CAS持续增值的数据内容与多元创新服务

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CAS
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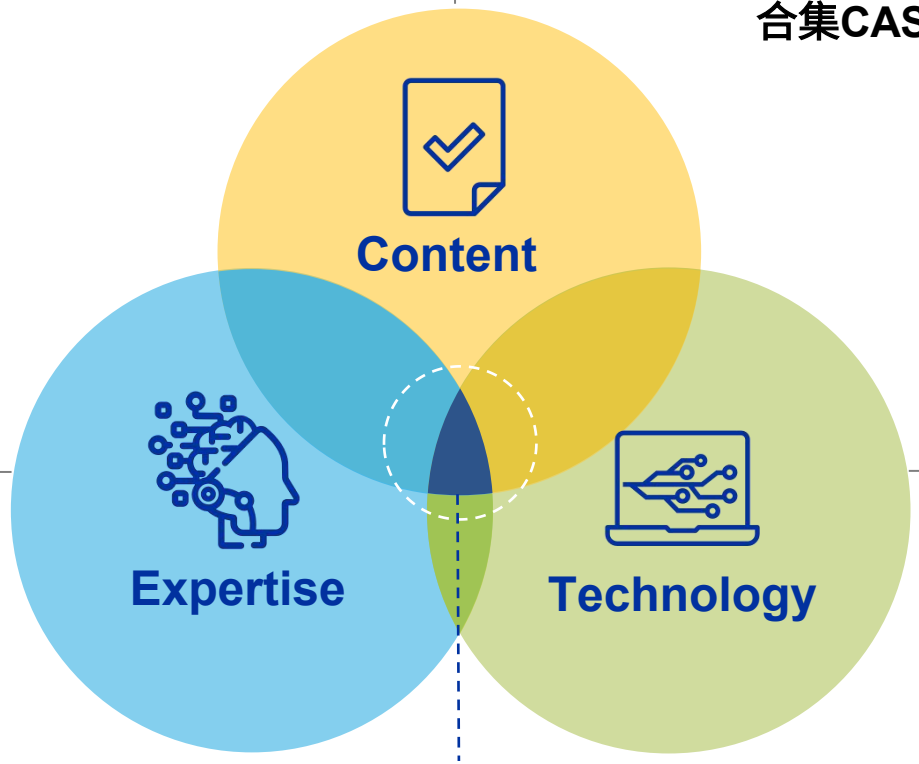
提纲

- 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

独特的内容 | 全球领先的科学数据合集CAS Content Collection™



专业知识 | 多学科背景的科学家和技术专家，精通50多国语言

专业技术 | 在数据管理、搜索和检索方面领先的创新者

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

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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[1]

TOP 25
CHEMICAL COMPANIES[2]

TOP 25
UNIVERSITIES[3]

TOP 10
GLOBAL PATENT OFFICES[4]

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

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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

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109
109家
专利授权机构

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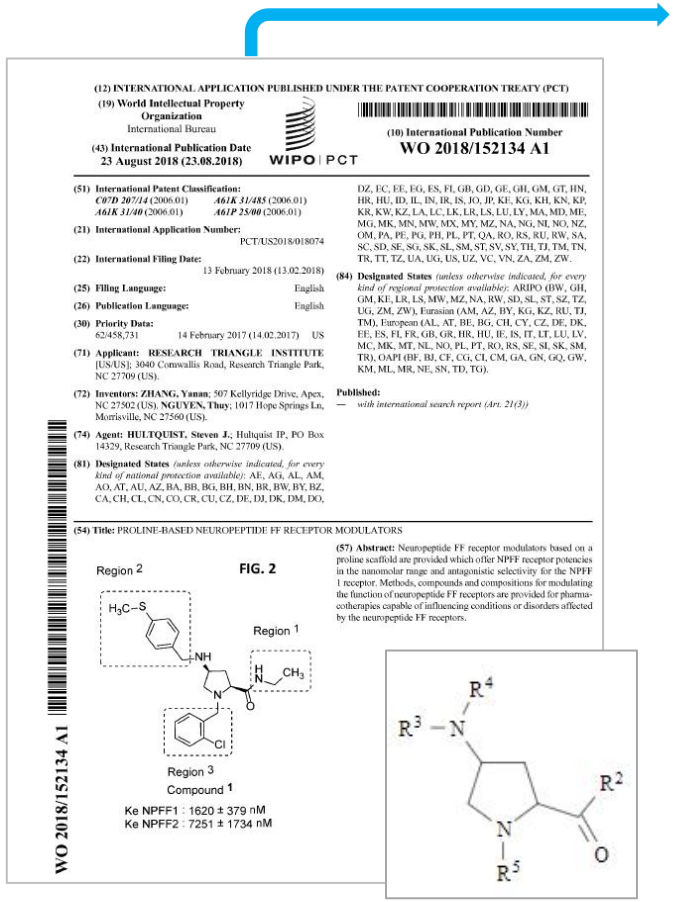
CAS 对文献的独特解读

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*



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

(54) 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 antagonistic 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

WO 2018/152134 A1

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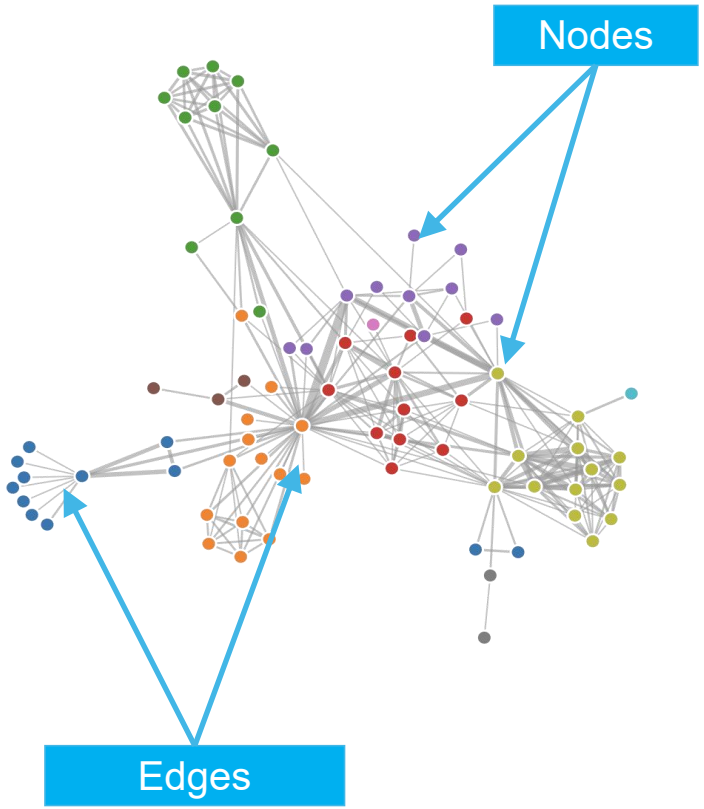

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CAS 持续开发新型解决方案，满足多元应用场景需求

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。

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CAS的解决方案持续进化发展

CAS Newton℠: 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 1.51×10^{-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

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_2/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

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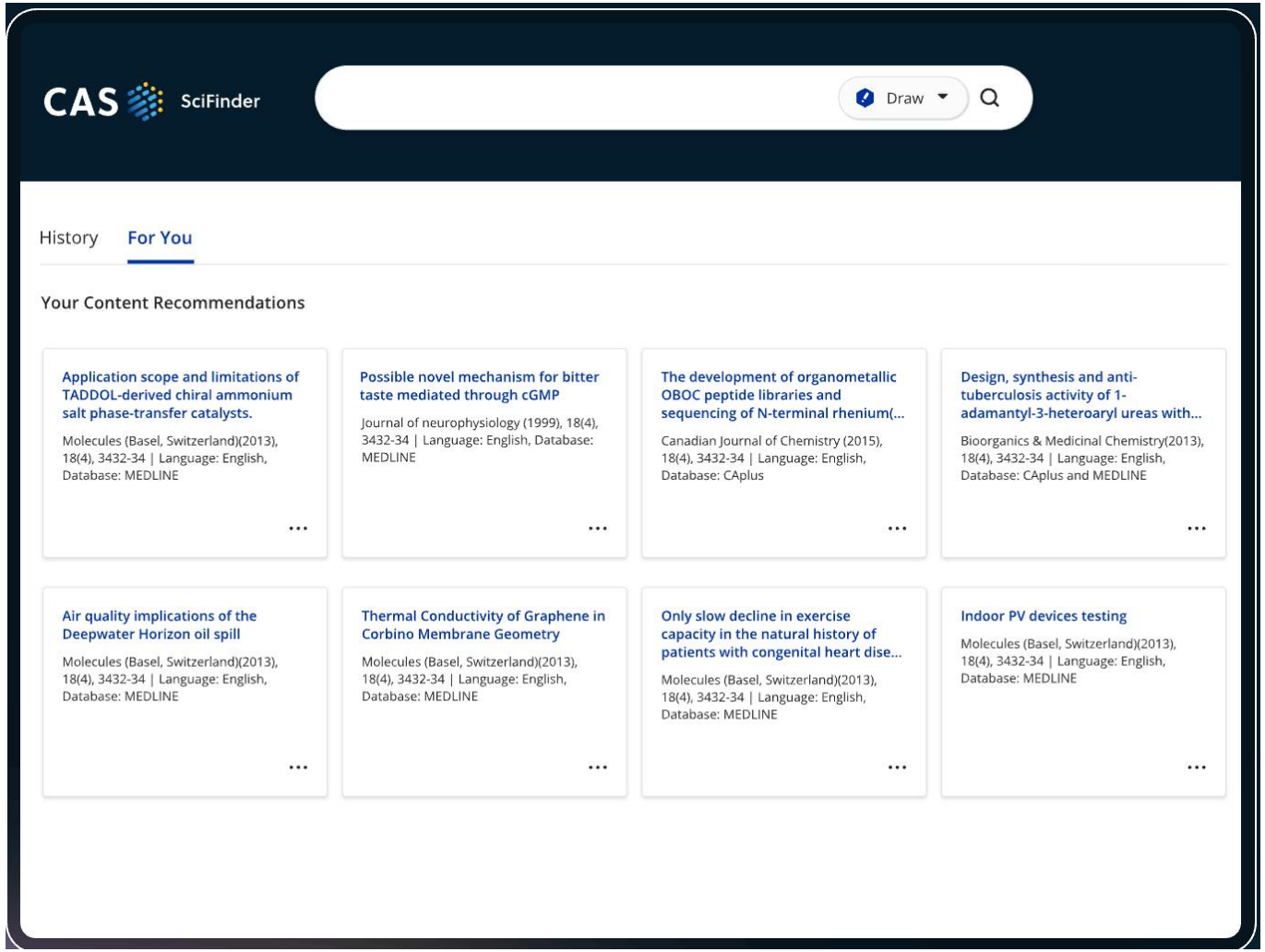
AI解析的自然语言检索，高效获取多类科研信息



- 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。

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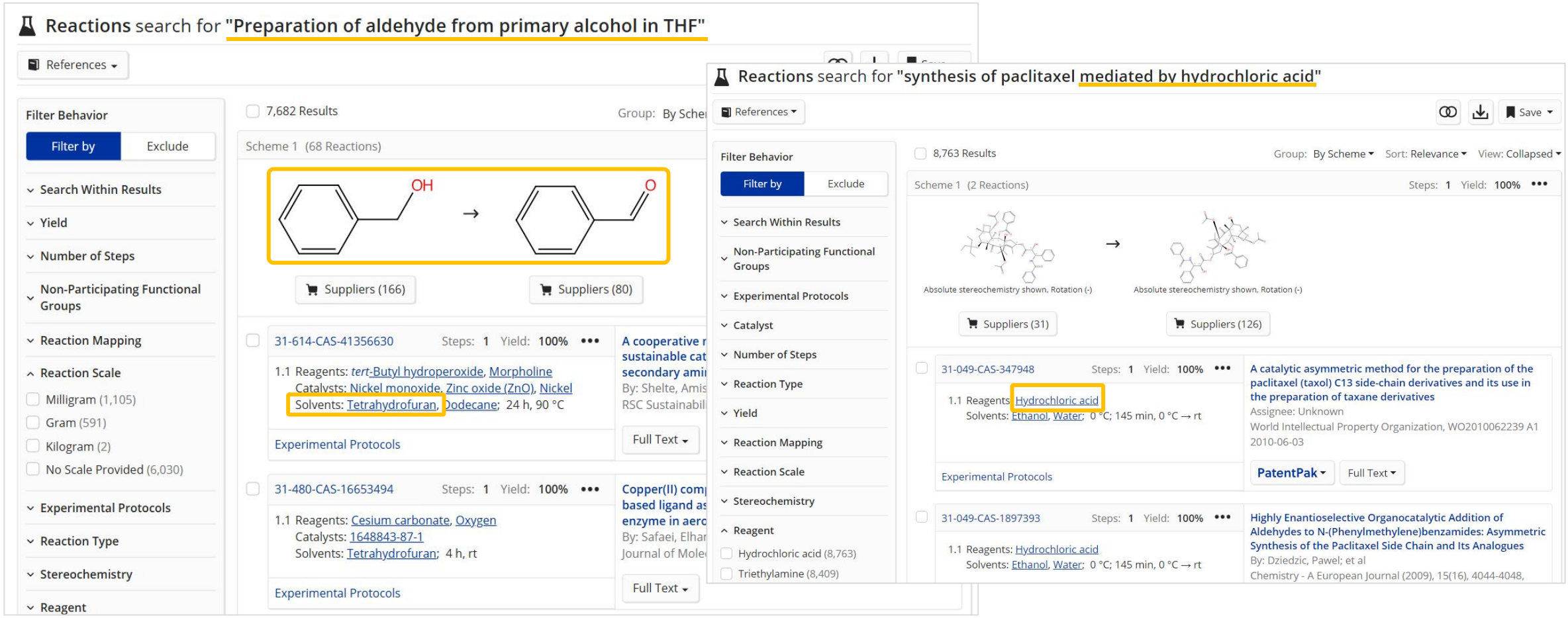
利用自然语言检索反应，降低检索难度



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

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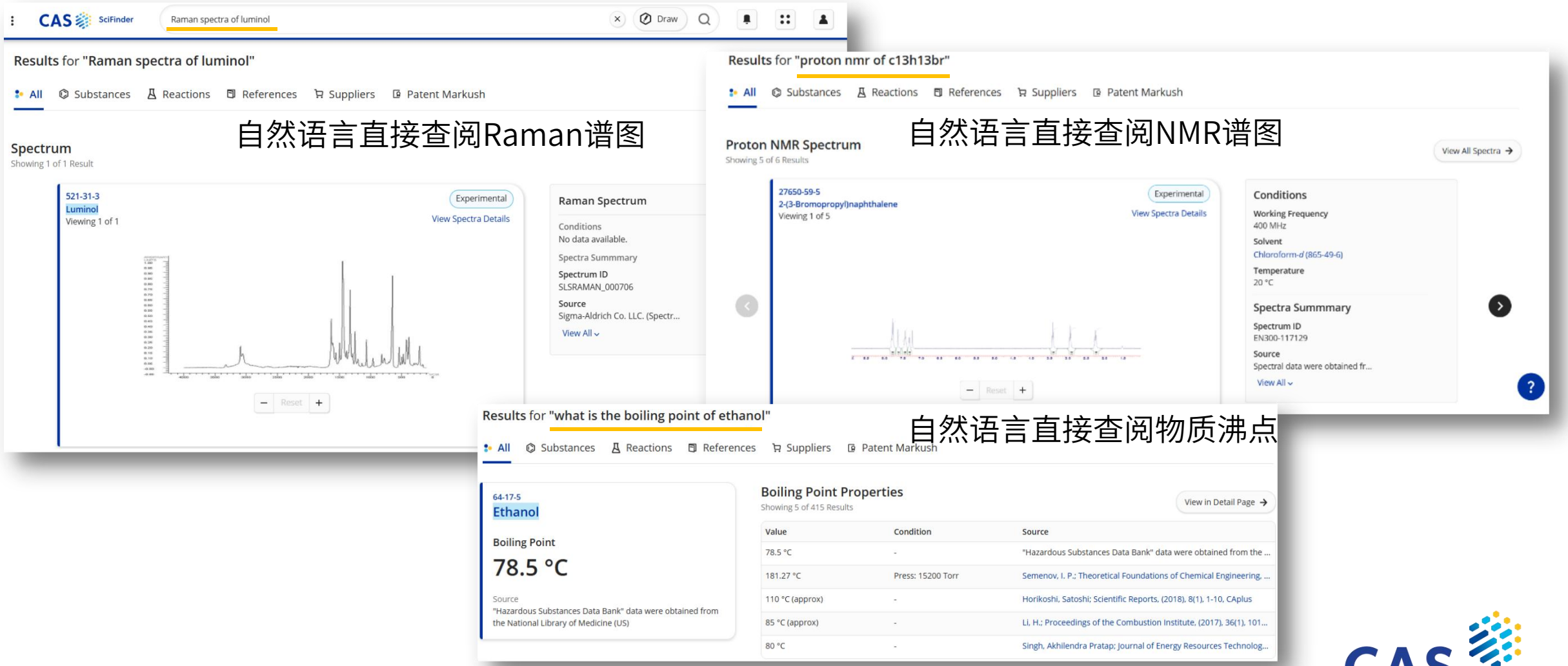
自然语言直接检索物质谱图和理化性质，直观高效

无需多次点击，直接展示目标结果



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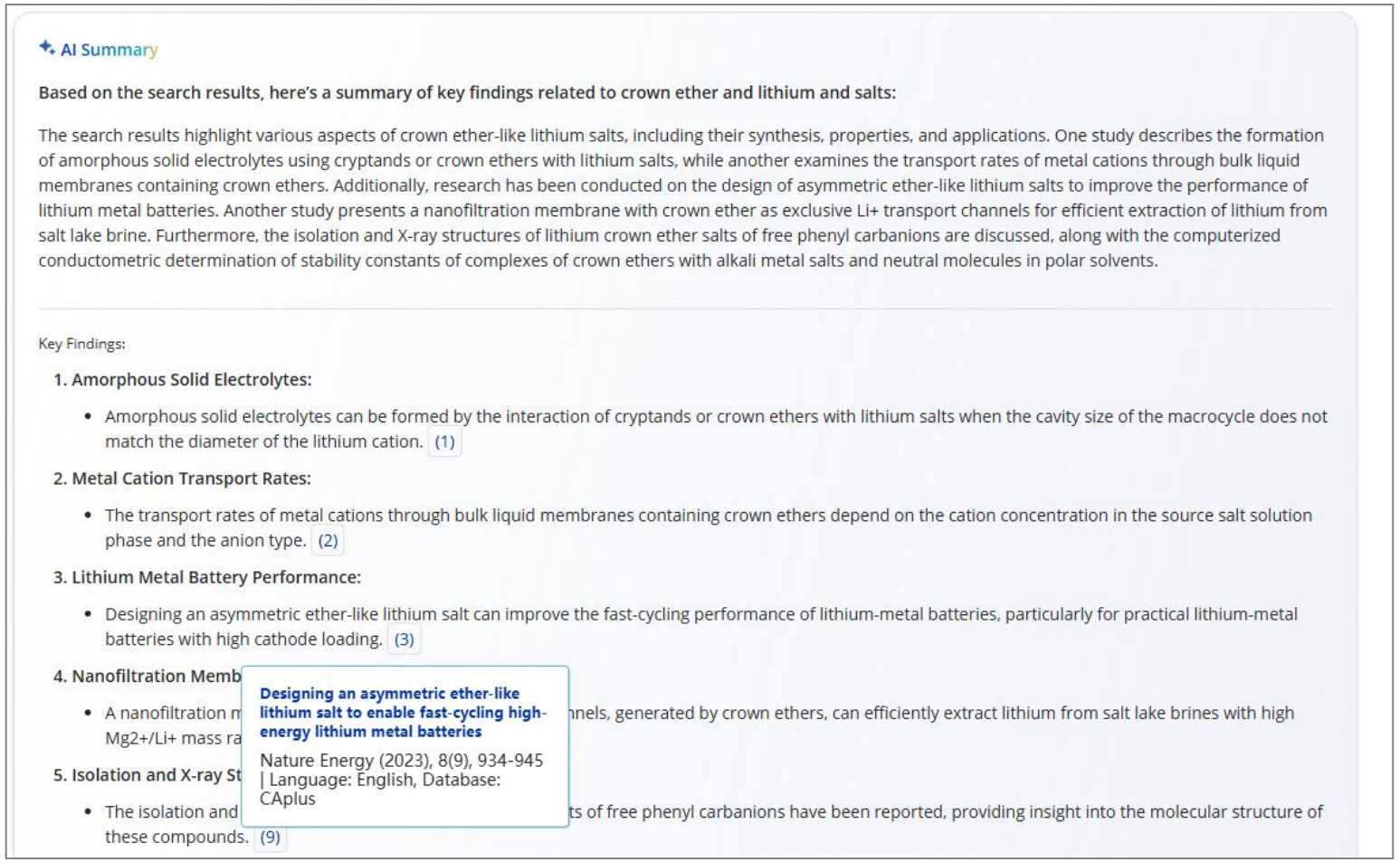
AI赋能的检索结果总结，助力快速掌握关键发现

在文献结果页面查看 AI Summary，更快理解文献中披露的信息。



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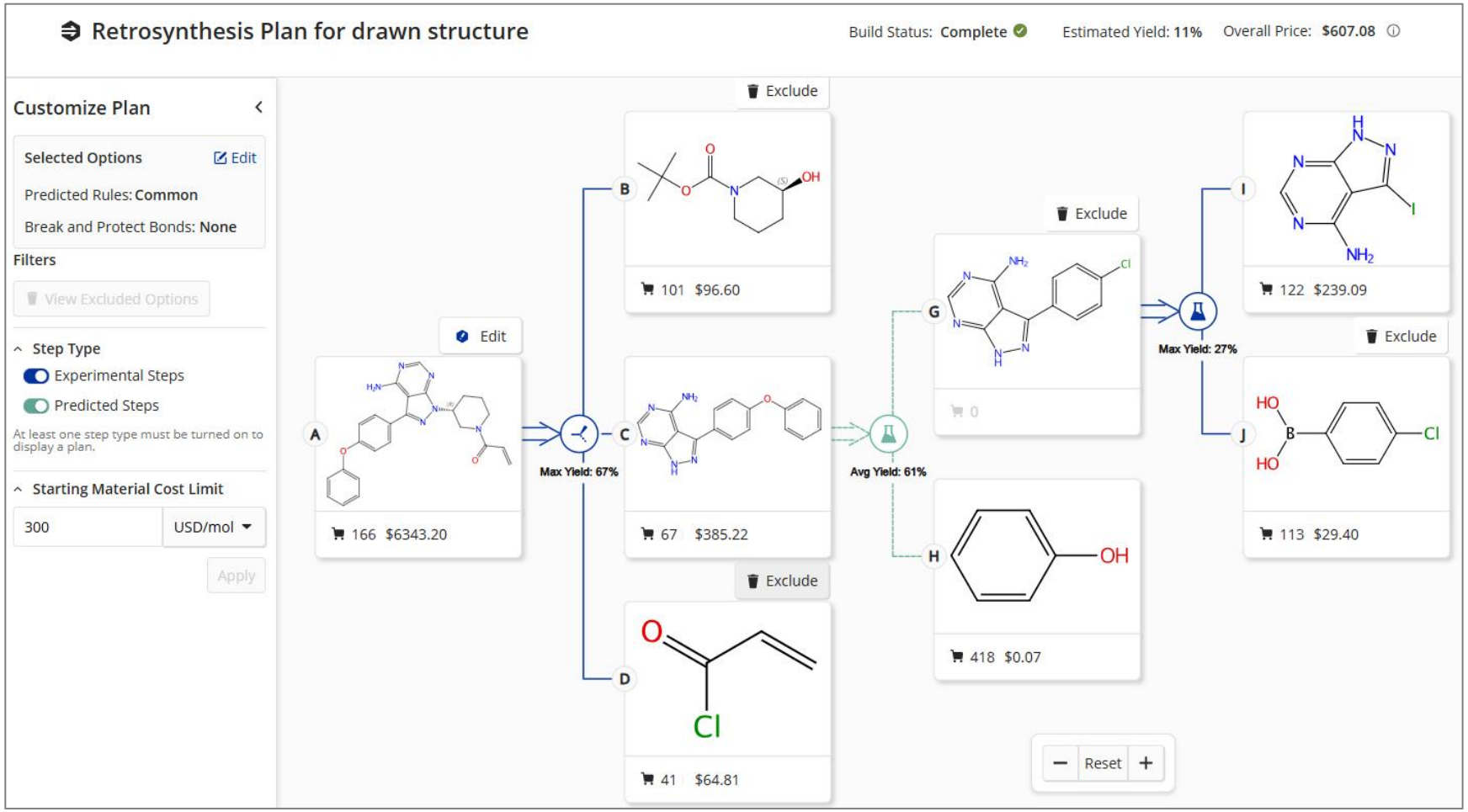
逆合成路线用时大幅减少，AI 和数据驱动高效研发



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

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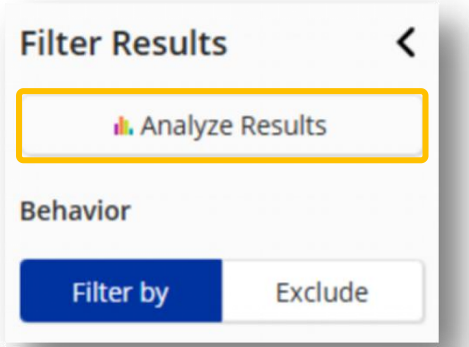
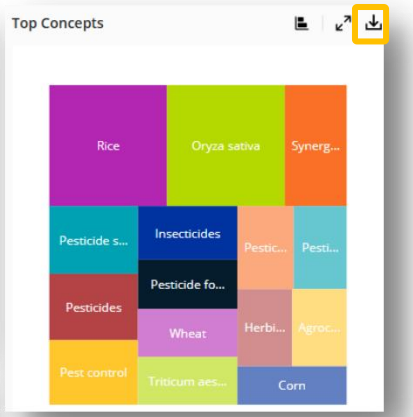
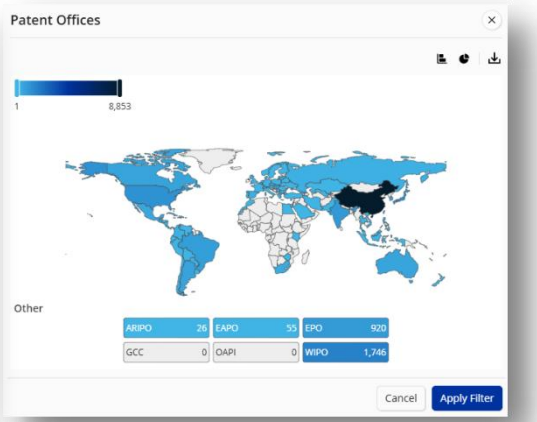
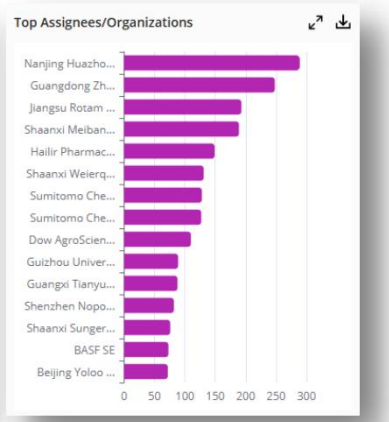
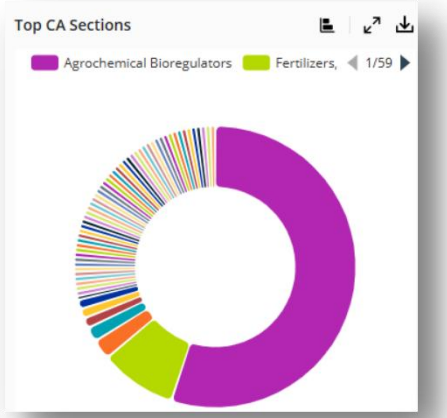
可视化的研究趋势和数据分析



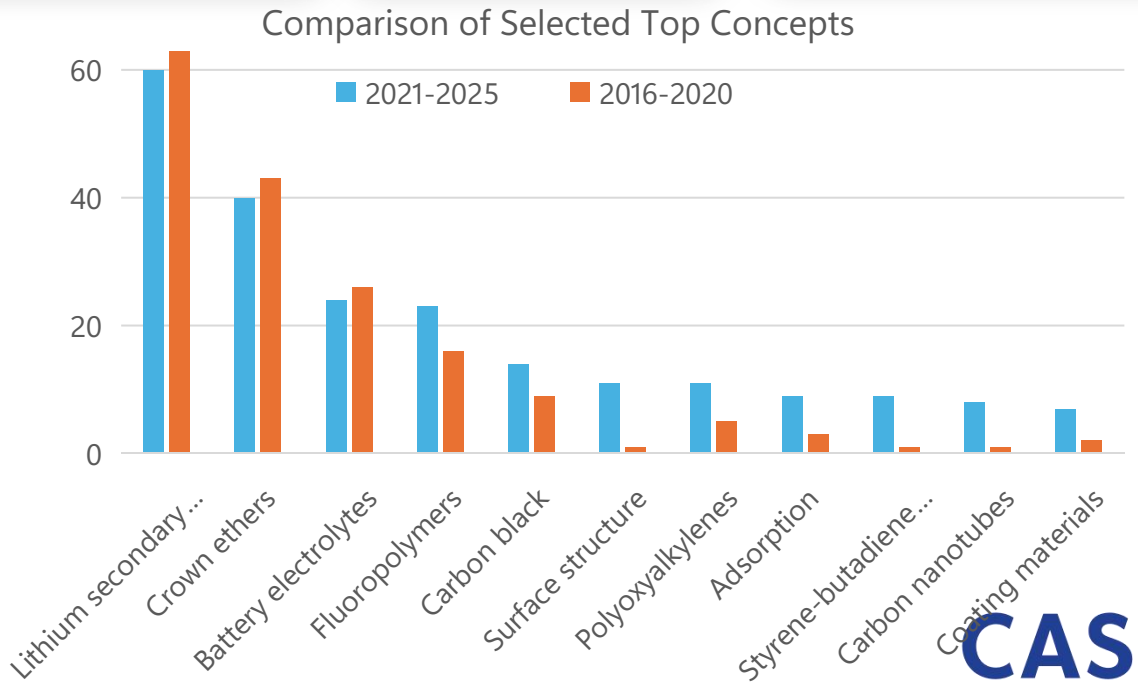








Top Concepts	2021-2025	Count	2016-2020	Count
1	Lithium secondary batteries	60	Lithium secondary batteries	63
2	Crown ethers	40	Crown ethers	43
3	Battery electrolytes	24	Battery electrolytes	26
4	Battery anodes	23	Battery anodes	25
5	Battery cathodes	23	Battery cathodes	18
6	Fluoropolymers	23	Fluoropolymers	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



示例：lithium batteries crown ether

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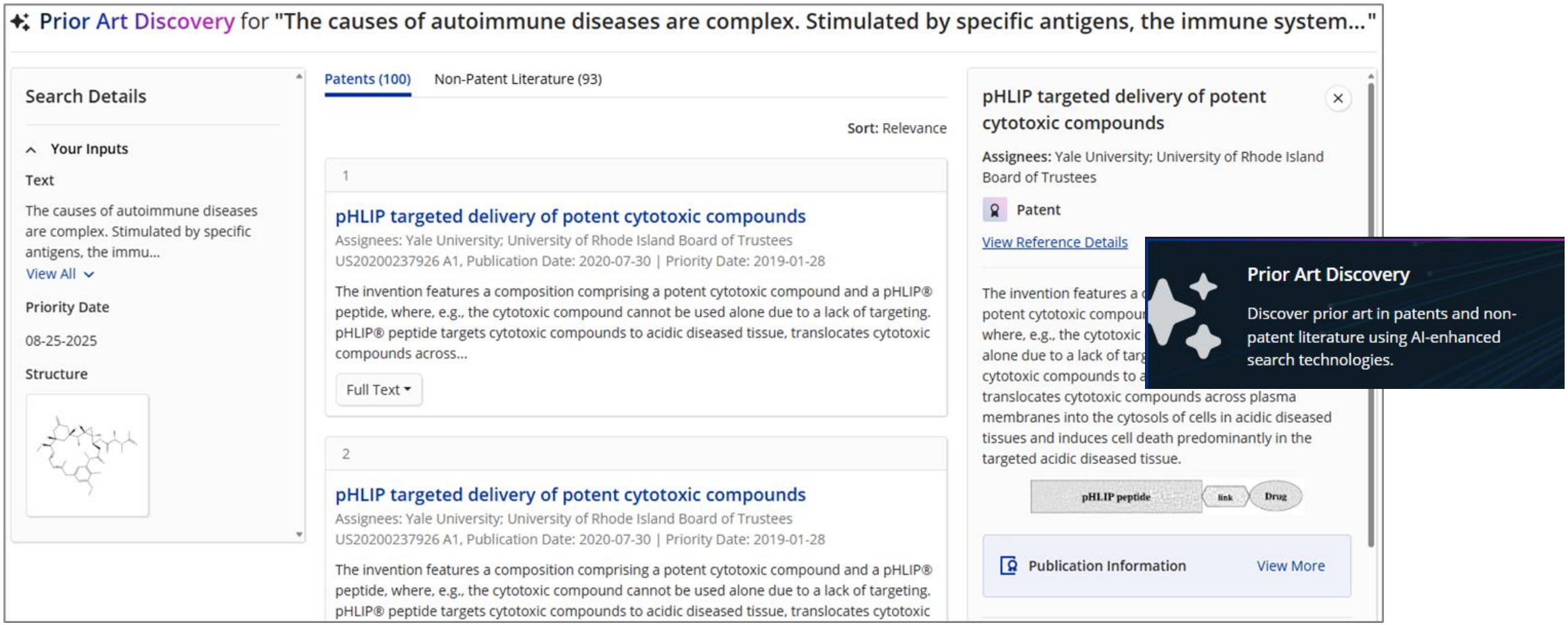
IP connections 专利检索，助力保护创新成果

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



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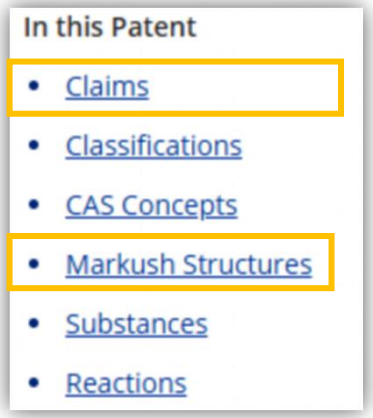
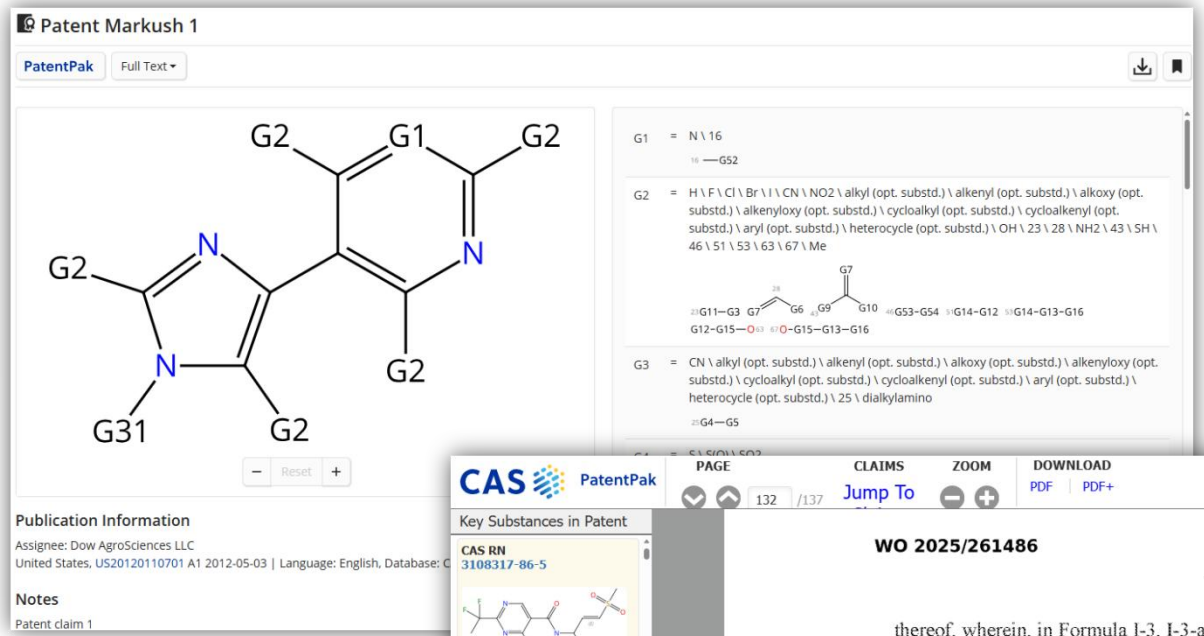
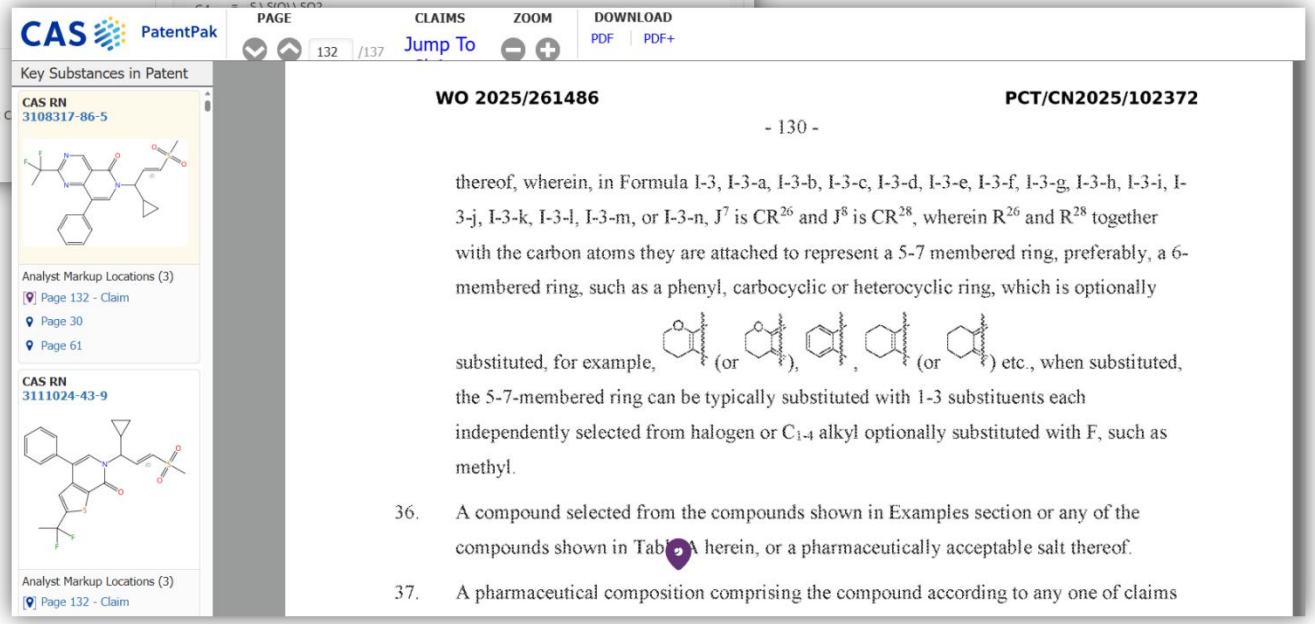
知识产权相关数据扩增，助力保护创新成果







- 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

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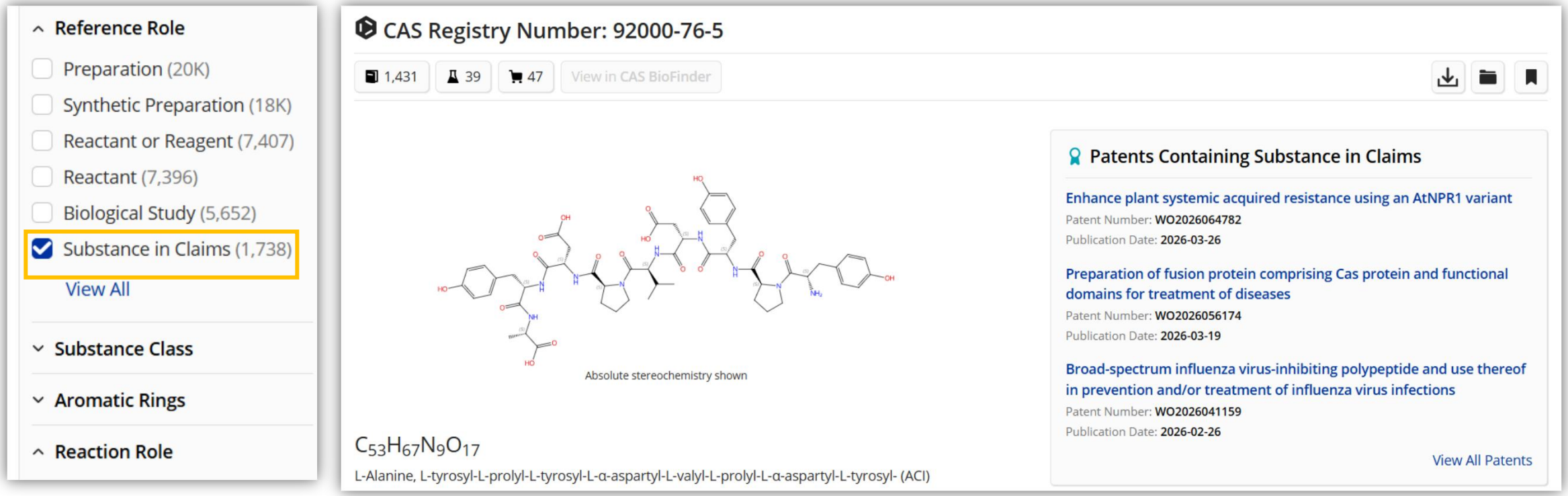
快速定位专利权利要求中的物质



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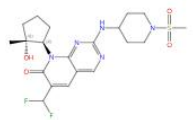
新增生命科学数据，便于挖掘隐藏的重要信息

Pharmacological Data

药理活性

CAS LIFE SCIENCES

2185857-97-8



Absolute stereochemistry shown

$C_{20}H_{27}F_2N_5O_4S$

6-(Difluoromethyl)-8-[(1*R*,2*R*)-2-hydroxy-2-methylcyclopentyl]-2-[[1-(methylsulfon...

Ligand	Target	Function	Parameter ^1	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

生物标志物

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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

毒性

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Ligand ^1	Target ^2	Function	Parameter ^3	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	-	View Detail
1092443-55-4	COLO 205	Inhibitor	LC50	0.637 µM	cancer	-	View Detail

ADME

代谢数据

CAS LIFE SCIENCES

Ligand ^1	Target ^2	Function	Parameter ^3	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

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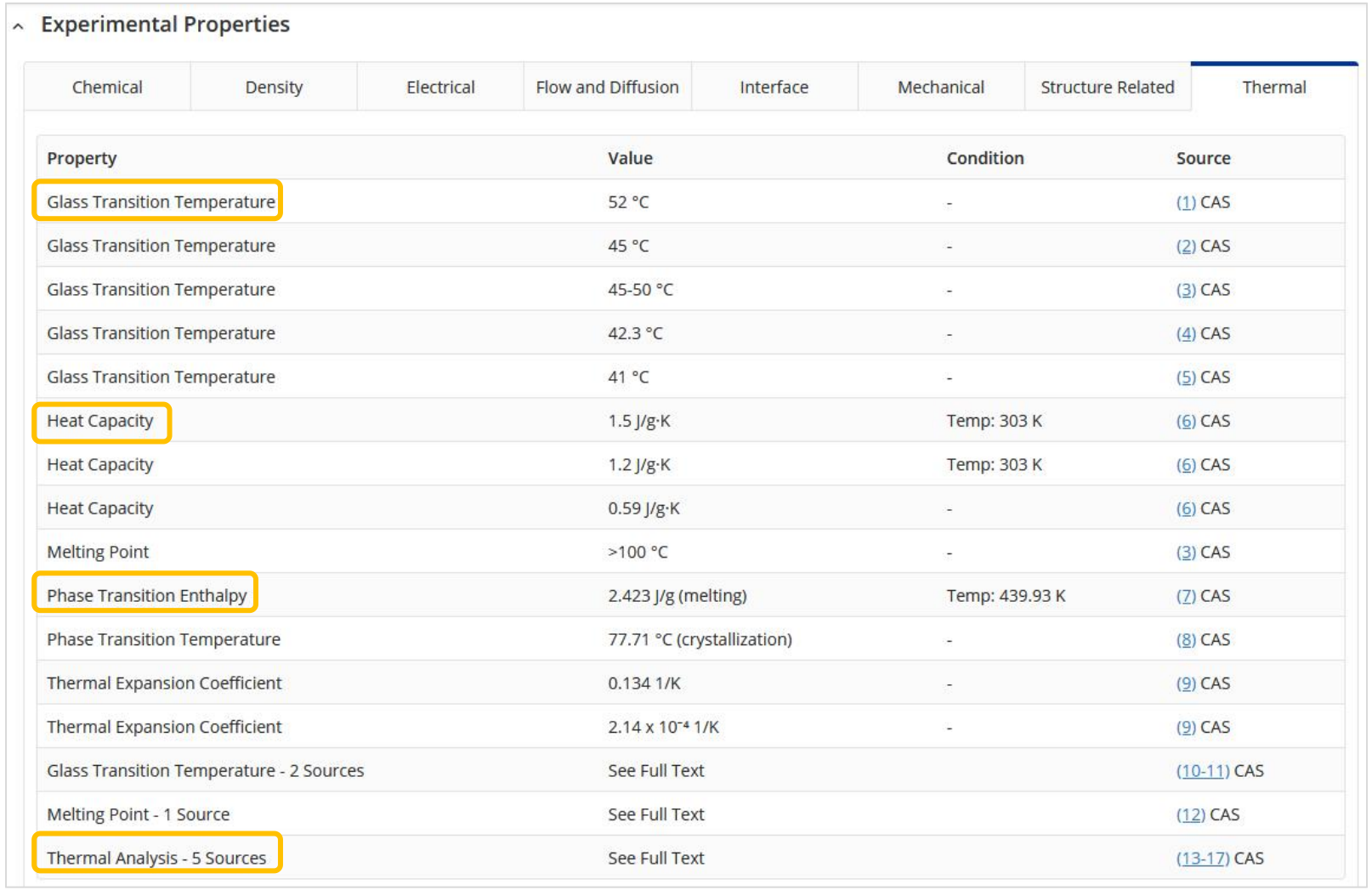
新增多种属性数据：助力材料、化学化工研究



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^{-4} 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

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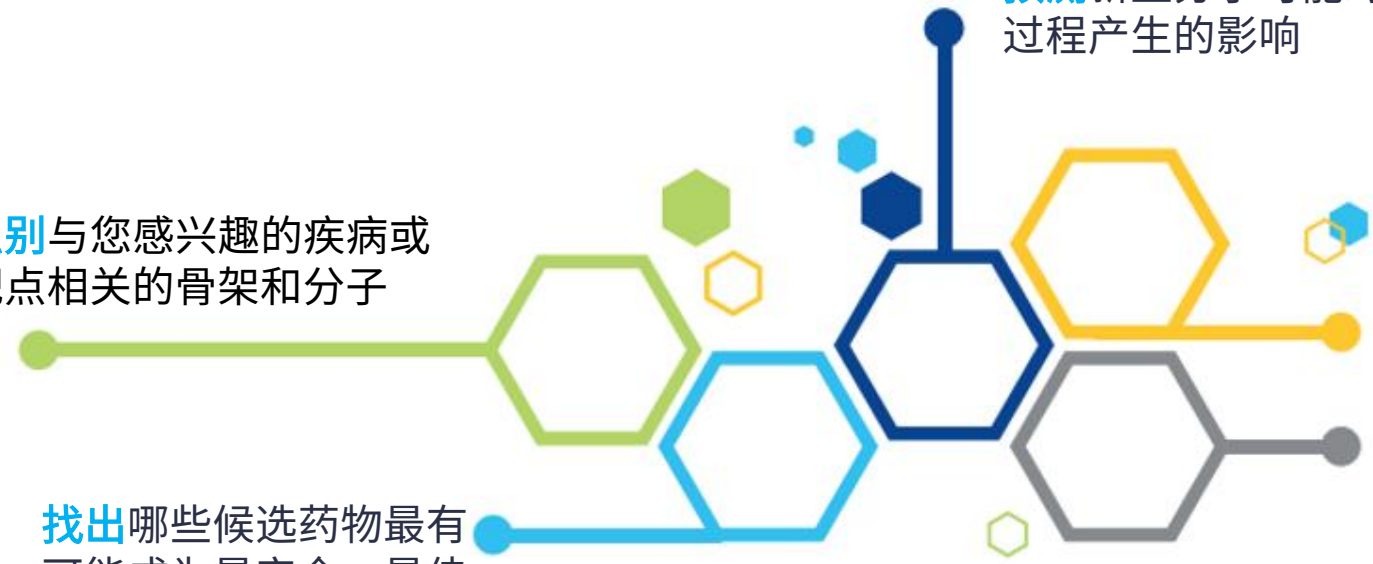
CAS BioFinder 加速早期药物研发



预测新型分子可能对生物过程产生的影响

识别与您感兴趣的疾病或靶点相关的骨架和分子

发现与您感兴趣的疾病相关的生物标志物

找出哪些候选药物最有可能成为最安全、最佳的先导化合物

持续开发中的更多内容与功能（序列、抗体、PDC、药物情报等）

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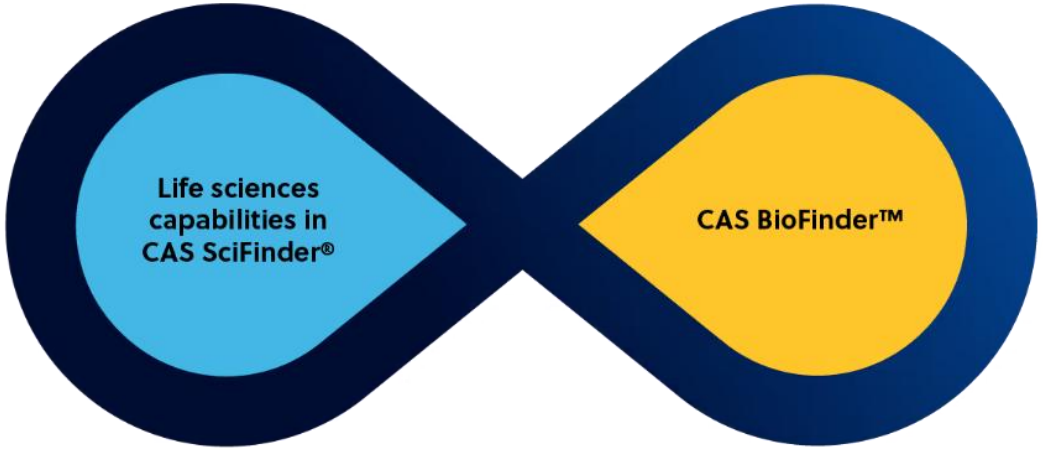
CAS生命科学领域的内容与创新赋能

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

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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

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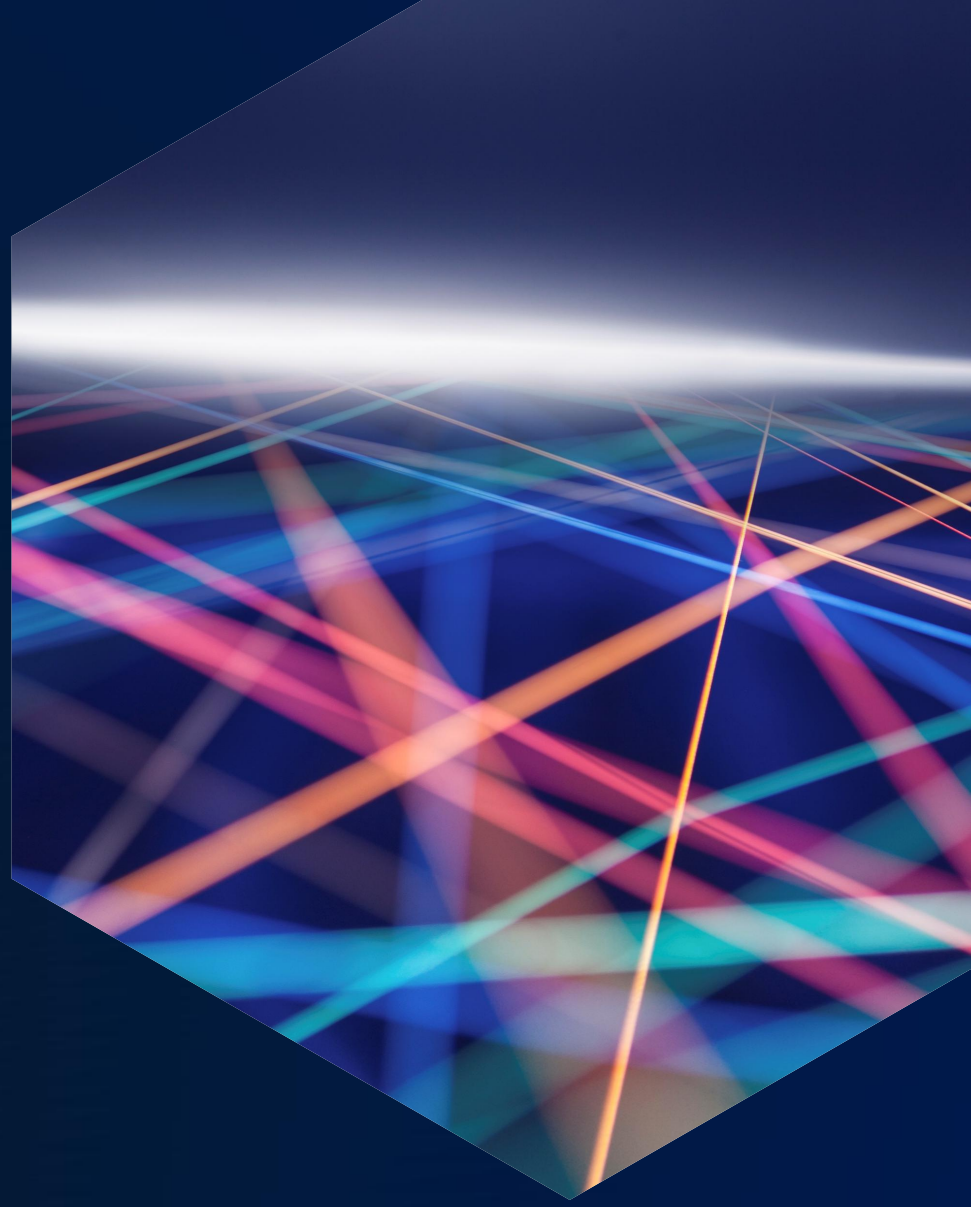
CAS SCIFINDER DISCOVERY PLATFORM

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。

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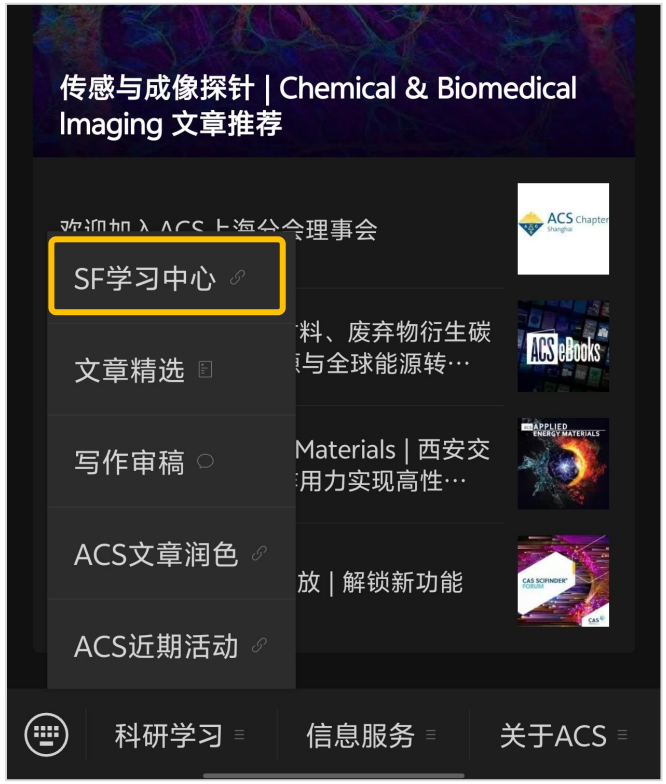
多学科、多形式的线上学习资源



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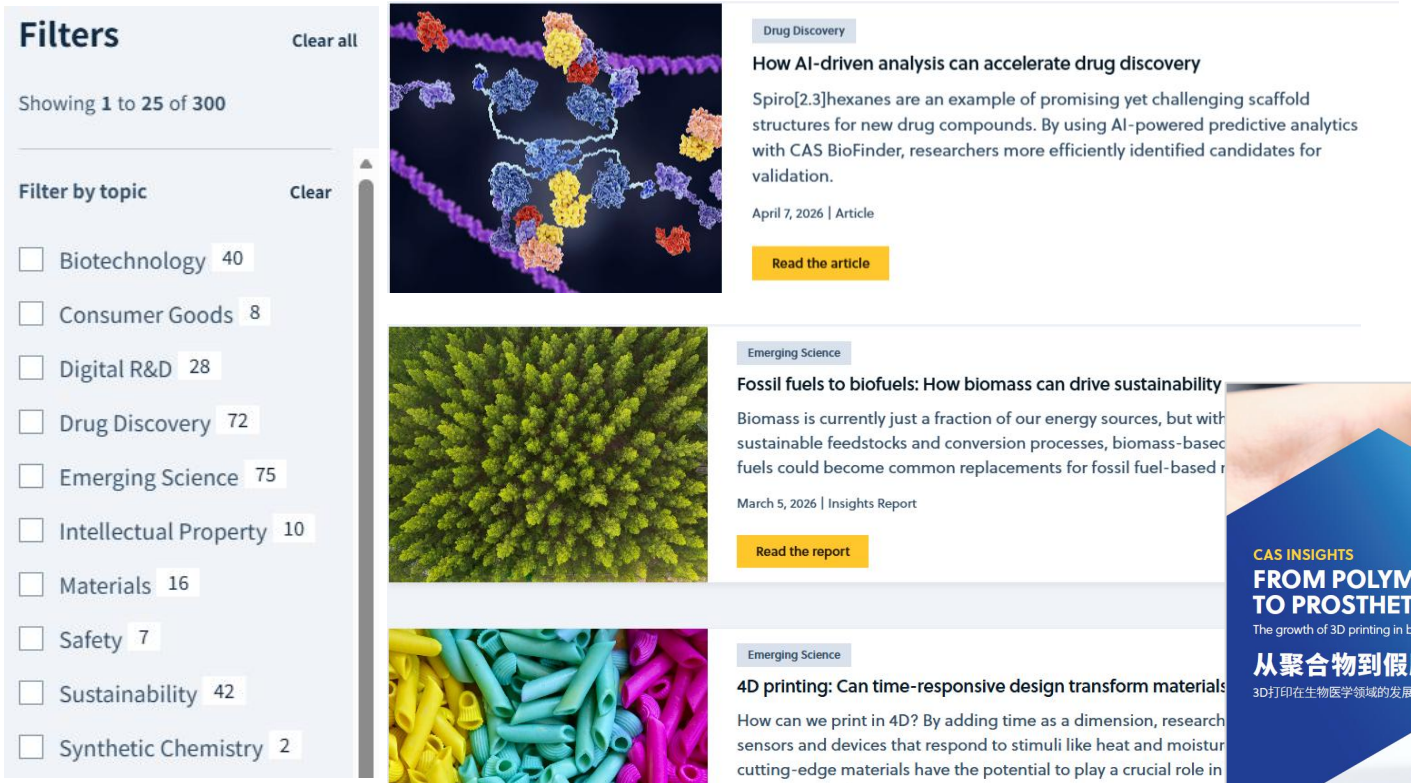
CAS 系列白皮书及洞察报告



来源：
https://www.cas.org/resources/white-papers
https://www.cas.org/resources/cas-insights

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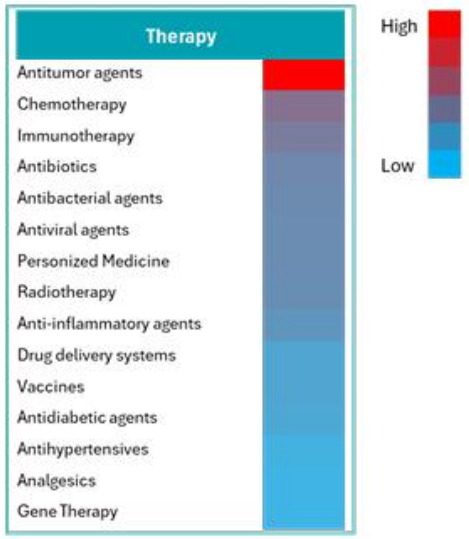
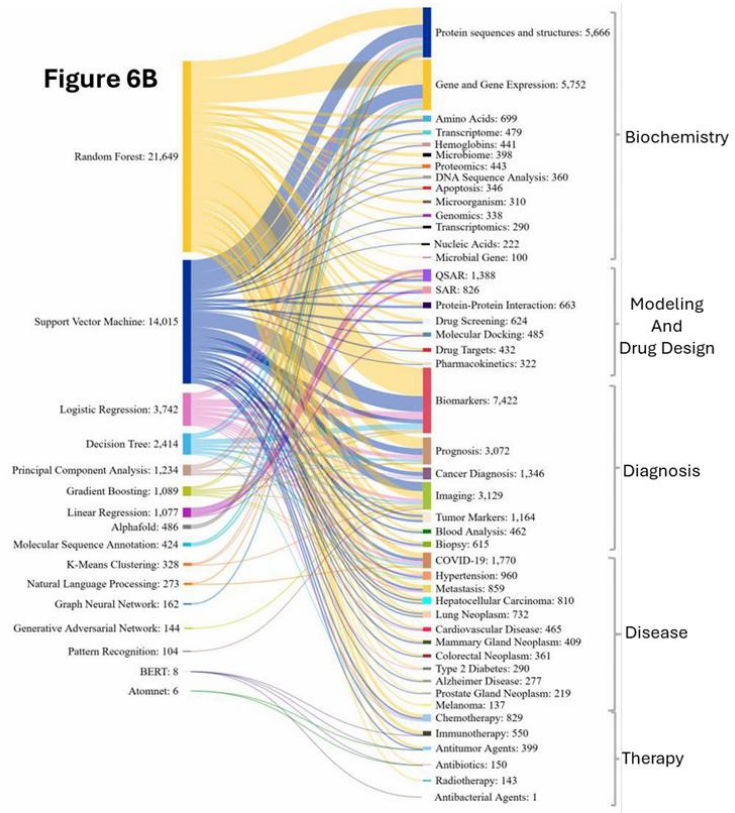
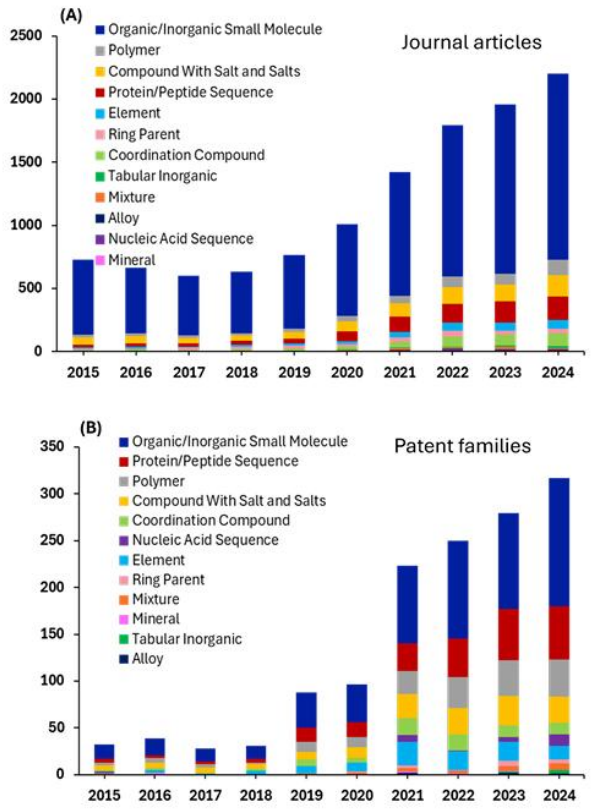
化学AI模型：绘制材料与生命科学领域的蓝图

- 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







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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

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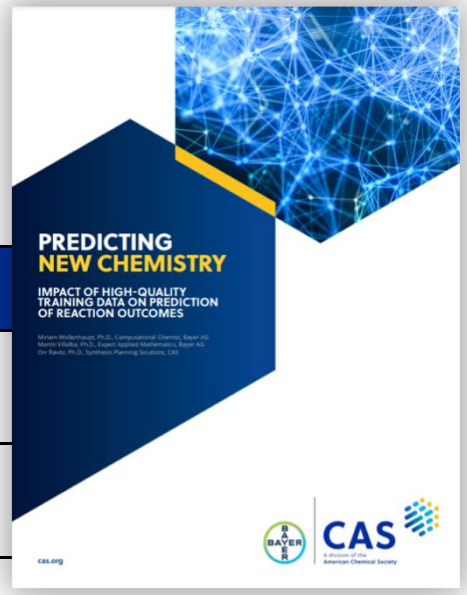
在极难突破的科学领域改进反应预测结果

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。

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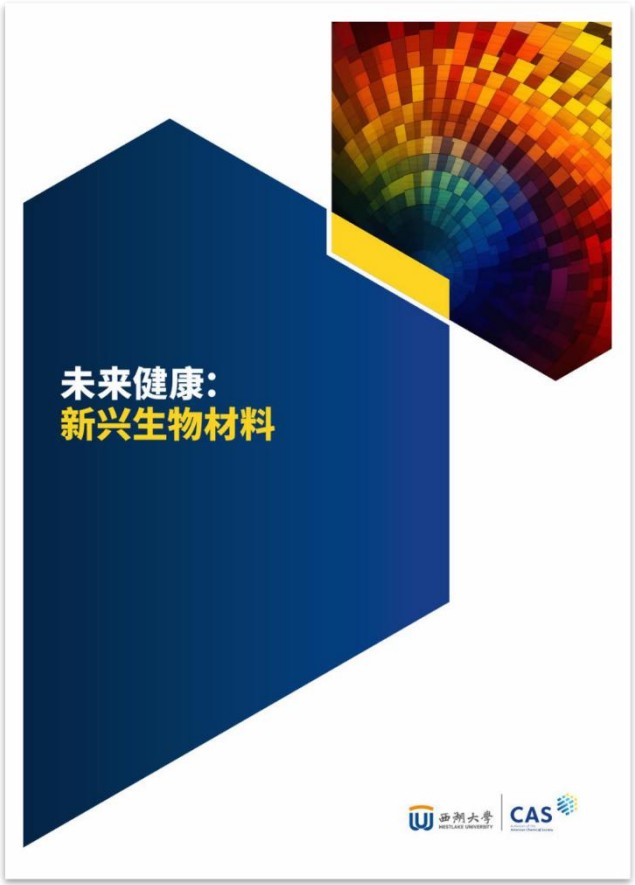
西湖大学分析报告《未来健康：新兴生物材料》

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

西湖大學 WESTLAKE UNIVERSITY
西湖大学未来产业研究中心 WESTLAKE UNIVERSITY RESEARCH CENTER FOR INDUSTRIES OF THE FUTURE
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提纲

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  - 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

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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

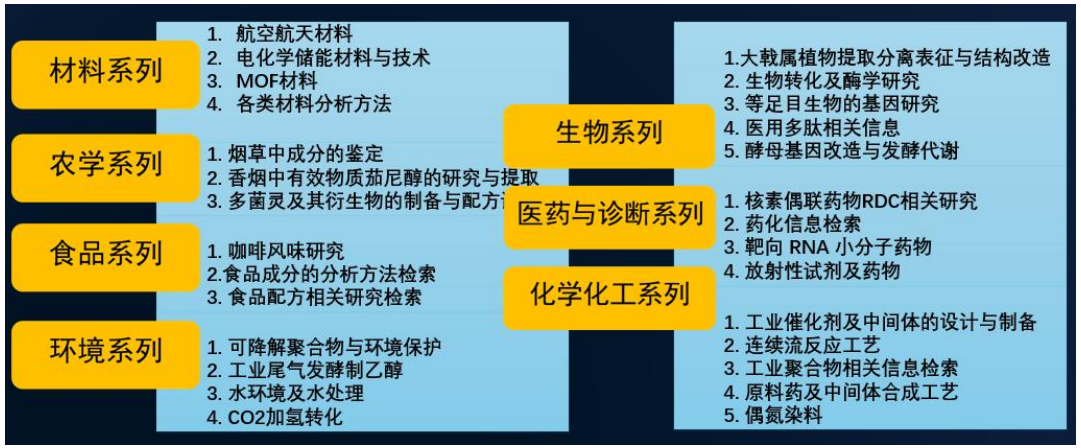
多学科的教学资源

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



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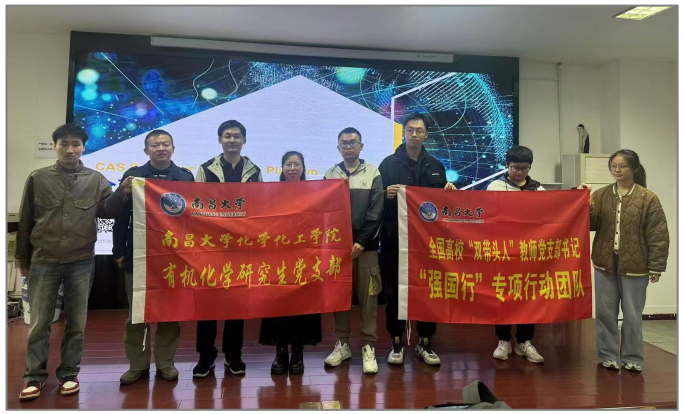
CAS 领先的技术培训团队

- 培训师均拥有国内外名校博士学位
- 每年为百余所学校提供数百场培训，参与人数超万人



培训互动及读书节小礼品

* 部分高校已将CAS SciFinder培训嵌入文检课程

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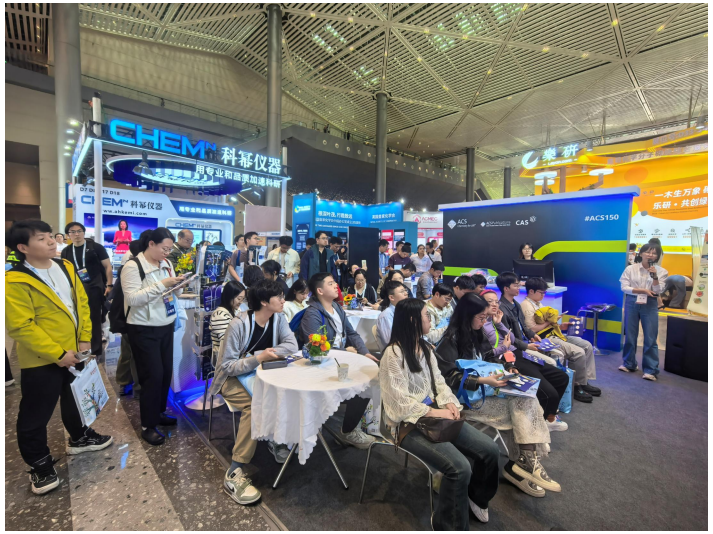
中国化学会第35届学术年会

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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2026 CAS SciFinder® 检索技能大赛

第一阶段：5月1日 – 6月14日

在线学习检索技能，并参加线上考试。

第二阶段：5月1日 – 6月14日*

分享检索体验，赢取全国大奖，通过第一轮考核后可随时提交第二轮的PPT

所有获奖者都将获得CAS官方获奖证书及ACS学生会员一年。

在第一轮中前300名85分以上的可额外获得CAS定制礼盒。

活动通知请关注公众号

ACS美国化学会

***参加第二轮需要完成第一阶段且成绩不低于85分，奖品颜色随机，最终解释权归CAS所有。**

一等奖：1名

MacBook Air

二等奖：3名

大疆 Osmo Action 5 pro 运动相机

三等奖：10名

Xiaomi 照片打印机 pro

入围奖：30名

罗技键鼠套装

K580键盘+Pebble鼠标（颜色随机）

大赛证书

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Between problems and progress are connections that matter

谢 谢!

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