

# CAS持续增值的数据内容 与多元创新服务

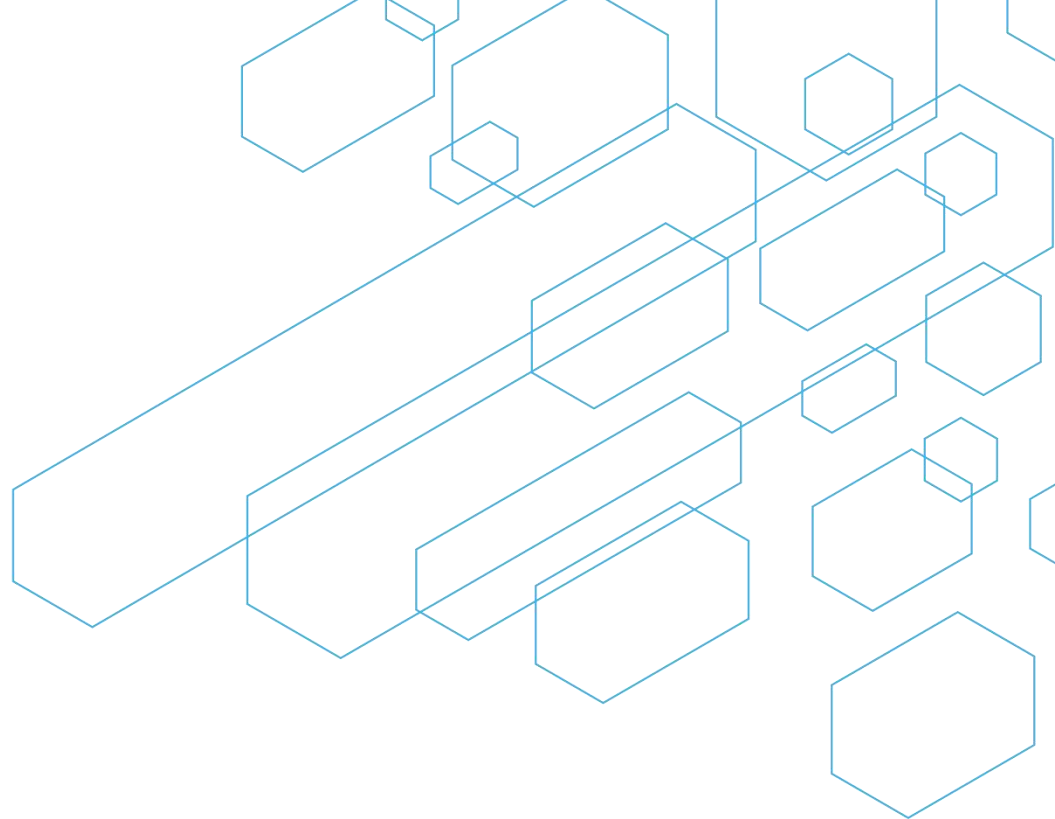


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美国化学文摘社 (CAS) 北京代表处



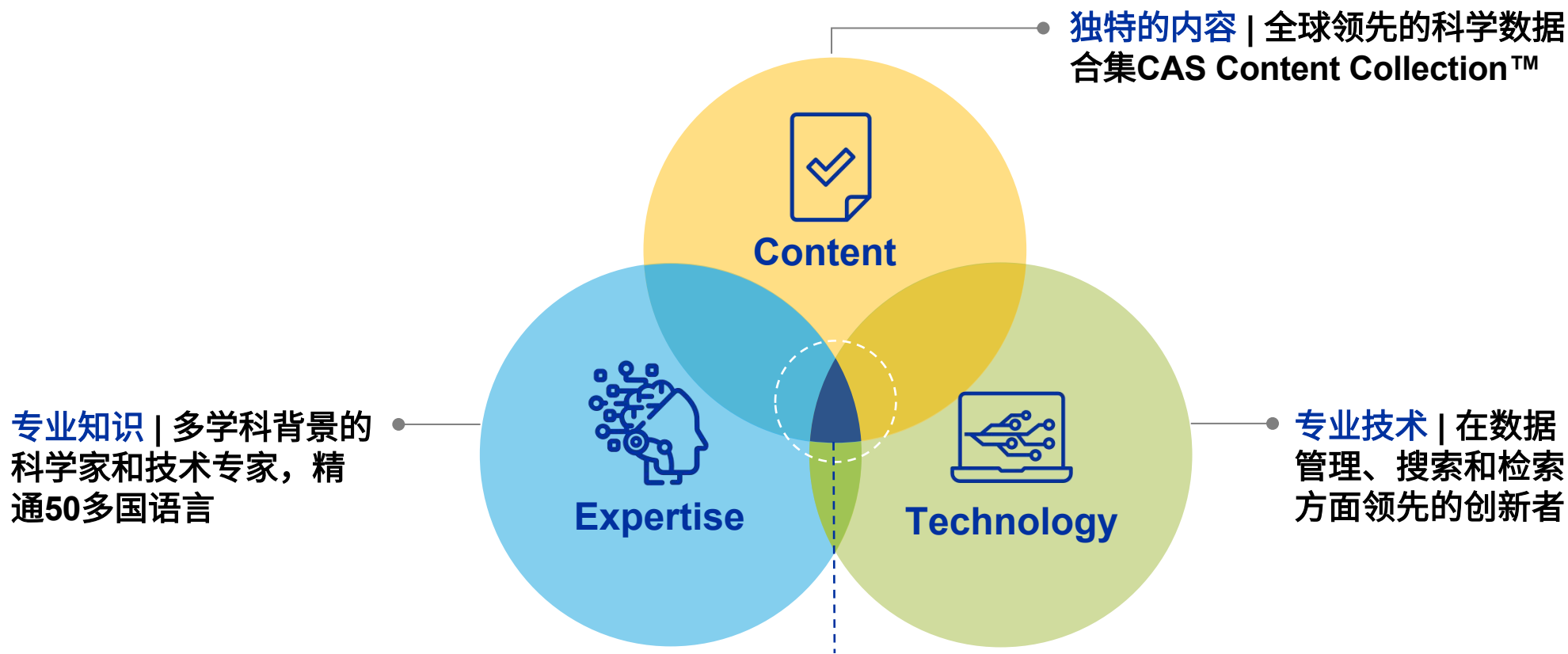
# 提纲

- CAS 简介
- CAS 持续增值的数据资源与创新服务
  - AI智能检索和内容增强赋能科研创新
  - 面向多学科的定制课程及数据服务
  - 持续创新的教学活动和服务流程



# 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

# CAS 值得信赖

生物、学术、生物技术、化学、全球专利局等各行业领先机构的选择



**TOP 25**  
**LIFE SCIENCES**  
**COMPANIES<sup>1</sup>**



**TOP 25**  
**CHEMICAL**  
**COMPANIES<sup>2</sup>**



**TOP 25**  
**UNIVERSITIES<sup>3</sup>**



**TOP 10**  
**GLOBAL PATENT**  
**OFFICES<sup>4</sup>**

1. <https://www.pharmexec.com/view/2024-pharm-exec-top-50-companies>
2. <https://www.chemanalyst.com/ChemAnalyst/ChemicalManufacturers>
3. <https://www.shanghairanking.com/rankings/gras/2024/RS0103>
4. <https://www.wipo.int/edocs/pubdocs/en/wipo-pub-941-2023-en-world-intellectual-property-indicators-2023.pdf>

# 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 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 技术概念

163 物质

625 反应

15 专利家族

3 配方

1 马库什结构

14 药理数据

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)  
(19) World Intellectual Property Organization  
International Bureau  
(43) International Publication Date  
23 August 2018 (23.08.2018) WIPO | PCT (10) International Publication Number  
WO 2018/152134 A1

(51) International Patent Classification:  
C07D 307.14 (2006.01) A61K 31.485 (2006.01)  
A61K 31/40 (2006.01) A61P 25/00 (2006.01)

(21) International Application Number:  
PCT/US2018/018074

(22) International Filing Date:  
13 February 2018 (13.02.2018)

(25) Filing Language:  
English

(26) Publication Language:  
English

(30) Priority Data:  
62458,731 14 February 2017 (14.02.2017) US

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(81) Designated States (unless otherwise indicated, for every  
kind of national protection available): AE, AG, AL, AM,  
AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ,  
CA, CH, CL, CN, CO, CR, CU, CZ, DE, DD, DK, DM, DO,  
DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN,  
HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP,  
KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME,  
MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ,  
OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA,  
SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN,  
TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every  
kind of regional protection available): ARIPO (BW, GH,  
GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ,  
UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ,  
TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK,  
EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LI, LU, LV,  
MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM,  
TR), OAPI (BF, BI, CF, CG, CI, CM, GN, GQ, GW,  
KM, ML, MR, NE, SN, TD, TG).

Published:  
with international search report (Art. 21(3)).

(74) Title: PROLINE-BASED NEUROPEPTIDE FF RECEPTOR MODULATORS

(57) Abstract: Neuropeptide FF receptor modulators based on a proline scaffold are provided which offer NPFF receptor potencies in the nanomolar range and antagonist selectivity for the NPFF 1 receptor. Methods, compounds and compositions for modulating the function of neuropeptide FF receptors are provided for pharmacotherapies capable of influencing conditions or disorders affected by the neuropeptide FF receptors.

FIG. 2

Region 2

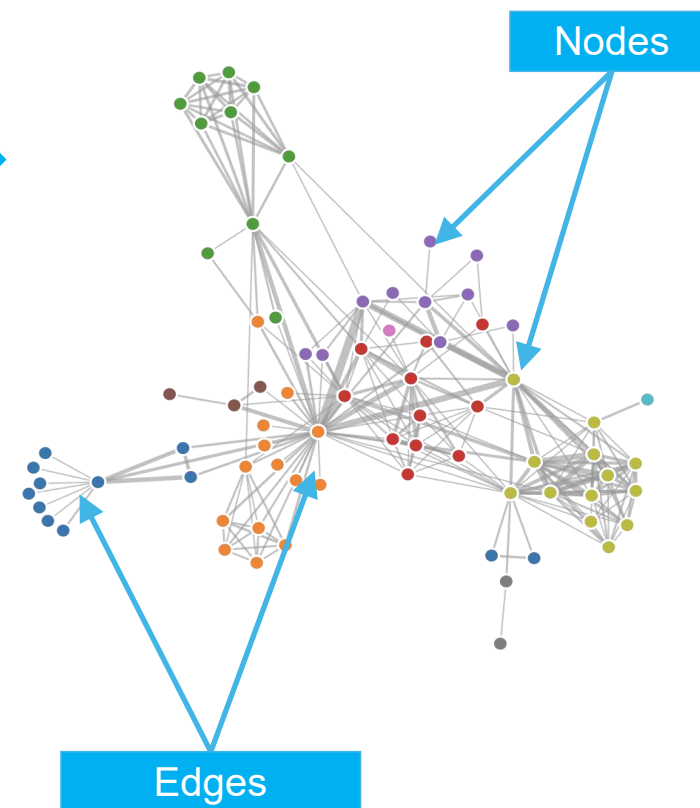
Region 1

Region 3

Compound 1

Ke NPFF1 : 1620 ± 379 nM  
Ke NPFF2 : 7251 ± 1734 nM

Click document to view on CAS SciFinder®



# CAS 持续开发新型解决方案，满足多元应用场景需求



Discovery

## CAS SciFinder Discovery Platform™

加速科学发现，  
加快科研转化。



Life sciences

## CAS BioFinder®

集成的数据推进药  
物及生命科学研究。



Intellectual property

## CAS IP Finder™ powered by STN

助力知识产权保护、  
查新及情报工作。



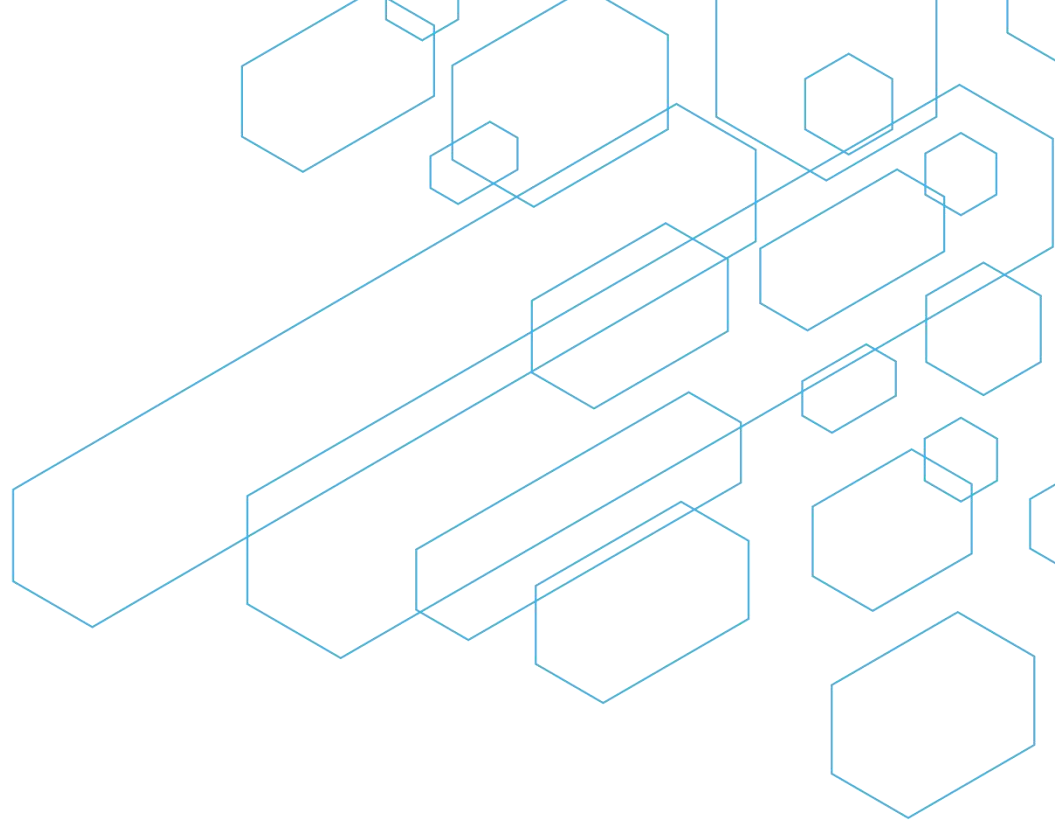
Custom solutions

## CAS Custom Services<sup>SM</sup>

CAS 定制服务为您提供  
数据、分析和洞察，  
发现机会，最大化投  
资回报率。

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# CAS的解决方案持续进化发展

CAS Newton<sup>SM</sup>: 利用自主代理和专家设计的工具，充分发挥CAS内容合集的潜力

March 23, 2026 9:48 AM

## Breakthroughs in flame-retardant materials for lithium batteries in the past three years

User

Breakthroughs in flame-retardant materials for lithium batteries in the past three years

CAS Newton

Based on my search of the CAS Content Collection, I found [1,152 references on flame-retardant materials for lithium batteries \(2022-2026\)](#) from the past three years. Here are the key breakthroughs:

### Major Research Directions

#### 1. Phosphorus-Based Flame Retardants

The most significant breakthrough is the shift toward **phosphorus-based flame retardants** as superior alternatives to fluorine-based compounds. A comprehensive [2025:709320](#) review highlights that P-based additives offer:

- Lower toxicity and reduced smoke generation
- High thermal and chemical stability
- Effectiveness at lower concentrations (reducing cost impact)
- Better compatibility with electrolyte properties

#### 2. Solid-State Polymer Electrolytes (SPEs)

Multiple breakthroughs in flame-retardant solid electrolytes:

- **Three-in-one polyphosphate electrolytes** [2023:401962](#): Integrated lithium salt, dissociation matrix, and flame retardant in one material, achieving a limiting oxygen index of 35.5% (non-ignitable)
- **Intrinsic flame-retardant polyurethane** [2022:212224](#): Novel flexible solid electrolyte with LOI of 27.6, excellent mechanical strength, and ionic conductivity of  $1.51 \times 10^{-4}$  S/cm at 70°C
- **Lithium bromide-induced organic-rich interphase** [2022:1304757](#): Achieved high-voltage resistance (up to 4.5V) with unprecedented flame-retardant properties in all-solid-state batteries

- AI生成式问答，基于CAS治理的干净数据，提供即时解答
- 提供来源可靠的答案，快速获得新的见解，避免AI幻觉问题

### 3. Advanced Separator Technologies

- **Water-soluble ammonium polyphosphate composites** [2023:68770](#): Bacterial cellulose-based separators that simultaneously enhance mechanical strength and flame retardancy
- **Nano-ceramic reinforced separators**: TiO<sub>2</sub>/polyimide and other ceramic-polymer composites providing thermal stability and dendrite suppression

### 4. Non-Coordinating Flame Retardants

A breakthrough approach using **non-coordinating flame retardants** (like hexafluorocyclotriphosphazene) that don't interfere with lithium-ion transport, maintaining battery performance while providing safety benefits.

### 5. Dual-Phase Fire Suppression

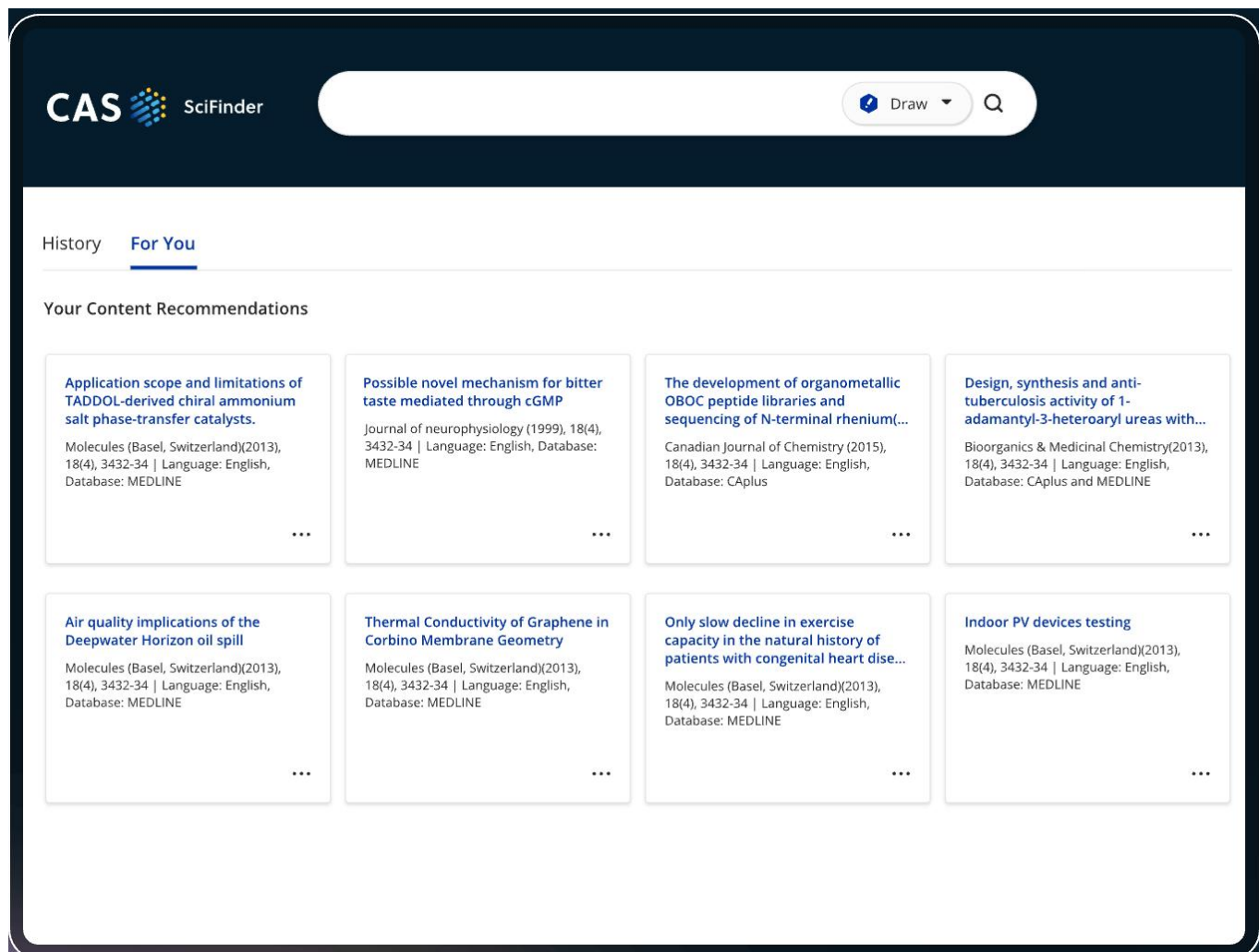
Recent innovations include **biphasic fire-extinguishing electrolytes** that suppress combustion in both gas and liquid phases during thermal runaway, using flame retardants with varied vapor pressures.

### Key Performance Achievements

- Limiting oxygen index values reaching **35-36%** (highly flame-retardant)
- Stable cycling for **1000-2000+ hours** in lithium metal batteries
- Capacity retention of **85-97%** after hundreds of cycles
- Temperature reduction during thermal runaway by **up to 300°C**
- UL-94 V-0 flame retardancy ratings

These breakthroughs represent a comprehensive approach to battery safety, addressing electrolytes, separators, and thermal management systems while maintaining or improving electrochemical performance.

# AI解析的自然语言检索，高效获取多类科研信息



The screenshot displays the CAS SciFinder homepage. At the top left is the CAS SciFinder logo. A search bar with a 'Draw' icon and a search icon is positioned at the top center. Below the search bar, there are tabs for 'History' and 'For You'. The main content area is titled 'Your Content Recommendations' and features a grid of eight article recommendations. Each recommendation card includes a title, a brief description, and publication details (journal, volume, issue, language, and database). The recommendations are:

- Application scope and limitations of TADDOL-derived chiral ammonium salt phase-transfer catalysts.** Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE
- Possible novel mechanism for bitter taste mediated through cGMP** Journal of neurophysiology (1999), 18(4), 3432-34 | Language: English, Database: MEDLINE
- The development of organometallic OBOC peptide libraries and sequencing of N-terminal rhenium(...)** Canadian Journal of Chemistry (2015), 18(4), 3432-34 | Language: English, Database: CAplus
- Design, synthesis and anti-tuberculosis activity of 1-adamantyl-3-heteroaryl ureas with...** Bioorganics & Medicinal Chemistry(2013), 18(4), 3432-34 | Language: English, Database: CAplus and MEDLINE
- Air quality implications of the Deepwater Horizon oil spill** Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE
- Thermal Conductivity of Graphene in Corbino Membrane Geometry** Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE
- Only slow decline in exercise capacity in the natural history of patients with congenital heart dise...** Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE
- Indoor PV devices testing** Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE

- 运用人工智能理解复杂查询，以自然语言检索为您精准呈现相关结果，助您节省宝贵时间。
- 检索结果个性化呈现，并随着您的每次使用而不断优化提升。

# 利用自然语言检索反应，降低检索难度

Reactions search for "Preparation of aldehyde from primary alcohol in THF"

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Milligram (1,105)

Gram (591)

Kilogram (2)

No Scale Provided (6,030)

Experimental Protocols

Reaction Type

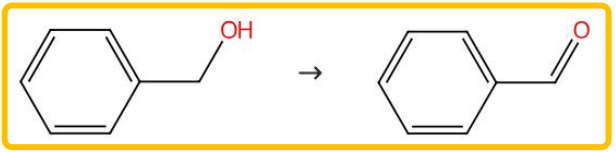
Stereochemistry

Reagent

7,682 Results

Group: By Scheme

Scheme 1 (68 Reactions)



Suppliers (166)

Suppliers (80)

31-614-CAS-41356630 Steps: 1 Yield: 100% ●●●

1.1 Reagents: [tert-Butyl hydroperoxide](#), [Morpholine](#)  
Catalysts: [Nickel monoxide](#), [Zinc oxide \(ZnO\)](#), [Nickel](#)  
Solvents: [Tetrahydrofuran](#), [Dodecane](#); 24 h, 90 °C

Experimental Protocols

Full Text

31-480-CAS-16653494 Steps: 1 Yield: 100% ●●●

1.1 Reagents: [Cesium carbonate](#), [Oxygen](#)  
Catalysts: [1648843-87-1](#)  
Solvents: [Tetrahydrofuran](#); 4 h, rt

Experimental Protocols

Full Text

Reagent

Hydrochloric acid (8,763)

Triethylamine (8,409)

Reactions search for "synthesis of paclitaxel mediated by hydrochloric acid"

References

Filter Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

Experimental Protocols

Catalyst

Number of Steps

Reaction Type

Yield

Reaction Mapping

Reaction Scale

Stereochemistry

Reagent

8,763 Results


Group: By Scheme

Sort: Relevance

View: Collapsed

Scheme 1 (2 Reactions)

Steps: 1 Yield: 100% ●●●



Suppliers (31)

Suppliers (126)

31-049-CAS-347948 Steps: 1 Yield: 100% ●●●

1.1 Reagents: [Hydrochloric acid](#)  
Solvents: [Ethanol](#), [Water](#); 0 °C; 145 min, 0 °C → rt

Experimental Protocols

PatentPak

Full Text

31-049-CAS-1897393 Steps: 1 Yield: 100% ●●●

1.1 Reagents: [Hydrochloric acid](#)  
Solvents: [Ethanol](#), [Water](#); 0 °C; 145 min, 0 °C → rt

Experimental Protocols

Full Text

Highly Enantioselective Organocatalytic Addition of Aldehydes to N-(Phenylmethylene)benzamides: Asymmetric Synthesis of the Paclitaxel Side Chain and Its Analogues  
By: Dziedzic, Pawel; et al  
Chemistry - A European Journal (2009), 15(16), 4044-4048.

智能识别反应的底物、产物、溶剂、试剂、催化剂、物质类别等信息，便捷反应检索

# 自然语言直接检索物质谱图和理化性质，直观高效

无需多次点击，直接展示目标结果

The image displays three overlapping screenshots of the CAS SciFinder web interface, illustrating natural language search capabilities. Each screenshot shows a search result card with a large, bolded title in Chinese and a corresponding scientific plot or table.

**Top Left Screenshot: Raman Spectra of Luminol**  
Search: "Raman spectra of luminol"  
Title: 自然语言直接查阅Raman谱图  
Content: Raman Spectrum plot for Luminol (521-31-3). Includes experimental details and a 'View All' link.

**Top Right Screenshot: Proton NMR of c13h13br**  
Search: "proton nmr of c13h13br"  
Title: 自然语言直接查阅NMR谱图  
Content: Proton NMR Spectrum plot for 2-(3-Bromopropyl)naphthalene (27650-59-5). Includes experimental conditions and a 'View All Spectra' link.

**Bottom Screenshot: Boiling Point of Ethanol**  
Search: "what is the boiling point of ethanol"  
Title: 自然语言直接查阅物质沸点  
Content: Boiling Point Properties table for Ethanol (64-17-5). The boiling point is highlighted as 78.5 °C. Includes a 'View in Detail Page' link.

# AI赋能的检索结果总结，助力快速掌握关键发现

在文献结果页面查看 AI Summary，更快理解文献中披露的信息。

**AI Summary**

Based on the search results, here's a summary of key findings related to crown ether and lithium and salts:

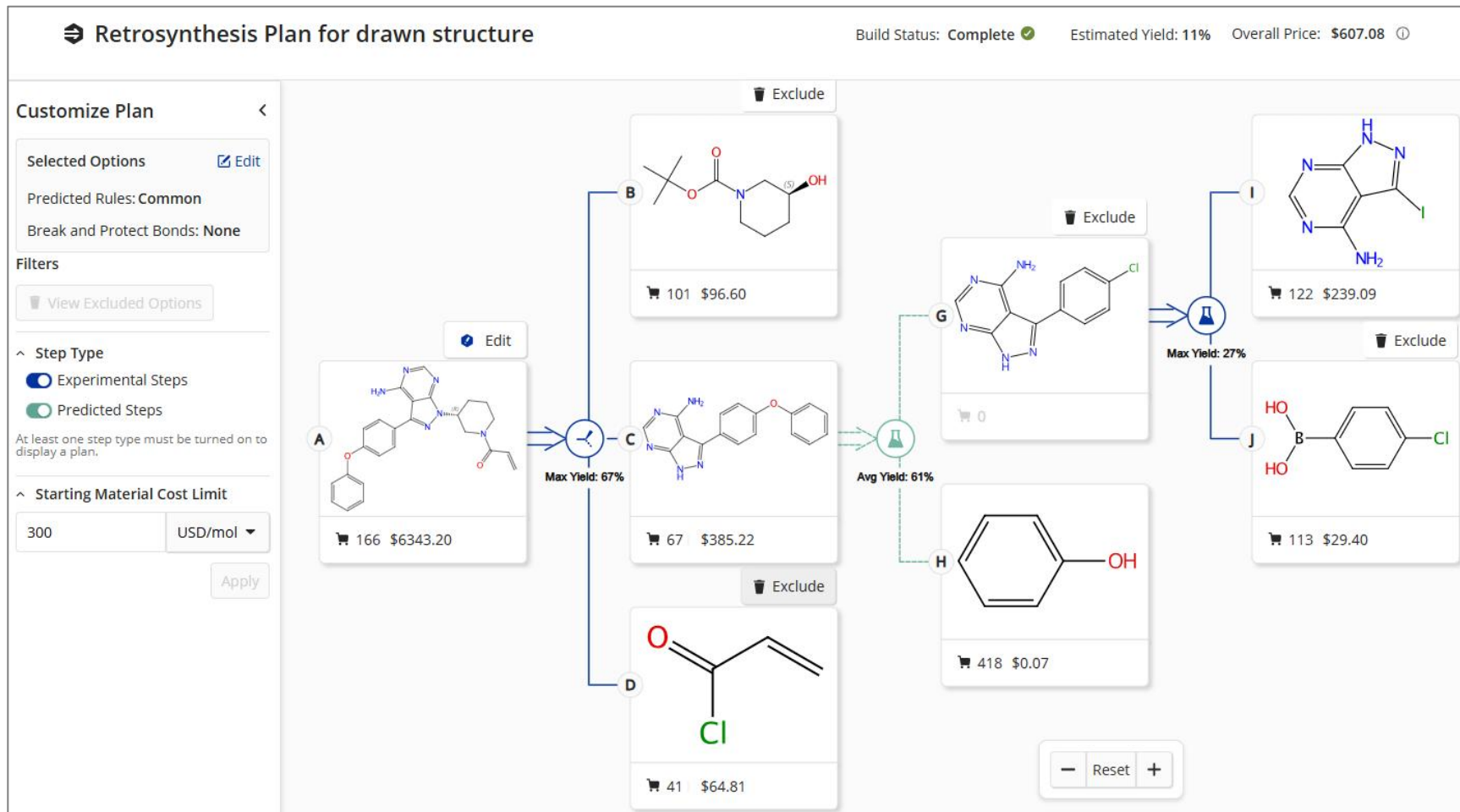
The search results highlight various aspects of crown ether-like lithium salts, including their synthesis, properties, and applications. One study describes the formation of amorphous solid electrolytes using cryptands or crown ethers with lithium salts, while another examines the transport rates of metal cations through bulk liquid membranes containing crown ethers. Additionally, research has been conducted on the design of asymmetric ether-like lithium salts to improve the performance of lithium metal batteries. Another study presents a nanofiltration membrane with crown ether as exclusive Li<sup>+</sup> transport channels for efficient extraction of lithium from salt lake brine. Furthermore, the isolation and X-ray structures of lithium crown ether salts of free phenyl carbanions are discussed, along with the computerized conductometric determination of stability constants of complexes of crown ethers with alkali metal salts and neutral molecules in polar solvents.

Key Findings:

- 1. Amorphous Solid Electrolytes:**
  - Amorphous solid electrolytes can be formed by the interaction of cryptands or crown ethers with lithium salts when the cavity size of the macrocycle does not match the diameter of the lithium cation. (1)
- 2. Metal Cation Transport Rates:**
  - The transport rates of metal cations through bulk liquid membranes containing crown ethers depend on the cation concentration in the source salt solution phase and the anion type. (2)
- 3. Lithium Metal Battery Performance:**
  - Designing an asymmetric ether-like lithium salt can improve the fast-cycling performance of lithium-metal batteries, particularly for practical lithium-metal batteries with high cathode loading. (3)
- 4. Nanofiltration Membranes:**
  - A nanofiltration membrane with crown ether as exclusive Li<sup>+</sup> transport channels, generated by crown ethers, can efficiently extract lithium from salt lake brines with high Mg<sup>2+</sup>/Li<sup>+</sup> mass ratio. (4)
- 5. Isolation and X-ray Structures:**
  - The isolation and X-ray structures of lithium crown ether salts of free phenyl carbanions have been reported, providing insight into the molecular structure of these compounds. (9)

**Designing an asymmetric ether-like lithium salt to enable fast-cycling high-energy lithium metal batteries**  
Nature Energy (2023), 8(9), 934-945  
| Language: English, Database: CAplus

# 逆合成路线用时大幅减少，AI 和数据驱动高效研发



**Retrosynthetic Analysis**

Make reaction plans with conditions, yields, catalysts, and experimental procedures.

- 即时获得逆合成路线
- 可自主调整的逆合成路线
- 增强的立体化学信息

# 可视化的研究趋势和数据分析

**Filter Results**

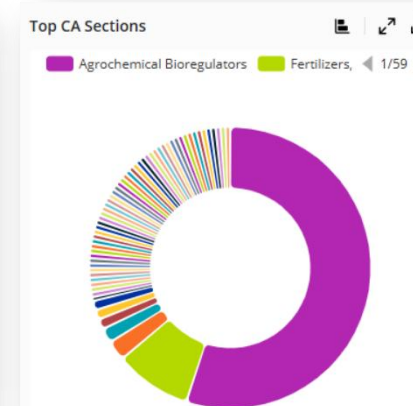
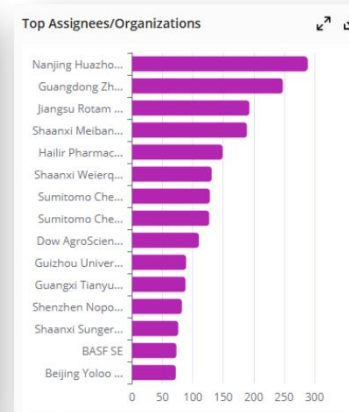
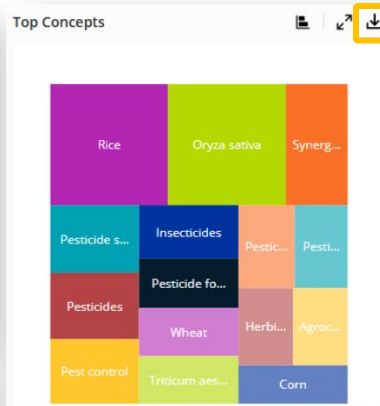
Analyze Results

**Behavior**

Filter by Exclude

**Filter Content Report**

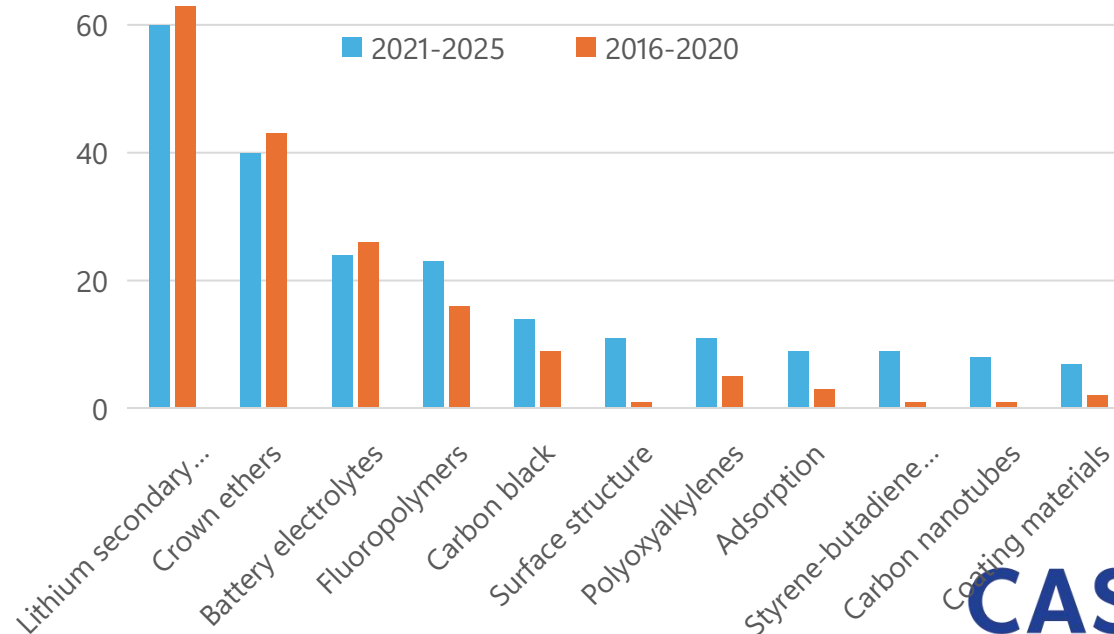
Download filter data from this result set.



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| Top Concepts | 2021-2025                   | Count | 2016-2020                       | Count |
|--------------|-----------------------------|-------|---------------------------------|-------|
| 1            | Lithium secondary batteries | 60    | Lithium secondary batteries     | 63    |
| 2            | Crown ethers                | 40    | Crown ethers                    | 43    |
| 3            | Battery electrolytes        | 24    | Battery electrolytes            | 26    |
| 4            | Battery anodes              | 23    | Battery anodes                  | 25    |
| 5            | Battery cathodes            | 23    | Battery cathodes                | 18    |
| 6            | Fluoropolymers              | 23    | Fluoropolymers                  | 16    |
| 7            | Carbon black                | 14    | Carbon black                    | 9     |
| 8            | Polyoxyalkylenes            | 11    | Electrode-electrolyte interface | 8     |
| 9            | Surface structure           | 11    | Electrolytes                    | 8     |
| 10           | Adsorption                  | 9     | Battery electrodes              | 7     |
| 11           | Styrene-butadiene rubber    | 9     | Electric impedance              | 6     |
| 12           | Carbon nanotubes            | 8     | Secondary battery separators    | 6     |
| 13           | Coating materials           | 7     | Composites                      | 5     |
| 14           | Current density             | 7     | Polyoxyalkylenes                | 5     |
| 15           | Density functional theory   | 7     | Polyolefins                     | 4     |

Comparison of Selected Top Concepts



示例: lithium batteries crown ether

# IP connections 专利检索，助力保护创新成果

Prior Art Discovery 输入自然语言即可开展现有技术分析，智能识别技术相关的专利及非专利文献

✦ Prior Art Discovery for "The causes of autoimmune diseases are complex. Stimulated by specific antigens, the immune system..."

Search Details

^ Your Inputs

Text

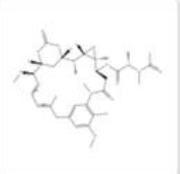
The causes of autoimmune diseases are complex. Stimulated by specific antigens, the immune system...

View All

Priority Date

08-25-2025

Structure



Patents (100) Non-Patent Literature (93)

Sort: Relevance

1

**pHLIP targeted delivery of potent cytotoxic compounds**

Assignees: Yale University; University of Rhode Island Board of Trustees  
US20200237926 A1, Publication Date: 2020-07-30 | Priority Date: 2019-01-28

The invention features a composition comprising a potent cytotoxic compound and a pHLIP® peptide, where, e.g., the cytotoxic compound cannot be used alone due to a lack of targeting. pHLIP® peptide targets cytotoxic compounds to acidic diseased tissue, translocates cytotoxic compounds across...

Full Text

2

**pHLIP targeted delivery of potent cytotoxic compounds**

Assignees: Yale University; University of Rhode Island Board of Trustees  
US20200237926 A1, Publication Date: 2020-07-30 | Priority Date: 2019-01-28

The invention features a composition comprising a potent cytotoxic compound and a pHLIP® peptide, where, e.g., the cytotoxic compound cannot be used alone due to a lack of targeting. pHLIP® peptide targets cytotoxic compounds to acidic diseased tissue, translocates cytotoxic

**pHLIP targeted delivery of potent cytotoxic compounds**

Assignees: Yale University; University of Rhode Island Board of Trustees

Patent

View Reference Details

The invention features a composition comprising a potent cytotoxic compound and a pHLIP® peptide, where, e.g., the cytotoxic compound cannot be used alone due to a lack of targeting. pHLIP® peptide targets cytotoxic compounds to acidic diseased tissue, translocates cytotoxic compounds across plasma membranes into the cytosols of cells in acidic diseased tissues and induces cell death predominantly in the targeted acidic diseased tissue.

pHLIP peptide link Drug

Publication Information View More

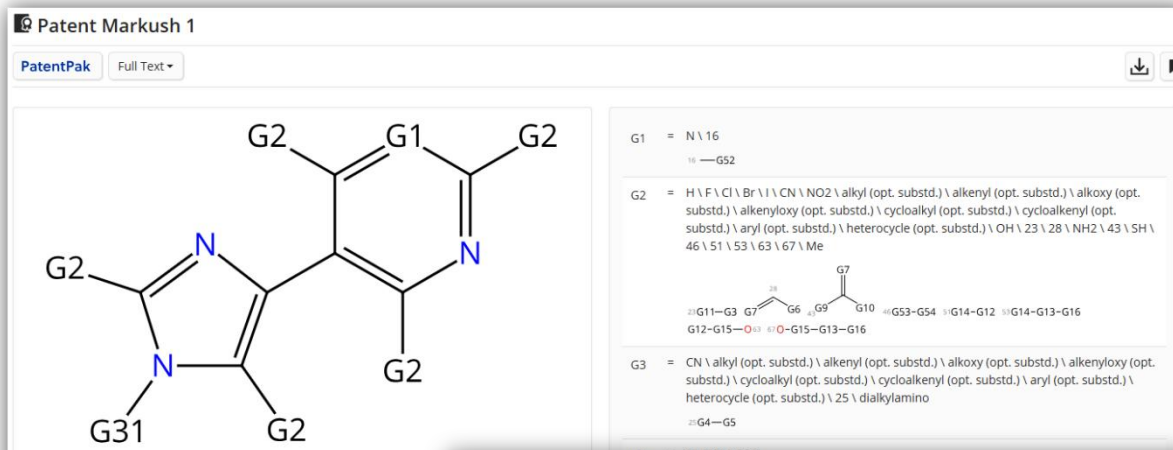
**Prior Art Discovery**

Discover prior art in patents and non-patent literature using AI-enhanced search technologies.

# 知识产权相关数据扩增，助力保护创新成果

## In this Patent

- [Claims](#)
- [Classifications](#)
- [CAS Concepts](#)
- [Markush Structures](#)
- [Substances](#)
- [Reactions](#)



## Publication Information

Assignee: Dow AgroSciences LLC  
United States, US20120110701 A1 2012-05-03 | Language: English, Database: C

## Notes

Patent claim 1

CAS PatentPak

PAGE 132 / 137 CLAIMS ZOOM DOWNLOAD Jump To PDF PDF+

Key Substances in Patent

CAS RN 3108317-86-5

Analyst Markup Locations (3)  
Page 132 - Claim  
Page 30  
Page 61

CAS RN 3111024-43-9

Analyst Markup Locations (3)  
Page 132 - Claim

WO 2025/261486 - 130 - PCT/CN2025/102372

thereof, wherein, in Formula I-3, I-3-a, I-3-b, I-3-c, I-3-d, I-3-e, I-3-f, I-3-g, I-3-h, I-3-i, I-3-j, I-3-k, I-3-l, I-3-m, or I-3-n, J<sup>7</sup> is CR<sup>26</sup> and J<sup>8</sup> is CR<sup>28</sup>, wherein R<sup>26</sup> and R<sup>28</sup> together with the carbon atoms they are attached to represent a 5-7 membered ring, preferably, a 6-membered ring, such as a phenyl, carbocyclic or heterocyclic ring, which is optionally substituted, for example, (or) etc., when substituted, the 5-7-membered ring can be typically substituted with 1-3 substituents each independently selected from halogen or C<sub>1-4</sub> alkyl optionally substituted with F, such as methyl.

36. A compound selected from the compounds shown in Examples section or any of the compounds shown in Table A herein, or a pharmaceutically acceptable salt thereof.

37. A pharmaceutical composition comprising the compound according to any one of claims

- 专利的权利要求
- 专利要求中的物质
- CAS科学家解读的马库什结构

# 快速定位专利权利要求中的物质

^ Reference Role

- Preparation (20K)
- Synthetic Preparation (18K)
- Reactant or Reagent (7,407)
- Reactant (7,396)
- Biological Study (5,652)
- Substance in Claims (1,738)

[View All](#)

^ Substance Class

^ Aromatic Rings

^ Reaction Role

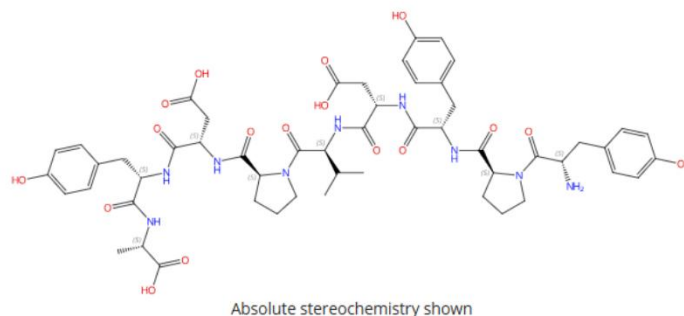
CAS Registry Number: 92000-76-5

1,431

39

47

[View in CAS BioFinder](#)



$C_{53}H_{67}N_9O_{17}$

L-Alanine, L-tyrosyl-L-prolyl-L-tyrosyl-L-α-aspartyl-L-valyl-L-prolyl-L-α-aspartyl-L-tyrosyl- (ACI)

## Patents Containing Substance in Claims

### Enhance plant systemic acquired resistance using an AtNPR1 variant

Patent Number: WO2026064782

Publication Date: 2026-03-26

### Preparation of fusion protein comprising Cas protein and functional domains for treatment of diseases

Patent Number: WO2026056174

Publication Date: 2026-03-19

### Broad-spectrum influenza virus-inhibiting polypeptide and use thereof in prevention and/or treatment of influenza virus infections

Patent Number: WO2026041159

Publication Date: 2026-02-26

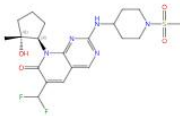
[View All Patents](#)

# 新增生命科学数据，便于挖掘隐藏的重要信息

Pharmacological Data CAS LIFE SCIENCES

**药理活性**

2185857-97-8



Absolute stereochemistry shown  
C20H27F2N5O4S  
 6-(Difluoromethyl)-8-[[1R,2R]-2-hydroxy-2-methylcyclopentyl]-2-[[1-(methylsulfonyl)...

| Ligand       | Target                            | Function  | Parameter | Value   | Disease | Organism     | Assay       |
|--------------|-----------------------------------|-----------|-----------|---------|---------|--------------|-------------|
| 2185857-97-8 | Cyclin-dependent kinase 1         | -         | EC50      |         |         |              |             |
| 2185859-32-7 | Cyclin-dependent kinase 2         | -         | EC50      |         |         |              |             |
| 2185857-97-8 | Cyclin-dependent kinase 2         | -         | EC50      |         |         |              |             |
| 2185859-32-7 | Cyclin-dependent kinase 1         | -         | EC50      |         |         |              |             |
| 2185857-97-8 | Retinoblastoma-associated protein | -         | EC50      |         |         |              |             |
| 571190-30-2  | Retinoblastoma-associated protein | Inhibitor | IC50      |         |         |              |             |
| 2185859-32-7 | Retinoblastoma-associated protein | Inhibitor | IC50      | 0.27 μM |         | Homo sapiens | View Detail |

Biomarkers CAS LIFE SCIENCES

**生物标志物**

| Biomarker  | Biomarker Type | Disease             | Category   | Measurement       | Details     |
|------------|----------------|---------------------|--|-------------------|-------------|
| CDK4 (DNA) | Molecular      | Cancer, Breast      | Gene-disease association linked with genetic variation | Association score | View Detail |
| CDK4 (DNA) | Molecular      | Breast Neoplasms    | Gene-disease association linked with genetic variation | Association score | View Detail |
| CDK4 (DNA) | Molecular      | CARCINOMA OF BREAST | Gene-disease association linked with genetic variation | Association score | View Detail |

Toxicity CAS LIFE SCIENCES

**毒性**

| Ligand       | Target   | Function  | Parameter | Value    | Disease |
|--------------|----------|-----------|-----------|----------|---------|
| 1092443-55-4 | 786-O    | Inhibitor | LC50      | > 100 μM | cancer  |
| 1092443-55-4 | A498     | Inhibitor | LC50      | > 100 μM | cancer  |
| 1092443-55-4 | A549     | Inhibitor | LC50      | > 100 μM | cancer  |
| 1092443-55-4 | ACHN     | Inhibitor | LC50      | > 100 μM | cancer  |
| 1092443-55-4 | BT-549   | Inhibitor | LC50      | > 100 μM | cancer  |
| 1092443-55-4 | CAKI-1   | Inhibitor | LC50      | > 100 μM | cancer  |
| 1092443-55-4 | CCRF-CEM | Inhibitor | LC50      | > 100 μM | cancer  |
| 1092443-55-4 | COLO 205 | Inhibitor | LC50      | 0.637 μM | cancer  |

ADME CAS LIFE SCIENCES

**代谢数据**

| Ligand      | Target | Function  | Parameter       | Value      | Disease | Organism | Assay       |
|-------------|--------|-----------|-----------------|------------|---------|----------|-------------|
| 571190-30-2 | -      | Inhibitor | Bioavailability | 56.1 %     | cancer  | -        | View Detail |
| 571190-30-2 | -      | Inhibitor | t1/2            | 2.1 hr     | cancer  | -        | View Detail |
| 363621-34-5 | -      | Inhibitor | AUC             | 12.1 μM.hr | cancer  | -        | View Detail |
| 363621-34-5 | -      | Inhibitor | Cmax            | 2.99 μM    | cancer  | -        | View Detail |
| 328061-69-4 | -      | Inhibitor | Cmax            | 3.2 μM     | cancer  | -        | View Detail |
| 328061-69-4 | -      | Inhibitor | t1/2            | 3 hr       | cancer  | -        | View Detail |

# 新增多种属性数据：助力材料、化学化工研究

Experimental Properties

| Chemical                                 | Density                     | Electrical     | Flow and Diffusion | Interface | Mechanical | Structure Related | Thermal |
|--|-----------------------------|----------------|--------------------|-----------|------------|-------------------|---------|
| Property                                 | Value                       | Condition      | Source             |           |            |                   |         |
| Glass Transition Temperature             | 52 °C                       | -              | (1) CAS            |           |            |                   |         |
| Glass Transition Temperature             | 45 °C                       | -              | (2) CAS            |           |            |                   |         |
| Glass Transition Temperature             | 45-50 °C                    | -              | (3) CAS            |           |            |                   |         |
| Glass Transition Temperature             | 42.3 °C                     | -              | (4) CAS            |           |            |                   |         |
| Glass Transition Temperature             | 41 °C                       | -              | (5) CAS            |           |            |                   |         |
| Heat Capacity                            | 1.5 J/g·K                   | Temp: 303 K    | (6) CAS            |           |            |                   |         |
| Heat Capacity                            | 1.2 J/g·K                   | Temp: 303 K    | (6) CAS            |           |            |                   |         |
| Heat Capacity                            | 0.59 J/g·K                  | -              | (6) CAS            |           |            |                   |         |
| Melting Point                            | >100 °C                     | -              | (3) CAS            |           |            |                   |         |
| Phase Transition Enthalpy                | 2.423 J/g (melting)         | Temp: 439.93 K | (7) CAS            |           |            |                   |         |
| Phase Transition Temperature             | 77.71 °C (crystallization)  | -              | (8) CAS            |           |            |                   |         |
| Thermal Expansion Coefficient            | 0.134 1/K                   | -              | (9) CAS            |           |            |                   |         |
| Thermal Expansion Coefficient            | 2.14 x 10 <sup>-4</sup> 1/K | -              | (9) CAS            |           |            |                   |         |
| Glass Transition Temperature - 2 Sources | See Full Text               |                | (10-11) CAS        |           |            |                   |         |
| Melting Point - 1 Source                 | See Full Text               |                | (12) CAS           |           |            |                   |         |
| Thermal Analysis - 5 Sources             | See Full Text               |                | (13-17) CAS        |           |            |                   |         |

## 新增实验属性：

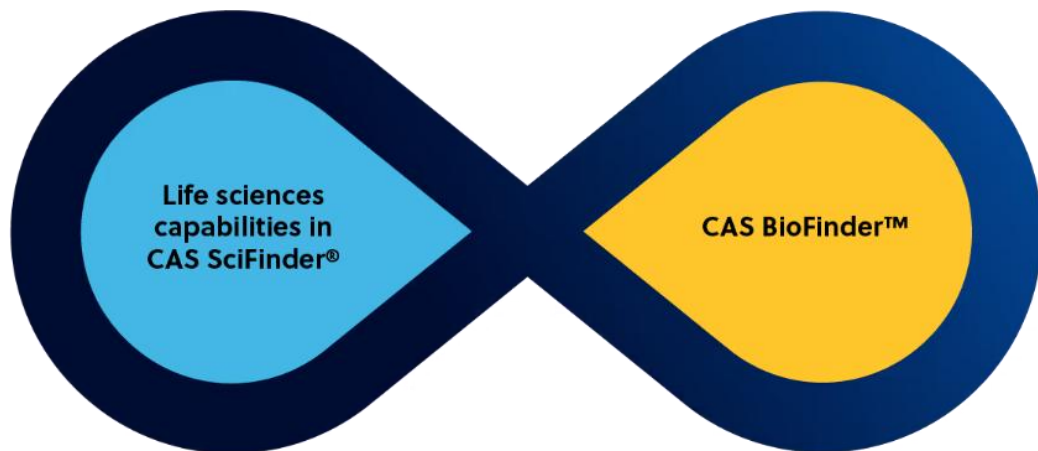
玻璃化转变温度、热分析动力学参数、相点、焓、自由能、热容、流体属性、溶解度、解离常数、偶极距数据等

# CAS BioFinder 加速早期药物研发



# CAS生命科学领域的内容与创新赋能

自信、高效地推进药物研究



## Life sciences capabilities in CAS SciFinder

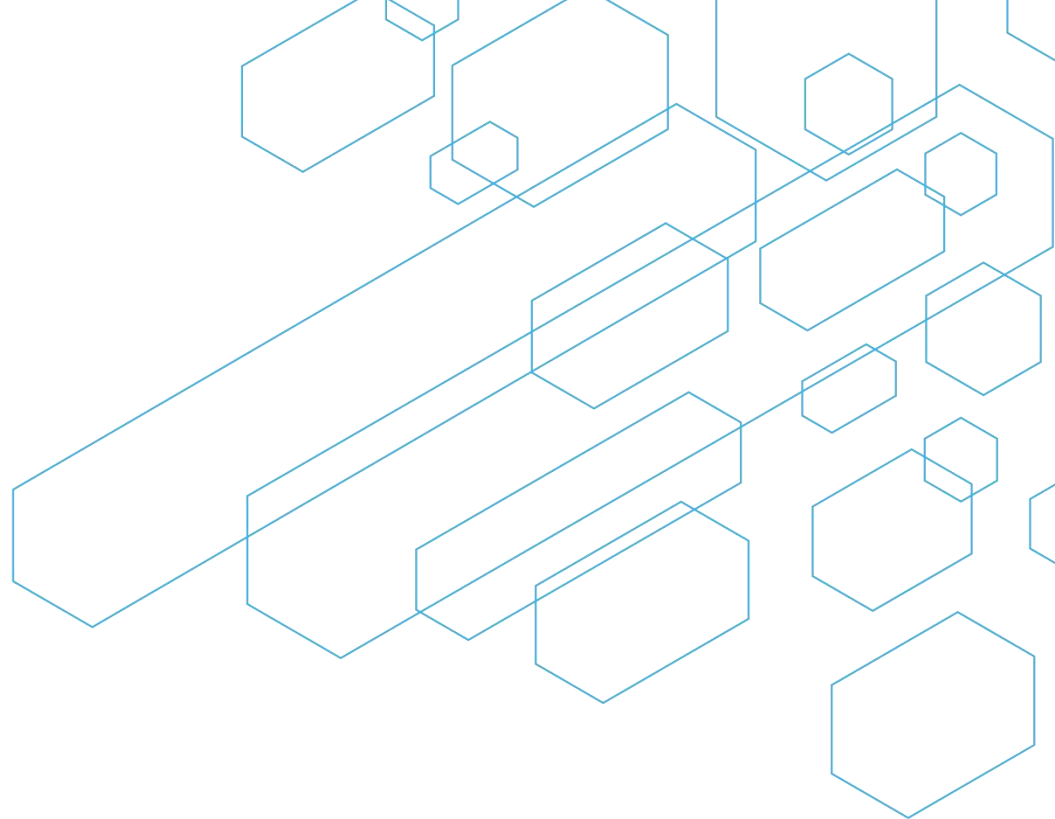
CAS SciFinder 中拓展了系列生命科学数据内容和检索功能，包括药理活性数据、ADME、生物标记物、序列信息等，并且与 CAS BioFinder 检索无缝集成。

## CAS BioFinder

- 探索配体或骨架结构、靶标和疾病之间的关联
- 已报道的和预测的生物活性与代谢数据
- 配体、序列、疾病、通路、生物标志物等数据及彼此关联的生命科学知识图谱
- 利用现有文献中的数据运行AI增强的预测生物活性模型，获得最相关的结果
- 集成了三维蛋白质模型等结构相关信息
- 集成了权威来源的药物情报信息
- 涵盖小分子药物、抗体、ADC等大分子药物研究所需要的生物学数据信息
- 持续增加的临床和序列相关信息

# 提纲

- CAS 简介
- CAS持续增值的数据资源与创新服务
  - AI智能检索和内容增强赋能科研创新
  - 面向多学科的定制课程及数据服务
  - 持续创新的教学活动和服务流程

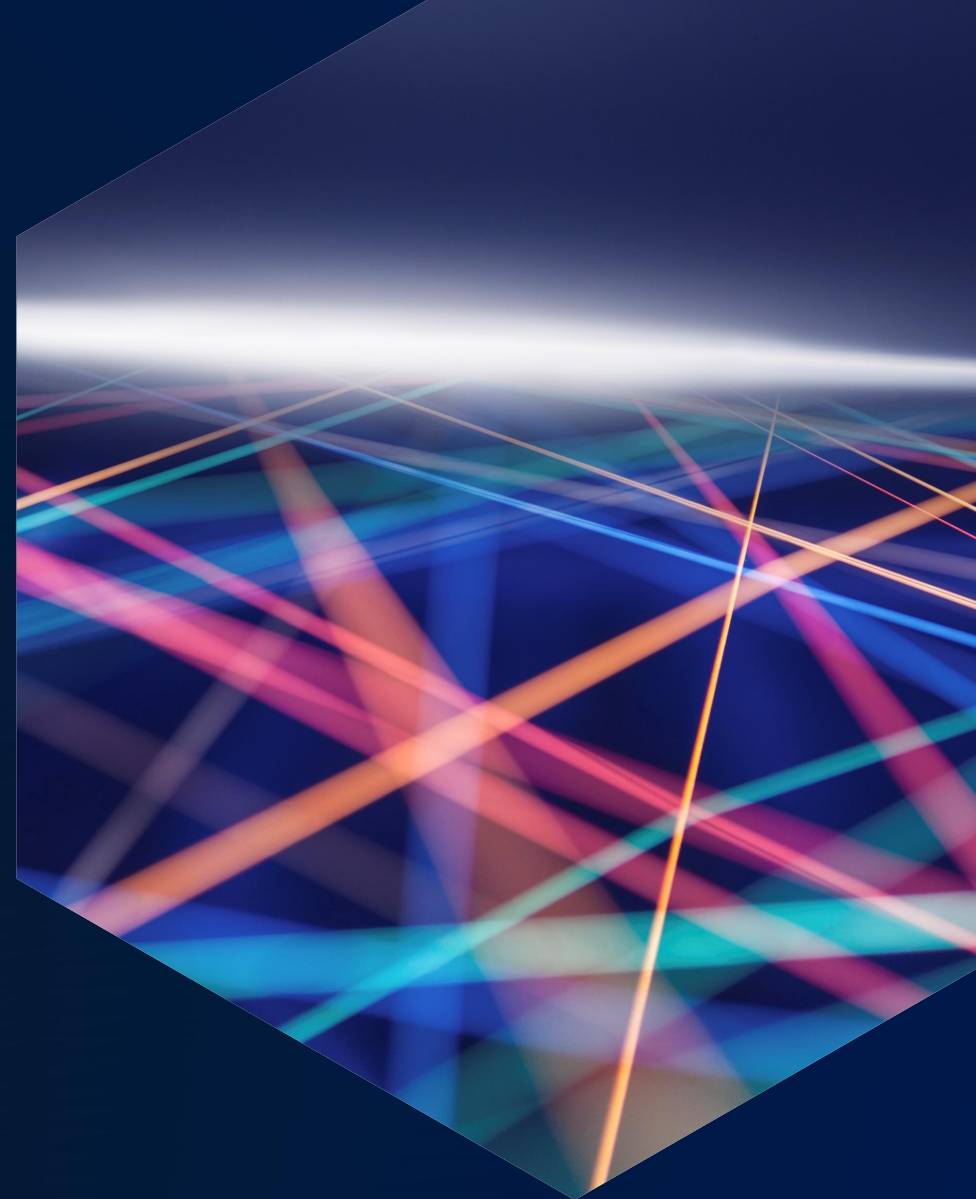


# CAS SCIFINDER DISCOVERY PLATFORM

## 2026 春季专题论坛

无论您的研究方向是**化学、化工、材料、高分子**，还是**医药、农化、环境、食品**等相关领域，从基础操作到应用案例的论坛内容，本次春季专题论坛将助您轻松掌握平台的核心功能和检索技巧，提升科研效率。

2026年3月至5月，CAS SciFinder Discovery Platform 四场专题论坛直播时间为**周四 15:00 - 16:00**。扫描二维码注册，观看直播有机会获得**CAS定制纪念品**，欢迎在直播中提问互动。



# 多学科、多形式的线上学习资源



ACS美国化学会 ★  
美国艾赛思国际有限公司北京代表处 北京

ACS作为权威科学信息的主要来源，是全球化学企业、化学家、化学工程师和相关人员的职业家园。 >

5292篇原创内容  
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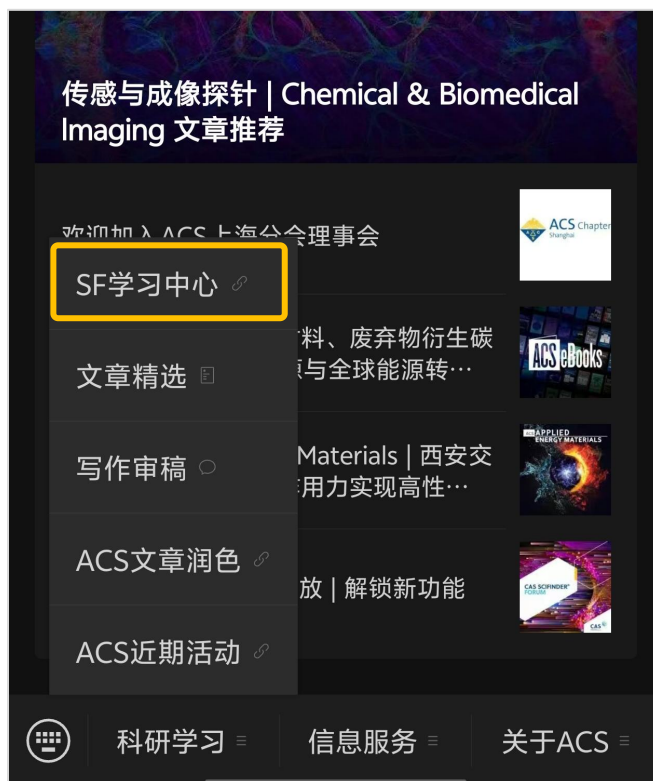
#每周分子 235 #CAS SciFinder Tips 99  
#JACS 63 #ACS环境 621 #检索案例精选 71  
#ACS年会 375 #CAS SciFinder常见问题解答 9  
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放 | 解锁新功能

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# 检索案例精选 订阅

ACS美国化学会

71篇内容

正序

材料系列：生物可降解材料 | CAS SciFinder Discovery Platform 检索案例  
03/04 阅读 204

医药系列：API表征属性与DMPK调研 | CAS SciFinder Discovery Platform  
02/18 阅读 86

医药系列：缓释药制剂配方的检索与调研 | CAS SciFinder Discovery Platform  
02/09 阅读 186

材料系列：3D打印聚合物材料 | CAS SciFinder Discovery Platform 检索  
01/26 阅读 308

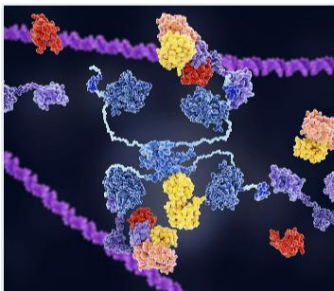
# CAS 系列白皮书及洞察报告

**Filters** Clear all

Showing 1 to 25 of 300

**Filter by topic** Clear

- Biotechnology 40
- Consumer Goods 8
- Digital R&D 28
- Drug Discovery 72
- Emerging Science 75
- Intellectual Property 10
- Materials 16
- Safety 7
- Sustainability 42
- Synthetic Chemistry 2



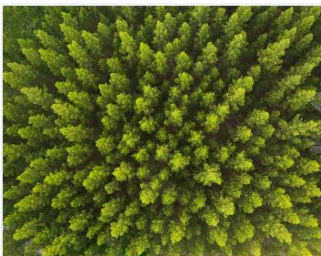
**Drug Discovery**

### How AI-driven analysis can accelerate drug discovery

Spiro[2.3]hexanes are an example of promising yet challenging scaffold structures for new drug compounds. By using AI-powered predictive analytics with CAS BioFinder, researchers more efficiently identified candidates for validation.

April 7, 2026 | Article

[Read the article](#)




**Emerging Science**

### Fossil fuels to biofuels: How biomass can drive sustainability

Biomass is currently just a fraction of our energy sources, but with sustainable feedstocks and conversion processes, biomass-based fuels could become common replacements for fossil fuel-based fuels.

March 5, 2026 | Insights Report

[Read the report](#)



**Emerging Science**

### 4D printing: Can time-responsive design transform materials

How can we print in 4D? By adding time as a dimension, research sensors and devices that respond to stimuli like heat and moisture cutting-edge materials have the potential to play a crucial role in aerospace, and more.

February 25, 2026 | Article

[Read the article](#)

来源:

<https://www.cas.org/resources/white-papers>

<https://www.cas.org/resources/cas-insights>



**CAS INSIGHTS™ 报告**

## 化学 AI 模型： 绘制 材料与生命科学 领域的蓝图

**锂离子电池回收**  
面向绿色未来的市场  
及创新趋势

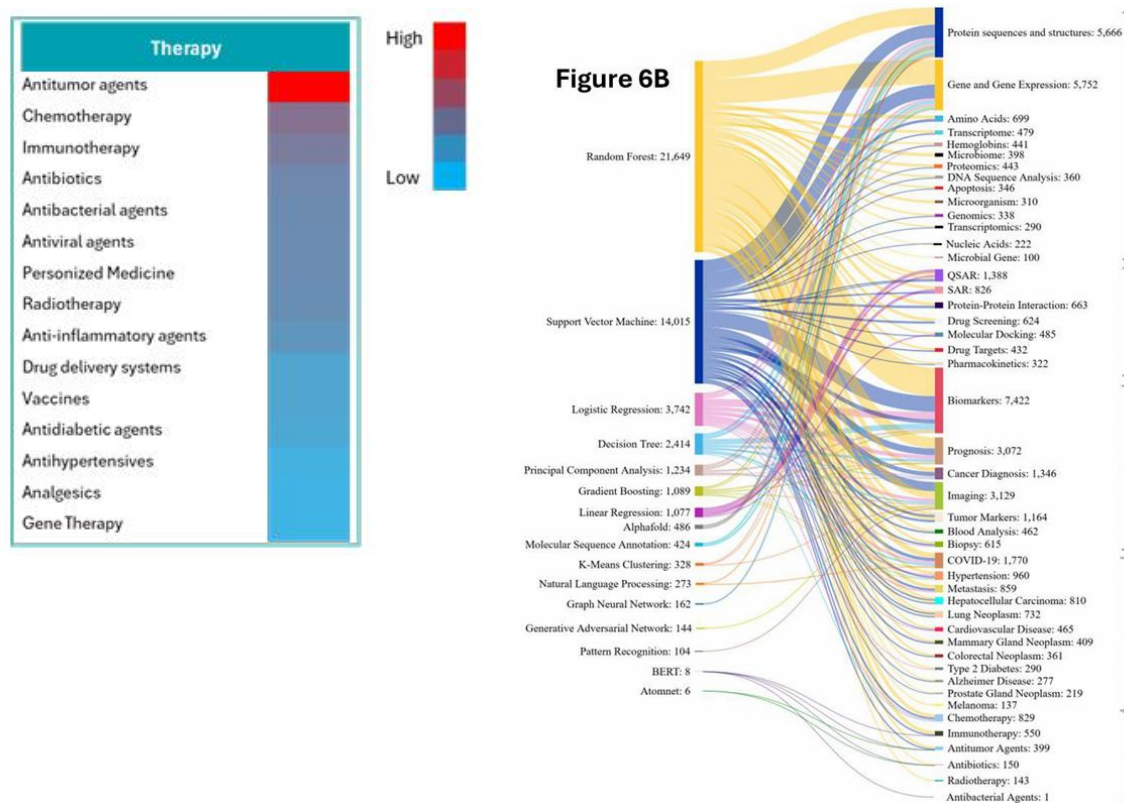
**CAS INSIGHTS**  
**FROM POLYMERS  
TO PROSTHETICS**  
The growth of 3D printing in biomedicine  
**从聚合物到假肢**  
3D打印在生物医学领域的发展

**CAS**  
A Division of the  
American Chemical Society

**Deloitte**

# 化学AI模型：绘制材料与生命科学领域的蓝图

- AI 驱动的出版物概念图谱，识别备受关注且研究投入集中的关键概念
- AI/ML方法与研究领域概念的共现分析，揭示主要的应用模式
- 具有公认治疗应用潜力的 CAS 索引物质分类



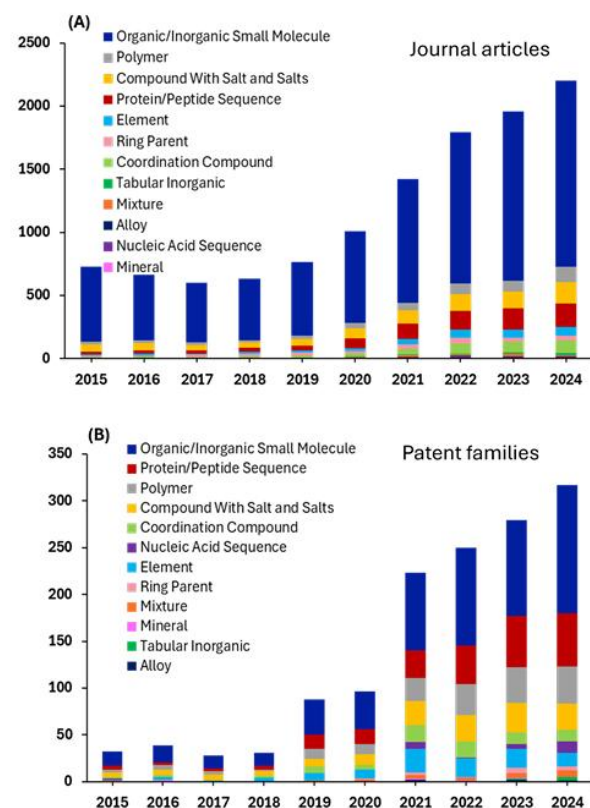
Biochemistry

Modeling And Drug Design

Diagnosis

Disease

Therapy



# CAS 数据服务助您解决独特挑战



## 内容管理： 内部数据治理

数字化

数据提取

数据标准化

数据分类标准制定

检索系统



## 知识管理： 数据设计

物质登记

领域知识建模与治理

物质结构标准化

数据迁移

内容审计

外部数据源对接



## 预测： 人工智能

定制训练数据集  
(算法开发)

定制AI数据

AI数据支持

领域检索增强生成  
(RAG) 技术方案

基于AI的研究领域评估  
报告



## 数据驱动的风险管理

可行的合成路线分析与  
设计

物质供应链分析

物质监管状态与安全性

毒理评估分析

可靠供应商信息

替代品分析



## 检索

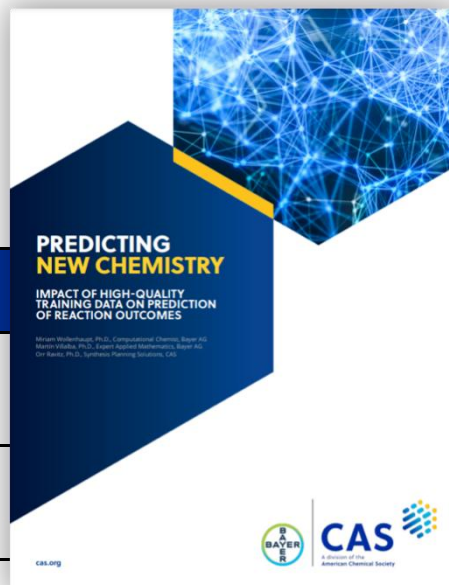
专利定制检索

- 全景分析
- 现有技术分析
- 自由实施检索
- 新颖性检索
- 预审
- 检索策略评估

# 在极难突破的科学领域 改进反应预测结果

## 案例分享

| 训练数据集     | 预测精度 |
|-----------|------|
| 基准数据集     | 16%  |
| +CAS反应数据集 | 48%  |



Click to view on CAS SciFinder®

| 训练数据集     | 数据组成                              |
|-----------|-----------------------------------|
| 基准数据集     | 商业可获得的正样本数据（800万）和负样本数据（2400万）    |
| +CAS反应数据集 | 拜尔的3200万基准数据+CAS定制的14,500条特定的反应数据 |

## 影响

用CAS科学家标引的反应数据集进行训练时，准确率提高到48%——提高了32个百分点。

这种在“罕见”反应类别中增强的预测能力贡献了新的、有用的结果，为极难突破的科学领域开辟了道路。

# 西湖大学分析报告 《未来健康：新兴生物材料》

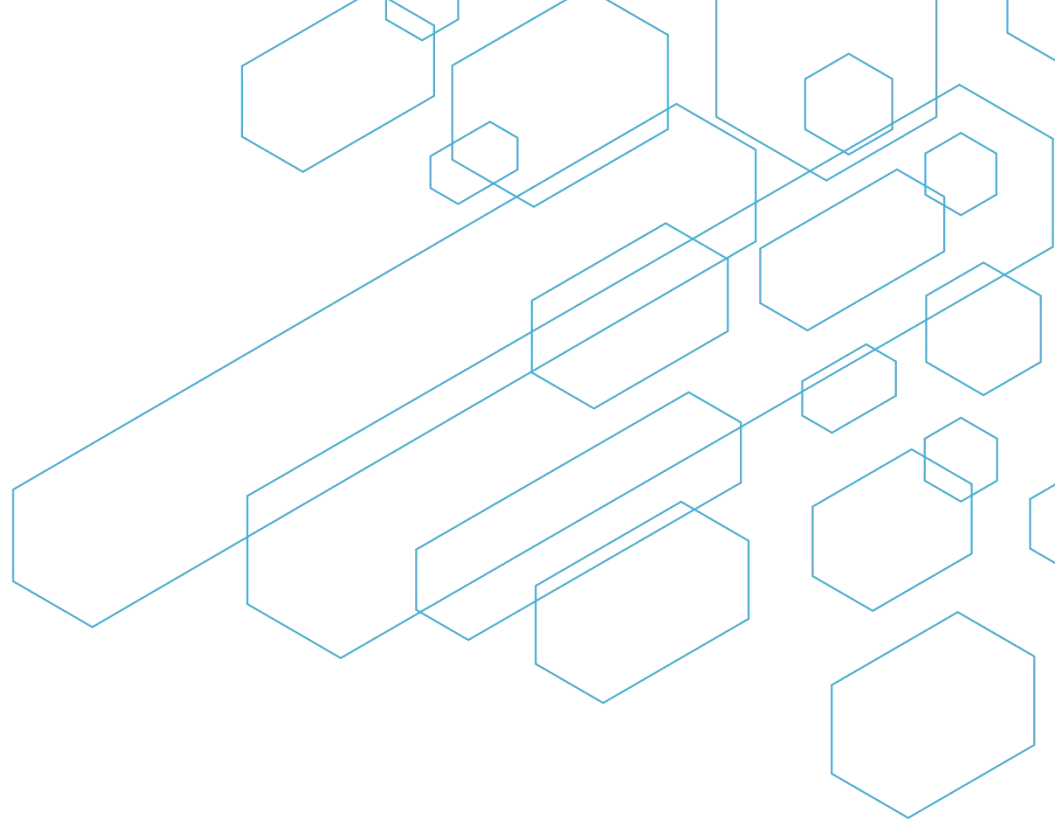
案例分享



报告免费下载：  
英文版：[Trailblazing the future with emerging biomaterials](#)  
中文版：[未来健康：新兴生物材料](#)

# 提纲

- CAS 简介
- CAS持续增值的数据资源与创新服务
  - AI智能检索和内容增强赋能科研创新
  - 面向多学科的定制课程及数据服务
  - 持续创新的教学活动和服务流程



# 服务创新——CAS SciFinder 教学沙龙

面向学科馆员、信息素养课程教师，旨在推动CAS SciFinder课程的创新共建和教学资源的共享  
多主题的内容分享



## 多学科的教学资源

### 文本教学资源

- 通用系统课件
- 简短通用示例
- 学科应用案例
- 检索习题

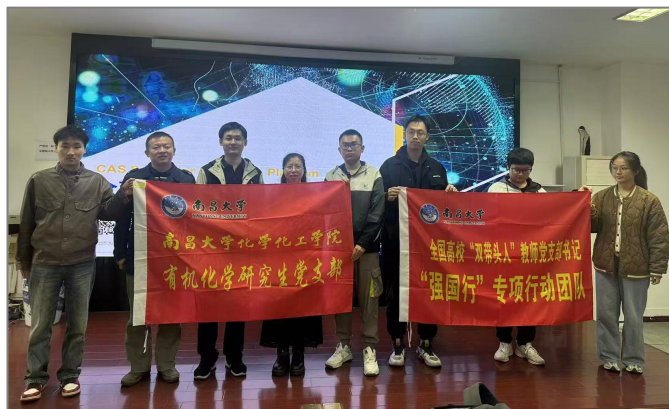
### 视频教学资源

- 检索短视频
- 系列专题视频

|             |   |                |   |
|-------------|---|----------------|---|
| <b>材料系列</b> | <ol style="list-style-type: none"><li>1. 航空航天材料</li><li>2. 电化学储能材料与技术</li><li>3. MOF材料</li><li>4. 各类材料分析方法</li></ol>      | <b>生物系列</b>    | <ol style="list-style-type: none"><li>1. 大戟属植物提取分离表征与结构改造</li><li>2. 生物转化及酶学研究</li><li>3. 等足目生物的基因研究</li><li>4. 医用多肽相关信息</li><li>5. 酵母基因改造与发酵代谢</li></ol> |
| <b>农学系列</b> | <ol style="list-style-type: none"><li>1. 烟草中成分的鉴定</li><li>2. 香烟中有效物质茄尼醇的研究与提取</li><li>3. 多菌灵及其衍生物的制备与配方</li></ol>         | <b>医药与诊断系列</b> | <ol style="list-style-type: none"><li>1. 核素偶联药物RDC相关研究</li><li>2. 药化信息检索</li><li>3. 靶向 RNA 小分子药物</li><li>4. 放射性试剂及药物</li></ol>                            |
| <b>食品系列</b> | <ol style="list-style-type: none"><li>1. 咖啡风味研究</li><li>2. 食品成分的分析方法检索</li><li>3. 食品配方相关研究检索</li></ol>                    | <b>化学化工系列</b>  | <ol style="list-style-type: none"><li>1. 工业催化剂及中间体的设计与制备</li><li>2. 连续流反应工艺</li><li>3. 工业聚合物相关信息检索</li><li>4. 原料药及中间体合成工艺</li><li>5. 偶氮染料</li></ol>       |
| <b>环境系列</b> | <ol style="list-style-type: none"><li>1. 可降解聚合物与环境保护</li><li>2. 工业尾气发酵制乙醇</li><li>3. 水环境及水处理</li><li>4. CO2加氢转化</li></ol> |                |   |

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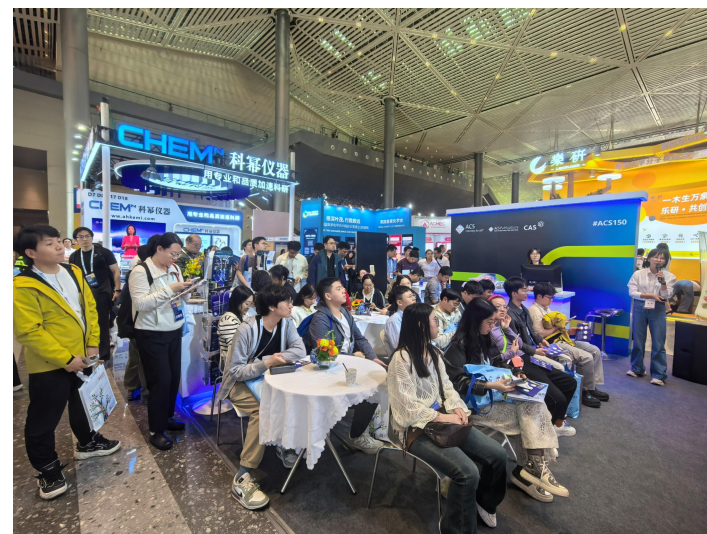
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# 中国化学会第35届学术年会

## CAS展位及活动照片



深入了解科研神器CAS SciFinder的功能和检索技巧，学习如何拆解检索问题思路开启检索，将丰富的功能和自己的研究课题更好的结合，又快又准地查到需要的结果。

鼓励同学们来现场注册CAS SciFinder春季论坛，答题，聆听2026 CAS SciFinder大赛宣讲并参与抽奖活动，更有资深检索专家进行现场检索指导。



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