



SciFinderⁿ 使用技巧手册

美国化学文摘社

CAS, a division of American Chemical Society

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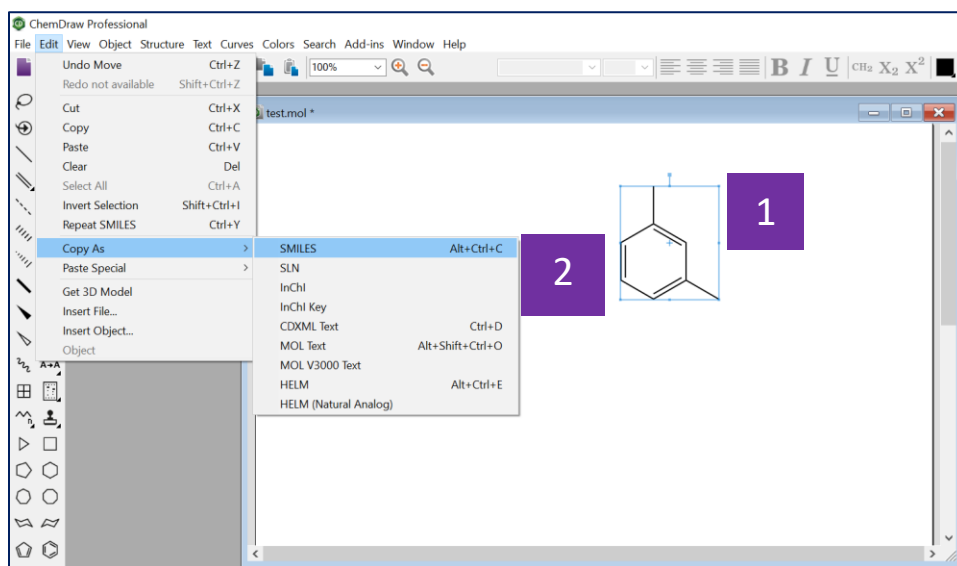
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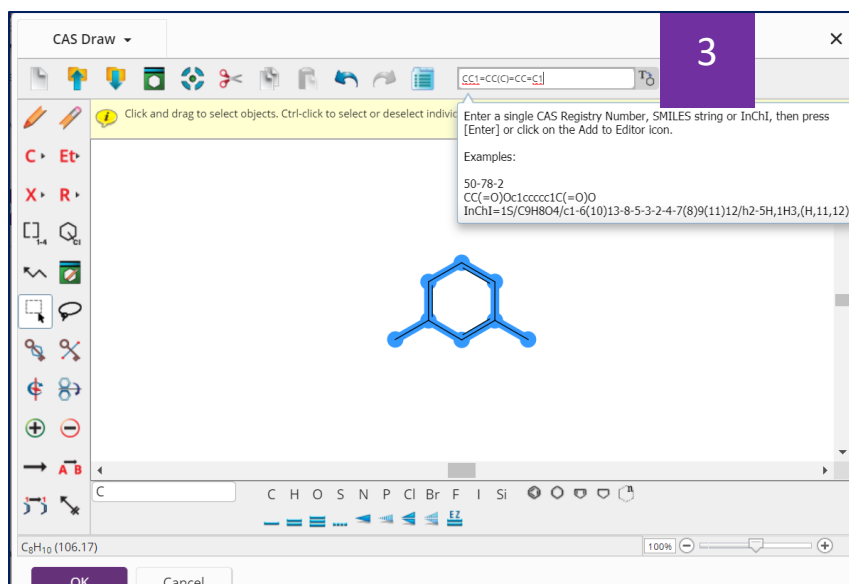
物质检索

与 ChemDraw 联用

可通过以下三种方式利用 ChemDraw 所绘制的结构在 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 SciFinder[®] 的结构编辑器中。





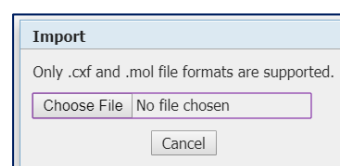
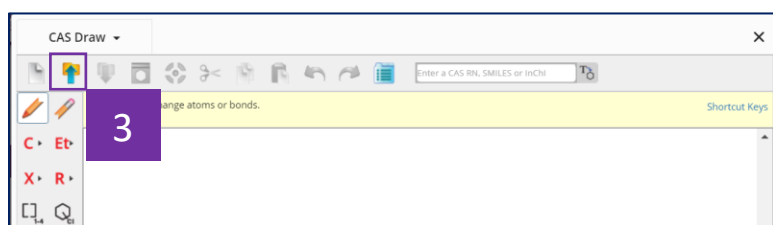
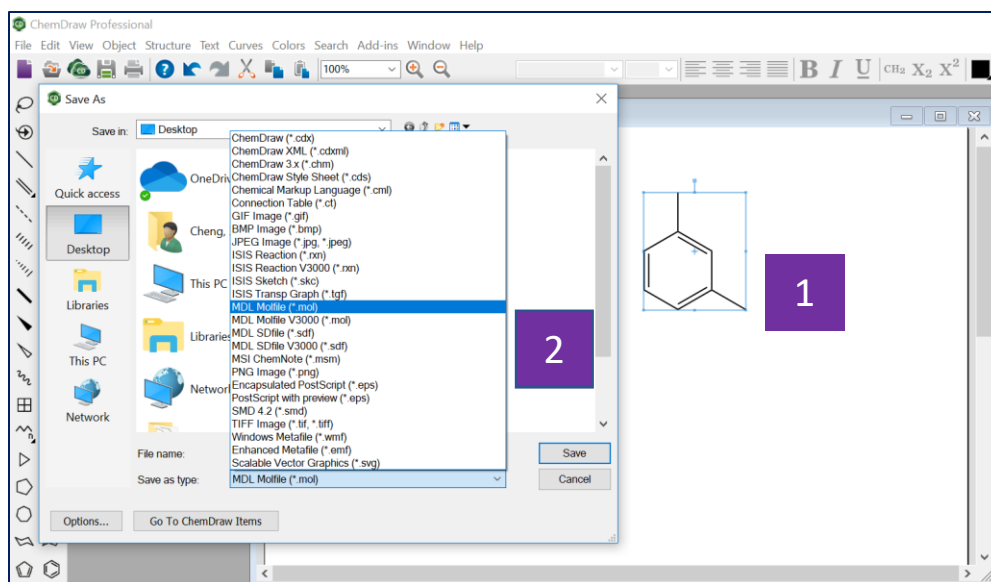
1 在ChemDraw中绘制好结构，并选中

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。



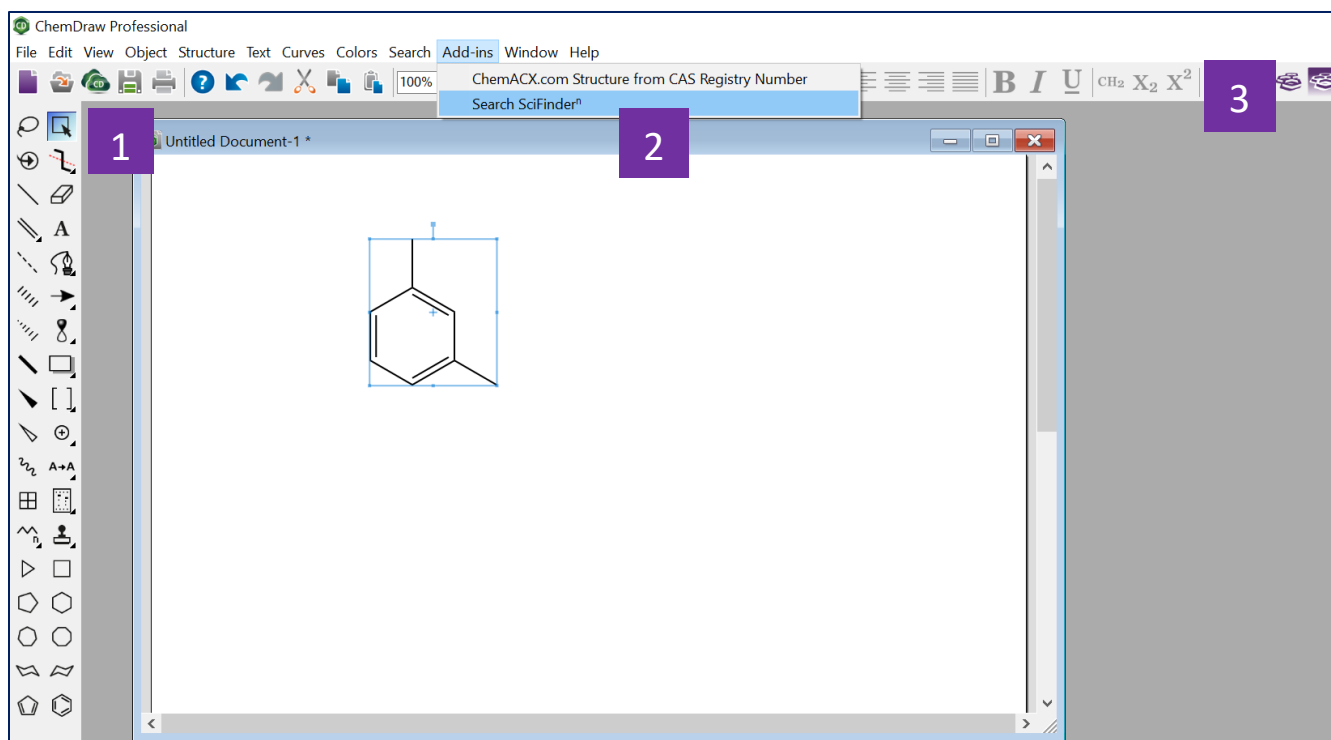
1 在ChemDraw中绘制好结构，并选中

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 18.0 以上版本中，点击 Search SciFinderⁿ 或点击右上角的 SciFinderⁿ 标识图标在 SciFindern 中进行检索。



- 1 在ChemDraw18.0以上的版本中绘制结构，并选中该结构
- 2 点击上方菜单中的Add-ins，并选中Search SciFinder[®]，开始在SciFinder[®]中进行检索
- 3 也可以直接点击右上角SciFinder[®]的标识图，开始在SciFinder[®]中进行检索

通过核磁谱图获得物质

The screenshot shows the SciFinder search interface. On the left, there is a vertical menu with options: All, Substances, Reactions, References, and Suppliers. The 'Substances' option is highlighted with a purple arrow and a purple box containing the number '1'. To the right of the menu, there is a search bar with the text 'Enter a query...' and a 'Draw' button with a search icon. Below the search bar, there is a link for 'Advanced Search' for Molecular Formula, Substance Property, or Experimental Spectra, which is highlighted with a purple box containing the number '2'. The search bar also contains the text 'Search by Substance Name, CAS RN, Patent Number, etc.' and a 'Draw' button with a search icon.

1 选择Substances

2 点击Advanced Search

[← Return to Home Page](#)

Substances

References

Advanced Substance Search

Molecular Formula

Enter one Molecular Formula.

Ex: C₆H₆
(C₈H₈)_x
C₂₂H₂₆CuN₂O₅.C₂H₃N

Add Another Molecular Formula

— AND —

Substance Property

Select Property

- Select One -

Enter Value

Add Another Property

AND

Experimental Spectra

Select Spectrum

1 Carbon-13 NMR

Enter Value

2 155.02, 127.6 to 129.01

(Search includes allowance of ± 2 ppm)

Example: 152.3, 127.6, 133.1
155.02 to 207.59
187

Add Another Spectra 3

4

Clear All

1 选择具体的核磁谱类型

2 输入核磁谱峰值

3 可继续添加其他核磁谱值

4 开始检索

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
 - Carbon-13 NMR (11K)
 - Proton NMR (3,196)
 - Mass (2,364)
 - IR Absorption (420)
 - Nitrogen-15 NMR (195)
 - Fluorine-19 NMR (156)
 - UV and Visible Absorption (112)
 - Raman (106)
 - Phosphorus-31 NMR (89)
 - Oxygen-17 NMR (61)
 - Silicon-29 NMR (18)
 - Boron-11 NMR (1)
- View Fewer
- Regulatory Information
- Bioactivity Indicator
- Target Indicator
- Search Within Results

1

Substances (11,384) Sort: Relevance View Partial

References Reactions Suppliers Save

2

108-95-2 View Detail
Oc1ccccc1
 C₆H₆O
 Phenol
 198K References 76K Reactions 199 Suppliers

50-28-2 View Detail
OCC12CC[C@H]3[C@@H]([C@@H]1CC[C@@H]2O)CCC4=CC(=C(O)C=C4
 C₁₈H₂₄O₂
 Estradiol
 178K References 828 Reactions 156 Suppliers

83-88-5 View Detail
O=C1NC(=O)NC2=C1C(=O)N(C)C2=O
 C₁₇H₂₀N₄O₆
 Riboflavin
 51K References 440 Reactions 150 Suppliers

50-24-8 View Detail
CC12CC[C@H]3[C@@H]([C@@H]1CC[C@@H]2O)CCC4=CC(=O)C=C4
 C₂₁H₂₈O₅
 Prednisolone
 51K References 421 Reactions 113 Suppliers

117-39-5 View Detail
O=C1C(=C(O)C=C(O)C=C1O)C2=CC(=C(O)C=C2O
 C₁₅H₁₀O₇
 Quercetin
 50K References 871 Reactions 110 Suppliers

50-56-6 View Detail
NC(CCC(C)C)C(=O)O
 C₄₃H₆₆N₁₂O₁₂S₂
 Oxytocin
 Protein/Peptide Sequence
 Sequence Length: 9
 37K References 349 Reactions 76 Suppliers

121-33-5 View Detail
COc1cc(O)ccc1C=O
 C₈H₈O₃
 Vanillin
 154-23-4 View Detail
O=C1C(=C(O)C=C(O)C=C1O)C2=CC(=C(O)C=C2O
 C₁₅H₁₄O₆
 Absolute stereochemistry shown, Rotation (+)

50-55-5 View Detail
O=C1C(=C(O)C=C(O)C=C1O)C2=CC(=C(O)C=C2O
 C₃₃H₄₀N₂O₉
 Absolute stereochemistry shown, Rotation (-)

1 通过实验谱图聚类物质

2 点击物质CAS登记号查看物质详情

Experimental Spectra **1**

¹ H NMR	¹³ C NMR	Hetero NMR	IR	Mass	UV and Visible	Additional Spectra
						Source
View Carbon-13 NMR Spectrum						(1) BIORAD
View Carbon-13 NMR Spectrum 2						(2) ACD-A
View Carbon-13 NMR Spectrum						(3) ACD
View Carbon-13 NMR Spectrum						(3) ACD
View Carbon-13 NMR Spectrum						(3) ACD
Carbon-13 NMR Spectrum - 4 Sources						(4-7) CAS

Sources **3**

(1) Copyright [redacted] Laboratories. All Rights Reserved.
 (2) Sigma-Aldrich (Spectral data were obtained from Advanced Chemistry Development, Inc.)
 (3) Spectral data were obtained from Advanced Chemistry Development, Inc.
 (4) Wang, Xingbin; Journal of Chemical Research, (2011), 35(5), 291-293, CAplus
 (5) Wang, Bijia; Organic Letters, (2010), 12(15), 3352-3355, CAplus
 (6) Commodari, Fernando; Magnetic Resonance in Chemistry, (2005), 43(6), 444-450, CAplus
 (7) Boovanahalli, Shanthaveerappa K.; Journal of Organic Chemistry, (2004), 69(10), 3340-3344, CAplus

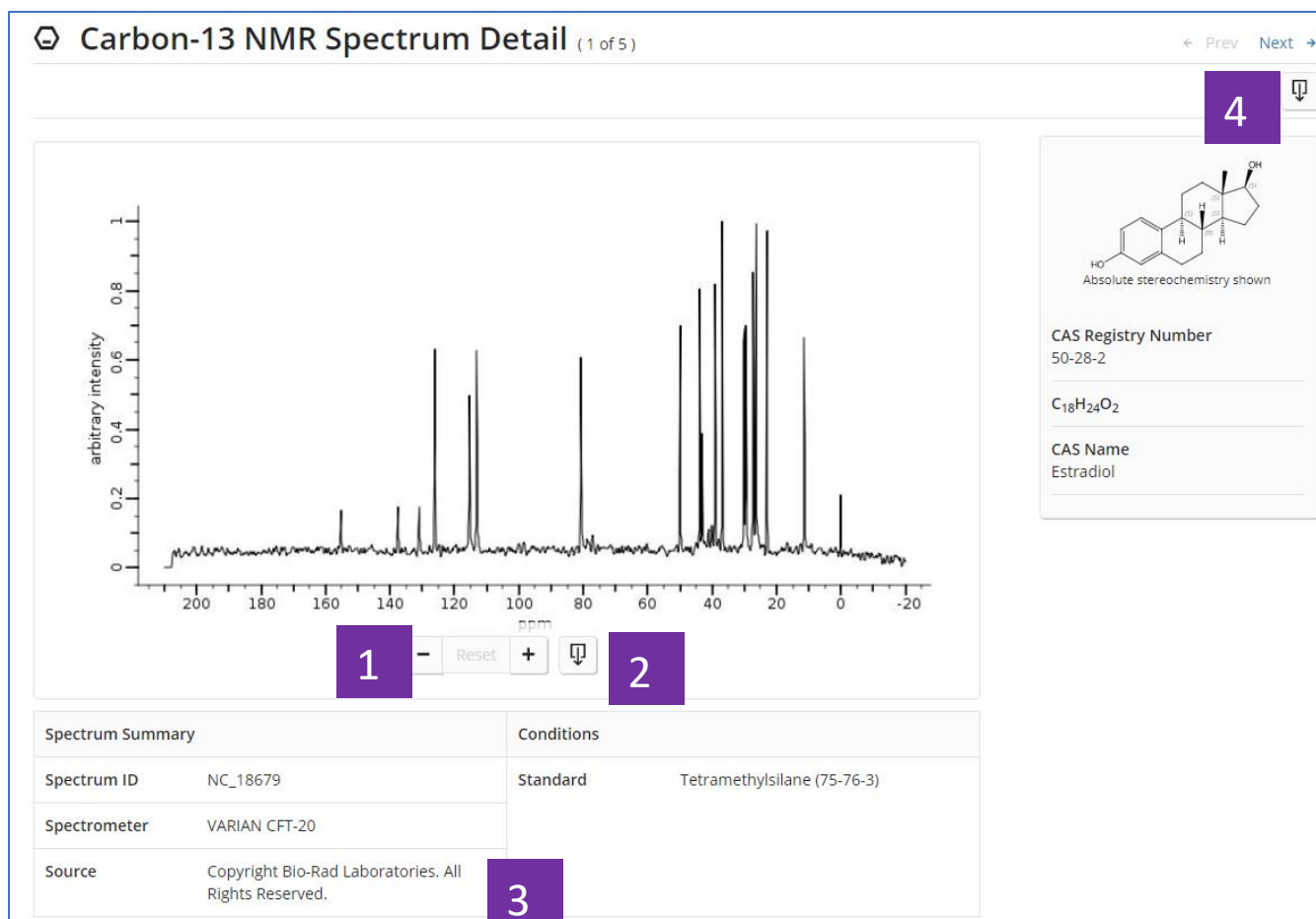
✓ Predicted Properties

✓ Predicted Spectra

1 物质详情中的实验谱图

2 点击超链接，查看核磁谱图

3 谱图信息的文献来源



1 缩放谱图

2 下载谱图图片

3 谱图概览：测试仪器、条件、来源等

4 下载谱图详情

通过生物活性、靶点筛选物质

The screenshot displays the SciFinder search results page. On the left, there are three main filter sections: 'Experimental Spectrum', 'Regulatory Information', and 'Bioactivity Indicator'. The 'Bioactivity Indicator' section is highlighted with a purple box and the number '1'. It includes a checked option for 'Anti-infective agents (131)' and several unchecked options for other categories like 'Pharmaceutical immune agents (6,787)', 'Antitumor agents (5,691)', 'Nervous system agents (4,700)', and 'Anti-inflammatory agents (3,963)'. Below this is the 'Target Indicator' section, highlighted with a purple box and the number '2', which includes a checked option for 'Enzymes (13K)' and several unchecked options for 'Viral proteins (6,217)', 'Ligand-binding proteins (3,517)', 'Blood proteins (3,456)', and 'Metalloproteins (3,338)'. At the bottom of the filters is a 'Search Within Results' section. The main content area shows a grid of chemical compounds. The first compound, Emtricitabine (CAS 143491-57-0), is highlighted with a purple box and the number '3'. Its chemical structure is shown with absolute stereochemistry and rotation (-). Below the structure are buttons for 'References' (4,133), 'Reactions' (220), and 'Suppliers' (103). Other compounds shown include Raltegravir (CAS 518048-05-0), Rilpivirine (CAS 500287-72-9), Atazanavir (CAS 198904-31-3), and Daclatasvir (CAS 1009119-64-5). Each compound entry includes its chemical structure, CAS number, name, and buttons for 'References', 'Reactions', and 'Suppliers'.

1 在物质结果集页面，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

Bioactivity Indicator X

By Count | Alphanumeric

1

- Anti-infective agents (13K)
- Pharmaceutical immune agents (6,787)
- Antitumor agents (5,691)
- Nervous system agents (4,700)
- Anti-inflammatory agents (3,963)
- Cytoprotective agents (3,455)
- Enzyme inhibitors (3,315)
- Cardiovascular agents (3,021)
- Antidiabetic agents (3,004)
- Gastrointestinal agents (2,876)
- Hematologic agents (2,851)
- Respiratory system agents (2,786)
- Renal agents (2,711)
- Peptide analogs (1,657)
- Receptor antagonists (1,620)
- Membrane transport modulators (1,237)
- Receptor agonists (444)
- Cytotoxic agents (386)
- Pharmaceutical natural products (371)
- Hormone antagonists (288)
- Antiproliferative agents (278)
- Lipid-regulating agents (229)
- Pharmaceutical adjuvants (198)
- Neuromuscular agents (142)
- Antiulcer agents (103)
- Antiosteoporotic agents (96)
- Biopharmaceuticals (66)
- Radioprotectants (43)
- Reproductive control agents (38)
- Receptor modulators (33)
- Peroxisome proliferators (25)
- Pharmaceutical photosensitizers (24)
- Hair growth stimulants (13)
- Ion channel openers (7)
- Antianemic agents (6)
- Antigout agents (5)
- Cell differentiation inducers (5)
- Anabolic agents (3)
- Antidotes (3)

2 Apply Cancel

1 在点击View All获得的所有适应症信息后，可根据研究密集程度或适应症字母顺序进行排序

2 选择感兴趣的适应症，然后点击Apply，即可获得针对某适应症的物质

^ Bioactivity Indicators

Anti-infective agents (56)

1

Anti-HIV agents (1498)

Antibacterial agents (76)

Antibiotics (87)

Antiviral agents (1050)

Fungicides (62)

Highly active antiretroviral therapy agents (161)

Integrase inhibitors (150)

Virus entry inhibitors (89)

Anti-inflammatory agents (96)

Antitumor agents (193)

Enzyme inhibitors

HIV protease inhibitors (289)

Integrase inhibitors (150)

Non-nucleoside reverse transcriptase inhibitors (485)

Nucleoside reverse transcriptase inhibitors (552)

Nucleotide reverse transcriptase inhibitors (120)

Reverse transcriptase inhibitors (221)

Pharmaceutical immune agents

Immunomodulators (80)

Immunosuppressants (50)

^ Target Indicators

Apoproteins

Apolipoprotein A-I (10)

2

Apoptosis-regulating proteins

Programmed cell death protein 1 (23)

Programmed death-ligand 1 (13)

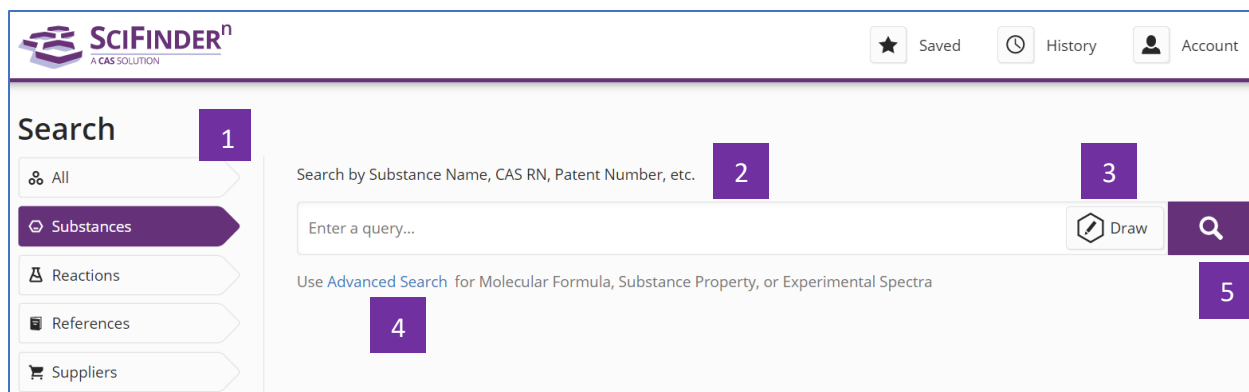
1

点击物质的CAS登记号，即可获得物质详情，在物质详情页面，点击蓝色超链接的适应症，即可获得相应的研究文献

2

在物质详情页面，点击蓝色超链接的靶点，获得相应的研究文献

获取物质信息



- 1 选择**Substances**，进行物质检索
- 2 输入检索文本：物质名称、**CAS**登记号、专利号等
- 3 点击**Draw**，绘制结构
- 4 点击**Advanced Search**，进行分子式、物质属性和实验谱图等检索
- 5 点击搜索图标，开始检索

The screenshot displays the SciFinder search results page for 'Morphine'. The interface includes a search bar at the top with a search icon (5) and a 'Substances' dropdown (4). Below the search bar, there are filters for 'Structure Match' (1) with options like 'As Drawn (8)', 'Substructure (30K)', and 'Similarity (32K)'. A button for 'Analyze Structure Precision' (2) is also present. On the left, a 'Filter by' sidebar (3) allows filtering by 'Commercial Availability', 'Reaction Role', 'Reference Role', 'Stereochemistry', and other criteria. The main results area shows a list of entries (6), each with a chemical structure, name, and a table of 'Key Physical Properties' (7, 10). Callouts 8, 9, and 10 point to specific details within the result cards, such as the chemical structure, the 'References', 'Reactions', and 'Suppliers' buttons, and the property table header.

1 结构匹配程度：As Drawn精确结构，Substructure亚结构，Similarity相似结构

2 点击Analyze Structure Precision，对精确结构和亚结构的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

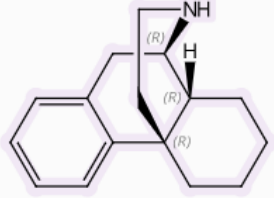
学、组份数、物质类型、同位素、金属、分子量、实验属性、实验谱图、
管控信息、生物活性、靶点、二次筛选

- 4 相关的文献、反应和供应
- 5 重新排序
- 6 选择是否展示物质的物理属性信息
- 7 下载、邮件、保存并设置提醒
- 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
- 10 此物质的物理属性信息

Substance Detail (1 of 30,974) ← Prev Next →

References (397) Reactions (0) Suppliers (3) 2 3 ↓ ✉ ★ Save

CAS Registry Number
468-10-0



Absolute stereochemistry shown

$C_{16}H_{21}N$
Morphinan 4

Key Physical Properties	Value	Condition
Molecular Weight	227.34	-
Melting Point (Experimental)	<25 °C	-
Boiling Point (Experimental)	115 °C	-
Density (Predicted)	1.09±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.11±0.20	Most Basic Temp: 25 °C

[Experimental Properties](#) | [Spectra](#)

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

- ▼ Other Names 5
- ▼ Experimental Properties
- ▼ Experimental Spectra
- ▼ Predicted Properties
- ▼ Predicted Spectra
- ▼ Regulatory Information
- ▼ Additional Details

1 点击左右箭头，查看前一个或后一个物质详情

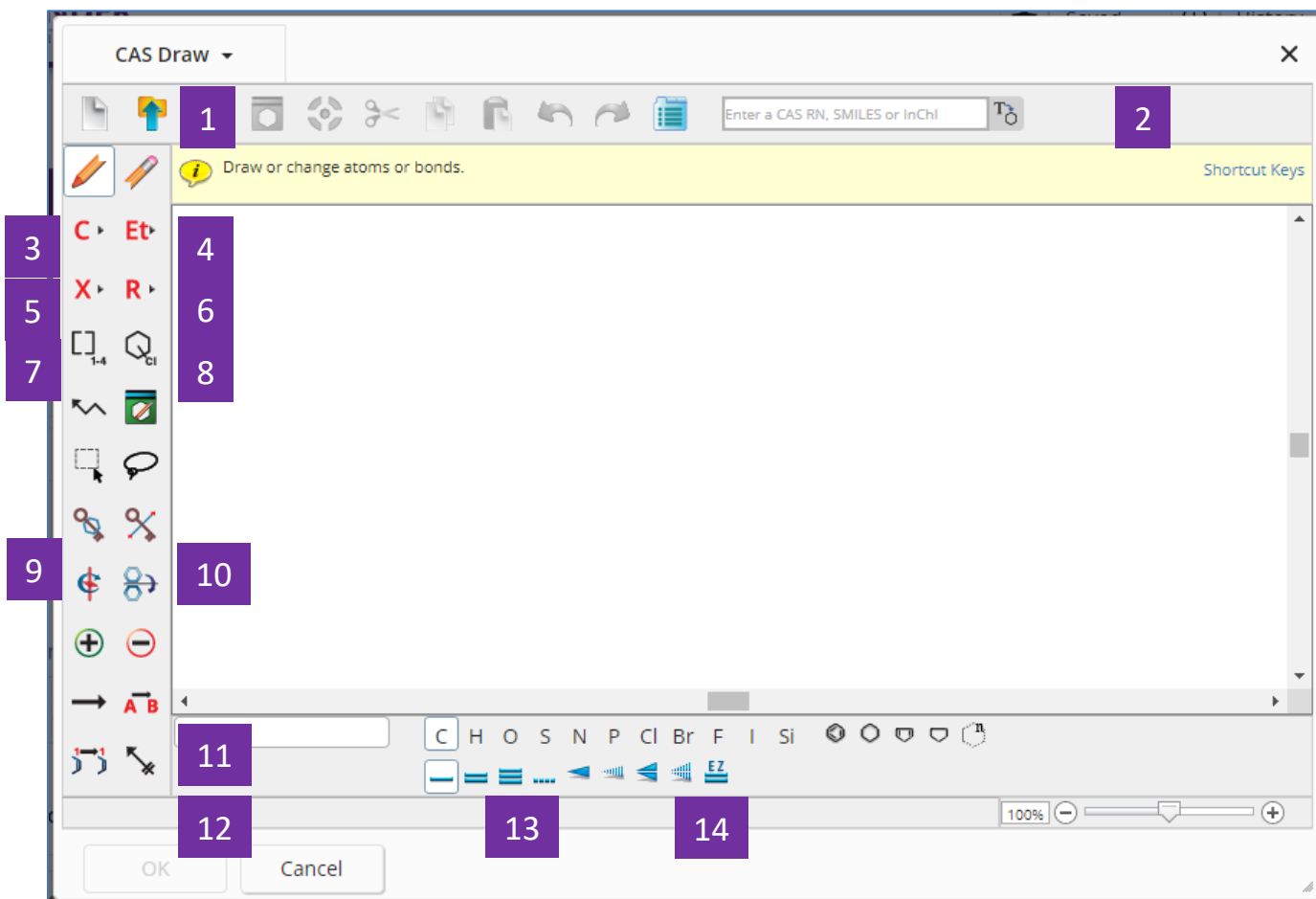
2 此物质相关的文献、反应和供应商


3 下载、分享及保存物质详情

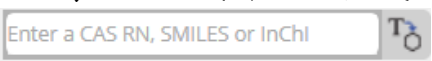
4 物质的物理属性信息


5 物质名称、实验属性、实验谱图、预测属性、预测谱图、管控信息及其他补充细节


结构编辑器

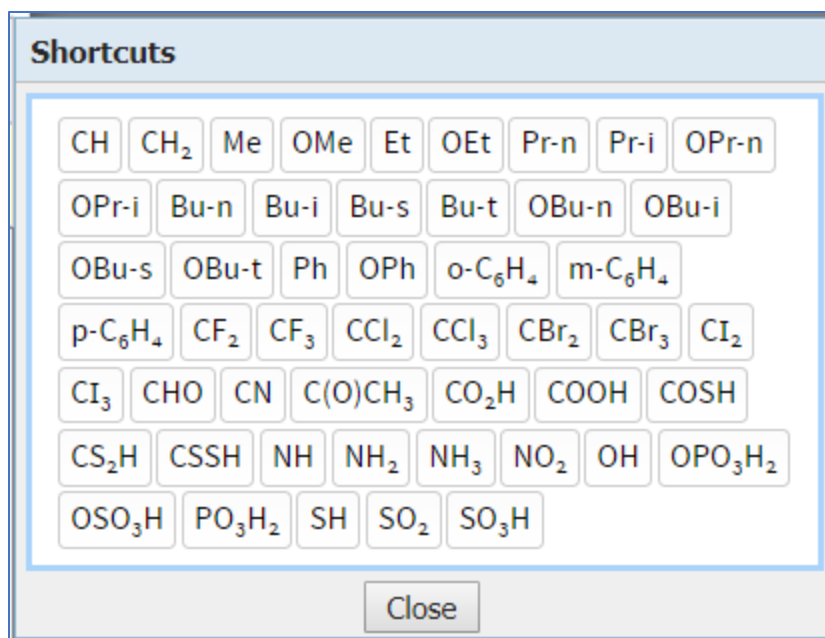


1  导入.cxf或者.mol格式文件。

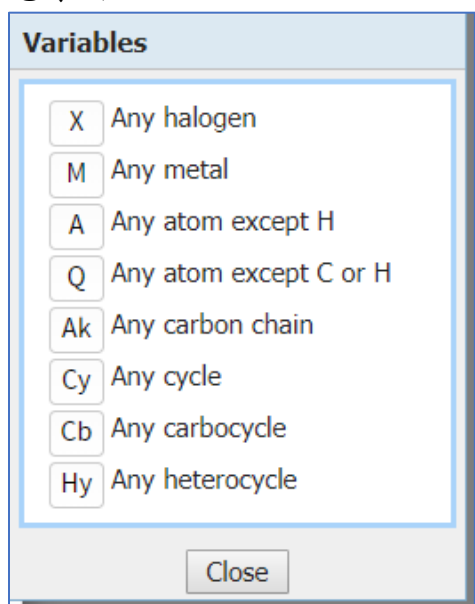
2  , 可以直接输入物质的CAS登记号、SMILES或者InChI
直接转化为结构。

3  为元素周期表。

4  为常用官能团列表。



5 **X** 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。



6 **R** 定义R基团，可以设置R为 **C**，**Et** 或者 **X** 的任意组合。

R-group Definitions

◀ R1 R2 R3 R4 R5 R6 R7 R8 R9 R10 ▶

R1 =

▼ Atoms

H																			He
Li	Be									B	C	N	O	F					Ne
Na	Mg									Al	Si	P	S	Cl					Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br			Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I			Xe
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At			Rn
Fr	Ra	**																	

* Lanthanides

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
----	----	----	----	----	----	----	----	----	----	----	----	----	----	----

** Actinides

Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
----	----	----	---	----	----	----	----	----	----	----	----	----	----	----

▶ Variables

▶ Shortcuts

7



重复原子或者基团。

CAS Draw

Enter a CAS RN, SMILES or InChI

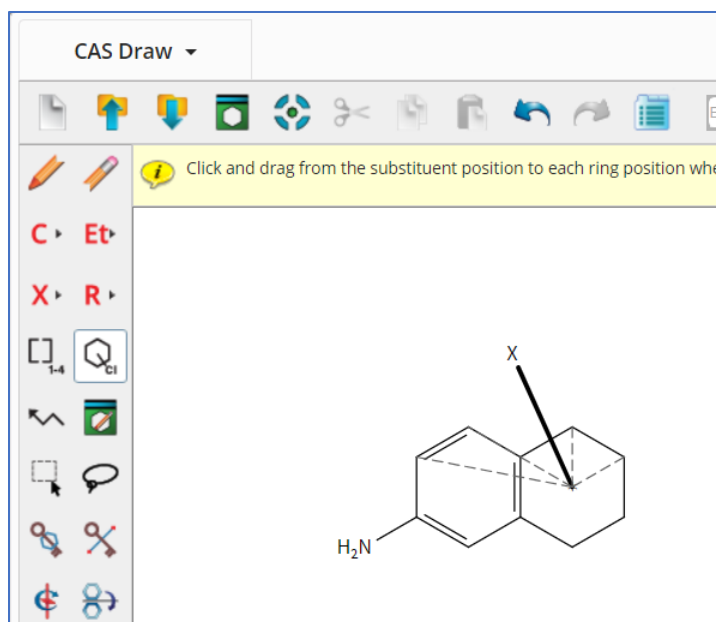
Click to select an atom to be repeated or drag to select a group to be repeated. Enter the number of repetitions. From 1 To 4 Apply


C ▶ Et
X ▶ R

8

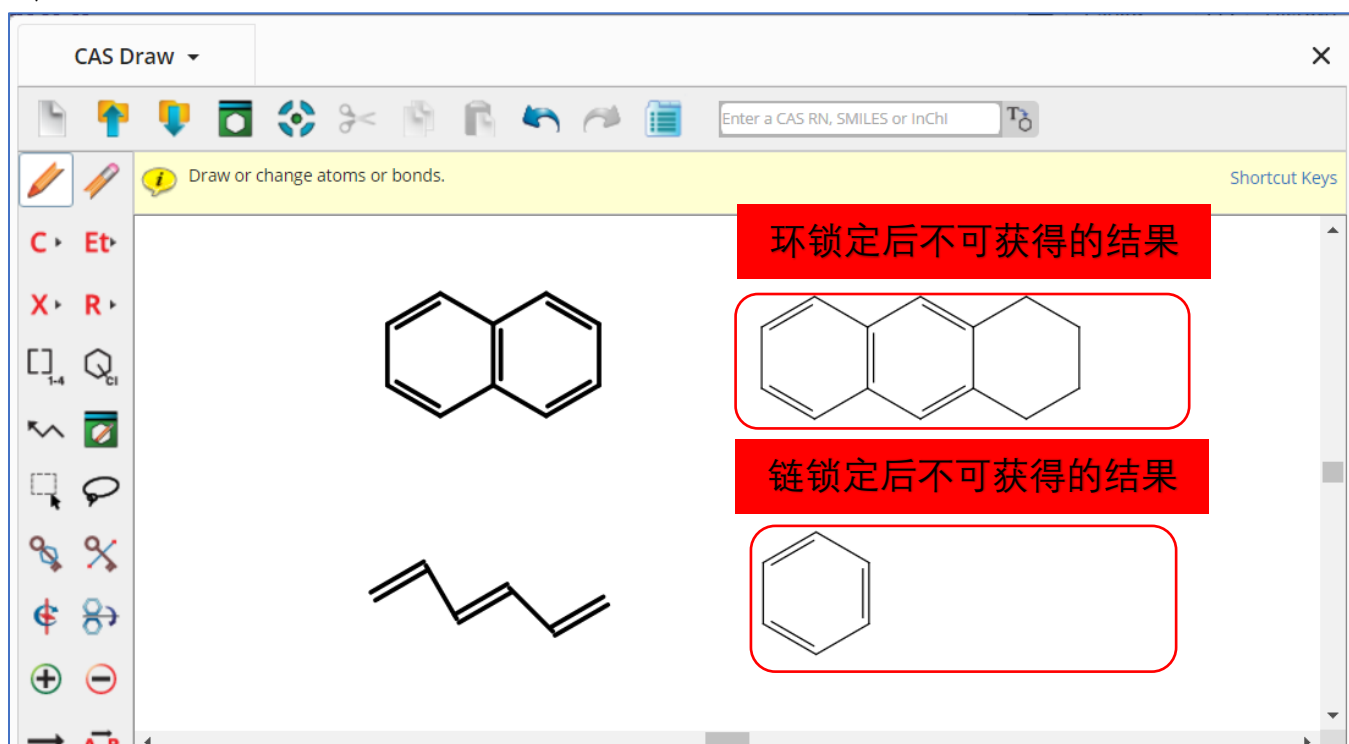



环上的取代位点不固定。



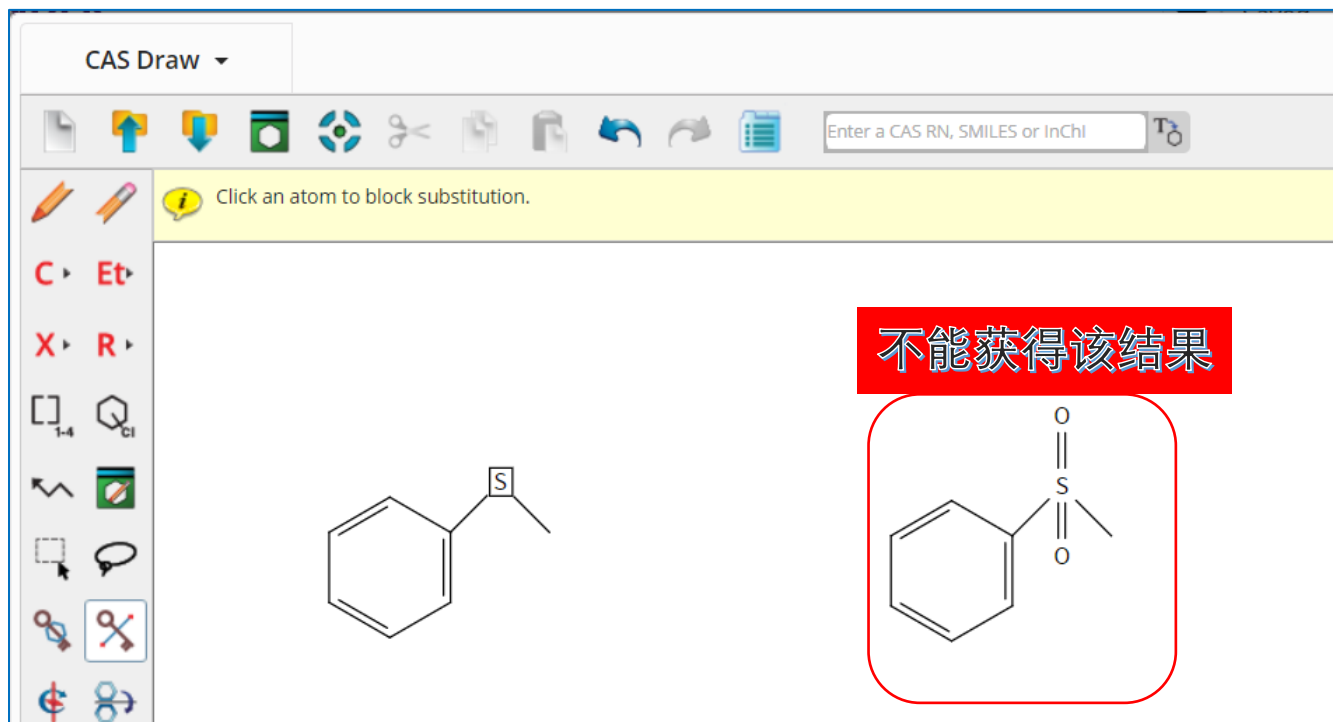
9  环锁定。当用该功能锁定某个环（系），表示该环（系）不能成为更大环系的一部分；如果用该功能锁定某个链，则表示该链不能成为某个环（系）的一部分。



例：

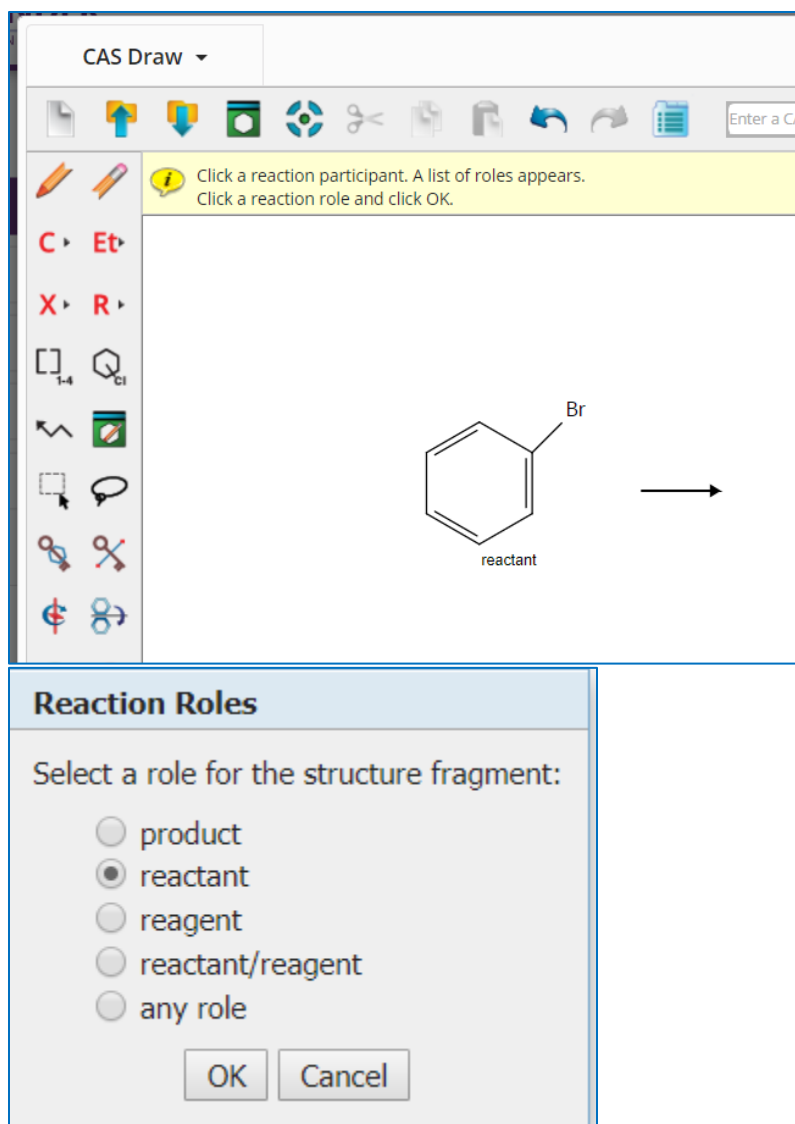




10  锁定原子。若某原子被锁定，则表明该原子只能连接氢原子。

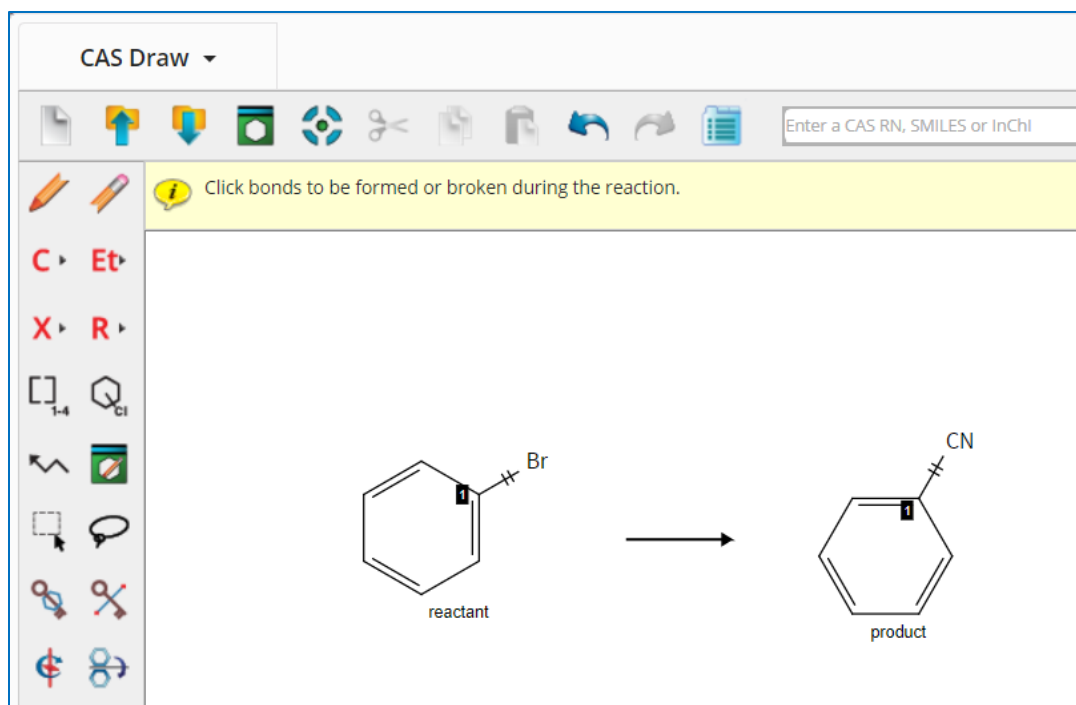
例：



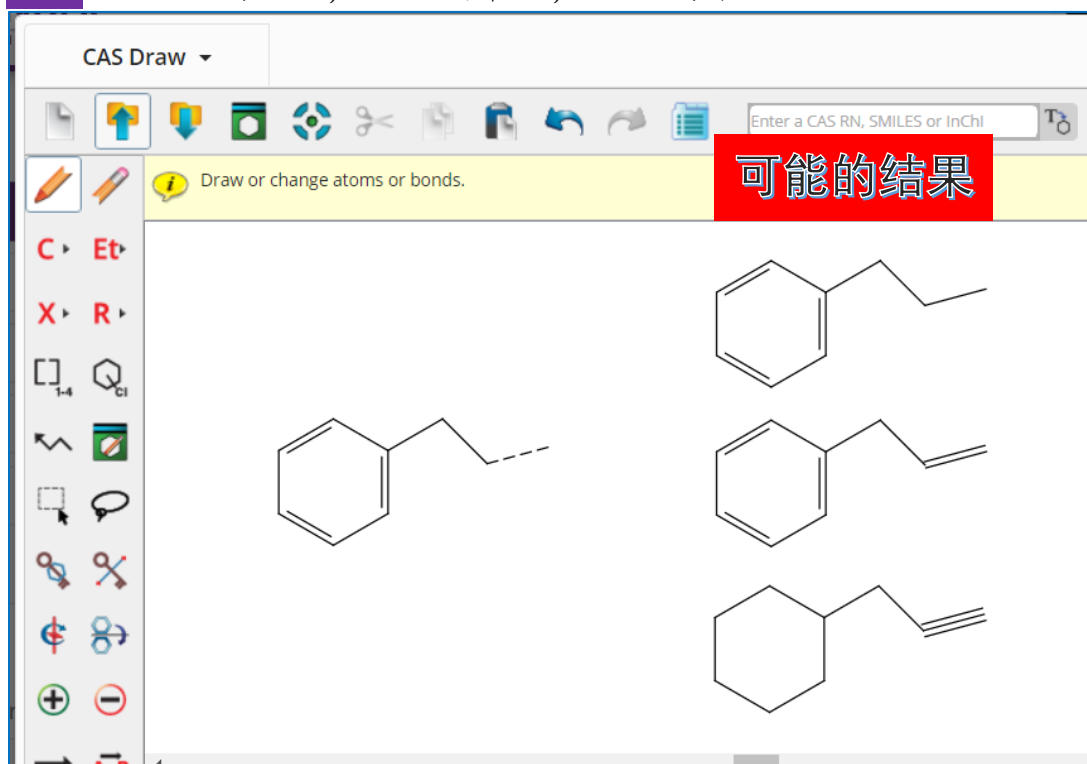
11  反应箭头。箭头左边的物质是起始物或者试剂，右边为产物。 为反应角色定义工具，用于定义物质在反应中的角色。




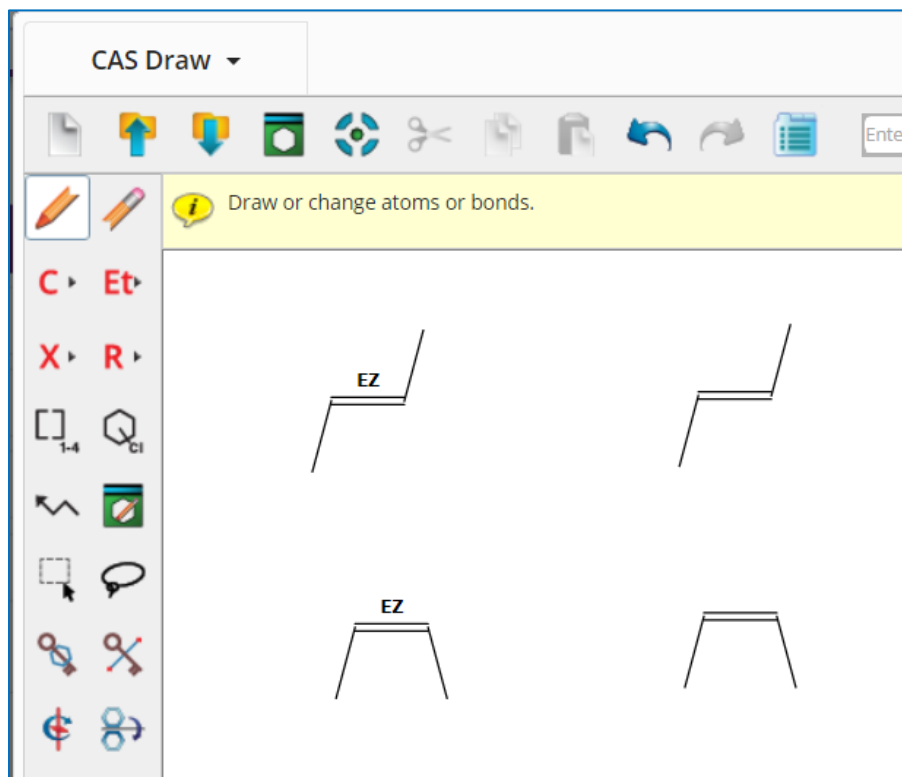
12  为反应原子标记工具。在原料和产物中以相同数字被标记的原子，表明其反应前后为同一原子。 为反应键标记工具，起始物的某键被标记，则表明此键在反应过程中发生断开等变化；产物的某键被标记，则表明此键在反应过程中是新生成的键。



13 为不确定键，可以指单键，双键或者三键。



14  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。



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

Structure Match

As Drawn (250)

Substructure (4.7M)

Similarity (15K)

Analyze Structure Precision

Filter by

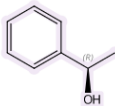
- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
 - Absolute Stereo Match (53) **4**
 - Absolute Stereo Mirror Image (53)
 - Stereo that Doesn't Match Query (29)
 - No Stereo in Answer Structure (112)
- Number of Components
- Substance Class

Substances (56)

Sort: Relevance View Partial

References Reactions Suppliers

1517-69-7
View Detail

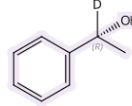


Absolute stereochemistry shown, Rotation (+)

$C_8H_{10}O$
(+)-1-Phenylethanol

3,701 References 9,271 Reactions 92 Suppliers

71886-65-2
View Detail

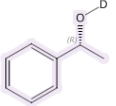


Absolute stereochemistry shown

C_8H_9DO
(αR)-α-Methylbenzenemethanol-d

14 References 19 Reactions 1 Supplier

1246182-86-4
View Detail

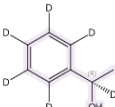


Absolute stereochemistry shown

C_8H_9DO
(αR)-α-Methylbenzenemethanol-d

6 References 13 Reactions 0 Suppliers

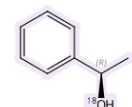
159146-97-1
View Detail



Absolute stereochemistry shown

$C_8H_4D_6O$
Benzene-*d*₅-methanol-*d*-ol, α-methyl-, (R)-

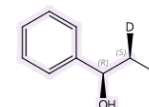
155797-94-7
View Detail



Absolute stereochemistry shown

$C_8H_{10}O$
Benzenemethanol-¹⁸O, α-methyl-, (R)-

101860-64-4
View Detail



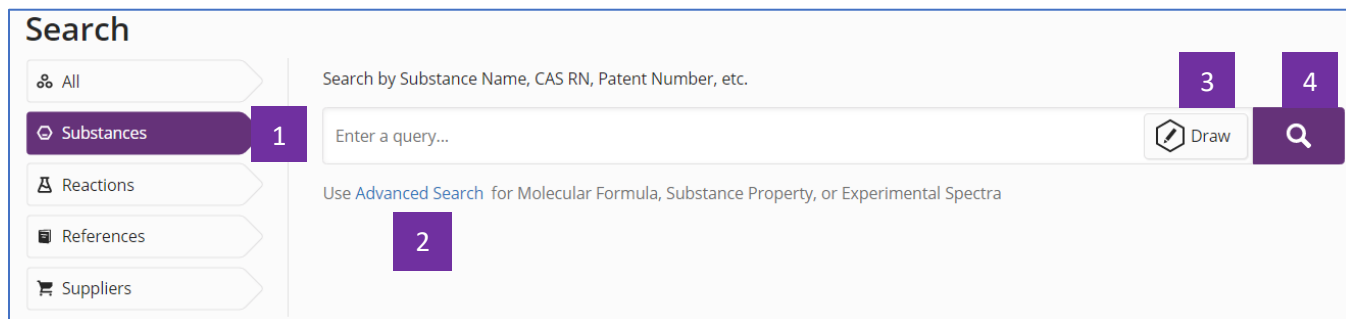
Absolute stereochemistry shown

C_8H_8DOT
Benzenemethanol, α-(methyl-*d*-1)-, [R-(R*,S*)]-

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

同位素化合物的检索



- 1 选择Substances，进行物质检索
- 2 点击Advanced Search，根据分子式、属性或实验谱图来检索物质
- 3 点击Draw，进行结构检索
- 4 点击放大镜，开始物质检索

Substances

References

Advanced Substance Search

Molecular Formula 1

Enter one Molecular Formula.

C6D6

Ex: C6H6
(C8H8)_x
C22H26CuN2O5.C2H3N

Add Another Molecular Formula

— AND —

Substance Property

Select Property Enter Value

- Select One -

Add Another Property

— AND —

Experimental Spectra

Select Spectrum Enter Value

- Select One -

Add Another Spectra

2

Clear All

1 可以通过分子式输入H的同位素（D或T），进行同位素化合物检索

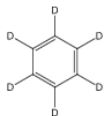
2 点击放大镜，开始检索

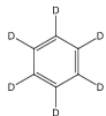
Filter by

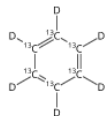
- Commercial Availability
 - Available (4)
 - Not Available (15)
- Reaction Role
- Reference Role
- Number of Components
- Substance Class **1**
- Isotopes
 - Containing Isotopes (19)
- Metals
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Search Within Results

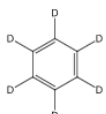
Substances (19) Sort: Relevance View Partial


References Reactions Suppliers

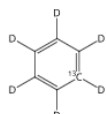
1076-43-3 View Detail

 C_6D_6
 Benzene- d_6
 2,823 References 27K Reactions 134 Suppliers

38091-14-4 View Detail

 C_6D_6
 Benzene- d_6 , radical ion(1+)
 45 References 0 Reactions 0 Suppliers

32602-97-4 View Detail

 C_6D_6
 Benzene-1,2,3,4,5,6- $^{13}C_6$ -1,2,3,4,5,6- d_6 **2**
 9 References 0 Reactions 4 Suppliers

34525-57-0 View Detail

 C_6D_6
 Benzene- d_6 , radical ion(1-)
 8 References 0 Reactions 0 Suppliers

73113-25-4 View Detail

 C_6D_6
 2,4-Hexadiyne-1,1,1,6,6,6- d_6 , radical ion(1+)
 7 References 0 Reactions 0 Suppliers

55153-53-2 View Detail

 C_6D_6
 Benzene- ^{13}C - d_6
 6 References 0 Reactions 1 Supplier

1 获得符合输入分子式的同位素标记物质

2 浏览并选择需要获取的物质结果

Substances (725)

Structure Match

- As Drawn (11K)
- Substructure (109.1M)
- Similarity (7,034)

Analyze Structure Precision

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
 - Containing Isotopes (725)
 - Not Containing Isotopes (10...)
- Metals
- Experimental Property
- Experimental Spectrum

1076-43-3
Benzene-*d*₆
C₆D₆
2,823 References, 27K Reactions, 134 Suppliers

1120-89-4
Benzene-*d*
C₆H₅D
377 References, 144 Reactions, 14 Suppliers

34-47-5
Benzene-1,3,5-*d*₃
C₆H₃D₃
176 References, 11 Reactions, 12 Suppliers

13657-09-5
Benzene-1,2,3,4,5-*d*₅
C₆HD₅
130 References, 29 Reactions, 12 Suppliers

1684-46-4
Benzene-1,4-*d*₂
C₆H₄D₂
117 References, 11 Reactions, 6 Suppliers

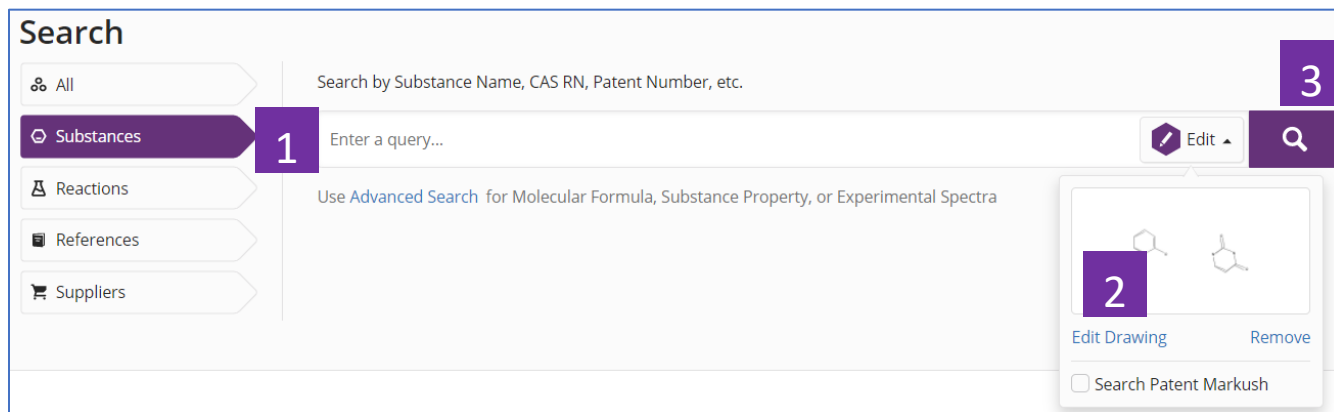
32488-44-1
Benzene-1,2,3,4,5,6-¹³C₆
C₆H₆
98 References, 47 Reactions, 20 Suppliers

1 根据结构式来检索物质

2 在物质结果中，通过左侧Isotopes选择containing isotopes，获取含有同位素标记的物质结果

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SciFinder[®]中用片段结构检索来实现。



The screenshot shows the SciFinder search interface. On the left, there is a navigation menu with options: All, Substances (selected), Reactions, References, and Suppliers. The main search area has a search bar with the text "Enter a query..." and a search button. Above the search bar, there is a prompt: "Search by Substance Name, CAS RN, Patent Number, etc." and a "3" in a purple box. Below the search bar, there is a prompt: "Use Advanced Search for Molecular Formula, Substance Property, or Experimental Spectra". On the right side of the search bar, there is an "Edit" button and a search button. Below the search bar, there is a drawing tool with two chemical structures and a "2" in a purple box. The drawing tool has buttons for "Edit Drawing" and "Remove". At the bottom of the drawing tool, there is a checkbox for "Search Patent Markush".

1 选择Substances检索

2 绘制片段结构

3 点击检索

The screenshot displays the SciFinder search results page. On the left, the 'Number of Components' filter is set to 1, and the 'Substance Class' filter is set to 'Organic/Inorganic Small Molecule'. The main results area shows a grid of chemical structures. The first result is '99361-68-9', a 5-pyrimidinesulfonic acid derivative. The second is '211449-01-3', a mercury complex. The third is '211449-03-5', another mercury complex. The fourth is '515824-66-5', a pyrimidinedione derivative. The fifth is '29050-86-0', a diazenyl-substituted pyrimidinedione. A purple box with the number '3' is overlaid on the top right of the results grid, indicating the third step in the tutorial.

1 通过Number of Components，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）

2 可继续通过Substance Class，筛选物质类型

3 查看物质详情

获取化学品供应商信息

在SciFindern中可通过以下三种方式获取化学品供应商的信息：

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

方法一

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

The screenshot shows the SciFinder search interface. On the left, there is a navigation menu with options: All, Substances, Reactions, References, and Suppliers. The Suppliers option is highlighted with a purple arrow and a '1' in a purple box. The main search area has a search bar with the text 'sudan red' and a '2' in a purple box. Below the search bar is a dropdown menu listing search results: Sudan Red, Sudan Red III, Sudan Red 380, Sudan Red 4BA, Sudan Red BB, Sudan Red BBA (highlighted), Sudan Red IV, Sudan Red I, Sudan Red II, and Sudan Red 290. The top right of the interface includes 'Saved', 'History', and 'Account' buttons. The bottom left shows 'Recent Search History' with the date 'October 30, 2019'.

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

化学品供应商信息结果集

SciFINDERⁿ A CAS SOLUTION

Suppliers Sudan Red BBA

Draw

Return to Home

Filter by 1

Preferred Suppliers

No Preference (69)

Supplier

Synovator Product List (3)

Carbosynth Product List (2)

FUJIFILM Wako Chemicals Europe GmbH Product List (2)

FUJIFILM Wako Chemicals U.S.A. Corporation Product List (2)

FUJIFILM Wako Pure Chemical Corporation Product List (2)

View All

Purity

≥99% (1)

95-98% (32)

90-94% (5)

<90% (1)

Quantity

Milligrams (17)

Grams (48)

Kilograms or greater (10)

Bulk (35)

Screening (9)

Ships Within

1 week (24)

2 weeks (12)

4 weeks (6)

8 weeks (1)

Suppliers (69)

Sort: Supplier: A to Z

Supplier: A to Z

Supplier: Z to A

Ships Within Purity

Supplier	Substance	Purity	Purchasing D	
1Click CHEMISTRY 1Click Chemistry Stock Products United States	2	95-98%	Order From Supplier 25.00 G, USD 250.00 G, USD 97.40 1.00 KG, USD 230.80 2.50 KG, USD 461.60 View all Bulk	Maintained in stock Ships within 1 week
aablocks AA BLOCKS LLC Product List United States	85-83-6 2-Naphthalenol, 1-[[2-methyl-4-[[2-methylphenyl]azo]phenyl]azo]-	95-98%	Order From Supplier 25g, USD 39 100g, USD 75	Maintained in stock Ships within 1 week
abcr abcr GmbH Product List Germany	85-83-6 Sudan IV		Product Information 100.0 g, EUR 79.20 EUR EUR 284.10	
Accel Pharmtech Accel Pharmtech Product List United States	85-83-6 1-((2-Methyl-4-(o-tolyl(diazenyl)phenyl)diazenyl)naphthalen-2-ol	95-98%	1g 10g 100g 1kg	
AK Scientific AK Scientific Product Catalog United States	85-83-6 Solvent Red 24	95-98%	Order From Supplier 25g, USD 21 100g, USD 54	Maintained in stock Ships within
			Bulk Screening	1 week
aldlab Aldlab Chemicals In Stock Product List United States	85-83-6 Sudan IV; Solvent red 24	95-98%	1g 5g Bulk	Typically in stock Ships within 2 weeks
Merck KGaA Darmstadt, Germany ALDRICH United States	85-83-6 Sudan IV		Order From Supplier 25 g 100 g Bulk	Maintained in stock
Alfa Aesar Alfa Aesar United States	85-83-6 Sudan IV		Order From Supplier 25g, USD 25.10 100g, USD 63.20 Bulk Screening	Typically in stock Ships within 1 week

Stock Status

Maintained in stock (34)

Typically in stock (17)

Intermittently available (3)

Synthesis on demand (3)

Order From Supplier

Link Available (30)

Country

United States (48)



Germany (12)

Japan (12)

China (10)

United Kingdom (10)

View All

- 1 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。
- 2 可以选择  或  来设置优选或者非优选供应商。
- 3 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。
- 4 点击order from suppliers，直接访问产品订购页面。
- 5 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

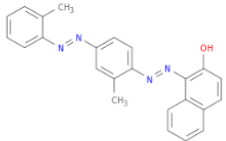
sales@aablocks.com +1 858-523-8231 Login Register

aablocks Search

Home About Us Products Support Contact Us

Home / Other Building Blocks / 85-83-6


Catalog No.:AA00IDF7 **85-83-6 | 2-Naphthalenol, 1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]azo]-**



Pack Size	Purity	Availability	Price(USD)	Quantity		
25g	≥88% (dye content)	1 week	\$52.00	- 1 +	Add To Cart	Order Now
100g	≥88% (dye content)	1 week	\$66.00	- 1 +	Add To Cart	Order Now
250g	≥88% (dye content)	1 week	\$93.00	- 1 +	Add To Cart	Order Now

Technical Information	Technical Information
Properties	Catalog Number: AA00IDF7
Literature	Chemical Name: 2-Naphthalenol, 1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]azo]-
	CAS Number: 85-83-6
Request for Quotation	Molecular Formula: C24H20N4O

点击 Product Information 所获界面



SEARCH

Home
About Us
Products v
Services v
Resources v
Order Center
Contact Us


NAVIGATION

- > Products
- > Services
- > Hot Products HOT
- > Order

CONTACT US


Email: info@alfa-chemistry.com
Tel: 1-201-478-8534
 1-516-662-5404
Fax: 1-516-927-0118
Address: 2200 Smithtown
 Avenue, Room 1 Ronkonkoma,
 NY 11779-7329 USA

For product inquiries, please use
 our online system or send an
 email to
inquiry@alfa-chemistry.com



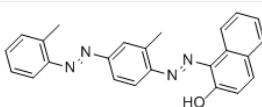
CHEMISTRY
PARTNER

Aims to be your chemistry
partner in custom
synthesis



Home > Product > Dyes > Solvent Dyes > Solvent Red 24
< >

Solvent Red 24
PRICE INQUIRY

Catalog Number	ACM85836
Product Name	Solvent Red 24
Structure	
CAS Number	85-83-6
IUPAC Name	(1Z)-1-[[[2-methyl-4-(2-methylphenyl)diazenylphenyl]hydrazinylidene]naphthalen-2-one
Synonyms	Scharlachrot, Lipid crimson, Scarlet oil, Scarlet red, Oil Scarlet, Hidaco Oil Red, Resoform Red G, Waxoline Red O, Fat Ponceau R, Lacquer Red V, Organol Red B, Rubrum scarlatinum, Waxoline Red OM, Waxoline Red OS, Candle Scarlet B, Candle Scarlet G, Tetrogras Red N, Lacquer Red VS, Somalia Red IV, Sudan P
Molecular Formula	C ₂₄ H ₂₀ N ₄ O
Molecular Weight	380.45
Exact Mass	380.16400
Boiling Point	260°C
Melting Point	199°C
Flash Point	424.365°C
Density	1.192 g/cm ³
Purity	PURIFIED
Appearance	dark red to brown crystals or powder
InChIKey	KMDLOETUWUPGMB-BXCCFQQFSA-N

H-Bond Donor	1
H-Bond Acceptor	5
Safety Description	S24/25
Hazard Statements	Xi: Irritant; T: Toxic;
WGK Germany	3
Stability	Stable. Incompatible with strong oxidizing agents.
MSDS	Download MSDS
COA	Download COA
Spec Sheet	Download Spec Sheet

← Return to Home

Suppliers (69) Sort: Supplier: A to Z

1

2

Download Results
Excel (.xlsx) (max 100)
PDF

Supplier	Substance	Pur	Price	Availability
<input type="checkbox"/> 1CLICK CHEMISTRY 1Click Chemistry Stock Products United States	<input type="checkbox"/> 85-83-6 1-((2-Methylphenyl)diazenyl)-phenyl)diazenyl)-2-naphthol	95-9	25.00 G, USD 54.30 100.00 G, USD 65.70 250.00 G, USD 97.40 1.00 KG, USD 230.80 2.50 KG, USD 461.60 View all Bulk	Ships within 1 week

1 供应商结果集可以导出为Excel或者PDF格式文件。

2 点击CAS登记号，查看物质信息详情。

点击 CAS 登记号所获界面

CAS RN
85-83-6
[View Detail](#)

CAS Name
Solvent Red 24

Substance Detail

Reactions (22)

Synthesize (2)

Create Retrosynthesis Plan

References (1,301)

Suppliers (69)

Edit Structure - Reset +

方法二

在物质结果集页面，点击相应的suppliers获得供应商信息。

The screenshot shows the SciFinder interface for a search of substances. The left sidebar includes filters for 'Structure Match' (As Drawn, Substructure, Similarity) and 'Filter by' (Commercial Availability, Reaction Role, Reference Role, Stereochemistry, etc.). The main area displays a grid of substance cards. Two cards are highlighted with red boxes and numbered 1 and 2. Card 1 is for 'L-Alanine, 1-methylethyl ester' (C₆H₁₃NO₂) and card 2 is for 'D-Alanine, 1-methylethyl ester' (C₆H₁₃NO₂). Both cards show a 'Suppliers' button with a shopping cart icon.

1 在物质结果集中，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

在反应结果集中页面点击相应的Suppliers获取供应商信息。

Filter by

- Substance Role
- Yield
- Number of Steps
- Experimental Protocols
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst
- Solvent
- Commercial Availability **1**
 - Products (1,693)
 - All Starting Materials (3,042)
- Reaction Notes
- Search Within Results

Source Reference

- Publication Year
- Document Type
- Language

Reactions (4,604) View Expanded

References

Scheme 1 (1 Reaction) View

Steps: 1
Yield: 100%

Suppliers (2) **2** Suppliers (110)

Reaction Summary

Reagents	-	Steps: 1
Catalysts	-	Yield: 100%
Solvents	-	
Conditions	-	

View Reaction Detail

View 1 Reaction

Collapse Scheme

Scheme 2 (1 Reaction) View

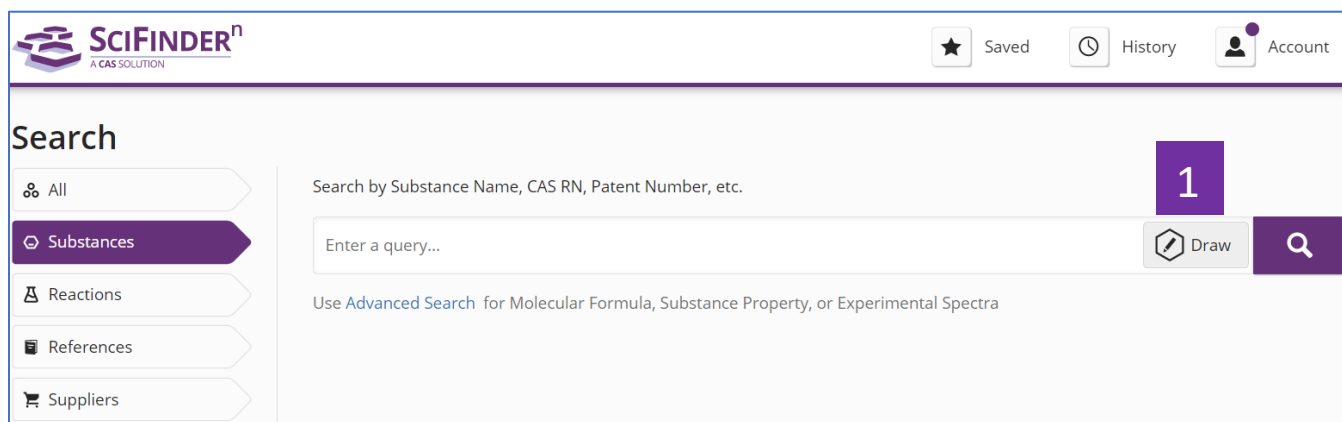
7,7a-Dihydroimidazo[1,2-d]-1,2,4-oxadiazoles from imidazoles and benzonitrile oxide
View Reference Detail
By: Foti, Francesco; et al
Journal of Chemical Research, Synopses (1983), (9), 230-1
Full Text

1 在反应结果集中，筛选起始物或者产物有供应商信息的反应

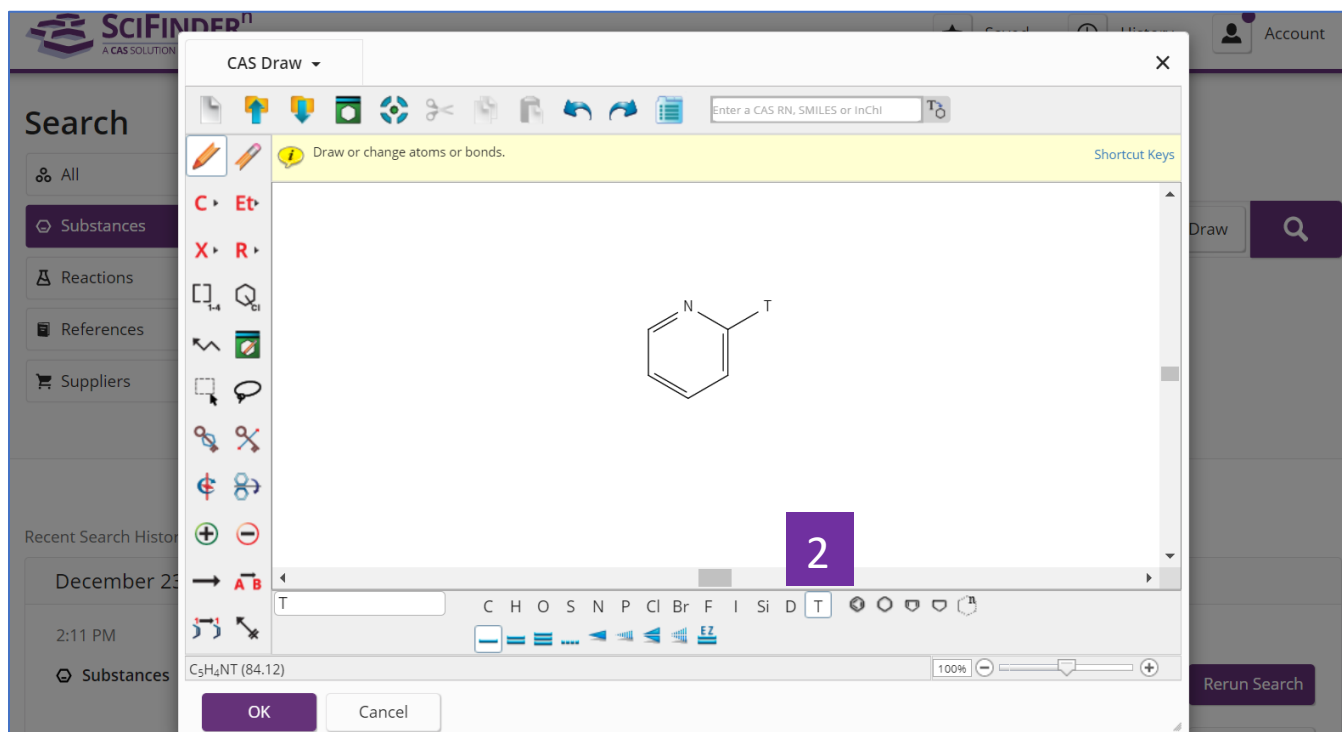
2 点击Suppliers按钮，查看供应商信息

直接在结构中绘制氢的同位素 D 和 T 原子

在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 点击结构编辑器下方的原子D或T，直接用于结构绘制

Search

All

Substances

Reactions

References

Suppliers

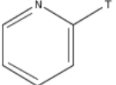
Search by Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use [Advanced Search](#) for Molecular Formula, Substance Property, or Experimental Spectra

3

Edit



Edit Drawing Remove

Search Patent Markush

3 开始检索

SciFINDERⁿ
A CAS SOLUTION

Substances ▾ Enter a query...

Edit ▾ 🔍 ★ 🕒 👤

← Return to Home

Structure Match

As Drawn (1)

Substructure (101)

Similarity (8,190)

Analyze Structure Precision

Filter by

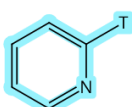
- Commercial Availability
- Reaction Role
- Reference Role
- Number of Components
- Substance Class
- Isotopes
- Containing Isotopes (1)

Substances (1) View Partial ▾

References ▾ Reactions ▾ Suppliers ▾

1

133181-95-0 View Detail



4

C₅H₄NT
Pyridine-2-t

2 References 1 Reaction 0 Suppliers

4 获得同位素标记的物质

先导化合物发现攻略 I

先导化合物发现通常包括：同系物结构修饰；高通量筛选；基于蛋白结构的药物从头设计；基于构效关系的药物发现；药物重利用等等¹。

SciFinderⁿ通过以上方法为先导化合物的发现与发展提供极大便利，接下来几章我们会介绍一些关于如上方法的具体操作技巧。

I. 同系物结构修饰

下面通过2个案例介绍在SciFinderⁿ中怎样找到相应物质的结构同系物：

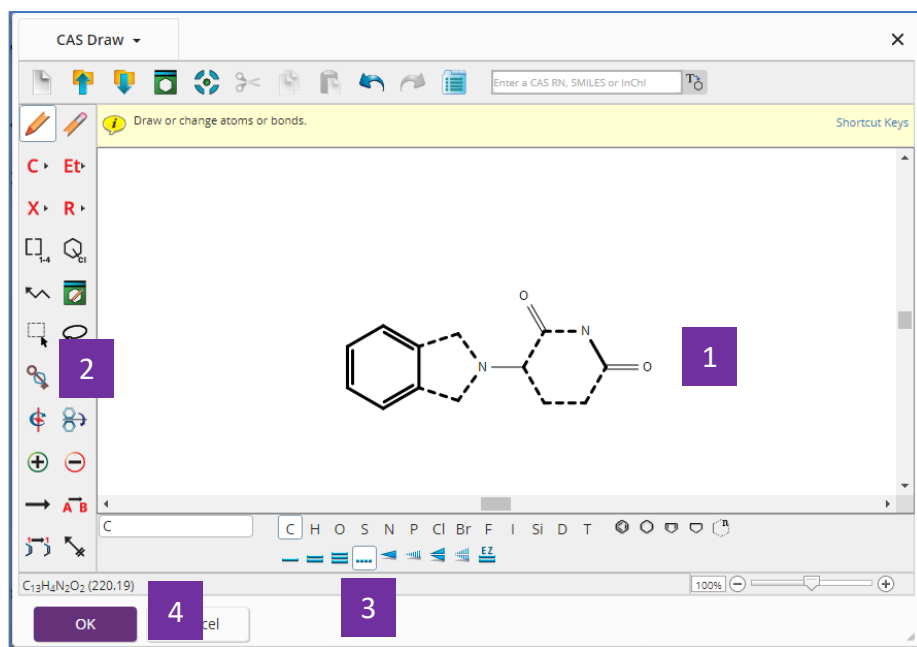
案例一

以沙利度胺（thalidomide）为例。沙利度胺早期被用于镇静、催眠和治疗妇女孕期反应，随后被发现对孕妇的严重致畸作用而撤市，近年来人们又发现其具有抗炎、免疫调节，抗肿瘤等生理活性。那么在SciFinderⁿ中怎样找到沙利度胺的结构同系物呢？

获取沙利度胺结构同系物的检索策略：

首先在SciFinderⁿ的结构编辑中绘制沙利度胺的母核结构，然后在物质结果集中，通过适应症筛选沙利度胺的结构同系物（如同样也具有抗炎和免疫调节效果的来那度胺，以及其他具有药用潜力的候选分子等）。（本示例中的检索结果数量获得日期为：2020-1-15）

¹ Fischer, János et al. (2018) Successful drug discovery. Volume 3. Weinheim, Germany: Wiley-VCH.



- 1 绘制母核结构，可以考虑略去非必要官能团
- 2 (可以) 使用环锁定功能键去除结果中的并环结构
- 3 (可以) 使用不确定键 (虚线) 获得饱和或不饱和的环系
- 4 检索

Structure Match

As Drawn (2)

Substructure (18K)

Similarity (373)

Analyze Structure Precision

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator **1**
 - Antitumor agents (13K)
 - Enzyme inhibitors (4,361)
 - Anti-inflammatory agents (3,990)
 - Pharmaceutical immune agents (3,147)
 - Anti-infective agents (2,661)

Substances (5,798) Sort: Number of References View Partial

References Reactions Suppliers

1 **50-35-1** View Detail
C13H10N2O4
 Thalidomide
 16K References 187 Reactions 108 Suppliers

2 **191732-72-6** View Detail
C13H13N3O3
 Lenalidomide
 7,081 References 1,040 Reactions 113 Suppliers

3 **19171-19-8** View Detail
C13H11N3O4
 Pomalidomide
 1,546 References 366 Reactions 103 Suppliers

4 **1323403-33-3** View Detail
C25H27N3O5
 (S)-3-(4-((4-(Morpholinomethyl)benzyl)oxy)-1-oxoisindolin-2-yl)piperidine-2,6-d...
 Absolute stereochemistry shown
 35 References 63 Reactions 36 Suppliers

5 **202271-89-4** View Detail
C13H11N3O4
 4-Amino-2-[(3S)-2,6-dioxo-3-piperidinyl]-1H-isindole-1,3(2H)-dione
 Absolute stereochemistry shown, Rotation (-)
 28 References 56 Reactions 10 Suppliers

6 **220460-55-9** View Detail
C13H9FN2O4
 1,3-Dioxo-2-(2,6-dioxo-3-fluoropiperidin-3-yl)isindoline
 25 References 43 Reactions 5 Suppliers

7 **1323402-36-3** View Detail

8 **202271-90-7** View Detail

9 **874946-00-6** View Detail

1 根据适应症进一步筛选结果

2 浏览结果集，可以发现沙利度胺的结构同系物，同样具备抗炎或免疫调节活性的成药：lenalidomide, pomalidomide等

案例二

以喜树碱(camptothecin)为例。喜树碱及其衍生物是一类广谱抗癌药物。

获取喜树碱及其衍生物的检索策略：

在SciFinder[®]中使用“text+structure”的联合检索，可以快速获得具有抗癌活性的

喜树碱同系物结构，还可以进一步获取其衍生物制备反应等信息。（本示例中的检索结果数量获得日期为：2020-1-15）

The screenshot displays the SciFinder search interface. On the left, a vertical menu contains options: All, Substances, Reactions, References (highlighted with a purple arrow and a '1' in a purple box), and Suppliers. The main search area has a header 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.' and a search bar containing the text 'anticancer' (with a '2' in a purple box). Below the search bar, there is a prompt 'Use Advanced Search for Author, Journal, or Organization'. To the right of the search bar, there is an 'Edit' button and a search icon (with a '4' in a purple box). Below the search bar, a chemical structure drawing of a complex polycyclic molecule is shown (with a '3' in a purple box). Below the drawing are two buttons: 'Edit Drawing' and 'Remove'.

- 1 选择Reference
- 2 输入关键文本词
- 3 绘制喜树碱母核结构
- 4 检索

通过“text+structure”检索获得的文献结果，文献的题目/摘要/Concept中会包含输入的文本，文献中的物质会包含所绘制的结构。

Structure Match

As Drawn (2) **1**

Substructure (23K) **2**

Filter by **3**

- Document Type
- Substance Role
- Language
- Publication Year
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
- CAS Solutions
- Formulation Purpose
- Database
- Search Within Results

References (23,506) Sort: Relevance View: Full Abstract

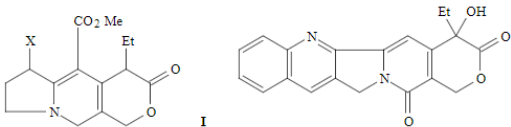
Substances **4** Reactions Cited By

1

Concise total syntheses of *dl*-camptothecin and related anticancer drugs

By: Shen, Wang; Coburn, Craig A.; Bornmann, William G.; Danishefsky, Samuel J.
Journal of Organic Chemistry (1993), 58(3), 611-17 | Language: English, Database: CPlus
[View Reference Detail](#)

Abstract: The readily available tricyclic ester I (X = H₂) was converted to *dl*-camptothecin (II) in 39% yield. With the C₅ carbomethoxy group in place, the C₆ benzylic position of I (X = H₂) (pyridone numbering) is selectively deprotonated by sodium hexamethyldisilazide. This allows for condensation with benzaldehyde, followed by ozonolysis and methylation to give the tricyclic keto ester I (X = O). The latter is smoothly converted to camptothecin, 10-hydroxycamptothecin, and 7-ethyl-10-hydroxycamptothecin via (i) Friedlaender condensation with appropriate aminobenzaldehydes, (ii) HBR-induced decarbomethoxylation, and (iii) hydroxylation at C₂₀. In the case of the two analog syntheses, the HBR step also accomplishes concurrent demethylation of the C₁₀ methoxyl group.



I II

Full Text Substances (32) Reactions (59) Cited By (101) Citation Map

2

Structure-activity study of the actions of camptothecin derivatives on mammalian topoisomerase I: evidence for a specific receptor site and a relation to antitumor activity

By: Jaxel, Christine; Kohn, Kurt W.; Wani, Mansukh C.; Wall, Monroe E.; Pommier, Yves

1 包含所绘制结构的精确结构的文献结果

2 包含所绘制结构的亚结构的文献结果

3 文献结果筛选选项

4 筛选文献后，点击get substance

Substances (462,916) Sort: Relevance View Full

References Reactions Suppliers

1

50-00-0
View Detail

C=O

CH₂O
Formaldehyde

236K References 184K Reactions 152 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	30.03	-
Melting Point (Experimental)	-92 °C	-
Boiling Point (Experimental)	-19.5 °C	-
Density (Experimental)	0.8 g/cm ³	-

Experimental Properties | Spectra

2

100-52-7
View Detail

c1ccccc1C=O

C₇H₆O
Benzaldehyde

154K References 206K Reactions 67 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	106.12	-
Melting Point (Experimental)	-26 °C	-
Boiling Point (Experimental)	179 °C	-
Density (Experimental)	1.050 g/cm ³	Temp: 15 °C

Experimental Properties | Spectra

3

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator
- Target Indicator
- Search Within Results

1

Edit Drawing Remove

As Drawn Substructure Find

1 用目标结构（喜树碱）筛选物质结果

Filter by

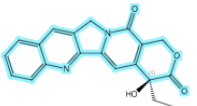
- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator
 - Antitumor agents (6,508) **1**
 - Cytotoxic agents (672)
 - Anti-infective agents (627)
 - Cardiovascular agents (481)
 - Anti-inflammatory agents (369)
 - [View All](#)
- Target Indicator
- Search Within Results

Substances (6,508) Sort: Number of References View Partial

References Reactions **3** Suppliers

1

7689-03-4
View Detail



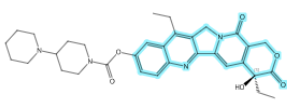
Absolute stereochemistry shown, Rotation (+)

$C_{20}H_{16}N_2O_4$
Camptothecin

21K References 2,193 Reactions 138 Suppliers

2

97682-44-5
View Detail



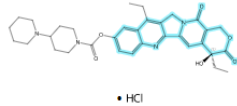
Absolute stereochemistry shown, Rotation (+)

$C_{33}H_{38}N_4O_6$
Irinotecan

10K References **2** Suppliers

3

100286-90-6
View Detail



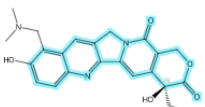
Absolute stereochemistry shown, Rotation (+)

$C_{33}H_{38}N_4O_6 \cdot ClH$
Irinotecan hydrochloride

9,051 References 77 Reactions 83 Suppliers

4

123948-87-8
View Detail

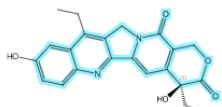


Absolute stereochemistry shown

$C_{23}H_{23}N_3O_5$
Topotecan

5

86639-52-3
View Detail

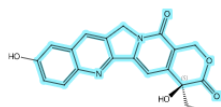


Absolute stereochemistry shown, Rotation (+)

$C_{22}H_{20}N_2O_5$
7-Ethyl-10-hydroxycamptothecin

6

19685-09-7
View Detail



Absolute stereochemistry shown, Rotation (+)

$C_{20}H_{16}N_2O_5$
Hydroxycamptothecin

1 用目标适应症筛选筛选物质结果

2 基于喜树碱母核结构，具有抗癌活性的物质结果集

3 点击获取反应

Filter by

- Substance Role
- Yield
- Number of Steps
- Experimental Protocols
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
- Search Within Results **1**

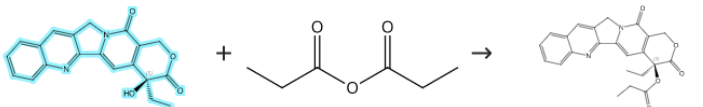
Source Reference

- Document Type
- Language
- Publication Year
- Publication Name

Reactions (3,425) View Collapsed

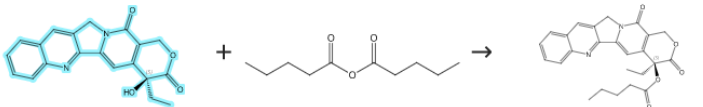
References

Scheme 1 (5 Reactions)



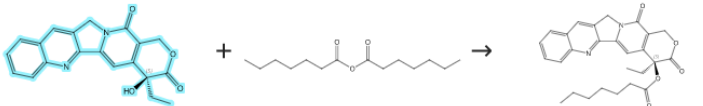
Absolute stereochemistry shown, Rotation (+) Steps: 1
Yield: 99%

Scheme 2 (5 Reactions)



Absolute stereochemistry shown, Rotation (+) Steps: 1
Yield: 99%

Scheme 3 (5 Reactions)



Absolute stereochemistry shown, Rotation (+) Steps: 1
Yield: 99%

1

用目标结构（喜树碱）作为起始物，限定反应结果。（查找如何从喜树碱合成喜树碱衍生物）

药物重定位

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SciFinder[®]中检索药物的重利用信息。

The screenshot displays the SciFinder interface for the substance Cinanserin. At the top, there are navigation buttons for 'References', 'Reactions', and 'Suppliers'. Below this, the substance is identified by its CAS number '1166-34-3' and name 'Cinanserin' with the molecular formula $C_{20}H_{24}N_2OS$. The chemical structure is shown with a purple box '1' next to it. Below the structure, there are three buttons: 'References' with the number '455' and a purple box '2' next to it, 'Reactions' with the number '2', and 'Suppliers' with the number '14'. The interface also includes a 'View Detail' link and a search icon.

- 1 通过肉桂硫胺的CAS登记号、化学名称或者结构式等多种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

Filter by

- Document Type
- Substance Role
- Language
- Publication Year **3**
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
 - 5-HT antagonists (46)
 - Brain (39)

References (455) Sort: Relevance View: Full Abstract

Substances Reactions Cited By Save

1

123I-ADAM binding to serotonin transporters in patients with major depression and healthy controls: a preliminary study.

By: Newberg, Andrew B; Amsterdam, Jay D; Wintering, Nancy; Ploessl, Karl; Swanson, Randel L; Shults, Justine; Alavi, Abass
Journal of nuclear medicine : official publication, Society of Nuclear Medicine (2005), 46(6), 973-7 | Language: English, Database: MEDLINE
[View Reference Detail](#)

Abstract: The serotonergic system may play an important role in the pathophysiology of major depressive disorder (MDD). Few imaging studies have examined serotonin transporter (SERT) binding in patients with MDD. We hypothesized that SERT binding activity may be altered in patients with MDD. This study compared SERT binding in patients with MDD with that in healthy controls. METHODS: We studied SERT activity in 7 patients (22-50 y old) with moderate to severe MDD and 6 healthy controls (24-56 y old) using (123I)-labeled 2-((2-((dimethylamino)methyl) phenyl)thio)-5-iodophenylamine (ADAM) and SPECT brain imaging. Subjects underwent SPECT 4 h after intravenous administration of 185 MBq (5 mCi) of (123I)-ADAM. Images were reconstructed in the axial plane, and region-of-interest demarcations were placed on the midbrain, medial temporal region, and basal ganglia region. RESULTS: (123I)-ADAM binding to SERT in the midbrain was significantly lower ($P = 0.01$) in MDD patients (1.81 ± 0.07) than in controls (1.95 ± 0.13). Age-adjusted (123I)-ADAM binding in the midbrain correlated significantly with scores on the Hamilton Depression Rating Scale ($r = 0.82$; $P = 0.02$). A significant negative correlation was observed between (123I)-ADAM SERT binding in the midbrain and age in the healthy control group ($r = 0.98$; $P = 0.0002$). SERT binding in the basal ganglia or medial temporal regions of interest did not significantly differ between groups. CONCLUSION: The findings from this preliminary study suggest the possibility of decreased SERT binding in the midbrain region of patients with MDD, with the degree of decrease correlating with the severity of depressive symptoms. There also appears to be an age-related decline in midbrain (123I)-ADAM SERT binding in healthy subjects.

3 按照Publication Year限定文献结果，如：筛选2000年以前发表的文献

Filter by

- Document Type
- Substance Role
- Language
- Publication Year
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
 - 5-HT antagonists (37)
 - Brain (33)
 - 5-HT receptors (31)
 - 5-HT agonists (16)
 - 5-HT2 receptors (12)
- Database
- Search Within Results

References (319) Sort: Relevance View: Full Abstract

Substances Reactions Cited By Save

1

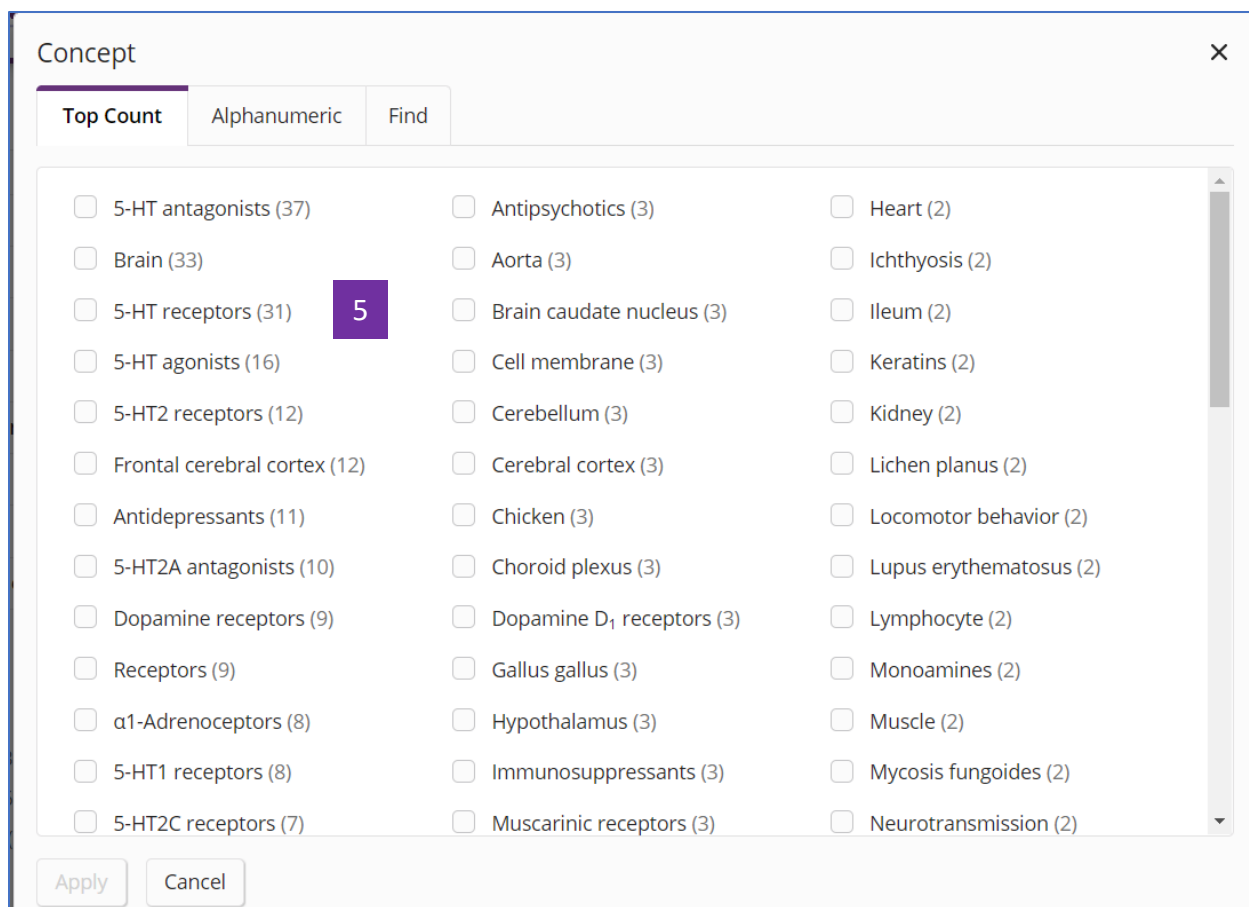
2-((2-((dimethylamino)methyl)phenyl)thio)-5-iodophenylamine (ADAM): an improved serotonin transporter ligand.

By: Oya, S; Choi, S R; Hou, C; Mu, M; Kung, M P; Acton, P D; Siciliano, M; Kung, H F
Nuclear medicine and biology (2000), 27(3), 249-54 | Language: English, Database: MEDLINE
[View Reference Detail](#)

Abstract: Serotonin transporters (SERT) are target-sites for commonly used antidepressants, such as fluoxetine, paroxetine, sertraline, and so on. Imaging of these sites in the living human brain may provide an important tool to evaluate the mechanisms of action as well as to monitor the treatment of depressed patients. Synthesis and characterization of an improved SERT imaging agent, ADAM (2-((2-((dimethylamino)methyl)phenyl)thio)-5-iodophenylamine)(7) was achieved. The new compound, ADAM(7), displayed an extremely potent binding affinity toward SERT ($K(i)=0.013$ nM, in membrane preparations of LLC-PK(1)-cloned cell lines expressing the specific monoamine transporter). ADAM(7) also showed more than 1,000-fold selectivity for SERT over norepinephrine transporter (NET) and dopamine transporter (DAT) ($K(i)=699$ and 840 nM, for NET and DAT, respectively). The radiolabeled compound $[(125)I]ADAM(7)$ showed an excellent brain uptake in rats (1.41% dose at 2 min post intravenous [IV] injection), and consistently displayed the highest uptake (between 60-240 min post IV injection) in hypothalamus, a region with the highest density of SERT. The specific uptake of $[(125)I]ADAM(7)$ in the hypothalamus exhibited the highest target-to-nontarget ratio (hypothalamus - cerebellum/cerebellum was 3.97 at 120 min post IV injection). The preliminary imaging study of $[(123)I]ADAM$ in the brain of a baboon by single photon emission computed tomography (SPECT) at 180-240 min post IV injection indicated a specific uptake in midbrain region rich in SERT. These data suggest that the new ligand $[(123)I]ADAM(7)$ may be useful for SPECT imaging of SERT binding sites in the human brain.

Full Text Substances (4) Reactions (0) Cited By (149) Citation Map

4 点击View All，查看所有Concept

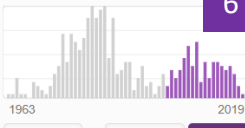


5

查看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。

Filter by

- Document Type
- Substance Role
- Language
- Publication Year



1963 to 2019

2001 to No Max Apply

[Reset](#) [View Larger](#)
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
- CAS Solutions

References (136)

Sort: Relevance View: Full Abstract

Substances
 Reactions
 Cited By

1

123I-ADAM binding to serotonin transporters in patients with major depression and healthy controls: a preliminary study.

By: Newberg, Andrew B; Amsterdam, Jay D; Wintering, Nancy; Ploessl, Karl; Swanson, Randel L; Shults, Justine; Alavi, Abass
 Journal of nuclear medicine : official publication, Society of Nuclear Medicine (2005), 46(6), 973-7 | Language: English, Database: MEDLINE

[View Reference Detail](#)

Abstract: The serotonergic system may play an important role in the pathophysiology of major depressive disorder (MDD). Few imaging studies have examined serotonin transporter (SERT) binding in patients with MDD. We hypothesized that SERT binding activity may be altered in patients with MDD. This study compared SERT binding in patients with MDD with that in healthy controls. **METHODS:** We studied SERT activity in 7 patients (22-50 y old) with moderate to severe MDD and 6 healthy controls (24-56 y old) using (123I)-labeled 2-((2-(dimethylamino)methyl) phenyl)thio)-5-iodophenylamine (ADAM) and SPECT brain imaging. Subjects underwent SPECT 4 h after intravenous administration of 185 MBq (5 mCi) of (123I)-ADAM. Images were reconstructed in the axial plane, and region-of-interest demarcations were placed on the midbrain, medial temporal region, and basal ganglia region. **RESULTS:** (123I)-ADAM binding to SERT in the midbrain was significantly lower ($P = 0.01$) in MDD patients (1.81 ± 0.07) than in controls (1.95 ± 0.13). Age-adjusted (123I)-ADAM binding in the midbrain correlated significantly with scores on the Hamilton Depression Rating Scale ($r = 0.82$; $P = 0.02$). A significant negative correlation was observed between (123I)-ADAM SERT binding in the midbrain and age in the healthy control group ($r = 0.98$; $P = 0.0002$). SERT binding in the basal ganglia or medial temporal regions of interest did not significantly differ between groups. **CONCLUSION:** The findings from this preliminary study suggest the possibility of decreased SERT binding in the midbrain region of patients with MDD, with the degree of decrease correlating with the severity of depressive symptoms. There also appears to be an age-related decline in midbrain (123I)-ADAM SERT binding in healthy

6

将肉桂硫胺文献结果集的发表年限定为2000年之后

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53

Concept

Top Count Alphanumeric Find **7**

<input type="checkbox"/> Homo sapiens (30)	<input type="checkbox"/> Locomotor behavior (5)	<input type="checkbox"/> Blood-brain barrier (3)
<input type="checkbox"/> Human (30)	<input type="checkbox"/> Schizophrenia (5)	<input type="checkbox"/> Blood plasma (3)
<input type="checkbox"/> Drug screening (11)	<input type="checkbox"/> Signal transduction (5)	<input type="checkbox"/> Brain hippocampus (3)
<input type="checkbox"/> 5-HT _{2C} receptors (10)	<input type="checkbox"/> 5-HT ₁ receptors (4)	<input type="checkbox"/> Calcium channels (3)
<input type="checkbox"/> 5-HT ₂ receptors (9)	<input type="checkbox"/> 5-HT ₆ receptors (4)	<input type="checkbox"/> Climbing (3)
<input type="checkbox"/> 5-HT antagonists (9)	<input type="checkbox"/> Alzheimer disease (4)	<input type="checkbox"/> Cognition enhancers (3)
<input type="checkbox"/> Antiviral agents (9) 8	<input type="checkbox"/> Brain corpus striatum (4)	<input type="checkbox"/> Demyelination (3)
<input type="checkbox"/> 5-HT _{1A} receptors (8)	<input type="checkbox"/> Coronavirus (4)	<input type="checkbox"/> Dopamine antagonists (3)
<input type="checkbox"/> 5-HT ₇ receptors (8)	<input type="checkbox"/> Drug delivery systems (4)	<input type="checkbox"/> Dopamine D ₃ receptors (3)
<input type="checkbox"/> Combination chemotherapy (8)	<input type="checkbox"/> Drug interactions (4)	<input type="checkbox"/> Drug bioavailability (3)
<input type="checkbox"/> 5-HT ₃ receptors (7)	<input type="checkbox"/> Hyperkinesia (4)	<input type="checkbox"/> Drug toxicity (3)
<input type="checkbox"/> 5-HT reuptake inhibitors (7)	<input type="checkbox"/> Muscarinic antagonists (4)	<input type="checkbox"/> Epilepsy (3)
	<input type="checkbox"/> Myelination (4)	<input type="checkbox"/> Guillain-Barre syndrome (3)

Apply **9** Cancel

7 可以浏览，或者在Find中输入关注的适应症

8 发现Antiviral agents的研究结果呈现上升趋势，勾选此词条

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 SciFinder search results page. On the left, a 'Filter by' sidebar is visible, with the 'Publication Year' filter selected. A bar chart shows the distribution of results from 1998 to 2019. A purple box with the number '10' is positioned over the 'Apply' button in the filter sidebar. The main area shows a search result for 'screening of anti-SARS coronavirus agents targeting protease 3CL'. The authors listed are Shen, Jianhua; Jiang, Hualiang; Shen, Xu; Zuo, Jianping; Luo, Xiaomin; Bai, Donglu; Shen, Jingkang; Chen, Kaixian; Gui, Chunshan; Chen, Lili. The abstract describes the use of protease 3CL as a target for screening anti-SARS CoV agents. A chemical structure of the compound is shown, featuring a benzene ring with a propylsulfanyl group and a propionamide side chain. A purple box with the number '11' is located above the result count. At the bottom of the result card, a purple box with the number '12' is positioned over the 'PATENTPAK' 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 Year: Oldest，将文献结果集按照发表年限重新排序

12 点击PatentPak，获取专利全文

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

13

S N I 0 0 8 - 4 2 7 4

13

在 SciFinderⁿ 中通过 PatentPak 直接下载的专利原文

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；且用于词中或者词尾。

The screenshot displays the SciFinder search results for the query 'La*chol'. The search bar at the top shows 'Substances' and 'La*chol' with a search count of 1. The results are sorted by 'Relevance' and shown in a grid of three cards. The first card, labeled '1', shows the chemical structure of Lapachol (C₁₅H₁₄O₃) and lists 997 references, 384 reactions, and 49 suppliers. The second card, labeled '2', shows '8038-34-4' with 'Image Not Available' and notes that it is an unspecified Lanochol, with 1 reference, 0 reactions, and 0 suppliers. The third card, labeled '3', shows '8006-54-0' with 'Image Not Available' and notes that it is an unspecified Lanichol, with 423 references, 0 reactions, and 22 suppliers. The interface includes navigation options like 'References', 'Reactions', and 'Suppliers' for each result, as well as global options like 'Sort: Relevance', 'View: Partial', and 'Save'.

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

2 此处输入Lapacho*，可以检索到Lapachol, Lapachol, Be deriv., Lapachol, Co deriv.等。

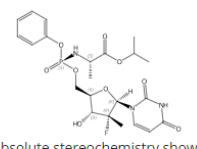
反应检索

逆合成路线的获取——Retrosynthesis 的使用

Substances (1)

References Reactions

1190307-88-0
View Detail



Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$
Sofosbuvir

2,644 References 567 Reactions 75 Suppliers

CAS RN
1190307-88-0
View Detail
CAS Name
Sofosbuvir

Substance Detail

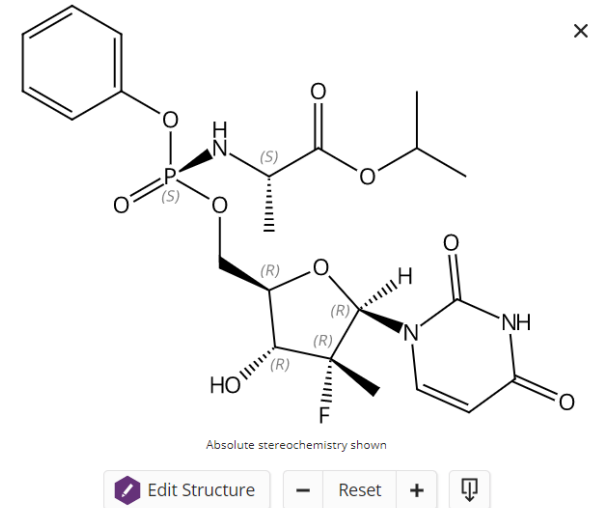
Reactions (567)

Synthesize (498)

Create Retrosynthesis Plan

References (2,644)

Suppliers (75)



Absolute stereochemistry shown

Edit Structure - Reset +

1 在SciFinderⁿ中找到所需合成物质后，点击物质结构

2 在弹出窗口中点击：Create Retrosynthesis Plan

The screenshot shows the CAS Draw software interface. On the left, a toolbar contains various drawing tools. The main workspace displays a complex chemical structure with a retrosynthetic arrow pointing to the left. A purple box with the number '1' is overlaid on the structure. On the right, a context menu is open, featuring an 'Edit' button with a pencil icon, a search icon, and a 'Create Retrosynthesis Plan' button with a retrosynthetic arrow icon. A purple box with the number '2' is overlaid on the 'Create Retrosynthesis Plan' button.

1 在结构编辑器中绘制所需合成结构

2 点击: Create Retrosynthesis Plan

The screenshot shows a dialog box titled 'Plan in progress...' in the SciFinder interface. The dialog contains the text: 'It's taking a little longer than expected to generate your plan. Click the OK button to return to the Home page where you can check the status of your plan under Recent Search History.' Below the text is an 'OK' button. A purple box with the number '1' is overlaid on the 'OK' button.

The screenshot shows the 'Recent Search History' page in SciFinder. It displays a search entry for 'June 18, 2019' at '10:30 AM'. The entry is labeled 'Retrosynthesis:' and includes a thumbnail of the chemical structure. To the right of the thumbnail is a purple box with the number '2'. Further right are two buttons: 'Open Plan' and 'Complete'.

1 如果出现这种提示，点击OK

2 稍后点击Recent Search History中的Open Plan

Retrosynthesis

Overview **1**

Plan Information

Estimated Yield: 25%
Overall Price: \$29,718.09
(USD per 100 grams)

Commercially Available:
A, B, C, D, E, F, G, H, I, J, K

Suppliers (75) Max. Yield: -

Suppliers (61) Max. Yield: 99%

Suppliers (135)

Suppliers (69)

Suppliers (12) Max. Yield: 92%

Suppliers (58) Max. Yield: 59%

Suppliers (101)

Suppliers (87) Max. Yield: 93%

Suppliers (56)

Suppliers (105)

Reset

1 Overview显示完整逆合成路线，预估产率和成本

Retrosynthesis

Overview Steps

1 A \Rightarrow B + C
Maximum Yield: -
Evidence (1)
Alternative Steps (51)

2 B \Rightarrow D + E + F
Maximum Yield: 99%
Evidence (28)
Alternative Steps (9)

3 C \Rightarrow G
Maximum Yield: 92%
Evidence (2)
Alternative Steps (6)

4 G \Rightarrow H + I
Maximum Yield: 59%
Evidence (3)
Alternative Steps (21)

I \Rightarrow J + K
Maximum Yield: 93%

Suppliers (75) Max. Yield: -

Suppliers (61) Max. Yield: 99%

Suppliers (135)

Suppliers (69)

Suppliers (12) Max. Yield: 92%

Suppliers (58) Max. Yield: 59%

Suppliers (101)

Suppliers (87) Max. Yield: 93%

Suppliers (56)

Suppliers (105)

Reset

1 精确匹配反应物和产物结构的反应，点击即获得反应信息详情

2 可替代步骤

3 当鼠标移到某一步骤时

4 右侧路线图中该反应的反应物和产物标识转为高亮

The screenshot displays the SciFinder interface with the following elements:

- Overview/Steps Panel:** Lists reaction steps:
 - A → B + C:** Maximum Yield: -, Evidence (1), Alternative Steps (51). A purple box labeled '1' highlights the 'Evidence (1)' link.
 - B → D + E + F:** Maximum Yield: 99%, Evidence (28), Alternative Steps (9).
 - C → G:** Maximum Yield: 92%, Evidence (2), Alternative Steps (6).
 - G → H + I:** Maximum Yield: 59%, Evidence (3), Alternative Steps (21).
- Filter by Panel:** Includes filters for Yield, Number of Steps, Reaction Type, Stereochemistry, Reagent, Solvent, Commercial Availability, and Search Within Results.
- Reactions (1) Section:** Shows 'Scheme 1 (1 Reaction) View' with chemical structures and reagents. A purple box labeled '2' highlights this section. Below the scheme are 'Suppliers' buttons for 61, 12, and 75 items.
- Reaction Summary Table:**

Reagents	Water	Steps: 1
Catalysts	-	
Solvents	Tetrahydrofuran	
- Reference Information:**
 - Process for synthesizing Sofosbuvir from cytidine
 - View Reference Detail
 - By: Liu, Ke
 - China, CN105646626 A 2016-06-08
 - Buttons: PATENTPAK, Full Text

1 点击Evidence

2 查看反应信息详情

Alternative Steps (51)

A → B + C
Maximum Yield: -
Evidence (1)
Alternative Steps (51)

B → D + E + F
Maximum Yield: 99%
Evidence (28)
Alternative Steps (9)

C → G
Maximum Yield: 92%
Evidence (2)
Alternative Steps (6)

G → H + I
Maximum Yield: 59%
Evidence (3)
Alternative Steps (21)

Alternative Step 1: Select Evidence (2) Maximum Yield: -

Alternative Step 2: Select Evidence (8) Maximum Yield: 88%

Retrosynthesis

Overview Steps

Plan Information

Estimated Yield: 38%
Overall Price: \$19,855.91
(USD per 100 grams)

Commercially Available:
A, B, C, D, E, F, G, H, I, J, K

Suppliers (75) Max. Yield: 88%

Suppliers (61) Max. Yield: 99%

Suppliers (135)

Suppliers (69)

Suppliers (94) Max. Yield: 78%

Suppliers (58) Max. Yield: 59%

Suppliers

Reset

1 点击Alternative Steps,查看其他可能的路线

2 点击Select, 结果将更换成新路线

3 自动生成新路线

#	Step	Yield	Evidence	Alternative Steps	Commercially Available
1	A → B + C	Max.: -	1	51	A, B, C
2	B → D + E + F	Max.: 99%	28	9	B, D, E, F
3	C → G	Max.: 92%	2	6	C, G
4	G → H + I	Max.: 59%	3	21	G, H, I
5	I → J + K	Max.: 93%	19	13	I, J, K

1 将路线结果导出为pdf格式文件，查看反应路线及反应信息

2 点击: View Retrosynthesis Plan in SciFinderⁿ 在线查看路线详情

逆合成路线中增加立体选择性反应

Retrosynthesis

Powered by ChemPlann

Overview Steps Scoring

$A \Rightarrow B + C$
 Average Yield: 71%
 Evidence (1,230)
 Alternative Steps (29)

$B \Rightarrow D + E$
 Average Yield: 60%
 Evidence (2,884)
 Alternative Steps (43)

$C \Rightarrow F$ *Stereoselective* **2**
 Maximum Yield: 69%
 Evidence (1)
 Alternative Steps (13)

$E \Rightarrow G + H$
 Maximum Yield: 94%
 Evidence (2)
 Alternative Steps (18)

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。

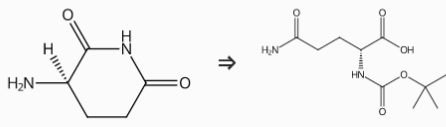
SciFINDERⁿ

Alternative Steps (13)

Filter by

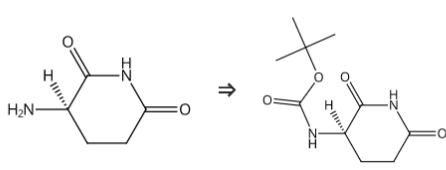
- Alternative Step Type
 - Experimental (3)
 - Predicted (10)
- Stereochemistry **4**
 - Selective (2)
 - Non-Selective (11)

1 of 13 *Stereoselective*



Selected Experimental Step Evidence (1) Maximum Yield: 69%

2 of 13 *Stereoselective*



Select Experimental Step Evidence (1) Maximum Yield: -

Overview Steps Scoring

A ⇒ B + C
Average Yield: 71%
Evidence (1,230)
Alternative Steps (29)

B ⇒ D + E
Average Yield: 60%
Evidence (2,884)
Alternative Steps (43)

C ⇒ F *Stereoselective*
Maximum Yield: 69%
Evidence (1)
Alternative Steps (13) **3**

E ⇒ G + H
Maximum Yield: 94%
Evidence (2)
Alternative Steps (18)

3 点击 **Alternative Steps** 查看替代路线。

4 在替代路线结果集页面，可通过 **Stereochemistry** 选择立体选择性反应。

逆合成路线增加自定义权重 (Scoring) 功能

The screenshot shows the 'Retrosynthesis' interface in SciFinder. The 'Scoring' tab is active, indicated by a purple box with the number '1'. On the left, the 'Scoring Profiles' sidebar is visible, with a purple box '2' highlighting the sliders for Complexity Reduction, Convergence, Evidence, Yield, and Atom Efficiency. At the bottom of the sidebar, a purple box '3' highlights the 'Apply' button. The main workspace shows a retrosynthetic pathway starting from target molecule A (Avg. Yield: 71%). It branches into two paths: one through B (Avg. Yield: 60%) and D (Suppliers: 93), and another through C (Suppliers: 46) and F (Max. Yield: 69%, Suppliers: 72). Both paths converge at E (Suppliers: 6), which then leads to G (Suppliers: 73) and H (Suppliers: 85) with a Max. Yield of 94%. A 'Reset Scoring' button is located at the bottom right of the main workspace.

1 在预测的逆合成路线结果中，点击左侧**Scoring**进行自定义评分

2 一共有5项，每项有4个设置（off, low, medium, high）。

Complexity Reduction降低每步前体的复杂度；**Convergence**可调整逆合成路线中前体的数量；**Evidence**每步反应的支持文献数量；**Yield**即每一步反应的产率，对目标分子的产率有影响；**Atom Efficiency**反应物中原子转化经济性。

以上选项，**Retrosynthesis**默认设置为**Medium**，如果需要更改，则用鼠标拖动滚动条进行自定义设置。

以上五项选择的相信信息，可在SciFinder-n help中获得：https://scifinder-n.cas.org/help/#t=Working_with_Search_Results%2FRetrosynthesis%2FRetrosynthesis_Page_-_Options_Tab.htm&rhsearch=retrosynthesis%20scoring&rhhlterm=retrosynthesis%20scoring&rhsyns=%20

3 点击**Apply**，完成设置

合成实验详情的获取

The screenshot displays the SciFinder interface for a chemical reaction. The main area shows a reaction scheme (Scheme 1) with a yield of 72% and 1 step. The reaction involves the synthesis of a quinazolinone derivative from an amide and TBHP. Below the scheme is a table with reaction details:

Reaction Summary		Steps: 1
Reagents	Cesium carbonate	Yield: 72%
Catalysts	-	
Solvents	Acetonitrile Water	
Conditions	rt; 10 h, 80 °C	

Additional information includes the reference: "TBHP as Methyl Source under Metal-Free Aerobic Conditions To Synthesize Quinazolin-4(3H)-ones and Quinazolines by Oxidative Amination of C(sp³)-H Bond" by Mukhopadhyay, Sushobhan; et al, published in the European Journal of Organic Chemistry (2018), 2018(22), 2784-2794.

Reaction Detail (Scheme 1, Reaction 1 of 1)

7

Steps: 1
Yield: 72%

Suppliers (7) Suppliers (56) 72%

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Cesium carbonate	-	Acetonitrile Water	rt; 10 h, 80 °C

CAS Reaction Number: Not assigned

Experimental Protocols

MethodsNow™ 3

Products 4(3H)-Quinazolinone, 5-chloro-3-phenyl-, Yield: 72%

Reactants tert-Butyl hydroperoxide
2-Amino-6-chloro-N-phenylbenzamide

Reagents Cesium carbonate

Solvents Acetonitrile
Water

Procedure

4

1. Add Cs₂CO₃ (0.74 mmol) and TBHP (70% aqueous solution, 7.4 mmol) in a round-bottom flask that contained amide (0.2 g, 0.74 mmol) in MeCN (6 mL) at room temperature.
2. Heat the mixture at 80 °C for 10 h under air.
3. Monitor the reaction progress by TLC analysis and remove the solvent under vacuum.
4. Dilute the residue with H₂O (20 mL) and extract the resulting mixture with EtOAc (3 × 20 mL).
5. Dry the combine organic layers with anhydrous Na₂SO₄ and filter.
6. Evaporate the filtrate under reduced pressure to obtain the crude residue.
7. Purify the crude residue by column chromatography over silica gel (hexanes/EtOAc, 7:3 v/v) to obtain the product.

Scale gram

Characterization Data

5

4(3H)-Quinazolinone, 5-chloro-3-phenyl-

Proton NMR Spectrum (400 MHz, [D₆]DMSO): δ = 7.33–7.42 (m, 2 H), 7.60–7.64 (m, 2 H), 7.74–7.78 (m, 3 H), 7.86–7.89 (m, 1 H), 8.00 (s, 1 H) ppm.

Carbon-13 NMR (100 MHz, [D₆]DMSO): δ = 124.9, 127.0, 127.7, 128.4, 129.2, 129.3, 132.7, 134.5, 136.9, 145.9, 147.2, 160.4 ppm.

IR Absorption Spectrum (KBr): ν_{max} = 1680 (CO) cm⁻¹.

HRMS (ESI): calcd. for C₁₅H₉ClN₂O [M+H]⁺ 257.0482; found 257.0480.

Mass Spectrum MS (ESI+): = 257.1.

Melting Point 167–169 °C.

R_f 0.61.

State white solid

6

Reference

TBHP as Methyl Source under Metal-Free Aerobic Conditions To Synthesize Quinazolin-4(3H)-ones and Quinazolines by Oxidative Amination of C(sp²)-H Bond

View Reference Detail

By: Mukhopadhyay, Sushobhan; et al

View All ▾

European Journal of Organic Chemistry (2018), 2018(22), 2784-2794

Full Text ▾

Company/Organization

Medicinal and Process Chemistry Division
CSIR Central Drug Research Institute
Lucknow 226031
India

- 1 在反应结果集中选择Experimental Protocols中的MethodsNow: Synthesis
- 2 点击Experimental Protocols获取增值标引的实验详情
- 3 实验中涉及的所有物质及其在反应中的角色
- 4 实验中涉及的所有实验步骤
- 5 产物的谱图表征信息及属性特征
- 6 产物的形态
- 7 下载、分享或保存实验详情

特定反应类型的获取及指定反应信息来源

The screenshot displays the SciFinder interface for searching reactions related to sofosbuvir. The left sidebar includes the following filters:

- Reaction Type:**
 - Full (545)
 - Product Only (32)
- Reaction Notes:**
 - Stereoselective (134)
 - Regioselective (33)
 - Prophetic Reaction (13)
 - High Pressure (10)
 - Anaerobic (6)
 - Biotransformation (1)
 - Enzymic (1)

Two reaction schemes are shown:

- Scheme 1:** Shows a reaction with 100% yield. A purple box with the number '1' highlights the 'Reaction Type' filter.
- Scheme 2:** Shows a reaction with 89% yield. A purple box with the number '2' highlights the 'Reaction Notes' filter.

1 在反应结果集页面，通过左侧Reaction Type，查看反应性质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，浏览或选择感兴趣的反应类型

Reactions 1190307-88-0

Document Type

Language

Publication Name **1**

- World Intellectual Property Organization (266)
- China (138)
- United States (73)
- India (43)
- European Journal of Organic Chemistry (36)
- Bioorganic & Medicinal Chemistry (5)
- Journal of Organic Chemistry (4)
- Organic Letters (4)
- Journal of Medicinal Chemistry (3)
- European Patent Organization (2)
- IP.com Journal (2)
- Czech Republic (1)
- Journal of the American Chemical Society (1)
- Topics in Heterocyclic Chemistry (1)

View Fewer

Yield: 89%

Suppliers (77)

Expand Scheme

Scheme 4 (8 Reactions) View All

Steps: 1
Yield: 83-88%

Suppliers (63) Suppliers (102) Suppliers (77)

Expand Scheme

Scheme 5 (1 Reaction) View

Steps: 1
Yield: 87%

1 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来源

相似反应检索

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

Reaction Summary		Steps: 1
Reagents	Methanesulfonic acid Sodium hydroxide	Yield: 12%
Catalysts	-	
Solvents	Dichloromethane Water	
Conditions	2 stages	

Preparation of 4-phenyl substituted tetrahydroisoquinolines and their therapeutic use to block reuptake of norepinephrine, dopamine, and serotonin for the treatment of neurological and psychological disorders
[View Reference Detail](#)
 By: Molino, Bruce F.; et al
 United States, US20060111385 A1 2006-05-25
[PATENTPAK](#) [Full Text](#)

- 1 根据Structure Match, 选择Similarity的反应结果
- 2 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

预测逆合成路线设计工具

Predicted Retrosynthesis Tool in SciFinder[®]

预测版逆合成路线设计工具（计算机辅助合成路线设计工具）

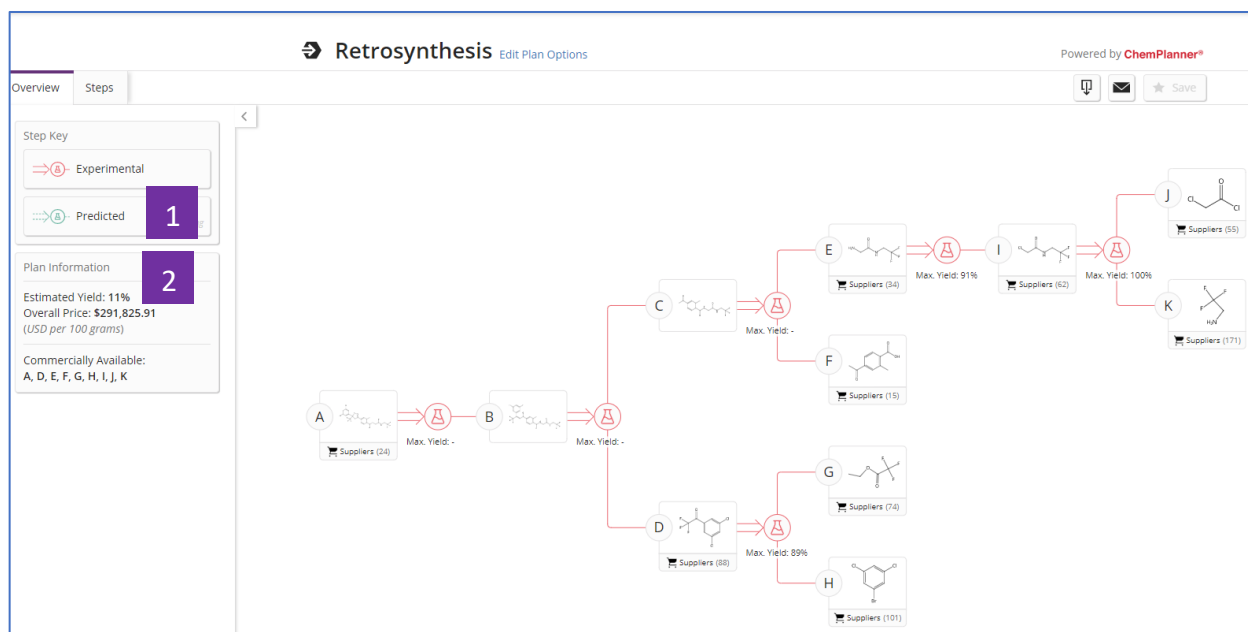
Retrosynthesis的运算基于世界上最大，更新速度最快，最权威的反应数据 ASREACT，加之先进的AI-搜索引擎技术，确保结果的质量和可靠性。通过 Retrosynthesis，您可以在数分钟内获得新分子的预测合成路线，或查找已知分子的新合成路线，从而获得创新所需要的新想法。Retrosynthesis综合考虑合成人员在设计合成路线中必需考量的因素（收率、绿色、成本、原料是否易得等），设计出增值的反应路线。

预测合成路线获取示例：获取 Fluralaner（CAS RN 864731-61-3）的预测合成路线

The image displays two screenshots from the SciFinder interface. The left screenshot shows the 'Substances' list with the entry for Fluralaner (CAS RN 864731-61-3) highlighted with a purple box labeled '1'. The right screenshot shows the 'Substance Detail' view for Fluralaner, with the 'Create Retrosynthesis Plan' button highlighted with a purple box labeled '2'.

1 点击物质结构

2 在弹出窗口中点击：Create Retrosynthesis Plan



1 基于文献报道的已知反应的优化路线

2 预测反应路线（一般需要10分钟左右完成，一旦完成，系统会向注册SciFinder[®]账号的邮箱发送通知）

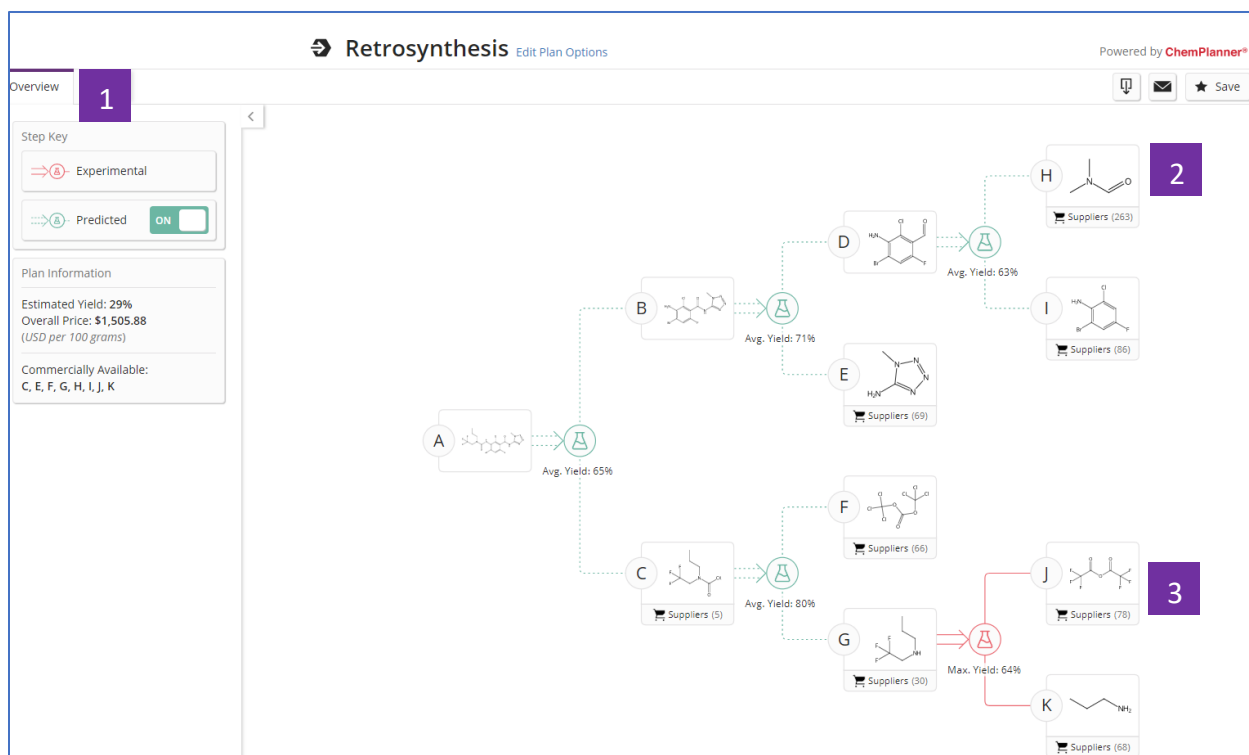
Your retrosynthesis plan is complete!

The retrosynthesis plan you recently submitted is ready to be viewed. Use the button below to access your plan directly or visit your [Search History](#) page to see all of your retrosynthesis plans.

Open

1

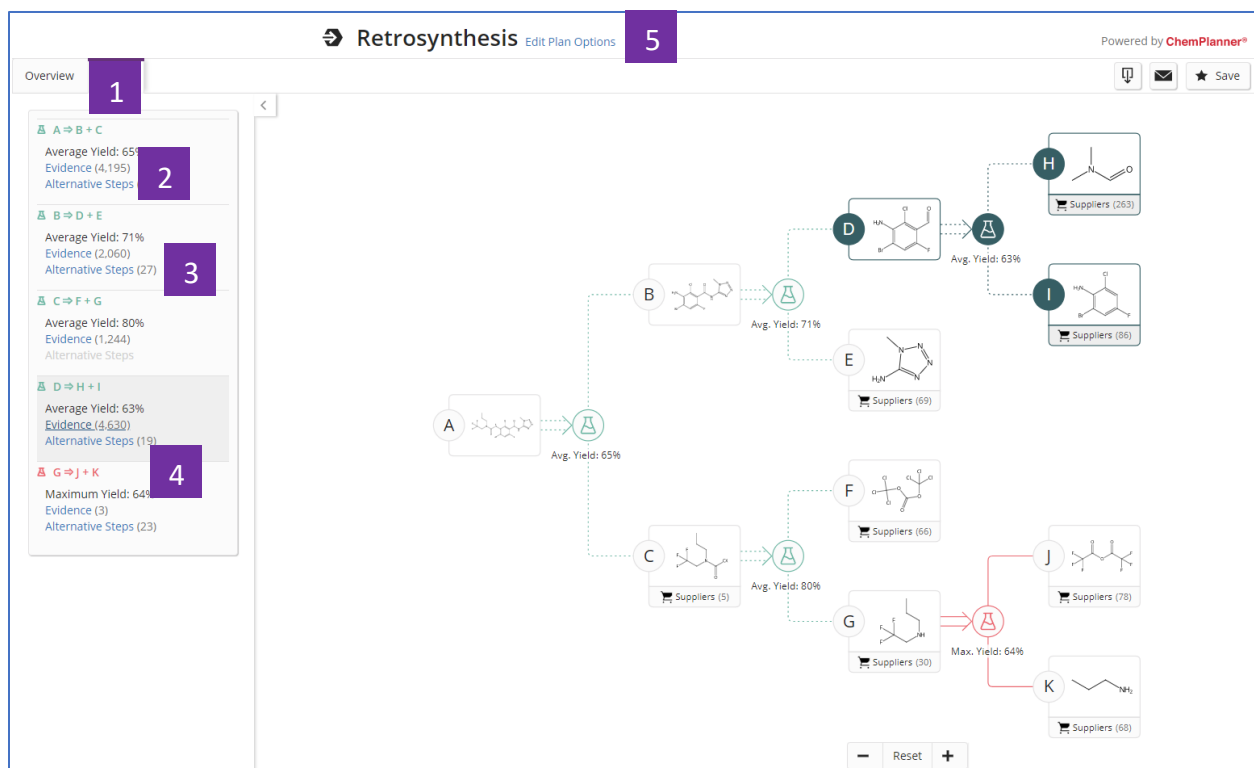
1 1. 打开注册SciFinder[®]账号邮箱，查找到系统发送的Retrosynthesis plan已经完成的电子邮件，点击Open，打开预测合成路线。



1 结果呈现：Overview显示完整逆合成路线，预估产率和成本

2 Predicted Plan (绿色代表预测步骤)

3 Experimental Plan (红色代表来源于已经报道的反应)



- 1 结果呈现：Steps显示合成路线中具体步骤信息，产率及可替代步骤
- 2 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
- 3 可替代反应步骤
- 4 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
- 5 编辑路线选项

Filter by

- Yield
 - 90-100% (541)
 - 80-89% (709)
 - 70-79% (672)
 - 50-69% (854)
 - 30-49% (403)
 - [View All](#)
- Number of Steps
 - 1 (4,630)
- Experimental Protocols
 - MethodsNow: Synthesis (890)
 - Experimental Procedure (1,102)
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst
- Solvent

Reactions (4,630) **1** View Expanded

References

Scheme 1 (1 Reaction)

Suppliers (86) Suppliers (263) Suppliers (28)

Steps: 1
Yield: 47%

Reaction Summary

Reagents	Lithium diisopropylamide Ammonium chloride	Steps: 1 Yield: 47%
Catalysts	-	
Solvents	Tetrahydrofuran Water	
Conditions	3 stages	

[View Reaction Detail](#)

Preparation of peptide macrocycles as antibacterial agents against acinetobacter baumannii

By: Alanine, Alexander; et al
World Intellectual Property Organization, WO2017072062 A1 2017-05-04

[PATENTPAK](#) [Full Text](#)

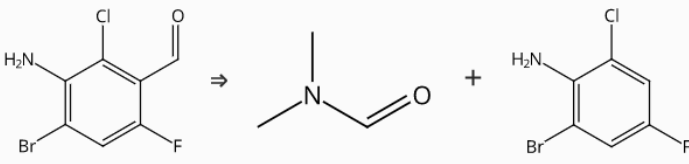
1

支持此反应 (D = H + J) 步骤的反应和文献信息

Alternative Steps (19) ×

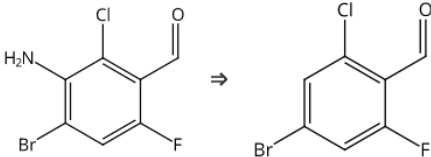
Filter by
^ Alternative Step Type
 Predicted (19)

1 of 19



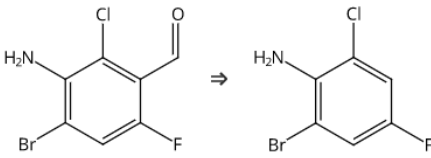
Evidence (4,630) Average Yield: 63%

2 of 19



1 Evidence (543) Average Yield: 48%

3 of 19



Evidence (629) Average Yield: 37%

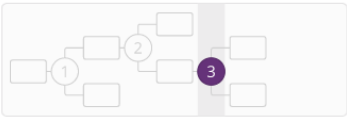
1 其他可选的反应步骤，点击后将更新为新路线

➔ Plan Options
Powered by ChemPlanner[®]

Select Synthetic Depth 1

Synthetic depth restricts the number of steps generated in the plan. [Learn More.](#)

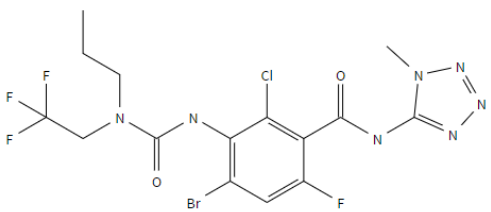
1
 2
 3
 4



Break and Protect Bonds 3

You may select one bond to break in the first step of the plan. Any bonds you protect will not break, though their order may change. [Learn More.](#)

Break Bond Protect Bond [Clear All Bond Selections](#)



➔ Create Retrosynthesis Plan

1 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

2 选择运行规则：

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。

3 标记断裂和被保护的键

筛选不参与反应的官能团

Search

All
Substances
Reactions
References
Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

1

2

3

Edit

Edit Drawing Remove

Create Retrosynthesis Plan

Set Plan Options

Recent Search History

1 点击Reactions进行反应检索

2 点击结构编辑器输入反应式

3 点击开始检索反应

Structure Match

As Drawn (2,594)
Substructure (533K)
Similarity (178K)

Filter by

Yield

Number of Steps

Non-Participating Functional Groups

Alkene (23)
Cyclic alkene (20)
Amine (16)
Secondary amine (15)
Tertiary amine (15)

View All

4

Reactions (2,594)

References

View Collapsed

Save

Scheme 1 (2 Reactions)

Steps: 1
Yield: 100%

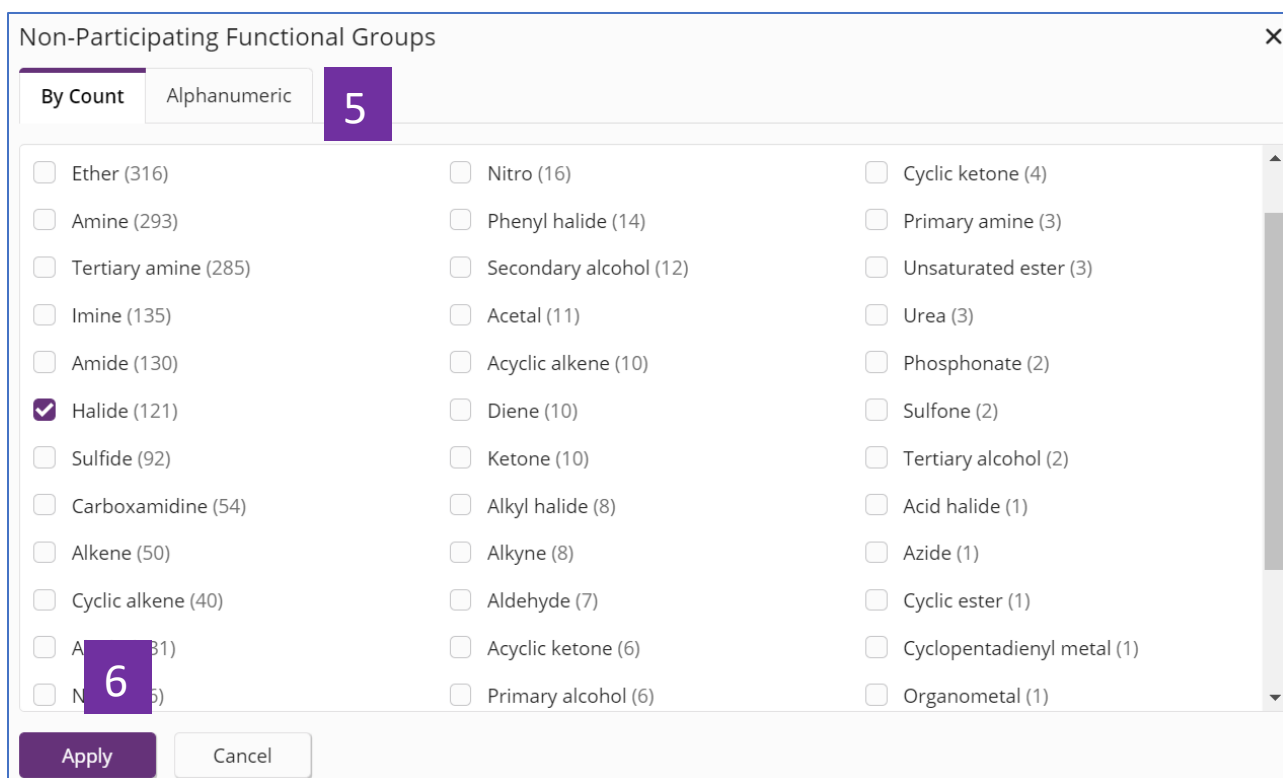
Suppliers (7)

Expand Scheme

Scheme 2 (1,907 Reactions)

Steps: 1
Yield: 100%

4 查看Non-Participating Functional Groups，点击View All查看官能团列表



5 可根据反应数量或官能团名称的字母顺序进行排序

6 勾选不参与反应的官能团后，点击Apply，获得选定官能团不参与反应果集（如下图）

Structure Match

As Drawn (48)

Substructure (4,118)

Similarity (617)

Filter by

- Yield
- Number of Steps
- Non-Participating Functional Groups
 - Ether (316)
 - Amine (293)
 - Tertiary amine (285)
 - Imine (135)
 - Amide (130)
 - Halide (121)
- View All
- Experimental Protocols
 - MethodsNow: Synthesis (15)


Reactions (121)

View Collapsed ▾

References ▾

📄 📧 ★ Save


Scheme 1 (3 Reactions) Steps: 1 Yield: 73-88%



🛒 Suppliers (70) 🛒 Suppliers (14)

Expand Scheme ▾

Scheme 2 (1 Reaction) Steps: 1 Yield: 59%



🛒 Suppliers (92) 🛒 Suppliers (17)

Expand Scheme ▾

在 PatentPak Viewer 中使用 Retrosynthesis

1 在 PatentPak Viewer 中，点击物质结构

2 弹出物质相关信息窗口

3 在弹出窗口中点击 Create Retrosynthesis Plan，对此物质进行逆合成反应路线设计

US005703247A

5,703,247
Dec. 30, 1997

Reaction of Taxol
Protic and Protic

Analog of Taxol
Binding Site on
5 (1993).

Studies of
Derivatives.”

mac. Ther., 52.

otere): A Semi-
inst., 4, 288-291

between the Struc-
totic Activity”. J.

Deacylation and
L., 56, 884-898

[03] Continuation-in-part of Ser. No. 30,612, Mar. 11, 1993,
abandoned, and Ser. No. 29,759, Mar. 11, 1993, abandoned.
[51] Int. Cl.⁶ C07D 305/14
[52] U.S. Cl. 548/962; 549/510; 549/511

(Jul. 1993).
Deutsch et al., “Synthesis of Congeners and Prodrugs 3.
Water-Soluble Prodrugs of Taxol With Potent Antitumor
Activity”. J. Med. Chem., 32, 788-792 (1989).

1 在 PatentPak Viewer 中，点击物质结构

2 弹出物质相关信息窗口

3 在弹出窗口中点击 Create Retrosynthesis Plan，对此物质进行逆合成反应路线设计

反应结果集的排序

在 SciFinderⁿ 反应结果集页面，提供两种结果排列方式：

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

The screenshot shows the SciFinderⁿ interface for searching reactions. At the top, there is a search bar with 'Reactions' selected and a search icon. Below the search bar, there are navigation options like 'Return to Home' and a filter panel on the left. The main area displays 'Reactions (86)' with a dropdown menu set to 'References'. A dropdown menu is open, showing 'By Scheme' and 'By Document' options, with a large purple box containing the number '1' highlighting the 'By Scheme' option. Below this, a reaction scheme is shown for 'Scheme 1 (4 Reactions)' with 'Steps: 1' and 'Yield: 85-99%'. The reaction shows a reactant with a hydroxyl group and a product with a spiro ring system. Below the scheme, there are buttons for 'Suppliers (6)' and 'Suppliers (9)'. A reaction summary is visible, including reagents (p-Toluenesulfonic acid) and solvents (Toluene). The summary also includes the title 'Synthesis and photoreactions of some spiro[cycloal kanephenalenes]' and the author 'By: Hempenius, M. A.; et al'.

1

根据需要进行选择 By Scheme 或 By Document 对反应进行排序

[← Return to Home](#)

Filter by

- Substance Role
 - Product (45)
 - Reactant (45)
- Yield
 - 90-100% (5)
 - 80-89% (7)
 - 70-79% (5)
 - 50-69% (5)
 - 30-49% (3)
 - [View All](#)
- Number of Steps
 - 1 (58)
 - 2 (7)
 - 3 (1)
- Non-Participating Functional Groups

Reactions (86)

Group: By Document ▾ View: Expanded ▾

References ▾

1

Synthesis and photoreactions of some spiro[cycloalkanephenalenes]

By: Hempenius, M. A.; Lugtenburg, J.; Cornelisse, J.
Recueil des Travaux Chimiques des Pays-Bas (1990), 109(7-8), 403-9 | Language: English, Database: CPlus

Full Text ▾ [View All Related Reactions](#)

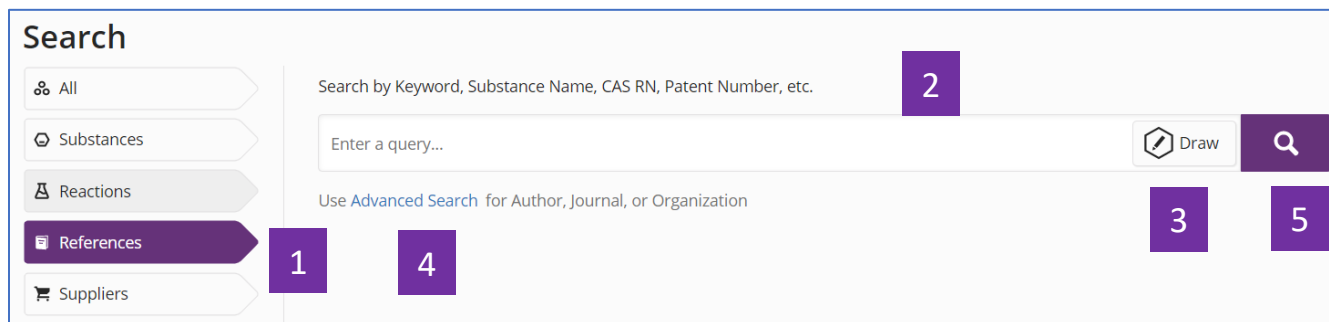
Suppliers (6) Suppliers (9)

2

当选择按照 By Document 时，点击 View All Related Reactions 查看该文献报道的所有反应

文献检索

文献信息的获取



- 1 选择 References，进行文献检索
- 2 输入检索信息：关键词、物质名称、CAS 登记号和专利号等
- 3 点击 Draw，绘制检索。并在 2 所示的文本框中输入相应文本，获取相关文献，所得文献结果包含输入文本及绘制的物质（反应）结构
- 4 点击 Advanced Search，进行作者、期刊名或组织机构名检索
- 5 点击放大镜，开始检索

The screenshot shows the SciFinder interface with the following callouts:

- 1: Sort dropdown menu
- 2: View dropdown menu
- 3: Filter by section
- 4: Download icon
- 5: Email icon
- 6: Save icon
- 7: Abstract text
- 8: Full Text dropdown
- 9: Substances button
- 10: Reactions button
- 11: Cited By button
- 12: Citation Map button
- 13: Return to Home link

1 点击 Sort 右侧小箭头，对结果按照引用次数，公开年份等重新进行排序

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选项

4 通过PDF、rtf、ris、txt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，并可同时设定信息更新提醒

7 查看文献详情

8 获取全文链接

9 获取文献中的物质

10 获取文献中的反应

- 11 获取被引用文献
- 12 引文地图，获取引用及被引用文献
- 13 回到首页界面

← Return to Results **1** **4**

Reference Detail (1 of 664) ← Prev Next →

Substances (10) Reactions (8) Cited By (14) Citation Map **3** Save

Journal **2**

Source
Journal of Surfactants and Detergents
Volume: 16
Issue: 3
Pages: 333-342
Journal
2013
DOI:
10.1007/s11743-012-1412-6

Database Information
AN: 2013:619398
CAN: 160:596744
CAplus

Company/Organization **7**
Petrochemicals Department
Egyptian Petroleum Research Institute
Cairo
Egypt

Publisher
Springer

Language
English

Synthesis, Surface and Thermodynamic Properties of Substituted Polytriethanolamine Nonionic Surfactants

By: Negm, Nabel A.; El-Faragy, Ahmed F.; Tawfik, Salah M.; Abdelnour, Ahmad M.; Hefni, Hassan H.; Khowdiary, Manal M.

Abstract: Three series of nonionic surfactants derived from polytriethanolamine containing 8, 10, and 12 units of triethanolamine were synthesized. Structural assignment of the different compounds was made on the basis of FTIR and ¹H-NMR spectroscopic data. The surface parameters of these surfactants included critical micelle concentration (CMC), surface tension at the CMC (γ_{CMC}), surfactant concentration required to reduce the surface tension of the solvent by 20 mN m⁻¹ (pC_{20}), maximum surface excess (Γ_{max}), and the interfacial area occupied by the surfactant mols. (A_{min}) using surface tension measurements. The micellization and adsorption free energies were calculated at 25 °C.

Full Text **5**

Expand All | Collapse All

- ▼ Concepts **6**
- ▼ Substances
- ▲ Citations **8**

Citations (37)

- 1) Wong, S; J Surf Deterg, 2012, 15, 593
- 2) Pegiadou, S; J Surf Deterg, 2000, 3, 517
- 3) Yakimchuk, O; Russian J Appl Chem, 2004, 77, 2001
- 4) Chao, Y; J Surf Deterg, 2012, 15, 299
- 5) Fekarcha, L; J Surf Deterg, 2012, 15, 419
- 6) Hill, K; Alkyl polyglucosides-technology, properties and applications, 1997
- 7) Laska, U; J Surf Deterg, 2006, 9, 115
- 8) Augu, L; Carbohydr Chem, 2000, 19, 379

- 1** 返回至文献结果集界面
- 2** 文献书目信息
- 3** 文献相关信息：物质、反应、引文
- 4** 点击左右箭头，查看上一篇或下一篇文献详情

5 全文链接

6 概念词语

7 文献中报道的物质

8 引文信息

作者名/期刊名/机构名检索

← Return to Home Page **1**

Substances

References

Advanced Reference Search

Author **2**

Author Name (Last, First Middle)

Nakamura, Eiichi

Ex: Schubert, J A

Add Another Author **3**

— AND —

1 回到首页界面

2 在文本框输入作者名，按照“姓，名（中间名）”的格式输入，姓需要输入完整，名可以简写为首字母

3 可以添加其他作者姓名

Advanced Reference Search

Author

Author Name (Last, First Middle)

Ex: Schubert, J A

— AND —

Journal 1

Journal Name

Volume Issue Starting Page 2

Title Word(s) 3

Ex: Antibiotic

— AND —

Organization 4

Organization Name

Ex: Bayer, Dupont

5

1

在文本框中输入期刊名称，推荐输入完整期刊名称

- 2 若有“卷”、“期”或者“起始页”信息，可以在文本框中输入
- 3 可以输入希望在题名中出现的关键词
- 4 (选填) 可以输入研究机构名称与期刊名或作者名联合检索，也可以直接按照研究机构名称进行文献检索
- 5 点击进行检索

← Return to Home

Filter by

- Document Type
- Language
- Publication Year
 - 1975 to 2019
 - No Min to No Max Apply
 - [View Larger](#)
- Available at My Institution
- Author
 - Nakamura, Eiichi (255)
 - Matsuo, Yutaka (66)
 - Nakamura, Masaharu (38)
 - Ilies, Laurean (35)
 - Tsuji, Hayato (26)
 - [View All](#)
- Organization
- Publication Name
 - Journal of the American Chemical Society (256)
- Concept
- Database
- Search Within Results

References (256) Sort: Relevance View: Full Abstract

Substances Reactions **1** Cited By Save

Enantioselective synthesis of alpha-substituted ketones by asymmetric addition of chiral zinc enamides to 1-alkenes.

By: Nakamura, Masaharu; Hatakeyama, Takuji; Hara, Kenji; **Nakamura, Eiichi**
 Journal of the American Chemical Society (2003), 125(21), 6362-3 | Language: English, Database: MEDLINE
[View Reference Detail](#)

Abstract: A zinc enamide of a chiral imine derived from a **2** and (S)-valinol or (S)-leucinol undergoes addition to 1-alkene to generate a gamma-zincioimine intermediate, which reacts with a carbon electrophile to give upon hydrolysis an optically active alpha-substituted ketone in good yield. The stereoselectivity of the addition reaction may reach 99% for the reaction of a cyclohexanone imine with ethylene.

Full Text Substances (0) Reactions (0) **“ Cited By (51)** Citation Map

Synthesis, structure, and aromaticity of a hoop-shaped cyclic benzenoid [10]cyclophenacene.

By: **Nakamura, Eiichi**; Tahara, Kazukuni; Matsuo, Yutaka; Sawamura, Masaya
 Journal of the American Chemical Society (2003), 125(10), 2834-5 | Language: English, Database: MEDLINE
[View Reference Detail](#)

Abstract: The first hoop-shaped cyclic benzenoid compounds, [10]cyclophenacene derivatives that contain 40 pi electrons, have been synthesized in three or four steps from [60]fullerene by rationally designed chemical modification. The compounds thus synthesized are chemically stable, yellow-colored, luminescent, and EPR-silent. X-ray crystallographic analysis provided high precision structural data sets. On the basis of these results and theoretical investigations, the new cyclic benzenoid molecules were proven to be aromatic.

Full Text Substances (0) Reactions (0) **“ Cited By (134)** Citation Map

Reaction pathways of the Simmons-Smith reaction.

By: Nakamura, Masaharu; Hirai, Atsushi; **Nakamura, Eiichi**
 Journal of the American Chemical Society (2003), 125(8), 2341-50 | Language: English, Database: MEDLINE
[View Reference Detail](#)

Abstract: The cyclopropanation reaction of α -alkenes with a metal carbenoid has been studied by means of the D3VP hybrid

- 1 查看文献结果集
- 2 输入的信息在结果中会被高亮显示

获取制剂（配方）信息

在SciFinder[®]中可通过以下2种方式获取制剂（配方）信息：

1. 直接在Reference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。
2. 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Reference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（以获取依托必利缓释剂为例）：

References (60,082) Sort: Relevance View: Full Abstract

Substances Reactions Cited By Save

Formulation & evaluation of itopride HCl sustained release pellets P

By: Rao, P. Sambha Siva; Babu, G. Raveendra; Praveen, T. Kala; Surekha, P. Sri Lakshmi; Shekhar, M. Chandra
International Journal of Pharmaceutical Sciences and Research (2014), 5(5), 2074-2083, 10 pp. | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: The present work is aimed to formulate itopride HCl sustained release pellets using Et cellulose N50 such as hydrophobic polymer by employing the solution/suspension layer technique. The drug excipients compatibility study was carried out by Furor Transform IR spectroscopy (FTIR) which reveals no interaction between drug and excipients. Total 12 batches were formulated. Six formulations were prepared by using each natural polymer like Et cellulose N50. All the formulations were evaluated for micromeritic properties, phys. evaluation, which includes particle size anal., percentage yield, drug content, drug entrapment efficacy, percent moisture loss and swelling index, in vitro dissolution studies, SEM, and drug polymer interaction studies. The formulated pellets were evaluated for various pellet properties, like hardness, bulk d., tapped d., cars index and dissolution rate. Comparative evaluation of the above-mentioned parameters established the superiority of the pellets formulated with Et cellulose those formulated with different grades. The Optimized batch F3 was found to release the drug for 12 h (96.46%) and follows Higuchi Matrix model in dissolution studies, indicating the matrix-forming potential of natural polymer and diffusion controlled release mechanism.

Full Text Substances (4) Reactions (0) Cited By (2) Citation Map

Sustained release itopride hydrochloride matrix tablet

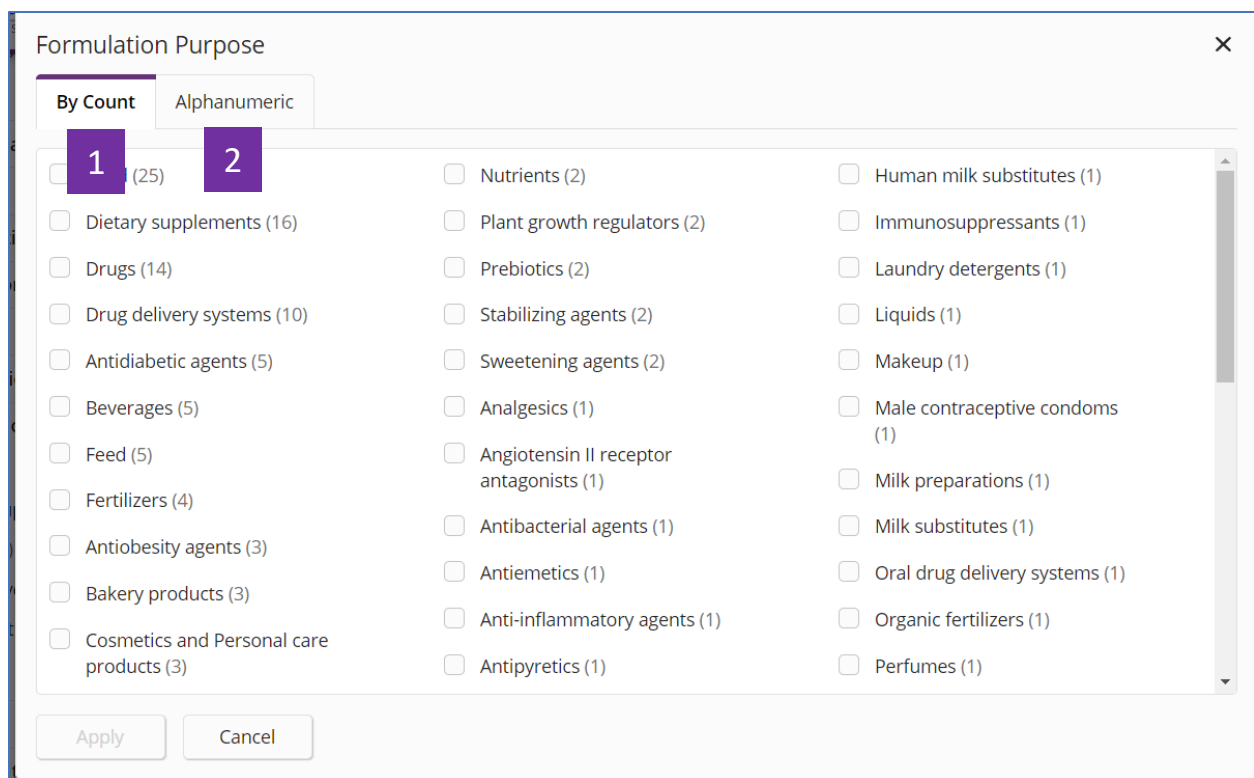
By: Prajapati, Bhupendra G.; Patel, Niklesh; Patel, Hitesh K.
Journal of Pharmaceutical Research and Health Care (2010), 2(1), 75-83 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: Oral route gets the highest priority for the delivery of the drug as well as better patient compliance in case of self delivery dosage formulation. The aim of present investigation was undertaken with the objective of formulating sustain release formulation of utopride hydrochloride for oral drug delivery. Itopride hydrochloride is highly water soluble prokinetic drug. Hydroxypropyl methylcellulose K4M (lower viscosity grade) and K100M (higher viscosity grade) were used as a matrix forming agents to control the release of drug. HPMC K4M and HPMC K100M were used individually as well as in combination with different proportion in the preparation of the Sustained release formulation. 3² Factorial designs were applied to the polymer concentration that affects the drug release profile. Reduced equation for drug release at 2hr, 6hr, and 10h were Q₂ = 37.644-5.41X₁-3.25X₂-2.017X₂², Q₆ = 72.367-8.05X₁-4.4X₂-3.75X₂², and Q₁₀ = 90.844-5.8X₁-2.633X₂-2.8X₁X₂ resp. Optimized batch F019 shows good tablet properties like hardness (7.9kg/cm²), thickness (4.48mm), friability (0.024%), assay (99.3%) and nearly similar

1 直接进行文献检索

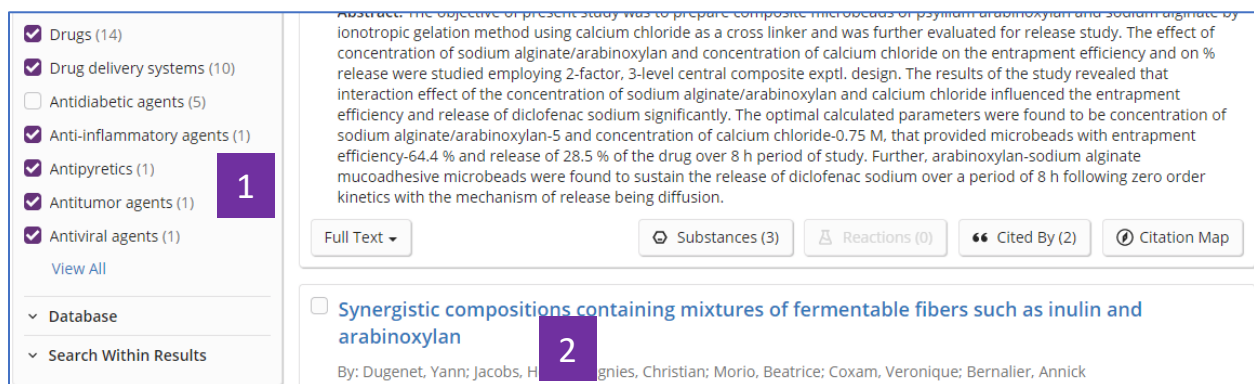
2 点击 Formulus, 可以获得制剂 (配方) 的更多信息 (请咨询美国化学文摘社北京代表处 china@acs-i.org 获取更多有关 Formulus 的信息)

3 在 Formulation Purpose 进行勾选感兴趣的制剂 (配方) 信息, 点击 View All 查看全部选项



1 根据文献数量对选项进行排序

2 根据选项字母顺序排序



1 可以选择一个或者几个选项

2 点击题目查看文献信息详情

Hydrolyzed protein-polysaccharide complexes

By: Schmitt, Christophe Joseph Etienne

Abstract: Hydrolyzed protein-polysaccharide complexes, and more specifically those complexes formed by complex formation of a protein with a polysaccharide followed by hydrolysis are presented. The resulting complexes have good emulsifying and stabilizing properties and can be used in food, cosmetic or pharmaceutical products. The invention further relates to the method of manufacture of such complexes.

PATENTPAK Viewer Full Text ▾

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
EP2196097	English	A1	PDF PDF+ Viewer	2010-06-16	EP2008-170653	2008-12-04
EP2196097	English	B1	PDF	2014-06-18	EP2008-170653	2008-12-04
ES2488098	Spanish	T3	PDF	2014-08-26	ES2008-170653	2008-12-04
AU2009324245	English	A1	PDF	2010-06-10	AU2009-324245	2009-11-30
CA2743101	English	A1		2010-06-10	CA2009-2743101	2009-11-30
WO2010063669	English	A1	PDF PDF+ Viewer	2010-06-10	WO2009-EP66038	2009-11-30
CN102227170	Chinese	A	PDF	2011-10-26	CN2009-80147598	2009-11-30
IL211972	English	A		2012-12-31	IL2009-211972	2009-11-30
NZ591979	English	A		2013-01-25	NZ2009-591979	2009-11-30
AU2009324245	English	B2	PDF	2014-11-20	AU2009-324245	2009-11-30
CN102227170	Chinese	B	PDF	2014-12-10	CN2009-80147598	2009-11-30
BR2009022290	Portuguese	A2		2015-08-11	BR2009-22290	2009-11-30
MY158625	English	A		2016-10-31	MY2011-1385	2009-11-30
US20110236554	English	A1	PDF	2011-09-29	US2011-13129501	2011-06-06
US8728556	English	B2	PDF PDF+ Viewer	2014-05-20	US2011-13129501	2011-06-06

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

▾ Concepts

▾ Substances

▾ Formulations **2**

1 点击PatentPak可以直接阅读或者获取专利的PDF全文

2 点击Formulations查看制剂（配方）信息

Hydrolyzed Protein-Polysaccharide Complex: Pharmaceutical Products or Cosmetic, Etc. **1**

[View Formulus® Detail](#) **2**

Location: example 3 **2**

Purpose: Cosmetics and Personal care products, Drugs **3**

Component 4	Function 5	Amount Reported 6
Whey proteins	active agent	1 w %
Gum arabic 7	active agent	1 w %
Enzeco bromelain enzyme	enzymes	1 w %
Sunflower oil	-	10 g

Additional Components Reported in Full Text

- 1** 点击View Formulus将进入CAS另一个解决方案Formulus ([请咨询美国化学文摘社北京代表处china@acs-i.org](#)获取更多有关Formulus的信息)
- 2** 该制剂（配方）在原文中出现的位置（示例为在实施例3中）
- 3** 制剂（配方）用途
- 4** 制剂（配方）中的成分
- 5** 各成分所起的作用
- 6** 成分含量
- 7** 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 SciFinder search results for 'arabinoxylan'. At the top left is the SciFinder logo with the text 'A CAS SOLUTION'. To the right of the logo is a search bar containing 'arabinoxylan' and a dropdown menu set to 'All'. Below the search bar is a navigation bar with a 'Return to Home' link. On the left side, there is a 'Show only' filter menu with the following options: 'Substances (1)' (highlighted with a purple box containing the number 1), 'Reactions (20)', 'References (5,458)', and 'Suppliers (3)'. The main content area is titled 'All Answer Types' and includes the text 'Top two answers by relevance from each answer type.'. Below this, there is a section for 'Substances (1)' which displays a result for '9040-27-1'. This result includes a 'View Detail' link, a placeholder for an image ('Image Not Available'), and the name 'Unspecified Arabinoxylan'. At the bottom of the result card, there are three buttons: 'References' with a count of 3,515 (highlighted with a purple box containing the number 2), 'Reactions' with a count of 20, and 'Suppliers' with a count of 3.

1 进行物质检索，获得物质检索结果集

2 由物质获得文献结果集

The screenshot displays the SciFinderⁿ web interface. At the top, there is a search bar with the text 'Enter a query...' and a 'References' dropdown menu. To the right of the search bar are icons for 'Draw', a search magnifying glass, a star, a clock, and a user profile. Below the search bar, the main content area is titled 'References (3,515)'. On the left, a 'Filter by' sidebar lists various categories: Document Type, Substance Role, Language, Publication Year, Available at My Institution, Author, Organization, Publication Name, Concept, CAS Solutions, and Formulation Purpose. The 'Formulation Purpose' category is highlighted with a purple box and a white number '1'. Under 'Formulation Purpose', several options are listed with checkboxes: Food (25), Dietary supplements (16), Drugs (14), Drug delivery systems (10), and Antidiabetic agents (5). The main search results area shows two entries. The first entry, 'Cereal arabinoxylans: advances in structure and physiochemical properties', is selected and expanded. It includes the authors 'Izydorczyk, Marta S.; Biliaderis, Costas G.', the journal 'Carbohydrate Polymers (1995), 28(1), 33-48', and a detailed abstract. Below the abstract are buttons for 'Full Text', 'Substance (1)', 'Reactions (0)', 'Cited By (502)', and 'Citation Map'. The second entry, 'Arabinoxylans and Endoxylanases in Wheat Flour Bread-making', is also visible but not expanded.

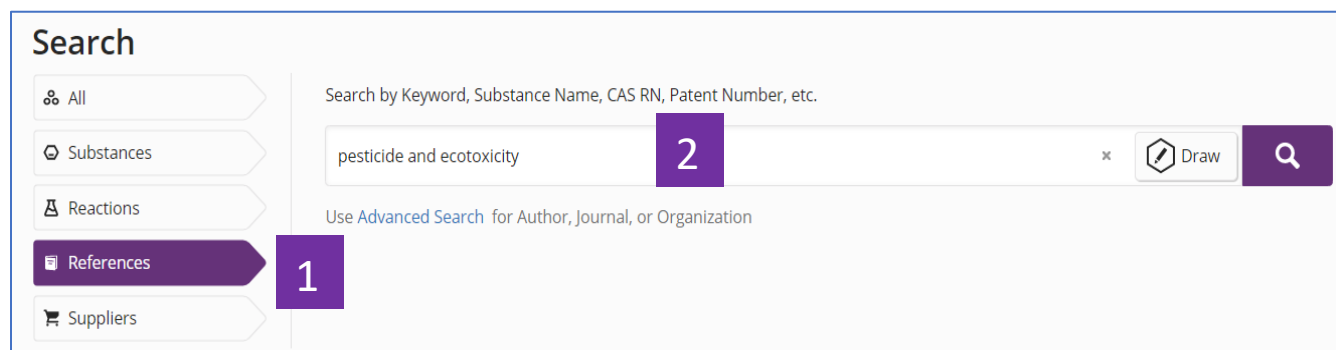
1

在Formulation Purpose中勾选所需目标制剂信息

布尔逻辑运算符在文献检索中的应用

在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检索结果中；
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。



1 点击References开始文献检索

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

The screenshot shows the SciFinder search page. On the left, there are navigation buttons for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The 'References' button is highlighted in purple. The main search area has a text input field containing 'ipatasertib or gdc 0068'. A purple callout box with the number '3' is positioned over the 'or' operator. To the right of the input field are buttons for 'Draw' and a search icon. Below the input field, there is a link for 'Advanced Search'.

3 使用OR连接两个检索词，如ipatasertib or gdc 0068，表示ipatasertib 和 gdc 0068任意一个出现即可

The screenshot shows the SciFinder search page with a search query 'thermally conductive not halogen-containing pd'. A purple callout box with the number '4' is positioned over the 'not' operator. A dropdown menu is open below the input field, showing several search suggestions. The first suggestion is 'thermally conductive not Halogen-containing polymers', which is highlighted in purple. Other suggestions include 'thermally conductive not Halogen-containing polyamide-polyesters', 'thermally conductive not Halogen-containing polycarbonate-polysulfones', and others. The 'References' button on the left is highlighted in purple. Below the search area, there is a 'Recent Search History' section showing the date 'October 12, 2019'.

4 使用NOT连接两个单词或词组，如**thermally conductive not halogen-containing polymers**，则只能得到**thermally conductive**出现的结果。

5 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。

6 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

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation tools like 'References', 'Draw', search, star, clock, and user icons are on the right. The search query is '"total synthesis" and taxol'. Below the search bar, there's a 'Return to Home' link. The main content area is titled 'References (298)' and includes sorting and viewing options. A left sidebar contains filters for Relevance, Document Type, Language, and Publication Year. The search results list two entries for 'Total synthesis of taxol', each with an abstract and associated buttons for 'Full Text', 'Substances', 'Reactions', 'Cited By', and 'Citation Map'.

References (298) Sort: Relevance View: Partial Abstract

Filter by

- Relevance
 - Best (69)
 - Good (174)
 - Fair (55)
 - Learn more about Relevance...
- Document Type
 - Journal (222)
 - Patent (11)
 - Review (86)
 - Commentary (1)
 - Conference (42)
 - View All
- Language
 - English (256)
 - Japanese (15)
 - Chinese (12)
 - German (4)
 - French (2)
 - View All
- Publication Year

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; Paulvannan, K Nature (1994), 367(6464), 630-4 | Language: English, Database: MEDLINE
View Reference Detail

Abstract: Taxol, a substance originally isolated from the Pacific yew tree (*Taxus brevifolia*) more than two decades ago, has recently been approved for the clinical treatment of cancer patients. Hailed as having provided one of the most significant advances in cancer therapy, this molecule exerts its anticancer activity by inhibiting mitosis through enhancement of the polymerization of tubulin and consequent stabilization of microtubules. The scarcity of taxol and the ecological impact of harvesting it have prompted extensive searches for alternative sources including semisynthesis, cellular culture pro...

View More

Full Text Substance (1) Reactions (0) Cited By (718) Citation Map

Total synthesis of taxol

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

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

View More

Full Text Substances (26) Reactions (23) Cited By (718) Citation Map

通配符的使用

在 SciFinder[®] 中用主题词进行文献检索时，可考虑使用通配符*和?。

通配符*代表 0 或多个字符；通配符? 代表 0 或一个字符。

通配符可位于词中间或词尾，不可用于词首。

通配符支持的主题检索会在文献的标题、摘要、关键词和 Concept Modifiers 处进行识别。

References ▾ synth* 1 × Draw 🔍 ★ ⌚ 👤

A planning strategy for diversity-oriented synthesis
 By: Burke, Martin D.; Schreiber, Stuart L.
 Angewandte Chemie, International Edition (2004), 43(1), 46-58 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: A review. In contrast to target-oriented **synthesis** (TOS) and medicinal or combinatorial chem., which aim to access precise or dense regions of chem. space, diversity-oriented **synthesis** (DOS) populates chem. space broadly with small-mols., having diverse structures. The goals of DOS include the development of pathways leading to the efficient (three- to five-step) **synthesis** of collections of small mols. having skeletal and stereochem. diversity with defined coordinates in chem. space. Ideally, these pathways also yield compounds having the potential to attach appendages site- and stereoselectively to a variety of attachment sites during a post-screening, maturation stage. The diverse skeletons and stereochemistries ensure that the appendages can be positioned in multiple orientations about the surface of the mols. TOS as well as medicinal and combinatorial chemistries have been advanced by the development of retrosynthetic anal. Although the distinct goals of DOS do not permit the application of retrosynthetic concepts and thinking, these foundations are being built on, by using parallel logic, to develop a complementary procedure known as forward-**synthetic** anal. This anal. facilitates **synthetic** planning, communication, and teaching in this evolving discipline.

Full Text ▾ Substances (0) Reactions (0) Cited By (1,299) Citation Map

6

Zeolite and molecular sieve synthesis
 By: Davis, Mark E.; Lobo, Raul F.
 Chemistry of Materials (1992), 4(4), 756-68 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: A review, with 107 references, of zeolite and mol. sieve **syntheses**. The **syntheses** of Al-rich zeolites, high-silica zeolites, and phosphate-based mol. sieves are evaluated. Unresolved mechanistic issues are outlined, and areas for exploration suggested. The ability to plan zeolite and mol. sieve **syntheses** is discussed, and a strategy for **synthesizing** a chiral zeolite is used to demonstrate the current limitations in designing new mol. sieves.

Full Text ▾ Substances (0) Reactions (0) Cited By (1,005) Citation Map

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

2

The screenshot shows the SciFinder interface with the search bar containing 'alumin?um'. The search results are displayed in a list format. The first result (ID 38) is titled 'Aluminum tolerance in wheat (Triticum aestivum L.). I. Uptake and distribution of aluminum in root apices' by Delhaize, Emmanuel; Craig, Stuart; Beaton, Colin D.; Bennet, Robin J.; Jagadish, Vidya C.; Randall, Peter J. The second result (ID 39) is titled 'Aluminium(III) as a promoter of cellular oxidation' by Zatta, Paolo; Kiss, Tamas; Suwalsky, Mario; Berthon, Guy. Both results include buttons for 'Full Text', 'Substance', 'Reactions', 'Cited By', and 'Citation Map'.

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

注意:

1. 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；
2. 一个检索词中最好只用一个通配符，否则 SciFinderⁿ 会忽略通配符，如输入 (R*,S*,R*,S*)-2,3,6,7-Tetrachlorooctane，则得到的检索结果则为 (R*,S*,R*,S*)-2,3,6,7-Tetrachlorooctane；
3. 一个检索式中不可超过 5 个通配符,否则会出错。

The screenshot shows the SciFinder search bar with the query 'tot* synth* nat* prod* terpen* last*'. A red error message box is displayed below the search bar, stating: 'Your query cannot contain more than 5 wildcard (?, *) characters. Learn more about wildcard searching.'

更详细说明可参考 https://scifinder-n.cas.org/help/#t=About_SciFinder-n%2FSciFinderN_Release_Notes%2FJanuary_15%2C_2020.htm%23SyntacticRefWildcard

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。

China (4,129)

Bioorganic & medicinal chemistry letters (2,773)

Journal of medicinal chemistry (2,609)

European journal of medicinal chemistry (2,308)

[View All](#)

^ Concept

Antiviral agents (30K)

Homo sapiens (12K)

Human (12K)

Humans (11K)

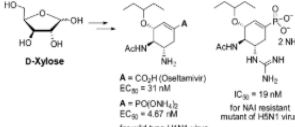
Structure-activity relationship (10K)

[View All](#)

Synthesis of Tamiflu and its Phosphonate Congeners Possessing Potent Anti-Influenza Activity

By: Shie, Jiun-Jie; Fang, Jim-Min; Wang, Shi-Yun; Tsai, Keng-Chang; Cheng, Yih-Shyun E.; Yang, An-Suei; Hsiao, Shih-Chia; Su, Ching-Yao; Wong, Chi-Huey

Journal of the American Chemical Society (2007), 129(39), 11892-11893 | Language: English, Database: CPlus



Using D-xylose as an appropriate chiral precursor, we have synthesized active neuraminidase inhibitor oseltamivir, antifu **drug** Tamiflu, and novel phosphonate congeners I [R = H, C(NH₂):NH] that exhibit even stronger antifu activities by inhibiting the neuraminidases of the wild-type and H274Y mutant of H1N1 and H5N1 viruses. Mol. modeling of the neuraminidase-phosphonate complex indicates a pertinent binding mode of the phosphonate with three arginine residues in the active site. Discovery of such potent neuraminidase inhibitors will offer an opportunity to development of new anti-influenza...

[View More](#)

Full Text
Substances (50)
Reactions (188)
Cited By (190)
Citation Map

5

Asymmetric synthesis of 1,3-dioxolane-pyrimidine nucleosides and their anti-HIV activity.

By: Kim, Hea O.; Ahn, Soon K.; Alves, Antonio J.; Beach, I. Warren; Jeong, Lak S.; Choi, Bo G.; Van Roey, Patrick; Schinazi, Raymond

1 点击View All，展开所有选项

Concept

Top Count Alphanumeric Search **2**

Concept Name

inhibit* **3** Search

110 Selected

- Growth Inhibitors (30)
- Growth inhibitors, animal (7)
- Hair growth inhibitors (32)
- HCV proteinase inhibitors (9)
- Heat-shock protein 70 inhibitors (1)
- Heat-shock protein 90 inhibitors (10)
- Helicase inhibitors (1)
- Hemagglutination Inhibition Tests (6)
- Leukemia inhibitory factor (29)
- lipid peroxidation inhibitor (2)
- lipoprotein-associated coagulation inhibitor (2)
- Lipoxygenase Inhibitors (56)
- Lysine-specific demethylase 1 inhibitors (2)
- Macrophage migration inhibitory factor (26)
- Macrophage Migration-Inhibitory Factors (1)
- Matrix metalloproteinase
- Nucleotide reverse transcriptase inhibitors (28)
- Ornithine decarboxylase-inhibiting proteins (2)
- Ornithine decarboxylase inhibitors (3)
- Phosphatidylinositol 3-kinase inhibitors (23)
- Phosphodiesterase 2 inhibitors (1)
- Phosphodiesterase 3 inhibitors (14)
- Phosphodiesterase 4

< Prev 1 2 3 Next >

4 Apply Cancel

2 点击 Search

3 输入检索词。可以添加星号 (*) 进行扩词，比如 `inhibit*`，可以检索到 `inhibiting`, `inhibitor`, `inhibitory` 等概念词。

4 点击 Apply，获得筛选后的文献结果。

文献结果集的聚类筛选项中增添全选功能

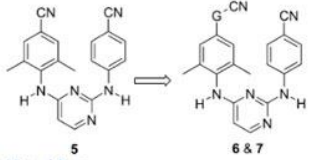
在文献检索结果集左侧的聚类筛选项里，点击View All展开所有的子项后，可以通过点击Search在所有子项中进行检索，并且可以通过Select All on Page全部选中检索到的子项。在Concept, Organization, Publication Name, Author等分析项中都增添了子项全选功能。

如下所示的是在Concept概念词库中对检索得到的子项进行全选的操作：

- ▼ Author
- ▲ Organization
 - Chinese Academy of Sciences (285)
 - Bristol-Myers Squibb Company (281)
 - Gilead Sciences, Inc. (186)
 - Nankai University (168)
 - Russian Academy of Sciences (149)
 - [View All](#)
- ▼ Publication Name
- ▲ Concept
 - Antiviral agents (30K)
 - Homo sapiens (12K)
 - Human (12K)
 - Humans (11K)
 - Structure-activity relationship (10K)
 - [View All](#) **1**
- ▼ CAS Solutions
- ▼ Formulation Purpose

Synthesis of novel diarylpyrimidine analogues and their antiviral activity against human immunodeficiency virus type 1

By: Guillemont, Jerome; Pasquier, Elisabeth; Palandjian, Patrice; Vernier, Daniel; Gaurrand, Sandrine; Lewi, Paul J.; Heeres, Jan; de Jonge, Marc R.; Koymans, Lucien M. H.; Daeyaert, Frits F. D.; et al
Journal of Medicinal Chemistry (2005), 48(6), 2072-2079 | Language: English, Database: CAplus



The **synthesis** and the **antiviral** properties of di(arylamino)pyrimidines (DAPY), e.g., **1**, as nonnucleoside reverse transcriptase inhibitors (NNRTIs), is reported. The **synthesis** program around this DAPY series was further optimized to produce compounds displaying improved activity against a panel of eight clin. relevant single and double mutant strains of human immunodeficiency virus type 1 (HIV-1).

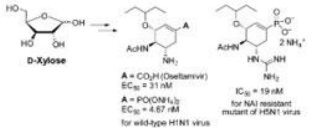
[View More](#) ▼

Full Text ▼
Substances (36)
Reactions (72)
Cited By (104)
Citation Map

4

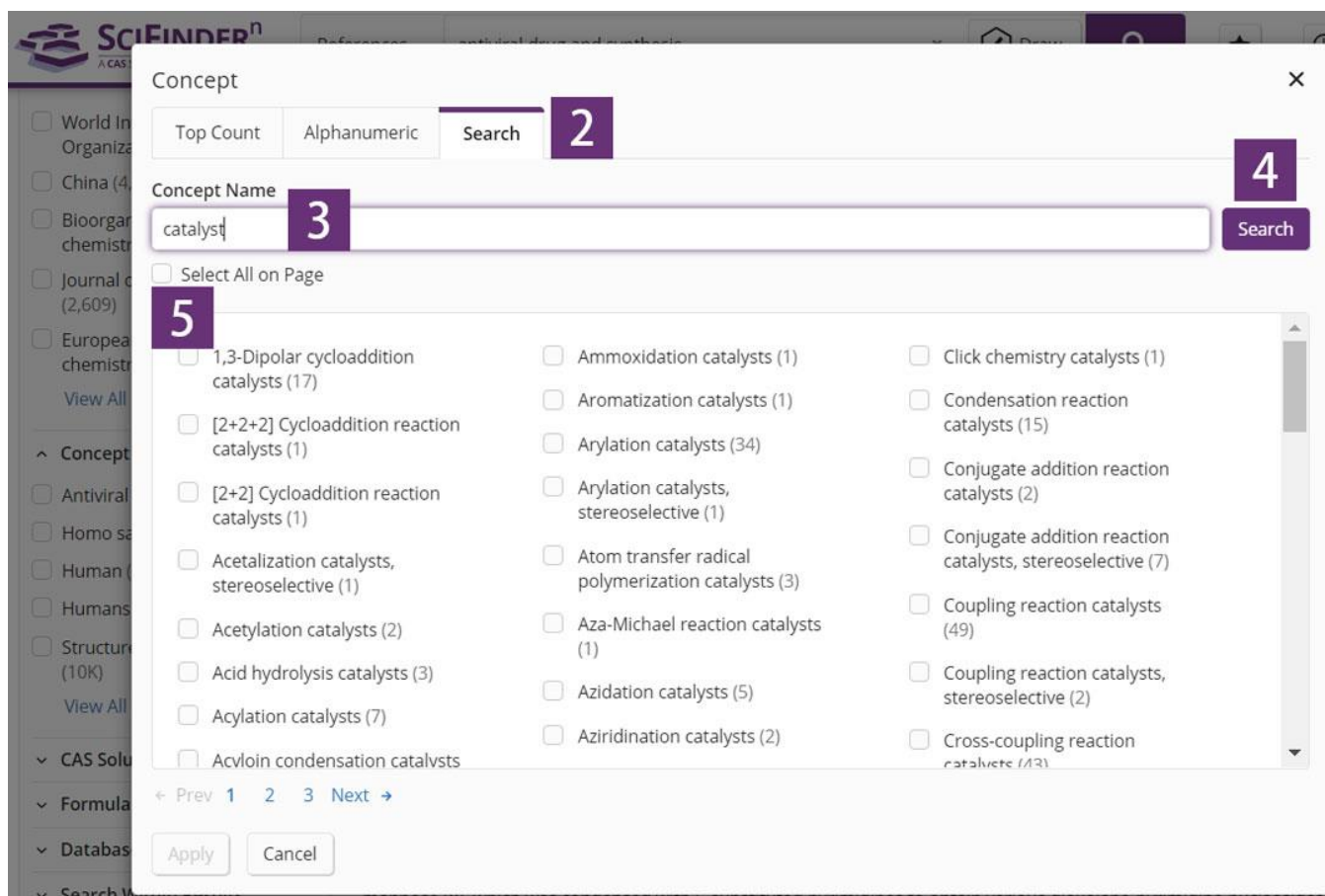
Synthesis of Tamiflu and its Phosphonate Congeners Possessing Potent Anti-Influenza Activity

By: Shie, Jiun-Jie; Fang, Jim-Min; Wang, Shi-Yun; Tsai, Keng-Chang; Cheng, Yih-Shyun E.; Yang, An-Suei; Hsiao, Shih-Chia; Su, Ching-Yao; Wong, Chi-Huey
Journal of the American Chemical Society (2007), 129(39), 11892-11893 | Language: English, Database: CAplus



Using D-xylose as an appropriate chiral precursor, we have synthesized active neuraminidase inhibitor oseltamivir, anti-flu **drug** Tamiflu, and novel phosphonate congeners **1** [R = H, C(NH₂);NH] that exhibit even stronger anti-flu activities by inhibiting the neuraminidases of the wild-type and H274Y mutant of H1N1 and H5N1 viruses. Mol. modeling of the neuraminidase-phosphonate complex indicates a pertinent binding mode of the phosphonate with three arginine residues in the active site. Discovery of such potent neuraminidase inhibitors will offer an opportunity to development of new anti-influenza **1**.

1 点击View All，展开所有的子项

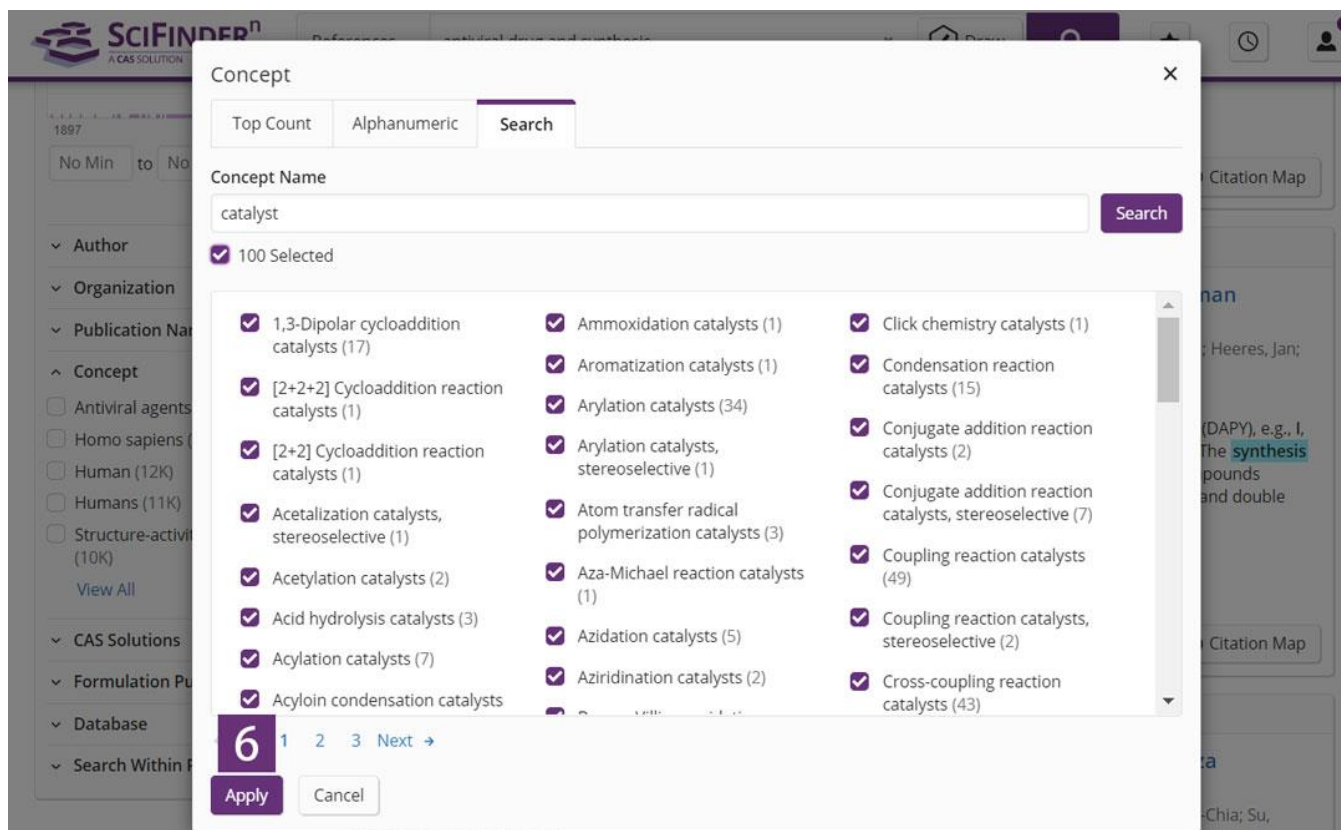


2 点击**Search**，在展开所有子项中进行检索

3 输入检索词

4 点击**Search**开始检索

5 点击**Select All on Page**，可以全部选中检索得到的子项



6 选中全部子项后，点击Apply获得筛选后的结果集

专利检索

专利信息的获取——PatentPak 的使用

References ▾ pcsk9 inhibitors

Best (30)

Good (4,768)

Fair (267K)

Learn more about Relevance...

Document Type

Journal (2M)

Patent (271K) **1**

Review (234K)

Biography (79)

Book (684)

View All

Substance Role

Adverse Effect (19)

Analytical Study (123)

Biological Study (621)

Combinatorial Study (2)

Occurrence (2)

View All

Language

English (125K)

Chinese (53K)

Treating autosomal dominant hypercholesterolemia associated with PCSK9 gain-of-function mutations using a PCSK9 inhibitor, such as anti-PCSK9 antibody

By: Swergold, Gary; Mellis, Scott; Sasiela, William J.
World Intellectual Property Organization, WO2014194111 A1 2014-12-04 | Language: English, Database: CPlus
View Reference Detail

Abstract: The present invention provides methods for treating autosomal dominant hypercholesterolemia (ADH). According to certain embodiments, the ADH is caused by or associated with a gain-of-function mutation (GOFm) in a gene encoding PCSK9. The GOFm encodes a PCSK9 variant protein comprising an amino acid substitution of V4I, E32K, D35Y, E48K, P71L, R96C, L108R, S127R, D129N, R215H, F216L, R218S, R357H, D374H, D374Y, S465L or R496W. The present invention therefore includes methods comprising selecting a patient who carries a GOFm in one or both alleles of the PCSK9 gene, and administering to the patient a pharmaceutical composition comprising a PCSK9 inhibitor. In certain embodiments, the PCSK9 inhibitor is an anti-PCSK9 antibody such as the exemplary antibody referred to herein as mAb316P (Alirocumab).

PATENTPAK ▾ **2** Text ▾ Substances (22) Reactions (0) Cited By (7) Citation Map

Patent	Language	Kind Code	PDF	PDF+	Viewer
WO2014194111	English	A1	PDF	PDF+	Viewer
US20140356370	English	A1	PDF		
AU2014274077	English	A1	PDF		
CN105263963	Chinese	A	PDF		
KR2016013046	Korean	A	PDF		
JP2016522211	Japanese	T	PDF		
JP6423868	Japanese	B2	PDF		

3 **4** **5**

3 PDF: 获取专利 PDF 全文

4 PDF+: 获取附有物质标记信息的专利 PDF 全文

5 Viewer: 查看专利全文

- 1** 在文献结果集中选择文献类型为 Patent
- 2** 点击 PatentPak 旁的小箭头，查看专利族列表
- 3** PDF: 获取专利 PDF 全文
- 4** PDF+: 获取附有物质标记信息的专利 PDF 全文

5

Viewer: PatentPak 浏览器，在线快速阅读专利全文

PatentPak 浏览器

The screenshot shows the PatentPak browser interface. At the top, there is a navigation bar with 'PAGE' (76 / 86), 'ZOOM' (+/-), and 'DOWNLOAD' (PDF, PDF+) options. The main content area displays a list of chemical substances with their names and corresponding page numbers. A sidebar on the left shows 'Key Substances in Patent' with their CAS RNs and analyst markup locations. The interface is annotated with numbered callouts: 1 points to the analyst markup location, 2 points to the analyst markup location, 3 points to the CAS RN, and 4 points to the download options.

1

物质位置信息：点击页码定位符号，右侧 PDF 全文快速跳转至该物质出现的页码处，同时对应物质的位置符号由蓝色变为紫色。

2

PDF 全文中对应的物质位置符号

3

点击 CAS 登记号，获取物质详情

4

下载专利全文：PDF: 获取专利 PDF 全文；PDF+: 获取附有物质标记信息的专利 PDF 全文。

马库什结构检索

Search

All | Substances | Reactions | References | Suppliers

Search by Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use [Advanced Search](#) for Molecular Formula, Substance Property, or Experimental Spectra

Edit | Search

Chemical structure drawing area

Edit Drawing | Remove

Search Patent Markush

- 1 选择Substances，进行Markush结构检索
- 2 点击Draw，绘制检索结构
- 3 点击放大镜，开始检索
- 4 点击Edit Drawing，重新编辑结构
- 5 点击Remove，去除结构
- 6 勾选Search Patent Markush进行马库什检索

Patent Markush Match

As Drawn (1) | Substructure (34)

Filter by

Patent Office

Japan (1)

Patent Markush (1)

References

JP2003261514

View Reference Detail

Patent claim 1

PATENTPAK | Full Text

There are no notes to display for this structure.

Chemical structure with Markush symbols G4 and G23

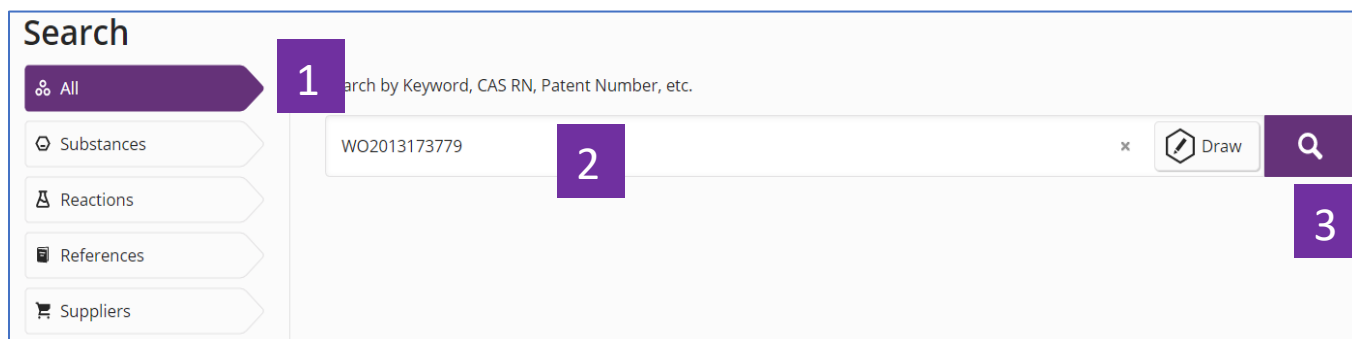
- 1 Markush结构检索的匹配程度：As Drawn，Substructure

- 2 击专利号，获取专利文献详情
- 3 该马库什结构在专利中出现的位置
- 4 PatantPak: 获取专利（同族）全文、定位专利中的重要物质
- 5 专利全文的链接
- 6 马库什结构详情

利用专利号进行检索

当用专利号进行检索时，可以选择**All**或分别选择**Substances**、**Reactions**和**References**进行检索。

注：专利号中的国家代码和数字间不能用空格隔开，如WO2013173779



- 1 选择**All**，同时获取该专利中披露的反应、物质、本专利文献及其披露的物质的供应商信息
- 2 输入专利号
- 3 进行检索

SciFinderⁿ A CAS SOLUTION

All WO2013173779 × Draw

← Return to Home

Show only

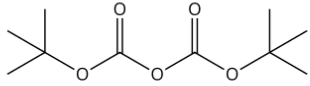
- Substances (18) **4**
- Reactions (35)
- References (2)
- Suppliers (0)

All Answer Types

Top two answers by relevance from each answer type.

Substances (18)

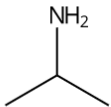
24424-99-5
View Detail



C₁₀H₁₈O₅
Di-*tert*-butyl dicarbonate

49K References 136K Reactions 144 Suppliers

75-31-0
View Detail




C₃H₉N
Isopropylamine

20K References 24K Reactions 68 Suppliers

[View All Substances](#)

Reactions (35)

Scheme 1 (1 Reaction) [View](#)



Steps: 1
Yield: 99%

Absolute stereochemistry shown

4

本专利披露的物质、反应和本专利文献信息及其披露的物质的供应商信息


SCIFINDERⁿ
A CAS SOLUTION

References WO2013173779

5

← Return to Home

Filter by

- Relevance
- Document Type
 - Patent (2)
- Language
- Publication Year
 

2009 to 2019

No Min to No Max Apply

[View Larger](#)
- Author
- Organization
- Publication Name
- Concept
- Database
- Search Within Results

References (2) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

Process for making amino acid compounds

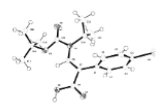
By: Remarchuk, Travis
United States, US9278917 B2 2016-03-08 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: 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) Cited By (0) Citation Map

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
[View Reference Detail](#)



Abstract: 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) Cited By (1) Citation Map

5 选择References，获得该专利及其同族信息

SciFinder[®] A CAS SOLUTION

Substances WO2013173779

Draw

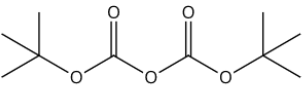
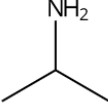
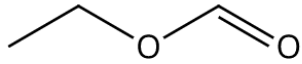
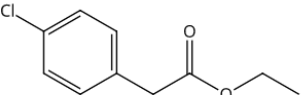
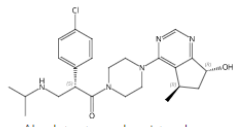
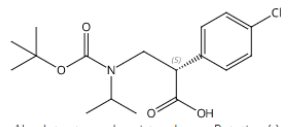
6 Substances (18)

Sort: Relevance View Partial

References Reactions Suppliers Save

Filter by

- Commercial Availability
- Reaction Role
 - Product (18)
 - Reactant (13)
 - Reagent (3)
 - Catalyst (4)
 - Solvent (3)
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator
- Target Indicator
- Search Within Results

<p><input type="checkbox"/> 24424-99-5 View Detail</p>  <p><chem>C10H18O5</chem> Di-tert-butyl dicarbonate</p> <p>49K References 136K Reactions 144 Suppliers</p>	<p><input type="checkbox"/> 75-31-0 View Detail</p>  <p><chem>C3H9N</chem> Isopropylamine</p> <p>20K References 24K Reactions 68 Suppliers</p>	<p><input type="checkbox"/> 109-94-4 View Detail</p>  <p><chem>C3H6O2</chem> Ethyl formate</p> <p>13K References 13K Reactions 72 Suppliers</p>
<p><input type="checkbox"/> 14062-24-9 View Detail</p>  <p><chem>C10H11ClO2</chem> Benzeneacetic acid, 4-chloro-, ethyl ester</p> <p>254 References 244 Reactions 68 Suppliers</p>	<p><input type="checkbox"/> 1001264-89-6 View Detail</p>  <p>Absolute stereochemistry shown</p> <p><chem>C24H32ClN5O2</chem> GDC 0068</p> <p>131 References 254 Reactions 71 Suppliers</p>	<p><input type="checkbox"/> 1001179-33-4 View Detail</p>  <p>Absolute stereochemistry shown, Rotation (-)</p> <p><chem>C17H24ClNO4</chem> (αS)-4-Chloro-α-[[[(1,1-dimethylethoxy) carbonyl]](1-methylethyl)amino]methyl] benz...</p> <p>24 References 156 Reactions 9 Suppliers</p>

6

选择Substances，获得该专利披露的物质信息

SciFinderⁿ A CAS SOLUTION

Reactions WO2013173779

Draw

7

Return to Home

Filter by

- Yield
- Number of Steps
- Experimental Protocols
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
- Search Within Results

Source Reference

- Publication Year
- Document Type
- Language

Reactions (35)

References

View Collapsed

Save

Scheme 1 (1 Reaction) View

Steps: 1
Yield: 99%

Absolute stereochemistry shown

Expand Scheme

Scheme 2 (1 Reaction) View

Steps: 1
Yield: 91%

Double bond geometry shown

Supplier (1)

Suppliers (30)

7

选择Reactions，获得该专利披露的反应信息

管理检索结果

设置 Alert

在SciFinder[®]中，可对以下几种结果集设置Alert：

1. Markush结构检索结果集
2. 文献检索结果集
3. 物质检索结果集
4. 反应检索结果集

1. 设置Markush结构检索结果集的Alert

The screenshot displays the 'Patent Markush Match' search results page. On the left, there are filter options for 'As Drawn (1)' and 'Substructure (34)'. The main search results area shows a chemical structure for patent JP2003261514. A 'Save Search' dialog box is overlaid on the right side of the page. The dialog box contains the following elements:

- 1**: A 'Save' button in the top right corner of the search results area.
- 2**: The 'Name' input field containing the text 'Markush alert'.
- 3**: The 'Tags (optional)' input field, which is currently empty.
- 4**: The 'Save' button within the 'Save Search' dialog box.

1 在Markush检索结果集中点击Save

- 2 输入保存文件的名称
- 3 点击Weekly或者Monthly设置提醒频率
- 4 点击Save完成设置

如果在保存结果集的过程中未设置Alert,则可以通过以下方法进行设置:

The screenshot shows the SciFinder interface with a search bar at the top. On the left, there are filter options for 'Result Type' (Patent Markush, References, Retrosynthesis, Substances) and buttons for 'Combine Saved Results' and 'Migrate Alerts & Saved Results'. The main area shows a 'Saved' section with 12 items. One item is a 'Markush alert' dated September 6, 2019, 2:32 PM, with the tag 'Patent Markush' and the text 'As Drawn'. A chemical structure is shown next to it. Below the alert, there are buttons for 'Alerts' (callout 2) and 'Add Tags'. At the bottom, there is a 'Frequency' dropdown menu with options 'No Alerts', 'Weekly' (callout 3), and 'Monthly'. A 'Rerun Search' button is visible on the right side of the alert card.

- 1 点击★，查看保存结果集
- 2 点击 Alerts，进行设置
- 3 设置发送频率

2. 设置文献检索结果集的Alert

The screenshot shows the SciFinderⁿ search results page for 'Programmed cell death protein 1'. The interface includes a search bar at the top with the query 'Programmed cell death protein 1'. Below the search bar, there are several filters and options. On the left, there is a 'Filter by' section with three categories: 'Relevance', 'Document Type', and 'Language'. Under 'Relevance', 'Best (9)' and 'Good (1,071)' are selected, and 'Fair (206K)' is unselected. A purple box with the number '1' highlights the 'Relevance' section. Below the filters, there is a 'References (1,080)' section. The first reference is 'Immunological reagents targeting programmed cell death 1 protein'. The abstract for this reference is visible. A purple box with the number '2' highlights the 'Save' button in the top right corner of the reference card. Another purple box with the number '3' highlights the star icon in the top navigation bar. The second reference is 'Methods for treatment of cancer with inhibitors of programmed cell death protein 1 (PD-1) pathway'.

1 根据需求，对文献结果集进行筛选

2 点击Save，保存文献

3 点击★，查看保存结果集

The screenshot shows a search result for 'PD-1' (Programmed cell death protein 1) with a timestamp of September 6, 2019, 4:07 PM. A 'Rerun Search' button is visible in the top right. Below the search result, there are controls for 'Alerts' and 'Add Tags'. A purple box with the number '1' highlights the 'Alerts' dropdown menu. Below it, a purple box with the number '2' highlights the 'Frequency' dropdown menu, which is currently set to 'Weekly'.

1 点击 Alerts ， 设置Alert

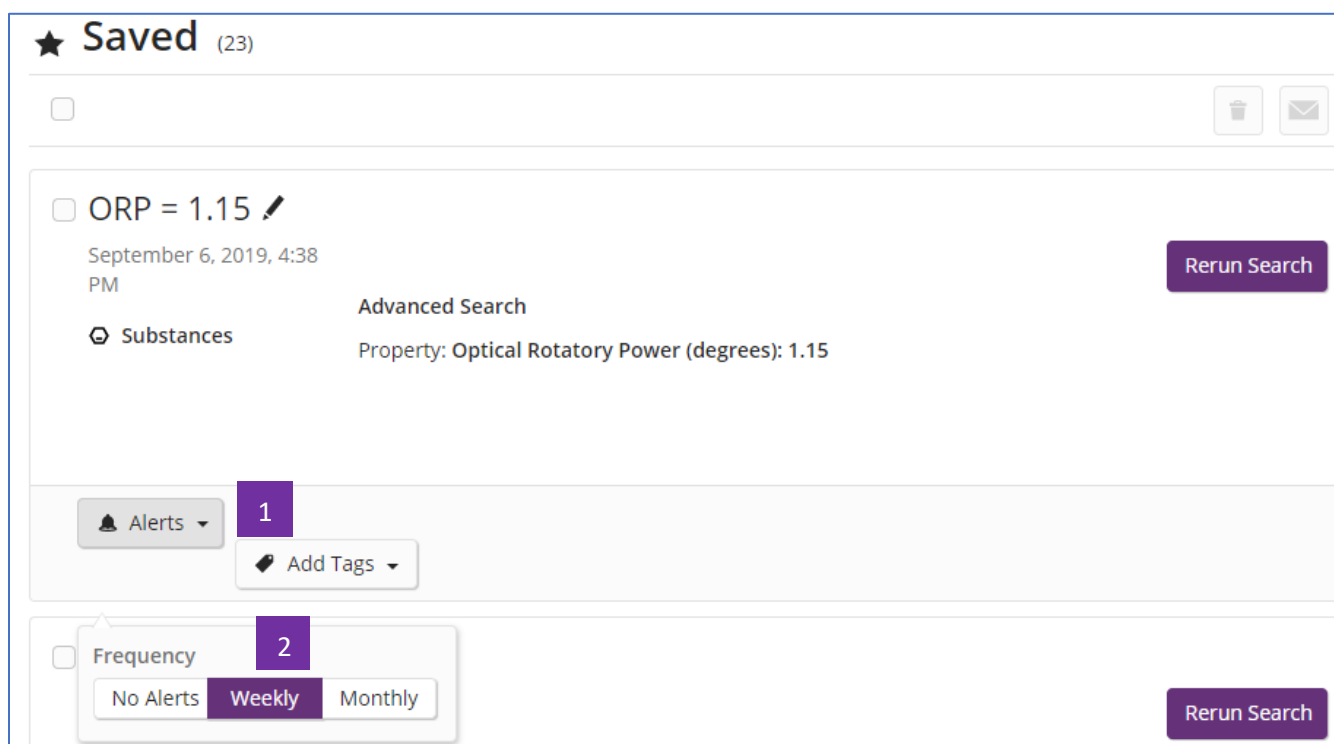
2 选择发送频率

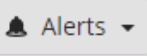
3. 设置物质检索结果集的Alert

The screenshot shows the SciFinder interface with a search for 'Substances' (108 results). A 'Save Search' dialog box is open, allowing the user to set up an alert. The dialog box has a 'Name' field containing 'ORP = |1.15', a 'Frequency' dropdown set to 'Weekly', and a 'Tags (optional)' field. A purple box with the number '2' highlights the 'Name' field, a purple box with the number '3' highlights the 'Tags' field, and a purple box with the number '4' highlights the 'Save' button. The background shows a list of substances, including '1179326-55-6' (D-Glucitol, 1,5-anhydro-1-C-[5-(4-nitrophenyl)-1,3,4-oxadiazol-2-yl]-, 2,3,4,6-t-...), '51-41-2' (Noradrenaline), and '1201917-29-4'.

- 1 在物质检索结果集中点击**Save**
- 2 在弹出窗口中输入保存名称
- 3 点击**Weekly**或者**Monthly**设置提醒频率
- 4 点击**Save**完成设置

如果保存过程中未设置**Alert**, 则可以打开已保存的结果集列表, 选择需要设置的结果集, 再进行设置:



- 1 然后点击 , 进行设置
- 2 选择发送频率

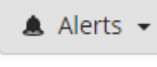
4. 设置反应检索结果集的Alert

The screenshot shows the SciFinder interface for searching reactions. On the left, there are filters for 'Structure Match' (As Drawn, Substructure, Similarity) and 'Yield' (90-100%, 80-89%, 70-79%, 50-69%, 30-49%). The main area displays 'Reactions (123)' with a 'Scheme 1' showing a reaction between a complex and a brominated benzene ring. A 'Save Search' dialog box is overlaid on the right, with four numbered callouts: 1 points to the 'Save' button in the top right of the main area; 2 points to the 'Name' input field containing 'ArCN'; 3 points to the 'Weekly' alert frequency button; 4 points to the 'Save' button at the bottom of the dialog.

- 1 在反应检索结果集中点击**Save**
- 2 在弹出窗口中输入保存名称
- 3 点击**Weekly**或者**Monthly**设置提醒频率
- 4 点击**Save**完成设置

如果保存过程中未设置Alert, 则可以打开已保存的结果集列表, 选择需要设置的结果集, 再进行设置:




The screenshot shows the 'Saved' section of the SciFinder interface. At the top, it says '★ Saved (24)'. Below this, there are two search results. The first result is for 'ArCN', dated 'September 6, 2019, 4:53 PM', with the label 'As Drawn'. It features a chemical reaction diagram showing a benzene ring with a cyano group (C≡N) and a hydrogen atom being added to form a benzene ring with a cyano group and a hydrogen atom. To the right of the diagram is a purple 'Rerun Search' button. Below the diagram, there is an 'Alerts' button with a bell icon and a dropdown arrow, and an 'Add Tags' button with a tag icon and a dropdown arrow. A purple box with the number '1' is placed over the 'Alerts' button. The second result is for 'Frequency', with options 'No Alerts', 'Weekly', and 'Monthly'. A purple box with the number '2' is placed over the 'Weekly' option. To the right of the 'Frequency' result is another purple 'Rerun Search' button.

1 点击 ，进行设置

2 选择发送频率

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：

1. 直接在物质结果集中点击 ，选择SDFFile，可以批量导出可编辑的结构数据文件。
2. 若需要导出某一物质结构数据文件，则可以点击该物质结构，在新窗口中点击 ，选择所需下载的结构数据文件格式(CXF, MOL, SDF)。
3. 若需要导出某一物质结构数据文件及其属性值，则可以点击substance detail，在新窗口中点击 ，同时下载的结构数据文件格式(CXF, MOL, SDF)和属性值(EXCEL)文件。

方法一


直接在物质结果集中点击 ，选择SDFFile，可以批量导出可编辑的结构数据文件。

The screenshot displays the SciFinder interface for searching substances. On the left, there are filter options for Commercial Availability, Reaction Role, Reference Role, Stereochemistry, Number of Components, Substance Class, Isotopes, and Metals. The main area shows a grid of substance cards. Each card includes a chemical structure, a name, a molecular formula (C₂₀H₃₄), and buttons for References, Reaction, and Suppliers. A dropdown menu is open over the first substance card, showing options: Download Results (PDF), Download Detailed Results (PDF (max 100)), SDFFile (.sdf), and Download Properties (Excel (.xlsx) (max 100)).

1 点击  按钮

2 选择SDF file

方法二


若需要导出某一物质结构数据文件，则可以点击该物质结构，在新窗口中点击  ，选择所需下载的结构数据文件格式(CXF, MOL, SDF)。

The screenshot displays the IDEK interface for the substance Ingenane (CAS RN 67707-88-4). The main window shows the chemical structure with absolute stereochemistry. A sidebar on the left contains navigation options like 'Substance Detail', 'Reactions (1)', and 'References (38)'. A dropdown menu is open over the 'Download Structure' button, with the 'SDFFile (.sdf)' option highlighted by a purple box labeled '2'. The download button icon itself is highlighted by a purple box labeled '1'.

1 点击  按钮

2 选择所需下载的结构数据文件格式 (CXF, MOL, SDF)

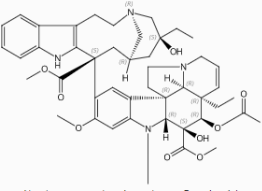
方法三

若需要导出某一物质结构数据文件及其属性值，则可以点击substance detail，在新窗口中点击 ，同时下载的结构数据文件格式(CXF, MOL, SDF)和属性值 (EXCEL) 文件。

Substance Detail (1 of 1)

References (23K) Reactions (400) Suppliers (41)

CAS Registry Number
865-21-4



Absolute stereochemistry shown, Rotation (-)

$C_{46}H_{58}N_4O_9$
Vincalukoblastine

Key Physical Properties	Value	Condition
Molecular Weight	810.97	-
Melting Point (Experimental)	211-216 °C	-
Density (Predicted)	1.37±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.36±0.60	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

Other Names

Experimental Properties

1 点击  按钮

2 所需下载的结构数据文件格式 (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。

结构式数据 SDF 文件下载示例：

```

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

```

```

57 58 2 0 0 0 0
M END
> <cas.rn>
865-21-4

> <cas.index.name>
Vincal leukoblastine

> <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:

							
Copyright © 2019 American Chemical Society (ACS). All Rights Reserved.							
CAS Registry Number:		865-21-4					
CAS Display Name:		Vinblastine					
Type	Category	Property	Value and Units	Temperature	Pressure	pH	
Experimental	Biological	Median Lethal Dose	15 mg/kg				
Experimental	Biological	Median Lethal Dose	15 mg/kg				
Experimental	Biological	Median Lethal Dose	7.3 mg/kg				
Experimental	Biological	Median Lethal Dose	5.6 mg/kg				
Experimental	Biological	Median Lethal Dose	3.12 mg/kg				
Experimental	Biological	Median Lethal Dose	0.34 mg/kg				
Experimental	Optical and Scattering	Optical Rotatory Power	+42 deg	26 °C			
Experimental	Optical and Scattering	Optical Rotatory Power	+42 deg	26 °C			
Experimental	Optical and Scattering	Optical Rotatory Power	+42 deg	26 °C			
Experimental	Optical and Scattering	Optical Rotatory Power	+40 deg	23 °C			
Experimental	Optical and Scattering	Optical Rotatory Power	+40 deg	23 °C			
Experimental	Optical and Scattering	Optical Rotatory Power	+31 deg	25 °C			
Experimental	Optical and Scattering	Optical Rotatory Power	-22 deg	25 °C			
Experimental	Optical and Scattering	Optical Rotatory Power	-32 deg	23 °C			
Experimental	Thermal	Melting Point	211-216 °C				
Experimental	Thermal	Melting Point	211-216 °C				
Experimental	Thermal	Melting Point	201-211 °C (decomp)				
Experimental	Thermal	Melting Point	201-211 °C				
Predicted	Biological	Bioconcentration Factor	1.0	25 °C		pH 1	
Predicted	Biological	Bioconcentration Factor	1.28	25 °C		pH 2	
Predicted	Biological	Bioconcentration Factor	1.50	25 °C		pH 3	
Predicted	Biological	Bioconcentration Factor	2.04	25 °C		pH 4	
Predicted	Biological	Bioconcentration Factor	13.9	25 °C		pH 5	

Combine 的应用

Combine功能：可用于对多个检索结果集（包括文献、物质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）。

The screenshot shows the SciFinderⁿ interface. At the top, there is a search bar with the text "Enter a query...". Below the search bar, there are several icons: a pencil for "Edit", a magnifying glass for search, a star for "Save", a clock for "History", and a user profile icon. The main content area is titled "Substances (143)". On the left, there are filters for "Structure Match" (As Drawn (3), Substructure (143), Similarity (1,841)) and "Analyze Structure Precision". Below these are "Filter by" options: "Commercial Availability" (Not Available (143)), "Reaction Role" (Product (110)), and "Reference Role". The main results area shows three substance cards. Each card has a chemical structure, a CAS number, a molecular formula, and a name. Below each card are buttons for "Reference", "Reactions", and "Suppliers". A purple box with the number "1" highlights the "Save" button in the top right corner of the results area. Another purple box with the number "2" highlights the "Combine" button in the top right corner of the results area.

1 点击Save，保存检索结果

2 打开保存的检索结果，进行Combine操作

SciFinderⁿ A CAS SOLUTION

References ▾ cataract and Metformin

Draw 🔍 ☆ 🕒 👤

Filter by

- Result Type
 - Patent Markush (2)
 - Reactions (38)
 - References (79)
 - Retrosynthesis (4)
 - Substances (46)
- Alerts
 - Unviewed (13)
- Tags
 - patent, Chinese, EOC (1)

Combine Saved Results **3**

Combine

★ Saved (169)

cataract and Metformin---Medline ✎

November 26, 2019, 12:08 PM

References cataract and Metformin + Filters

Rerun Search View Saved

Alerts Add Tags

cataract and Metformin---CPlus ✎

November 26, 2019, 12:05 PM

References cataract and Metformin + Filters

Rerun Search View Saved

3 点击Combine, 进行多个结果的逻辑处理

Combine Saved Results ✕

1 2 3

Select a Result Type:

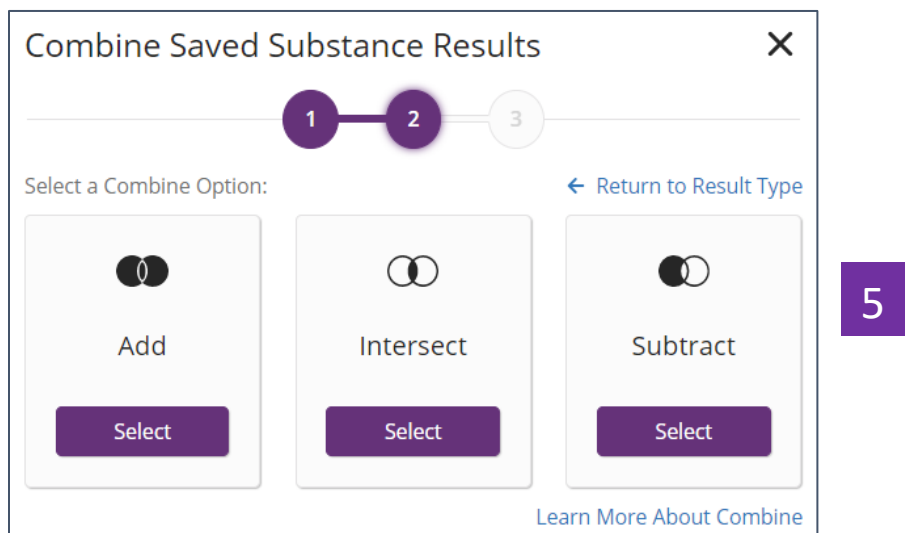
Substances Reactions References

Select Select Select

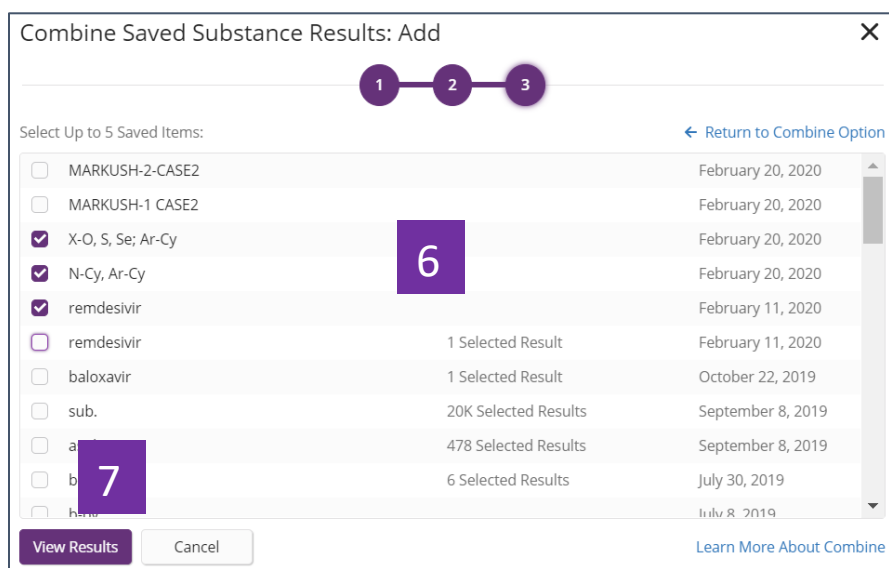
Learn More About Combine

4

4 选择需要处理的结果集类型



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

Alert 新增即时更新提醒设置

The screenshot shows the SciFinderⁿ interface with the search query "synthesis and antiviral prodrug". The "References" section displays 15,609 results. A "Save Search" dialog box is open, showing the search name "synthesis and antiviral prodrug" and alert frequency options: "No Alerts", "As Available" (selected), "Weekly", and "Monthly". The dialog also includes a "Tags (optional)" field with "patent, Chinese, EC" and a "New Tag (optional)" field. The "Save" button in the dialog is highlighted with a purple box and the number 3. The "Save" button in the top right of the search results is highlighted with a purple box and the number 1. The "As Available" option in the dialog is highlighted with a purple box and the number 2.

1 在检索结果集页面，点击右上角Save

2 在弹出窗口中点击As Available

3 点击Save，完成即时更新提醒功能的设置

The screenshot shows the SciFinder interface with a search for "synthesis and antiviral prodrug". The search results are displayed under a "Saved" folder. A purple box labeled "4" highlights the search title, and another purple box labeled "5" highlights the "Alerts" dropdown menu. The interface includes a search bar, a filter sidebar, and a frequency selection dropdown.

4 点击保存的文件夹，查看设置提醒的保存项

5 点击Alerts查看或更改设置提醒频率。更新的结果可以在此处查看，也会发送至账号对应的注册邮箱中

Alert 增添分类选项

The screenshot shows the SciFinder interface with the following elements:

- Top Bar:** SciFinder logo, search bar with "Reactions" dropdown and "Enter a query..." text, "Edit" button, search icon, star icon (highlighted with callout 1), clock icon, and user profile icon.
- Filter by sidebar:**
 - Result Type:** Reactions (1), References (19), Substances (4).
 - Alerts:** Unviewed (24) (highlighted with callout 2), Alerts Set (28), No Alerts (219).
 - Tags:** 29 as drawn (1), as drawn 23 (1).
- Combine Saved Results:** A "Combine" button.
- Migrate Alerts & Saved Results:** A "Migrate" button.
- Alerts List:**
 - Alert 1:** "phosphorescent material and OLED" (highlighted with callout 3), dated March 24, 2020, 11:54 AM. Category: References. Includes a "Rerun Search" button and an "Alerts" button with a notification icon.
 - Alert 2:** "X-O, S, Se; Ar-Cy", dated February 20, 2020, 9:57 AM. Category: Substances. Includes a "Rerun Search" button and a chemical structure image.

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（更新）信息），Alerts Set（已设置新增（更新），No Alerts（未设置新增（更新）提醒）

3 点击Alerts查看新增（更新）的信息

文献详情 Excel 格式导出

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 (15,609) Sort: Relevance View: Partial Abstract

50 Selected Substances Reactions Cited By

1

Download Results

- PDF
- Rich Text (.rtf)
- Download Detailed Results
- Citation (.ris)
- Excel (.xlsx)**
- PDF (max 100)
- Quoted (.txt)
- Rich Text (.rtf)
- Tagged (.txt)

2

Metabolism, Biochemical Actions, and Chemical Synthesis of Nucleosides, and Base Analogs

By: Shelton, Jadd; Lu, Xiao; Hollenbaugh, Joseph A.; Cho, Jong Hyun; Ambler, David L. Chemical Reviews (Washington, DC, United States) (2016), 116(23), 14379-14455.

A review. Nucleoside, nucleotide, and base analogs are used to treat both bacterial and viral pathogens and neoplasms. More than 200 analogs have been treated with one or more of these analogs. This review covers the anticancer nucleoside, nucleotide, and base analogs since 2000. The authors highlight the cellular mechanisms, and compound specificity toward various targets. Explore analog synthesis...

View More

Full Text Substances (0) Reactions (0) Cited By (86) Citation Map

1 在文献结果集页面，点击下载图标

2 选择Excel(.xlsx)，即可下载文献详情的Excel文件

Database	Title	Abstract	Author	Document Type	ISSN	Journal Title	Language	Volume	Issue	Page	Publication Year	Concepts	CAS Registry	Supplementary	Accession Num.	Chemical	Section	Section Cross	CODEN
Caplus	Metabolism, Biochemical Actions, and Chemical Synthesis of Nucleosides, and Base Analogs	A review. Nucleoside, nucleotide, and base analogs are used to treat both bacterial and viral pathogens and neoplasms. More than 200 analogs have been treated with one or more of these analogs. This review covers the anticancer nucleoside, nucleotide, and base analogs since 2000. The authors highlight the cellular mechanisms, and compound specificity toward various targets. Explore analog synthesis...	Shelton, Jadd; Lu, Xiao; Hollenbaugh, Joseph A.; Cho, Jong Hyun; Ambler, David L.	Journal, General Review	0009-2665	Chemical Reviews (Washington, DC, United States)	English	116	23	14379-14455	2016	Antitumor agents; Antiviral agents; AIDS (disease); Antiviral agents; Prodrugs	125780-98-5 ([1,1,1-trimethyl-2-(2-oxoethyl)pyrrolidine] hydrochloride)	1990198959	CAN 112198959	Carbohydrates; Nucleosides and Nucleotides; Cobalamins; Riboflavin	Pharmacology Reviews	Carbohydrates	JMCMAR
Caplus	Synthesis and evaluation of novel amide prodrugs of PMEA and PMPA	Some novel amide prodrugs of PMEA and PMPA have been synthesized and tested in vitro for their biol. activity.	Balatore, C.; McGuigan, C.; De Baiterni, J.	Journal	0960-894X	Bioorganic & Medicinal Chemistry Letters	English	11	6	1053-1056	2001	Antiviral agents; Nucleosides	942631-80-5 ([L-Alanine, N-[[[2-(6-amino-9H-purin-9-yl)-3-methylthio]methyl]amino]propanoic acid])	2001279043	CAN 13519860	Carbohydrates; Nucleosides and Nucleotides; Cobalamins; Riboflavin	Pharmacology; Amino Acids, Peptides, and Proteins	BIACLEB	
Caplus	Discovery of the First Cytosine Nucleoside HIV Nucleoside Polymerase Inhibitor (GS-6620) with Demonstrated Antiviral Response in HIV-1 Infected	Hepatitis C virus (HCV) infection presents an unmet medical need requiring more effective treatment options.	Cho, Aesop; Zhang, Lijun; Xu, Jie; Lee, Rick; Butler, Thomas; Mersbo, Sammy; Alkoudanakis, Vangelis; Lew, Willard; Ye, Hong; Clarke, Michael; et al.	Journal	0022-2623	Journal of Medicinal Chemistry	English	57	5	1812-1825	2014	Additivity (antiviral synergism for drug combinations); Antiviral agents; Biological permeation (of phosphoramidate prodrugs); Cytosine nucleosides	1431392-99-8 ([L-Alanine, (1S)-2-(2-chlorophenyl)-3-methylpropyl ester])	2013509459	CAN 160356475	Carbohydrates; Nucleosides and Nucleotides; Cobalamins; Riboflavin	Pharmacology	JMCMAR	

3 查看文献详情Excel文件

在导出的文件中查看检索过程

SciFinder®

Page 1

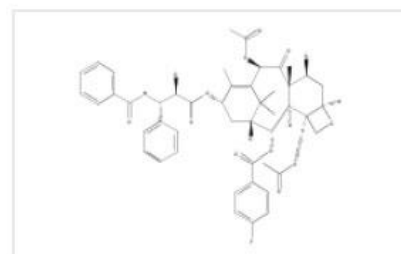


Task History

Initiating Search **1**

January 16, 2020, 11:10AM

References: 33069-62-4 docetaxel



Search Tasks **2**

Task	Search Type	View 3
Returned Reference Results	References	View Results
Viewed Reference Detail	References	View Detail
Exported: Retrieved Related Substance Results	Substances	View Results

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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，点击View Detail打开该记录的详情页面

其他

利用 Retrosynthesis 的产品反馈功能

为了提升客户的使用体验，CAS 诚挚欢迎您的使用反馈，以便我们根据您的需要不断提升 Retrosynthesis 的能力。

The screenshot displays the Retrosynthesis interface. On the left, there is a 'Step Key' section with 'Experimental' (red circle with arrow) and 'Predicted' (green circle with arrow) options, and a 'Plan Information' section showing 'Estimated Yield: 24%', 'Overall Price: \$358.10 (USD per 100 grams)', and 'Commercially Available: C, D, E, F, G'. The main area shows a reaction plan starting with a target molecule (A) and branching into reagents B, C, D, E, F, and G. A 'Feedback' button is located in the bottom right corner of the interface.


1 可以在Retrosynthesis的结果页面，点击Feedback图标，进行使用反馈

Plan Options
Powered by **ChemPlanner[®]**

Select Synthetic Depth

Synthetic depth restricts the number of steps generated in the plan. [Learn More.](#)

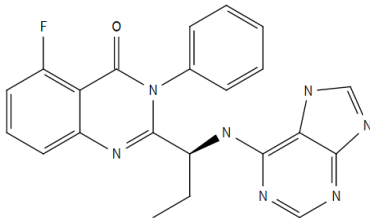
1
 2
 3
 4



Break and Protect Bonds

You may select one bond to break in the first step of the plan. Any bonds you protect will not break, though their order may change. [Learn More.](#)

Break Bond Protect Bond [Clear All Bond Selections](#)




Set Rules Supporting Predicted Reactions

Common rules are supported by many literature examples. Uncommon and Rare rules are supported by fewer examples, but may expose novel approaches. [Learn More.](#)

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

[Create Retrosynthesis Plan](#)

2


Feedback


2 也可在Retrosynthesis的Plan option页面点击Feedback图标，进行使用反馈

SciFinder[®] Feedback

We appreciate your feedback.
How can we improve your experience?

1000 Characters Remaining

3




SciFinder[®] Feedback


We appreciate your feedback.
How can we improve your experience?

992 Characters Remaining

Feedback|



4



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



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