

CAS SciFinder<sup>n</sup> 论坛

# 物质信息的获取

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ACS  
International



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# 提纲

- CAS和CAS SciFinder<sup>n</sup>简介
- CAS SciFinder<sup>n</sup> 物质检索方式
- 物质属性或谱图查询
- 在线演示以及Q&A

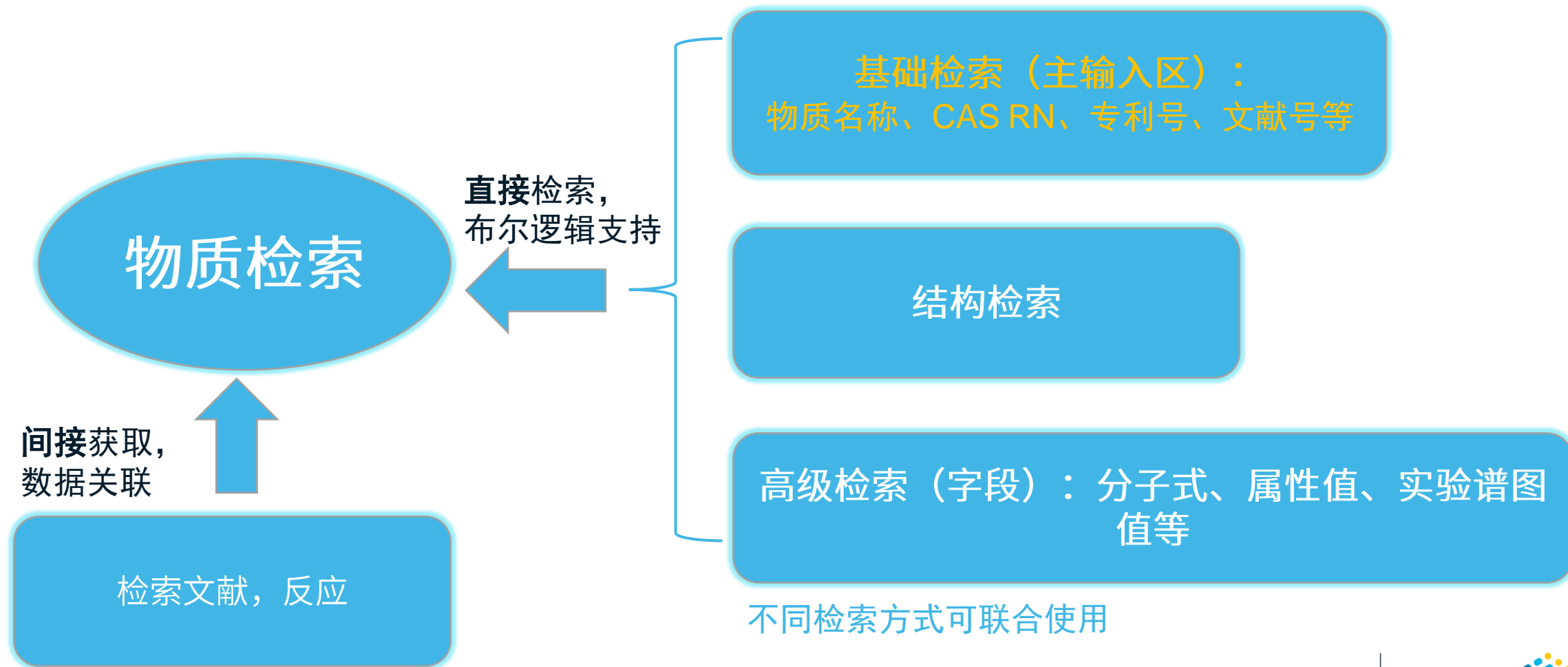


# CAS SciFinder<sup>n</sup>中覆盖的内容合集



来源: <https://www.cas.org/cas-data>和<https://www.cas.org/about/cas-content>

# 物质检索方法





# 丰富的物质检索方式




Searching for...

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


## Substances

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

Enter a query...  Draw 

 Molecular Formula   结构编辑器

在此输入物质名称, CAS号, 专利号或者其他文献ID号

 Add Advanced Search Field [Learn more about SciFinder<sup>®</sup> Advanced Search.](#)

Examples: C6H6 | (C8H8)<sub>x</sub> | C22H26CuN2O5.C2H3N

# 物质名称、CAS号检索

### Searching for...

All

**Substances**

Reactions

References

Suppliers

### Substances

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

kapton

Kapton

Kapton 100EN

Kapton 100H

Kapton 100VN

### Filter Behavior

Filter by Exclude

Commercial Availability

Reaction Role

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

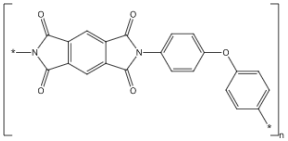
Reference Role

- Technical or Engineered Material Use (12)
- Uses (12)
- Properties (3)

### Substances (12)

Sort: Relevance View: Partial

References Reactions Suppliers Save And Alerts

<p>1</p> <p>25036-53-7</p>  <p><math>(C_{22}H_{10}N_2O_5)_n</math> Kapton</p> <p>14K References 2,102 Reactions 2 Suppliers</p>	<p>2</p> <p>240402-77-1</p> <p>Image Not Available</p> <p>Notes: Described as a Kapton Teflon coat material (Du Pont)</p> <p>Unspecified 120HR616</p> <p>1 Reference 0 Reactions 0 Suppliers</p>	<p>3</p> <p>2413839-54-8</p> <p>Image Not Available</p> <p>Notes: A Kapton type adhesive tape (As One Corp., Japan)</p> <p>Unspecified KS 100055</p> <p>1 Reference 0 Reactions 0 Suppliers</p>
--	--	---

### Searching for...

All

**Substances**

Reactions

References

Suppliers

### Substances

Search by Substance Name

25036-53-7

AND Molecular Formula

+ Add Advanced Search Field

# 由文献号或者专利号获取

## Searching for...

- All
- Substances**
- Reactions
- References
- Suppliers

## Substances

Search by Substance Name, CAS RN, Patent

10.1021/acs.jmedchem.5b01168

AND

+ Add A

CAS SciFinder<sup>®</sup> Substances 10.1021/acs.jmedchem.5b01168

Return to Home

### Substances (14)

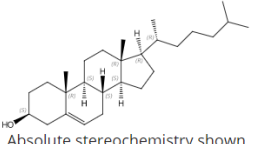
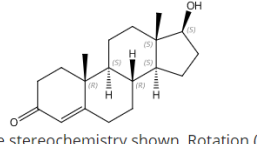

Sort: Relevance View: Partial

References Reactions Suppliers Save And Alerts

#### Filter Behavior

Filter by Exclude

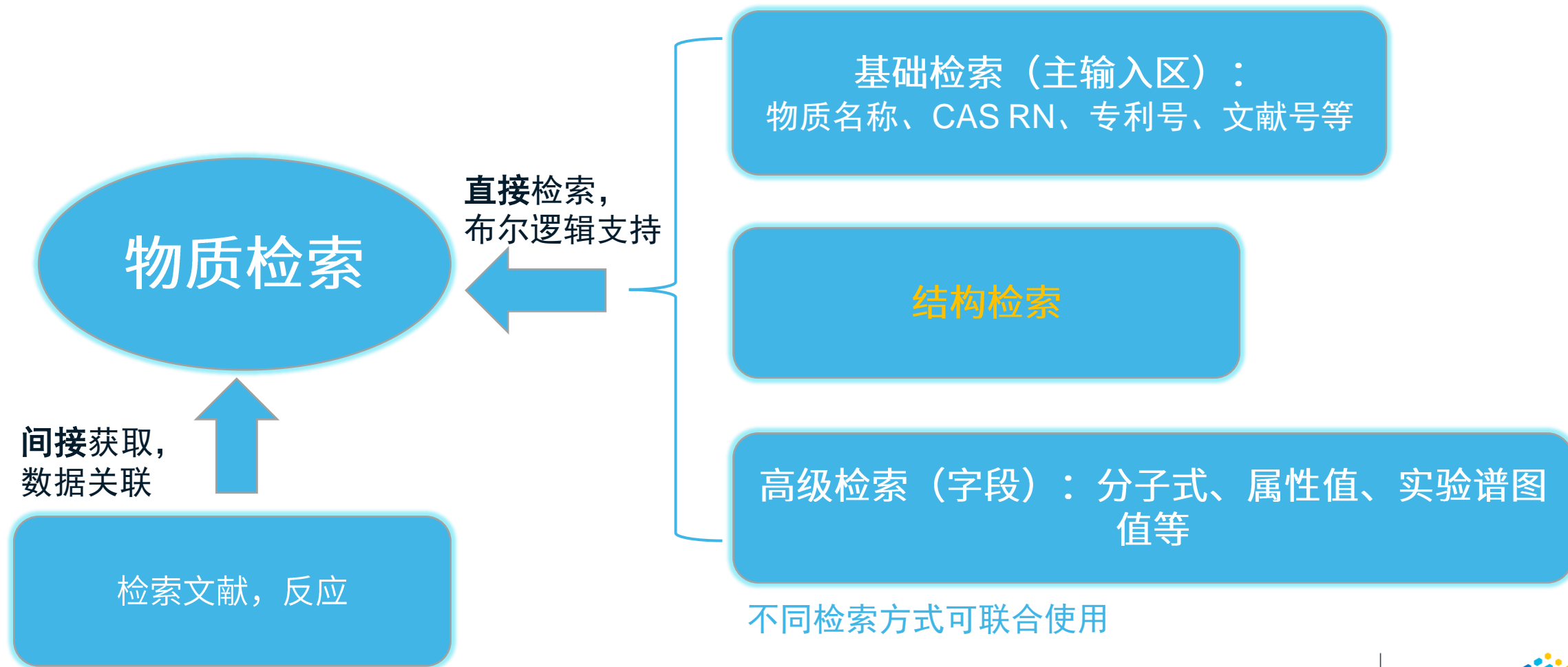
- Commercial Availability
  - Available (14)
- Reaction Role
  - Product (14)
  - Reactant (9)
  - Reagent (4)
  - Catalyst (2)
  - Solvent (2)
- Reference Role
  - Preparation (14)
  - Synthetic Preparation (14)
  - Uses (12)
  - Biological Study (11)

<input type="checkbox"/> 1 <b>57-88-5</b>  Absolute stereochemistry shown <b>C<sub>27</sub>H<sub>46</sub>O</b> Cholesterol 388K References 4,833 Reactions 157 Suppliers	<input type="checkbox"/> 2 <b>58-22-0</b>  Absolute stereochemistry shown, Rotation (+) <b>C<sub>19</sub>H<sub>28</sub>O<sub>2</sub></b> Testosterone 123K References 1,285 Reactions 83 Suppliers	<input type="checkbox"/> 3 <b>74-88-4</b>  <b>CH<sub>3</sub>I</b> Methyl iodide 120K References 264K Reactions 86 Suppliers
<input type="checkbox"/> 4	<input type="checkbox"/> 5	<input type="checkbox"/> 6

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Feedback

# 物质检索方法





# 结构绘制面板的介绍

## 重要绘制工具注释

**X** 选择可变基团

**R** 自定义R基团

[ ]<sub>1-4</sub> 重复工具

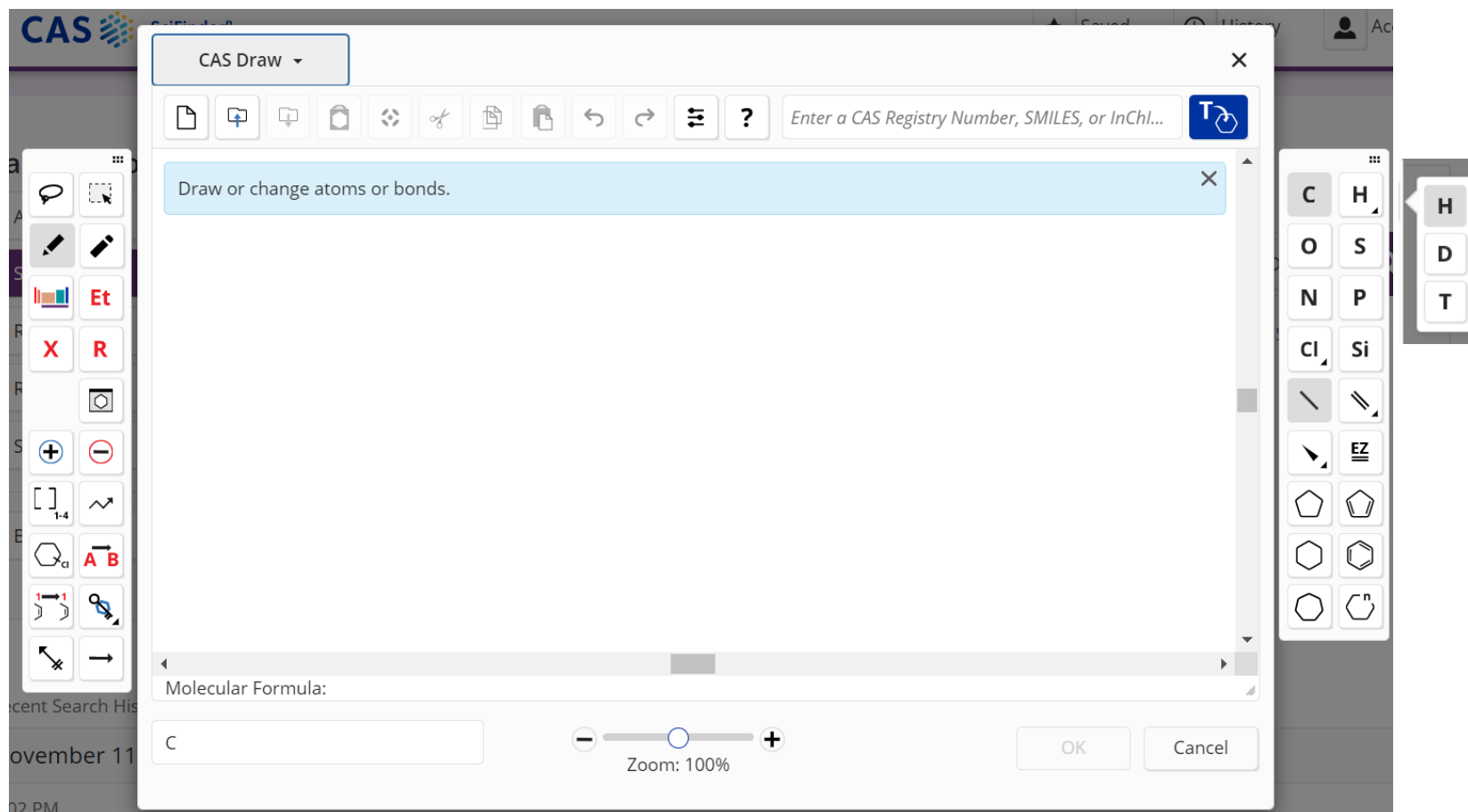
 取代位置可变

 锁定工具

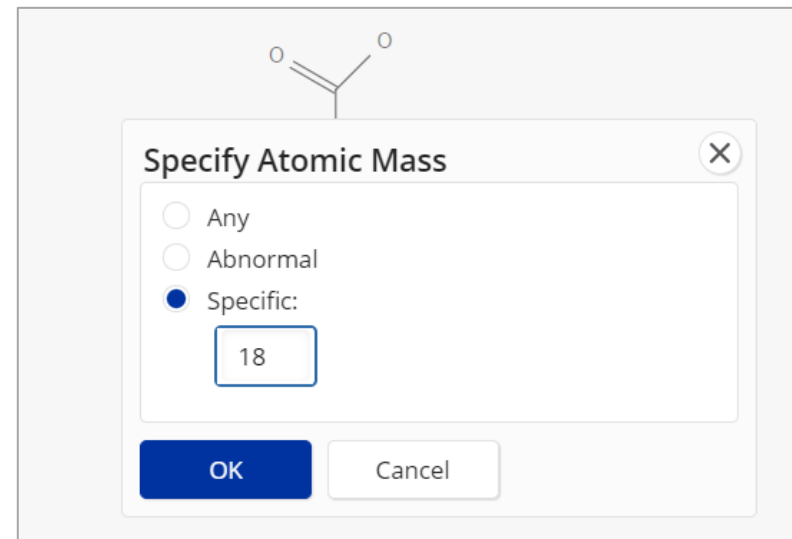
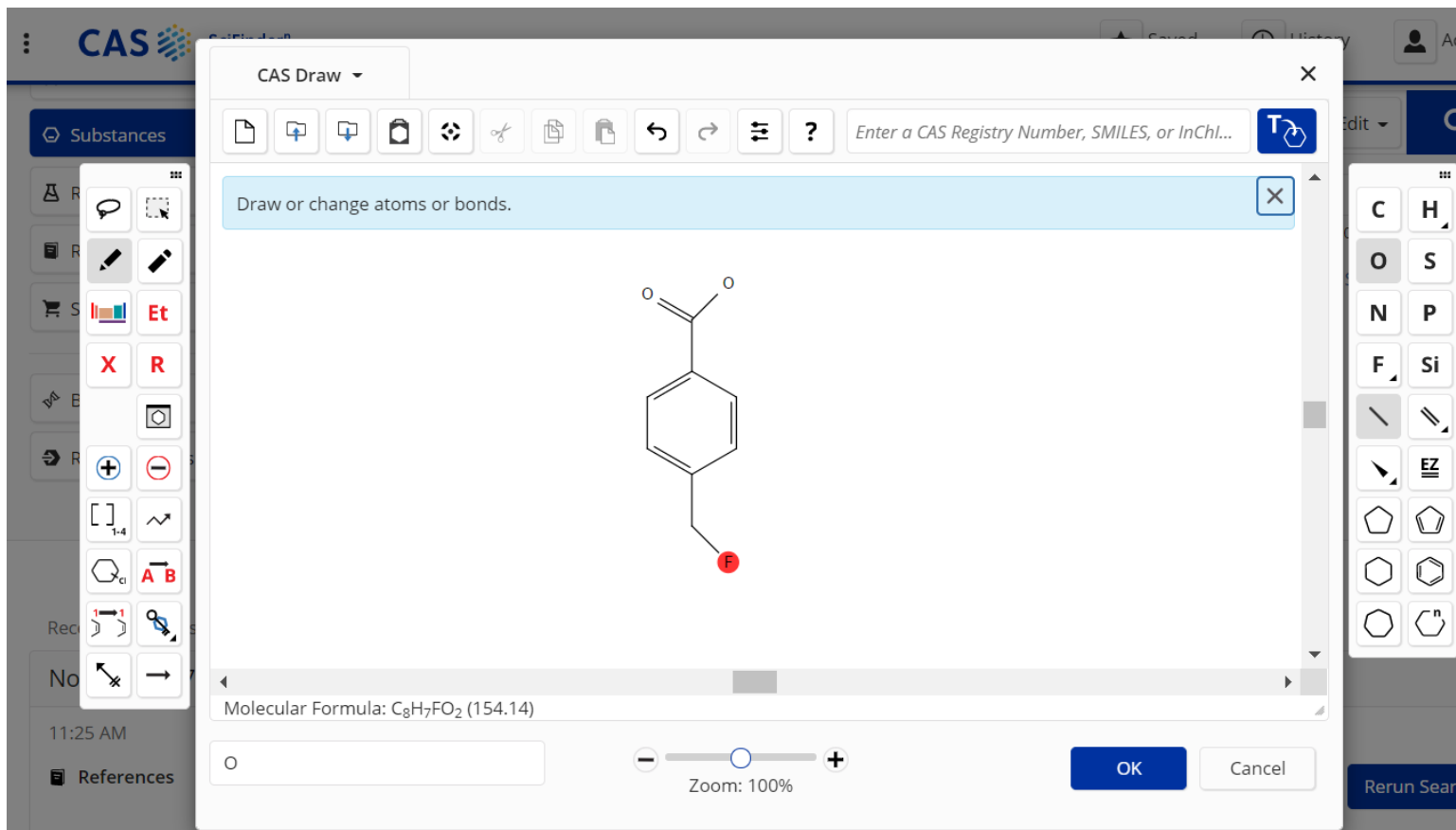
**A B** 反应角色标记

 原子标记

 化学键标记



# 结构绘图工具的使用：同位素原子的绘制



鼠标右键点击某原子，选中Abnormal获取其各种同位素的化合物，选择Specific可以精准输入具体的同位素质量数

# ChemDraw与SciFinder<sup>n</sup>联用检索的方法

- (1) 通过SMILES或InChI字符串切换
- (2) 直接在ChemDraw中Add-in SciFinder<sup>n</sup> (ChemDraw 18.2及以上版)
- (3) 通过MDL Molfile (.mol)文件导入

# (1)通过SMILES或InChI字符串切换

ChemDraw Professional - [Untitled Document-1 \*]

File Edit View Object Structure Text Curves Colors Search Add-ins Window Help

Undo Move Ctrl+Z  
Redo not available Shift+Ctrl+Z  
Cut Ctrl+X  
Copy Ctrl+C  
Paste Ctrl+V  
Clear Del  
Select All Ctrl+A  
Invert Selection Shift+Ctrl+I  
Repeat SMILES Ctrl+Y

Copy As > SMILES Alt+Ctrl+C  
Paste Special > SLN  
InChI  
InChI Key  
CDXML Text Ctrl+D  
MOL Text Alt+Shift+Ctrl+O  
MOL V3000 Text Alt+Ctrl+O  
HELM Alt+Ctrl+E  
HELM (Natural Analog)

Get 3D Model  
Insert File...  
Insert Object...  
Object

100%  
Arial 10  
B I U CH<sub>2</sub> X<sub>2</sub> X<sup>2</sup>

Chemical structure: Indole

C12=CC=CC=C1NC=C2

CAS Draw

Enter a single CAS Registry Number, SMILES string or InChI, then press [Enter] or click on the Add to Editor icon.

Examples:  
50-78-2  
CC(=O)Oc1ccccc1C(=O)O  
InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)

Click and drag to select objects. Ctrl-click to select or deselect individual objects.

Chemical structure: Indole

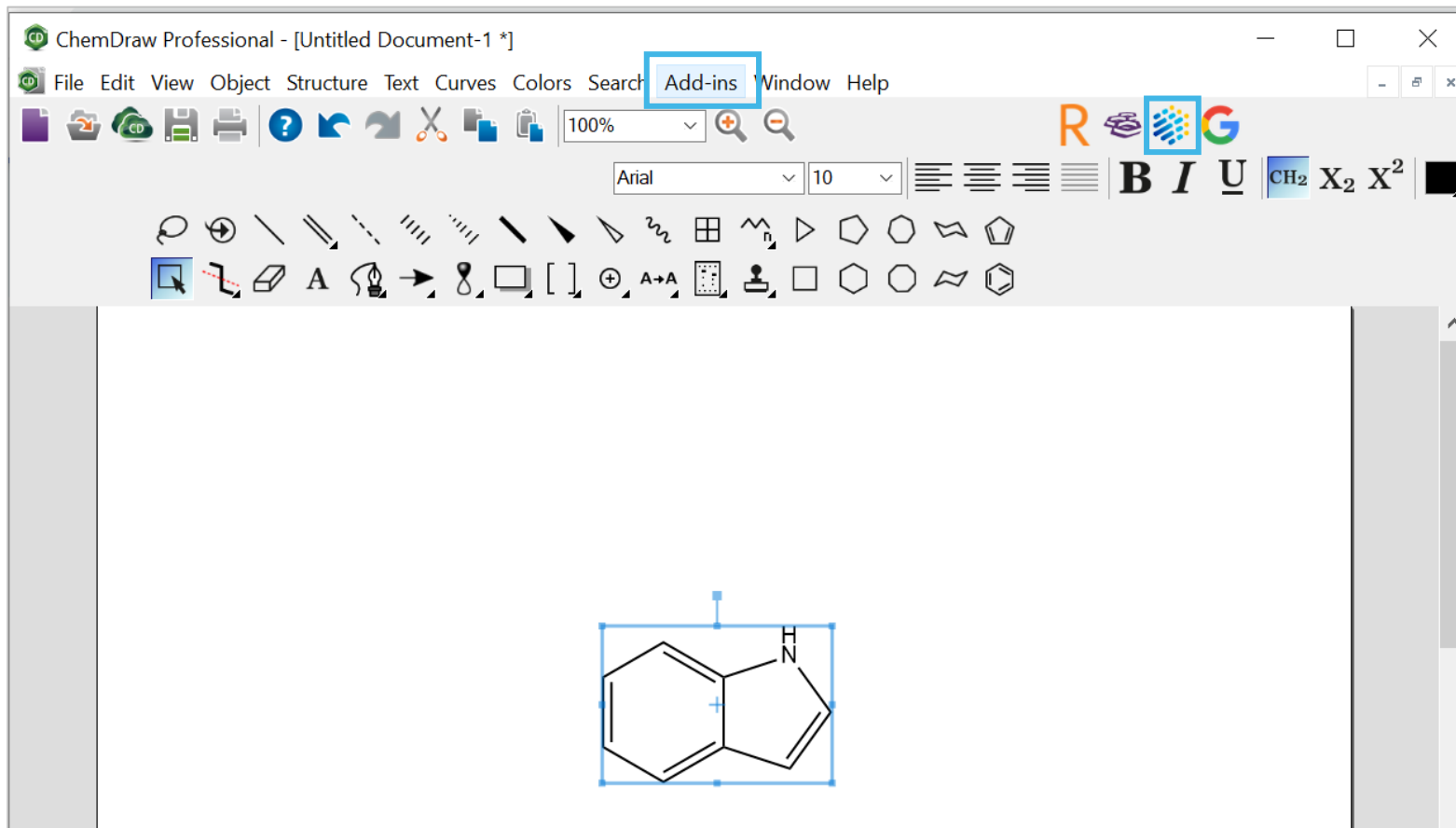
Molecular Formula: C<sub>8</sub>H<sub>7</sub>N (117.15)

Zoom: 100%

OK Cancel

## (2) 直接在ChemDraw中进入SciFinder<sup>n</sup>联用检索

点击ChemDraw菜单Add-ins列表中Search SciFinder<sup>n</sup>这项; 或点击CAS SciFinder<sup>n</sup>的新Logo



ChemDraw Add-in - Search SciFinder<sup>n</sup>

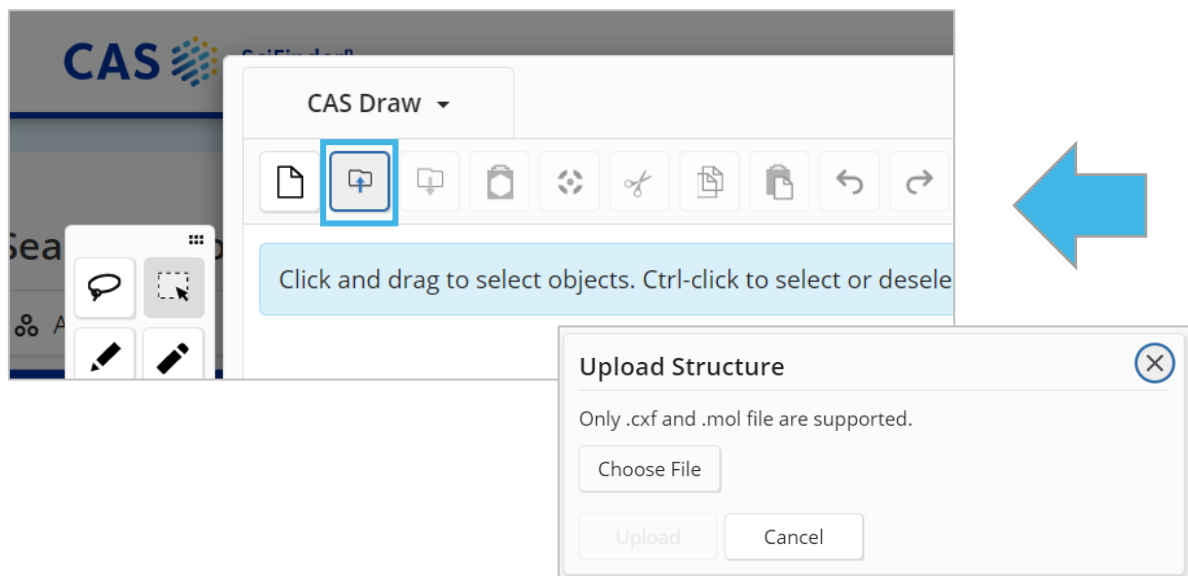
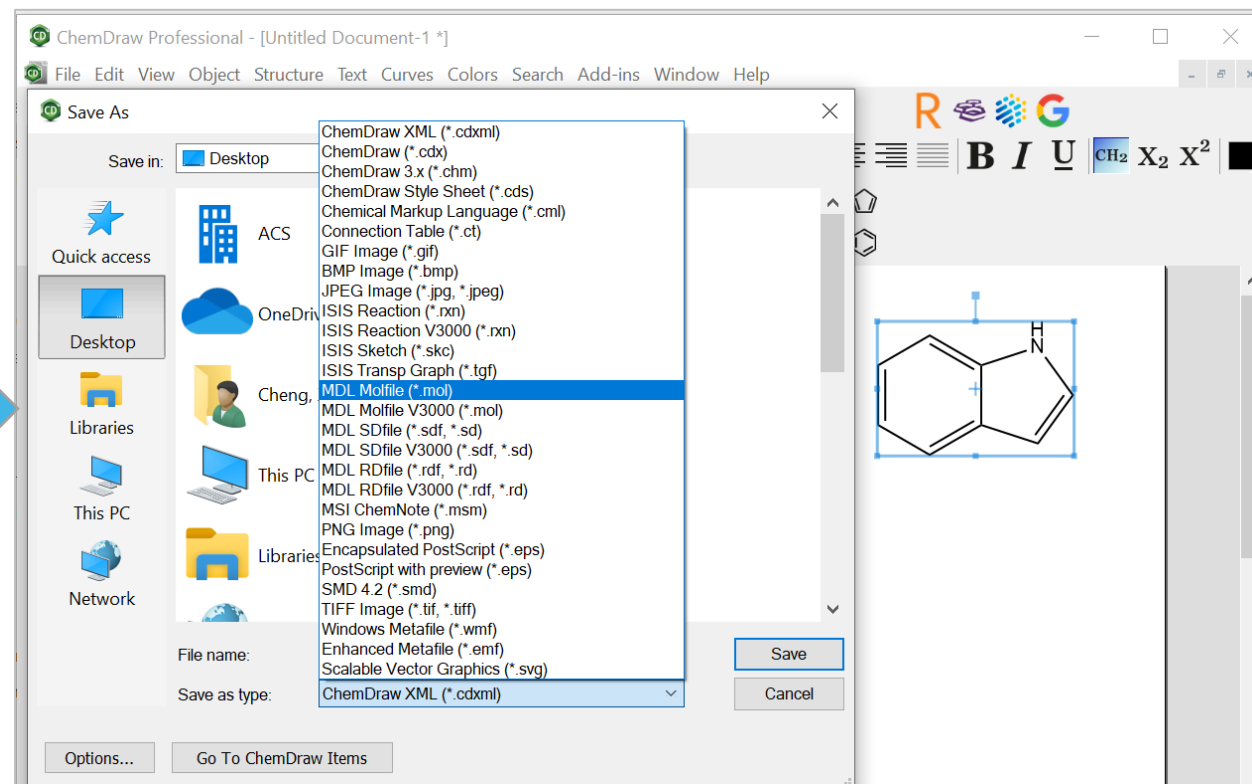
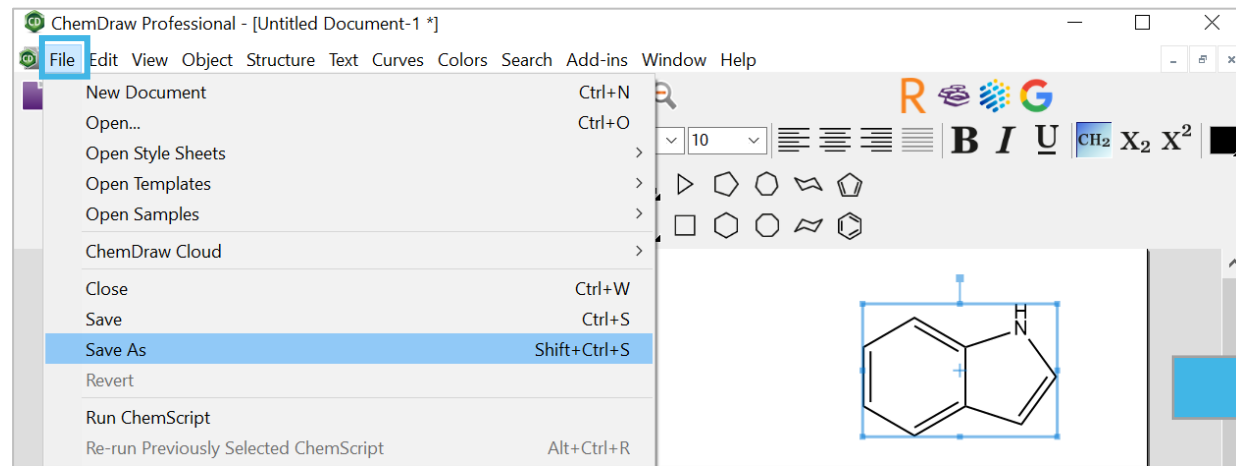
CAS SciFinder<sup>n</sup>

C1=CN=C2C=CC=CC2=C1

Search for...  
- Select -

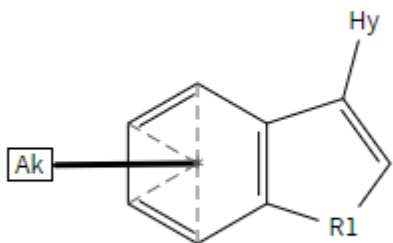
- Substances
- Reactions
- References
- Suppliers

# (3) 通过MDL Molfile 文件导入



# 结构式检索

获取物质结果集文献，反应和供应商信息



R1 = O, N, B



Structure Match

As Drawn (617)

**Substructure (28K)**

Similarity (73)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

[Learn more about Chemscape.](#)

**Create Chemscape Analysis**

Filter Behavior

**Filter by** Exclude

Commercial Availability

Available (14K)

Not Available (13K)

**Substances** (28,125)

References Reactions Suppliers

同时获取三个精准度的物质检索结果

1809096-52-9

C<sub>13</sub>H<sub>11</sub>NO  
3-(3-Furanyl)-5-methyl-1H-indole

1 Reference 5 Reactions 0 Suppliers

2559515-15-2

C<sub>14</sub>H<sub>13</sub>NO  
1H-Indole, 3-(2-furanyl)-2,6-dimethyl-

0 References 0 Reactions 1 Supplier

2477823-84-8

C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O  
Furo[3,2-c]pyridine, 4,5,6,7-tetrahydro-4-(6-methyl-1H-indol-3-yl)-

0 References 0 Reactions 1 Supplier

1443502-17-7

2535031-21-9

2110044-55-6

# 结构检索匹配维度

## ■ As Drawn:

绘制结构中可出现R基团、可变基团。绘制结构中价态未达饱和的原子只能接氢，环系（如有）不能与其他的环稠合或成桥环

## ■ Substructure:

包括As Drawn的检索稠合或成桥环结果，另外价态未达饱和的原子可以连接氢以外的其他原子，环系（如有）可以与其他环

## ■ Similarity:

绘制结构中不能出现R基团、可变基团，绘制的结构必须是一个确定的结构。获得片段或整体结构与被检索结构相似的物质，母体结构可以被取代，也可以被改变



# Filter by从物质角色、属性、活性、结构等多方面对结果进行分析

丰富直观的聚类分析，  
高效直观地纵览结果，  
便捷地选择或排除结果

The screenshot displays a search interface with a 'Filter Behavior' panel on the left and search results on the right. The 'Filter Behavior' panel includes a 'Filter by' button (highlighted in blue) and an 'Exclude' button. Below these are several expandable filter categories: Commercial Availability, Reaction Role, Reference Role, Stereochemistry, Number of Components, Substance Class, Isotopes, Metals, Molecular Weight, Experimental Property, Experimental Spectrum, Regulatory Data by Country, Regulatory Data by List, Bioactivity Indicator, Target Indicator, and Search Within Results. The search results are organized into a table with columns for 'Reference', 'Reactions', and 'Suppliers'. Two results are visible: 1) Reference 1443502-17-7, showing a chemical structure of 7-Methyl-3-(3-methyl-2-furanyl)-1H-indole with a molecular formula of C<sub>14</sub>H<sub>13</sub>NO, 1 Reference, 5 Reactions, and 0 Suppliers. 2) Reference 2534033-51-5, showing a chemical structure of Furo[2,3-c]pyridine, 4,5,6,7-tetrahydro-7-(6-methyl-1H-indol-3-yl)- with a molecular formula of C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O, 7 References, 5 Reactions, and 0 Suppliers.

# As Draw——检索盐或者同位素标记物

As Draw (16)

Substructure (24)

Similarity (24K)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
  - Salt and Compound With (8)
  - Organic/Inorganic Small Molecule (8)
- Isotopes
  - Containing Isotopes (7)
  - Not Containing Isotopes (9)

References Reactions Suppliers

1 610798-31-7  
  
C<sub>22</sub>H<sub>21</sub>N<sub>3</sub>O<sub>4</sub>  
Icotinib  
564 References 133 Reactions 39 Suppliers

2 1567366-94-2  
  
C<sub>22</sub>H<sub>16</sub>D<sub>5</sub>N<sub>3</sub>O<sub>4</sub>  
N-[3-(Ethynyl-2-d)phenyl]-7,8,10,11,13,14-hexahydro-10,11-d<sub>2</sub>[1,4,7,10]tetraoxacyclododecine  
2 References 22 Reactions 0 Suppliers

4 1567366-92-0  
  
C<sub>22</sub>H<sub>12</sub>D<sub>9</sub>N<sub>3</sub>O<sub>4</sub>  
N-[3-(Ethynyl-2-d)phenyl]-7,8,10,11,13,14-hexahydro-7,8,13,14-d<sub>4</sub>[1,4,7,10]tetraoxacyclododecine  
2 References 19 Reactions 0 Suppliers

5 1567366-91-9  
  
C<sub>22</sub>H<sub>20</sub>D<sub>N</sub>3O<sub>4</sub>  
N-[3-(Ethynyl-2-d)phenyl]-7,8,10,11,13,14-hexahydro[1,4,7,10]tetraoxacyclododecine  
2 References 2 Reactions 0 Suppliers

6 1567366-91-9  
  
C<sub>22</sub>H<sub>13</sub>D<sub>8</sub>N<sub>3</sub>O<sub>4</sub>  
N-[3-(Ethynyl-2-d)phenyl]-7,8,10,11,13,14-hexahydro[1,4,7,10]tetraoxacyclododecine  
2 Reference

7

8

9

# 片段结构的物质检索——亚结构

CAS SciFinder<sup>®</sup> Substances Enter a query... Edit

Return to Home

Structure Match

- As Drawn (0)
- Substructure (6,297)**
- Similarity (7,022)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components**
  - 1 (6,221)
  - 2 (73)
  - 3 (2)
  - 4 (1)
- Substance Class

Substances (6,221)

References Reactions Suppliers

Filtering: Number of Components: 1

Relevance View: Partial

Edit Drawing Remove

Search Patent Markush Clear All Filters

Number	CAS Number	Molecular Formula	Name	References	Reactions	Suppliers
1	2504948-44-9	C <sub>19</sub> H <sub>13</sub> NO <sub>2</sub>	4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-7-[2-(1 <i>H</i> -indol-6-yl)ethynyl]-	0	0	1
2	2605148-54-5	C <sub>17</sub> H <sub>13</sub> NO <sub>2</sub>	4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-2-(1 <i>H</i> -indol-4-yl)-	0	0	1
3	2536496-10-1	C <sub>19</sub> H <sub>13</sub> NO <sub>2</sub>	4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-7-[2-(1 <i>H</i> -indol-5-yl)ethynyl]-	0	0	1
4	2515451-53-1	C <sub>17</sub> H <sub>13</sub> NO <sub>2</sub>	4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-2-(1 <i>H</i> -indol-6-yl)-	0	0	1
5	725252-13-1	C <sub>17</sub> H <sub>13</sub> NO <sub>2</sub>	2,3-Dihydro-3-(1 <i>H</i> -indol-3-yl)-4 <i>H</i> -1-benzopyran-4-one	2	2	0
6	2576898-59-2	C <sub>19</sub> H <sub>13</sub> NO <sub>2</sub>	4 <i>H</i> -1-Benzopyran-4-one, 2,3-dihydro-6-[2-(1 <i>H</i> -indol-6-yl)ethynyl]-	0	0	1

# 相似结构检索

推荐使用确定的结构进行Similarity检索

CAS SciFinder<sup>®</sup> Substances Enter a query... Edit

Similarity (600K)

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Similarity

- $\geq 99$  (1)
- 90-94 (11)
- 85-89 (231)
- 80-84 (3,271)
- 75-79 (17K)

1 100

2259861-89-5

C59H34F2N2O  
N-Benzo[*b*]naphtho[2,1-*d*]furan-9-yl-*N*-(2',7'-difluoro-9,9'-spirobi[9*H*-fluoren]-3-

2 100

2200307-54-4

C57H34F2N2O  
Spiro[acridine-9(10*H*),7'-[7*H*]dibenzo[*c,g*]fluoren]-5'-amine, *N*-(6-fluoro-4-dibenz...

3 100

93

93-33-3

C56H34F2N2O  
9*H*-Carbazol-2-amine, *N*-(2',7'-difluoroospiro[7*H*-benzo[*b*]fluoreno[3,4-*d*]furan-7,9'...

4 92

2740545-65-5

5 92

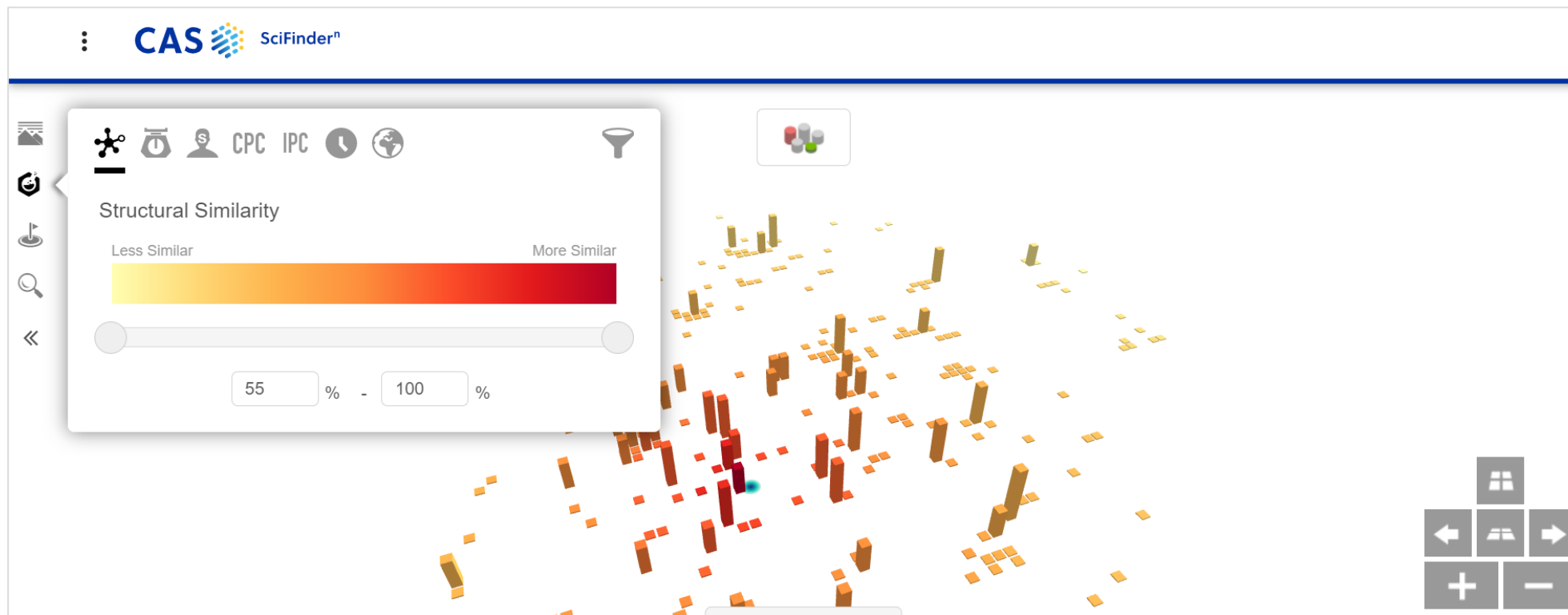
2699902-30-0

6

2200307-34-0

Feedback

# 对结构检索结果集进行可视化分析：发现物质研究空白及专利布局

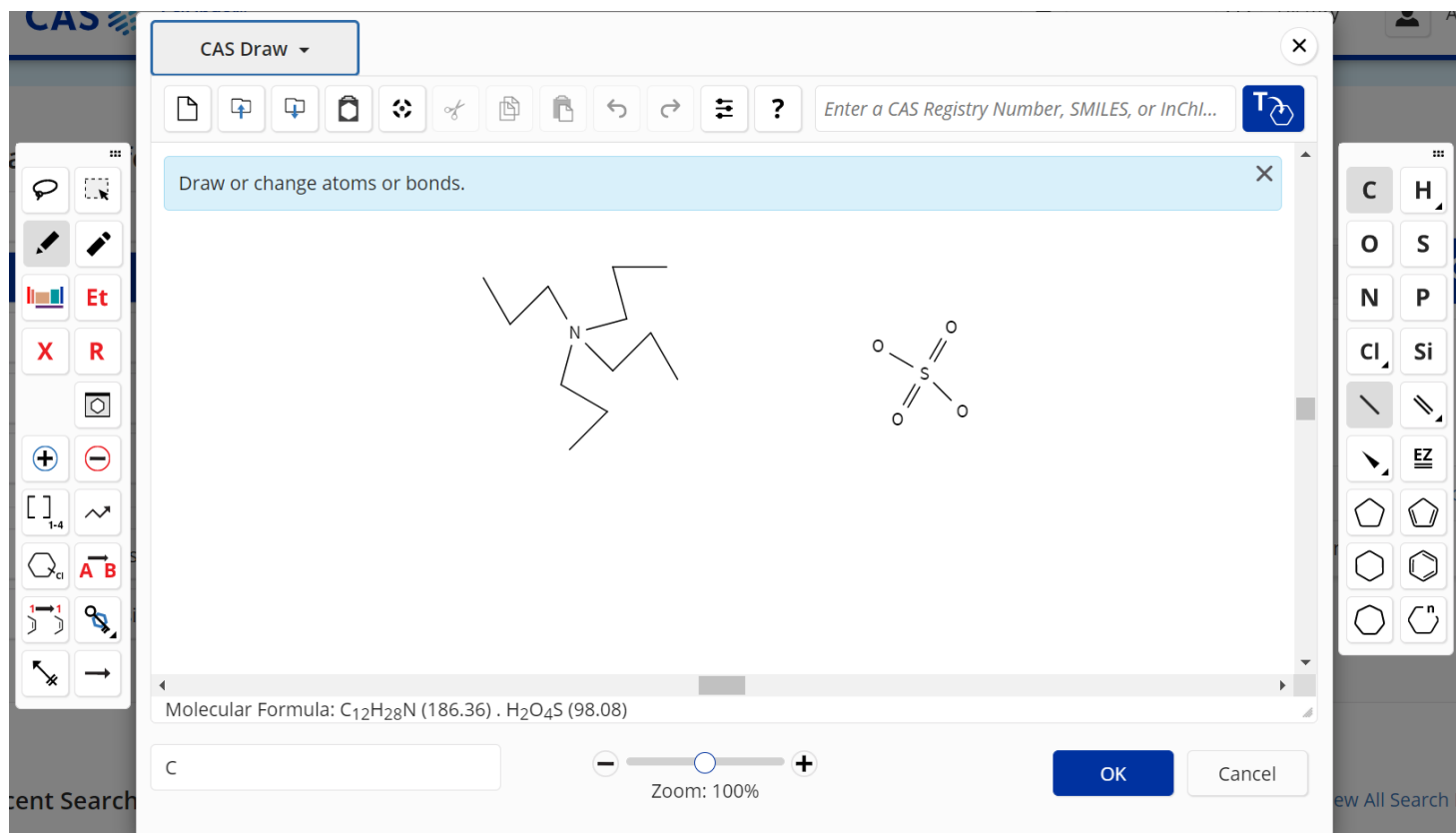


# 对结构检索结果集进行可视化分析：发现物质研究空白及专利布局



# 案例1：季铵盐的检索

方法一：绘制不同组分，忽略化合价



# 获得所需结果

Number of Components

- 2 (672)
- 3 (206)
- 4 (35)
- 5 or more (6)

Substance Class

- Salt and Compound With (672)
- Coordination Compound (60)
- Protein/Peptide Sequence (15)
- Polymer (5)

CAS SciFinder®

Substances

References  Reactions  Suppliers

Filtering: Number of Components: 2  Substance Class: Salt and Compound With  [Clear All Filters](#)

AS Drawn (3)  Substructure (1,094)  Similarity (18K)

Analyze Structure Precision

Chemscape Analysis

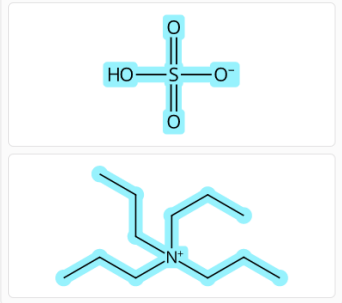
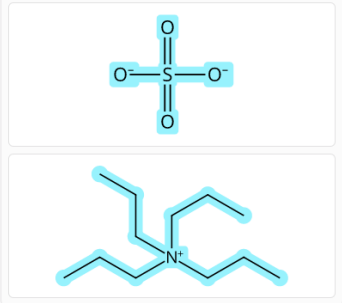
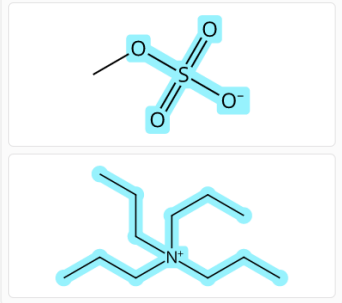
Visually explore structure similarity with a powerful new tool. [Learn more about Chemscape.](#)

[Create Chemscape Analysis](#)

Filter Behavior

Commercial Availability

- Available (39)
- Not Available (633)

1	2	3
		
<b>56211-70-2</b>	<b>28462-80-8</b>	<b>1242155-35-6</b>
$C_{12}H_{28}N.HO_4S$ Components: 2 Tetrapropylammonium hydrogen sulfate	$C_{12}H_{28}N.^{1/2}O_4S$ Components: 2 1-Propanaminium, <i>N,N,N</i> -tripropyl-, sulfate (2:1)	$C_{12}H_{28}N.CH_3O_4S$ Components: 2 1-Propanaminium, <i>N,N,N</i> -tripropyl-, methyl sulfate (1:1)

[Feedback](#)



# 方法二：绘制其中一部分结构



# 在结果集中通过另外组分结构筛选

^ Number of Components


- 2 (677)
- 3 (206)
- 4 (35)
- 5 or more (6)

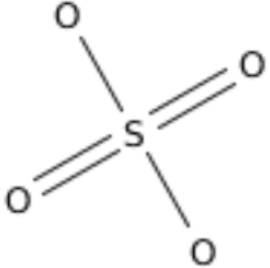
^ Substance Class

- Salt and Compound With (677)
- Coordination Compound (60)
- Protein/Peptide Sequence (15)
- Polymer (5)

^ Search Within Results

Search for up to 3 structures within the result set.

 Edit



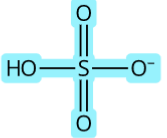
As Drawn

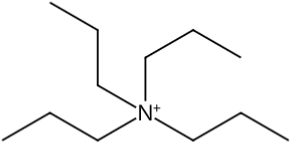
Substructure

Search

1

56211-70-2



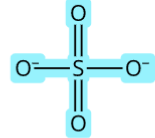


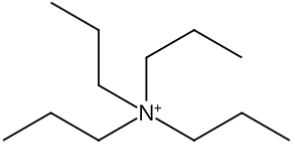
$C_{12}H_{28}N.HO_4S$   
Components: 2  
Tetrapropylammonium hydrogen sulfate

33 References 6 Reactions 49 Suppliers

2

28462-80-8



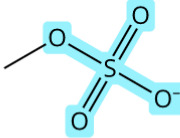


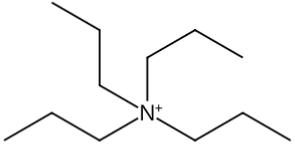
$C_{12}H_{28}N.^{1/2}O_4S$   
Components: 2  
1-Propanaminium, *N,N,N*-tripropyl-, sulfate (2:1)

13 References 2 Reactions 2 Suppliers

3


1242155-35-6





$C_{12}H_{28}N.CH_3O_4S$   
Components: 2  
1-Propanaminium, *N,N,N*-tripropyl-, methyl sulfate (1:1)

1 Reference 0 Reactions 0 Suppliers

 Feedback

# 案例2：双膦配体-镍基手性催化剂检索

Searching for...

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

## Substances

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

Enter a query...

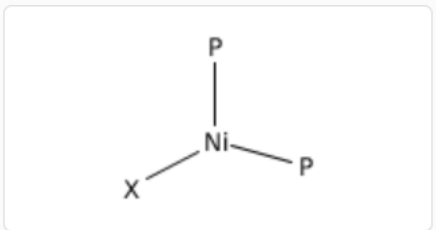
AND Molecular Formula

[+ Add Advanced Search Field](#)

Examples: C<sub>6</sub>H<sub>6</sub> | (C<sub>8</sub>H<sub>8</sub>)<sub>x</sub> | C<sub>2</sub>

[Learn more about SciFinder](#)

Edit



Edit Drawing Remove

Search Patent Markush

# 选择物质结果集中带有立体键的结果

Properties (110)

Catalyst Use (77)

Uses (77)

[View All](#)

^ Stereochemistry

Stereo in Answer Structure (238)

No Stereo in Answer Structure (13K)

^ Number of Components

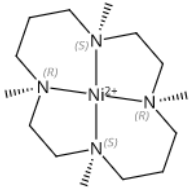
^ Substance Class

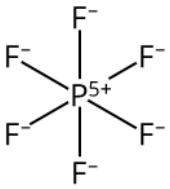
Coordination Compound (238)

^ Isotopes

^ Metals

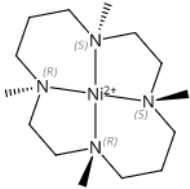
^ Molecular Weight

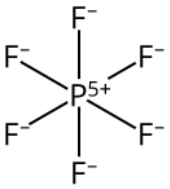
  
Relative stereochemistry shown



**C<sub>14</sub>H<sub>32</sub>N<sub>4</sub>Ni.2F<sub>6</sub>P**  
Components: 2  
Nickel(2+), (1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane-κN<sup>1</sup>,κN<sup>4</sup>,κN<sup>8</sup>,...

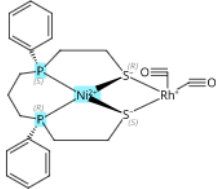
4 References   1 Reaction   0 Suppliers

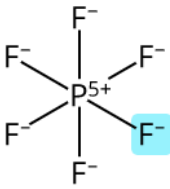
  
Relative stereochemistry shown



**C<sub>14</sub>H<sub>32</sub>N<sub>4</sub>Ni.2F<sub>6</sub>P**  
Components: 2  
Nickel(2+), (1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane-κN<sup>1</sup>,κN<sup>4</sup>,κN<sup>8</sup>,...


2 References   0 Reactions   0 Suppliers

  
Relative stereochemistry shown



**C<sub>21</sub>H<sub>24</sub>NiO<sub>2</sub>P<sub>2</sub>RhS<sub>2</sub>.F<sub>6</sub>P**  
Components: 2

1 Reference   2 Reactions   0 Suppliers

 Feedback

# 可通过物质的Reaction role或者Reference role筛选物质

Reaction Role

- Product (62)
- Reactant (15)
- Catalyst (57)

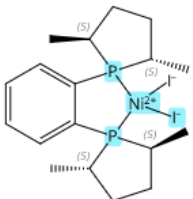
Reference Role

- Catalyst Use (57)
- Uses (57)
- Preparation (49)
- Synthetic Preparation (48)
- Properties (23)

[View All](#)

4

220502-56-7



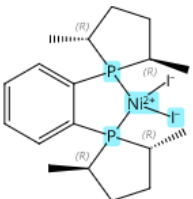
Absolute stereochemistry shown

**C<sub>18</sub>H<sub>28</sub>I<sub>2</sub>NiP<sub>2</sub>**  
(*SP*-4-2)-Diiodo[(*2S,2'S,5S,5'S*)-1,1'-(1,2-phenylene)bis[2,5-dimethylphospholane-...]]

3 References   5 Reactions   0 Suppliers

5

332131-31-4



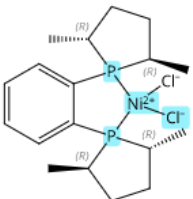
Absolute stereochemistry shown

**C<sub>18</sub>H<sub>28</sub>I<sub>2</sub>NiP<sub>2</sub>**  
(*SP*-4-2)-Diiodo[(*2R,2'R,5R,5'R*)-1,1'-(1,2-phenylene)bis[2,5-dimethylphospholane-...]]

2 References   5 Reactions   0 Suppliers

6

332131-30-3



Absolute stereochemistry shown


**C<sub>18</sub>H<sub>28</sub>Cl<sub>2</sub>NiP<sub>2</sub>**  
Nickel, dichloro[(*2R,2'R,5R,5'R*)-1,1'-(1,2-phenylene)bis[2,5-dimethylphospholane-...]]

3 References   3 Reactions   0 Suppliers

Feedback

# 结果符合检索需求

Scheme 1 (1 Reaction) Steps: 1 Yield: 83%



Suppliers (2)

Absolute stereochemistry shown,  
Rotation (-)

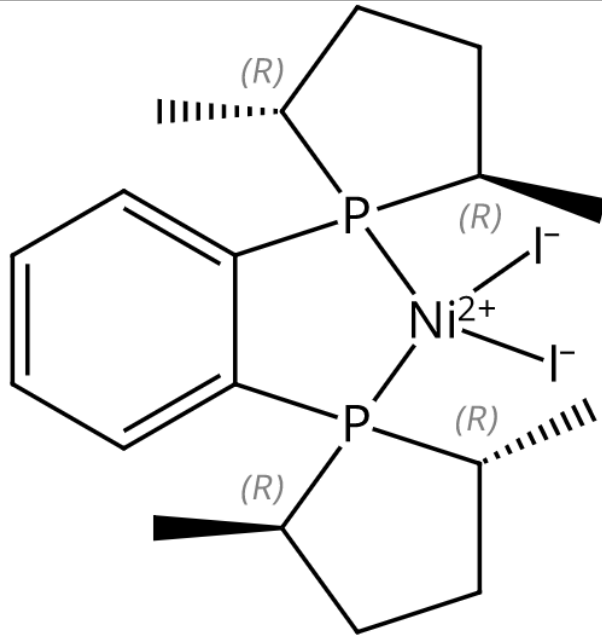
Reaction Summary Steps: 1 Yield: 83%

1.1 Reagents: [Lithium triethylborohydride](#)  
Catalysts: [\(SP-4-2\)-Diiodo\[\(2R,2'R,5R,5'R\)-1,1'-\(1,2-phenylene\)bis\[2,5-dimethylphospholane-...\]](#)  
Solvents: [Toluene](#), [Tetrahydrofuran](#); 72 h, -20 °C

CAS RN  
**332131-31-4**

CAS Name  
[\(SP-4-2\)-Diiodo\[\(2R,2'R,5R,5'R\)-1,1'-\(1,2-phenylene\)bis\[2,5-dimethylphospholane-...\]](#)

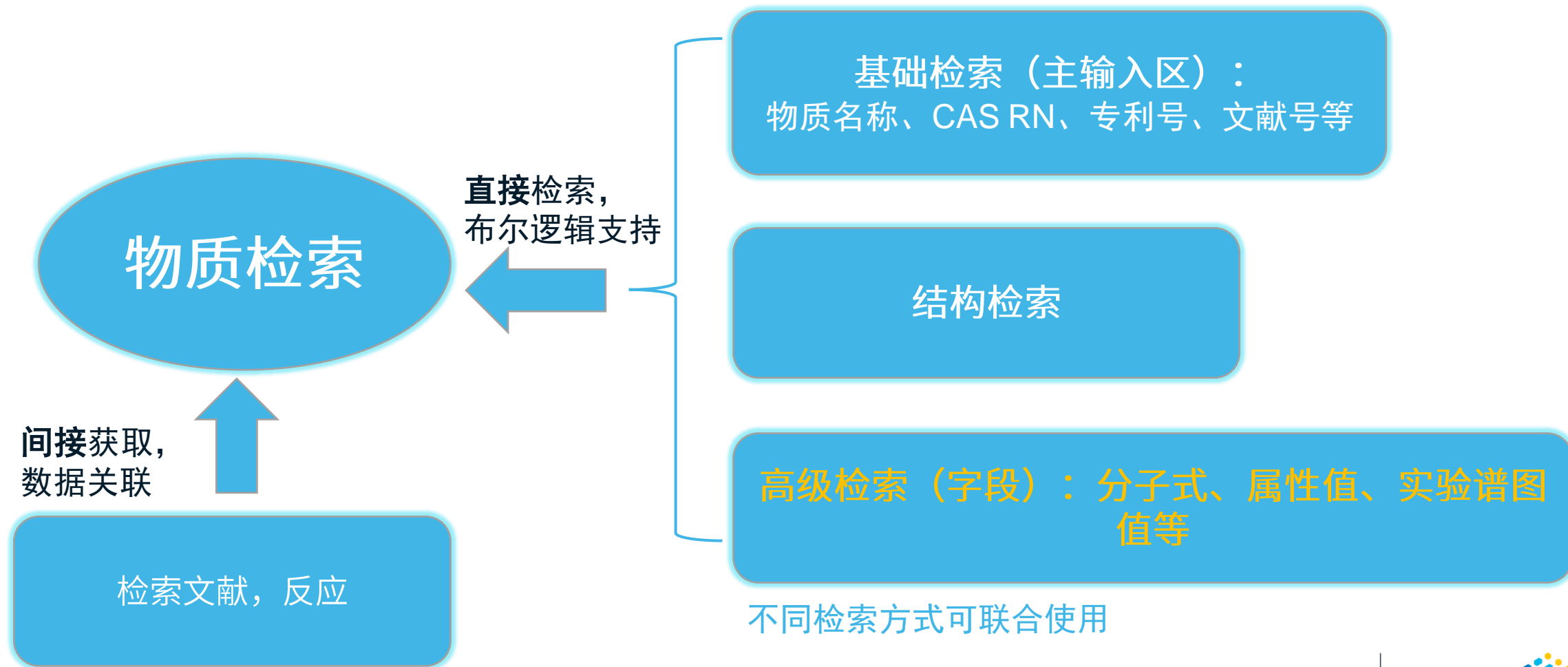
- [Substance Detail](#)
- [Reactions \(5\)](#)
- [Synthesize \(0\)](#)
- [Start Retrosynthetic Analysis](#)
- [References \(2\)](#)
- [Suppliers \(0\)](#)



Absolute stereochemistry shown

Edit Structure    -    Reset    +    Download

# 物质检索方法





# 物质检索-高级检索


Searching for...

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

Substances

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

Enter a query...  Draw 

Molecular Formula 

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

Learn more about SciFinder<sup>®</sup> Advanced Search.


通过运算符连接不同的字段进行高级检索

- Molecular Formula
- CAS Registry Number
- Chemical Name
- Document Identifier
- Patent Identifier
- Experimental Spectra >
- Biological >
- Chemical Properties >
- Density >
- Electrical >
- Lipinski >
- Magnetic >
- Mechanical >
- Optical and Scattering >
- Structure Related >
- Thermal >

Recent Search History

November 26, 2021

12:46 PM

 References (tlr or "toll like re

Rerun Search

Edit Search



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

满足要求的结果

Searching for...

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

Substances

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

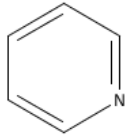
Enter a query...

AND Molecular Weight 125 to 349  
Predicted values only. *Examples: 46.*

AND Carbon-13 NMR 115,141  
Allowance of  $\pm 2$  ppm. *Examples: 152.3, 127.6, 133.1*

[Add Advanced Search Field](#)

[Edit](#) [Search](#)



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

Search Patent Markush

[Learn more about SciFinder](#)

Structure Match

- As Drawn (0)
- Substructure (647)**
- Similarity (0)

Analyze Structure Precision

Chemscape Analysis

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

[Create Chemscape Analysis](#)

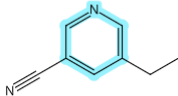
Filter Behavior

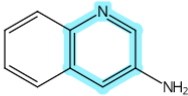
[Filter by](#) [Exclude](#)

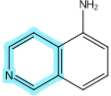
Substances (647)

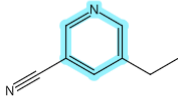
Sort: Relevance View: Partial

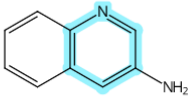
References  Reactions  Suppliers

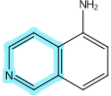
1 61391-07-9   
C8H8N2  
5-Ethyl-3-pyridinecarbonitrile  
4 References 2 Reactions 15 Suppliers

2 580-17-6   
C9H8N2  
3-Aminoquinoline  
1,605 References 1,877 Reactions 81 Suppliers

3 1125-60-6   
C9H8N2  
5-Aminoisoquinoline  
668 References 1,147 Reactions 111 Suppliers

4 55758-02-6   
C8H8N2  
5-Ethyl-3-pyridinecarbonitrile  
4 References 2 Reactions 15 Suppliers

5 51984-46-4   
C9H8N2  
3-Aminoquinoline  
1,605 References 1,877 Reactions 81 Suppliers

6 211371-96-9   
C9H8N2  
5-Aminoisoquinoline  
668 References 1,147 Reactions 111 Suppliers

# 案例2：获取玻璃体转化温度在50-100摄氏度之间；密度小于1.5g/cm<sup>3</sup>的聚合物

Searching for...

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

## Substances

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

poly\* ✕ Draw 🔍

AND ▼ Glass Transition Temperature (°C) ▼ 50 to 100 ✕  
Experimental values only. *Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2*

AND ▼ Density (g/cm<sup>3</sup>) ▼ <1.5 ✕  
 Include predicted values. *Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2*

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

# 获得的结果均满足检索需求

### Filter Behavior

**Filter by** Exclude

Commercial Availability

- Available (98)
- Not Available (10)

Reaction Role

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

Reference Role

- Preparation (108)

## Substances (108)

References Reactions Suppliers

25248-42-4

$(C_6H_{10}O_2)_n$   
**Polycaprolactone**

38K References 3,224 Reactions

### Substance Detail (1 of 107)

References (37K) Reactions (3,067) Suppliers (8)

CAS Registry Number  
25248-42-4

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

Polymer Class Terms  
Polyester

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

Experimental Properties

Biological	Chemical	Density	Electrical	Flow and Diffusion	Interface	Mechanical	Optical and Scattering	Structure Related	Thermal
Property	Value	Condition	Source						
Glass Transition Temperature	63.6 °C	-	(1) CAS						
Glass Transition Temperature	62.8 °C	-	(1) CAS						
Glass Transition Temperature	62.0 °C	-	(1) CAS						
Glass Transition Temperature	61.8 °C	-	(1) CAS						
Glass Transition Temperature	60.4 °C	-	(1) CAS						

# 分子式检索化合物

Searching for...

All

Substances

Reactions

References

Suppliers

## Substances

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

Enter a query...

Draw



Molecular Formula



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

+ Add Advanced Search Field

[Learn more about SciFinder<sup>®</sup> Advanced Search.](#)

适用于分子式检索的物质类型包括：

1. 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
2. 聚合物

# 分子式检索化合物检索规则

- 不含碳化合物，按照元素符号的首字母顺序进行排列，如：氯化钠NaCl

The screenshot shows the 'Substances' search section. The 'Searching for...' sidebar has 'Substances' selected. The 'Molecular Formula' dropdown is set to 'CINa', which is highlighted with a blue box.

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列，如：碳酸 $\text{H}_2\text{CO}_3$

The screenshot shows the 'Substances' search section. The 'Searching for...' sidebar has 'Substances' selected. The 'Molecular Formula' dropdown is set to 'CH2O3', which is highlighted with a blue box.

- 不同组分之间用“.”隔开，如：铁钴镍合金

The screenshot shows the 'Substances' search section. The 'Searching for...' sidebar has 'Substances' selected. The 'Molecular Formula' dropdown is set to 'Co.Fe.Ni', which is highlighted with a blue box.

# 分子式检索化合物检索规则

- 无机含氧酸盐，标引规则为金属离子和相应的含氧酸的混合物，即：在分子式中，需要补充和阳离子等同个数的氢原子，如：磷酸钠 $\text{Na}_3\text{PO}_4$

The screenshot shows a search interface with two main sections: 'Searching for...' and 'Substances'.

**Searching for...**

- All
- Substances** (highlighted)
- Reactions
- References

**Substances**

Search by Substance Name, CAS RN, Patent Number, Pu

Enter a query...

-

Molecular Formula

# 案例：碳氮化钛化合物检索

Searching for...

- All
- Substances**
- Reactions
- References
- Suppliers

Substances

Search by Substance Name, CAS RN, Patent Number, F

Enter a query...

- Molecular Formula C.N.Ti

+ Add Advanced Search Field

分子式检索是查找合金，无机表格化合物的好选择

# 可通过物质的文献角色或者物质类别筛选结果

CAS SciFinder<sup>®</sup> Substances

References  Reactions  Suppliers

1  2  3  4  5

**12627-33-7**  
Image Not Available  
**Unspecified**  
Titanium carbide nitride  
5,909 References 5 Reactions 4 Suppliers

**12347-09-0**  

Component	Ratio
Ti	1
N	0-1
C	0-1

**C.N.Ti**  
Components: 3  
Titanium carbide nitride (Ti(C,N))  
3,627 References 0 Reactions 0 Suppliers

**106698-99-1** **110686-85-6**

**Substance Detail** (2 of 559)

References (3,627)  Reactions (0)  Suppliers (0)

CAS Registry Number  
12347-09-0

Component	Ratio	CAS RN
Ti	1	7440-32-6
N	0-1	17778-88-0
C	0-1	7440-44-0

**C.N.Ti**  
Components: 3  
Co-1No-1Ti  
Titanium carbide nitride (Ti(C,N)) (9CI, ACI)

Other Names and Identifiers

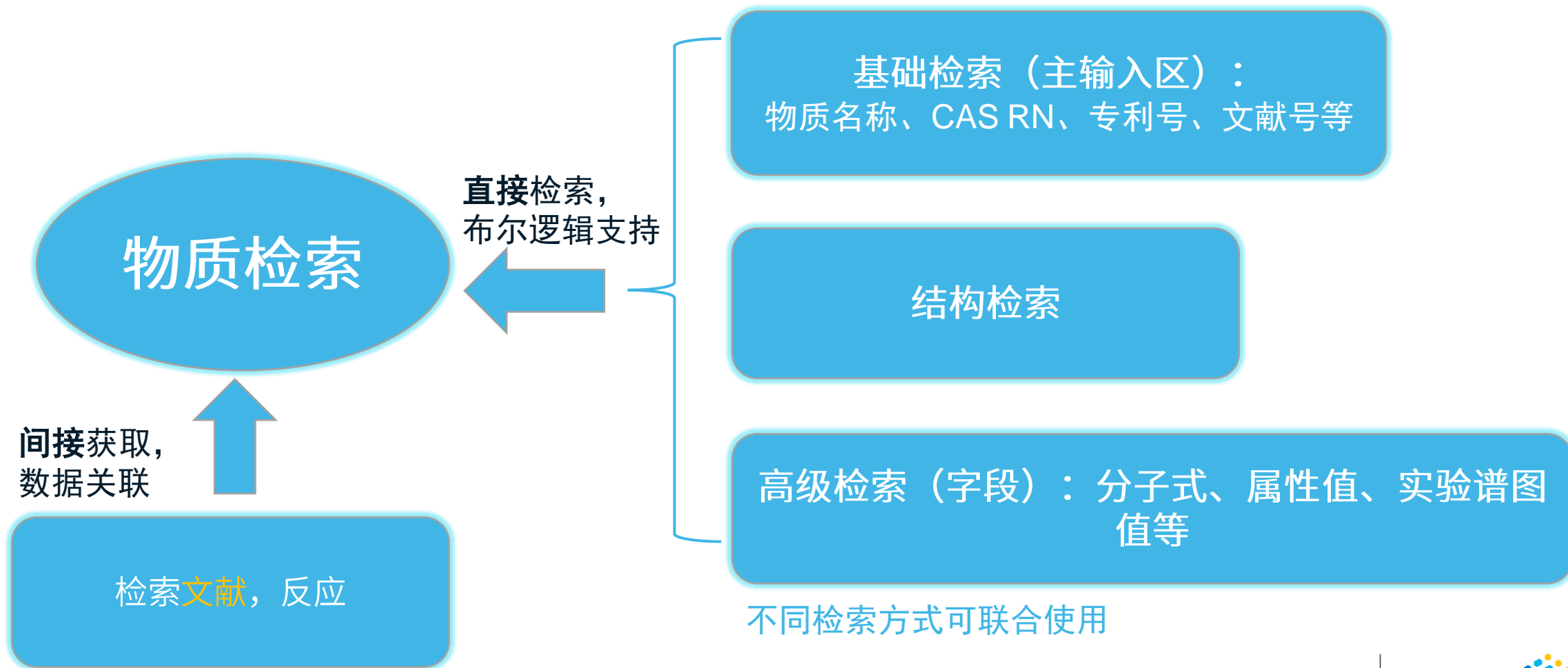
Experimental Properties

Mechanical  Structure Related  Thermal

Property	Value	Condition	Source
Tensile Strength	1251.9 MPa (None)	-	(1) CAS
Tensile Strength	1230.0 MPa (None)	-	(1) CAS
Tensile Strength	1221.3 MPa (Yield)	-	(1) CAS
Tensile Strength	1207.8 MPa (Yield)	-	(1) CAS
Tensile Strength	1207.4 MPa (None)	-	(1) CAS
Tensile Strength	1207.1 MPa (Yield)	-	(1) CAS



# 物质检索方法



# 案例：含Ti或者Zr的耐磨陶瓷复合材料

## Searching for...

All

Substances

Reactions

References

Suppliers

Biosequences

## References

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

"ceramic-metal composites" and wear-resistance

AND

Author Name

Enter last name, first name middle name.

+

文献检索支持布尔逻辑运算符(and, or, not)和

“” 表示双引号中的内容不作同义词，相关词拓展。

[Learn more about SciFinder](#)

R<sub>1</sub>

设置R1为Ti, Zr

Edit Drawing

Remove

Feedback

# 可通过物质角色筛选选项快速筛选文献

The screenshot displays a search interface for references. On the left, a sidebar contains filter options: 'Structure Match' (As Drawn (118), Substructure (168)), 'Filter Behavior' (Filter by, Exclude), and 'Document Type' (Substance Role). The 'Substance Role' section is expanded, showing options: Uses (92), Process (56), Properties (37), Preparation (14), and Formation, Non-preparative (4). A blue box highlights this section. The main area shows 'References (118)' with a 'Sort: Relevance' and 'View: Full Abstract' dropdown. A 'Substances' dropdown menu is open, showing 'Get Substances from References' and 'Selected Results' buttons. A blue box highlights the 'Substances' dropdown and the text '由文献获得物质'. Below, a reference entry is shown: 'logical properties of plasma sprayed TiCN-Mo based composite' by Zhang, Fanyong; Li, Chao; Yan, Shu; He, Jining; Liu, Baoxi; Yin, Fuxing. The abstract text includes terms like 'ceramic-metal composite', 'wear resistance', and 'wear' highlighted in blue. At the bottom, there are buttons for 'Full Text', 'Substances (5)', 'Reactions (0)', 'Citing (23)', and 'Citation Map'. A 'Feedback' icon is also present.

Substance role为物质在文献中的研究角色，如uses表明物质在文献中作应用研究；process作工艺研究等

# 物质结果集中，用结构筛选出包含Ti或者Zr的结果

R-Group Definitions

R1: Ti, Zr

Atoms

H				
Li	Be			
Na	Mg			
K	Ca	Sc	Ti	V
Rb	Sr	Y	Zr	Nb
Cs	Ba	*	Hf	Ta
Fr	Ra	**		

\*Lanthanides: La, Ce  
\*\*Actinides: Ac, Th  
Isotopes: D, T

Zoom: 100%

Substances (128) Sort: Relevance View: Partial

References Reactions Suppliers Save And Alerts

Filtering: Search Within Results: Drawn Structure Clear All Filters

1 7440-32-6 **Ti**  
Titanium  
455K References 3,283 Reactions 890 Suppliers

2 12347-09-0  
Component Ratio  
Ti 1  
N 0-1  
C 0-1  
C.N.Ti  
Components: 3  
Titanium carbide nitride (Ti(C,N))  
3,627 References 0 Reactions 0 Suppliers

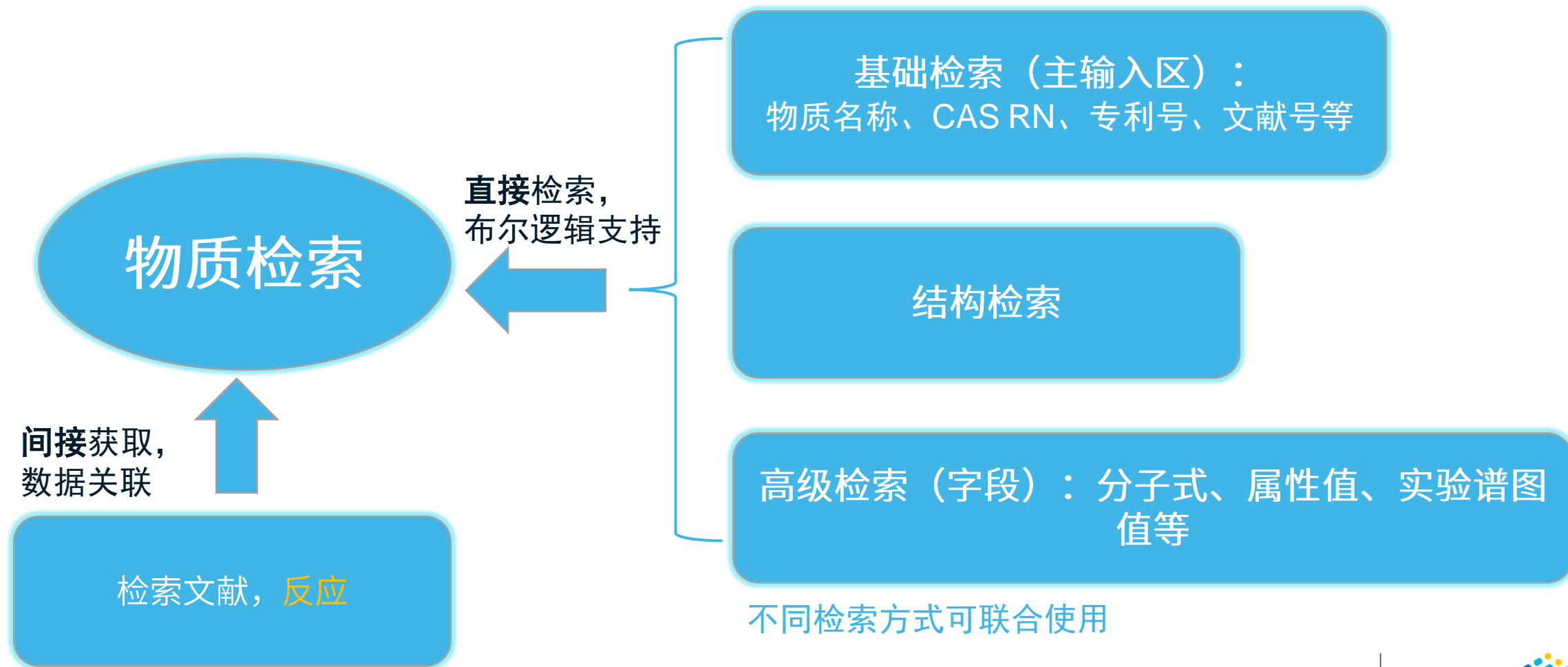
3 7440-67-7 **Zr**  
Zirconium  
157K References 1,412 Reactions 442 Suppliers

4 1374584-70-9  
Component Percent  
Ni 30-50  
Al 20-70  
Ti 5-20

5 12045-63-5  
**B≡Ti≡B**

6 14940-68-2  
O[Si](O)(O)O  
• **Zr(IV)**

# 物质检索方法



# 案例：乙烯加成反应中，铁/钴/镍基催化剂检索

The screenshot displays the CAS Draw software interface. At the top, there is a toolbar with various drawing tools and a search bar labeled "Enter a CAS Registry Number, SMILES, or InChI...". Below the toolbar, a blue instruction box reads: "Click an atom in the reactant and its corresponding atom in the product." The main workspace shows a chemical reaction: ethylene (reactant) with atoms 1 and 2 highlighted, reacting to form ethane (product) with atoms 1 and 2 highlighted. A "Variables" menu is open on the right, listing options: X (Any halogen), M (Any metal), A (Any atom except H), Q (Any atom except C or H), Ak (Any carbon chain), Cy (Any cycle), Cb (Any carbocycle), and Hy (Any heterocycle). The "A" option is selected. At the bottom, there is a text input field containing "A", a zoom slider set to 100%, and "OK" and "Cancel" buttons.

# 在反应结果集中，可通过Catalyst直接查看，筛选催化剂

CAS SciFinder<sup>®</sup> Reactions  Edit Search

Structure Match

- As Drawn (893)
- Substructure (1.6M)
- Similarity (0)

Filter Behavior


Filter by Exclude

- Yield
- Number of Steps
- Non-Participating Functional Groups
- Reaction Mapping
- Experimental Protocols
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst**
  - Poly[oxy(methylaluminum)] (66)
  - Ethylaluminum dichloride (52)
  - Triethylaluminum (37)
  - Alumina (32)
  - Cupric chloride (30)

Reactions (893) Group: By Scheme View: Expanded

References **由反应获取文献**

Scheme 1 (15 Reactions) Steps: 1 Yield: 23-100%



Suppliers (17) Suppliers (65)

Reaction Summary	Steps	Yield	Details
1.1 Reagents: <a href="#">Bromine</a> Solvents: <a href="#">Water</a> ; 24 d, cooled	1	100%	Device having absorption kettle with metering tank and method for batch-series industrial production of 1,2-dibromoethane By: Luo, Zhifeng; et al China, CN113087594 A 2021-07-09 <a href="#">PatentPak</a> <a href="#">Full Text</a>
1.1 Reagents: <a href="#">Bromine</a> ; 40 - 60 min, -5 °C	1	91%	Facile Preparation of Λ-Shaped Building Blocks: Hunlich Base Derivatization By: Kazem-Rostami, Masoud Synlett (2017), 28(13), 1641-1645 <a href="#">Full Text</a>
1.1 Reagents: <a href="#">Bromine</a>	1	23%	Metalation of o-halostyrene oxides. Preparation of benzocyclobutenols By: Alqahtani, Fawzan et al.

Catalyst

Top Count Alphanumeric **Search**

Catalyst Name  **Search**

Select All on Page

<input type="checkbox"/> Bismuth cobalt iron molybdenum oxide (BiCo <sub>9</sub> Fe <sub>3</sub> Mo <sub>12</sub> O <sub>51</sub> ) (1)	<input type="checkbox"/> Iron, bis[4-nitro-2-[[[3-(triethoxy)silyl]propyl]imino-κN]methyl]phenolato-κO]- (2)	<input type="checkbox"/> Iron, chlorobis(dimethylcarbomethioato-5,5')- (1)
<input type="checkbox"/> Dichloro[2,4,6-trimethyl-N-[1-(2-quinolinyl-κN)ethylidene]benzenamine-κN]iron (1)	<input type="checkbox"/> Iron, bis[bis(1-methylethyl)carbomethioato-5,5']bromo-, (SP-5-12)- (1)	<input type="checkbox"/> Iron, iodobis(1-pyrrolidincarbothioato-κS <sup>1</sup> ,κS <sup>1</sup> )-, (SP-5-12)- (1)
<input type="checkbox"/> Dichloro[2,6-diethyl-4-methyl-N-[1-(2-quinolinyl-κN)ethylidene]benzenamine-κN]iron (1)	<input type="checkbox"/> Iron, bis[bis(1-methylethyl)carbomethioato-5,5']chloro-, (SP-5-12)- (2)	<input type="checkbox"/> (SP-5-13)-Dichloro[N,N'-[(2,6-pyridinediyl-κN)diethylidene]bis[2,6-dimethylbenzenamine-κN]]iron (1)
<input type="checkbox"/> Dichloro[2,6-diethyl-N-[1-(2-quinolinyl-κN)ethylidene]benzenamine-κN]iron (1)	<input type="checkbox"/> Iron, bis[bis(1-methylethyl)carbomethioato-5,5']iodo-, (SP-5-12)- (1)	<input type="checkbox"/> (T-4)-Dichloro[2-(1-methylethoxy)-N-[2-(2-pyridinyl-κN)-1-(trimethylsilyl)ethylidene]benzenamine-κN]iron (1)
<input type="checkbox"/> Dichloro[2,6-dimethyl-N-[1-(2-quinolinyl-κN)ethylidene]benzenamine-κN]iron (1)	<input type="checkbox"/> Iron, bis(dimethylcarbomethioato-κS,κS')iodo-, (SP-5-12)- (1)	<input type="checkbox"/> (T-4)-Dichloro[2-(phenylmethoxy)-N-[2-(2-pyridinyl-κN)-1-(trimethylsilyl)ethylidene]benzenamine-κN]iron (1)

Apply Cancel

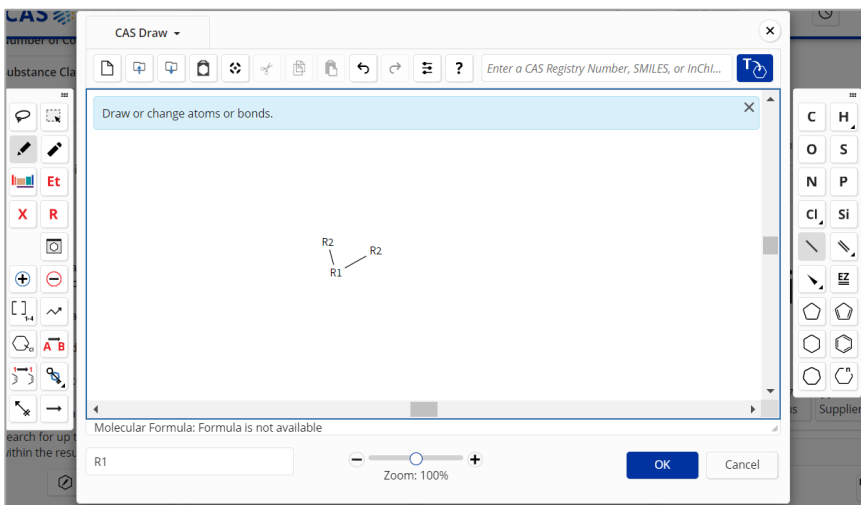
# 获得文献后，经过筛选再获取物质

The image displays the CAS SciFinder interface. On the left is a 'Filter Behavior' sidebar with options like 'Filter by' and 'Exclude', and various filters such as 'Document Type', 'Language', 'Publication Year', etc. The main area shows a 'References (512)' list. A pop-up window titled 'Get Substances from References' is open, showing 'All Results' and 'Selected Results' tabs. The selected result is a patent document: 'kettle with metering tank and method for batch-series industrial... ethane'. Below this, a 'PatentPak' button and 'Full Text' option are visible. On the right, a 'CAS SciFinder' search bar is present. Below it, a 'Search Within Results' sidebar lists various filters like 'Commercial Availability', 'Reaction Role', 'Reference Role', etc. The main content area shows a grid of substance cards. Each card includes a CAS number, a chemical structure, the substance name, and statistics for references, reactions, and suppliers.

CAS Number	Chemical Structure	Substance Name	References	Reactions	Suppliers
7631-86-9	<chem>O=Si=O</chem>	O <sub>2</sub> Si Silica	1.2M	96K	659
7440-50-8	<chem>Cu</chem>	Cu Copper	1.2M	79K	2,658
7440-44-0	<chem>C</chem>	C Carbon	1.1M	26K	622
7782-44-7	<chem>O=O</chem>	O <sub>2</sub> Oxygen	1.1M	441K	9
7732-18-5	<chem>H2O</chem>	H <sub>2</sub> O Water	1M	9.8M	219
7440-21-3	<chem>Si</chem>	Si Silicon	1M	1,637	179



# 通过结构筛选物质



R1 = Fe, Co, Ni

R2 = N, P

Filter Behavior

Filter by Exclude

Commercial Availability

Reaction Role

- Product (308)
- Reactant (31)
- Reagent (13)
- Catalyst (246)
- Solvent (1)

Reference Role

- Catalyst Use (246)
- Preparation (246)
- Uses (246)
- Synthetic Preparation (243)
- Properties (119)

View All

Number of Components

Substance Class

- Coordination Compound (246)
- Salt and Compound With (4)
- Alloy (1)

Substances (246) Sort: Number of References: Descending View: Partial

References Reactions Suppliers

Filtering: Reaction Role: Catalyst Reference Role: Catalyst Use Substance Class: Coordination Compound Search Within Results: Drawn Structure Clear All Filters

1	2	3
13478-93-8	15133-82-1	14126-37-5
<b>C<sub>8</sub>H<sub>14</sub>N<sub>4</sub>NiO<sub>4</sub></b> Bis(dimethylglyoximate)nickel	<b>C<sub>72</sub>H<sub>60</sub>NiP<sub>4</sub></b> (7-4)-Tetrakis(triphenylphosphine)nickel	<b>C<sub>36</sub>H<sub>30</sub>Br<sub>2</sub>NiP<sub>2</sub></b> Bis(triphenylphosphine) nickel dibromide
700 References 45 Reactions 28 Suppliers	559 References 1,179 Reactions 28 Suppliers	534 References 2,530 Reactions 60 Suppliers

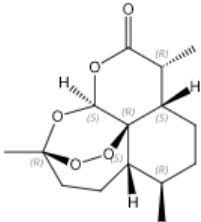
可以通过物质的反应角色或者文献角色筛选物质

4	5	6
13007-90-4	19999-87-2	15274-43-8

# 物质属性或者谱图查看

1 [点击物质CAS号](#)

**63968-64-9**



Absolute stereochemistry shown

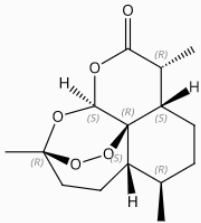
**C<sub>15</sub>H<sub>22</sub>O<sub>5</sub>**  
**Qinghaosu**

7,843 References   2,965 Reactions   95 Suppliers

## Substance Detail (1 of 1)

References (7,843)   Reactions (2,965)   Suppliers (95)

CAS Registry Number  
**63968-64-9**



Absolute stereochemistry shown

**C<sub>15</sub>H<sub>22</sub>O<sub>5</sub>**  
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)- (9CI, AC1)

Key Physical Properties	Value	Condition
Molecular Weight	282.33	-
Melting Point (Experimental)	156-157 °C	-
Boiling Point (Predicted)		
Density (Experimental)		

### Experimental Properties

Biological	Chemical	Density	Flow and Diffusion	Lipinski	Optical and Scattering
Property		Value	Condition		
Median Lethal Dose		5576 mg/kg	Organism: rat; Route: oral		
Median Lethal Dose		5105 mg/kg	Organism: mouse; Route: oral		
Median Lethal Dose		2800 mg/kg	Organism: mouse; Route: intraperitoneal		
Median Lethal Dose		2571 mg/kg	Organism: rat; Route: intraperitoneal		
Median Lethal Dose		1558 mg/kg	Organism: mouse; Route: intraperitoneal		

- Experimental Spectra
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- Additional Details

# 在反应方法中查看

Filter Behavior

[Filter by](#) [Exclude](#)

Substance Role

Yield

Number of Steps

Non-Participating Functional Groups

- Acetal (2)
- Ether (2)
- Carboxylic acid (1)

Experimental Protocols

- Synthetic Methods (66)
- Experimental Procedure (1,736)

Reaction Type

Stereochemistry

Scheme 2 (5 Reactions) Steps: 1 Yield: 41-66%

Absolute stereochemistry shown, Rotation (-)

Suppliers (42)

Suppliers (95)

<input type="checkbox"/>	Reaction Summary	Steps: 1 Yield: 66%	<a href="#">Applying green chemistry artemisinin</a>
	1.1 Reagents: <a href="#">Trifluoroacetic acid</a> , <a href="#">Carbon dioxide</a> , <a href="#">Oxygen</a>		By: Amara, Zacharias; et al Nature Chemistry (2015), 7
	Catalysts: <a href="#">Tris(2,2'-bipyridyl)ruthenium(II) chloride</a>		
	Solvents: <a href="#">Tetrahydrofuran</a> , <a href="#">Water</a> ; 8 h, 10 °C		<a href="#">Full Text</a>
	<a href="#">View Reaction Detail</a>	<a href="#">Experimental Protocols</a>	
<input type="checkbox"/>	Reaction Summary	Steps: 1 Yield: 50%	<a href="#">Continuous-Flow Synthesis of Artemisinin</a>
	1.1 Reagents: <a href="#">Oxygen</a>		By: Levesque, Francois; et al Angewandte Chemie, International Edition (2016), 55, 1706-1709, S1706/1-S1706/10
	Catalysts: <a href="#">Tetraphenylporphyrin</a>		
	Solvents: <a href="#">Dichloromethane</a> ; 11.5 bar, rt; 2 min, 1 atm, 0 °C		<a href="#">Full Text</a>
	1.2 Reagents: <a href="#">Trifluoroacetic acid</a> , <a href="#">Oxygen</a> ; 2 h, 1 atm, 0 °C		
	1.3 Reagents: <a href="#">Sodium bicarbonate</a>		
	Solvents: <a href="#">Water</a> ; rt		
	<a href="#">View Reaction Detail</a>	<a href="#">Experimental Protocols</a>	

Characterization Data

Artemisinin

Proton NMR Spectrum	(400 MHz, CDCl <sub>3</sub> ) δ 5.86 (s, 1H), 3.40 (dq, <i>J</i> = 7.3, 5.4 Hz, 1H), 2.47-2.39 (m, 1H), 2.08-1.98 (m, 2H), 1.91-1.86 (m, 1H), 1.81-1.74 (m, 2H), 1.51-1.34 (m, 3H), 1.45 (s, 3H), 1.21 (d, <i>J</i> = 7.3 Hz, 3H), 1.11-1.04 (m, 2H), 1.00 (d, <i>J</i> = 6.0 Hz, 3H).
Carbon-13 NMR	(101 MHz, CDCl <sub>3</sub> ) δ 172.2, 105.5, 93.9, 79.6, 50.2, 45.1, 37.7, 36.1, 33.8, 33.0, 25.4, 25.0, 23.6, 19.9, 12.7.
IR Absorption Spectrum	(film) 2960, 2933, 2860, 1731, 1112, 991 cm <sup>-1</sup> .
Optical Rotatory Power	[α] +66.3 ° (c 0.97, CHCl <sub>3</sub> ).
HRMS	calcd for C <sub>15</sub> H <sub>22</sub> O <sub>5</sub> (M <sup>+</sup> ) 282.1467, found 282.1463.
Mass Spectrum	MS (EI) 282 (1) [M <sup>+</sup> ], 250 (5), 192 (70), 150 (40), 55 (63), 43 (100).
Melting Point	153-154 °C.
State	yellow solid

# 总结：CAS SciFinder<sup>n</sup>支持多途径物质检索

- 基础检索：物质标识符；文献号
- 结构式检索：
  - 与Chemdraw联用
  - 有机化合物、盐类、金属有机化合物均支持结构式检索
- 高级检索：
  - 属性值检索：助力结构解析、快速检索功能材料
  - 分子式检索：无机盐、合金等
- 通过文献或者反应获取物质
- 点击物质CAS号，或者在反应方法中查看物质属性、谱图信息

# 学习资源

1. 关注“ACS美国化学会”微信公众号, 搜索SciFinder-n, 查看检索技巧、检索视频, 以及论坛回放视频



2. CAS SciFinder<sup>n</sup>网络在线演示培训资料

<https://www.cas.org/about/events/scifinder-webinars>

3. CAS官网上的培训资料

<https://www.cas.org/support/training/scifinder-n>

4. CAS SciFinder<sup>n</sup> Help使用指南

[https://scifinder-n.cas.org/help/#t=Searching\\_in\\_SciFinder-n%2FIntroduction\\_to\\_searching.htm](https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FIntroduction_to_searching.htm)