

CAS SCIFINDER DISCOVERY PLATFORM™

探索科研成果转化



[钱欣博士](#)

China@acs-i.org

美国化学文摘社中国代表处

4/25/2025

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CAS SCIFINDER DISCOVERY PLATFORM

2025 春季专题论坛直播时间表



3月21日 | 零基础入门

演讲人：刘子露 博士



3月28日 | 解锁新功能

演讲人：杜德鑫 博士



4月18日 | 助攻论文写作

演讲人：潘娜 博士



4月25日 | 探索科研成果转化

演讲人：钱欣 博士



5月9日 | 结构绘制面板
及案例详解

演讲人：刘子露 博士



5月23日 | 反应检索策略及典型
案例

演讲人：陈开乾 博士

“

扫描二维码，一键预约六场直播！

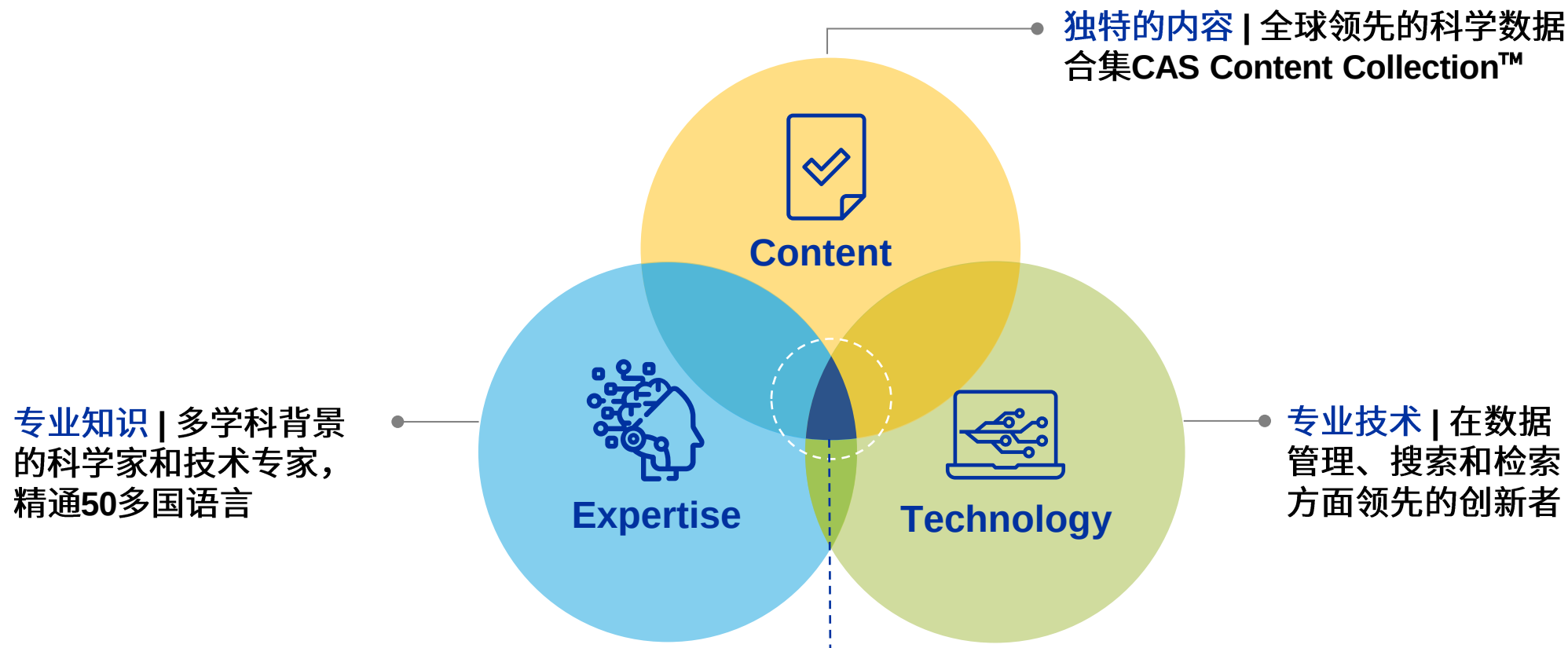


提纲

- CAS SciFinder Discovery Platform简介
- 科研成果转化：科学影响力、技术转化力与商业化潜力的实践探索
 - 技术成熟度高效评估
 - 技术空白精准定位
 - 技术瓶颈快速识别
 - 商业化潜力分析

关于 CAS

CAS 从专业知识、内容和技术三方面为全球创新保驾护航



我们在全球出版的科学数据间建立关联，
将科学数据转化为更好的洞察力

历经百年，CAS 始终如一 承担着连接全球科学知识的工作

协助科学家解决重大科学信息挑战



50K+

超过5万种科技期刊

50+

50多种语言

290+

超过2.9亿种物质

109

109家
专利授权机构

CAS独特的内容合集



来源：

<https://www.cas.org/cas-data>

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

CAS 对文献的独特解读

以专利WO2018152134为例

改写的标准和摘要，尽可能揭示专利核心价值

丰富的增值标引信息：

19 Concepts

163 Substances

625 Reactions

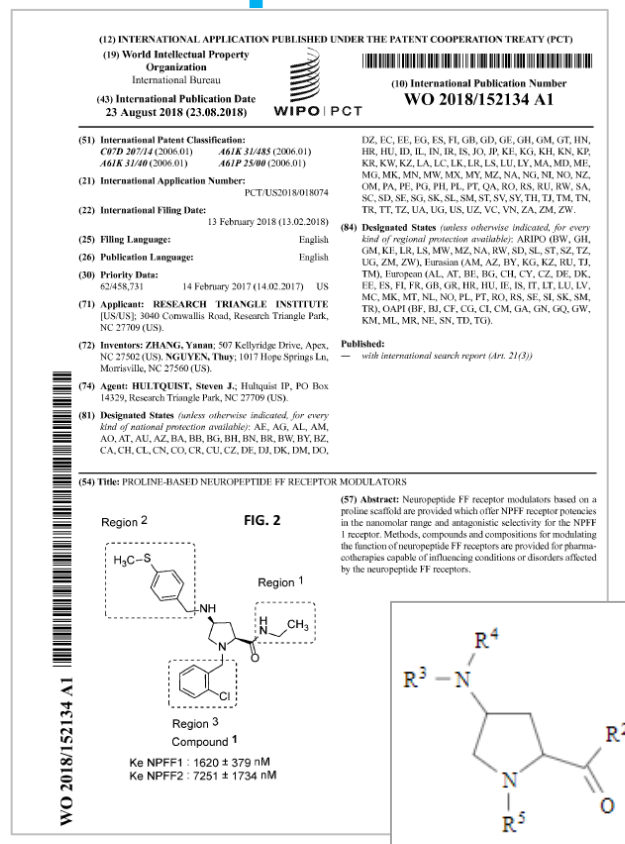
15 Patent Family Members

3 Formulations

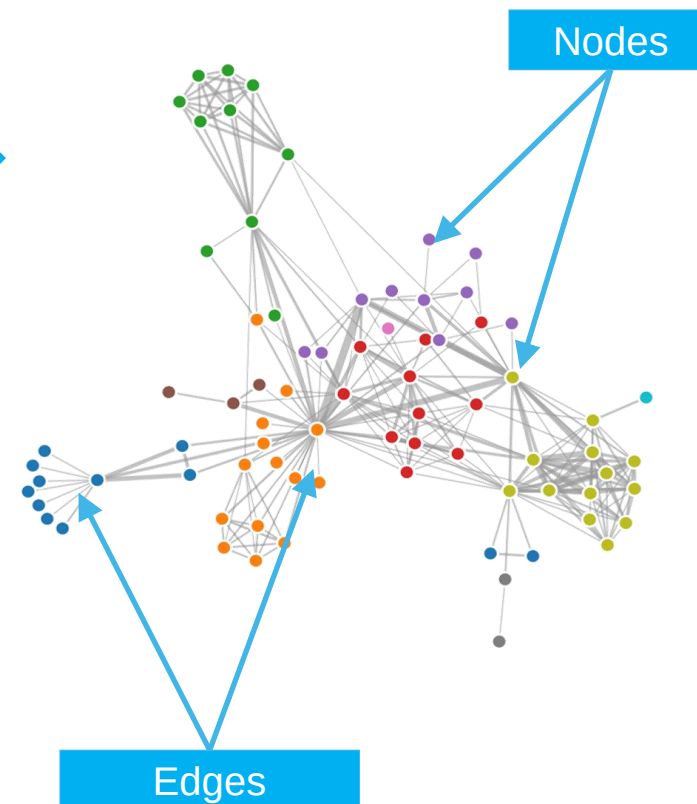
1 Markush structure

18 SAR data points

141 ADME data points



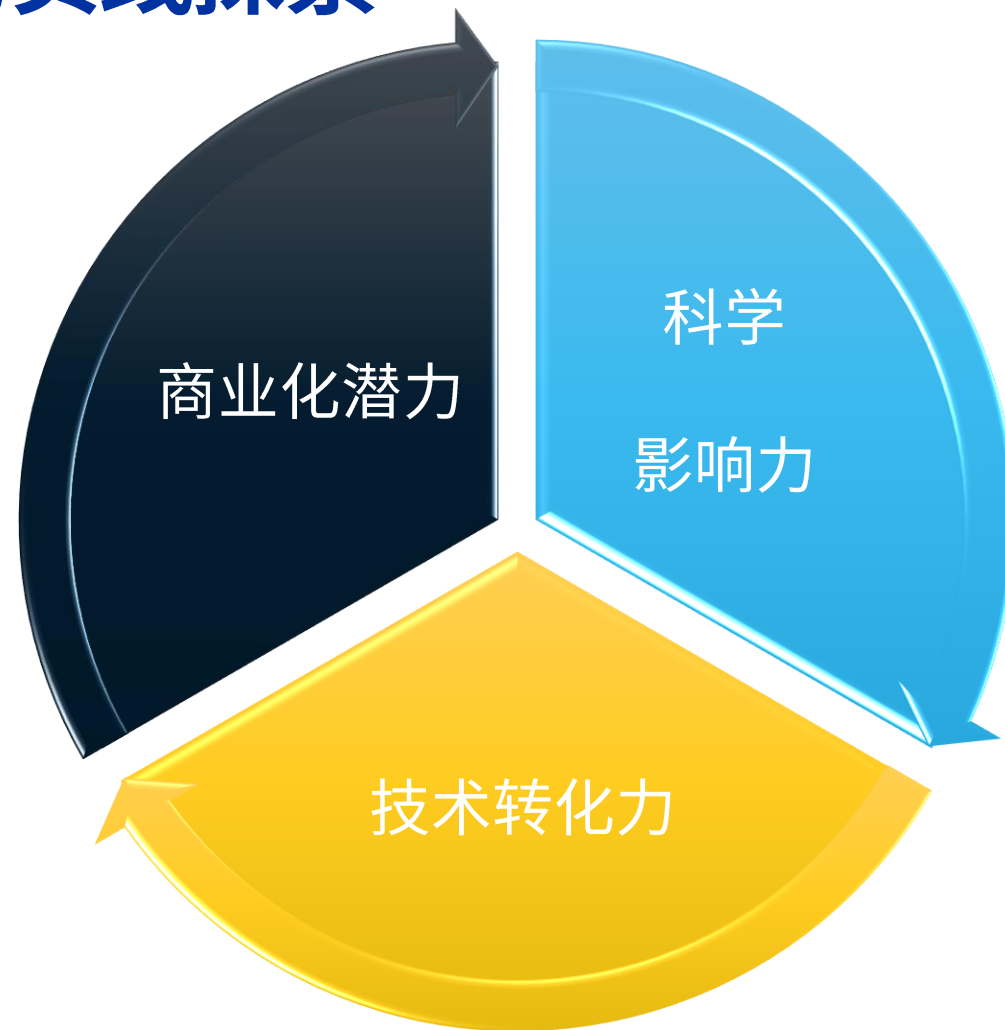
Click document to view on CAS SciFinder®



提纲

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 - 技术空白精准定位
 - 技术瓶颈快速识别
 - 商业化潜力分析

科技成果转化：科学影响力、技术转化力与商业化潜力的实践探索



示例一：技术成熟度评估——专利数量远高于期刊发表数量

CAS SciFinder

References ("Lithium-ion Battery" or "Li battery" or "Lithium battery")

Draw

6

Clear All Filters

We are displaying the most relevant results.
[Learn about result relevance.](#)

Load All Results

Filtering: Publication Year: 2014 to No Max

以锂电池回收领域为例

10,308 Results

Sort: Publication Date: Newest View: No Abstract

1

Method for recycling waste lithium battery positive electrode material
Assignee: Guangdong Ruichi New Energy Technology Co., Ltd.
China, CN119812547 A 2025-04-11 | Language: Chinese, Database: CAPLUS
[View Abstract](#)

Full Text

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

2

A method for recycling and repairing waste lithium iron phosphate positive electrode material and lithium iron phosphate finished product
Assignee: DFD New Energy Technology Co., Ltd.
China, CN119812543 A 2025-04-11 | Language: Chinese, Database: CAPLUS
[View Abstract](#)

Filter Behavior

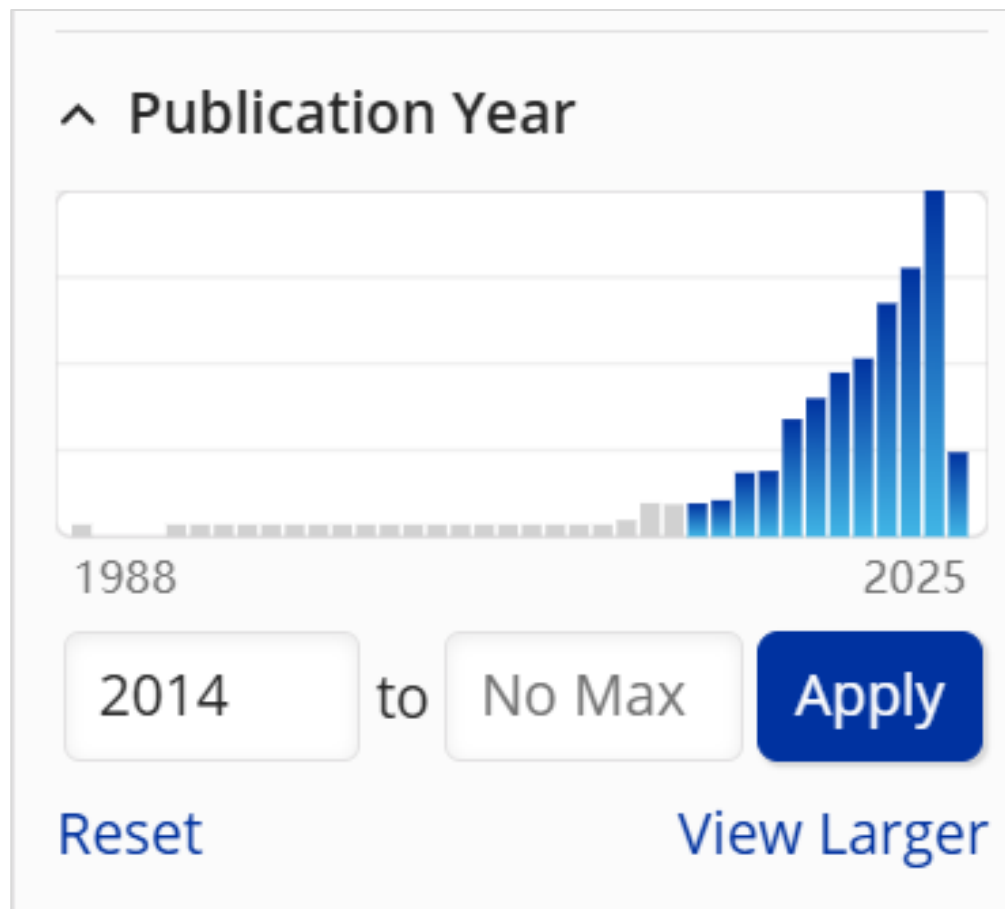
Filter by Exclude

Search Within Results

Document Type

- Journal (4,230)
- Patent (6,022)
- Review (502)
- Book (1)

数量增长显著，企业主导创新



Organization

Top Count Alphanumeric Search

0 Selected

☐ Hunan Brulp Recycling Technology Co., Ltd. (245)	☐ Changzhou University (18)	☐ Northeastern University (13)
☐ Guangdong Brulp Recycling Technology Co., Ltd. (244)	☐ GEM Co., Ltd. (18)	☐ Quannan Ruilong Technology Co., Ltd. (13)
☐ Central South University (164)	☐ Lanzhou University of Technology (18)	☐ Research Institute of Industrial Science & Technology (13)
☐ [NAME NOT TRANSLATED] (99)	☐ Xiangtan University (18)	☐ Taiheiyu Cement Corporation (13)
☐ Anhui Narada Huabo New Material Technology Co., Ltd. (73)	☐ Beijing Institute of Technology (17)	☐ Tongji University (13)
☐ Kunming University of Science and Technology (72)	☐ Jiangxi Ruida New Energy Technology Co., Ltd. (17)	☐ Tongji University (13)
☐ Hunan Brulp EV Recycling Co., Ltd. (68)	☐ Nanchang Hangkong University (17)	☐ Zhengzhou University (13)
☐ Institute of Process Engineering, Chinese Academy of Sciences (67)	☐ Beijing Institute of Technology (16)	☐ Zhengzhou University (13)
☐ Hefei Guoxuan High-tech Power Energy Co., Ltd. (64)	☐ Guangxi Normal University (16)	☐ China ENFI Engineering Corporation (12)
	☐ Hunan Brulp Automobile Recycling Co., Ltd. (16)	☐ Hefei University of Technology (12)
	☐ Wuhan Weineng Battery Asset	☐ Jiangsu University (12)

构建技术壁垒，提高市场竞争力，推动成果转化

CAS SciFinder

References ("Lithium-ion Battery" or "Li battery" or "Lithium battery")

Substances (29) Reactions (0) Citing (6) Citation Map

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

- ☐ Journal (4,230)
- ☒ Patent (6,022)
- ☐ Review (502)
- ☐ Book (1)
- ☐ Commentary (3)

View All

Language

- ☐ Chinese (5,131)
- ☐ English (404)

6

Processes for extracting metals from lithium-ion batteries

Assignee: Albemarle Corporation

World Intellectual Property Organization, WO2020092157 A1 2020-05-07 | Language: English, Database: CAplus

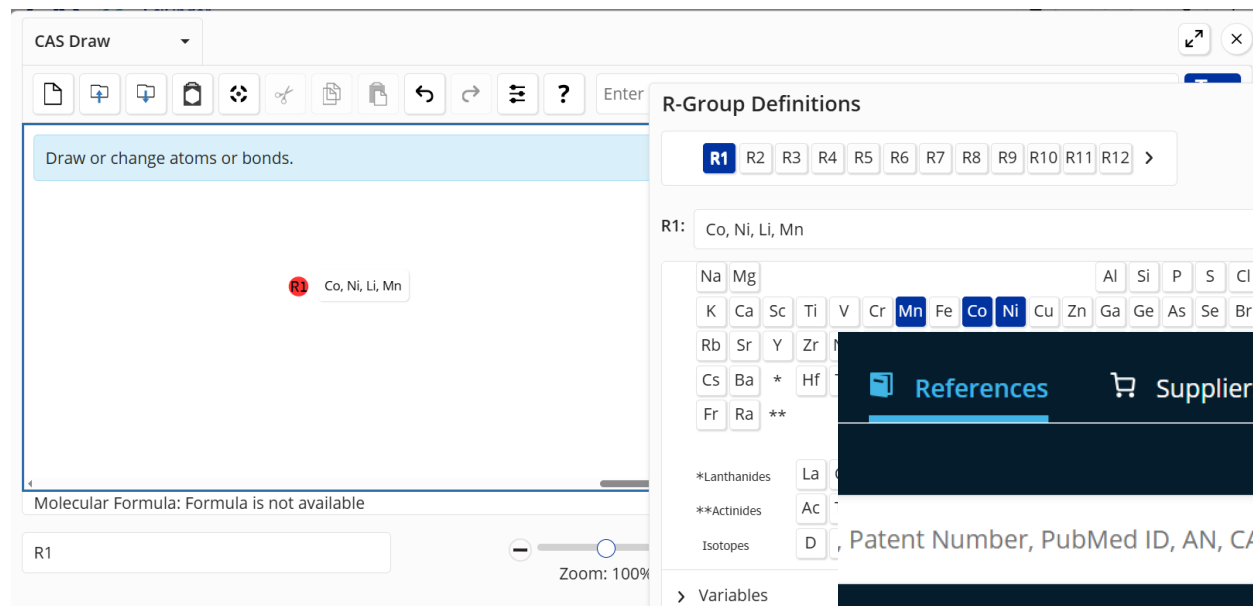
View Abstract

PatentPak Full Text

Substances (19) Reactions (0) Citing (5) Citation Map

Patent	Language	Kind Code	PatentPak Options
WO2020092157	English	A1	PDF PDF+ Viewer
AU2019373424	English	A1	PDF
CN113039295	Chinese	A	PDF
KR2021080379	Korean	A	PDF
JP2022507019	Japanese	T	PDF
JP7483700	Japanese	B2	PDF
US20210395859	English	A1	PDF

技术迁移：其他领域的金属回收方案是否适用于锂电池金属回收？



References Suppliers

For You NEW

Patent Number, PubMed ID, AN, CAN, and/or DOI.

Edit

name, first name middle name.

Example: Schubert, J A

R₁

Edit Drawing Remove

通过CAS Role获取所有关于给定金属回收的文献

References search for drawn structure

Substances

Reactions

Citing

Knowledge Graph

Structure Match

As Drawn (3.6M)

Substructure (4.3M)

Filter Behavior

Filter by

Exclude

Search Within Results

Document Type

Filtering: Substance Role: Purification or Recovery

32,355 Results

Sort: Publication Date: Newest

View: M

1

System and method for recycling magnetic material and rare earth elements contained therein

Assignee: Cyclic Materials Inc.

United States, US20250109454 A1 2025-04-03 | Language: English, Database: CAPLUS

View Abstract

PatentPak

Full Text

Substances (12)

Reactions (0)

Citing (0)

Cita

除去锂电池领域，依然有丰富的金属回收方法文献可借鉴

 **References search for drawn structure**

Substances ▾ Reactions ▾ Citing ▾ Knowledge Graph

Document Type

- ☐ Journal (12K)
- ☐ Patent (15K)
- ☐ Review (722)
- ☐ Book (11)
- ☐ Commentary (1)

[View All](#)

Substance Role

- ☐ Uses (2M)
- ☐ Properties (1.4M)

Filtering: Substance Role: Purification or Recovery ✕

Excluding: Search Within Results: lithium battery ✕

[Clear All Filters](#)

☐ 29,501 Results

Sort: Times Cited ▾ View: No Abstract ▾

☐ 1

Synthesis of hcp. Co nanodisks

By: Puentes, Victor F.; Zanchet, Daniela; Erdonmez, Can K.; Alivisatos, A. Paul

Journal of the American Chemical Society (2002), 124(43), 12874-12880 | Language: English, Database: CAPLUS and MEDLINE

[View Abstract ▾](#)

Full Text ▾

Substances (11) Reactions (0) Citing (612) Citation Map

示例二：技术成熟度评估

领域期刊发表数量远大于专利发表量，学术影响力大而专利转化有限

CAS SciFinder

References supramolecular and "self-assembly"

Draw

6

以超分子自组装为例

We are displaying the most relevant results.
Learn about result relevance.
Load All Results

Filter Behavior
Filter by Exclude

Search Within Results

Document Type

- ☐ Journal (28K)
- ☐ Patent (1,457)
- ☐ Review (4,570)
- ☐ Biography (3)

32,733 Results

1

Gold Nanoparticles: Assembly, Supramolecular Chemistry, Quantum-Size-Related Properties, and Applications toward Biology, Catalysis, and Nanotechnology.
By: Daniel, Marie-Christine; Astruc, Didier
Chemical Review

A review. An ex...
This will motiva...
components in

Full Text

2

Folding DN...
By: Rothemund...
Nature (London)

Publication Year

1977 2025

2014 to No Max Apply

Reset View Larger

Database: English, Database: CAPLUS and MEDLINE

old nanoparticles has become available recently.
of other mol., inorganic, and biol. nanomaterials
line.

Citing (11K) Citation Map

Database: CAPLUS and MEDLINE

to direct their self-organization is widely used to

学术领域繁荣

Publication Name

Top Count

Alphanumeric

Search

0 Selected

☐ Angewandte Chemie, International Edition (1,390)

☐ Chemistry - A European Journal (1,384)

☐ Journal of the American Chemical Society (1,332)

☐ Chemical Communications (Cambridge, United Kingdom) (1,108)

☐ Langmuir (688)

☐ ACS Applied Materials & Interfaces (449)

☐ Soft Matter (427)

☐ ACS Nano (413)

☐ Macromolecules (Washington, DC, United States) (392)

☐ RSC Advances (370)

☐ Nano Letters (169)

☐ Molecules (160)

☐ Proceedings of the National Academy of Sciences of the United States of America (160)

☐ Supramolecular Chemistry (153)

☐ Chemical Engineering Journal (Amsterdam, Netherlands) (149)

☐ Journal of Materials Chemistry B: Materials for Biology and Medicine (148)

☐ Colloids and Surfaces, A: Physicochemical and Engineering Aspects (145)

☐ Journal of Materials Chemistry C: Materials for Optical and

☐ Scientific Reports (81)

☐ Huaxue Jinzhan (79)

☐ Journal of Physical Chemistry Letters (78)

☐ Frontiers in Chemistry (Lausanne, Switzerland) (75)

☐ Polymers (Basel, Switzerland) (75)

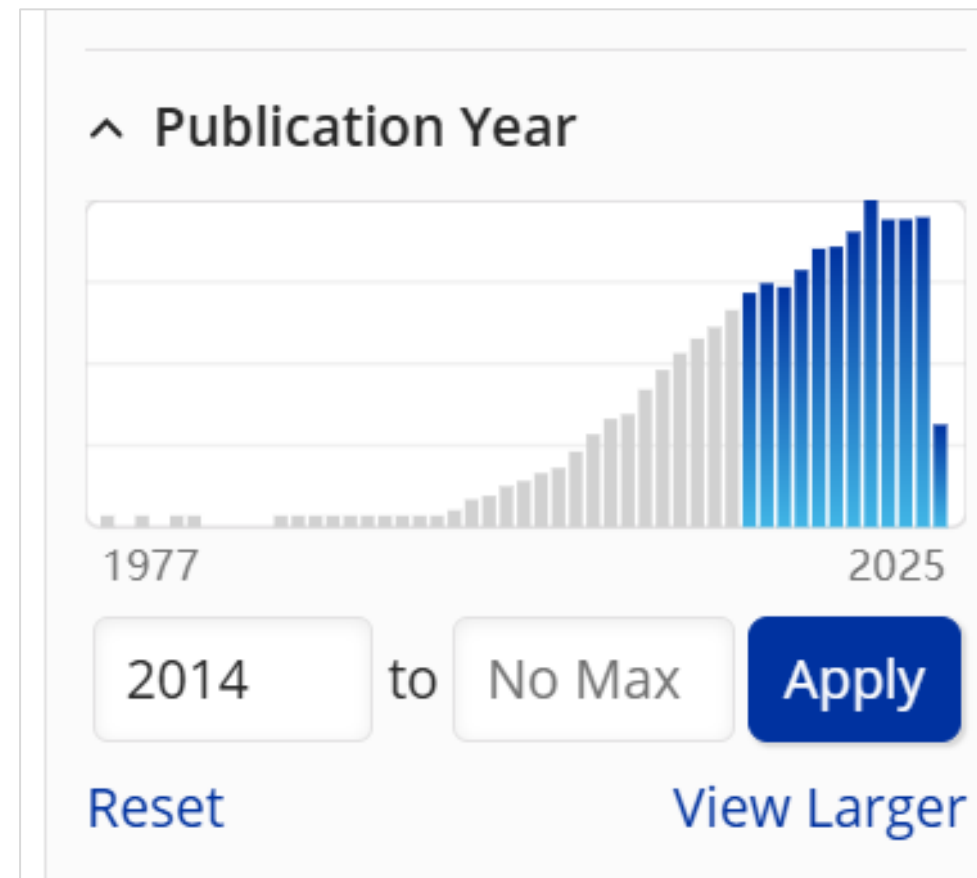
☐ Biomaterials (74)

☐ Analytical Chemistry (Washington, DC, United States) (70)

☐ Chemistry Letters (70)

☐ Advanced Healthcare Materials (69)

☐ ACS Applied Bio Materials (68)



专利引用次数少，专利布局没有高效构建技术壁垒

CAS SciFinder

References ▾ supramolecular and "self-assembly"

Sort: Times Cited ▾ View: No Abstract ↑

1,457 Results

1

Pyridazine and pyrrole compounds, particularly nonlinear oligopyridazines, pyridazinylpyrroles and oligopyrroles, processes for their preparation and uses in medicine, materials, environmental, electronic and optics field

Assignee: C.N.R.S.
World Intellectual Property Organization, WO2008012440 A2 2008-01-31 | Language: French, Database: CAplus

View Abstract ▾

PatentPak ▾ Full Text ▾ Substances (118) Reactions (150) Citing (14) Citation Map

Patent	Language	Kind Code	PatentPak Options
WO2008012440	French	A2	PDF
JP5564252	Japanese	B2	PDF
US9034873	English	B2	PDF

assembly of rationally designed peptides, and
ducts, tissue engineering scaffolds and drug

relevant results.
Learn about result relevance.
Load All Results

Search Within Results

Document Type

- ☐ Journal (28K)
- ☒ Patent (1,457)
- ☐ Review (4,570)
- ☐ Biography (3)
- ☐ Book (16)

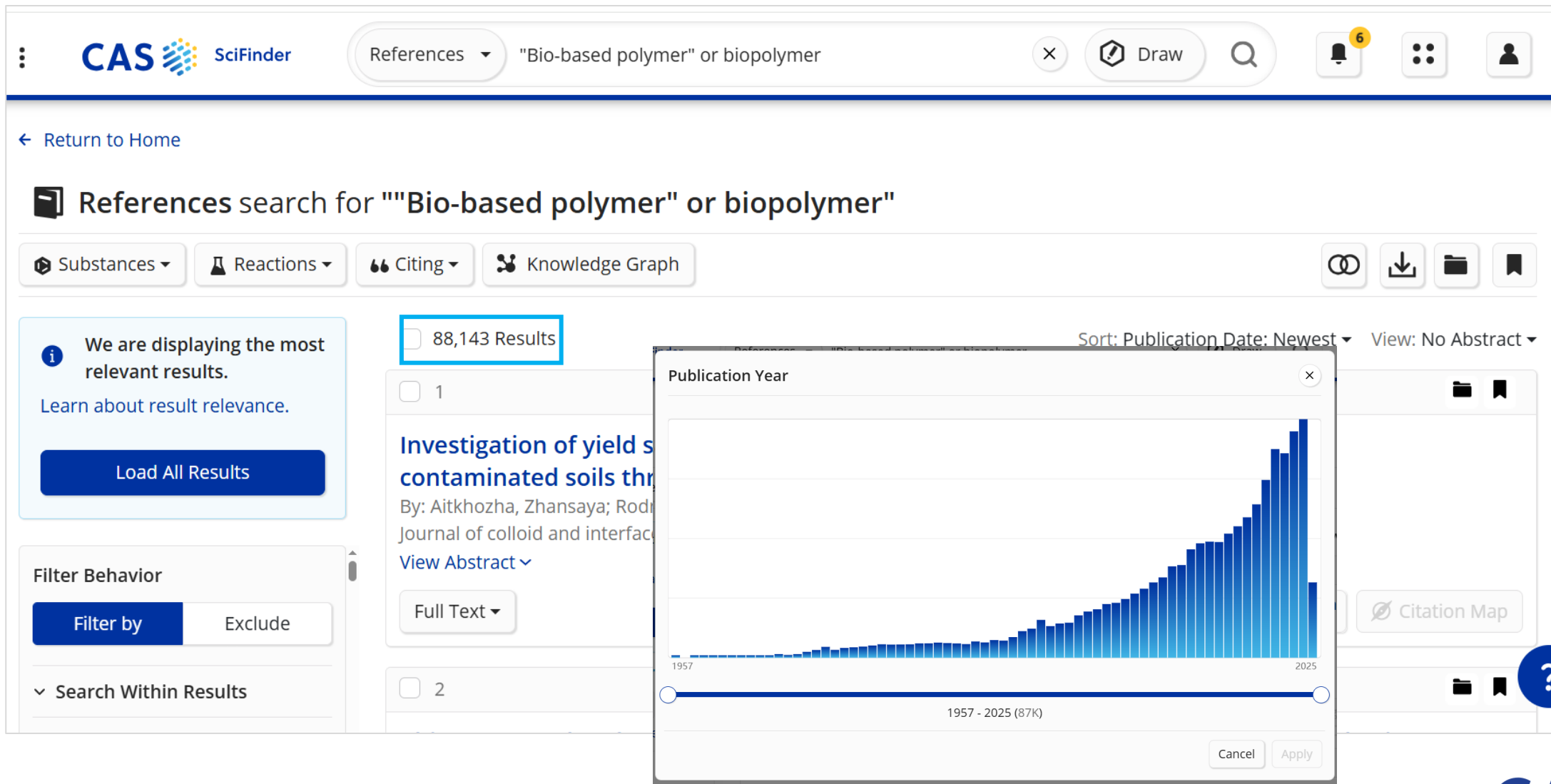
View All

Language

提纲

- CAS SciFinder Discovery Platform简介
- 科研成果转化：科学影响力、技术转化力与商业化潜力的实践探索
 - 技术成熟度高效评估
 - 技术空白精准定位
 - 技术瓶颈快速识别
 - 商业化潜力分析

示例一：技术空白精准定位：生物基聚合物论文爆炸式增长



但是耐热生物基聚合物报道却很少

CAS SciFinder

References ("Bio-based polymer" or biopolymer) and temperature and high and resistan*

Substances Reactions Citing Knowledge Graph

We are displaying the most relevant results.
Learn about result relevance.
Load All Results

664 Results

Sort: Publication Date: Newest View: No Abstract

1

Fully biomass porous photothermal composite material with enhanced microstructure and its preparation method and application thereof

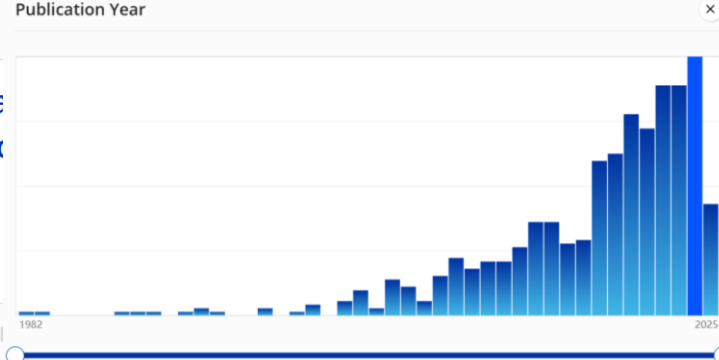
Assignee: Wuyi University
China, CN119637839 A 2025-03-18 | Language: Chinese, Database: CAPlus
View Abstract

PatentPak Full Text Substances (3) Reaction

2

Ionic liquid grafted modified high temperature resistant bio-based nylon and its preparation

Publication Year



1982 2025

1982 - 2025 (659)

Cancel Apply

具体以聚酰胺为例，由物质获取文献

The screenshot displays the CAS SciFinder web interface. At the top, the CAS logo and 'SciFinder' text are visible. A search bar contains 'Substances' and 'Enter a query...'. Below the search bar, there are tabs for 'References', 'Reactions', and 'Suppliers'. The main section is titled 'Substances search for drawn structure'. On the left, there are filters for 'Structure Match' (As Drawn (419K), Substructure (220.9M), Similarity (42K)) and 'Chemscape Analysis'. The main search results area shows 'Filtering: Polymer Class: Polyamide' and '161,566 Results'. A chemical structure is displayed with the ID '3079285-15-4'. On the right, a 'References from Substances' panel is open, showing '385,846 Results'. It includes a 'Filter Behavior' section with 'Filter by' and 'Exclude' options, and a 'Search Within Results' section. A reference entry is visible: 'Silica microparticles as guiding substrates for the fabrication of steel sheets by dip-coating technique: Application to the... samples by direct infusion mass spectrometry' by Pedraza-Soto, Ana M.; Lucena, Rafael; Cardenas, Soledad. The reference is from 'Analytica Chimica Acta (2025), 1348, 343814'. A 'Full Text' button is also present.

CAS SciFinder

Substances Enter a query...

Return to Home

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (419K)

Substructure (220.9M)

Similarity (42K)

Chemscape Analysis

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

Filtering: Polymer Class: Polyamide

161,566 Results

1

3079285-15-4

3079277

References from Substances

Substances Reactions Citing Knowledge Graph

385,846 Results

1

Silica microparticles as guiding substrates for the fabrication of steel sheets by dip-coating technique: Application to the... samples by direct infusion mass spectrometry

By: Pedraza-Soto, Ana M.; Lucena, Rafael; Cardenas, Soledad

Analytica Chimica Acta (2025), 1348, 343814 | Language: English, Database: CAS

View Abstract

Full Text

Substances (7)

聚酰胺耐热性文献报道广泛，其中石油基PA占主导

References from Substances

Substances ▾

Reactions ▾

Citing ▾

Knowledge Graph

Filter Behavior

Filter by

Exclude

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

Searching for...

Clear All

Filtering:

Search Within Results: heat resist* X

Clear All Filters

184,754 Results

Sort: Publication Date: Newest ▾ View: No Abstract ▾

1

Anode for lithium secondary battery, lithium secondary battery comprising same, and manufacturing method for anode for lithium secondary battery

Assignee: LG Energy Solution, Ltd.

World Intellectual Property Organization, WO2025071315 A1 2025-04-03 | Language: Korean, Database: CAPlus

View Abstract ▾

PatentPak ▾

Full Text ▾

Substances (12)

Reactions (0)

Citing (0)

Citation Map

23

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CAS
A division of the
American Chemical Society

如再用生物基限定，可见生物基耐热性聚酰胺报道极为有限



References

 Draw 

 6  

[Return to Home](#)

 **References from Substances**

Substances ▾

Reactions ▾

Citing ▾

Knowledge Graph

Filter Behavior

Filter by

Exclude

Search Within Results

Search for up to 3 text strings within the result set.

Searching for... [Clear All](#)

Filtering:

Search Within Results: 2 Selected ▾ ×

☒ heat resist*

☒ biopolymer or "bio-based polymer"

☐ 941 Res

Sort: Publication Date: Newest ▾

View: No Abstract ▾

☐ 1

Surface-modified fibers and articles and methods of making the same

Assignee: Origin Materials Operating, Inc.

World Intellectual Property Organization, WO2025064709 A1 2025-03-27 | Language: English, Database: CAplus

[View Abstract ▾](#)

PatentPak ▾

Full Text ▾

Substances (36)

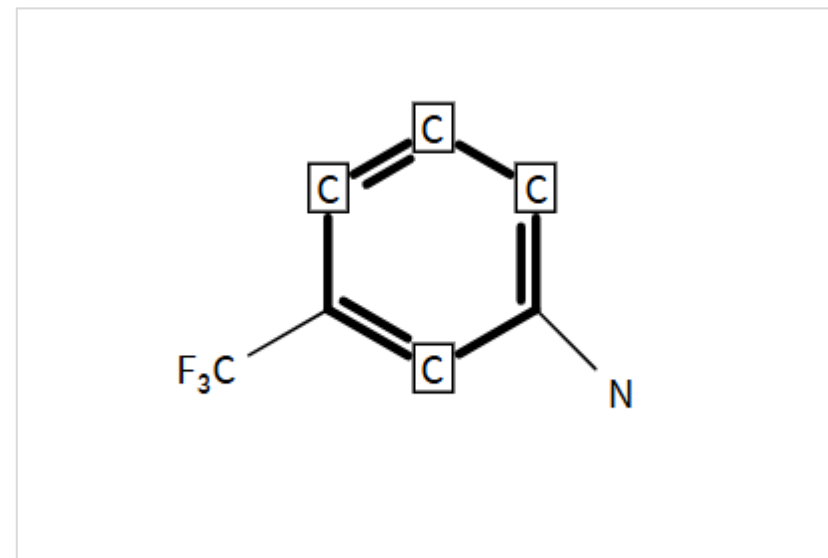
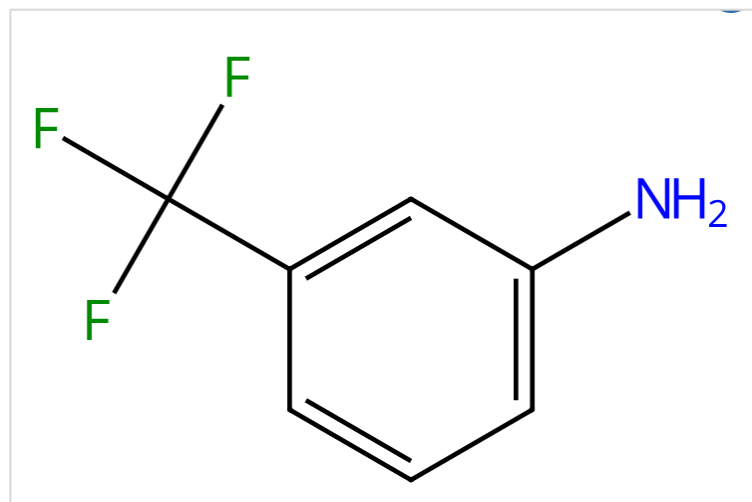
Reactions (0)

Citing (0)

Citation Map

示例二：技术空白精准定位——目标中间体转化高附加值产品

间三氟甲基苯胺可以转化为哪些农化用途分子？特别要求：只在氨基处修饰。



锁环锁原子，保证只有N为开放位点

物质结果集中，限定应用为Agricultural Use

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

- Product (4,118)
- Reactant (179)
- Reagent (1)
- Catalyst (3)
- Solvent (1)

Reference Role

- Preparation (98K)
- Synthetic Preparation (97K)
- Biological Study (86K)
- Uses (85K)
- Prophetic Synthesis or Use (61K)
- ☒ Agricultural Use (54K)

[View All](#)

References Reactions Suppliers

☒ Agricultural Use (54K) [View All](#)

Life Science Data

Commercial Availability

- ☐ Available (830)
- ☐ Not Available (53K)

Number of Components

Molecular Weight

LogP

Stereochemistry

Element

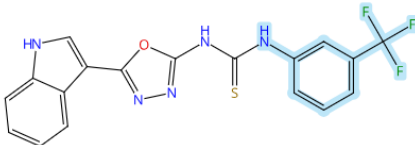
Filtering: Reference Role: Agricultural Use X [Clear All Filters](#)

54,224 Results

Sort: CAS RN: Descending View: Partial

1

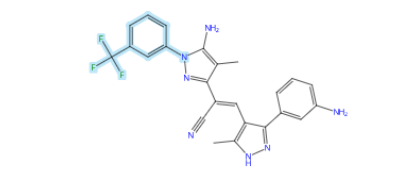
3076466-93-5



C18H12F3N5OS
Thiourea, N-[5-(1H-indol-3-yl)-1,3,4-oxadiazol-2-yl]-N'-[3-(trifluoromethyl)phenyl]...

2

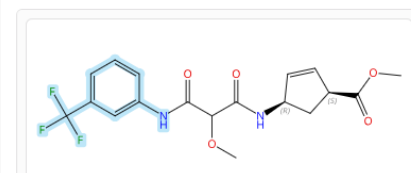
3075600-68-6



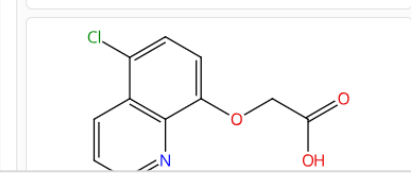
C24H20F3N7
1H-Pyrazole-3-acetonitrile, 5-amino-α-[[3-(3-aminophenyl)-5-methyl-1H-pyrazol-4-yl]...

3

3068688-99-0



Absolute stereochemistry shown



筛选由间三氟甲基苯胺转化的反应

^ Search Within Results

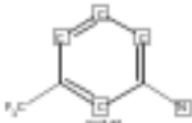
Search for up to 3 structures within the result set.

Draw

Search

Searching for... [Clear All](#)

Remove and Edit

 →

^ Substance Role

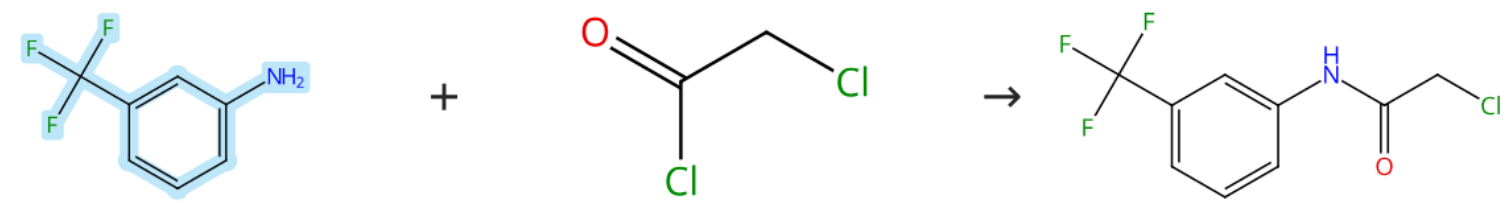
☒ Product (1,775)

1,775 Results

Group: By Scheme ▾ Sort: Publication Date: Newest ▾ View: Expanded ▾

Scheme 1 (68 Reactions)

Steps: 1 Yield: 61%



Suppliers (63)

Suppliers (44)

Suppliers (65)

☐ 31-614-CAS-41865402

Steps: 1

Synthesis, characterization and evaluation of novel isoquinoline analogues as anticancer agents

By: Ambati, Anna Reddy; et al

Journal of Molecular Structure (2025), 1321(Part_3), 139957

Full Text ▾

1.1 Reagents: [Triethylamine](#)

Solvents: [Dichloromethane](#); 4 - 5 h, 0 - 5 °C

Experimental Protocols

☐ 31-614-CAS-40553717

Steps: 1

Green preparation of pyrazoline-1,3,4-oxadiazole thioacetamide derivatives as pesticides

技术空白精准定位：还有哪些基于目标中间体的重要农化分子还没有合成报道？

Structure Match

As Drawn (65)

Substructure (351K)

Similarity (39K)

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

Filtering: Reference Role: Agricultural Use X

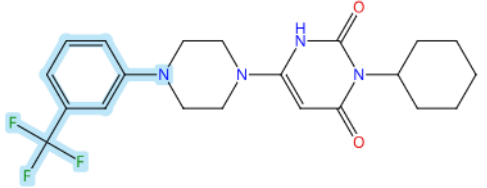
Excluding: Reaction Role: Product X

50,098 Results

Sort: Number of Suppliers View: Partial

1

1883548-87-5

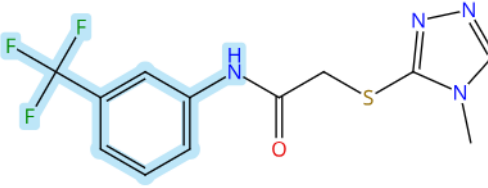


C₂₁H₂₅F₃N₄O₂
3-Cyclohexyl-6-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]-2,4(1H,3H)-pyrimidin-5(1H)-one

2 References 0 Reactions 47 Suppliers

2

328266-10-0

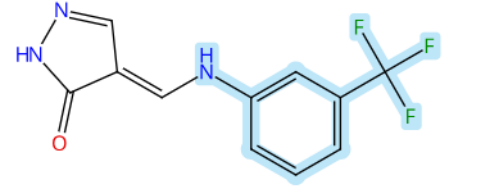


C₁₂H₁₁F₃N₄OS
2-[(4-Methyl-4H-1,2,4-triazol-3-yl)thio]-N-[3-(trifluoromethyl)phenyl]acetamide

1 Reference 0 Reactions 15 Suppliers

3

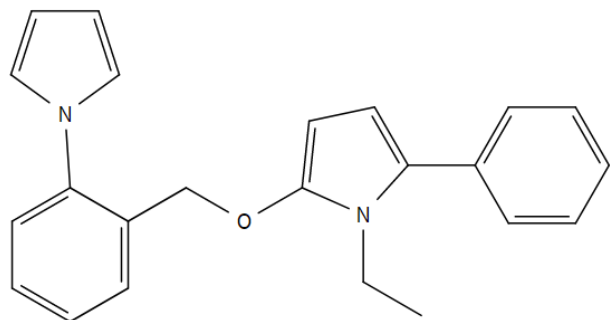
338777-72-3



C₁₁H₈F₃N₃O
2,4-Dihydro-4-[[[3-(trifluoromethyl)phenyl]amino]methylene]-3H-pyrazol-3-one

1 Reference 0 Reactions 14 Suppliers

示例三：技术空白精准定位——我设计的结构有哪些应用？应该做哪些活性测试？



As drawn, Substructure结果为0,
Similarity结果中物质最大相似度
仅为75-79%

该物质是否隐藏在Markush结构中?

CAS SciFinder[®]

Substances ▾

Enter a query...

Edit ▴

🔍

🔔

🔖

👤

← Return to Home

🔍 Patent Markush search for drawn structure

📖 References ▾

Patent Markush Match

As Drawn (1)

Substructure (1)

Filter Behavior

Filter by Exclude

Patent Office

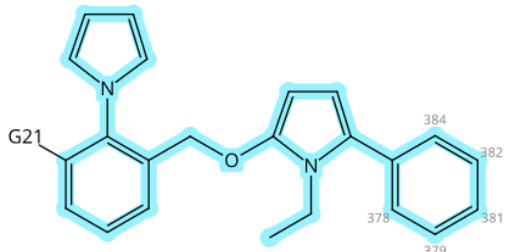
☐ World Intellectual Property Organization (1)

CA Section

1 Result

1

WO2018062978



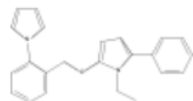
Preparation of heteroaryl compounds as antiviral agents

By: Min, Ji Young; Chang, So Young; Lee, Ji Hye; Kang, Sun Hee; Kong, Sun Ju; Jo, Su Yeon; Park, Kaapjoo; Kim, Young Mi; Choi, Junghwan
World Intellectual Property Organization, WO2018062978 A1 2018-04-05 |
Language: Korean, Database: CAPlus
Assignee: Institut Pasteur Korea

Patent claim 1

PatentPak ▾ Full Text ▾

378,379,381,382,384: opt. substd. by G16



Edit Drawing Remove

☒ Search Patent Markush

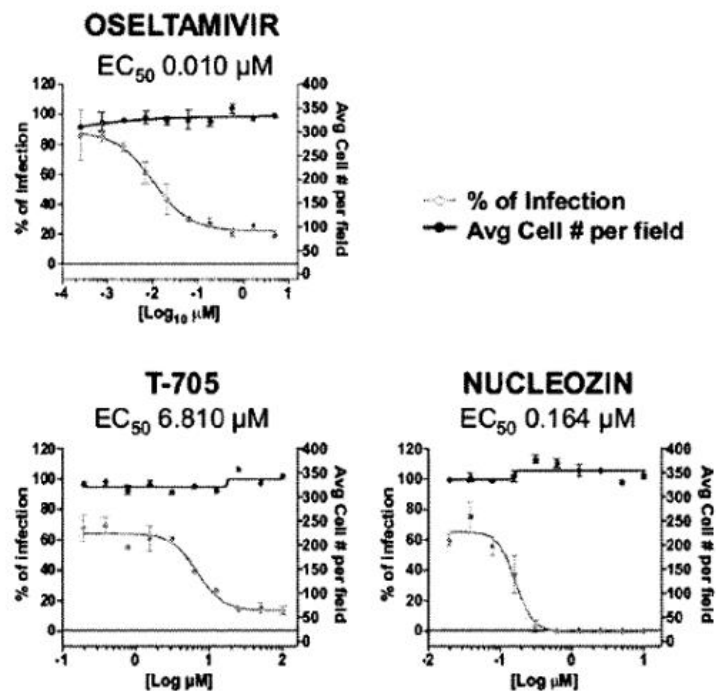
📧

🔔 Save and Alert

通过PatentPak直接获取专利PDF文件

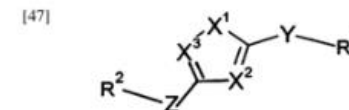
(54) Title: NOVEL HETEROARYL COMPOUND, ENANTIOMER, DIASTEREOMER OR PHARMACEUTICALLY ACCEPTABLE SALT THEREOF, AND ANTIVIRAL COMPOSITION CONTAINING SAME AS ACTIVE INGREDIENT

(54) 발명의 명칭: 신규 헤테로아릴 화합물, 이의 거울상 이성질체, 부분 입체 이성질체 또는 약학적으로 허용가능한 염, 및 이를 유효성분으로 함유하는 항바이러스용 조성물



WO 2018/062978

PCT/KR2017/011091



[48] 상기 식에서,

[49] X¹은 O, S 또는 -N(CH₂CH₃)- 이고,

[50] X² 및 Y는 각각 독립적으로 N 또는 CH 이며,

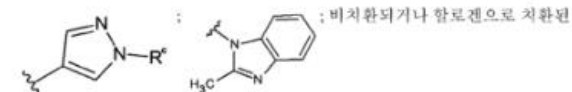
[51] Y는 존재하지 않거나; -CH₂-; -CH₂NH-; -C(=O)-; -CH₂CH₂-; -NH-; -NHC(=O)-; -C(=O)NH-; -CH(CH₃)-; -CF₂-; -CH(OCH₃)-; -CH₂O-; -N(CH₃)-; 또는 -CH₂NHC(=O)- 이고,

[52] Z는 존재하지 않거나; -CH₂S-; -CH₂S(=O)-; -CH₂NH-; -CH(R')S-; -CH₂CH₂S-; -CH₂N(CH₃)-; -CH₂N(CH₃)₂-; -CH=CH-; -S-; -CH₂-; -O-; -CH₂S(=O)₂-; -C(=O)-; -CH₂N(C(=O)CH₃)-; -SCH₂-; -CH₂CH₂-; -CH(OH)-; -CH(CH₃)CH₂-; -OCH₂-; -C(=O)CH₂S-; -C(=O)-NH-; -CH=C(CH₃)-; -CH₂-사이클로프로필-; -NH-S(=O)₂-; -S(=O)₂-NH-; -NH-C(=O)-이며,

[53] R'는 벤젠이고,

[54] R¹은 ; 비치환되거나, 할로겐, 직쇄 또는 분쇄형 C₁₋₄알킬, C₁₋₄

사이클로알킬, -OCF₃, -CF₃, -CHF₃, -OH, 페녹시, 페닐, C₁₋₄알콕시, -CN, -NH₂, 및 -N(CH₃)₂로 이루어진 군에서 선택한 1종 이상으로 치환된 벤젠; ;



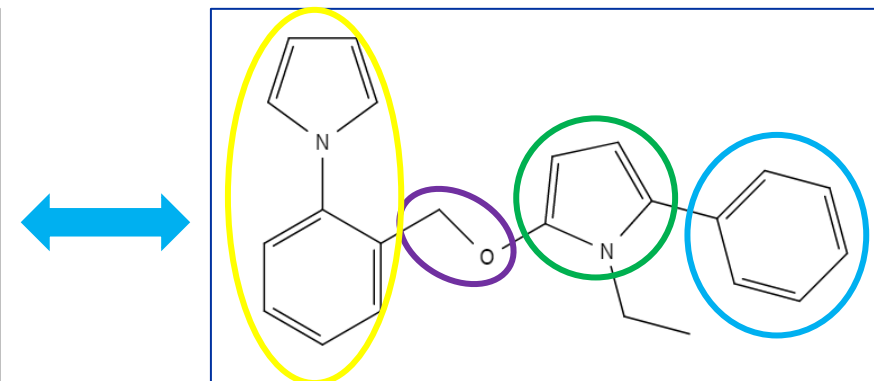
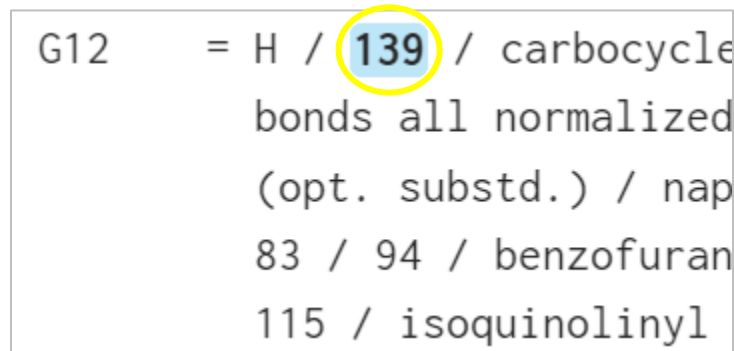
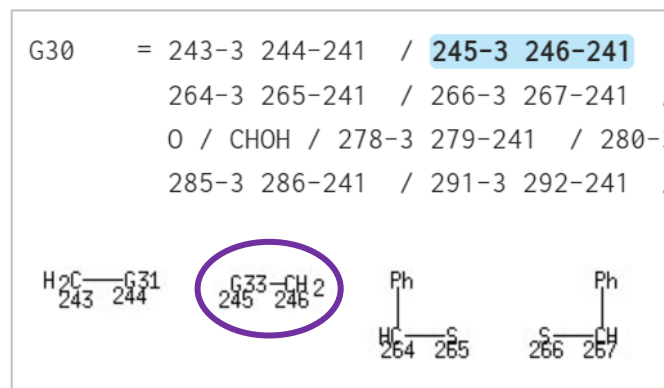
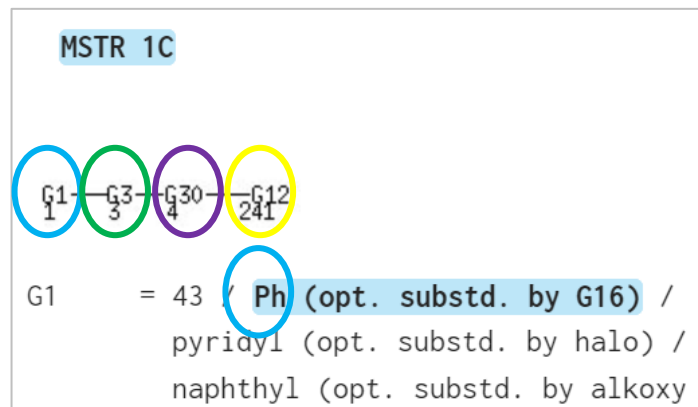
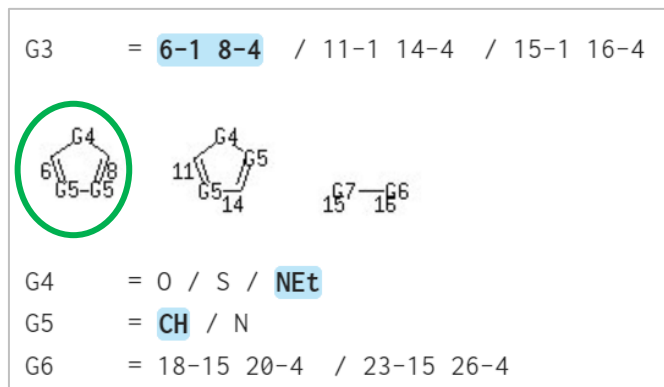
피리딘; 비치환되거나 C₁₋₄알콕시로 치환된 나프탈렌; 벤조트리아졸; 비치환되거나, C₁₋₄알킬, C₁₋₄알콕시 또는 할로겐으로 치환된 퀴놀린 또는 이소퀴놀린; 비치환되거나 C₁₋₄알킬로 치환된 인다졸; C₁₋₄ 사이클로알킬; 벤조티오펜; 벤조퓨란; 비치환되거나 C₁₋₄알킬로 치환된 인돌; 또는 티오벤이며,

[55] R²는 할로겐; 직쇄 또는 분쇄형 C₁₋₄알킬; OCF₃; CF₃; 또는 비치환된 벤젠이고,

[56] R²는 벤젠이며,

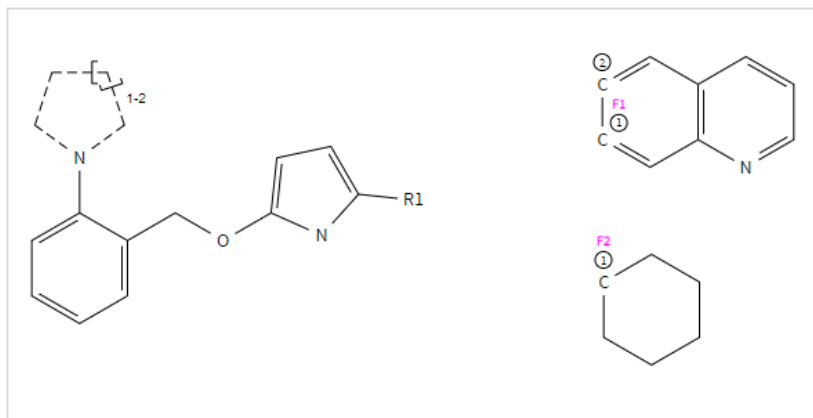
[57] n은 0 내지 3 범위의 정수이고,

清晰展示查询结构如何被专利原文中的 Markush 结构覆盖，提高专利阅读效率



查询结构如何被覆盖均可清晰展示

系列化合物可采取相同方式进行检索



R1 = F1, F2

R

自定义R基团

Fn

片段结构

[]
1-4

重复工具

...

不确定键级

CAS SciFinder

Substances Enter a query...

Return to Home

Patent Markush search for drawn structure

References

Patent Markush Match

As Drawn (0)

Substructure (1)

Filter Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (1)

CA Section

1 Result

1

WO2018062978

Preparation of heteroaryl compounds as antiviral agents

Assignee: Institut Pasteur Korea
World Intellectual Property Organization, WO2018062978 A1 2018-04-05 | Language: Korean, Database: CPlus

Patent claim 1

PatentPak Full Text

609,610,613,615,616,617: opt. substd. by G15

提纲

- CAS SciFinder Discovery Platform简介
- 科研成果转化：科学影响力、技术转化力与商业化潜力的实践探索
 - 技术成熟度高效评估
 - 技术空白精准定位
 - 技术瓶颈快速识别
 - 商业化潜力分析

示例一：技术瓶颈快速识别——合成工艺对比

是否全面获取工艺信息？工艺条件是否适配？

The screenshot displays the CAS Reactions search interface. At the top, there are navigation tabs: "All", "Substances", and "Reactions". Below these, a search bar contains the text "synthesis of 1818339-66-0". The main search results area shows "Reactions search for 'synthesis of 1818339-66-0'" with 67 results. On the left, a sidebar contains filters: "Non-Participating Functional Groups", "Reaction Mapping", "Reaction Scale", and "Experimental Protocols". The "Reaction Scale" filter is highlighted with a blue box and includes the following options: "Milligram (31)", "Gram (27)", "Kilogram (7)", and "No Scale Provided (29)". The main results area shows "Scheme 1 (3 Reactions)" with a chemical reaction scheme. The scheme shows a complex molecule with a fluorine atom and a nitrogen atom, reacting to form a product with a fluorine atom and a nitrogen atom. The product is labeled "Absolute stereochemistry shown, Rotation (-)". Below the scheme, there is a button labeled "Suppliers (37)".

不同量产规模的工艺对比

CAS SciFinder

Reactions synthesis of 1818339-66-0

7 results

Filter Behavior

Filter by Exclude

- Search Within Results
- Yield
- Number of Steps
- Non-Participating Functional Groups
- Reaction Mapping
- Reaction Scale**
 - ☐ Milligram (31)
 - ☐ Gram (27)
 - ☒ Kilogram (7)
 - ☐ No Scale Provided (29)

Scheme 1 (1 Reaction)

Absolute stereochemistry shown

	Products
	N-[2-((4aR,6S,8aR)-2-Amino-4,4a,5,6-tetrahydro-6-methylpyrano[3,4-d][1,3]thiazin-8a(8H)-yl]-4-thiazolyl]-5-(difluoromethoxy)-2-pyridinecarboxamide, Yield: 86%
	Reactants
	N-[2-((4aR,6S,8aR)-2-(Benzoylamino)-4,4a,5,6-tetrahydro-6-methylpyrano[3,4-d][1,3]thiazin-8a(8H)-yl]-4-thiazolyl]-5-(difluoromethoxy)-2-pyridinecarboxamide
	Reagents
	L-Lysine
	Solvents

31-353-CAS-23620715 Steps: 1 Yield: 86% ...

1.1 Reagents: [L-Lysine](#)
Solvents: [Isopropanol](#), [Water](#); 25 °C; 2 h, 90 °C; 30 min, 90 °C → 55 °C

1.2 Reagents: [Sodium hydroxide](#)
Solvents: [Water](#); 55 °C; 2 h, 55 °C → 20 °C; 20 °C → 55 °C; 2 h, 55 °C → 20 °C

[Experimental Protocols](#)

查看反应源文献

📄 Process Development of a Second Generation β -Amyloid-Cleaving Enzyme Inhibitor-Improving the Robustness of a Halogen-Metal Exchange Using Continuous Stirred-Tank Reactors

 13

29

“4

 Citation Map

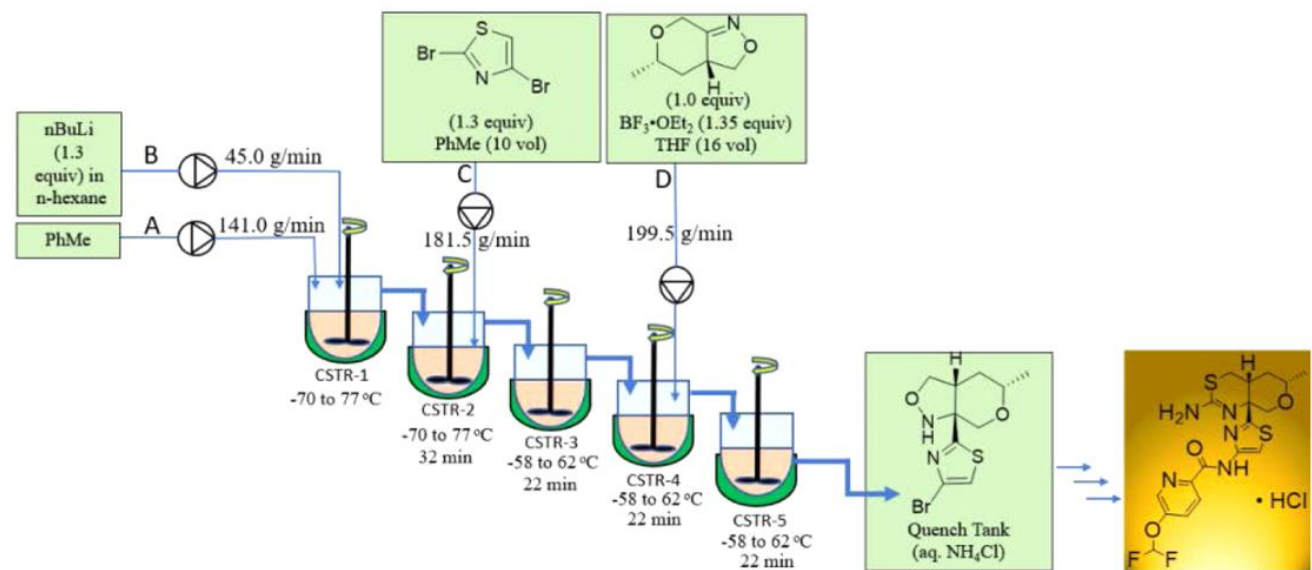
In this Reference

- [CAS Concepts](#)
- [Substances](#)
- [Reactions](#)
- [Cited Documents](#)

By: Li, Bryan ; Barnhart, R
Teresa; Maloney, Mark; Nels
[View All](#) 

DOI: 10.1021/acs.oprd.1c00

Process development for the
lithiothiazole addition to the



毫克级制备的方法

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

☒ Milligram (31)

☐ Gram (27)

☐ Kilogram (7)

☐ No Scale Provided (29)

☐ 31 Results

Group: By Scheme ▾ Sort: Publication Date: Newest ▾ View: Expanded ↑

Scheme 1 (1 Reaction) Steps: 1 Yield: 61% ⋮

Absolute stereochemistry shown

+

Suppliers (20)

→

Absolute stereochemistry shown, Rotation (-)

Suppliers (37)

☐ 31-172-CAS-19339935 Steps: 1 Yield: 61% ⋮

1.1 Reagents: [Lithium tert-butoxide](#)
Catalysts: [Tris\(dibenzylideneacetone\)dipalladium](#),
[\[3,6-Dimethoxy-2',4',6'-tris\(1-methylethyl\)\[1,1'-biphenyl\]-2-yl\]bis\(1,1-dimethyl...](#)
Solvents: [2-Methyl-1-butanol](#); 3 min, 95 °C

1.2 Solvents: [1,4-Dioxane](#), [2-Methyl-1-butanol](#); 1 h, 95 °C

Design and Synthesis of Clinical Candidate PF-06751979: A Potent, Brain Penetrant, β -Site Amyloid Precursor Protein Cleaving Enzyme 1 (BACE1) Inhibitor Lacking Hypopigmentation

By: O'Neill, Brian T.; et al

Journal of Medicinal Chemistry (2018), 61(10), 4476-4504

Full Text ▾

38

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CAS
A division of the
American Chemical Society

也可通过Retrosynthesis查看适配的工业方案

Retrosynthesis Plan for drawn structure Powered by **Che**

Key Experimental Steps Predicted Steps Edit Structure View Excluded Options Save

A Max Yield 86% View all alternatives (232) View evidence Exclude this step

B Max Yield 93%

C (10)

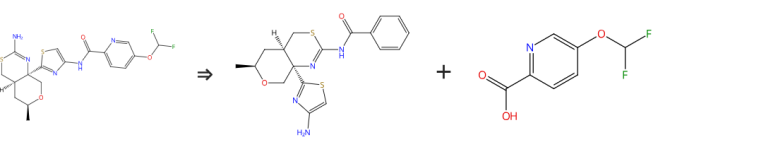
D (66)

A ⇒ B Alternative Steps (232)

Filter by

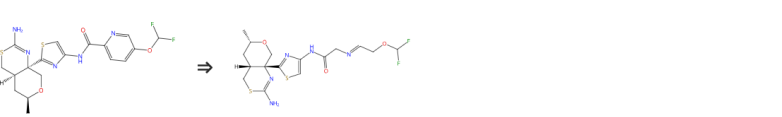
- Alternative Step Type
 - Experimental (2)
 - Predicted (230)
- Experimental Stereochemistry
 - Non-Selective (2)

3 of 65 Predicted Step



Select View 60 similar Alternatives View evidence Average yield: 61%

4 of 65 Predicted Step



持续助力杰出的EHS管理与规范，保障企业的可持续发展，并树立行业典范

CAS在数据内容上提供丰富的化学品危害、
管控、注册、安全和绿色化学等相关信息

- 提供GHS危害信息
- 提供化学品管控信息
- 提供实验安全及绿色化学相关信息
- CAS持续增加相关内容

^ CA Section

- ☐ Pharmaceuticals (586)
- ☒ Unit Operations and Processes (195)
- ☐ Biochemical Methods (102)
- ☐ Pharmacology (71)
- ☐ Pharmaceutical Analysis (49)

[View All](#)

CAS Registry Number: 1190307-88-0

References (4,279) Reactions (725) Suppliers (68)

GHS危害与合规管控信息

Reaction Notes

By Count Alphanu

8 Selected

- ☐ Stereoselective (101)
- ☐ Regioselective (97K)
- ☒ Safety (58K)
- ☐ Combinatorial (41K)
- ☐ Chemoselective (22K)
- ☐ Solid-Support
- ☐ Thermal (19K)
- ☒ Green Chemistry (10K)
- ☐ Photochemical (15K)
- ☐ Microwave Irradiation (11K)
- ☐ In The Dark (8K)

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)
 - ☐ H335: May cause respiratory irritation (1)
 - ☐ H319: Causes serious eye irritation (1)
 - ☐ H315: Causes skin irritation (1)
 - ☐ H302: Harmful if swallowed (1)
- ☐ Bioactivity Indicator
- ☐ Target Indicator
- ☐ Regulatory Data by Country/Region
- ☐ Reference Availability

Regulatory Information

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 serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria
H335	May cause respiratory irritation	Fisher Scientific

聚焦安全与绿色化学相关反应

CAS Method Number 3-513-CAS-7303816

Transformations

1. Reduction of Aldehydes and Ketones to Alcohols

Reaction Notes

high pressure, stereoselective, key intermediate, ee 87.8%, scale up, catalyst prepared and used, autoclave used

CAS
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American Chemical Society

示例二：工艺对比——配方对比

Formulations

Ingredients

Search by Formulations by Ingredients, Purpose, Form, Functions, etc.

Formulation Designer

Design custom formulation templates based on selections

Advanced Search

Search Formulations by criteria like ingredients, functions, etc.

Advanced Formulations Search

Searches the following content fields: Ingredient, Function, Form, etc.

At least two search terms are required.

Search For

Operator

Enter one term

All Fields

Required

Antibacterial

General search of all fields

Search For

Operator

Enter one term

Function

Required

mouthwash

Ex: binder, surfactant, carrier

CAS Formulus

Formulations + "Antibacterial " +Function:"mouthwash"

Delivery Route

Information Included

Document Type

Component

Function

Amount Reported

Group: ingredient

Breath fresheners

-

Antibacterial agents

Antibacterial agents

-

Breath fresheners

-

-

Thickening agents

-

-

flavors

-

-

Additional group components reported

Group: water-soluble/water-swallowable polymer

-

-

Acrylic acid

-

-

可将专利、产品说明书中的配方成分、工艺直接进行对比

	 Predicted value	
	Formulation 1	Formulation 2
	Nano-Emulsion Composite: Mouthwashes or Toothpastes, Etc.	Oral Antivavity Sodium Fluoride Mouthwash:
Purpose	Antiulcer agents, Oral hygiene products, To	
Target	Aphthous ulcer, Dental pain, Homo sapiens	
Delivery Route	Oral drug delivery systems	
Physical Form	Dental creams	
Experimental Activity	Not Available	
Components	Ocimum gratissimum oil Function: Anti-inflammatory agents, Anti- Essential oils, wintergreen Function: Antipruritic agents, Analgesics, Anti-inflammatory agents Amount Reported: 1 pbw Optionality: Mandatory Mentha Function: Antibacterial a Amount Reported: 3 pbw Optionality: Mandatory Essential oils, wintergreen Function: Antipruritic agents, Analgesics, Anti-inflammatory agents Amount Reported: 1 pbw Optionality: Mandatory	Water Function: Solvents Amount Reported: - Optionality: Mandatory Glycerol Function: Humectants Amount Reported: - Optionality: Mandatory Cetylpyridinium chloride Function: Antibacterial agents, Cationic surfactants Amount Reported: -
	Source	
		PATENT Nano-emulsion composite and preparation method and application thereof Assignee : Ningbo Liwah Pharmaceutical Co., Ltd. CN108938558 Language: Chinese Location: Example 1, Table 1 Patent PDF View in CAS SciFinder
		PRODUCT INSERT oral ANTIVAVITY sodium fluoride mouthwash Manufacturer : Vi-Jon, LLC NDC: 11822-5768-6 Location: Product insert

提纲

- CAS SciFinder Discovery Platform简介
- 科研成果转化：科学影响力、技术转化力与商业化潜力的实践探索
 - 技术成熟度高效评估
 - 技术空白精准定位
 - 技术瓶颈快速识别
 - 商业化潜力分析

商业化潜力分析

有哪些MOF材料制备技术较为成熟，并且有较强的商业化潜力？

Good Afternoon, Cyrene

All Substances Reactions References

"Metal-organic frameworks" or MOF

+ Add Advanced Search Field

References search for ""Metal-organic frameworks" or MOF"

Substances Reactions Citing Knowledge Graph

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

☐ Journal (124K)

☐ Patent (24K)

☐ Review (14K)

☐ 155,416 Results

☐ 1

Sustained antimicrobial polymer film from γ -CD-MOF hu preservation.

By: Yu, Wangfei; Wang, Guannan; Chen, Huizhi; Mu, Honglei; Niu, Ben; Han, Food chemistry (2025), 479, 143856 | Language: English, Database: MEDLIN

[View Abstract](#)

Full Text

Substances (2)

通过CAS Role获取可以工业化规模制备的MOF材料

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

☐ Preparation (46K)

☐ Synthetic Preparation (45K)

☐ Properties (42K)

☐ Process (16K)

☐ Physical, Engineering, or Chemical Process (16K)

☒ Industrial Manufacture (2,910)

Filtering:

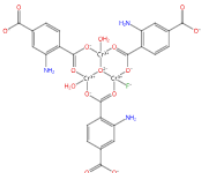
Reference Role: Industrial Manufacture X

Substance Class: Coordination Compound X

2,910 Results

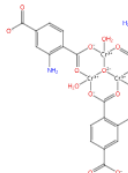
1

3079218-29-1

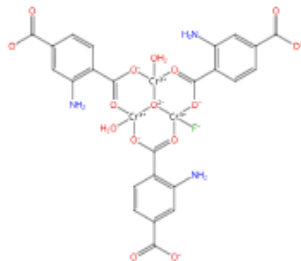


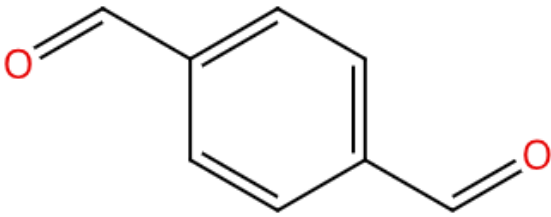
2

3079218-28-0



3079218-29-1





$$(\text{C}_{24}\text{H}_{19}\text{Cr}_3\text{FN}_3\text{O}_{15} \cdot \text{C}_8\text{H}_6\text{O}_2 \cdot \text{C}_3\text{H}_7\text{N})_x$$

Role: Industrial Manufacture, Polymer in Formulation, Technical or Engineered Material Use, Preparation, Uses

包含羧基配体的商业可获得MOF材料

CAS SciFinder

Substances Enter a query... Draw

6

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Searching for... Clear All

Remove and Edit

Reaction Role

Reference Role

Reference Role: Industrial Manufacture X

Commercial Availability: Available X

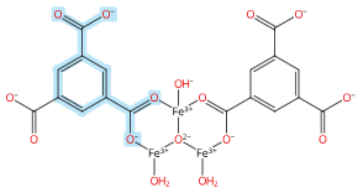
Substance Class: Coordination Compound X

51 Results

Sort: Number of Suppliers View: Partial

1

1257379-83-1

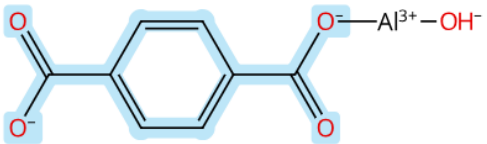


$C_{18}H_{11}Fe_3O_{16}$
Diaquabis[μ-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO¹]]hydroxy-μ₃-oxotriiron

54 References 56 Reactions 35 Suppliers

2

654061-20-8

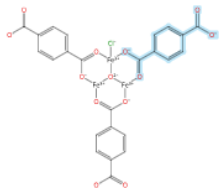


$C_8H_5AlO_5$
[1,4-Benzenedicarboxylato(2-)-κO¹]hydr oxyaluminum

1,283 References 470 Reactions 32 Suppliers

3

1189182-67-9



$C_{24}H_{12}ClFe_3O_{13}$
Tris[μ-[1,4-benzenedicarboxylato(2-)-κO¹:κO¹]]chloro-μ₃-oxotriiron

877 References 517 Reactions 30 Suppliers

包含羧基配体的商业不可获得MOF材料

CAS SciFinder

Substances Enter a query...

Draw

6

Clear All Filters

Return to Home

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Searching for... Clear All

Remove and Edit

HOOC

HOOC

Filtering:

Search Within Results: Drawn Structure

Reference Role: Industrial Manufacture

Commercial Availability: Not Available

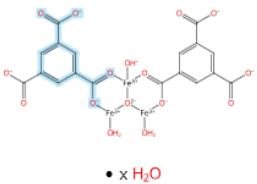
Substance Class: Coordination Compound

469 Results

Sort: Number of Suppliers View: Partial

1

1257297-80-5



$\text{C}_{18}\text{H}_{11}\text{Fe}_3\text{O}_{16} \cdot x\text{H}_2\text{O}$

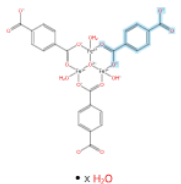
Components: 2

Component RN: 1257379-83-1

Iron, diaquabis[μ-[1,3,5-benzenetricarboxylato(2-)-κO¹:κO²]]tris[μ-[5'-(4-carboxyphenyl)-1,3,5-benzenetricarboxylato(2-)-κO¹:κO²]]]·x H₂O

2

1341133-27-4



$\text{C}_{24}\text{H}_{17}\text{Fe}_3\text{O}_{16} \cdot x\text{H}_2\text{O}$

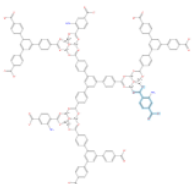
Components: 2

Component RN: 1341134-41-5

Iron, diaquatrakis[μ-[1,4-benzenedicarboxylato(2-)-κO¹:κO²]]]·x H₂O

3

1092659-25-0



$\text{C}_{132}\text{H}_{75}\text{N}_3\text{O}_{39}\text{Zn}_{12}$

Zinc, tris[μ-[2-amino-1,4-benzenedicarboxylato(2-)-κO¹:κO²]]]tris[μ-[5'-(4-carboxyphenyl)-1,3,5-benzenetricarboxylato(2-)-κO¹:κO²]]]·x H₂O

总结

- CAS收录完整的科技内容合集，并且具有独特的标引。确保检索结果全面，可靠。
- 技术成熟度评估：通过文献类型、研究机构、引文数量等揭示领域科技转化潜力。
- 技术空白定位：通过关键词限定、CAS Role、Markush检索等探索技术空白。
- 技术瓶颈识别：通过对比合成工艺、配方工艺等识别技术瓶颈。
- 商业化潜力分析：通过CAS数据关联，物质类别，供应商信息等分析材料的商业价值。

Between problems
and progress **are**
connections that
matter

are connections that
matter

谢谢!

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