

# 解锁 CAS SciFinder-n 新功能



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美国化学文摘社 (CAS) 北京代表处

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# 目录

## ➤ CAS SciFinder<sup>n</sup> 重要新功能

- 文献检索
- 物质检索
- 反应检索
- 设置、项目管理和历史记录

# 登录

CAS SciFinder<sup>n</sup>:

<https://scifinder-n.cas.org>



# 目录

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- 文献检索
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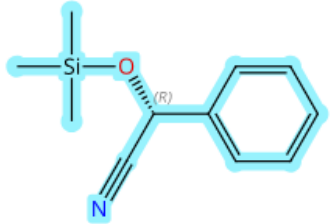


# 一站式检索功能增强

Results for drawn structure

All Substances Reactions References Suppliers

120443-82-5



Absolute stereochemistry shown, Rotation (+)

$C_{11}H_{15}NOSi$   
Benzeneacetonitrile,  $\alpha$ -[(trimethylsilyl)oxy]-, ( $\alpha R$ )-

97 349 4 View Spectra

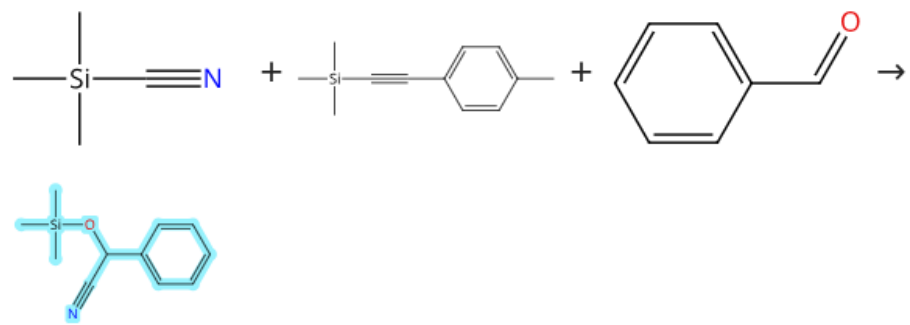
Key Physical Properties

|                  |                           |  |
|------------------|---------------------------|--|
| Molecular Weight | Boiling Point             | Density (Predicted)  |
| 205.33           | 68 °C<br>Press: 0.08 Torr | 0.987±0.06 g/cm <sup>3</sup><br>Temp: 20 °C; Press: 760 Torr |

More Substances for drawn structure  
View All (9)

Reactions for drawn structure  
View All (1,585)

31-614-CAS-36849237  
Steps: 1 Yield: 100%



References for drawn structure  
View All (143)

First structurally defined catalyst for the asymmetric addition of trimethylsilyl cyanide to benzaldehyde

By: Tararov, Vitali I.; Hibbs, David E.; Hursthouse, Michael B.; Ikonnikov, Nicolai S.; Abdul Malik, K. M.; North, Michael; Orizu, Charles; Belokon, Yuri N.  
Chemical Communications (Cambridge) (1998), (3), 387-388 | Language: English, Database: CPlus

Full Text 6 1 102

一站式检索“**All**”界面更新，最大限度地减少滚动页面的需要，提高界面整体可用性。

# 通过 IPC 分类号检索专利

高级检索项选择 Patent Identifier, 点击 IPC Code 检索专利

The screenshot displays the CAS search interface. At the top, navigation tabs include 'All', 'Substances', 'Reactions', 'References' (which is active), and 'Suppliers'. A search bar contains the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' Below the search bar, a dropdown menu is open for 'IPC Code', showing a list of search options: Authors, Publication Name, Organization, Title, Abstract/Keywords, Concept, Substances, Bioactivity Data (marked 'NEW'), Publication Year, Document Identifier, Patent Identifier (highlighted with a blue border), and Publisher. To the right of the dropdown, a search input field contains 'G21F'. Below the search bar, there are two promotional cards: 'Search CAS Lexicon' (Build powerful searches using CAS concepts, chemical classes, and taxonomy) and 'Search CAS Sequences' (Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences). At the bottom left, a 'Recent Searches' section is partially visible. At the bottom right, there are links for 'View All Search History' and 'Feedback'.



# 浏览 IPC Data 及其他专利信息

点击标题进入文献详情页面，查看 IPC Data 相关信息

## References search for "G21F" IPC Code

Substances Reactions Citing Knowledge Graph

Filter Behavior  
Filter by Exclude

Search Within Results

Document Type  
 Patent (705)

Language  
 English (238)  
 French (194)  
 German (194)  
 Japanese (20)  
 Italian (14)  
View All

Publication Year  
1968 to 2023  
View Larger

705 Results  
Sort: Times Cited View: Partial Abstract

1  
**Formulations for neutralization of chemical and biological toxicants**  
By: Tadros, Maher E.; Tucker, Mark D.  
United States, US6566574 B1 2003-05-20 | Language: English, Database: CAplus  
A formulation and method of making that neutralizes the adverse health effects of both chem. and biol. compounds, especially chem. warfare (CW) and biol. warfare (BW) agents. The formulation of the present invention non-toxic and non-corrosive and can be delivered by a variety of means and in different phases. The formulation provides solubilizing compounds that serve to effectively render the chem. and biol. compounds, particularly CW and BW compounds, susceptible to attack and at least one reactive compound that serves to attack (and detoxify or kill) the compound. The at least one reactive c...  
View More

PatentPak Full Text Substances (71) Reactions (0) Citing (29) Citation Map

2  
**Manufacture of pumpable/injectable phosphate-bonded ceramics**  
By: Singh, Dileep; Wagh, Arun S.; Perry, Lamar; Jeong, Seung-Young  
United States, US6204214 B1 2001-03-20 | Language: English, Database: CAplus  
The pumpable ceramic compositions comprise inorganic oxide (especially MgO), acidic potassium phosphate, and an oxide coating material containing polymer component. A method for preparing pumpable ceramic-based waste forms comprising selecting inorganic oxides is based on solubility, surface area and morphol. criteria and includes (a) mixing the selected oxides with phosphate solution and waste to form a first mixture; (b) combining an additive to the first mixture to create a second mixture; (c) adding water to the second mixture to create a reactive mixture; (d) homogenizing the reactive mix...  
View More

### IPC Data

| Patent       | Class | Patent Family Classification Codes   |
|--------------|-------|--|
| US6566574    | IPCI  | A62D 0003/00 A; B01F 0017/18 B; B01F 0017/38 B; C11D 0001/62 B; C11D 0003/39 B   |
| WO2002002192 | IPCI  | A62D 0003/00 A; B01F 0017/18 B; B01F 0017/38 B; C11D 0001/62 B; C11D 0003/39 B   |
| AU2001056947 | IPCI  | A62D 0003/00; A01N 0025/02; A01N 0025/10; A01N 0031/02; A01N 0033/12; A01N 0043/40; A01N 0059/00; A62D 0003/30; A62D 0003/36; A62D 0003/38; A62D 0101/02; A62D 0101/22; A62D 0101/26; A62D 0101/28; B01F 0017/18; B01F 0017/38; C11D 0001/62; C11D 0003/39; A62D 0003/00 B; B01F 0017/18 B; B01F 0017/38 B; C11D 0001/62 B; C11D 0003/39 B |
| BR2000017275 | IPCI  | A62D 0003/00 A; B01F 0017/18 B; B01F 0017/38 B; C11D 0001/62 B; C11D 0003/39 B   |
| ⋮            |       |  |
| WO2005055963 | IPCI  | A61K 0007/00 A   |
| WO2005057588 | IPCI  | G21F   |
| WO2005055963 | IPCI  | A61K 0007/00 A   |
| WO2005057588 | IPCI  | G21F   |
| WO2005089100 | IPCI  | A61K   |
| WO2005089100 | IPCI  | A62D 0003/00 A; B01F 0017/18 B; B01F 0017/38 B; C11D 0001/62 B; C11D 0003/39 B   |
| US7750199    | IPCI  | A62D 0003/38   |

# 文献检索支持根据生物活性数据检索文献

根据生物活性数据（靶点、疾病、配体/药物）等检索

The screenshot displays the CAS search interface. At the top, there are navigation tabs: All, Substances, Reactions, References (selected), and Suppliers. Below the tabs is a search bar with the text: "Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." To the right of the search bar is a "Draw" button and a search icon. Below the search bar is a dropdown menu for "Author Name" with the placeholder text "Enter last name, first name middle name." and an "Example: Schubert, J A". The dropdown menu is open, showing options: Authors, Publication Name, Organization, Title, Abstract/Keywords, Concept, Substances, Bioactivity Data (marked with a "NEW" badge), Publication Year, Document Identifier, Patent Identifier, and Publisher. The "Bioactivity Data" option is further expanded to show sub-options: Target, Ligand, and Disease. Below the search bar are two promotional cards: "Search CAS Lexicon" (Build powerful searches using CAS concepts, chemical classes, and taxonomy.) and "Search CAS Sequences" (Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.). At the bottom right, there is a link "View All Search History".

# 通过作者 ORCID iD 链接至其他出版物

The screenshot displays a search results interface. On the left, there are filter options under 'Filter by' and 'Exclude', including 'Search Within Results', 'Substance Role' (Biological Study (2), Uses (2)), 'Concept', 'CA Section', and 'Document Type' (Journal (1), Patent (1)). The main content area shows a search result for the paper: 'Probenecid Increases the Concentration of 7-Chlorokynurenic Acid Derived from the Prodrug 4-Chlorokynurenine within the Prefrontal Cortex'. The author is listed as 'Dickens, David' with an ORCID iD icon and the URL 'https://orcid.org/0000-0001-8295-0752'. A blue box highlights the ORCID iD, and a blue arrow points to a button labeled 'Get References for this ORCID iD'. Below the title, there is a 'View More' dropdown and a 'Full Text' button. At the bottom right, there are buttons for 'Substances (7)', 'Reactions (0)', 'Citing (7)', and 'Citation Map'. A chemical structure is visible below the author's name.

支持检索与作者 ORCID iD 相关的参考文献



# 获取引文地图中的关联文献

点击被引/施引文献上方数字获取文献结果集

**Filter By** Cited By Citing

**Filter Behavior**  
Filter by Exclude

**Document Type**

- Journal (14)
- Patent (27)
- Review (2)

**Author**

- Tucker, Mark D. (9)
- Betty, Rita G. (5)
- Brockmann, John E. (3)
- Lucero, Daniel A. (3)
- Boucher, Raymond M. (2)

[View All](#)

**Concept**

- Chemical warfare agents (16)
- Decontamination (11)

**Citation Map for Formulations for neutralization of chemical and biological toxicants**  
By: Tadros, Maher E.; Tucker, Mark D.  
United States, US6566574 B1 2003-05-20 | Language: English, Database: CPlus

PatentPak Full Text

Get References (12)

View 4 More (29)

Reset




**Citation Map Key**

- Cited by Root Document
- References Citing Root Document

# 获取文献知识谱图

点击 Knowledge Graph 获取文献知识谱图

## References cited by AN 2003:390868

Substances Reactions Citing Knowledge Graph    Save and Alert

Filter Behavior

Filter by Exclude

Search Within Results


Document Type

- Journal (8)
- Patent (4)
- Review (2)

Language

- English (12)

Publication Year



12 Results Sort: Times Cited View: Partial Abstract

1

**Synthesis of hybrid inorganic-organic mesoporous silica by co-condensation of siloxane and organosiloxane precursors**

By: Burkett, Sandra L.; Sims, Stephen D.; Mann, Stephen  
Chemical Communications (Cambridge) (1996), (11), 1367-1368 | Language: English, Database: CAPlus

Organically functionalized mesoporous silicas are prepared at room temperature by the co-condensation of tetraethoxysilane and organosiloxanes in the presence of surfactant templates; the resulting materials are the first examples of covalently linked, ordered, hybrid inorganic-organic networks.

Full Text Substances (4) Reactions (0) Citing (729) Citation Map

2

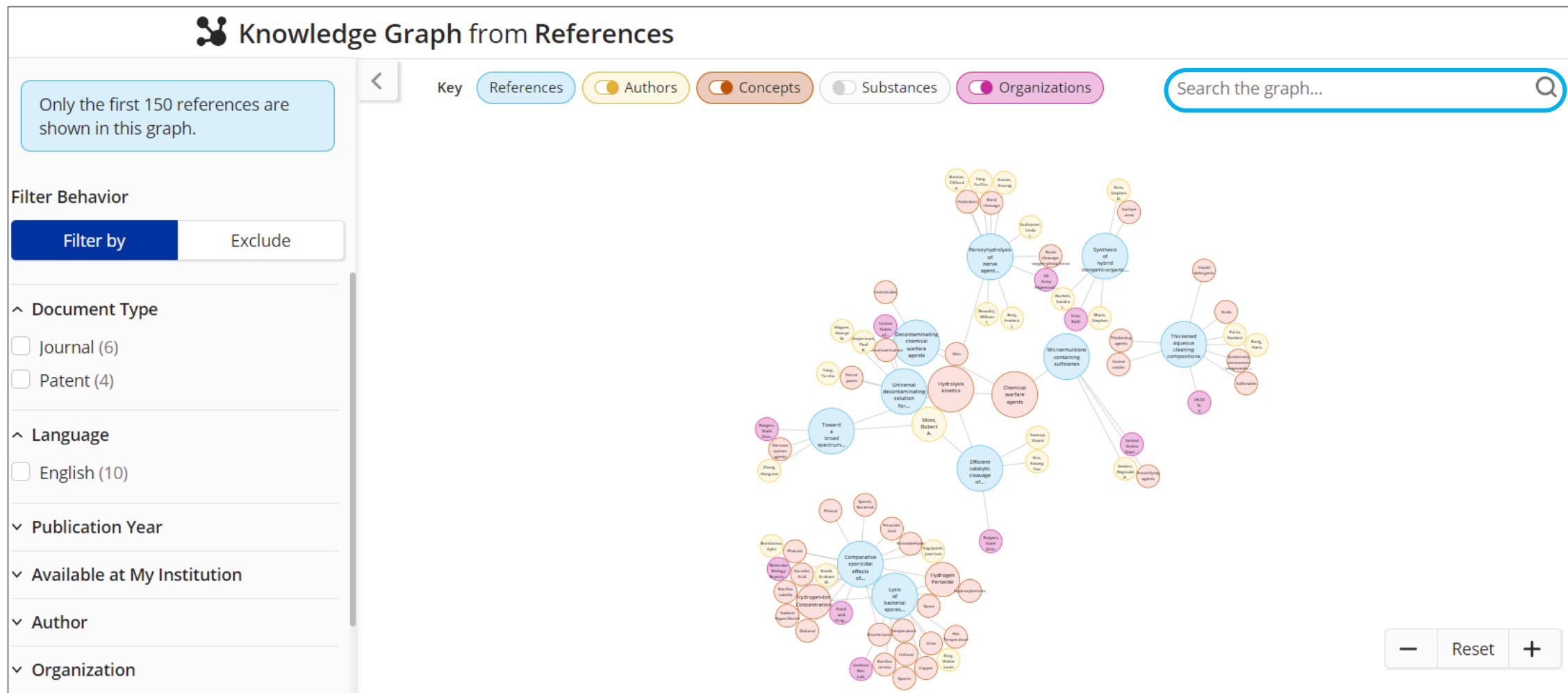
**Bacterial spores and chemical sporicidal agents.**

By: Russell, A D  
Clinical microbiology reviews (1990), 3(2), 99-119 | Language: English, Database: MEDLINE

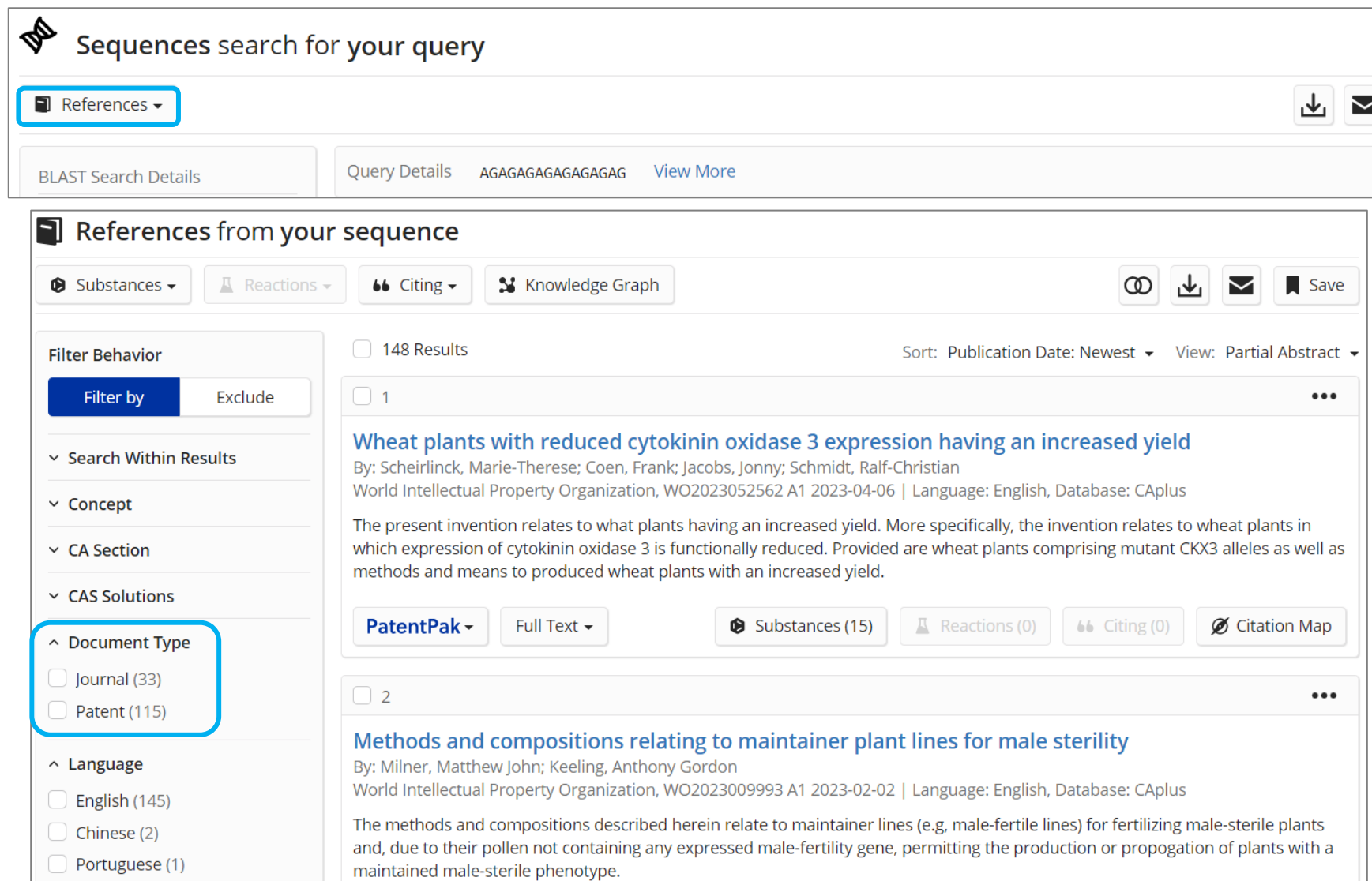
Bacterial spores are among the most resistant of all living cells to biocides, although the response depends on the stage of sporulation. The development of resistance to some agents such as chlorhexidine occurs much earlier in sporulation than does

# 检索文献知识谱图

通过输入框对图谱信息进行关键词检索



# 从序列结果获得的文献结果页面新增显示非专利文献



Sequences search for your query

References

BLAST Search Details Query Details AGAGAGAGAGAGAGAG View More

References from your sequence

Substances Reactions Citing Knowledge Graph

Filter Behavior

Filter by Exclude

Search Within Results

Concept

CA Section

CAS Solutions

Document Type

- Journal (33)
- Patent (115)

Language

- English (145)
- Chinese (2)
- Portuguese (1)

148 Results Sort: Publication Date: Newest View: Partial Abstract

1

**Wheat plants with reduced cytokinin oxidase 3 expression having an increased yield**

By: Scheirlinck, Marie-Therese; Coen, Frank; Jacobs, Jonny; Schmidt, Ralf-Christian  
World Intellectual Property Organization, WO2023052562 A1 2023-04-06 | Language: English, Database: CPlus

The present invention relates to what plants having an increased yield. More specifically, the invention relates to wheat plants in which expression of cytokinin oxidase 3 is functionally reduced. Provided are wheat plants comprising mutant CKX3 alleles as well as methods and means to produced wheat plants with an increased yield.

PatentPak Full Text Substances (15) Reactions (0) Citing (0) Citation Map

2

**Methods and compositions relating to maintainer plant lines for male sterility**

By: Milner, Matthew John; Keeling, Anthony Gordon  
World Intellectual Property Organization, WO2023009993 A1 2023-02-02 | Language: English, Database: CPlus

The methods and compositions described herein relate to maintainer lines (e.g. male-fertile lines) for fertilizing male-sterile plants and, due to their pollen not containing any expressed male-fertility gene, permitting the production or propogation of plants with a maintained male-sterile phenotype.

# 文献详情页面推荐相似文献

## Comparative analysis of syntenic genes in grass genomes reveals accelerated rates of gene structure and coding sequence evolution in polyploid wheat

Substances (19) Reactions (0) Citing (90) Citation Map

Download Email Save

### JOURNAL

**Source**  
Plant Physiology  
Volume: 161  
Issue: 1  
Pages: 252-265  
Journal: Comparative Study;  
Article: Research Support, Non-U.S. Gov't; Research Support, U.S. Gov't, Non-P.H.S.  
2013  
DOI:  
[10.1104/pp.112.205161](https://doi.org/10.1104/pp.112.205161)

CODEN: PLPHAY  
E-ISSN: 1532-2548  
ISSN-L: 0032-0889

### Database Information

AN: 2013:704699  
CAN: 160:481281  
PubMed ID: 23124323  
CAplus and MEDLINE

### Company/Organization

Department of Plant Pathology  
Kansas State University  
Manhattan, Kansas 66506  
United States

By: Akhunov, Eduard D.; Sehgal, Sunish; Liang, Hanquan; Wang, Shichen; Akhunova, Alina R.; Kaur, Gaganpreet; Li, Wanlong; Forrest, Kerrie L.; See, Deven; Simkova, Hana; et al  
[View All](#)

Cycles of whole-genome duplication (WGD) and diploidization are hallmarks of eukaryotic genome evolution and speciation. Polyploid wheat (*Triticum aestivum*) has had a massive increase in genome size largely due to recent WGDs. How these processes may impact the dynamics of gene evolution was studied by comparing the patterns of gene structure changes, alternative splicing (AS), and codon substitution rates among wheat and model grass genomes. In orthologous gene sets, significantly more acquired and lost exonic sequences were detected in wheat than in model grasses. In wheat, 35% of these gene structure rearrangements resulted in frame-shift mutations and premature termination codons. An increased codon mutation rate in the wheat lineage compared with *Brachypodium distachyon* was found for 17% of orthologs. The discovery of premature termination codons in 38% of expressed genes was consistent with ongoing pseudogenization of the wheat genome. The rates of AS within the individual wheat subgenomes (21%-25%) were similar to diploid plants. However, we uncovered a high level of AS pattern divergence between the duplicated homeologous copies of genes. Our results are consistent with the accelerated accumulation of AS isoforms, nonsynonymous mutations, and gene structure rearrangements in the wheat lineage, likely due to genetic redundancy created by WGDs. Whereas these processes mostly contribute to the degeneration of a duplicated genome and its diploidization, they have the potential to facilitate the origin of new functional variations, which, upon selection in the evolutionary lineage, may play an important role in the origin of novel traits.

**Keywords:** genome synteny sequence evolution polyploidy Triticum

Open Access Full Text

**Similar References** NEW [Get Similar References](#)

**Evolution of the glutamine synthetase gene in plants**  
Plant Science (Shannon, Ireland) (1997), 128(1), 51-58 | Language: English, Database: CAplus

**The effects of gene duplication modes on the evolution of regulatory divergence in wild and cultivated soybean**  
Frontiers in Genetics (2020), 11, 601003 | Language: English, Database: CAplus

**Megabase level sequencing reveals contrasted organization and evolution patterns of the wheat gene and transposable...**  
Plant Cell (2010), 22(6), 1686-1701 | Language: English, Database: CAplus

点击“get similar references”  
浏览最多500篇相似文献

# 目录

## ➤ CAS SciFinder<sup>n</sup> 重要新功能

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- **物质检索**
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# 物质检索支持根据生物活性数据检索物质

根据生物活性数据（靶点、疾病、配体/药物）等检索

The screenshot displays the CAS search interface. At the top, navigation tabs include 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. A search bar contains the text 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' To the right of the search bar is a 'Draw' button and a search icon. Below the search bar, a dropdown menu is open, showing 'Target' selected with the search term 'sonic'. The dropdown menu lists various search criteria: Molecular Formula, CAS Registry Number, Chemical Identifier, Document Identifier, Patent Identifier, Experimental Spectra, Bioactivity Data (marked with a 'NEW' badge), Biological, Chemical Properties, Density, and Electrical. The 'Bioactivity Data' section is further expanded to show 'Target', 'Ligand', and 'Disease'. Below the search bar, there are two promotional cards: 'Search CAS Lexicon' (Build powerful searches using CAS concepts, chemical classes, and taxonomy.) and 'Search CAS Sequences' (Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.). At the bottom right, there is a 'View All Search History' link.

# LogP 值筛选物质结果集

了解当前物质结果集 LogP 分布范围，输入范围或具体数值筛选物质

As Drawn (17)

Substructure (94)

Similarity (103K)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

Similarity

Reaction Role

Reference Role

Bioactivity Data

Commercial Availability

Number of Components

Molecular Weight

LogP

6.8 to 9.6

Available Range: -2.042 to 10.34

7,484 Results

Sort: Relevance View: Partial

1 100

1190307-88-0

Absolute stereochemistry shown

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

4,319 References 725 Reactions 69 Suppliers

2 100

1064684-44-1

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[2*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-L-alanine 1-methyl...

77 References 150 Reactions 20 Suppliers

3 100

1190308-01-0

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[*P*(*R*),2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-L-alanine 1-met...

34 References 197 Reactions 28 Suppliers

4 100

1496552-28-3

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[*P*(*S*),2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-D-alanine 1-met...

7 References 13 Reactions 17 Suppliers

5 100

1496552-16-9

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[*P*(*R*),2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-D-alanine 1-met...

7 References 16 Reactions 18 Suppliers

6 100

1064684-71-4

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-D-alanine 1-methyl...

7 References 6 Reactions 7 Suppliers

7 100

8 100

9 100

Filtering: Similarity: 4 Selected Number of Components: 1 LogP: 6.8 to 9.6 Clear All Filters

68 Results

Sort: Relevance View: Partial

1 92

1256490-35-3

Absolute stereochemistry shown

$C_{34}H_{57}FN_3O_{11}PSi_2$   
*N*-[[*P*(*S*),2'*R*]-2'-Deoxy-2'-fluoro-3'-O-[3-hydroxy-1,1,3,3-tetrakis(1-methylethyl)...

5 References 36 Reactions 0 Suppliers

2 91

2377915-18-7

Absolute stereochemistry shown

$C_{35}H_{63}FN_3O_{10}P$

1 Reference 0 Reactions 0 Suppliers

3 91

2377915-17-6

Absolute stereochemistry shown

$C_{35}H_{63}FN_3O_{10}P$

1 Reference 0 Reactions 0 Suppliers

Predicted Properties

| Biological             | Chemical    | Density     | Lipinski | Structure Related |
|------------------------|-------------|-------------|----------|-------------------|
| Property               | Value       | Condition   | Source   |                   |
| Freely Rotatable Bonds | 19          | -           | (1) ACD  |                   |
| H Acceptors            | 14          | -           | (1) ACD  |                   |
| H Donors               | 3           | -           | (1) ACD  |                   |
| H Donor/Acceptor Sum   | 17          | -           | (1) ACD  |                   |
| logP                   | 7.904±0.617 | Temp: 25 °C | (1) ACD  |                   |
| Molecular Weight       | 789.97      | -           |          |                   |

Sources

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2023 ACD/Labs)

# 官能团筛选物质结果集

查看或筛选包含特定官能团的物质

Search Within Results

Similarity

Reaction Role

Reference Role

Bioactivity Data

Commercial Availability

Number of Components

Molecular Weight

LogP

Stereochemistry

Element

**Functional Group**

- Alkene (7,419)
- Cyclic alkene (7,410)
- Urea (7,405)
- Carboxylic ester (7,395)
- Ether (7,203)
- [View All](#)

4 100

**1496552-28-3**

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[[*P*(*S*),2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-D-alanine 1-met...

7 References 13 Reactions 17 Suppliers

5 100

**1496552-16-9**

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[[*P*(*R*),2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-D-alanine 1-met...

7 References 16 Reactions 18 Suppliers

6 100

**1064684-71-4**

Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[[2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-D-alanine 1-methyl-...

7 References 6 Reactions 7 Suppliers

7 100

**1868134-97-7**

Absolute stereochemistry shown

$C_{22}H_{24}D_5FN_3O_9P$

8 100

**1631159-29-9**

Absolute stereochemistry shown

$C_{22}H_{27}D_2FN_3O_9P$

9 100

**1256490-44-4**

Absolute stereochemistry shown

$C_{22}H_{26}D_3FN_3O_9P$

Functional Group

By Count Alphanumeric

3 Selected

|  |  |   |
|--|--|---|
| <input type="checkbox"/> Alkene (7,419)                      | <input type="checkbox"/> Phenyl halide (475)   | <input type="checkbox"/> Phenol (17)              |
| <input type="checkbox"/> Cyclic alkene (7,410)               | <input type="checkbox"/> Primary alcohol (316) | <input type="checkbox"/> Secondary amine (17)     |
| <input type="checkbox"/> Urea (7,405)                        | <input type="checkbox"/> Nitrile (216)         | <input type="checkbox"/> Ketone (12)              |
| <input checked="" type="checkbox"/> Carboxylic ester (7,395) | <input type="checkbox"/> Acetal (157)          | <input type="checkbox"/> Aldehyde (9)             |
| <input type="checkbox"/> Ether (7,203)                       | <input type="checkbox"/> Azide (126)           | <input type="checkbox"/> Enol (9)                 |
| <input checked="" type="checkbox"/> Amide (6,559)            | <input type="checkbox"/> Hydroxylamine (102)   | <input type="checkbox"/> Unsaturated aldehyde (9) |
| <input type="checkbox"/> Halide (6,191)                      | <input type="checkbox"/> Thiocarbonyl (94)     | <input type="checkbox"/> Acyclic ketone (8)       |
| <input checked="" type="checkbox"/> Alcohol (5,965)          | <input type="checkbox"/> Sulfide (88)          | <input type="checkbox"/> Cyclic ester (4)         |
| <input type="checkbox"/> Cyclic alcohol (5,912)              | <input type="checkbox"/> Allyl alcohol (72)    | <input type="checkbox"/> Cyclic ketone (4)        |
| <input type="checkbox"/> Secondary alcohol (5,701)           | <input type="checkbox"/> Carboxylic acid (57)  | <input type="checkbox"/> Nitro (4)                |
| <input type="checkbox"/> Glycol (1,278)                      | <input type="checkbox"/> Thiocarboxy (52)      | <input type="checkbox"/> Unsaturated ester (3)    |

OK Cancel

# GHS 危害说明筛选物质结果集

支持根据 GHS 分类代码筛选结果

Experimental Property

Experimental Spectrum

**GHS Hazard Statements**

- H373: May cause damage to organs; through prolonged or repeated exposure (1)
- H372: Causes damage to organs through prolonged or repeated exposure (1)
- H361fd: Suspected of damaging fertility. Suspected of damaging the unborn child (1)
- H361f: Suspected of damaging fertility (1)
- H361d: Suspected of damaging the unborn child (1)

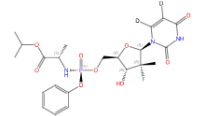
[View All](#)

Bioactivity Indicator

Target Indicator

Regulatory Data by Country/Region

1631159-27-7

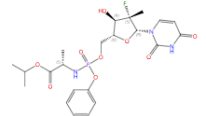


Absolute stereochemistry shown

$C_{22}H_{27}D_2FN_3O_9P$   
*N*-[[*P*(*S*),2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl-5,6-*d*<sub>2</sub>]-L-alanin...

4 References 16 Reactions 0 Suppliers

1987957-28-7

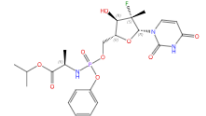


Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[2'*S*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-L-alanine 1-methylet...

3 References 34 Reactions 3 Suppliers

1987953-85-4

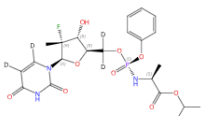


Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
*N*-[[2'*S*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-D-alanine 1-methylet...

3 References 23 Reactions 1 Supplier

1651206-09-5

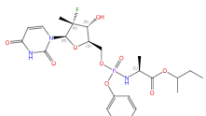


Absolute stereochemistry shown

$C_{22}H_{25}D_4FN_3O_9P$   
*N*-[[*P*(*S*),2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl-5,6-*d*<sub>2</sub>-5',5'-*C*-*d*...

13 100

1064684-43-0

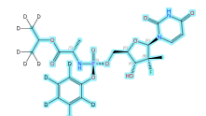


Absolute stereochemistry shown

$C_{23}H_{31}FN_3O_9P$   
*N*-[[2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-phenyl-5'-uridylyl]-L-alanine 1-

14 100

1868135-17-4



Absolute stereochemistry shown

$C_{22}H_{18}D_{11}FN_3O_9P$   
*N*-[[*P*(*S*),2'*R*]-2'-Deoxy-2'-fluoro-2'-methyl-*P*-(phenyl-2,3,4,5,6-*d*<sub>5</sub>)-5'-uridylyl]-...

15 100

Structure Match

As Drawn (17)

Substructure (94)

Similarity (103K)

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

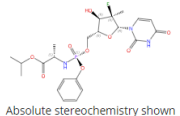
Filtering: Similarity: 4 Selected X Number of Components: 1 X

GHS Hazard Statements: H372: Causes damage to or... X

1 Result

1 100

1190307-88-0



Absolute stereochemistry shown

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

4,319 References 725 Reactions 69 Suppliers

GHS Hazard Statements

| Code | Hazard Statement   | Source  |
|------|--|---|
| H373 | May cause damage to organs; through prolonged or repeated exposure | European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most common notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria  |
| H372 | Causes damage to organs through prolonged or repeated exposure     | European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most common notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria |
| H335 | May cause respiratory irritation                                   | Fisher Scientific   |
| H319 | Causes serious eye irritation                                      | Fisher Scientific   |
| H315 | Causes skin irritation   | Fisher Scientific   |
| H302 | Harmful if swallowed   | European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most common notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria |

物质详情界面展示 GHS 标识图标和详细的危害说明

# 芳香环数量 & 是否有关联文献筛选物质结果集

Functional Group

Aromatic Rings

- No aromaticity (155)
- 1 (5,849)
- 2 (1,387)
- 3 (89)
- 4 (4)

Substance Class

Isotopes

Metals

Experimental Property

Experimental Spectrum

GHS Hazard Statements

Bioactivity Indicator

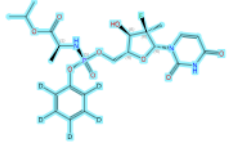
Target Indicator

Regulatory Data by Country/Region

Reference Availability

- Available (7,452)
- Not Available (32)

1868134-97-7

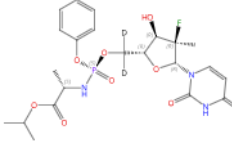


Absolute stereochemistry shown

$C_{22}H_{24}D_5FN_3O_9P$   
N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d<sub>5</sub>)-5'-uridylyl]-...

6 References 15 Reactions 0 Suppliers

1631159-29-9

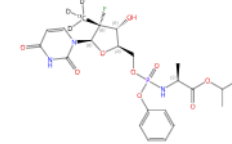


Absolute stereochemistry shown

$C_{22}H_{27}D_2FN_3O_9P$   
N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-phenyl-5'-uridylyl-5',5'-C-d<sub>2</sub>]-L-al...

6 References 27 Reactions 0 Suppliers

1256490-44-4

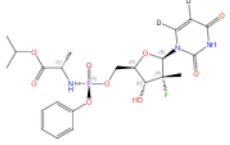


Absolute stereochemistry shown

$C_{22}H_{26}D_3FN_3O_9P$   
N-[(2'R)-2'-Deoxy-2'-fluoro-2'-(methyl-<sup>13</sup>C-d<sub>3</sub>)-P-phenyl-5'-uridylyl]-L-alanine 1...

5 References 38 Reactions 2 Suppliers

1631159-27-7

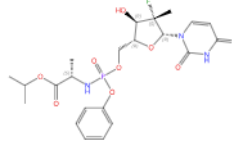


Absolute stereochemistry shown

$C_{22}H_{27}D_2FN_3O_9P$   
N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-phenyl-5'-uridylyl-5,6-d<sub>2</sub>]-L-alanin...

4 References 16 Reactions 0 Suppliers

1987957-28-7

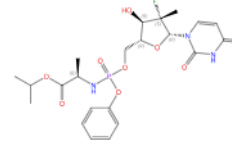


Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
N-[(2'S)-2'-Deoxy-2'-fluoro-2'-methyl-P-phenyl-5'-uridylyl]-L-alanine 1-methylet...

3 References 34 Reactions 3 Suppliers

1987953-85-4



Absolute stereochemistry shown

$C_{22}H_{29}FN_3O_9P$   
N-[(2'S)-2'-Deoxy-2'-fluoro-2'-methyl-P-phenyl-5'-uridylyl]-D-alanine 1-methylet...

3 References 23 Reactions 1 Supplier

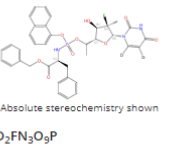
Filtering: Similarity: 4 Selected X Number of Components: 1 X Aromatic Rings: 4 X Clear All Filters

4 Results

Sort: Relevance View: Partial

1 88

1621166-85-5



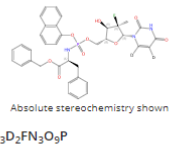
Absolute stereochemistry shown

$C_{37}H_{35}D_2FN_3O_9P$   
L-Phenylalanine, N-[hydroxy(1-naphthalenyloxy)phosphinyl]-, phenylmethyl ester, ...

2 References 2 Reactions 0 Suppliers

2 88

1621155-90-5



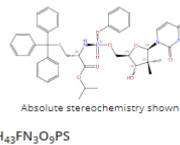
Absolute stereochemistry shown

$C_{36}H_{33}D_2FN_3O_9P$   
N-[(2'R)-2'-Deoxy-2'-fluoro-2'-methyl-P-1-naphthalenyl-5'-uridylyl-5,6-d<sub>2</sub>]-L-phe...

2 References 2 Reactions 0 Suppliers

3 86

2140231-76-9



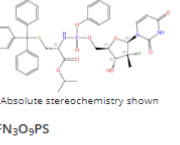
Absolute stereochemistry shown

$C_{41}H_{43}FN_3O_9PS$   
N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-phenyl-5'-uridylyl]-S-(triphenylmet...

1 Reference 1 Reaction 0 Suppliers

4 86

2140231-70-3






Absolute stereochemistry shown

$C_{41}H_{43}FN_3O_9PS$

1 Reference 6 Reactions 0 Suppliers


# 根据价格高低筛选供应商信息

 Suppliers from Substances








 

Filter Behavior

164 Results

Sort: Relevance 

1

| Supplier  | Substance  | Purity | Purchasing Det   |
|---|--|--------|--|
| <input type="checkbox"/> 1<br><br>Enamine Stock Building Blocks<br>United States<br>Last Updated: 20 Oct 2023                |  <br>102-54-5<br>1-ferra-1,1'-spirobi[pentacyclo<br>[2.2.0.0{1,3}.0{1,5}.0{2,6}]<br>hexane]-2,2',4,4'-tetraene | 95-98% | Order From Sup<br>100 mg, USD 19<br>250 mg, USD 19<br>500 mg, USD 19<br>1 g, USD 24.00<br>2.5 g, USD 25.00<br><a href="#">View all</a>   |
| <input type="checkbox"/> 2<br><br>Aaron Chem<br>Aaron Chemicals Product List<br>United States<br>Last Updated: 22 Nov 2023 |  <br>1282-37-7<br>Ferrocenium, tetrafluoroborate<br>(1-) (1:1)   | 95-98% | Order From Supplier <br>1 g, USD 44.00<br>5 g, USD 124.00<br>Maintained in stock<br>Ships within 1 week |

164 Results

Price: Low to High  
Price: High to Low  
Supplier: A to Z  
Supplier: Z to A  
Ships Within  
Purity

Preferred Suppliers

No Preference (164)

Supplier

Atomax Chemicals Product List (10)

KANTO CHEMICAL (6)

Alfa Chemistry Product List (5)

AURUM Pharmatech Product List (5)

A2B Chem Product List (4)

[View All](#)



# 新增多种物质实验属性

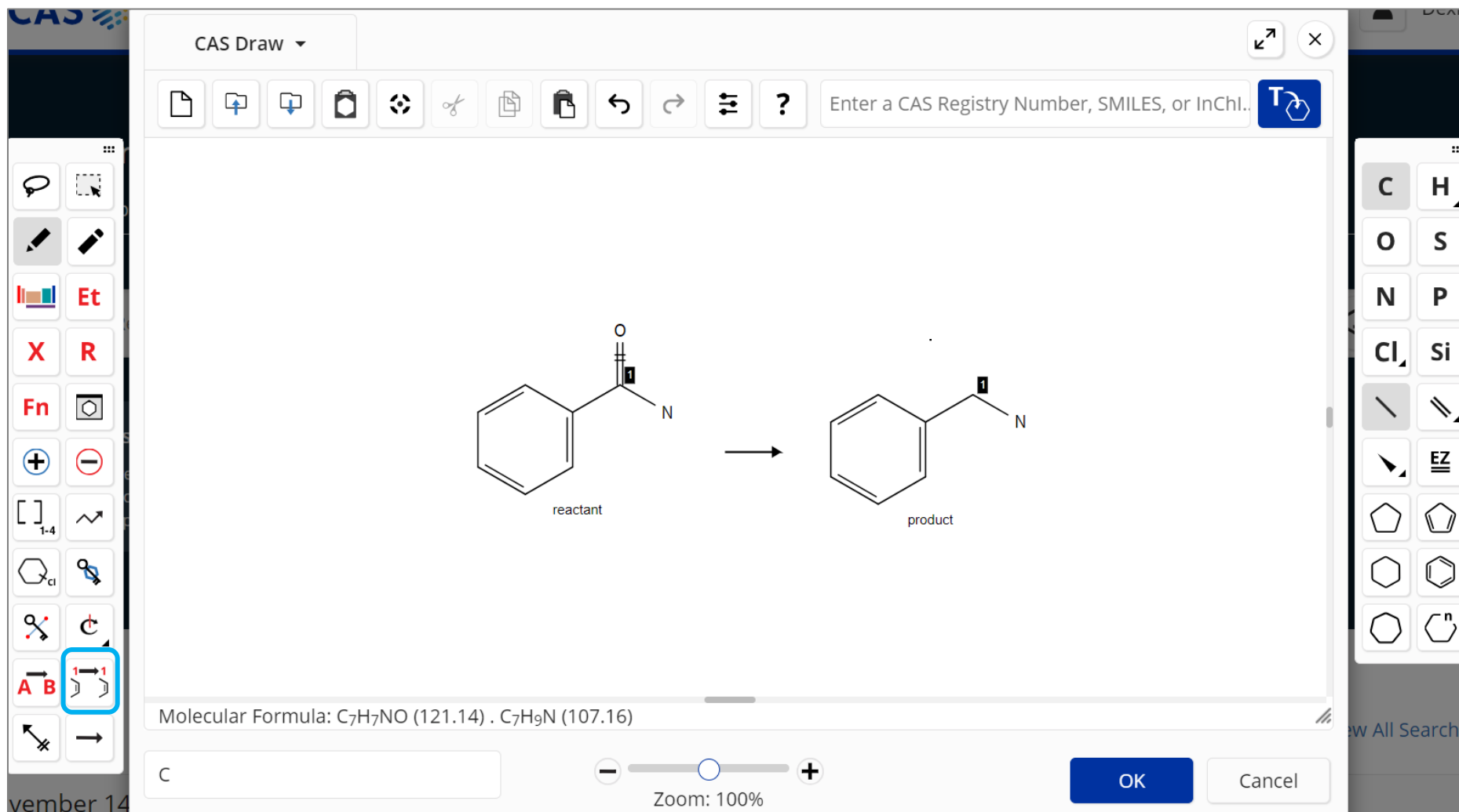
新增转化温度、流体属性、解离常数、偶极距数据，以及热力学参数等实验属性

| Acoustic            | Biological             | Chemical                         | Density | Electrical | Electronic | Flow and Diffusion | Interface | Lipinski | Mechanical | Optical and Scattering | Structure Related | Thermal |
|---------------------|------------------------|----------------------------------|---------|------------|------------|--------------------|-----------|----------|------------|------------------------|-------------------|---------|
| Property            | Value                  | Condition                        | Source  |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 6x10+5 mPa-s (dynamic) | Temp: 293 K; Press: Atm pressure | (1) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 5.189 mPa-s (dynamic)  | Temp: 333.15 K                   | (2) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 0.817 mPa-s (dynamic)  | Temp: 293 K                      | (3) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 0.6956 mPa-s (dynamic) | -                                | (4) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 0.6 mPa-s (dynamic)    | Temp: 293 K                      | (5) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 0.6 mPa-s (dynamic)    | Temp: 298 K                      | (6) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 0.60 mPa-s (dynamic)   | -                                | (7) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 0.5944 mPa-s (dynamic) | -                                | (8) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 0.5944 mPa-s (dynamic) | Temp: 293.15 K                   | (8) CAS |            |            |                    |           |          |            |                        |                   |         |
| Viscosity (Dynamic) | 0.594 mPa-s (dynamic)  | Temp: 293.15 K                   | (9) CAS |            |            |                    |           |          |            |                        |                   |         |



# 可对多步反应进行原子对标记筛选

在CAS SciFinder<sup>n</sup> 结构绘制面板的左侧工具栏中，使用原子标记工具对原料和产物中同一原子进行对应标记

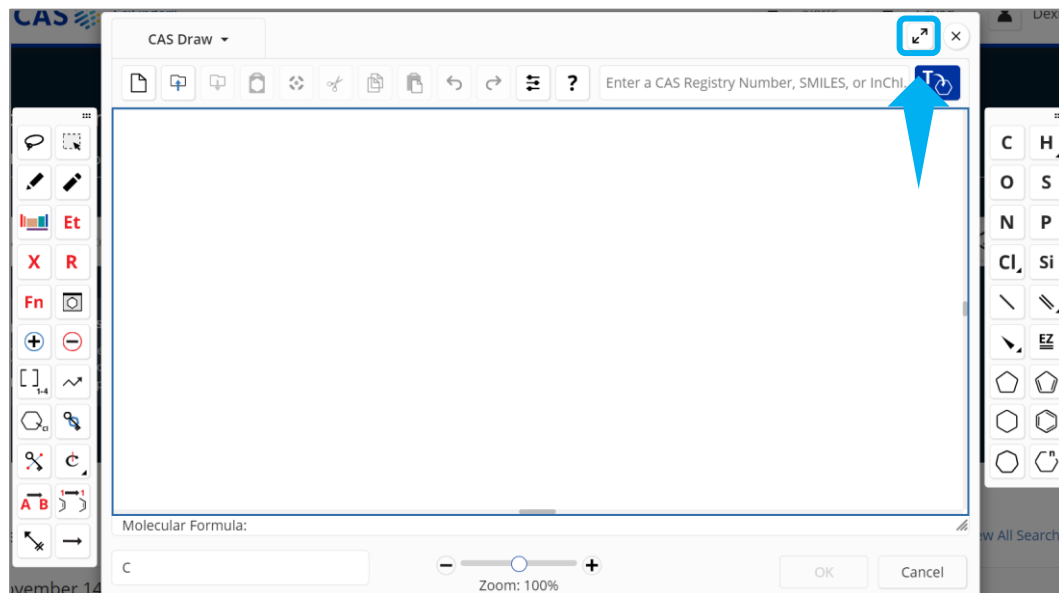


# 可对多步反应进行原子对标记筛选

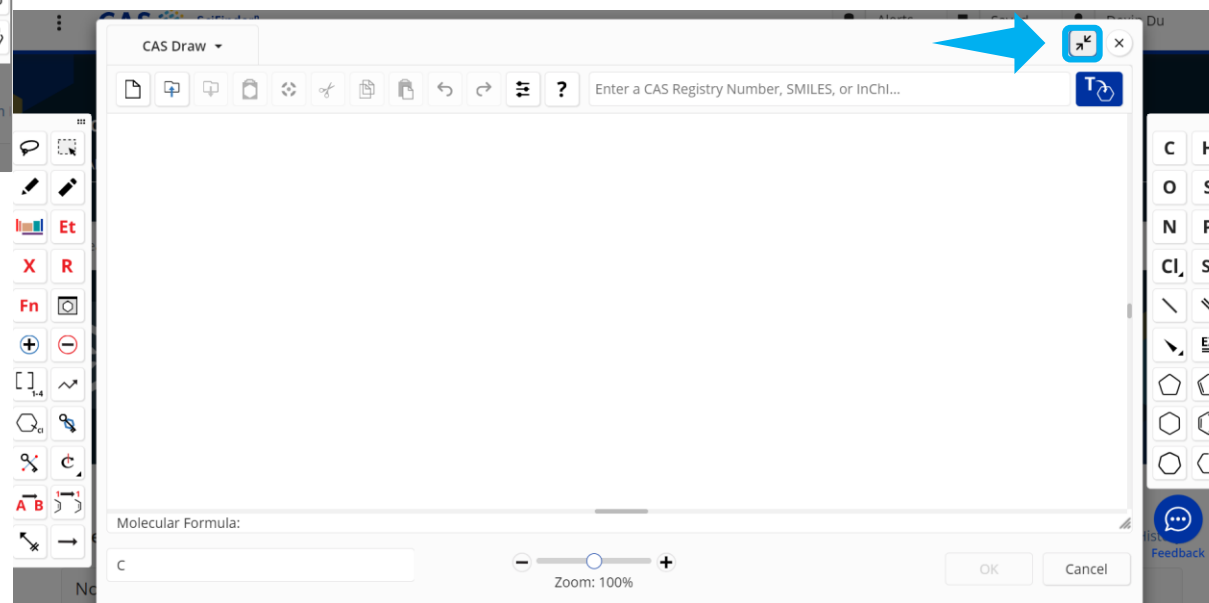
对是否含有原子对标记的反应进行分类，适用于单步和多步反应

The screenshot displays a search interface for chemical reactions. On the left, a sidebar contains several filter sections: 'Structure Match' with options 'As Drawn (106)', 'Substructure (777K)', and 'Similarity (108K)'; 'Filter Behavior' with 'Filter by' and 'Exclude' buttons; 'Search Within Results'; 'Non-Participating Functional Groups'; 'Experimental Protocols'; 'Catalyst'; 'Number of Steps' with radio buttons for '1 (93)' and '2 (13)'; 'Reaction Type'; 'Yield'; and 'Reaction Mapping' with a checked radio button for 'Mapping Data Available (106)'. The main area shows 'Filtering: Reaction Mapping: Mapping Data Available' and '106 Results'. Below this, a reaction scheme is shown: benzamide (with blue atom mapping) reacts to form N-benzylamine (with blue atom mapping). Below the scheme are 'Suppliers (109)' and 'Suppliers (83)' buttons. Two reaction detail cards are visible. The first card, titled 'View Reaction Detail', shows a 2-step process: 1.1 Catalysts: Phosphorus pentoxide; 0.3 h, < 500 mbar, 150 °C; 2.1 Reagents: Hydrogen; Catalysts: Nickel; Solvents: Ethanol; 0.5 h, 7 MPa, 100 °C. The second card, also titled 'View Reaction Detail', shows a 2-step process: 1.1 Reagents: Methyl-diethoxysilane; Catalysts: Ferrate(1-), μ-carbonyldecacarbonyl-μ-hydrotri-, triangulo, hydrogen, compd. wit...; Solvents: Toluene; 24 h, 100 °C; 2.1 Reagents: Methyl-diethoxysilane; Catalysts: 3,4,7,8-Tetramethyl-1,10-phenanthroline, Ferrous acetate; Solvents: Toluene; 24 h, 100 °C.

# 结构编辑器可自由缩放



- 点击右上角图标可将绘制面板最大化，再次点击可恢复初始大小
- 退出 CAS SciFinder<sup>n</sup> 后，再次访问时会默认使用上次的设置



# CAS Draw 对出错信息添加描述

增加出错信息描述，出错位置高亮显示

The screenshot displays the CAS Draw software interface. At the top, there is a search bar with the text "Enter a CAS Registry Number, SMILES, or InChI." and a search icon. Below the search bar, a red error message box is visible, containing the text: "R-groups must consist of at least 2 and at most 20 items. Show this error" and "A chiral node must have either three or four attachments. Show this error". The main drawing area shows a chemical structure of a chiral center (a carbon atom) bonded to a phenyl ring, a carbonyl group, and a methyl group. A red circle highlights the chiral center, and a blue arrow points to it from the right. The label "R1" is positioned above the chiral center. The bottom of the interface shows a text input field containing "R1", a zoom slider set to 100%, and "OK" and "Cancel" buttons.



# 目录

## ➤ CAS SciFinder<sup>n</sup> 重要新功能

- 文献检索
- 物质检索
- **反应检索**
- 设置、项目管理和历史记录



# 反应结果集排序和筛选新功能

按转化类型 (Transformation) 分组后, 可根据转化类型名称或反应数量排序

The screenshot shows a search interface with a left sidebar containing filters. The 'Reaction Scale' filter is highlighted with a blue box and contains two options: 'Milligram (4)' and 'No Scale Provided (105)'. The main results area shows two reaction categories:

- Formation of Nitrogen Heterocycles** (1 result): Shows two chemical transformations. The first is the cyclization of an amide-like structure to a nitrogen heterocycle. The second is the cyclization of an imine-like structure to a nitrogen heterocycle. Below the structures, it states 'Z = Electron withdrawing group'.
- Hydrolysis or Hydrogenolysis of Amides/ Imides/ Carbamates** (2 results): Shows a chemical reaction where an amide reacts with H<sub>2</sub>O to form a carboxylic acid and an amine, or with H<sub>2</sub> to form an amine.

Group: **By Transformation**

- By Scheme
- By Document
- By Transformation**

Sort: **Reaction Count: Descending**

- Reaction Count: Descending**
- Reaction Count: Ascending
- Transformation Name: A to Z
- Transformation Name: Z to A

反应规模 (Reaction Role) 筛选  
不同反应规模的反应结果

# 获取指定反应的相似反应结果

反应中心一致，周边原子和化学价特征较相似的反应

Reactions search for drawn structure

References

Structure Match

- As Drawn (4)
- Substructure (14K)

Filter Behavior

Filter by Exclude

Search Within Results

Number of Steps

- 1 (4)

Reaction Type

Yield

- 90-100% (1)

4 Results

Group: By Scheme Sort: Relevance View: Expanded

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

Suppliers (65) Suppliers (84) Supplier (1)

31-354-CAS-20403992 Steps: 1 Yield: 93% **Get Similar Reactions** Light-Stabilized Dynamic Materials

1.1 Reagents: [Triethylamine](#)  
Solvents: [Dichloromethane](#); 0 °C; overnight

1.2 Reagents: [Hydrochloric acid](#)  
Solvents: [Dichloromethane](#), [Water](#); rt

Full Text

Collapse Scheme

Get Similar Reactions

Set Reaction Similarity

Broad (176,834)  
Reaction centers only


Medium (40,847)  
Reaction centers plus adjacent atoms and bonds




Narrow (15,607)  
Reaction centers plus extended atoms and bonds

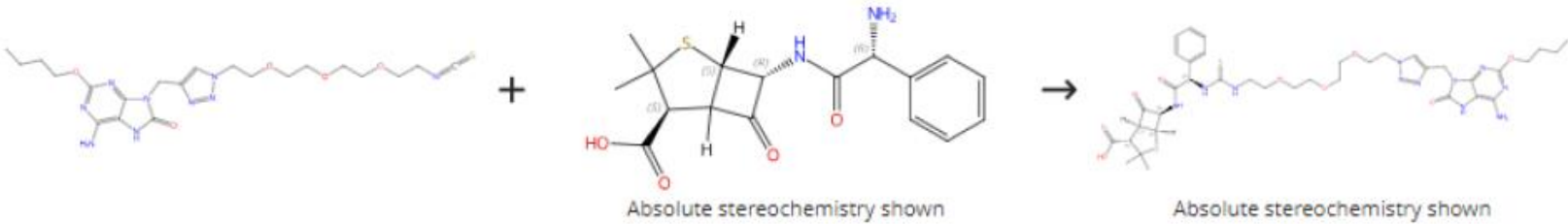
Get Reactions Cancel

选择相似度范围

# 反应详情页获取相似反应

 CAS Reaction Number: 31-316-CAS-23145310

[Get Similar Reactions](#)    Save



Absolute stereochemistry shown

Absolute stereochemistry shown

10%

**Reaction Overview**

Steps: 1      Yield: 10%

**PATENT**

[Preparation of purine derivatives as immune agonists](#)

**Step 1**

| Stage | Reagents                      | Catalysts | Solvents                           | Conditions    |
|-------|-------------------------------|-----------|------------------------------------|---------------|
| 1     | <a href="#">Triethylamine</a> | -         | <a href="#">Dimethyl sulfoxide</a> | overnight, rt |

[Alternative Steps \(0\)](#)

# 逆合成路线结果页面展示更新

CAS SciFinder<sup>®</sup> Reactions Enter a query... Draw

## Retrosynthesis Plan for drawn structure

Powered by ChemPlanner<sup>®</sup>

Key Experimental Steps Predicted Steps Edit Plan Options View Excluded Options Save

**Plan Information**  
Estimated Yield: 42%  
Overall Price: \$6,855.79 (USD per 100 grams)

**Scoring Profiles**  
Complexity Reduction  
Convergence  
Evidence  
Cost  
Yield

Avg. Yield 67% Avg. Yield 76% Max Yield 75%

Feedback

| Step   | Evidence  |
|--|---|
| A ⇒ B<br>Average Yield: 92%<br>Evidence (206,649)<br>Alternative Steps (3)   | 1.1 Reagents: Hydrogen<br>Catalysts: Palladium dihydroxide<br>Solvents: Tetrahydrofuran, Water:<br>2.5 h, 50 psi, rt<br>View All ▾      |
| B ⇒ C + D<br>Average Yield: 79%<br>Evidence (1,097,444)<br>Alternative Steps | 1.1 Reagents: Sodium bicarbonate,<br>Hydrochloric acid,<br>Methanamine, 1-chloro- <i>N,N</i> -<br>dimethyl-<br>Solvents: Acetone, Water |
| C ⇒ E<br>Average Yield: 90%<br>Evidence (5,016)<br>Alternative Steps (2)     | 1.1 Reagents: Trifluoroacetic acid<br>Solvents: Dichloromethane; 2 - 3 h,<br>rt<br>View All ▾   |
| D ⇒ F + G  | 1.1 Reagents: Sodium hydroxide  |

# 以可编辑的 RTF 格式下载反应检索结果

Download Reaction Results

File Type: Rich Text (.rtf)

Select Quantity:  All Results,  Selected Results,  Range (ex. 2 to 20)

Display:  Result Summary,  Result Details

File Name: Reactions

Download

View in SciFinder<sup>®</sup>

Reactions (30)

## 1. Scheme 1 (14 Reactions)



### Ultrasound mediated functional group reduction and chemoselective studies by DMAB

By: Jayakumar, Venkatesan; et al  
Chemical Science Transactions (2019), 8(3), 418-424.  
[10.7598/cst2019.1581](#)  
[View All Sources in SciFinder<sup>®</sup>](#)

Steps: 1-2, Yield: 29-96%

**CAS Reaction Number: 31-541-CAS-20665946**

- 1.1 **Reagents:** (*T*-4)-(*N,N*-Dimethylbenzenamine)trihydroboron  
**Solvents:** Tetrahydrofuran; 5 min; 21 min
- 1.2 **Reagents:** Potassium carbonate  
**Solvents:** Water

### A Convenient and General Reduction of Amides to Amines with Low-Valent Titanium

By: Zhang, Tongxin; et al  
Advanced Synthesis & Catalysis (2013), 355(14-15), 2775-2780.

# 目录

## ➤ CAS SciFinder<sup>n</sup> 重要新功能

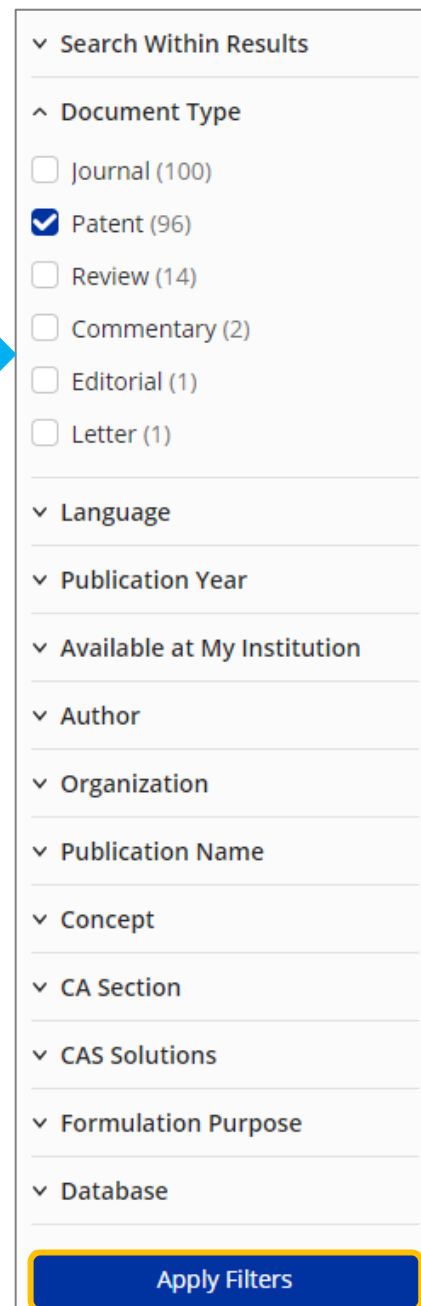
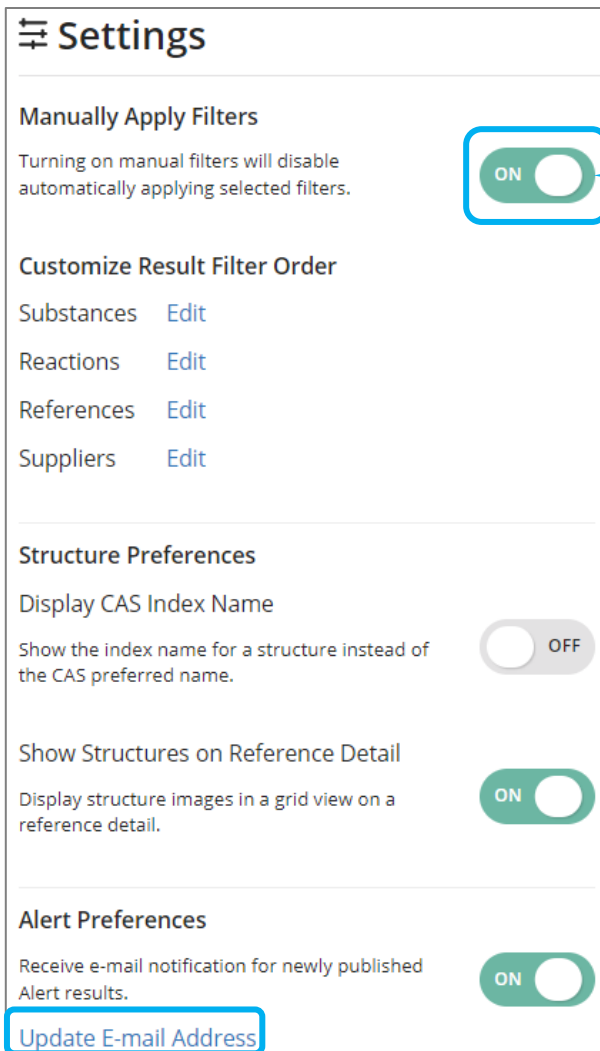
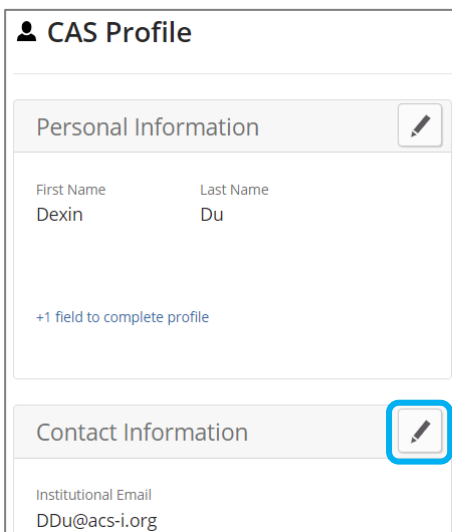
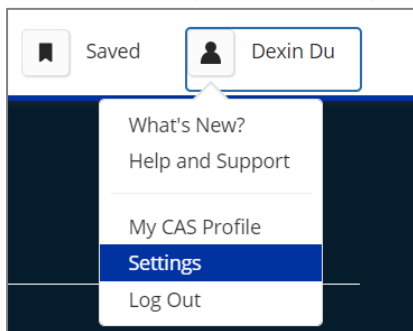
- 文献检索
- 物质检索
- 反应检索
- **设置、项目管理和历史记录**



# 自定义设置功能

Manually Apply Filters: 手动筛选检索结果

Alert Preferences: 更改提醒邮箱



# 自定义设置检索结果筛选项及排序

拖拽筛选项进行选择或排序

## Settings

**Manually Apply Filters**  
Turning on manual filters will disable automatically applying selected filters.

**Customize Result Filter Order**  
Substances [Edit](#)  
Reactions [Edit](#)  
References [Edit](#)  
Suppliers [Edit](#)

**Structure Preferences**  
Display CAS Index Name  
Show the index name for a structure instead of the CAS preferred name.

Show Structures on Reference Detail  
Display structure images in a grid view on a reference detail.

**Alert Preferences**  
Receive e-mail notification for newly published Alert results.

[Update E-mail Address](#)



## Customize Substance Filters

Drag and drop filter options to add, remove, or customize your preference on a Substance result set. You can also [reset substances filter order](#).

**Included Filters**

- Reaction Role
- Reference Role
- Bioactivity Data
- Number of Components
- Molecular Weight
- LogP
- Stereochemistry
- Element

**Unused and Available Filters**

- Commercial Price
- Commercial Availability

→ Drag ←

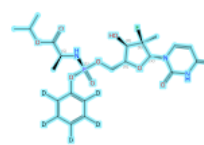
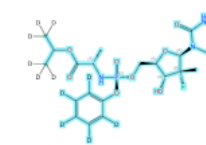
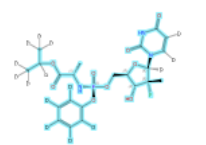
# 优先展示 CAS Index Name

## Structure Preferences

### Display CAS Index Name

Show the index name for a structure instead of the CAS preferred name.

ON

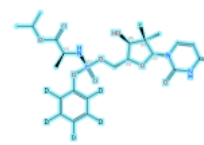
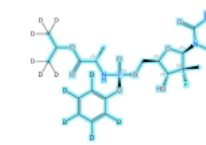
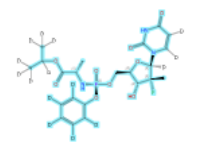
|  |   |   |
|--|---|---|
| <p>1</p> <p>1868134-97-7</p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>22</sub>H<sub>24</sub>D<sub>5</sub>FN<sub>3</sub>O<sub>9</sub>P</b><br/>L-Alanine, N-[[P(S),2'R]-2'-deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d<sub>5</sub>)-5'...</p> <p>6 References   15 Reactions   0 Suppliers</p> | <p>2</p> <p>1868135-17-4</p>  <p>Absolute stereochemistry shown</p> <p>C<sub>22</sub>H<sub>18</sub>D<sub>11</sub>FN<sub>3</sub>O<sub>9</sub>P<br/>L-Alanine, N-[[P(S),2'R]-2'-deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d<sub>5</sub>)-5'...</p> <p>2 References   4 Reactions   0 Suppliers</p> | <p>3</p> <p>1868135-82-3</p>  <p>Absolute stereochemistry shown</p> <p>C<sub>22</sub>H<sub>14</sub>D<sub>15</sub>FN<sub>3</sub>O<sub>9</sub>P<br/>L-Alanine, N-[[P(S),2'R]-2'-deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d<sub>5</sub>)-5'...</p> <p>1 Reference   1 Reaction   0 Suppliers</p> |
|--|---|---|

## Structure Preferences

### Display CAS Index Name

Show the index name for a structure instead of the CAS preferred name.

OFF

|   |  |  |
|---|--|--|
| <p>1</p> <p>1868134-97-7</p>  <p>Absolute stereochemistry shown</p> <p>C<sub>22</sub>H<sub>24</sub>D<sub>5</sub>FN<sub>3</sub>O<sub>9</sub>P<br/><b>N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d<sub>5</sub>)-5'-uridylyl]-...</b></p> <p>6 References   15 Reactions   0 Suppliers</p> | <p>2</p> <p>1868135-17-4</p>  <p>Absolute stereochemistry shown</p> <p>C<sub>22</sub>H<sub>18</sub>D<sub>11</sub>FN<sub>3</sub>O<sub>9</sub>P<br/>N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d<sub>5</sub>)-5'-uridylyl]-...</p> <p>2 References   4 Reactions   0 Suppliers</p> | <p>3</p> <p>1868135-82-3</p>  <p>Absolute stereochemistry shown</p> <p>C<sub>22</sub>H<sub>14</sub>D<sub>15</sub>FN<sub>3</sub>O<sub>9</sub>P<br/>N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d<sub>5</sub>)-5'-uridylyl]-5'...</p> <p>1 Reference   1 Reaction   0 Suppliers</p> |
|---|--|--|

# 文献详情页面物质信息展现形式

Show Structures on Reference Detail

Display structure images in a grid view on a reference detail.

ON

Show Structures on Reference Detail

Display structure images in a grid view on a reference detail.

OFF

## 带有结构图片的网格

Substances

Substances (59)

1868134-97-7

Absolute stereochemistry shown

**C<sub>22</sub>H<sub>24</sub>D<sub>5</sub>FN<sub>3</sub>O<sub>9</sub>P**  
N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d<sub>5</sub>)-5'-uridylyl]-...

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

2330911-13-0

• HCl

**C<sub>4</sub>H<sub>3</sub>D<sub>2</sub>N<sub>3</sub>O.C1H**

Role: Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

2330911-11-8

Absolute stereochemistry shown

**C<sub>18</sub>H<sub>10</sub>D<sub>7</sub>F<sub>5</sub>NO<sub>5</sub>P**

Role: Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

## 以列表形式展示

Substances

Substances (59)

| CAS RN                       | Chemical Name  | Role  |
|------------------------------|--|---|
| <a href="#">1868134-97-7</a> | N-[[P(S),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-(phenyl-2,3,4,5,6-d <sub>5</sub> )-5'-uridylyl]-... | Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses |
| <a href="#">2330911-13-0</a> |  | Reactant, Synthetic Preparation, Reactant or Reagent, Preparation                                     |
| <a href="#">2330911-11-8</a> |  | Reactant, Synthetic Preparation, Reactant or Reagent, Preparation                                     |
| <a href="#">2093595-25-4</a> | Phenyl-4-d phosphorodichloridate   | Reactant, Synthetic Preparation, Reactant or Reagent, Preparation                                     |
| <a href="#">2093595-17-4</a> | Phenyl-2,3,4,5,6-d <sub>5</sub> phosphorodichloridate  | Reactant, Synthetic Preparation, Reactant or Reagent, Preparation                                     |

# 结果项目管理

Alerts (0) Saved (12) History (769) **Projects (1)**

Saved and History

Alerts (0) Saved (12) History (769) **Projects (1)**

+

Start New Project

**EGFR inhibitor**

References searched by "EGFR or "Epidermal growth factor receptors" and inhibitor"

Updated on 1 September 2023

Edit Project Details 新建项目

Project Name

EGFR inhibitor

Project Color

Orange

Project Description (Optional)

References searched by "EGFR or "Epidermal growth factor receptors" and inhibitor"

Save Cancel

Edit Project

Change Color >

Delete Project

# 添加文献/物质检索结果到项目

## References search for "EGFR or "Epidermal growth factor receptors" and inhibitor"

Substances Reactions Citing Knowledge Graph

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

**Load More Results**

Filter Behavior  
**Filter by** Exclude

Search Within Results

Document Type  
 Journal (47K)  
 Patent (8,045)

56,039 Results Sort: Times Cited View: Partial Abstract

1

**Activating mutations in the epidermal growth factor receptor underlying response to gefitinib in non-small-cell lung cancer**  
By: Lynch, Thomas J.; Bell, Daphne W.; Sordella, Raffaella; Gurubhagavataiah, Patricia L.; Haseerlat, Sara M.; Supko, Jeffrey G.; Haluska, Frank G.; et al  
New England Journal of Medicine (2004), 350(21), 2129-2139 | Language: English

**EGFR inhibitor**

Most patients with non-small-cell lung cancer have no response to the tyrosine kinase inhibitor gefitinib, which targets the epidermal growth factor receptor (EGFR). However, about 10% of patients have a rapid and often dramatic clinical response. The molecular mechanisms underlying sensitivity to gefitinib are unknown. We searched for mutations in the EGFR gene in primary tumors from patients with non-small-cell lung cancer who had a response to gefitinib, those who did not have a response, and those who had not been exposed to gefitinib. The functional consequences of identified mutations were evaluated.

**Add to Project**

## Substances from References

References Reactions Suppliers

1,976,917 Results Sort: Relevance View: Partial

Filter Behavior  
**Filter by** Exclude

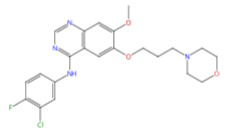
Search Within Results

Reaction Role  
 Product (392K)  
 Reactant (163K)  
 Reagent (10K)  
 Catalyst (7,539)  
 Solvent (2,950)

Reference Role  
 Biological Study (1.7M)

1

**184475-35-2**

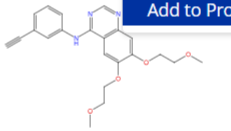


$C_{22}H_{24}ClFN_4O_3$   
4-Quinazolinamine, N-(3-chloro-4-fluorophenyl)-7-methoxy-6-[3-(4-morpholinyl)propyl]-

14K References 882 Reactions 119 Suppliers

2

**183321-74-6**

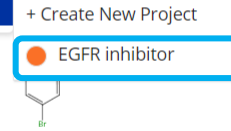


$C_{22}H_{23}N_3O_4$   
4-Quinazolinamine, N-(3-ethynylphenyl)-6,7-bis(2-methoxyethoxy)-

10K References 963 Reactions 78 Suppliers

3

**13-06-8**

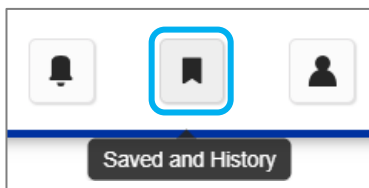


$C_{18}H_{13}BrN_4O$   
2-Butynamide, N-[4-[(3-bromophenyl)amino]-6-quinazolyl]-

111 References 56 Reactions 67 Suppliers

**EGFR inhibitor**

# 删除特定时间段历史记录



Alerts (0) Saved (12) **History (769)** Projects (1)

Filter by



Result Type

- All (19)
- Sequences (30)
- Patent Markush (20)
- Prior Art Analysis (4)
- Reactions (43)
- References (290)
- Retrosynthesis (26)
- Substances (336)
- Suppliers (1)

Date

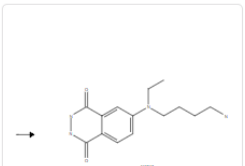
Start Date  to End Date

## Your Search History

769 Searches  


September 1, 2023

**References** 2:05 PM EGFR or "Epidermal growth factor receptors" and inhibitor (56K Results) [Rerun Search](#)  
[Edit Search](#)

**Reactions** 11:59 AM  As Drawn (28) Substructure (109) [Rerun Search](#)  
[Edit Search](#)

## Delete Your Search History

Select a Range

Date  

Time  AM  PM

Delete All

[Delete](#) [Cancel](#)



# CAS SciFinder<sup>n</sup> 新功能总结

## ➤ 文献检索

- 支持高级检索项 IPC Data 检索专利文献
- 文献结果页面支持检索与作者 ORCID iD 相关的参考文献
- 从序列结果获得的文献结果页面新增显示非专利文献
- 文献检索支持根据生物活性数据检索文献
- 文献详情页面推荐相似文献，引文地图可直接查看文献合集
- 知识谱图可直接搜索关注内容

## ➤ 物质检索

- 支持按 LogP 值、官能团、芳香环数量、GHS Code 和是否有文献关联等筛选结果
- 新增多种物质实验属性，核磁谱图支持显示溶剂信息
- 物质检索支持根据生物活性数据检索物质
- CAS Draw 对出错信息添加描述
- 支持根据价格高低筛选供应商信息

# CAS SciFinder<sup>n</sup> 新功能总结

## ➤ 反应检索

- 按转化类型 (Transformation) 分组后, 支持根据转化类型名称或反应数量排序
- 支持按反应规模筛选结果
- 可直接查看相似反应
- 支持对多步反应进行原子对标记和筛选
- 支持下载可编辑RTF格式的反应检索结果
- 逆合成路线结果页面展示更新

## ➤ 设置、项目管理和历史记录

- 支持自定义设置功能和排序
- 文献/物质结果集支持项目管理
- 支持删除特定时间历史记录

Between problems  
and progress  
are connections  
that matter



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