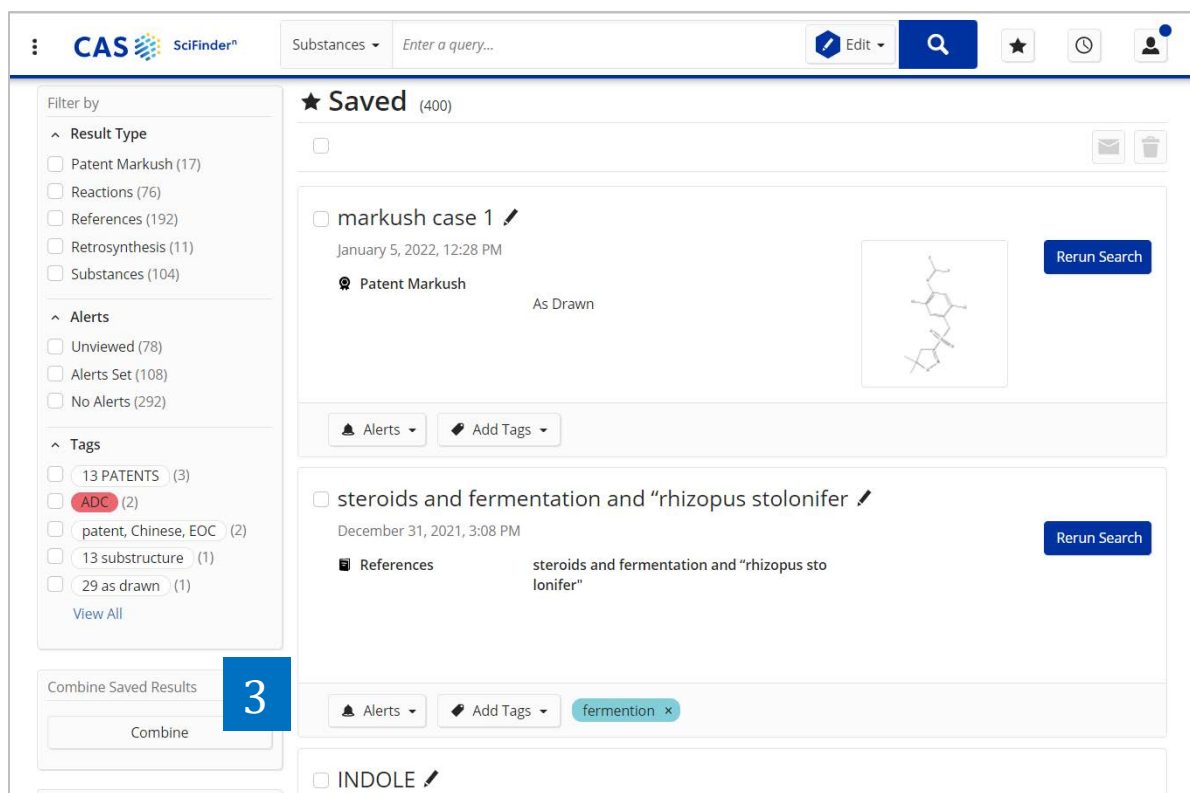
1. 在文献结果集页面，点击下载图标
2. 在弹出窗口中的 File Type 下选择 Excel(.xlsx)，即可使用 Excel 文件格式下载文献详情。

Combine 的应用

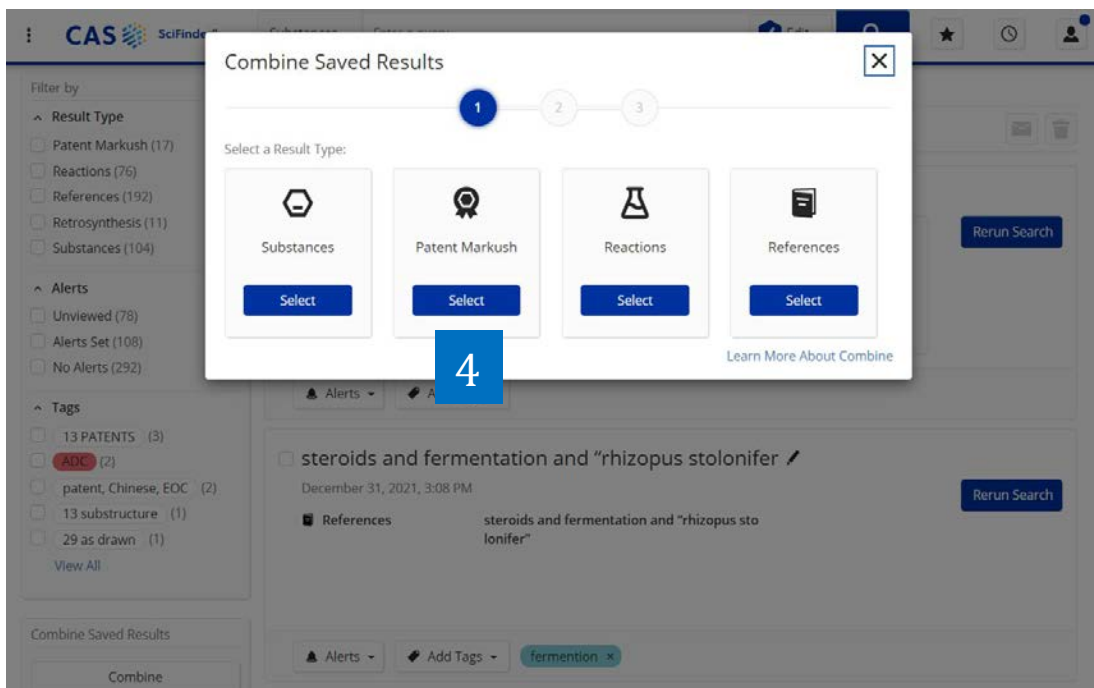
Combine 功能：可用于对多个检索结果集（包括文献、物质、Markush 和反应的检索结果集）进行逻辑处理（包括合并、取交集和排除）。



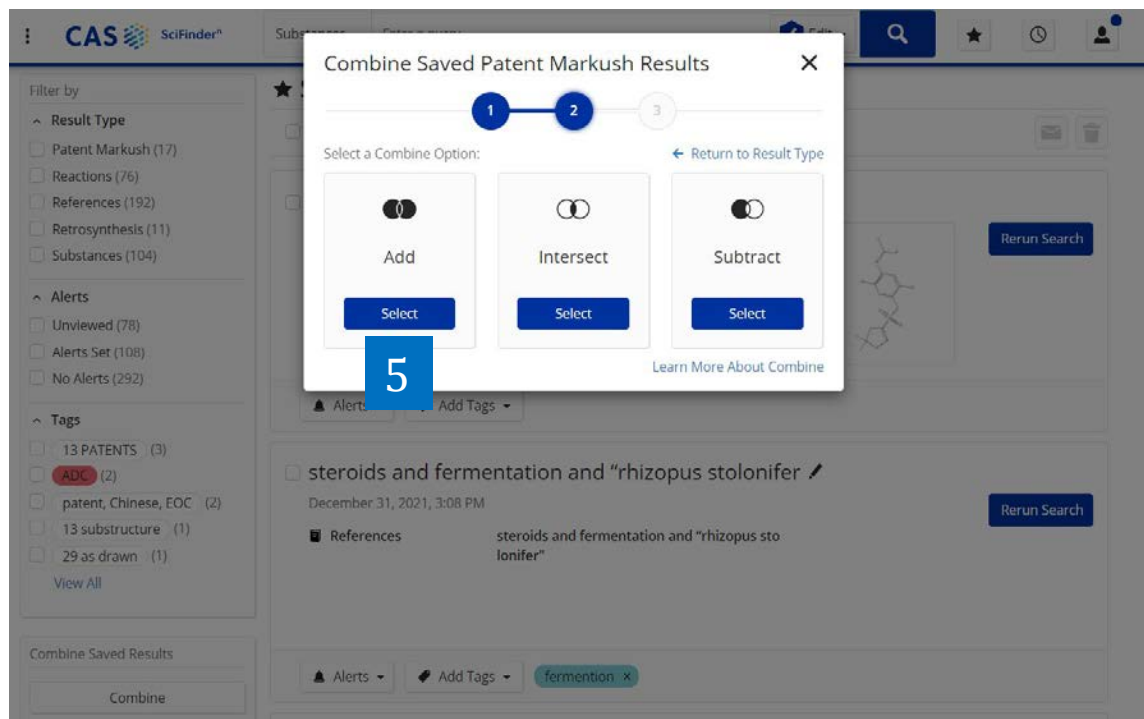
1. 点击 Save And Alerts，在弹出窗口中填写 Name，点击 Save，保存检索结果集。
2. 打开保存的检索结果集，进行 Combine 操作。



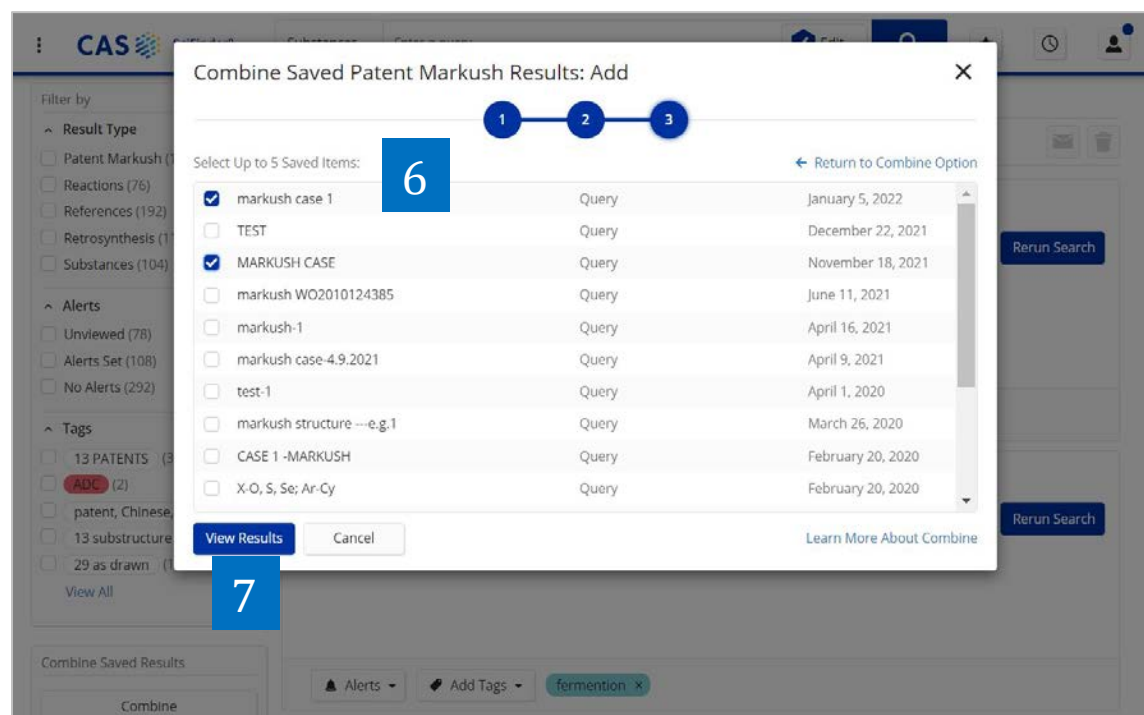
3. 点击 Combine, 进行多个结果集的逻辑处理。



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



5. 选择需要进行的逻辑操作。



6. 选择需要 combine 的结果集。

7. 点击 View Results, 获得 combine 后的结果集。

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

Return to Home

Filter Behavior

Filter by Exclude

Patent Office

- ☐ World Intellectual Property Organization (519)
- ☐ China (199)
- ☐ United States (105)
- ☐ Japan (69)
- ☐ Korea, Republic of (49)
- [View All](#)

CA Section

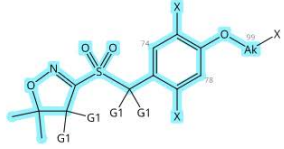
- ☐ Heterocyclic Compounds (More Than One Hetero Atom) (374)
- ☐ Heterocyclic Compounds (One Hetero Atom) (225)
- ☐ Optical, Electron, and Mass Spectroscopy and Other Related Properties (104)
- ☐ Pharmacology (77)
- ☐ Benzene, Its Derivatives, and Condensed Benzenoid Compounds (47)
- [View All](#)

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

References

1

WO2008152074



Herbicidal compositions containing piperazinediones, other active substances, and safeners

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

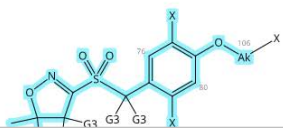
Patent claim 15

[PatentPak](#) [Full Text](#)

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

2

WO2010066679







Herbicidal mixtures of cellulose biosynthesis inhibitors with VLCF A inhibitors.

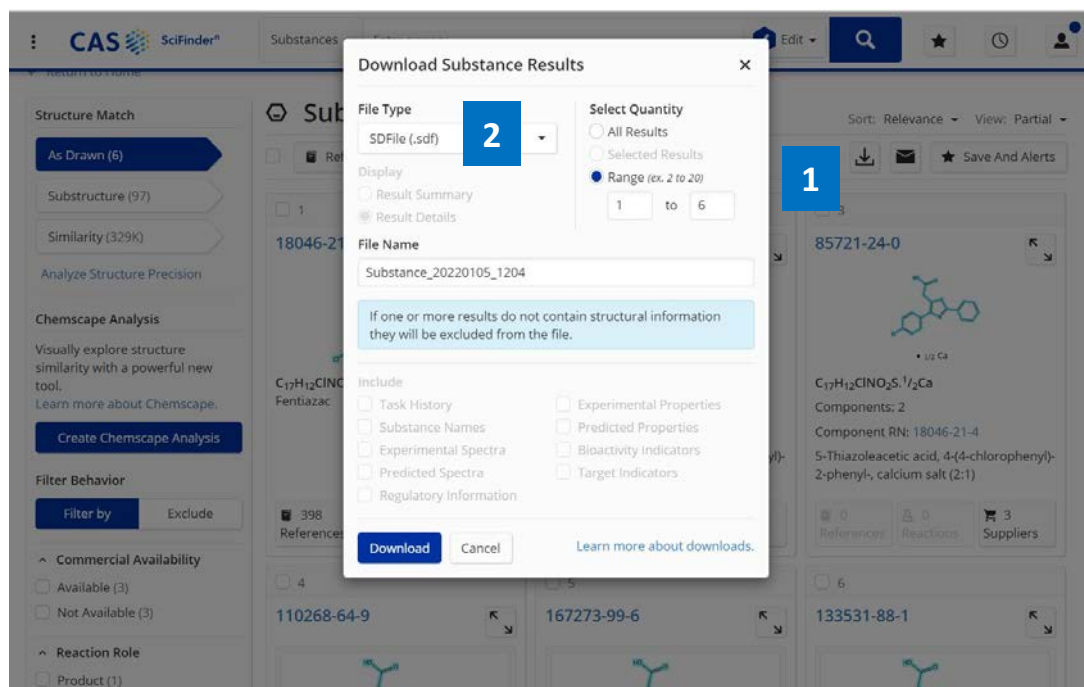
By: Parra Rapado, Liliana; Moberg, William Karl; Witschel, Matthias; Seitz, Thomas; Simon, Anja; Newton, Trevor William
World Intellectual Property Organization, WO2010066679 A2 2010-06-17 | Language: German, Database: CAplus
Assignee: BASF SE

将物质结果导出为可以编辑的结构数据文件

有以下三种方法可以将物质结果导出为可以编辑的结构数据文件：


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

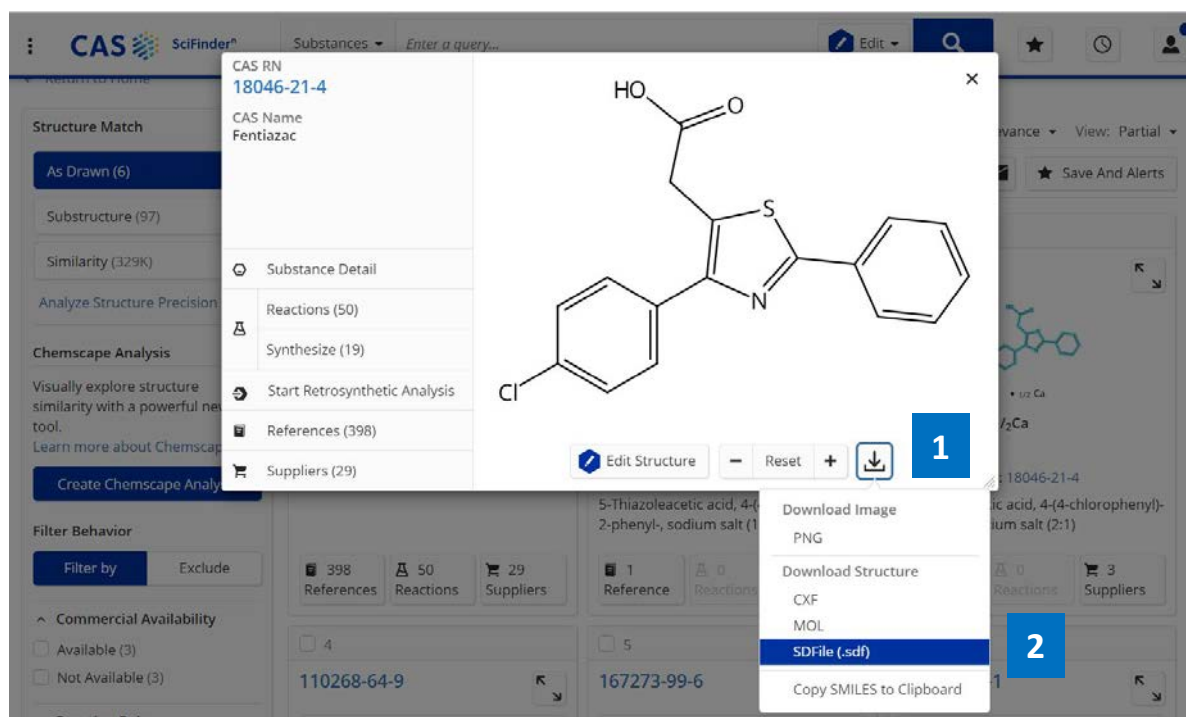
方法一：直接在物质结果集页面点击 ，选择 SDFFile，可以批量导出可编辑的结构数据文件。




1. 点击  按钮


2. 选择 SDFFile

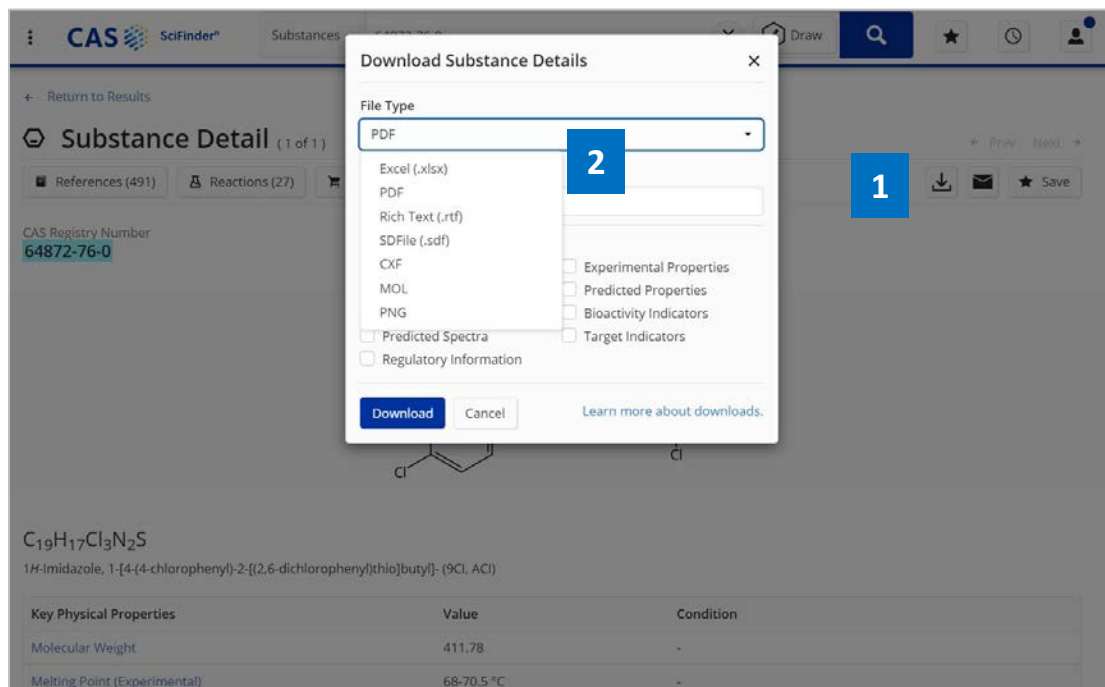
方法二：若需要导出某一选定物质的结构数据文件，则可以点击该物质的结构，在打开的新窗口中点击 ，选择所需下载的结构数据文件格式（CXF, MOL, SDF）。




The screenshot displays the CAS SciFinder web interface. A chemical structure of 5-(4-chlorophenyl)-2-phenylthiazole-3-carboxylic acid is shown in a central window. To the left, a sidebar lists various analysis tools like 'Structure Match', 'Similarity', and 'Chemscap Analysis'. Below the structure, a table lists search results with columns for CAS RN, CAS Name, and Suppliers. A dropdown menu is open over the structure, showing options: 'Download Image', 'Download Structure', and 'Copy SMILES to Clipboard'. The 'Download Structure' option is expanded, showing sub-options: 'CXF', 'MOL', and 'SDFFile (.sdf)'. A blue box with the number '1' highlights the download icon in the top right of the structure window, and another blue box with the number '2' highlights the 'SDFFile (.sdf)' option in the dropdown menu.

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
Vincalcukoblastine
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
80891.129029975.8065 0.0000 C 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
69024.1935 9308.4677 0.0000 O 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
74721.774212592.7419 0.0000 C 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
50969.7581 0.0000 0.0000 C 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
84302.419424750.0000 0.0000 C 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
84302.419431336.6935 0.0000 O 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
19306.451623788.3065 0.0000 C 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
14897.177440046.3710 0.0000 O 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
 8637.096836435.4839 0.0000 C 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
66592.741950806.4516 0.0000 C 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
57157.258129975.8065 0.0000 C 0 0 1 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
57157.258122772.1774 0.0000 C 0 0 1 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
50969.758133586.6935 0.0000 C 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
 57 58 2 0 0 0 0 0
M END
> <cas.rn>
865-21-4

> <cas.index.name>
Vincalcukoblastine

> <molecular.formula>
C46H58N4O9

> <molecular.weight>
810.97

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

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

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

$$$$

```


属性值 EXCEL 文件下载示例：

Substance_20220105_1216.xlsx

Cheng, Xiaoyan Z

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

Clipboard Font Alignment Number Styles Cells Editing Ideas Sensitivity

AutoSave On

Search

Share Comments

Calibri 11 A A

B I U

General

Conditional Formatting

Format as Table

Cell Styles

Insert

Delete

Format

Σ

Sort & Filter

Find & Select

Ideas

Sensitivity

A1

CAS SciFinder[®]

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CAS Registry Number: 64872-76-0

CAS Display Name: Butenonasole

Type	Category	Property	Value and Units	Temperature	Pressure	pH
Experimental	Thermal	Boiling Point	68-70.3 °C	25 °C		
Predicted	Biological	Bioconcentration Factor	184	25 °C		pH 1
Predicted	Biological	Bioconcentration Factor	155	25 °C		pH 2
Predicted	Biological	Bioconcentration Factor	155	25 °C		pH 3
Predicted	Biological	Bioconcentration Factor	155	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	57600	25 °C		pH 7
Predicted	Biological	Bioconcentration Factor	55200	25 °C		pH 8
Predicted	Biological	Bioconcentration Factor	57900	25 °C		pH 9

Substance Name 64872-76-0

Ready

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 displays the CAS SciFinderⁿ interface. A modal dialog titled "Save Results and Create Alert" is centered on the screen. The dialog contains the following elements:

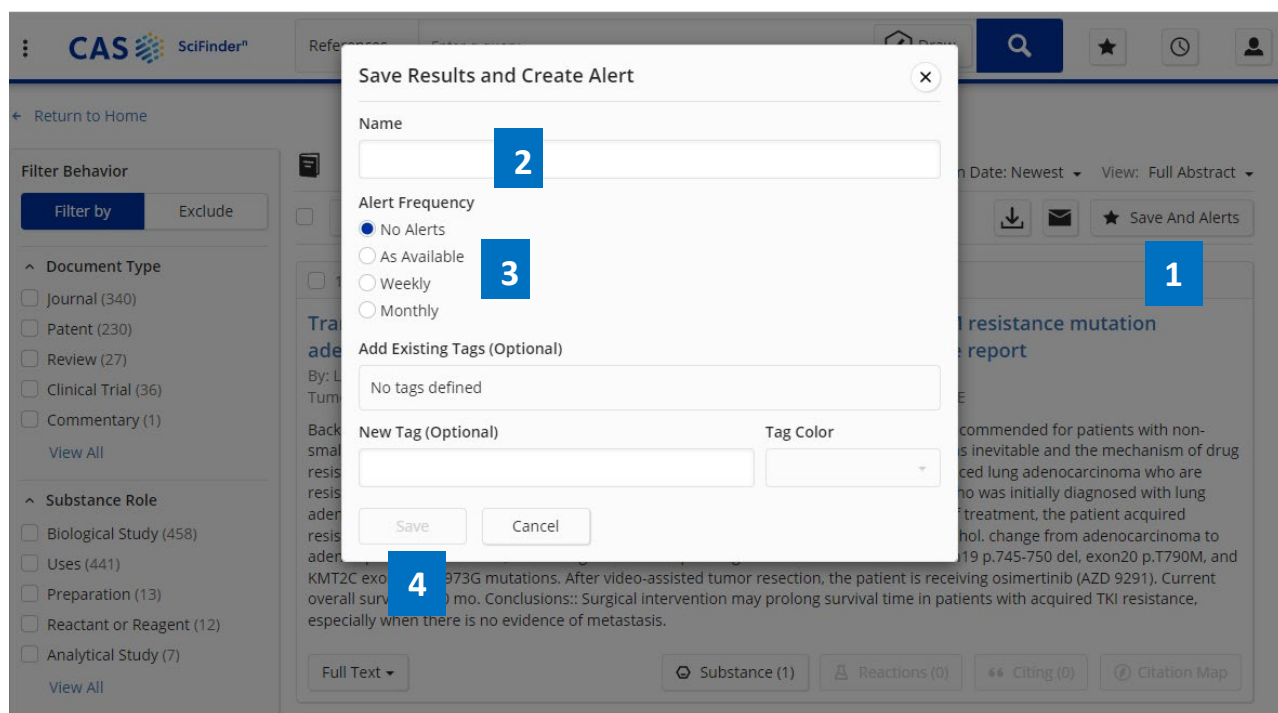
- Name:** A text input field containing "Icotinib Markush".
- Alert Frequency:** A group of radio buttons with options: "No Alerts" (selected), "As Available", "Weekly", and "Monthly".
- Add Existing Tags (Optional):** A text input field showing "No tags defined".
- New Tag (Optional):** A text input field.
- Tag Color:** A dropdown menu.
- Buttons:** "Save" and "Cancel" buttons at the bottom.

Numbered callouts (1-4) indicate the sequence of actions: 1. Click "Save And Alerts" in the top right of the search results page. 2. Enter the name of the alert in the "Name" field. 3. Select the desired alert frequency. 4. Click the "Save" button in the dialog.

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。

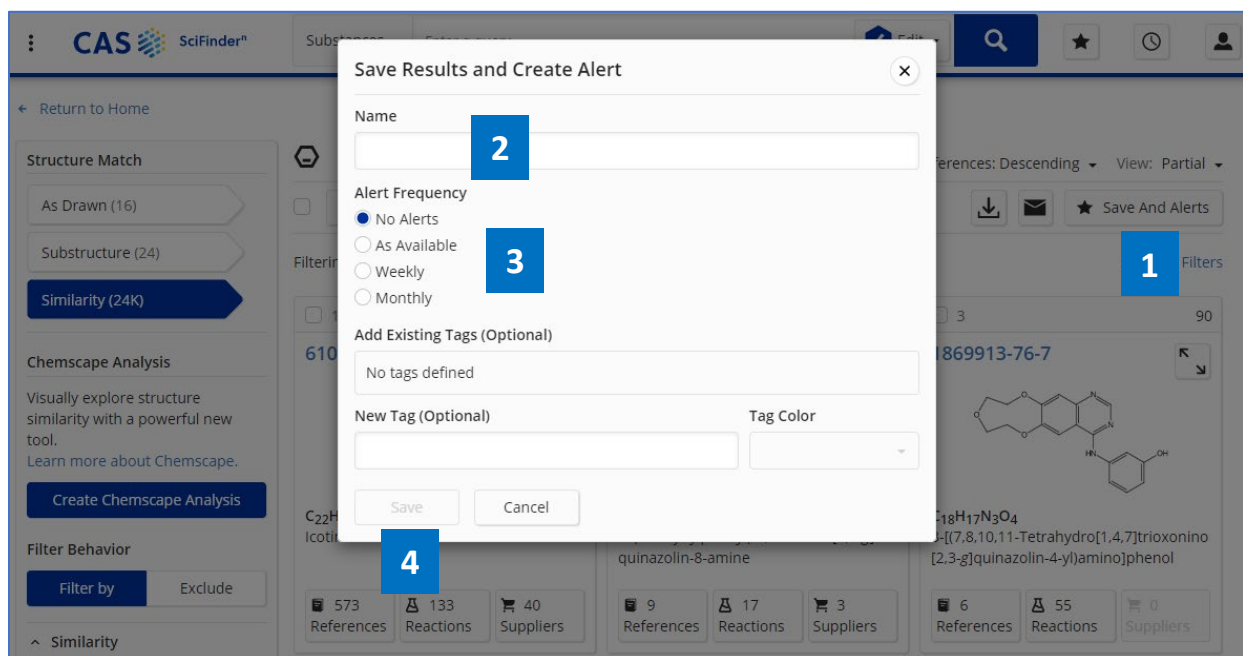
3. 选择 No Alerts 表示不设置提醒；选择 As Available、Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

二. 文献检索后，设置 Alert



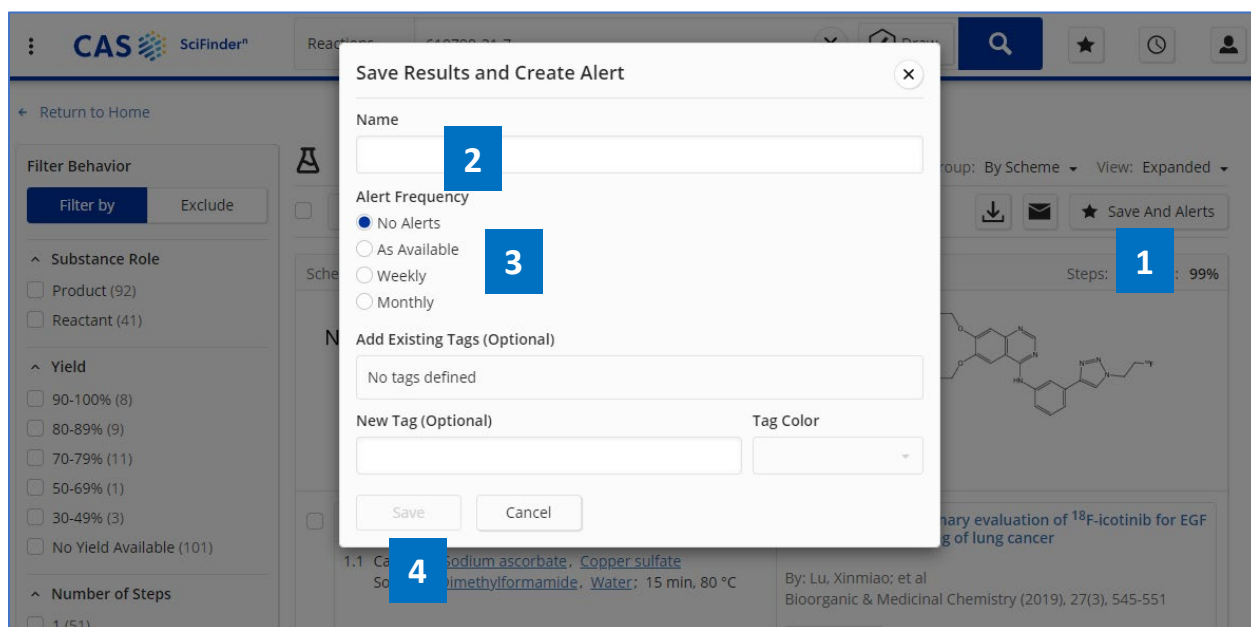
1. 在文献结果集页面点击 Save And Alerts。
2. 输入保存文件的名称。
3. 选择 No Alerts 表示不设置提醒；选择 As Available、Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

三. 物质检索后，设置 Alert



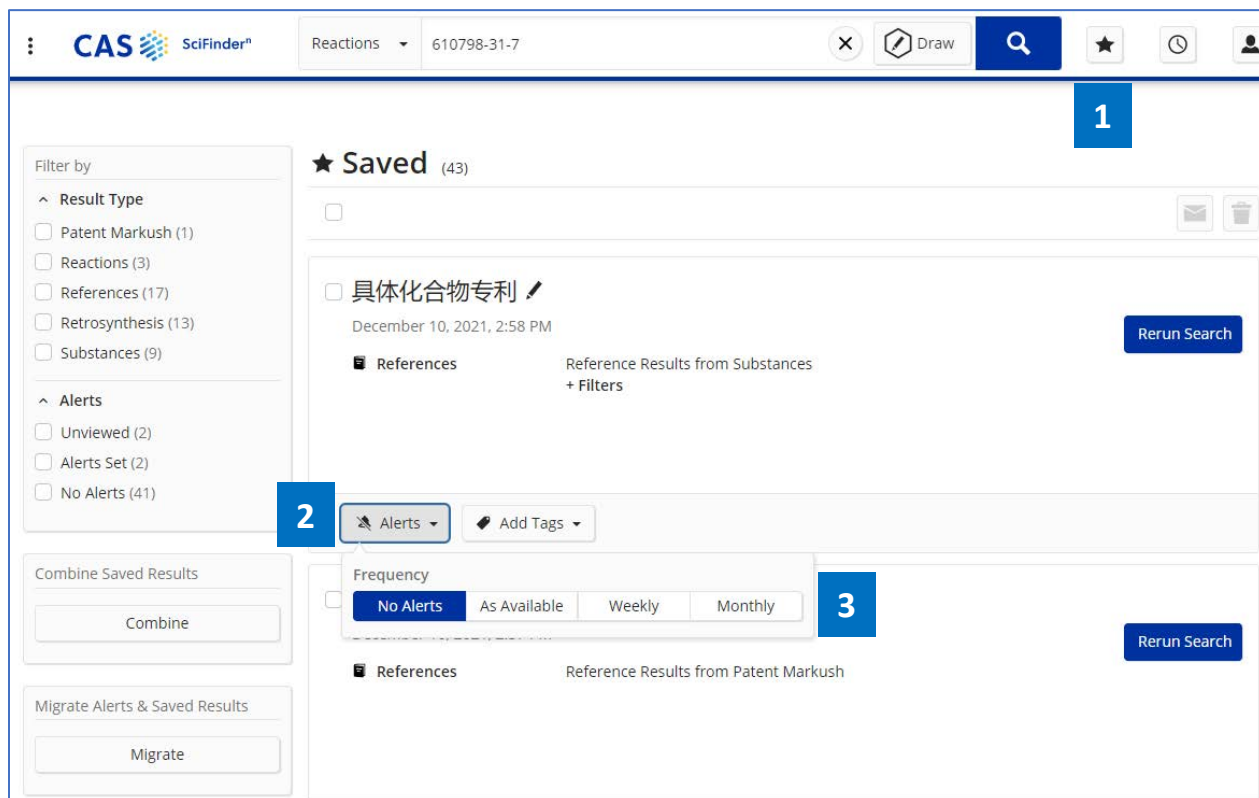
1. 在物质结果集页面点击 Save And Alerts。
2. 输入保存文件的名称。
3. 选择 No Alerts 表示不设置提醒；选择 As Available、Weekly 或 Monthly 表示设置提醒，并同时设置提醒频率。
4. 点击 Save 完成设置。

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：



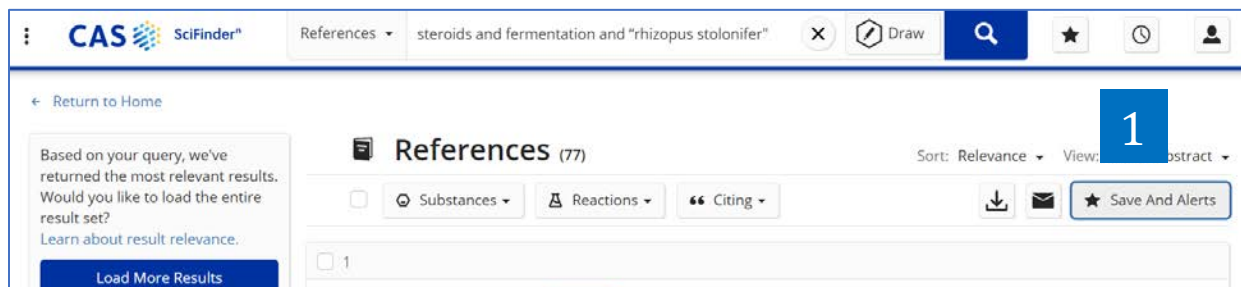
1. 点击 ，查看保存结果集。
2. 点击 ，进行设置。
3. 设置提醒频率。

Alerts 分类选项

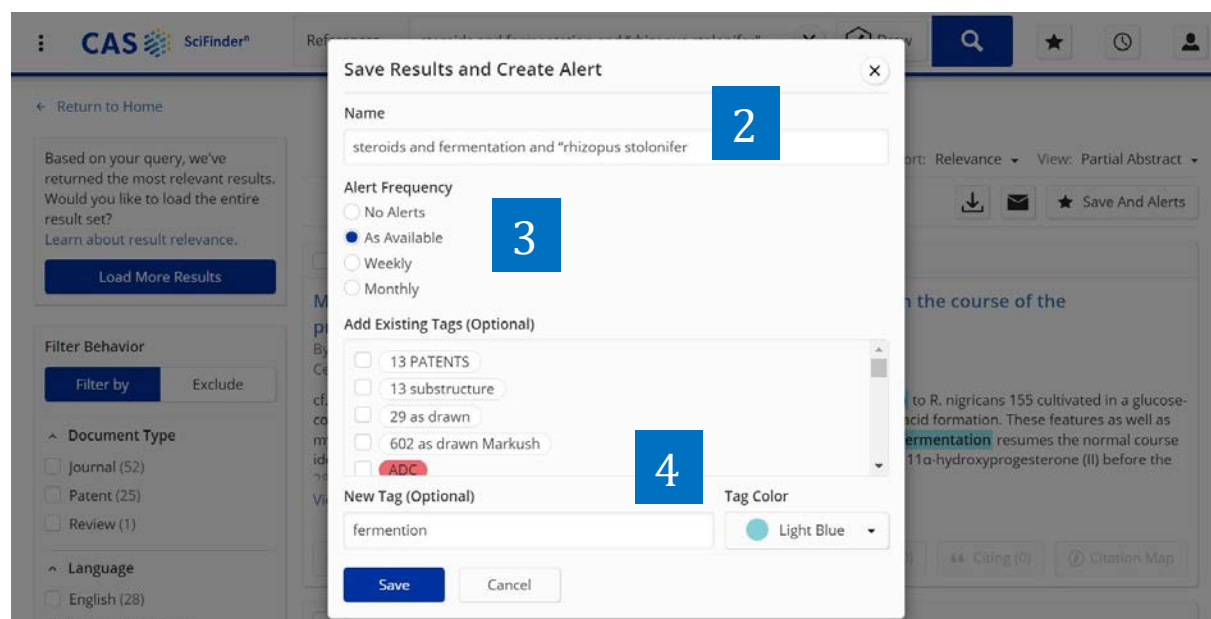
The screenshot shows the CAS SciFinder Alerts management page. On the left is a 'Filter by' sidebar with sections for 'Result Type' (Patent Markush, Reactions, References, Substances), 'Alerts' (Unviewed, Alerts Set, No Alerts), and 'Tags' (13 PATENTS, ADC, 29 as drawn, adhesive, ANTIBODY). The main area displays a 'Saved (78)' alert for 'TLR' with a timestamp of 'December 24, 2021, 9:42 AM'. Below this, there are sections for 'References', 'Frequency' (No Alerts, As Available, Weekly, Monthly), and 'Results' (listing dates and counts). Numbered callouts indicate: 1. Star icon in the top right; 2. Alerts filter section; 3. Alerts dropdown menu; 4. Alerts dropdown menu; 5. Frequency selection buttons; 6. Results list item; 7. Results list item.

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

最新信息提醒



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

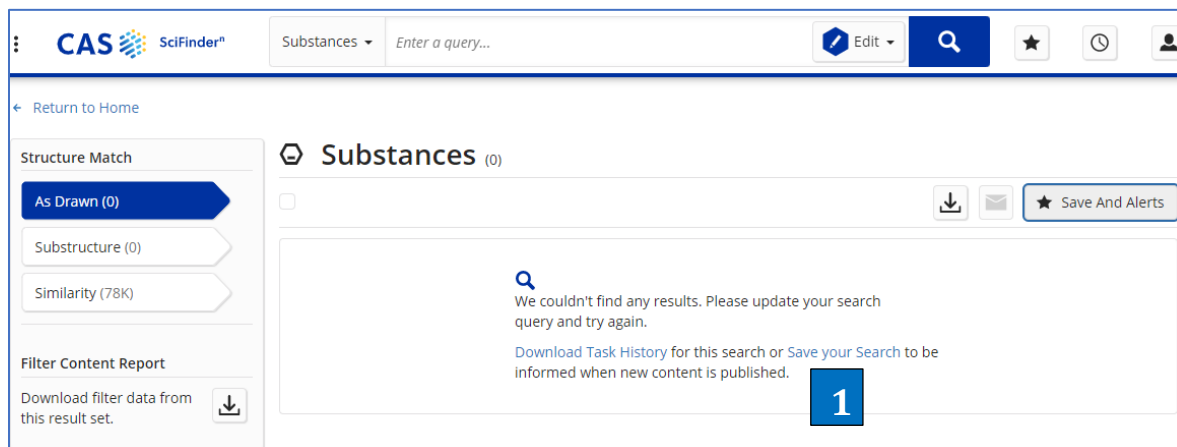


2. 输入本次保存&提醒的文件名。
3. 设置提醒频率：As Available 即时提醒、Weekly 每周提醒、Monthly 每月提醒。
4. 可根据需要标注标签(new tag)，并选择标签颜色(tag color)。

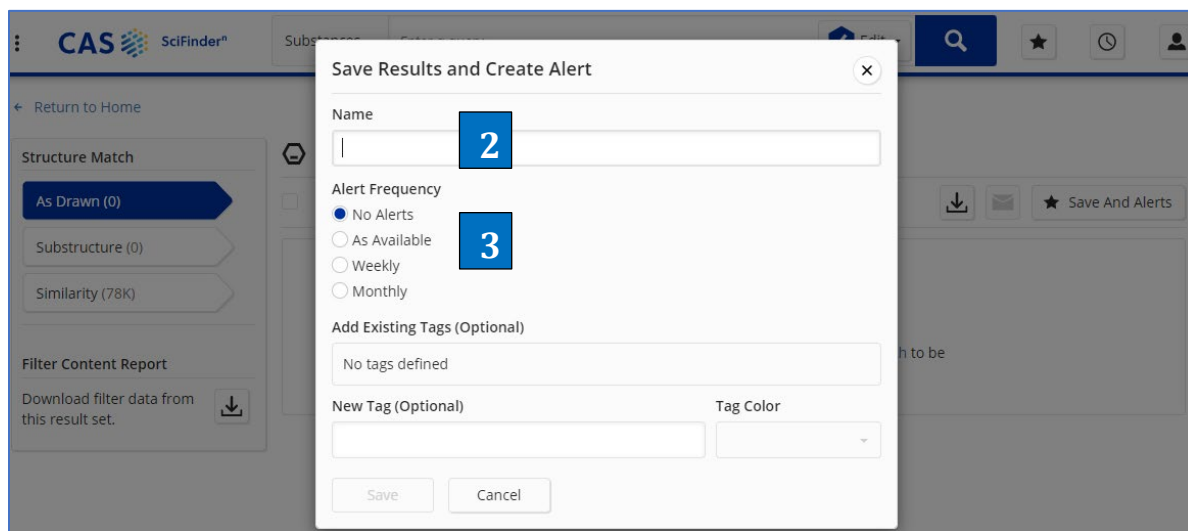
The screenshot shows the CAS SciFinder web interface. On the left, there is a sidebar with filter options. Under 'Filter by', there are sections for 'Result Type' (Patent Markush, Reactions, References, Retrosynthesis, Substances), 'Alerts' (Unviewed, Alerts Set, No Alerts), and 'Tags' (13 PATENTS, ADC, patent, Chinese, EOC, 13 substructure, 29 as drawn). The main area is titled '★ Saved (399)'. It lists two saved searches: 'steroids and fermentation and "rhizopus stolonifer"' and 'INDOLE'. Each search entry includes a date, a 'Rerun Search' button, and a 'References' or 'Reactions' section. A blue box with the number '5' is placed over the top right of the main area. A blue box with the number '6' is placed over the 'Alerts' button in the main area. A blue box with the number '7' is placed over the 'Alerts: Unviewed' option in the sidebar.

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

无检索结果时，如何设置 Alerts



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



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


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

在导出的文件中查看检索过程

SciFinder[®] Page 1

Task History

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




 References: **steroids and fermentation and "rhizopus stolonifer"**

Filtered By:

Publication Year: **2020**

Search Within Results: **intermediates**

Search Tasks 2

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

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

其他

从 CAS SciFinder[®] 链接至其他 CAS 解决方案

The first screenshot shows the CAS SciFinder[®] homepage. A blue banner at the top left contains a large number '1' and text: 'CAS Formulus[®] is available as a part of your CAS SciFinder[®] experience. [Launch Formulus](#) from references with formulations to help with ingredient identification, formulations search, and additional product development needs.' Below this, the 'Substances' search section is visible, with a search bar and a dropdown menu set to 'Molecular Formula'. A sidebar on the left lists search categories: All, Substances (selected), Reactions, References, Suppliers, Biosequences, and Retrosynthesis.

The second screenshot shows the CAS App Switcher interface. A blue banner at the top left contains a large number '2' and text: 'You can now use [@LAST search](#) to mine our newly enhanced collection of more than 500M proteins and nucleotides from 60+ patent authorities dating back to 1957. Plus [visually review sequence similarity and frequency](#) across your patent search results.' Below this, the 'Substances' search section is visible. A sidebar on the left lists various CAS solutions: CAS SciFinder[®], CAS Analytical Methods, CAS Formulus, STN IP PROTECTION SUITE, STNext, CAS Scientific Patent Explorer, REGULATORY, CAS Chemical Compliance Index, ACCOUNT MANAGEMENT, and CAS Profile.

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