CAS SciFinder Discovery Platform

全面高效获取科技信息

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美国化学文摘社(CAS)北京代表处

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大纲

CAS及CAS SciFinder Discovery Platform 简介

科研信息的高效查阅

- 全面的文献调研与拓展助力开题
- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

常见问题Q&A

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CAS SciFinder Discovery Platform 涵盖的工作流程解决方案

CAS SciFinder

新一代的权威科学研究工具，是化学及相关学科智能研究平台，提供全球全面、可靠的化学及相关学科研究信息和分析工具

CAS Analytical Methods

独特的分析方法详情数据库，有助于分析科学家快速获取详尽的分析方法信息、直接用于实验，并启发新方法的建立

CAS Formulus

专业的制剂/配方数据库， 助力配方研究科学家快速评估配方、寻找可替代供应商和探索监管信息

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CAS 内容合集来源于化学、超越化学

5大类80小类

- **有机化学各领域：**
  - 脂肪/环族化合物、杂环化合物、有机金属化合物、生物分子、碳水化合物
- **物理、无机、分析化学各领域：**
  - 电化学、表面化学、催化剂、相平衡、核现象
- **大分子化学各领域：**
  - 合成高聚物化学；塑料的制造、加工、成型与应用；涂料、墨水
  - 染料、有机颜料；合成橡胶；纺织品、纤维
- **应用化学各领域：**
  - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- **生物化学：**
  - 药理学、农化产品管控信息、生化遗传学、发酵、免疫化学

来源：https://www.cas.org/support/documentation/references/ca-sections

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CAS独特的内容合集

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

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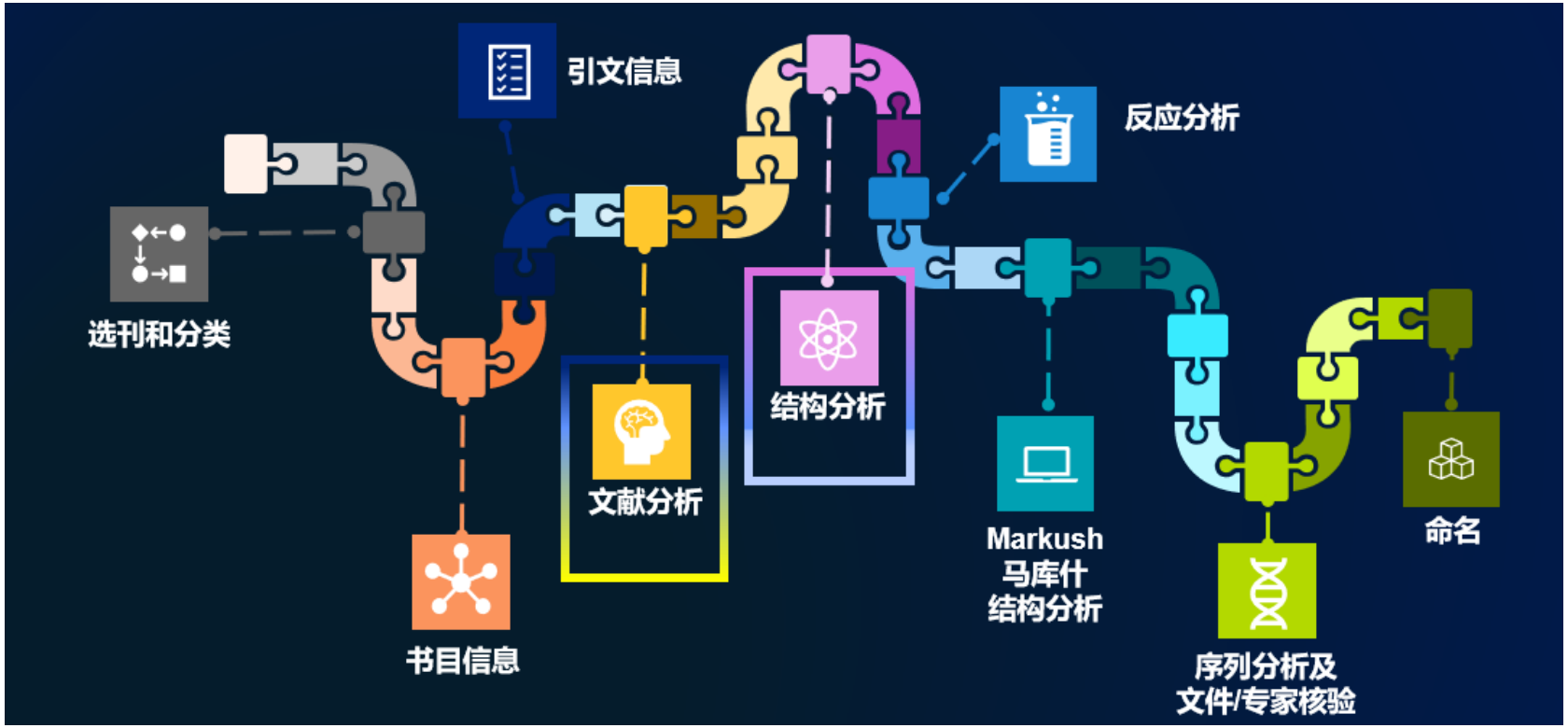
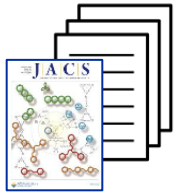
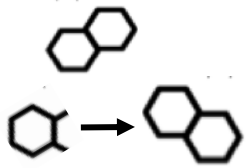
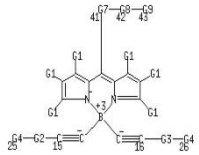
CAS科学家的智力标引





1990
Smith, M.
anthracene





Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

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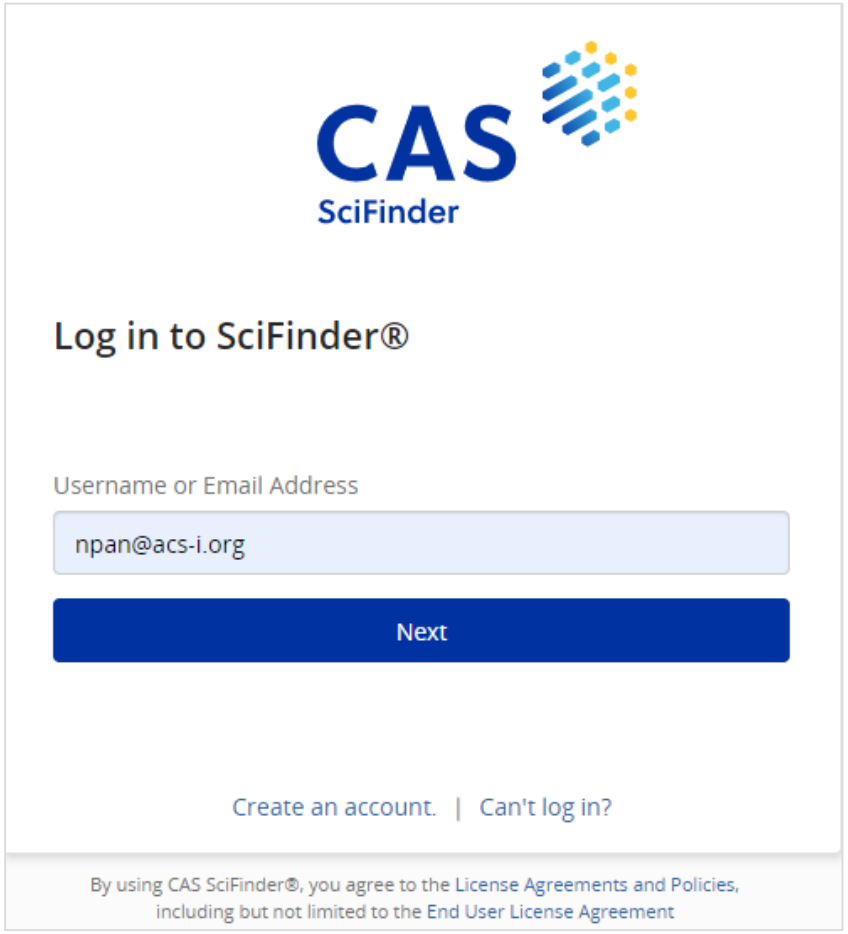

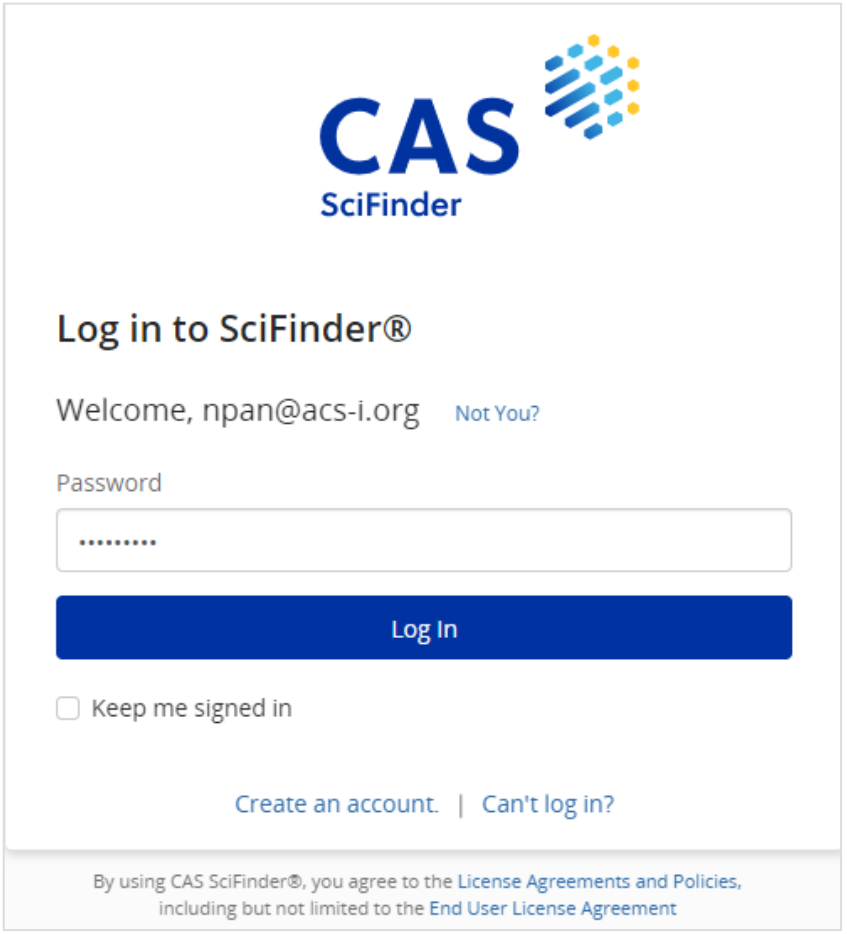

使用CAS SciFinder账号登录

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如何获取CAS SciFinder账号

登录本校图书馆网站，查看注册相关的链接和说明

https://lib.jiangnan.edu.cn/info/1131/1637.htm

使用说明：

1、CAS SciFinder-n 账号注册须知

读者在使用CAS SciFindern之前须用江南大学的学校域名邮箱地址注册账号（如果已经注册了CAS SciFinder账号，请用该账号直接登录CAS SciFinder-n），根据提示输入相应信息，提交注册申请后系统将自动发送一个链接到您所填写的邮箱中，进入邮箱激活此链接即可完成注册。

2、SciFinder账号注册链接

https://scifinder.cas.org/registration/index.html?corpKey=F1455EF5X86F35055X2E756CE85D18B16693

3、CAS SciFinder-n检索网址

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

4、CAS SciFinder-n培训材料及视频：

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

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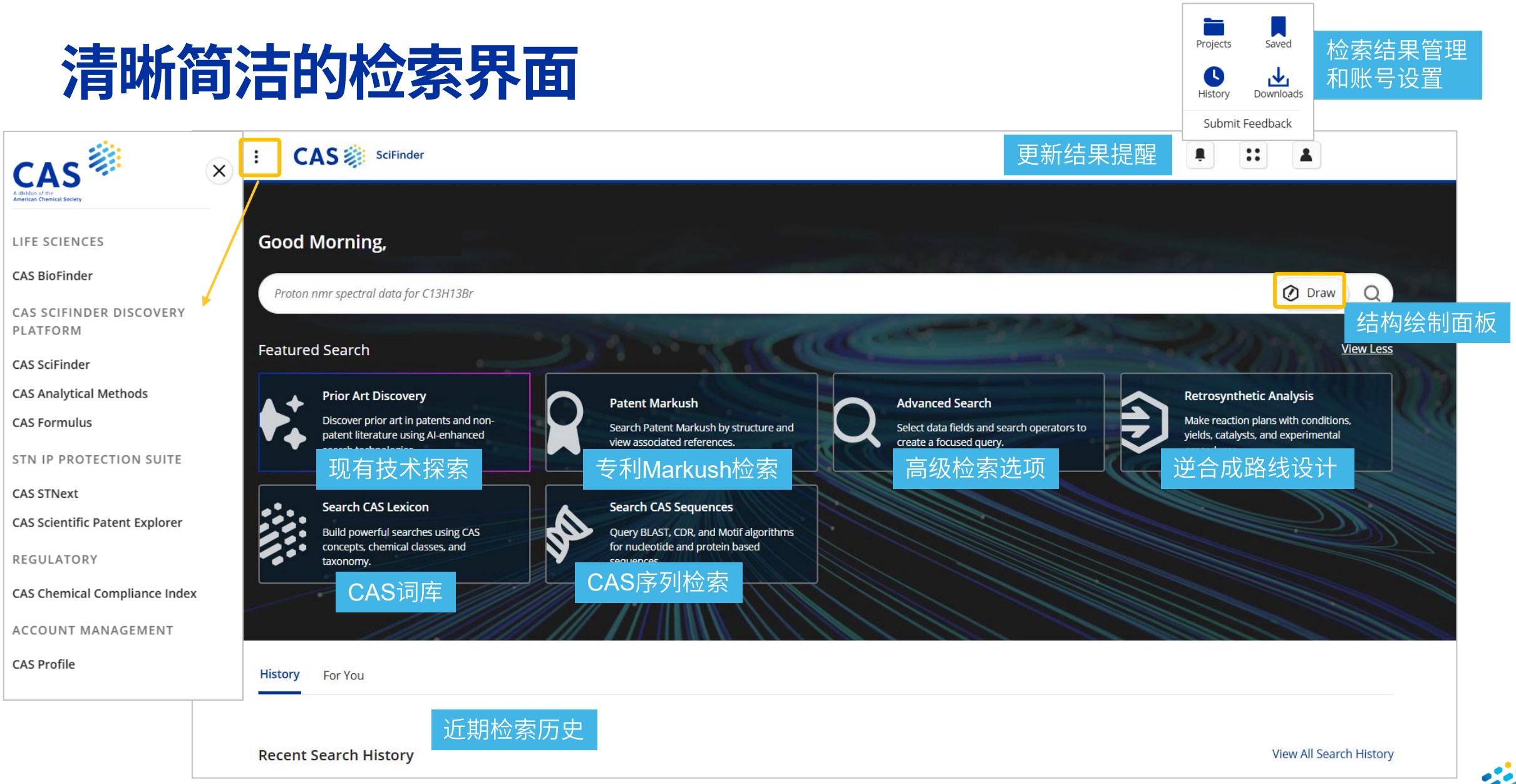
清晰简洁的检索界面



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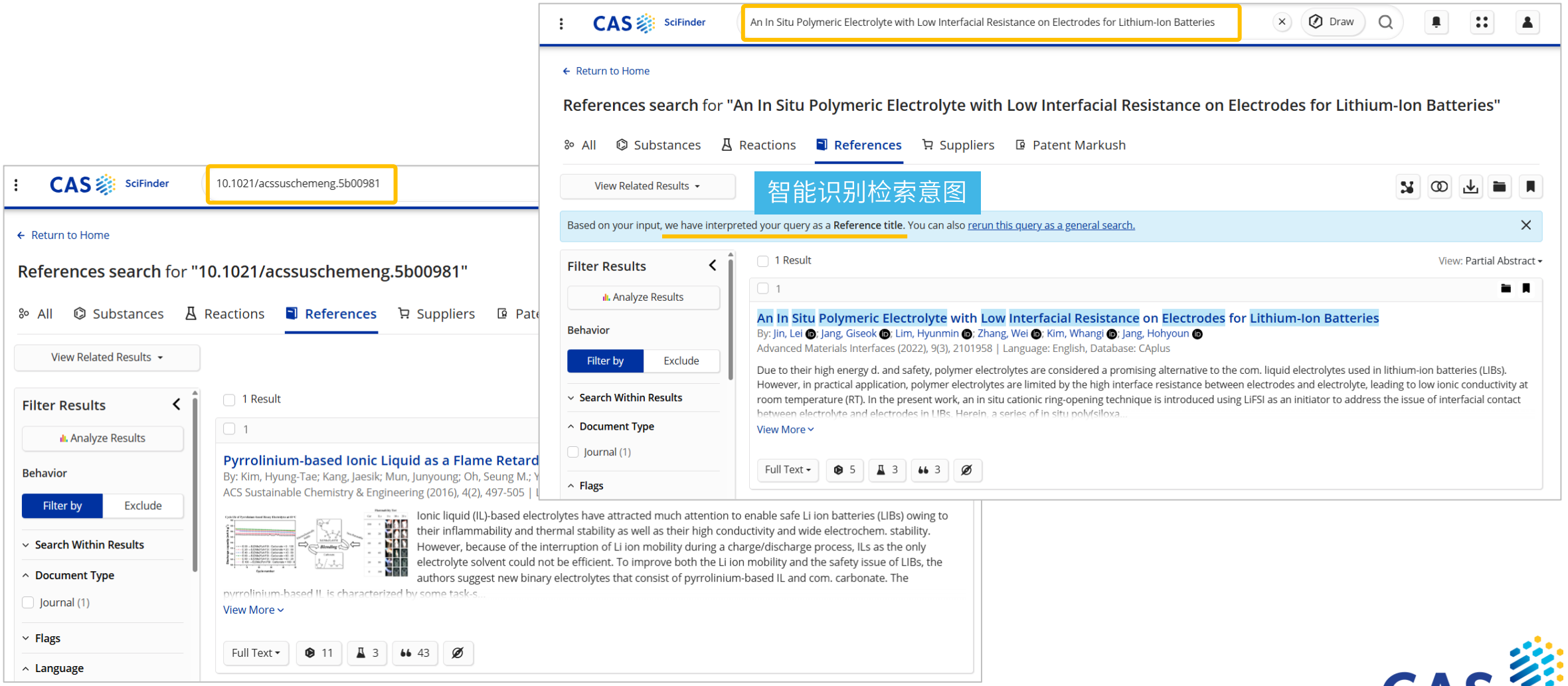
通过文献标识符快速获取文献

支持使用：主题词、DOI、文献号、专利号、物质名词、CAS登记号等



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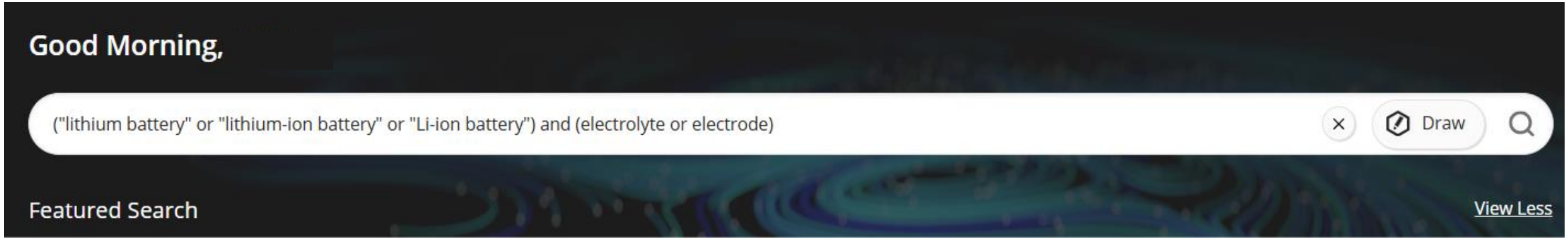
如何精准构建检索主题?

- 支持布尔逻辑运算符(and, or, not)
- 默认运算顺序or > and > not, ( )优先运算
- “”不允许词形变化，但可出现单数或复数
- 通配符*代表0或多个字符；?代表0或1个字符



示例：("lithium battery" or "lithium-ion battery" or "Li-ion battery") and (electrolyte or electrode)

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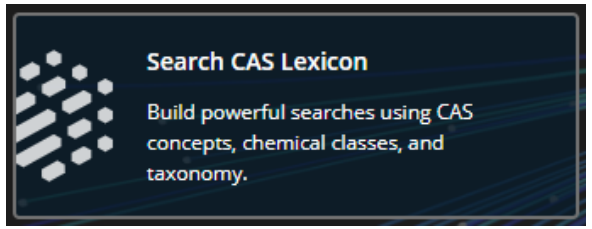
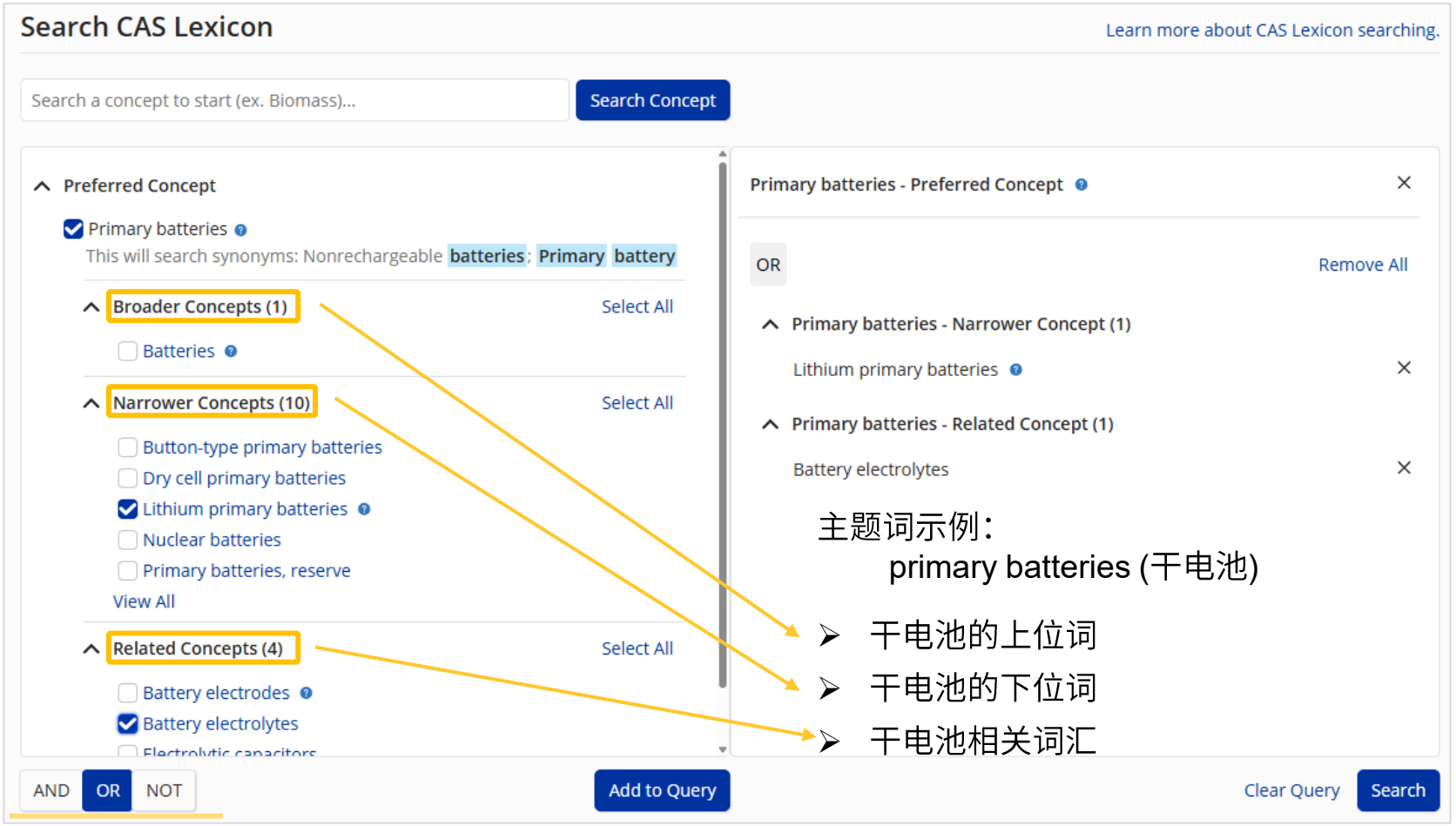
CAS Lexicon 快速开启检索

对新的研究方向了解不深，不知道从何入手？



- CAS科学家标引的概念词（Concepts）和重要物质
- 选择感兴趣的技术词来建立检索式（最多可用1000个词）



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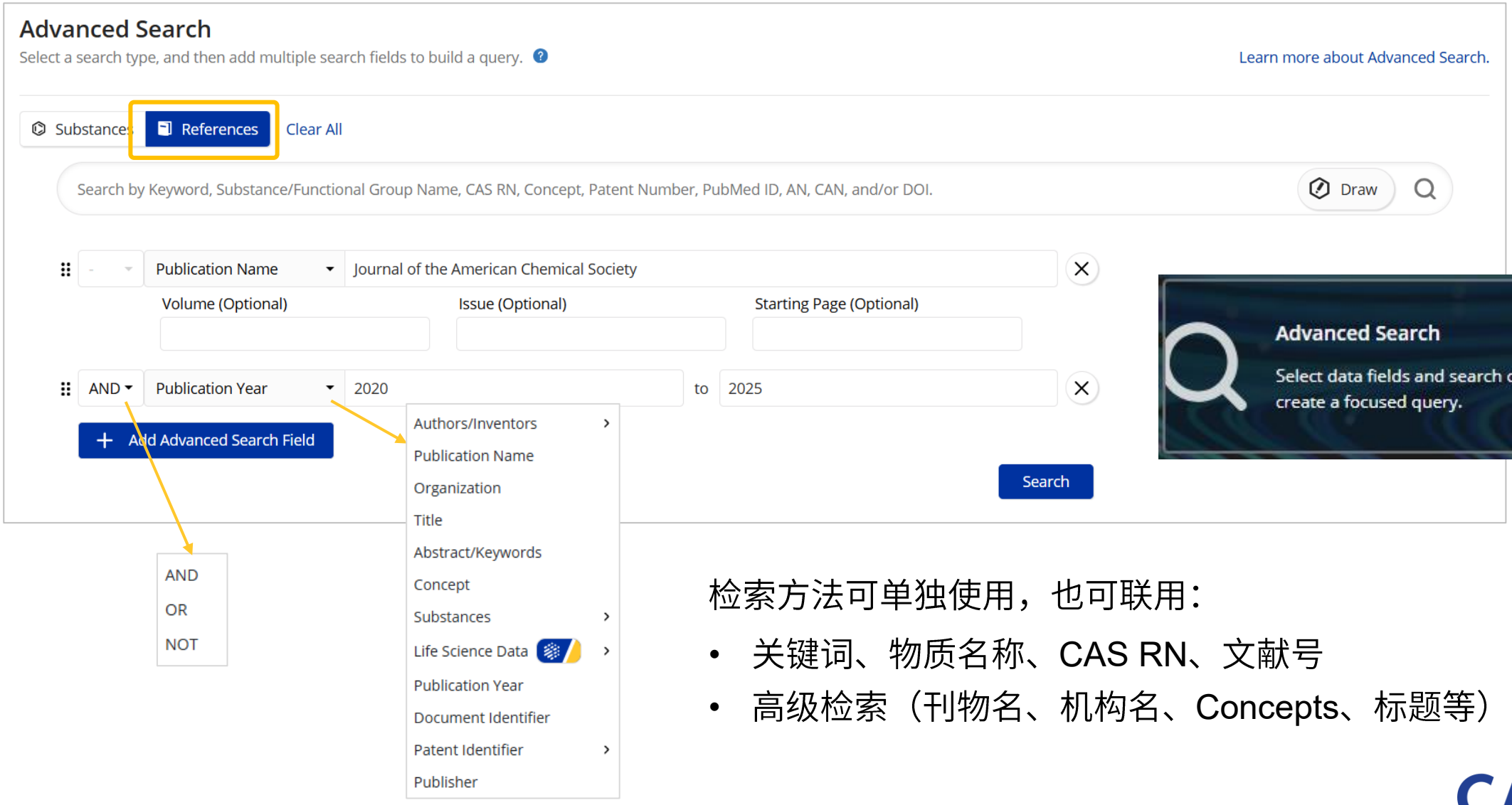
自定义组合检索



检索方法可单独使用，也可联用：

- 关键词、物质名称、CAS RN、文献号
- 高级检索（刊物名、机构名、Concepts、标题等）

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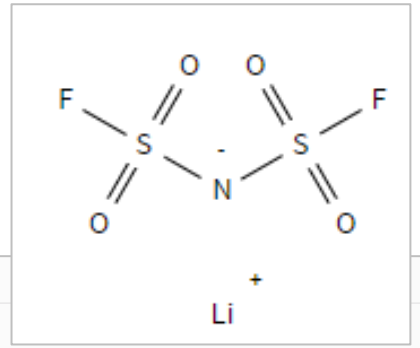
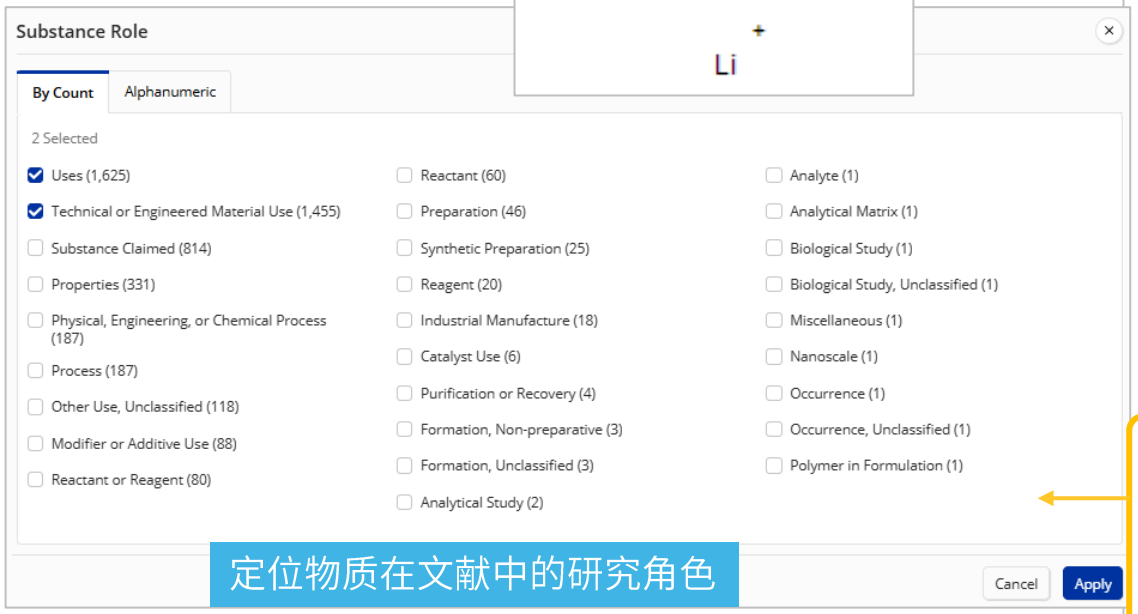
如何获得结构相关的文献?

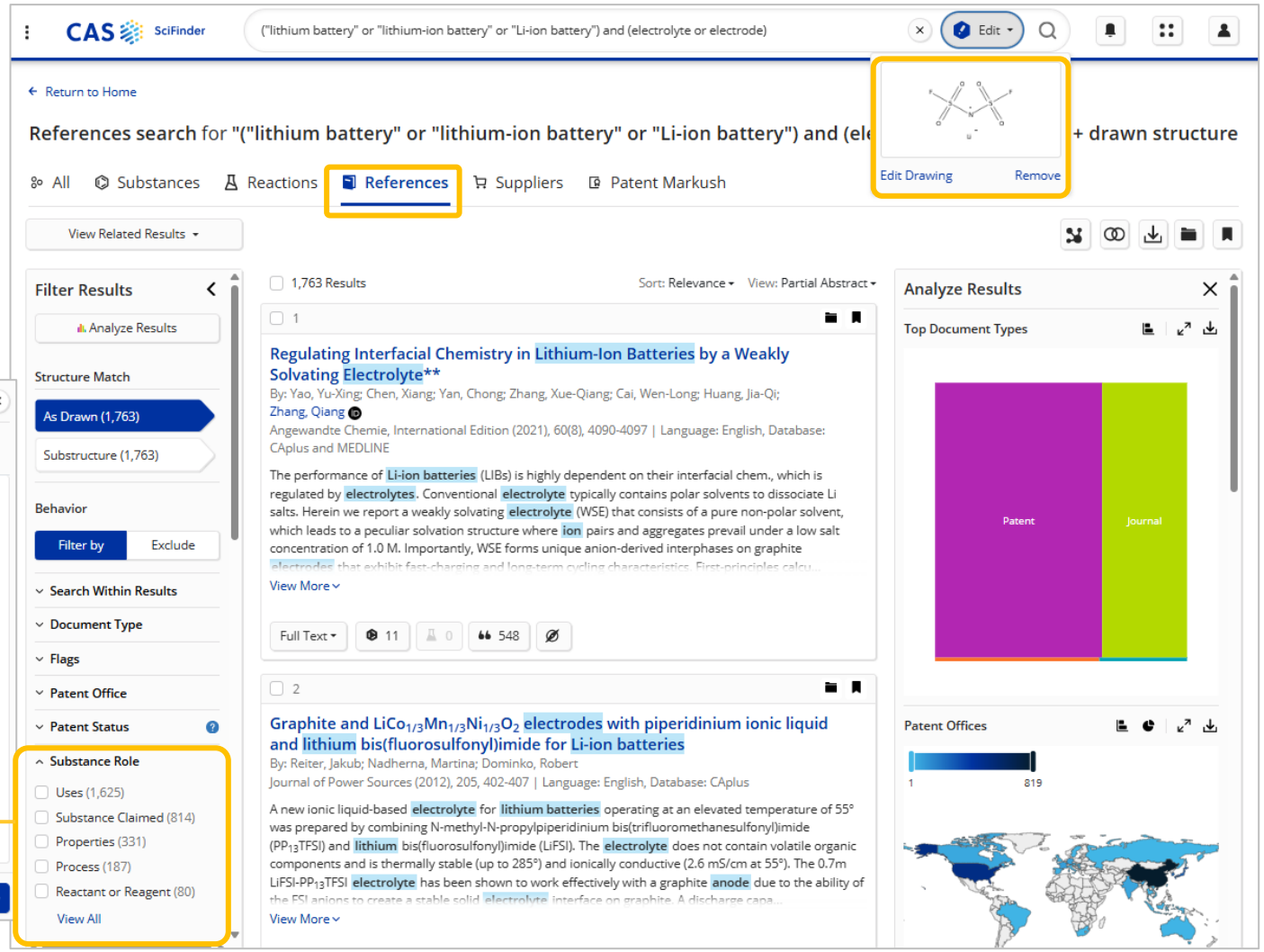
文本与结构是“and”关系

示例：关注锂电池技术中特定的热点材料
策略：从References出发，主题词+结构联用检索





定位物质在文献中的研究角色



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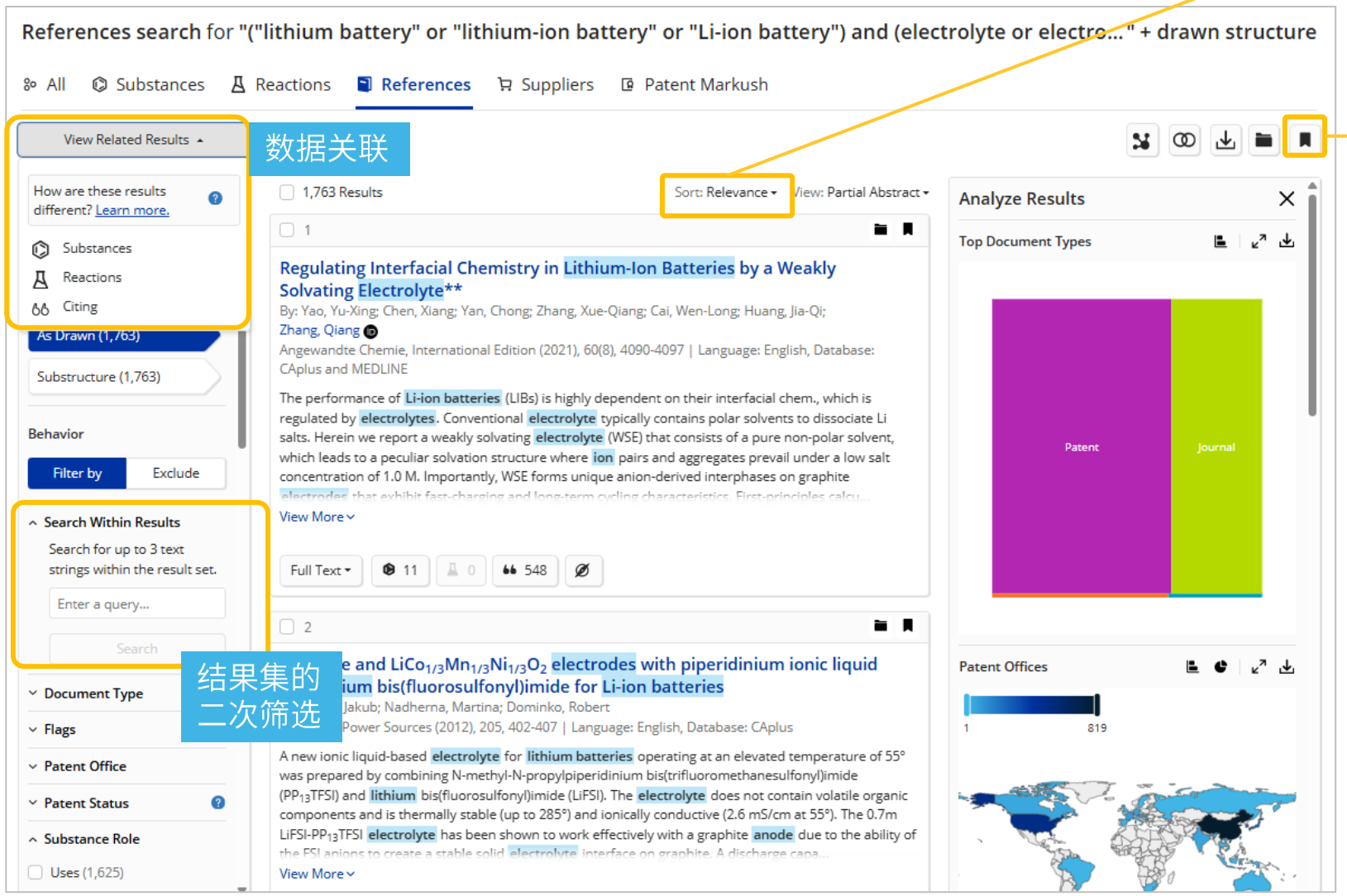
文献结果的筛选与定题追踪



排序方式

- Relevance
- Times Cited
- Accession Number: Ascending
- Accession Number: Descending
- Publication Date: Newest
- Publication Date: Oldest

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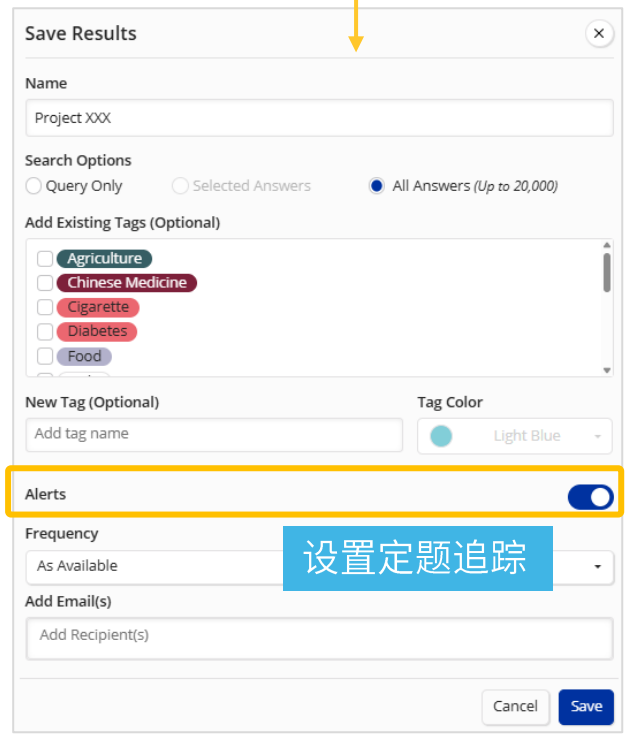
- Copy Search to Clipboard



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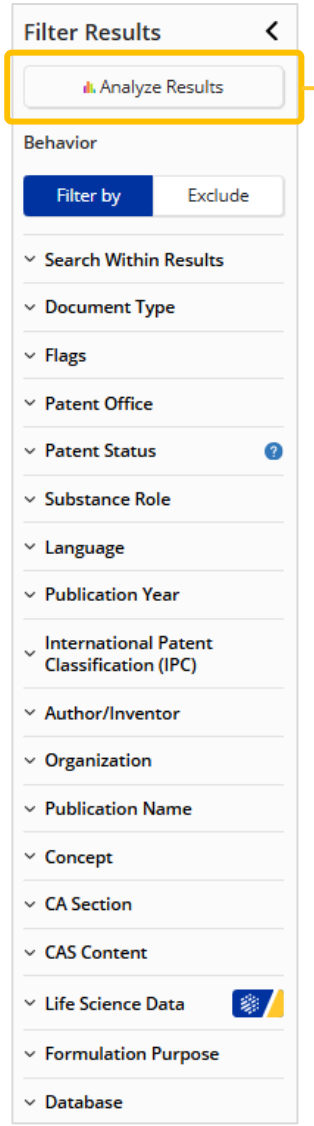
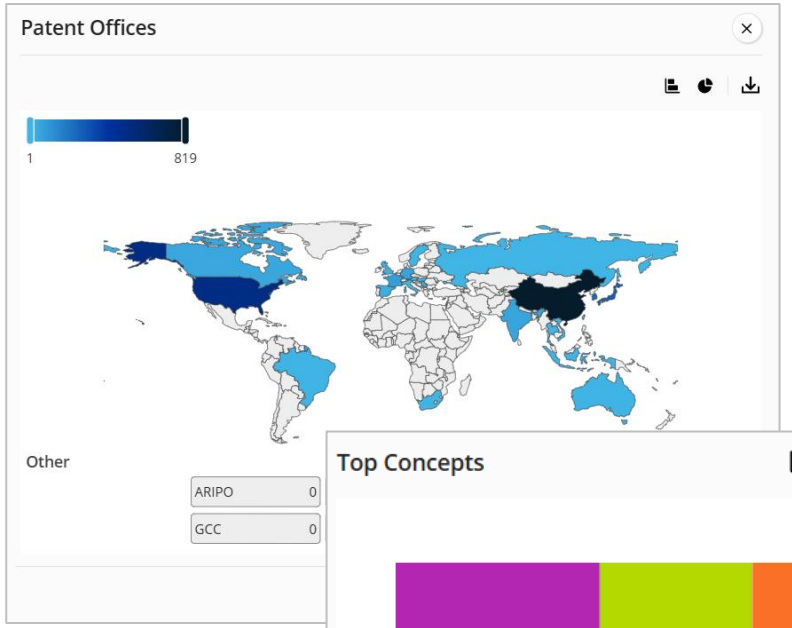
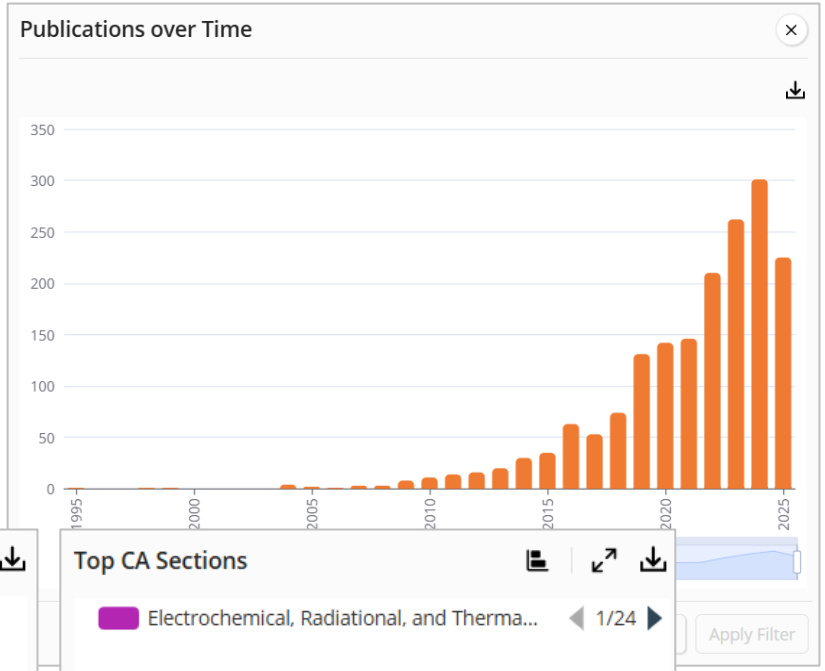
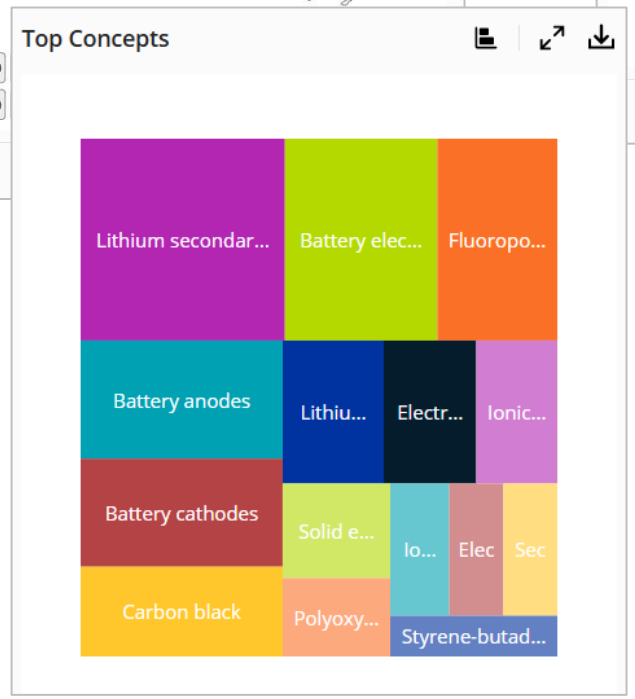
文献结果的筛选与可视化分析

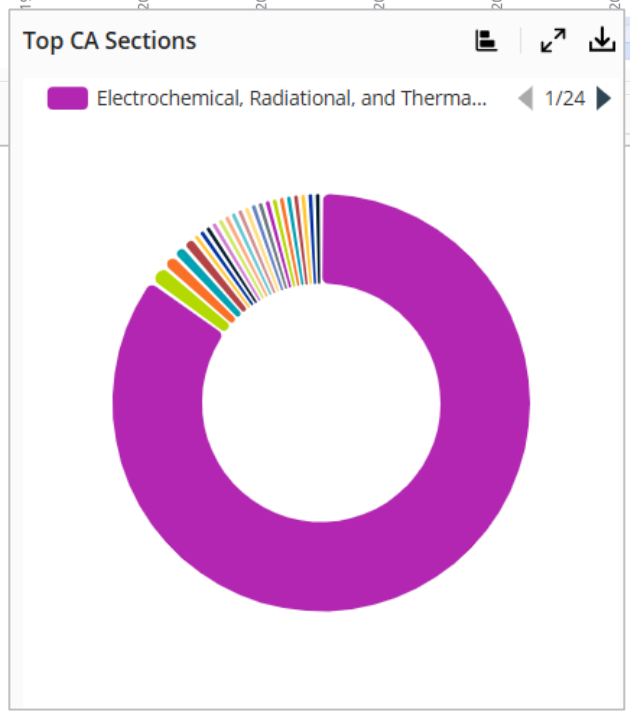






- 与筛选项联动的检索结果可视化分析
- 可自定义显示或隐藏





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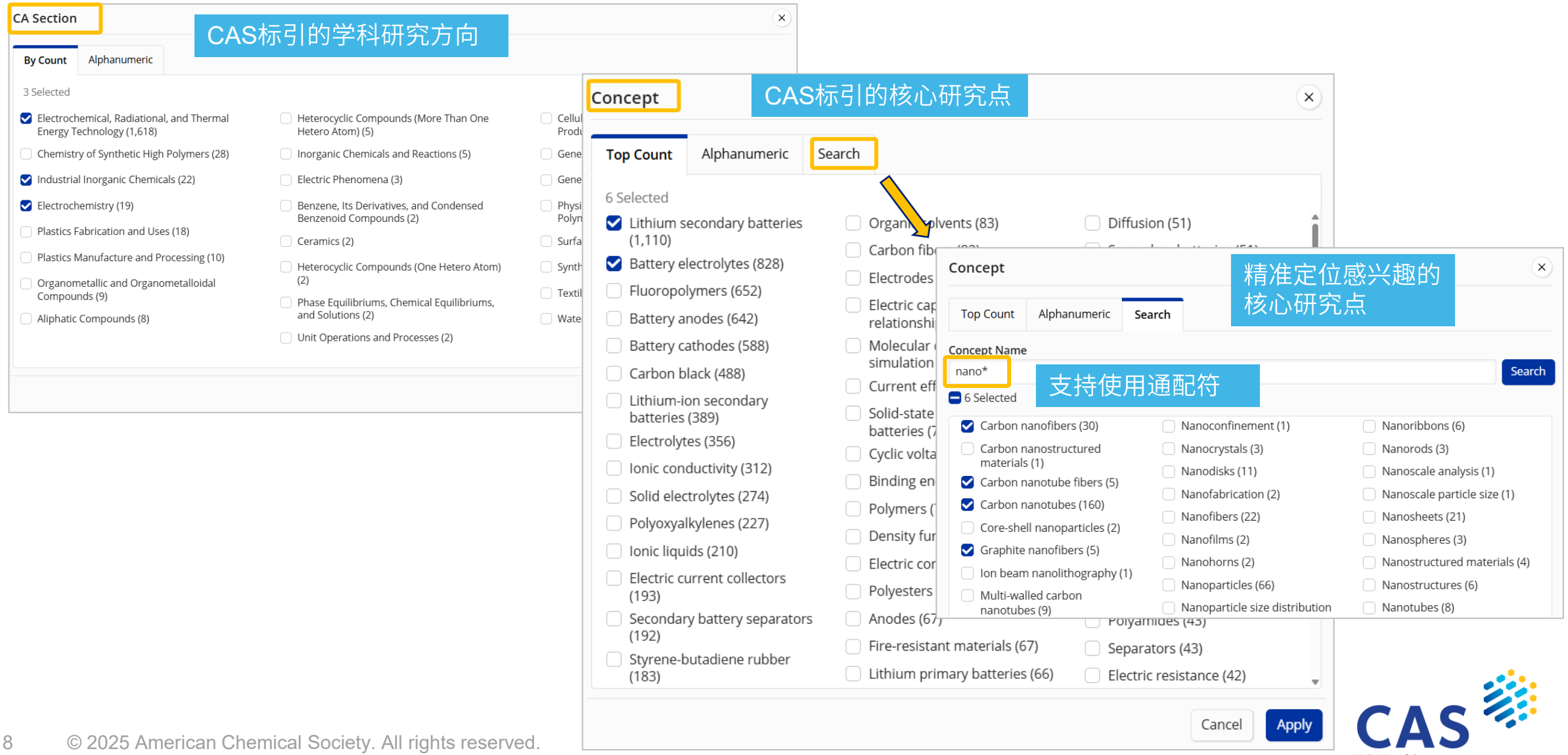
筛选工具 CA Section & Concept



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文献详情：通过CAS科学家的增值标引，快速概览重要信息

An In Situ Polymeric Electrolyte with Low Interfacial Resistance on Electrodes for Lithium-Ion Batteries

5 | 3 | 3 | Citation Map

In this Reference
- CAS Concepts
- Substances
- Reactions
- Cited Documents

导航速览

By: Jin, Lei; Jang, Giseok; Lim, Hyunmin; Zhang, Wei; Kim, Whangi; Jang, Hohyoun

DOI: 10.1002/admi.202101958

Due to their high energy d. and safety, polymer electrolytes are considered a promising alternative to the com. liquid electrolytes used in lithium-ion batteries (LIBs). However, in practical application, polymer electrolytes are limited by the high interface resistance between electrodes and electrolyte, leading to low ionic conductivity at room temperature (RT). In the present work, an in situ cationic ring-opening technique is introduced using LiFSI as an initiator to address the issue of interfacial contact between electrolyte and electrodes in LIBs. Herein, a series of in situ poly(siloxane-epoxy)-based polymer electrolytes (PSEPEs) are synthesized, which present good thermal stability (158°C), low glass transition temperature (T_g) (-42°C), high ionic conductivity of 1.16 x 10^{-4} S cm^{-1}, and good t_{Li+} of 0.61 at RT. The PSEPEs also show a wide electrochem. window (>4.7 V vs Li/Li+), and excellent compatibility with the lithium anode with an assembled $LiFePO_4$/ PSEPEs /Li cell. This work contributes to developing a new polymer electrolyte fabricated by in situ cationic polymerization, and its effects on the reduction of the interfacial resistance of electrodes-electrolyte.

Keywords: polysiloxane epoxy electrolyte lithium ion battery electrode thermal stability

View Source | Full Text

CAS Concepts

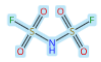
核心研究点

- Amorphous structure
- Battery anodes
- Battery cathodes
- Battery electrolytes

Substances

原文中重点研究的物质信息

171611-11-3



• Li

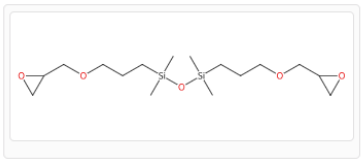
$F_2HNO_4S_2.Li$

Lithium bis(fluorosulfonyl)imide

Role: Technical or Engineered Material Use, Uses

物质研究角色

31305-85-8

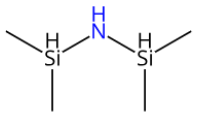


$(C_{16}H_{34}O_5Si_2)_x$

Disiloxane, 1,1,3,3-tetramethyl-1,3-bis[3-(2-oxiranylmethoxy)propyl]-, homopolym...

Role: Physical, Engineering or Chemical Process, Properties, Synthetic Preparation, Technical or Engineered Material Use, Process, Preparation, Uses

15933-59-2



$C_4H_{15}NSi_2$

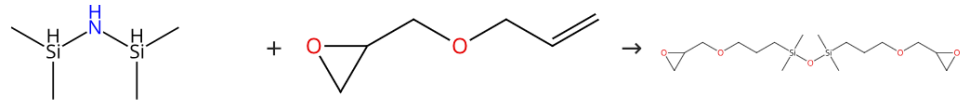
Tetramethyldisilazane

Role: Reactant, Reactant or Reagent

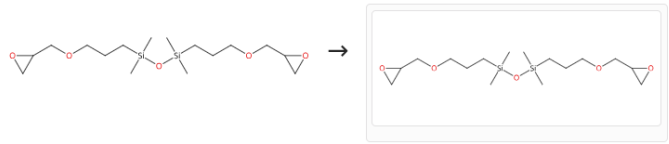
Reactions

涉及的反应

31-614-CAS-31042382



31-614-CAS-31042381



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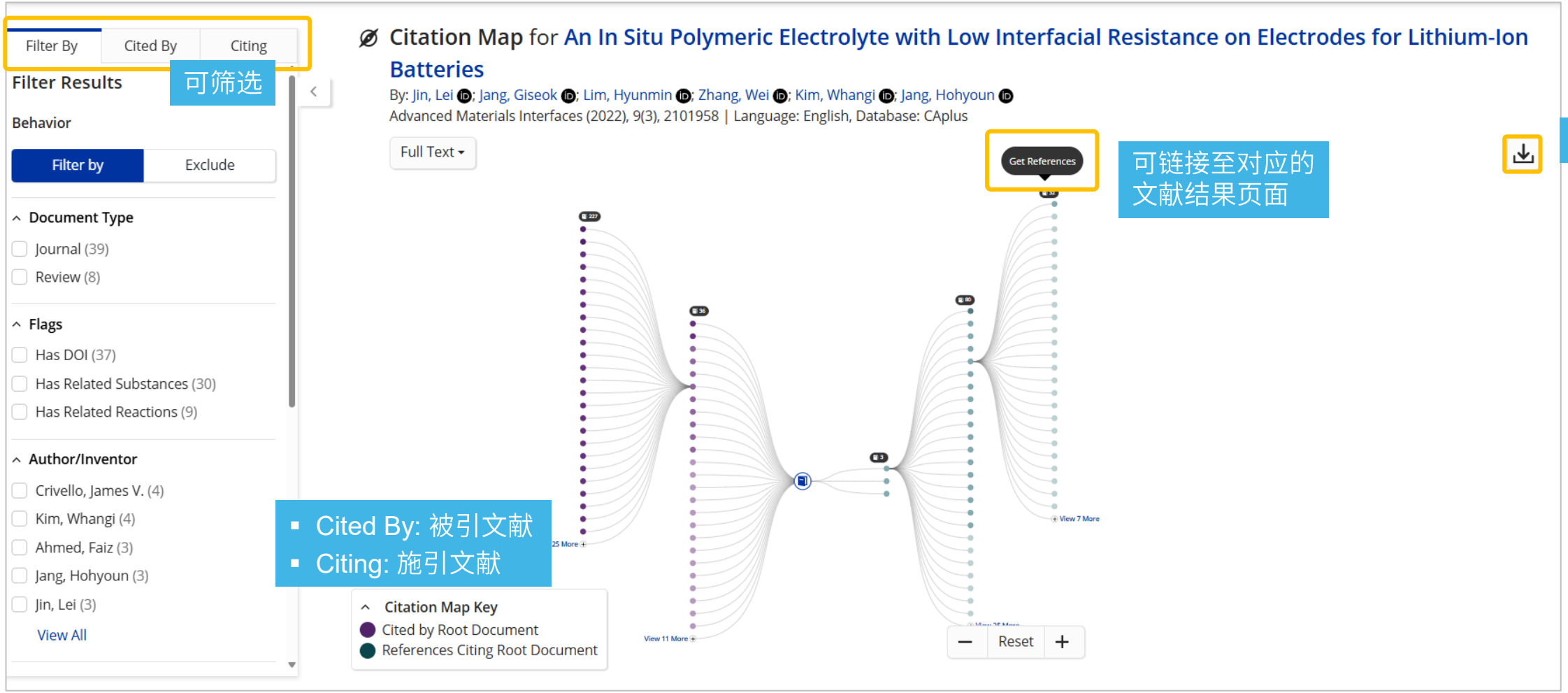
Citation Map



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深入专利文献详情

Claims

权利要求

Claims text may be based on automatic Optical Character Recognition processes.

1 What is claimed is:
A rechargeable lithium battery cell comprising an anode, a cathode, and a hybrid quasi-solid or solid-state electrolyte in ionic communication with the anode and the cathode, wherein:
the hybrid electrolyte, having a lithium ion conductivity from 10^{-5} S/cm to 5×10^{-2} S/cm, comprises a mixture of a polymer and an inorganic solid electrolyte;
the polymer is a polymerization or crosslinking product of a reactive additive, wherein the reactive additive comprises (i) a first liquid solvent that is polymerizable, (ii) an initiator or curing agent, and (iii) a lithium salt; wherein the first liquid solvent occupies from 1% to 99% by weight based on the total weight of the reactive additive;
the polymer is present in the anode, the cathode, the separator, an interface between the anode and the separator, and/or an interface between the cathode and the separator; and
the hybrid electrolyte forms a contiguous phase in the cathode or in the anode, and occupies from 3% to 40% by volume of the cathode or from 3% to 40% by volume of the anode.

2 The rechargeable lithium cell of claim 1 , wherein the inorganic solid electrolyte material is selected from an oxide type, sulfide type, hydride type, halide type, borate type, phosphate type, lithium phosphorus oxynitride (LiPON), garnet-type, lithium superionic conductor (LISICON) type, sodium superionic conductor (NASICON) type, or a combination thereof.

3 The rechargeable lithium cell of claim 1 , wherein the first liquid solvent is selected from the group consisting of vinylene carbonate, ethylene carbonate, fluoroethylene carbonate, ethylene glycol phenyl ether acrylate) (PEGPEA), ethoxylated trimethyl propyl triacrylate (ETPTA), tetrahydrofuran (THF), vinyl sulfite, vinyl ethylene sulfite, vinyl ethylene carbonate, 1,3-propyl sultone, 1,3,5-trioxane (TXE), 1,3-acrylic-sultones, methyl ethylene sulfone, methyl vinyl sulfone, ethyl vinyl sulfone, methyl methacrylate, vinyl acetate, acrylamide, 1,3-dioxolane (DOL), fluorinated ethers, fluorinated esters, sulfones, sulfides, dinitriles, acrylonitrile (AN), sulfates, siloxanes, silanes, N-methylacetamide, acrylates, ethylene glycols, phosphates, phosphonates, phosphinates, phosphines, phosphine oxides, phosphonic acids, phosphorous acid, phosphites, phosphoric acids, phosphazene compounds, derivatives thereof, and combinations thereof.

Patent Family

专利家族

专利状态

Patent	Language	Full Text	Publication Date	Application Number	Application Date	Patent Status	Status Date
US20230096724 A1	English	PatentPak PDF	2023-03-30	US2021-17410282	2021-08-24	Alive	2023-04-06
US12272791 B2	English	PatentPak PDF	2025-04-08	US2021-17410282	2021-08-24	Alive	2023-04-06
WO2023028514 A1	English	PatentPak PDF	2023-03-02	WO2022-US75385	2022-08-23	Alive	2023-03-09

Keywords: flame resistant solid state composite electrolyte lithium ion battery

PatentPak | Get Prior Art Analysis | Full Text

Classifications

分类信息

Patent	Classification	Codes
US20230096724 A1	IPCI	H01M 10/0569; H01M 10/0525
	CPCI	H01M 10/0569; H01M 10/0525; H01M 2300/0028
US12272791 B2	IPCI	H01M 4/62; H01M 10/0525; H01M 10/0569
	CPCI	H01M 10/0569; H01M 10/0525; H01M 2300/0028
WO2023028514 A1	IPCI	H01M 10/056; H01M 10/42; H01M 4/62; H01M 10/052; H01M 12/08

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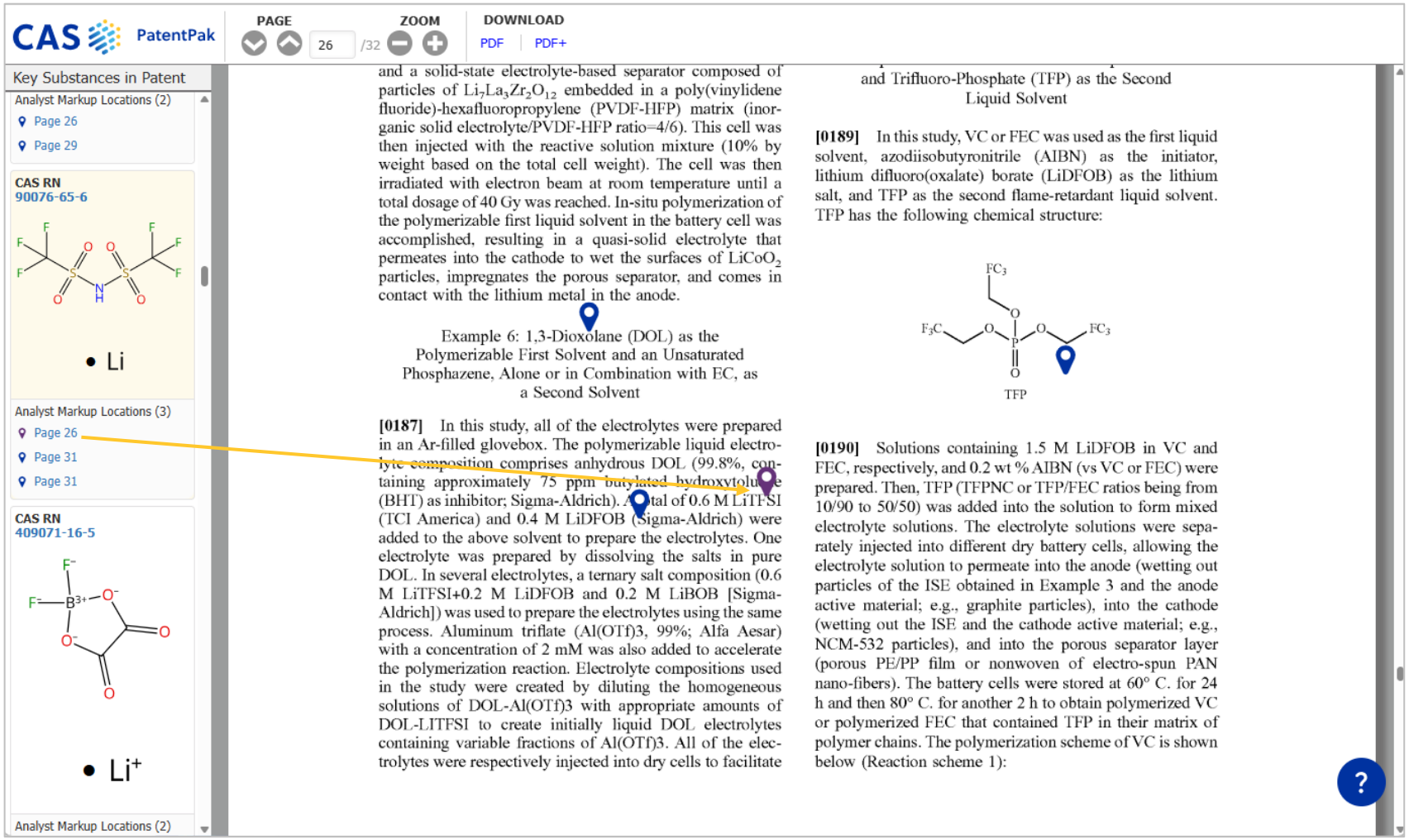
CAS PatentPak：高效浏览专利

一键定位专利原文中的核心研究物质



CAS PatentPak：

- 快速理解专利
- 一键下载原文
- 快速定位专利中的物质
- 阅读其他语言撰写的等同专利

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AI+科学家训练的模型，提升现有技术分析效率和精度

基于指定信息的现有技术探索

支持文本+结构检索，使结果更精准

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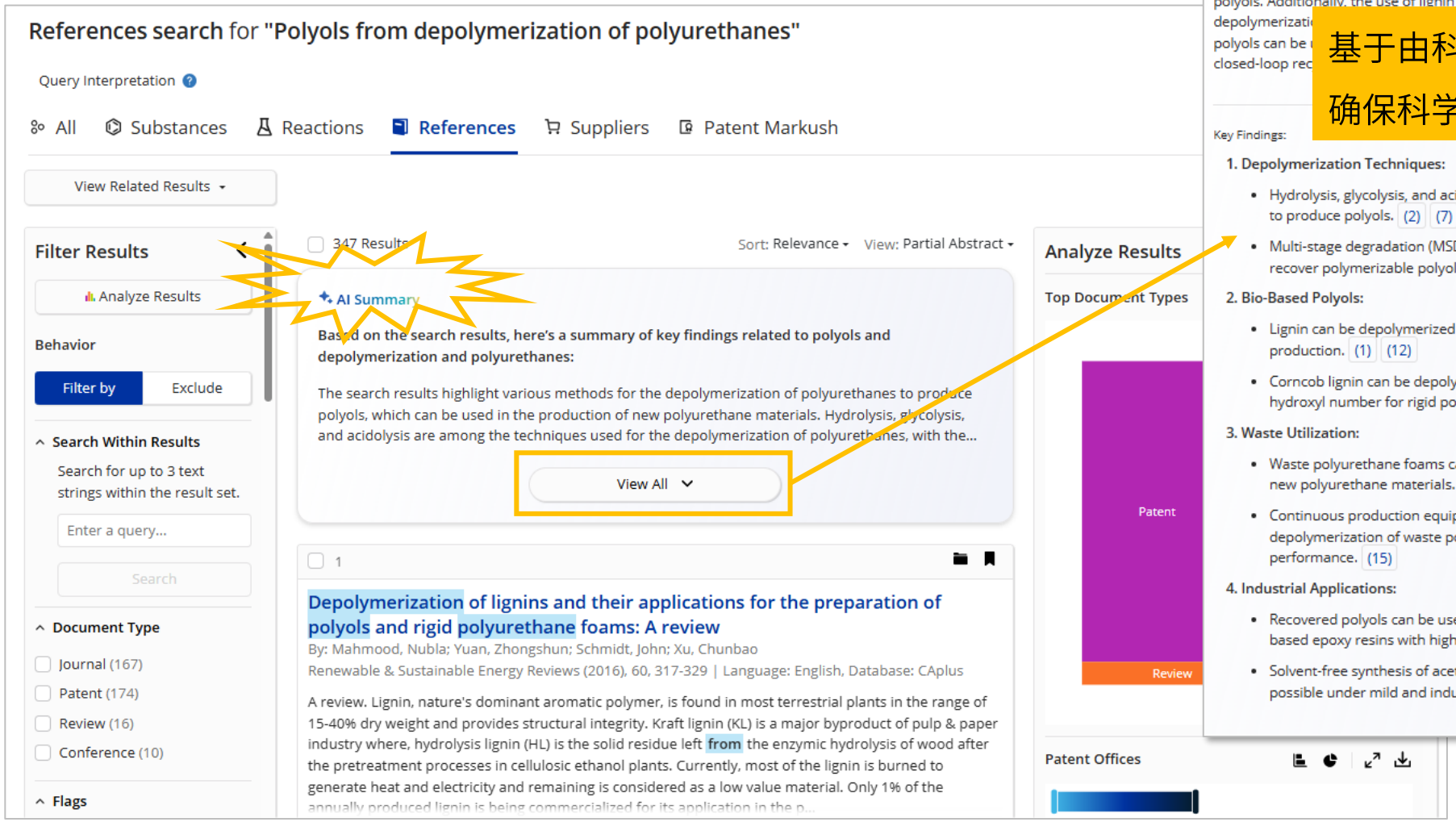
AI赋能自然语言便捷获取文献检索结果总结，快速掌握关键发现



基于由科学家训练的AI模型生成的总结，确保科学准确性并提供可追溯的引用来源

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小结

1. 检索主题的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符等工具灵活构建检索主题，利用高级检索选项进行自定义组合检索。
2. 主题词+结构联合检索，快速获得文献。
3. 利用多维的筛选工具，如Concept、CA Section等快速缩小范围，锁定目标文献。
4. 检索结果趋势分析、引文地图。
5. 文献详情中可快速获取关键信息，CAS PatentPak浏览专利详情。

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大纲

CAS及CAS SciFinder Discovery Platform 简介

科研信息的高效查阅

- 全面的文献调研与拓展助力开题
- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

常见问题Q&A

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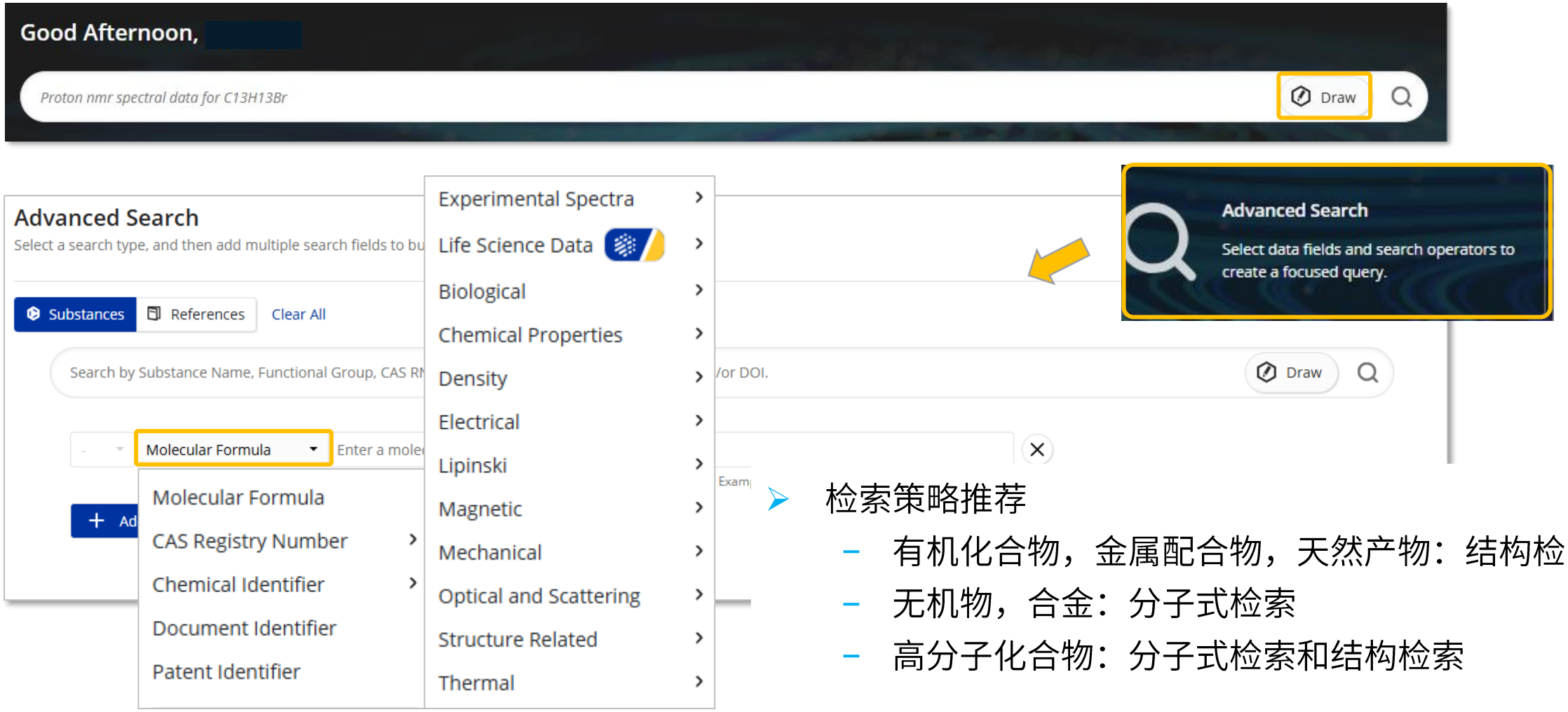
灵活的检索方式，满足各种物质类别的检索



- 检索策略推荐
  - 有机化合物，金属配合物，天然产物：结构检索
  - 无机物，合金：分子式检索
  - 高分子化合物：分子式检索和结构检索

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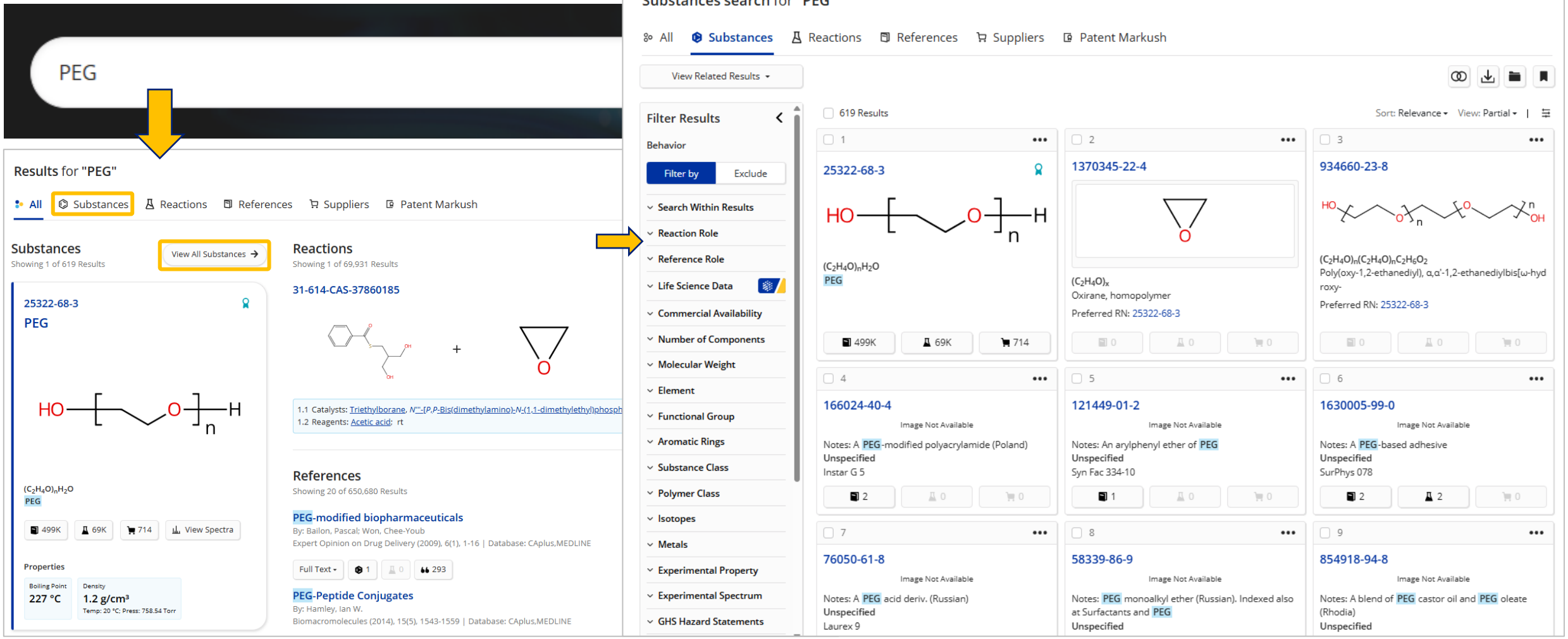
物质检索—物质标识符



- 可同时检索多个物质识别符（物质名称或CAS RN）
- 不同物质使用空格隔开（<2000个字符

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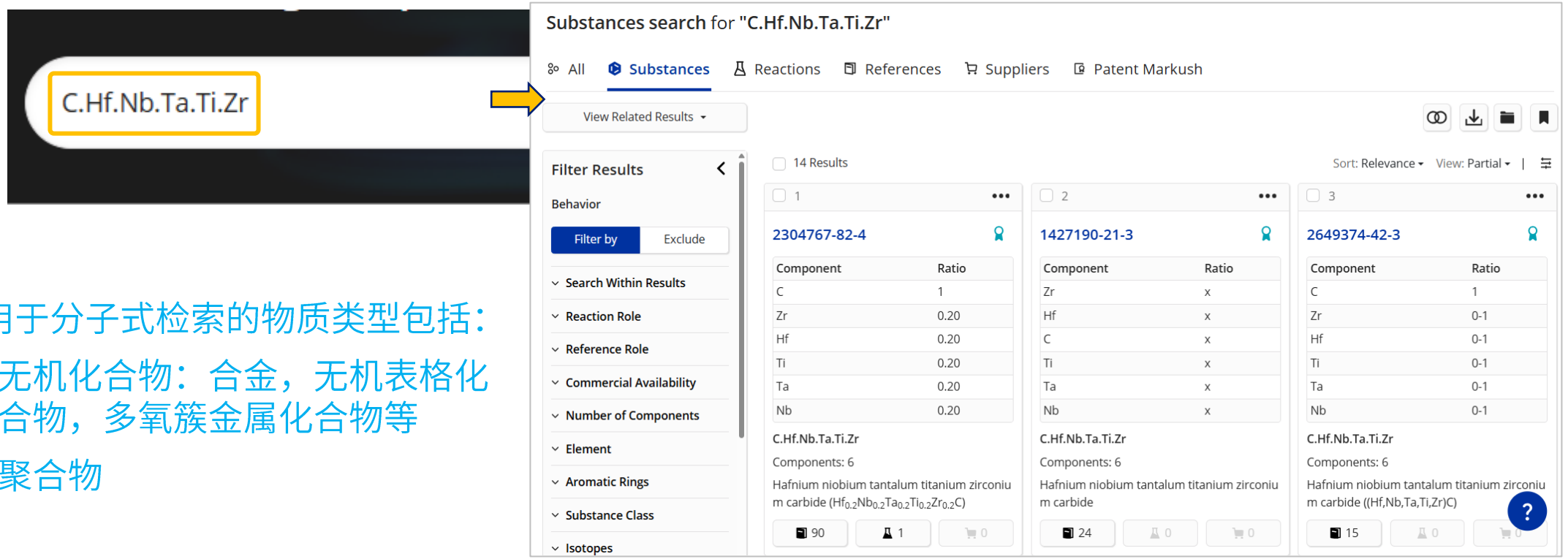
分子式检索：高效检索聚合物或无机化合物

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物 ，按照元素符号的首字母顺序进行排列
- 不同组分之间用 “.”隔开，如：高熵碳化物 C.Hf.Nb.Ta.Ti.Zr
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性　Na2SO4：H2O4S.2Na



适用于分子式检索的物质类型包括：

- 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
- 聚合物

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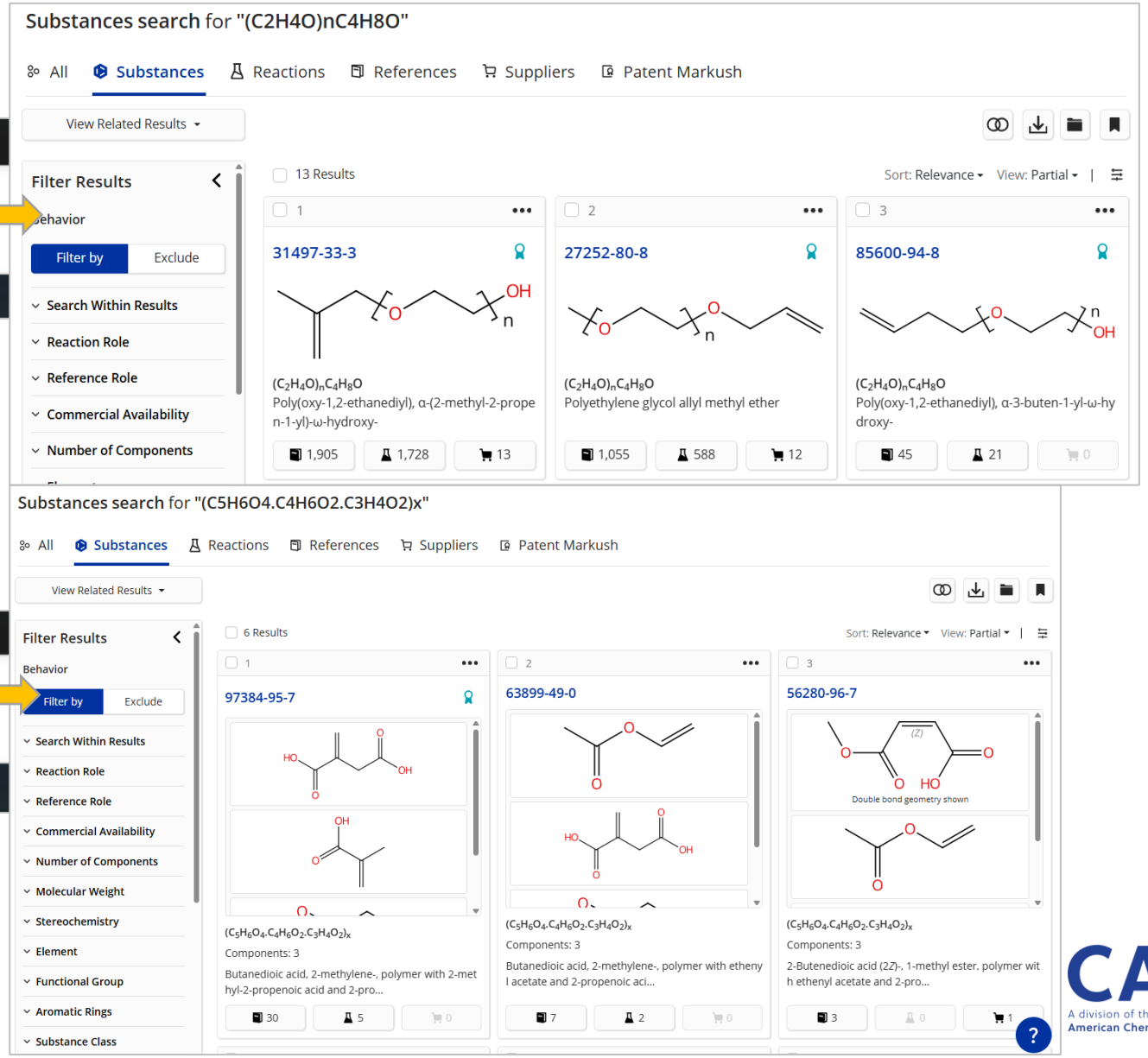
分子式检索：高效检索聚合物或无机化合物

(C2H4O)nC4H8O

- (C2H4O)nC4H8O: 括号中是重复结构单元，括号外为n
- (C5H6O4.C4H6O2.C3H4O2)x：括号中是单体，括号外为x

(C5H6O4.C4H6O2.C3H4O2)x



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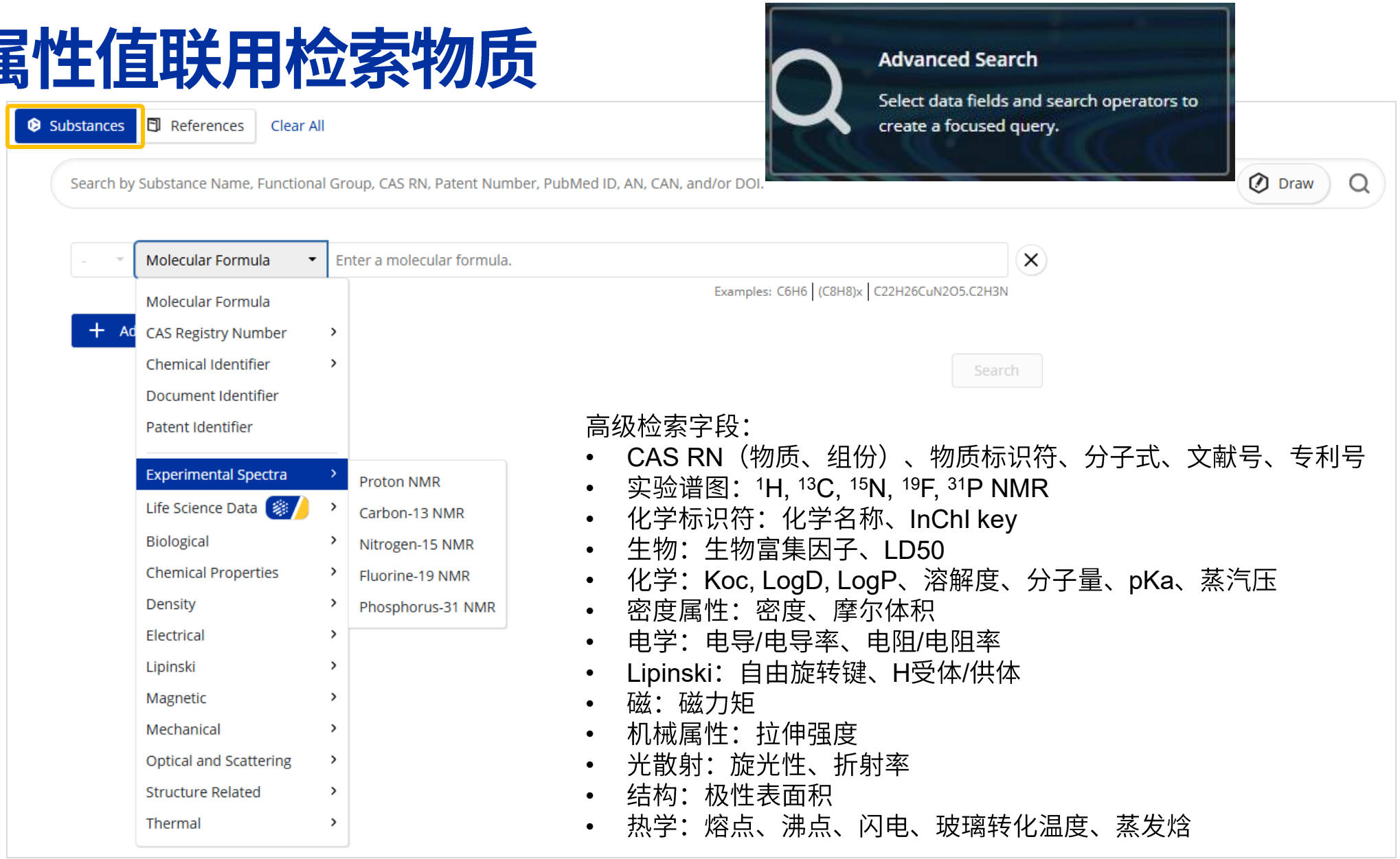
属性值联用检索物质



高级检索字段：

- CAS RN（物质、组份）、物质标识符、分子式、文献号、专利号
- 实验谱图：^{1}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P NMR
- 化学标识符：化学名称、InChI key
- 生物：生物富集因子、LD50
- 化学：Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压
- 密度属性：密度、摩尔体积
- 电学：电导/电导率、电阻/电阻率
- Lipinski：自由旋转键、H受体/供体
- 磁：磁力矩
- 机械属性：拉伸强度
- 光散射：旋光性、折射率
- 结构：极性表面积
- 热学：熔点、沸点、闪电、玻璃转化温度、蒸发焓

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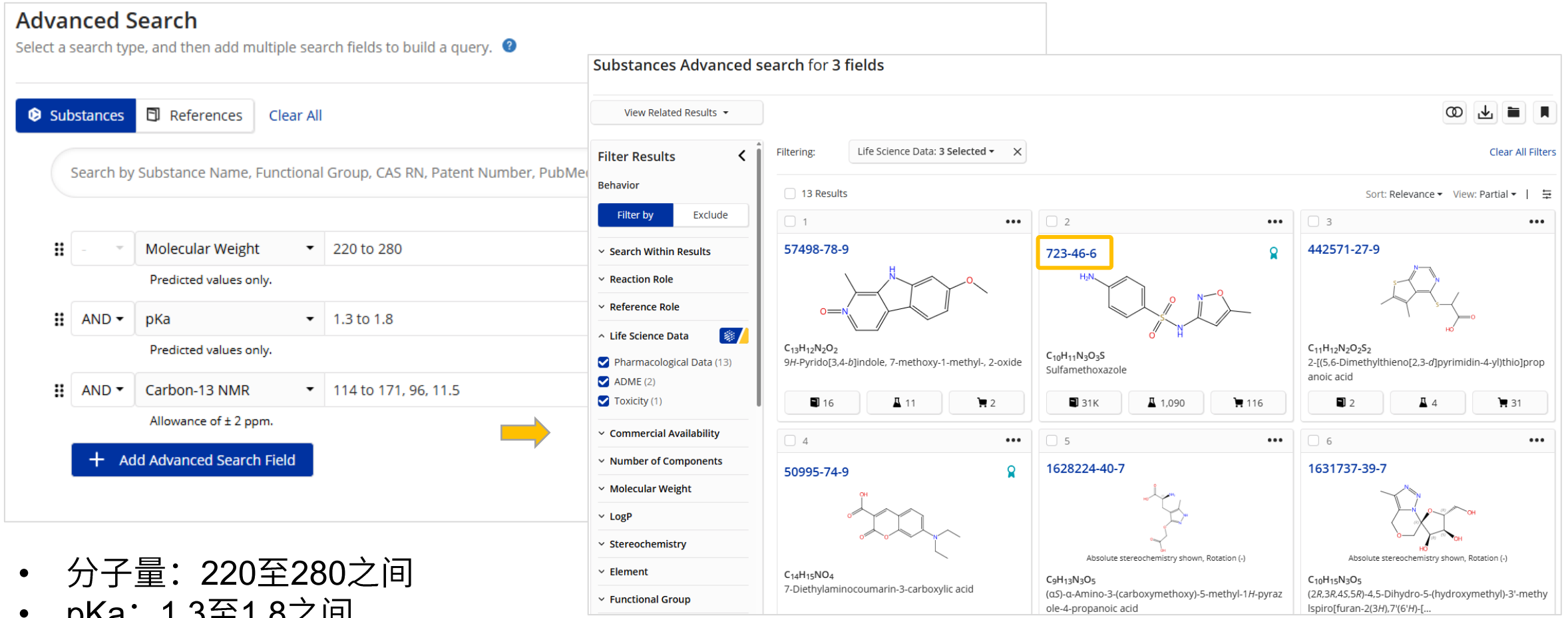
属性值、谱图数据联用检索物质



- 分子量：220至280之间
- pKa：1.3至1.8之间
- C谱特征峰：114至171之间，96，11.5

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物质的详情页

CAS Registry Number: 723-46-6

31K | 1,079 | 123 | View in CAS BioFinder

该物质被专利Claims保护的系列专利信息

Patents Claimed In

Triazine desulfurizer containing triazine methoxazole and tetracarboxylic acid oxazolide used for desulfurization of crude oil
Role: Reactant
Patent Number: CN120349810
Publication Date: 2025-07-22

Method for co-treating organic wastewater using peroxymonosulfate and peroxydisulfate
Role: Pollutant
Patent Number: CN120349021
Publication Date: 2025-07-22

External antibacterial liquid containing sulfamethoxazole, alcohol and water
Role: Therapeutic Use
CN120305271
2025-07-15

View All Pate

$C_{10}H_{11}N_3O_3S$

Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isox

Properties	Condition
Molecular Weight	-
Melting Point (Experimental)	-
Boiling Point (Predicted)	Press: 760.00 Torr
Density (Experimental)	
pKa (Experimental)	

Experimental Properties | Spectra

- Other Names and Identifiers
- Experimental Properties 实验属性
- Experimental Spectra 实验谱图
- Pharmacological Data
- ADME
- Toxicity
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements GHS危害信息
- Additional Details

723-46-6

$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

Working Frequency
400 MHz

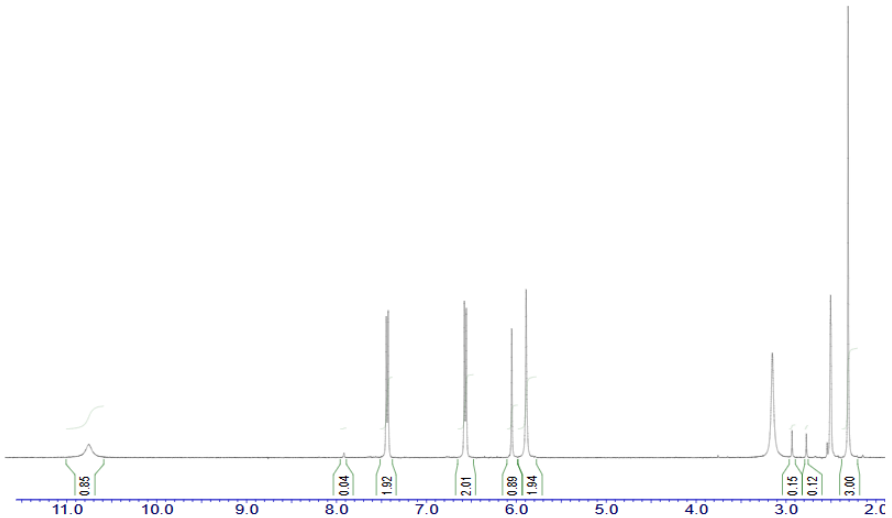
Solvent
Dimethyl sulfoxide (67-68-5)
Carbon tetrachloride (56-23-5)

Temperature
20 °C

Spectrum Summary

Spectrum ID
F0175-0013

Source
Spectral data were obtained from Life Chemicals



Reset

Experimental Spectra

^{1}H NMR | ^{13}C NMR | Hetero NMR

	Solvent	Source
View Proton NMR Spectrum (Image Available)	Dimethyl sulfoxide; Carbon tetrachloride	(1) LC
View Proton NMR Spectrum (Image Available)	-	(2) ENAMINE
View Proton NMR Spectrum (Image Available)	-	(2) ENAMINE
View Proton NMR Spectrum (Image Available)	-	(3) BIORAD
View Proton NMR Spectrum (Image Available)	Chloroform-*d*; DMSO-d_6 (1:1)	(3) BIORAD

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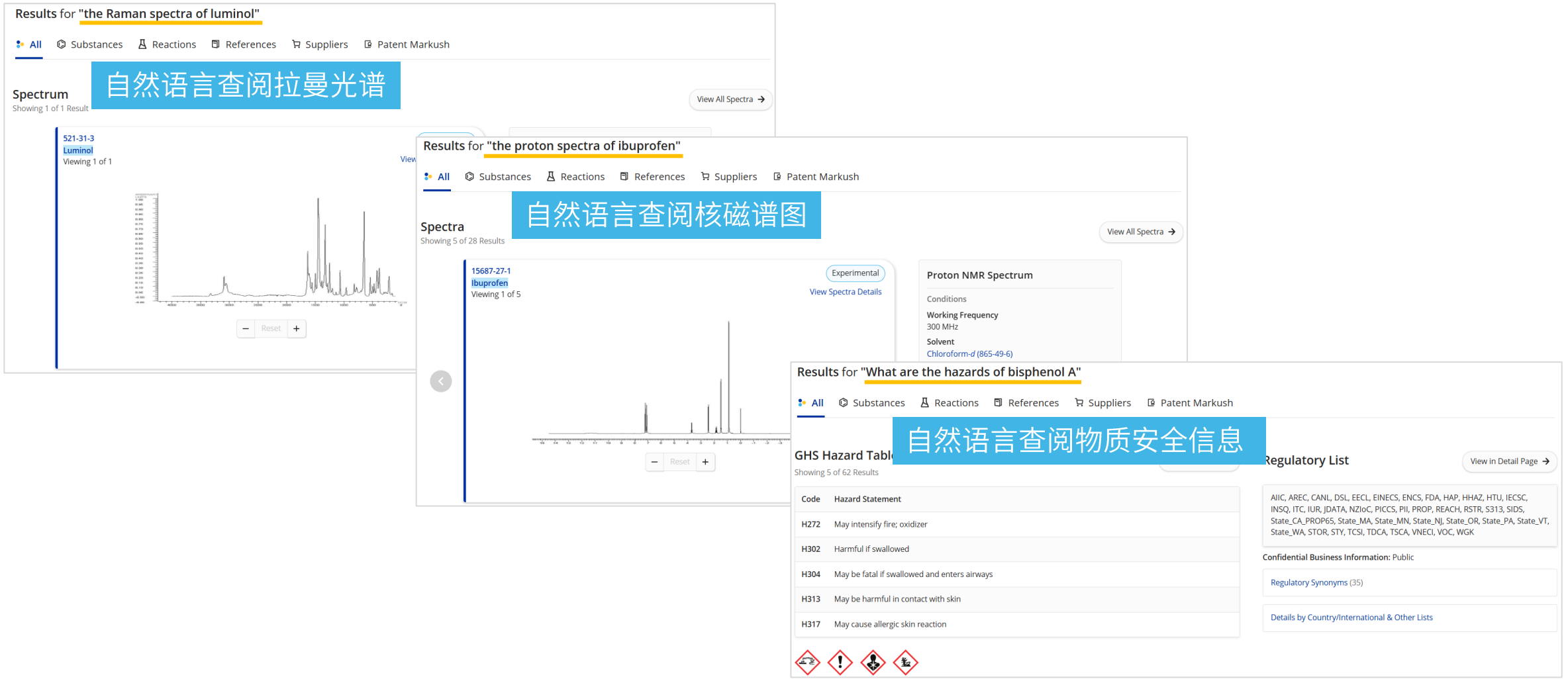
扩展问答类型，快速聚焦物质谱图和安全信息



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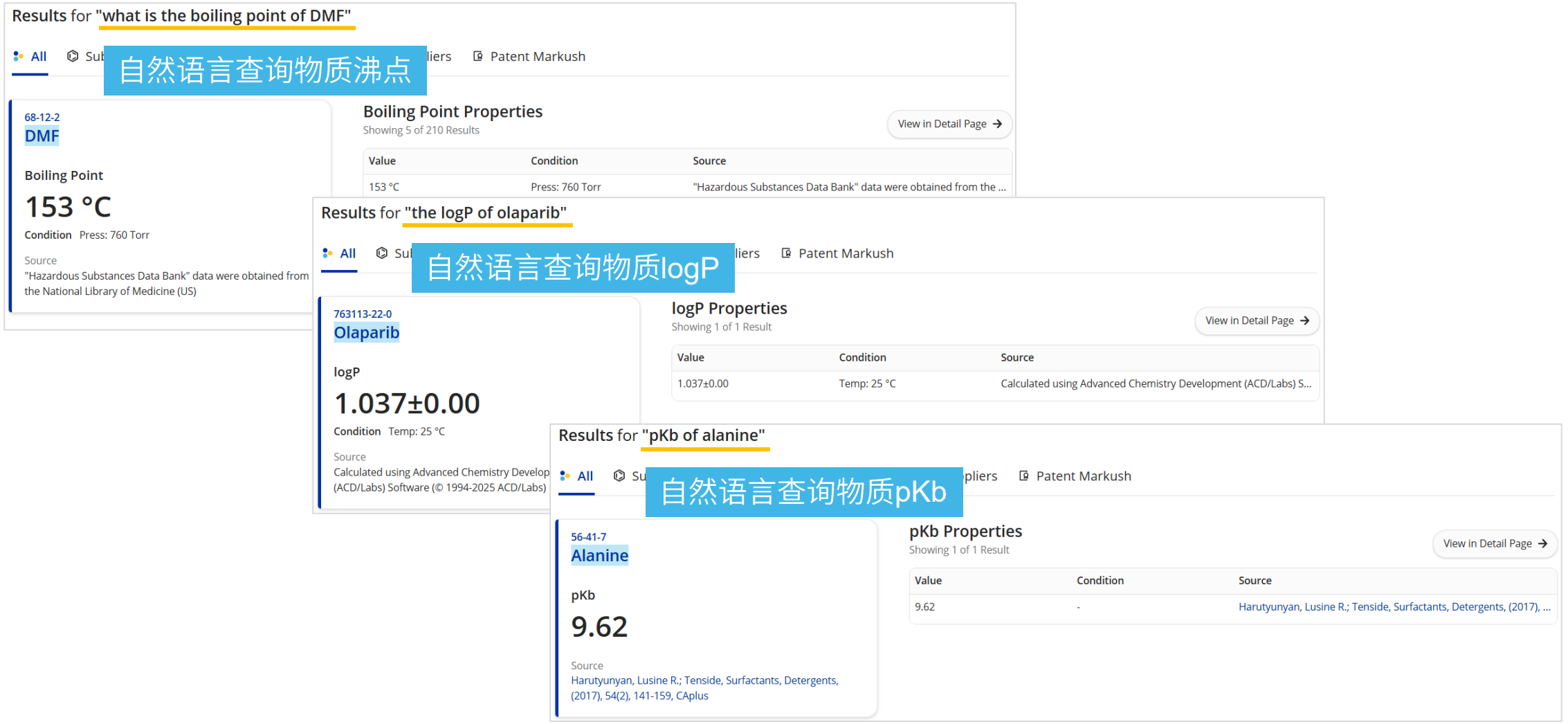
支持自然语言直接检索物质理化性质，直观高效



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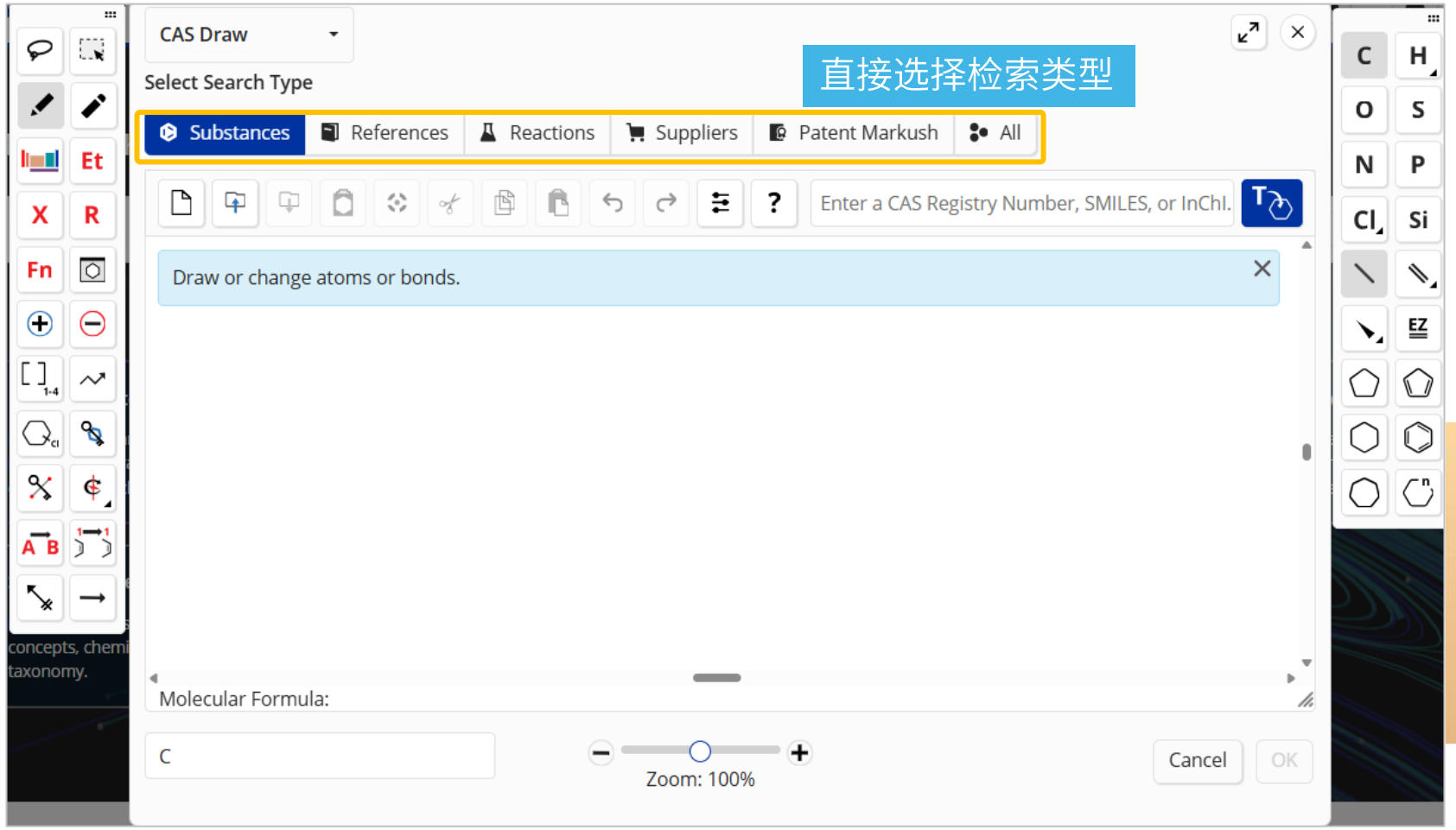
物质检索—CAS Draw：结构绘制面板

- 选择可变基团
- 自定义R基团
- 片段结构
- 重复工具
- 取代位置可变
- 环锁定工具
- 原子锁定工具



线上学习短视频：

CAS 美国化学文摘社

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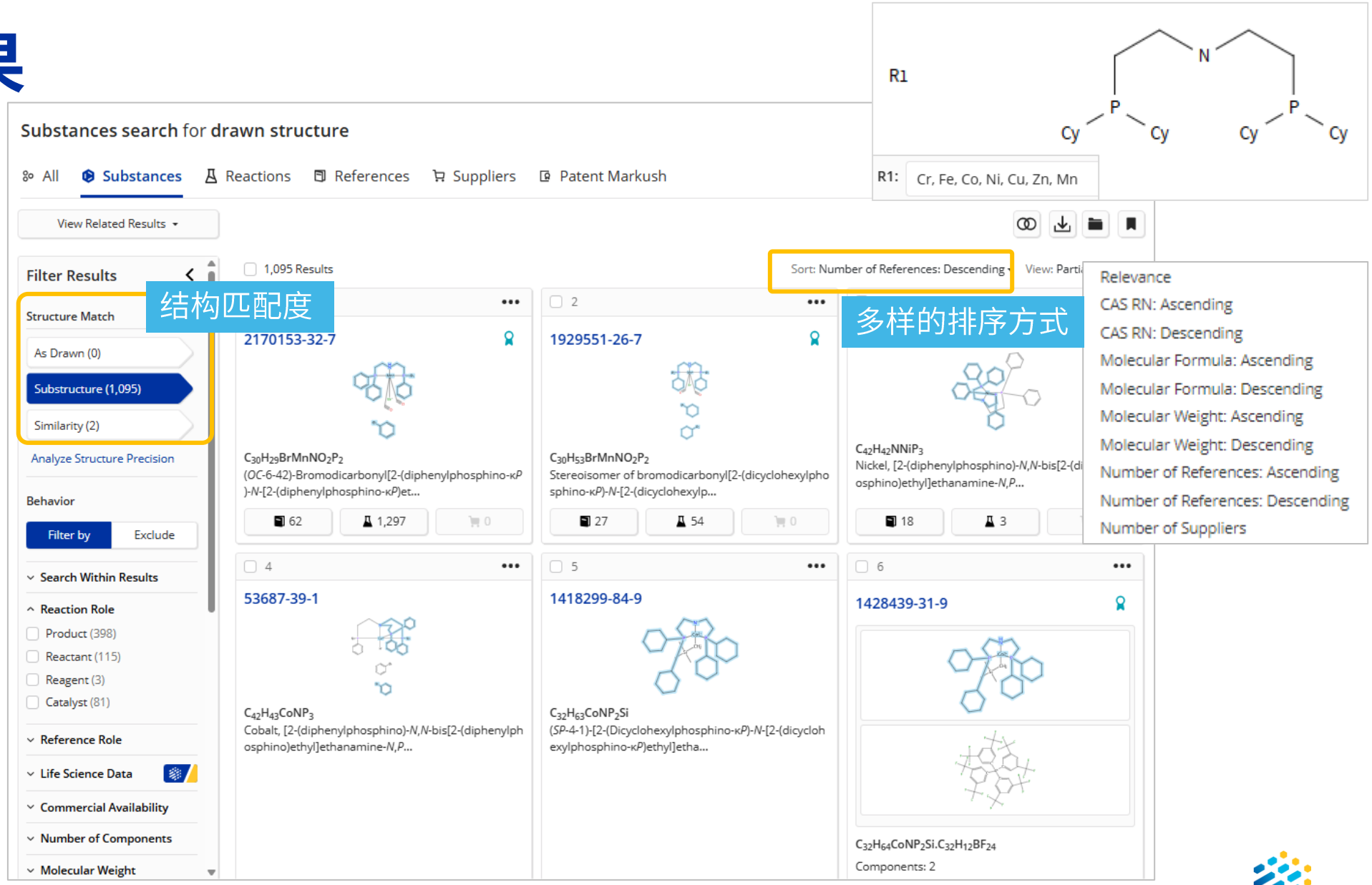
结构检索结果

结构检索类别：

- As Drawn：可变结构可变，其他位点锁环锁原子。
- Substructure 亚结构：包含As Drawn结果，有取代基。
- Similarity 相似结构：母体结构可以被取代，也可以被改变的相似结果。



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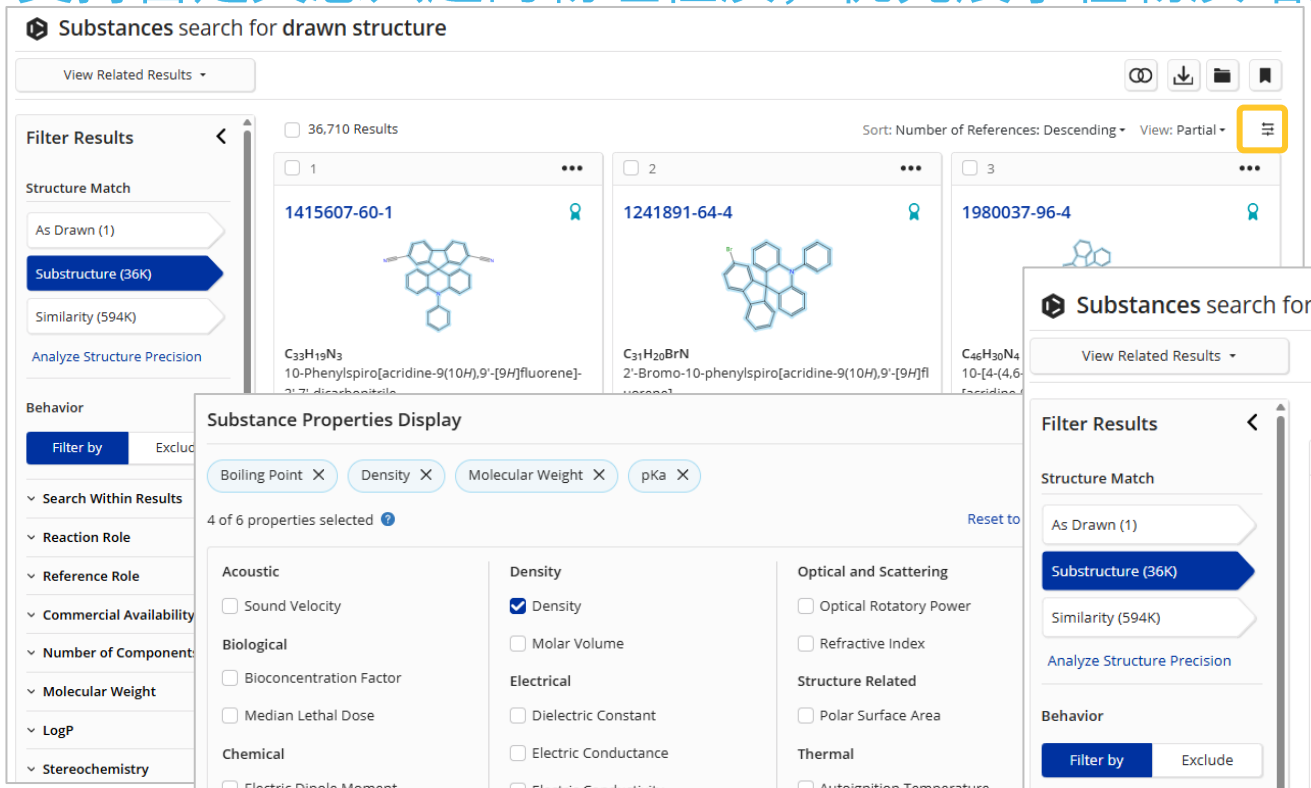
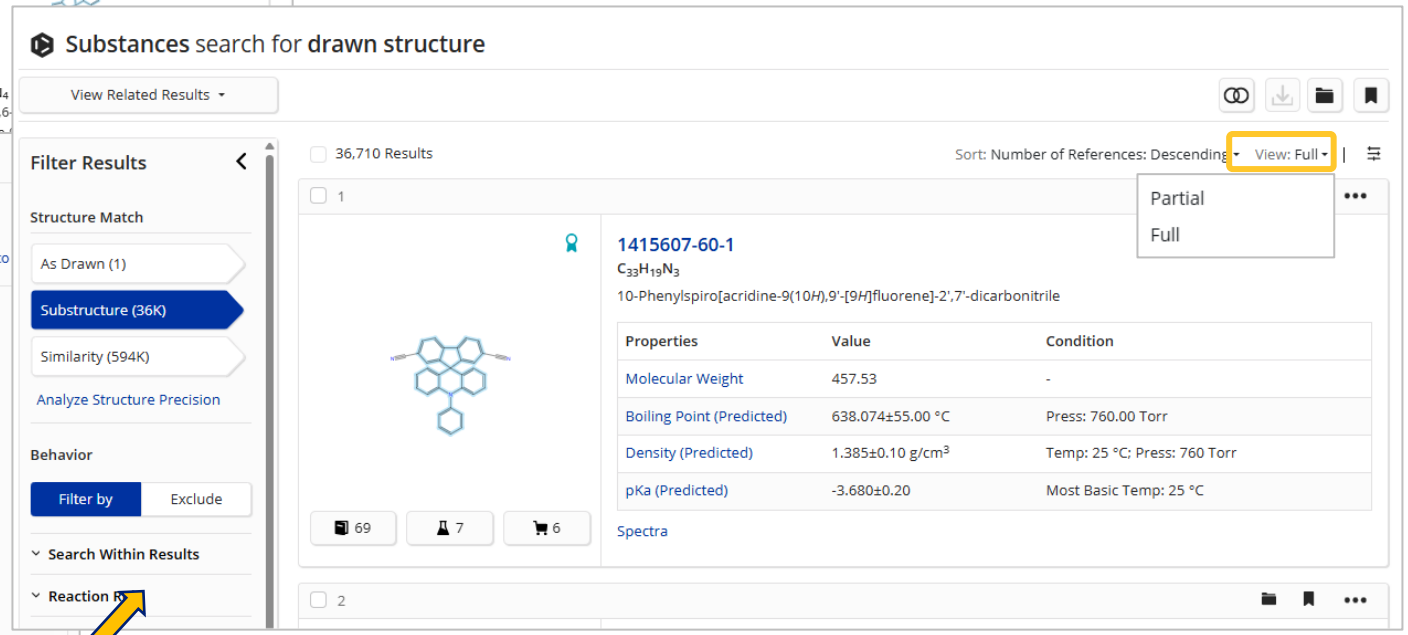
自定义关键物理性质的优先展示

支持自定义感兴趣的物理性质，优先展示在物质结果集上





可以选取最多六个性质在物质结果上显示

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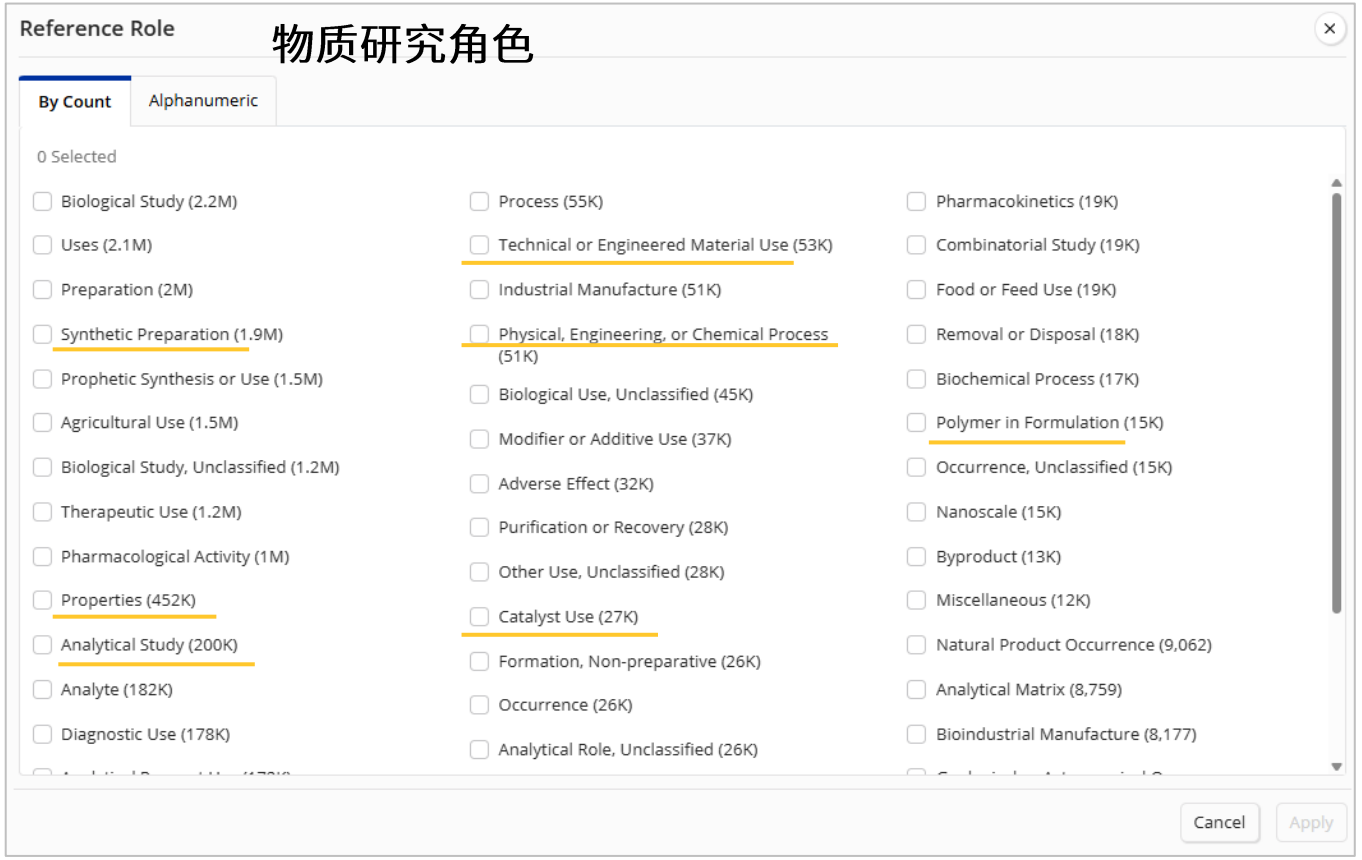
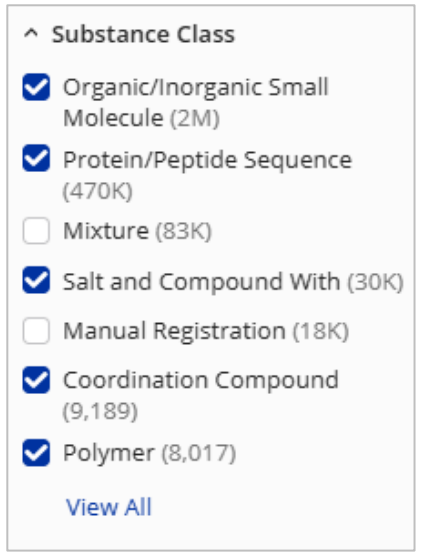
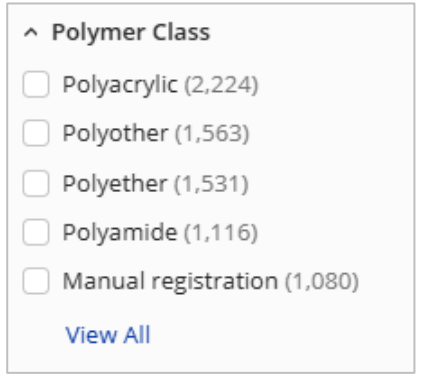
快速筛选物质结果集，助力聚焦领域核心技术



物质类别

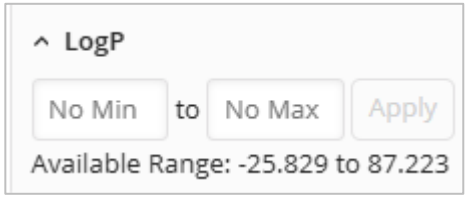


聚合物类别



芳环数量

官能团



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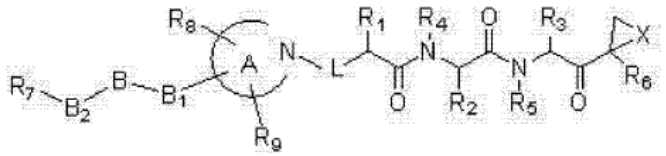
CAS Markush检索，助力结构查新

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



I

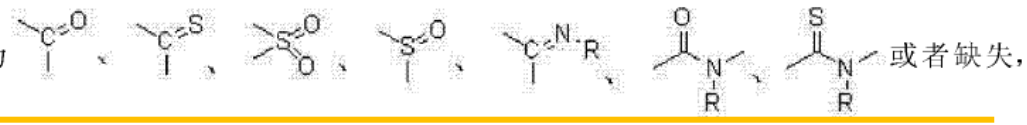
其中：

R_1，R_2，R_3 各自独立选自 H、C_{1-6} 烷基 -D、卤代的 C_{1-6} 烷基 -D、C_{1-6} 羟基烷基、C_{1-6} 巯基烷基、C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 $N(R_a)(R_b)$ 或缺失，R_a，R_b 各自独立选自 H、OH、C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4，R_5 各自独立选自 H、OH、C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H，C_{1-6} 烷基，卤代的 C_{1-6} 烷基，C_{1-6} 羟基烷基，C_{1-6} 烷氧基，卤代的 C_{1-6} 烷氧基，$C(O)O-C_{1-6}$ 烷基，$C(O)NH-C_{1-6}$ 烷基，芳烷基；

X 为 O、S、NH、$N-C_{1-6}$ 烷基或 N- 卤代的 C_{1-6} 烷基；

L 为  或者缺失，

其中 R 选自 H、C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

环 A 选自 5 ～ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ～ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ～ 3 个选自 O 、N 和 S 的杂原子并任选地被 R_8、R_9 和 B_1 基团取代；

R_8，R_9 分别独立选自 H、OH，C_{1-6} 烷基，C_{1-6} 烷氧基，C_{1-6} 羟基烷基，C_{1-6} 巯基烷基，C_{1-6} 烷

具体物质[Specific Substance]

- 以具体化学结构陈述的特定物质，会被分配CAS 登记号

预测性物质[Prophetic Substance]

- 使用Markush结构陈述的预测物质，一个Markush可以陈述上千甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS登记号
- Markush 检索，能检索到通过Substance可能检索不到的结构

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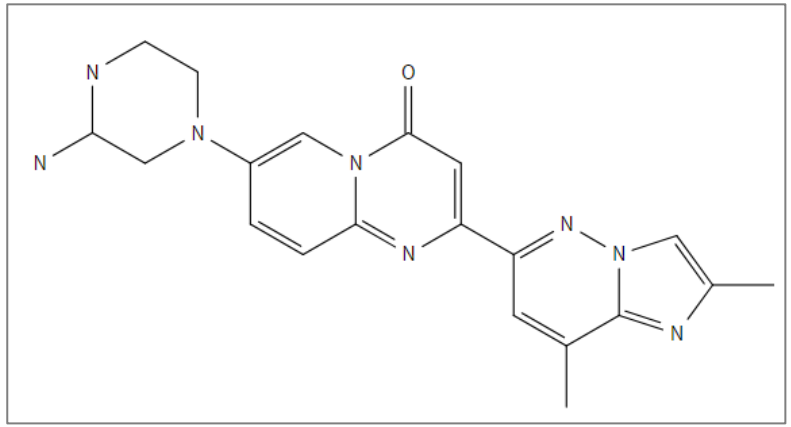
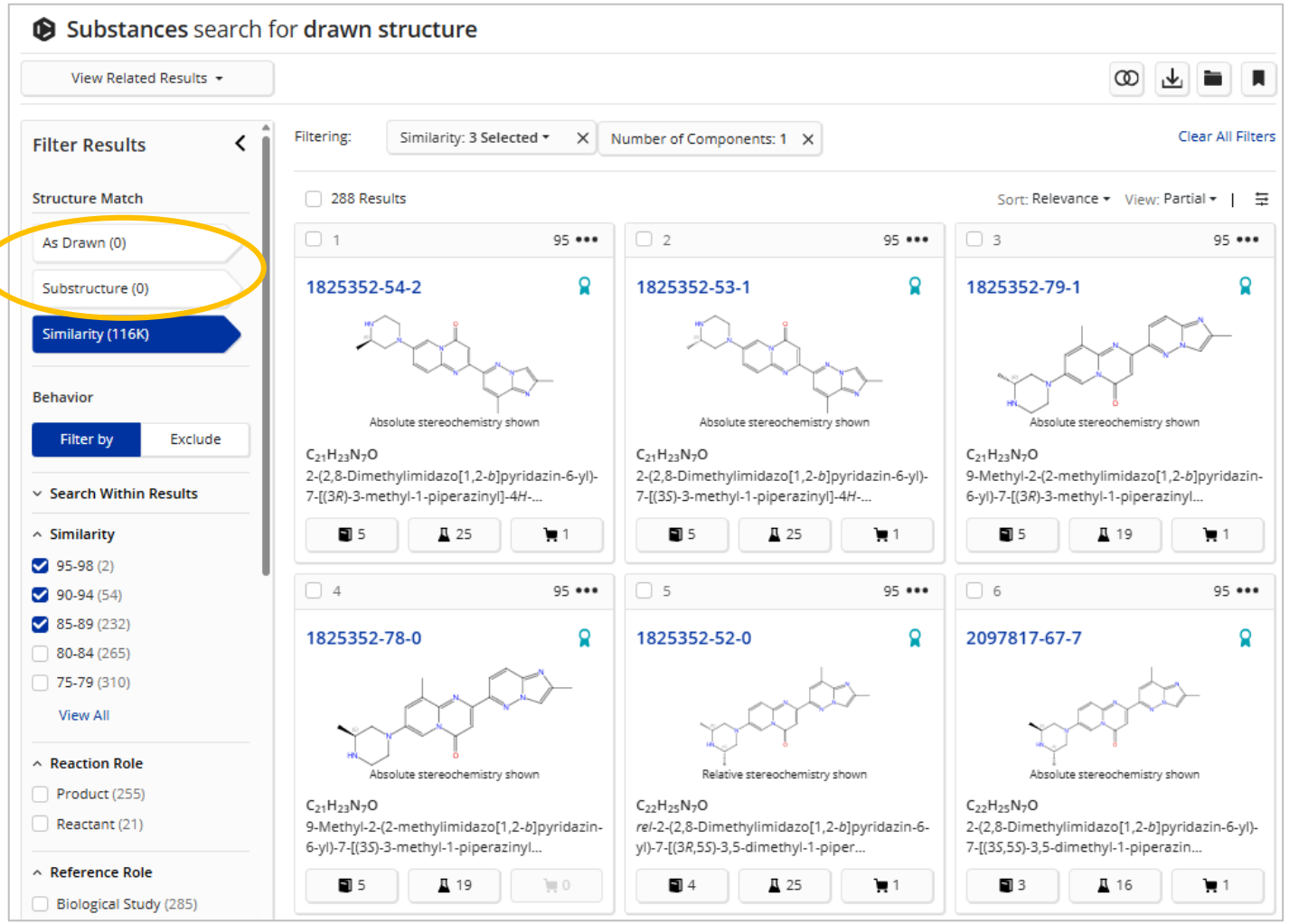
CAS Markush检索

该结构进行精准结构，亚结构均无结果，能够确定它没有被公开吗?



此时您检索的是CAS REGISTRY数据库，它是专利审查员的重要参考依据之一。



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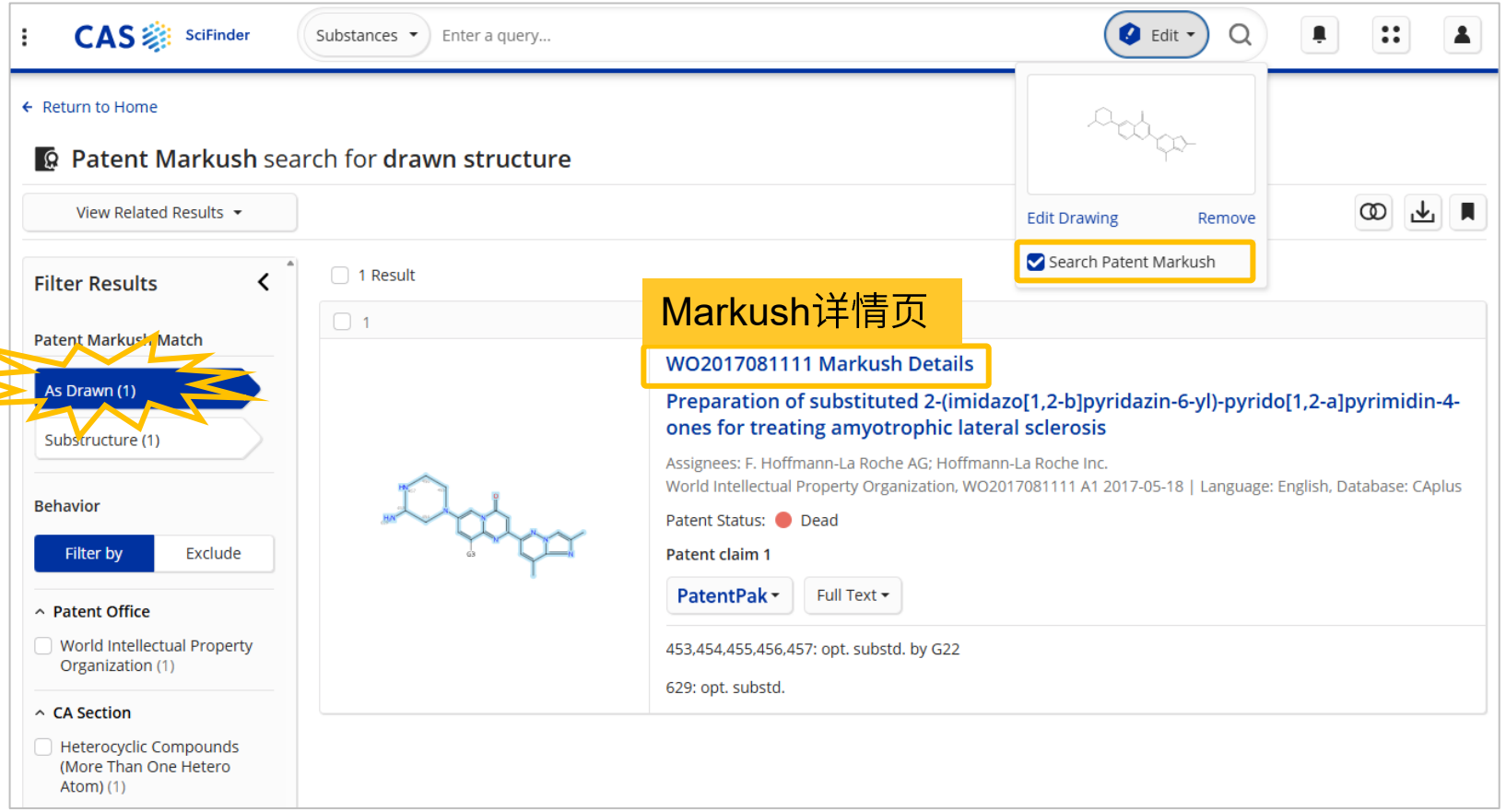
CAS Markush检索

- CAS专利马库什数据集，是专利审查员进行可专利性检索的重要参考依据。
- 马库什检索可以使用具体结构、骨架结构和通式结构来进行迭代检索，确保获得完整的公开结构信息
- 用户可以根据必要性使用 CAS 文献数据集 CAplus 进行文本检索补充



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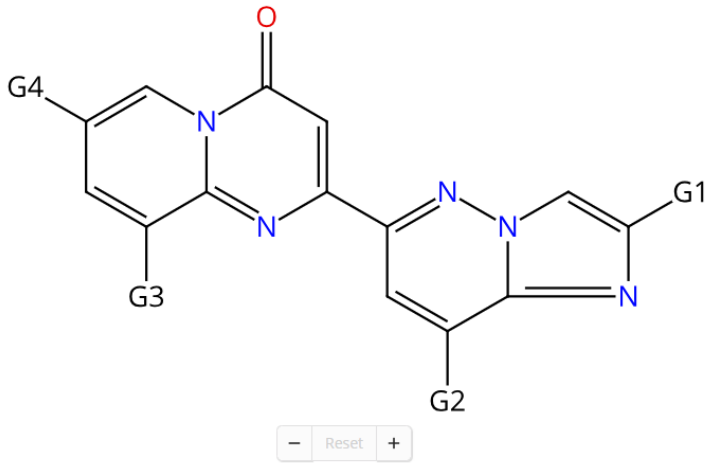
直观的 Markush 详情页

Patent Markush 1

PatentPak | Full Text



Publication Information

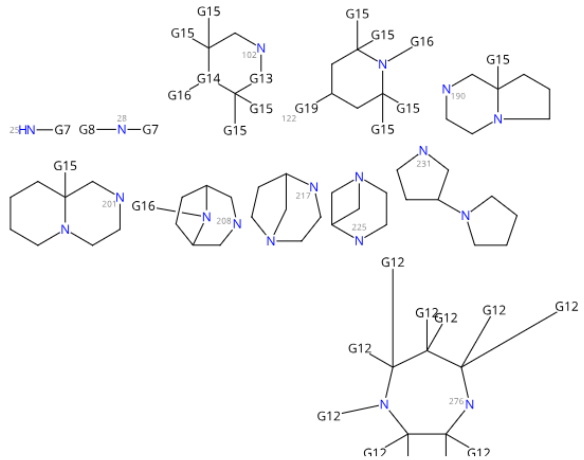
Assignees: F. Hoffmann-La Roche AG; Hoffmann-La Roche Inc.
World Intellectual Property Organization, WO2017081111 A1 2017-05-18 | Language: English, Database: CAplus

Notes

Patent claim 1

or pharmaceutically acceptable salts
substitution is restricted
additional ring formation also claimed

G1	=	H \ alkyl \ Me
G2	=	H \ CN \ alkyl (opt. substd. by G5) \ cycloalkyl \ Me
G3	=	H \ alkyl \ cycloalkyl \ Me
G4	=	heterocycle (opt. substd. by G6) \ 25 \ 28 \ 102 \ 122 \ 190 \ 201 \ 208 \ 217 \ 225 \ 231 \ 245 \ 250 \ piperazino (opt. substd. by G22) \ 276 \ 355 \ 374 \ pyrrolidino (opt. substd. by G22) \ 299 \ 318 \ 330 \ 339 \ 349

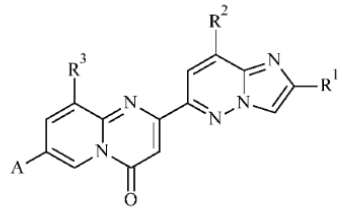


清晰直观展示原文中复杂Markush结构的拆解与解读，助力发现专利文件中隐藏的结构保护信息

原文中Markush结构

Claims

1. The compound of formula (I)



(I)

wherein

R^1 is hydrogen or C_{1-7}-alkyl;

R^2 is hydrogen, cyano, C_{1-7}-alkyl, C_{1-7}-haloalkyl or C_{3-8}-cycloalkyl;

R^3 is hydrogen, C_{1-7}-alkyl, or C_{3-8}-cycloalkyl;

A is N-heterocycloalkyl or $NR^{12}R^{13}$, wherein N-heterocycloalkyl comprises 1 or 2 nitrogen ring atoms and is optionally substituted with 1, 2, 3 or 4 substituents selected from R^{14};

R^{12} is heterocycloalkyl comprising 1 nitrogen ring atom, wherein heterocycloalkyl is optionally substituted with 1, 2, 3 or 4 substituents selected from R^{14};

R^{13} is hydrogen, C_{1-7}-alkyl or C_{3-8}-cycloalkyl;

R^{14} is independently selected from hydrogen, C_{1-7}-alkyl, amino, amino-C_{1-7}-alkyl, C_{3-8}-cycloalkyl and heterocycloalkyl or two R^{14} together form C_{1-7}-alkylene;

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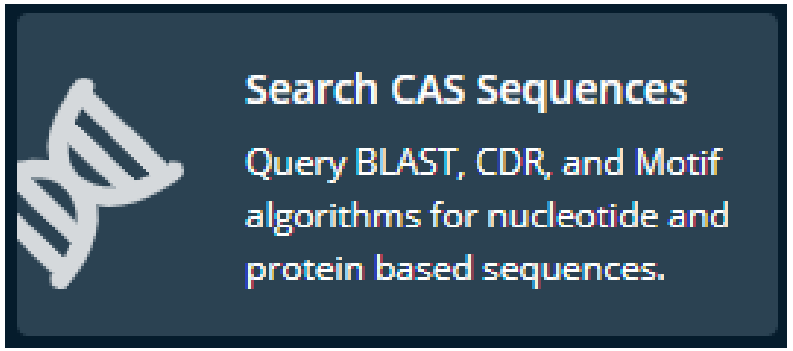
CAS SciFinder 中的序列检索

- BLAST
- CDR
- Motif



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小结

1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 使用自然语言检索，快速获取物质的理化性质、谱图数据等信息
3. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
4. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
5. 利用CAS Markush检索尽可能全面的获得结构的公开信息
6. 利用CAS Sequences高效获取生物序列检索结果。

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大纲

CAS及CAS SciFinder Discovery Platform 简介

科研信息的高效查阅

- 全面的文献调研与拓展助力开题
- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

常见问题Q&A

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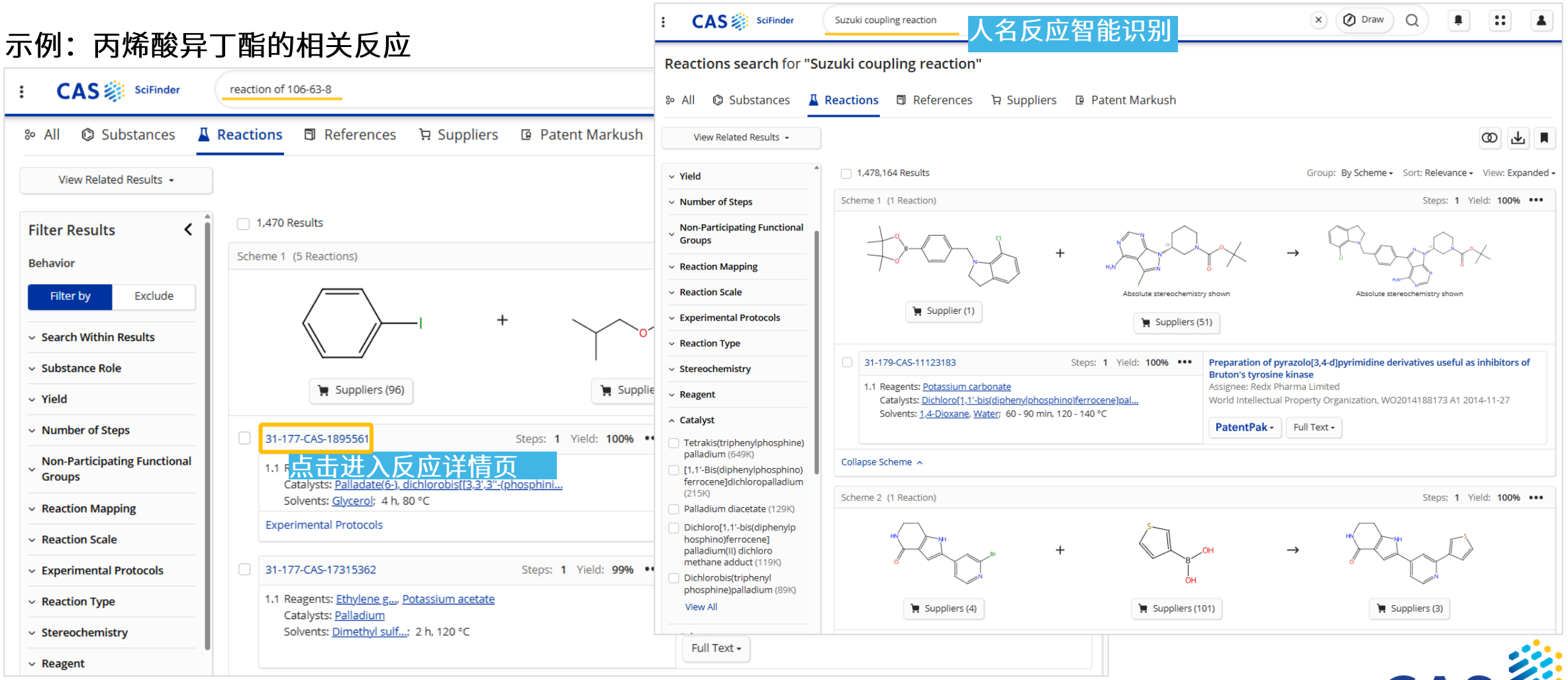
使用标识符直接检索

支持使用：CAS反应登记号、物质名称、CAS登记号、文献号等

示例：丙烯酸异丁酯的相关反应



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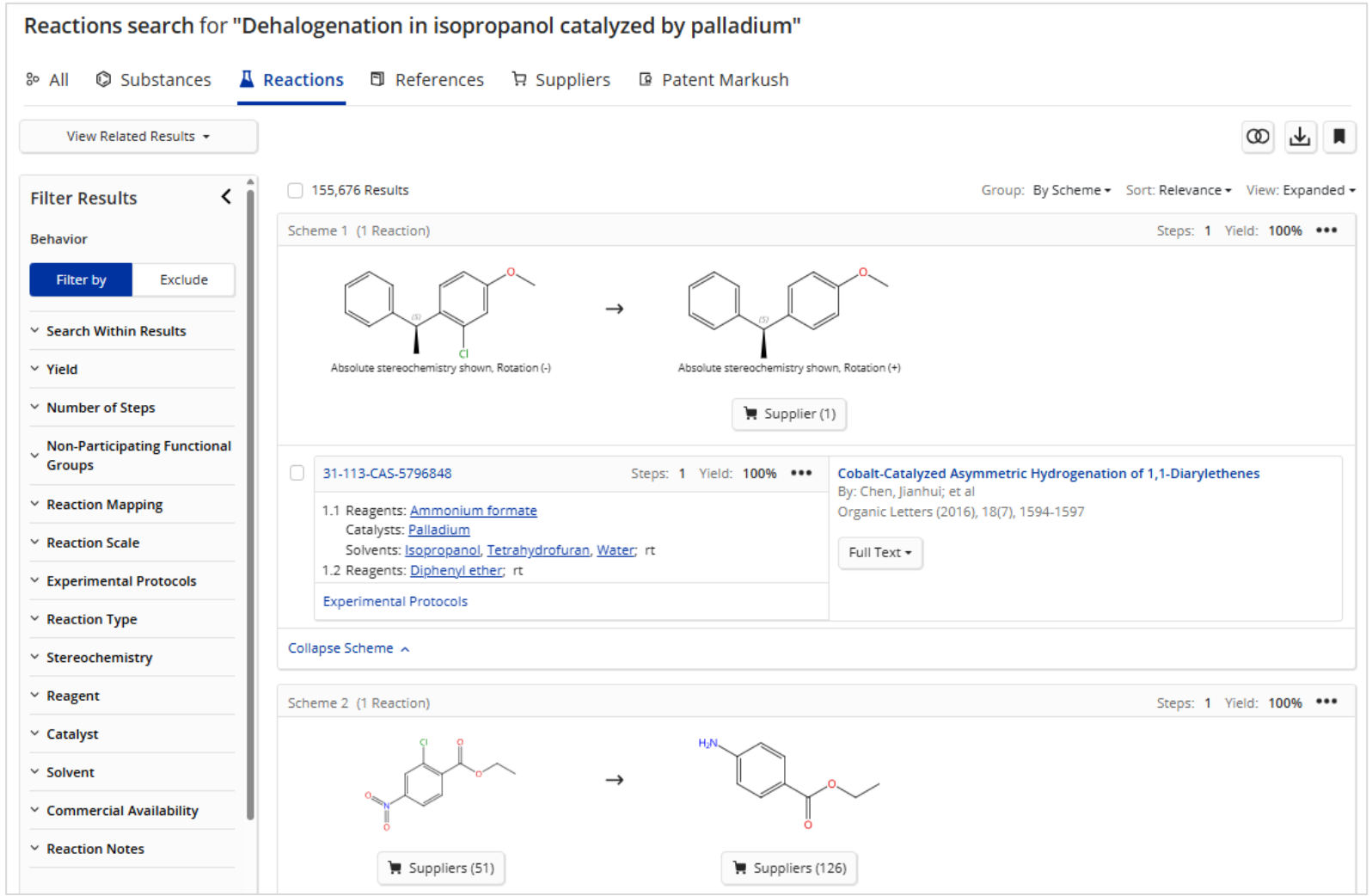
利用自然语言检索反应，降低检索难度

使用CAS数据训练的AI，智能识别检索意向，提供最相关反应检索结果



支持检索：

- 反应转化类型
- 物质类别和官能团
- 物质名称、CAS RN、分子式

支持指定反应参与角色：

- 产物 synthesis/preparation /manufacture of
- 反应物 from
- 溶剂 in
- 催化剂 catalyzed by
- 试剂 mediated by

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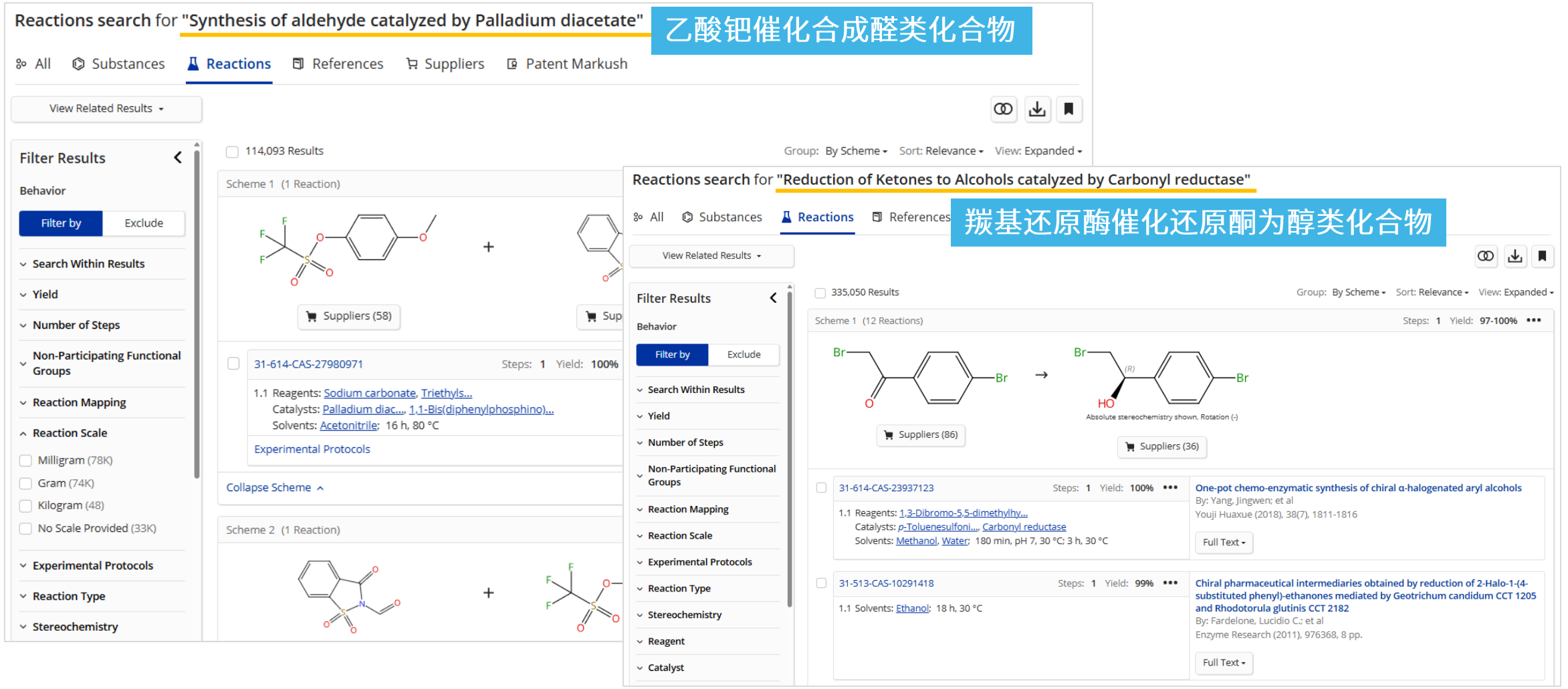
不止具体反应，还可便捷检索某一类反应



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直接绘制反应进行检索

Reactions search for drawn structure

All | Substances | Reactions | References | Suppliers | Patent Markush

View Related Results

Filter Results

Structure Match

As Drawn (34)

Substructure (8,161)

Similarity (0)

结构匹配度

Behavior

Filter by | Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

34 Results

Group: By Scheme | Sort: Relevance | View: Expanded

By Scheme

By Document

By Transformation

Relevance

Publication Date: Newest

Publication Date: Oldest

Yield

Number of Steps: Ascending

Number of Steps: Descending

Scheme 1 (5 Reactions) Steps: 1 Yield: 85%

Suppliers (79) Suppliers (13)

Expand Scheme

Scheme 2 (1 Reaction)

Suppliers (43) Suppliers (3)

31-614-CAS-28968228 Steps: 1 Yield: 76%

1.1 Reagents: O-Methylhydroxylamine hydro...
Solvents: Pyridine; rt; 1 h, 50 °C
1.2 Reagents: (T-4)-Trihydro(tetrahydrof...
Solvents: Tetrahydrofuran; rt; 3 h, reflux; reflux → 0 °C
1.3 Reagents: Sodium hydroxide
Solvents: Water; overnight, reflux; reflux → rt

Experimental Protocols

Preparation of heteroc... adrenergic agents
Assignee: Allergan, Inc.
World Intellectual Prope...

PatentPak

Filter Results

Structure Match

As Drawn (34)

Substructure (8,161)

Similarity (0)

Behavior

Filter by | Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

8,161 Results

Group: By Transformation | Sort: Reaction Count: Descending | View: Expanded

1

Reductive Alkylation of Ammonia or Amines

View 121 Related Reactions

聚焦反应类型

2

Formation of N/O/S Heterocycles

View 54 Related Reactions

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反应结果的筛选

筛选/排除，二次检索

Filter Behavior

Filter by | Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

反应规模

Reaction Scale

- Milligram (5,818)
- Gram (4,525)
- Kilogram (12)
- No Scale Provided (26K)

不参与反应官能团

Non-Participating Functional Groups

- Alkene (8,230)
- Cyclic alkene (8,230)
- Halide (4,370)
- Ether (2,466)
- Amine (2,197)

View All

反应注释

Reaction Notes

- Stereoselective (53) 立体选择性
- Chemoselective (25) 化学选择性
- Regioselective (10) 区域选择性
- Thermal (8)
- Photochemical (7) 光化学
- Prophetic Reaction (5)
- Combinatorial (4)
- Green Chemistry (3) 绿色化学
- Electrochemical (2) 电化学
- Green Chemistry-Process Simplification (1) 绿色化学-工艺简化

View Fewer

试剂

Reagent

- Sodium hydride (17K)
- Sodium hydroxide (9,054)
- Water (7,867)
- Hydrochloric acid (6,933)
- Triethylamine (6,070)

View All

催化剂

Catalyst

- Tetrabutylammonium hydrogen sulfate (3,656)
- 4-(Dimethylamino)pyridine (2,697)
- Tetrakis(triphenylphosphine) palladium (2,381)
- Palladium diacetate (1,455)
- Palladium (1,426)

View All

溶剂

Solvent

- Water (21K)
- Tetrahydrofuran (19K)
- Dichloromethane (15K)
- Dimethylformamide (13K)
- Methanol (5,501)

View All

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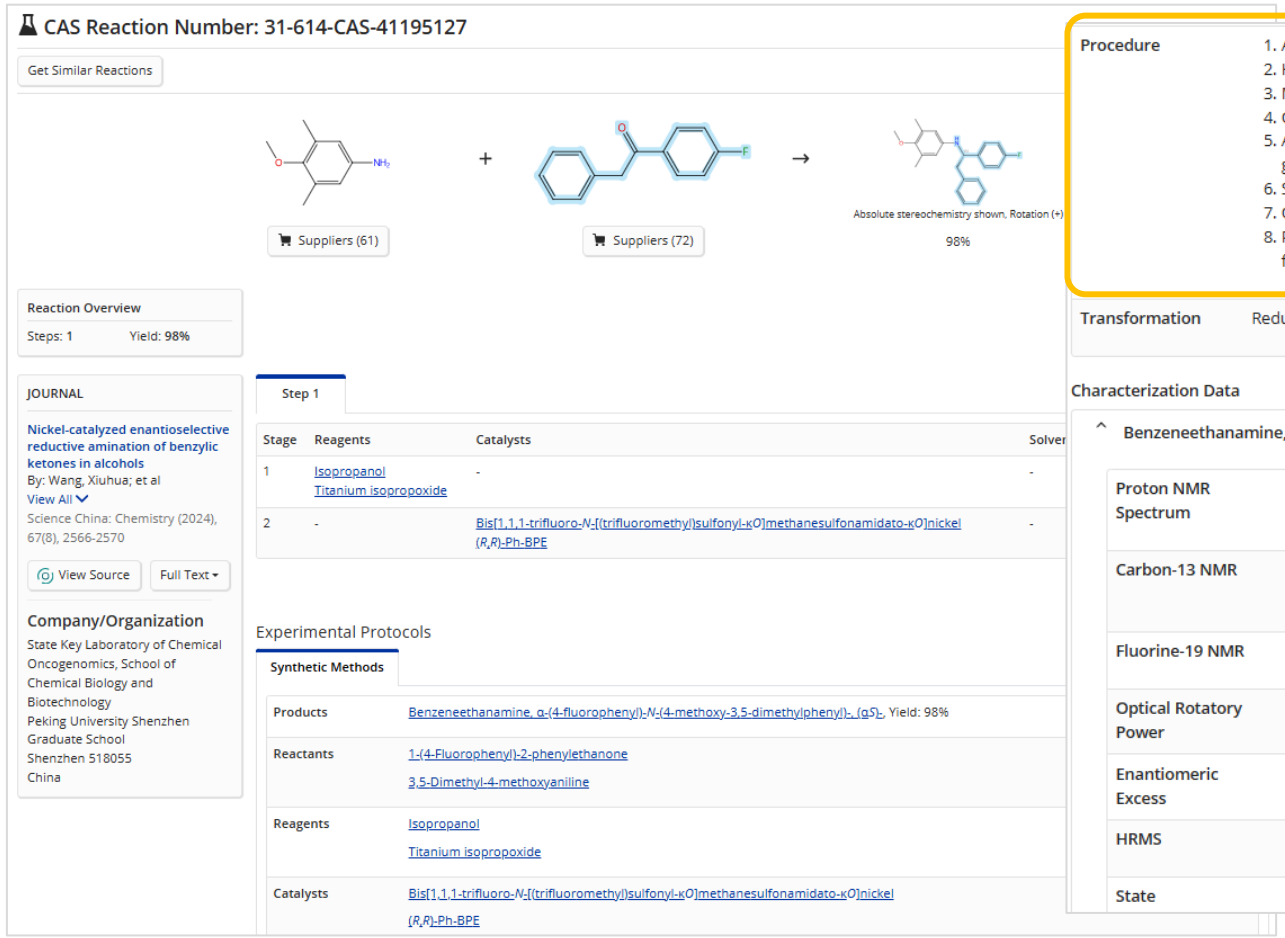
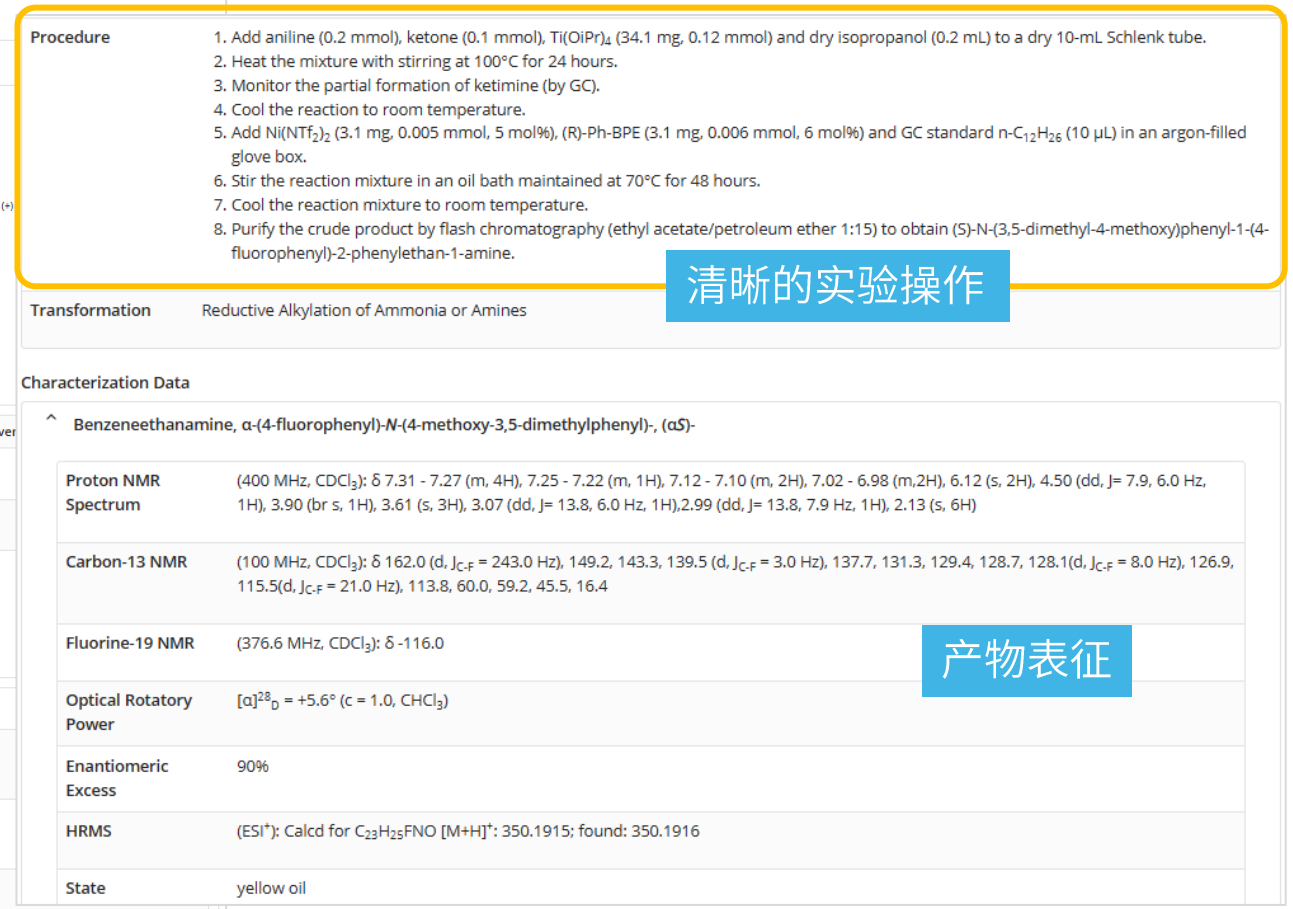
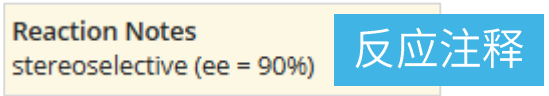
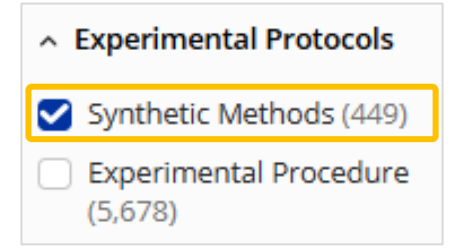
高效获取CAS科学家增值的合成路线详情

Synthetic Methods——CAS科学家增值标引的合成制备详情









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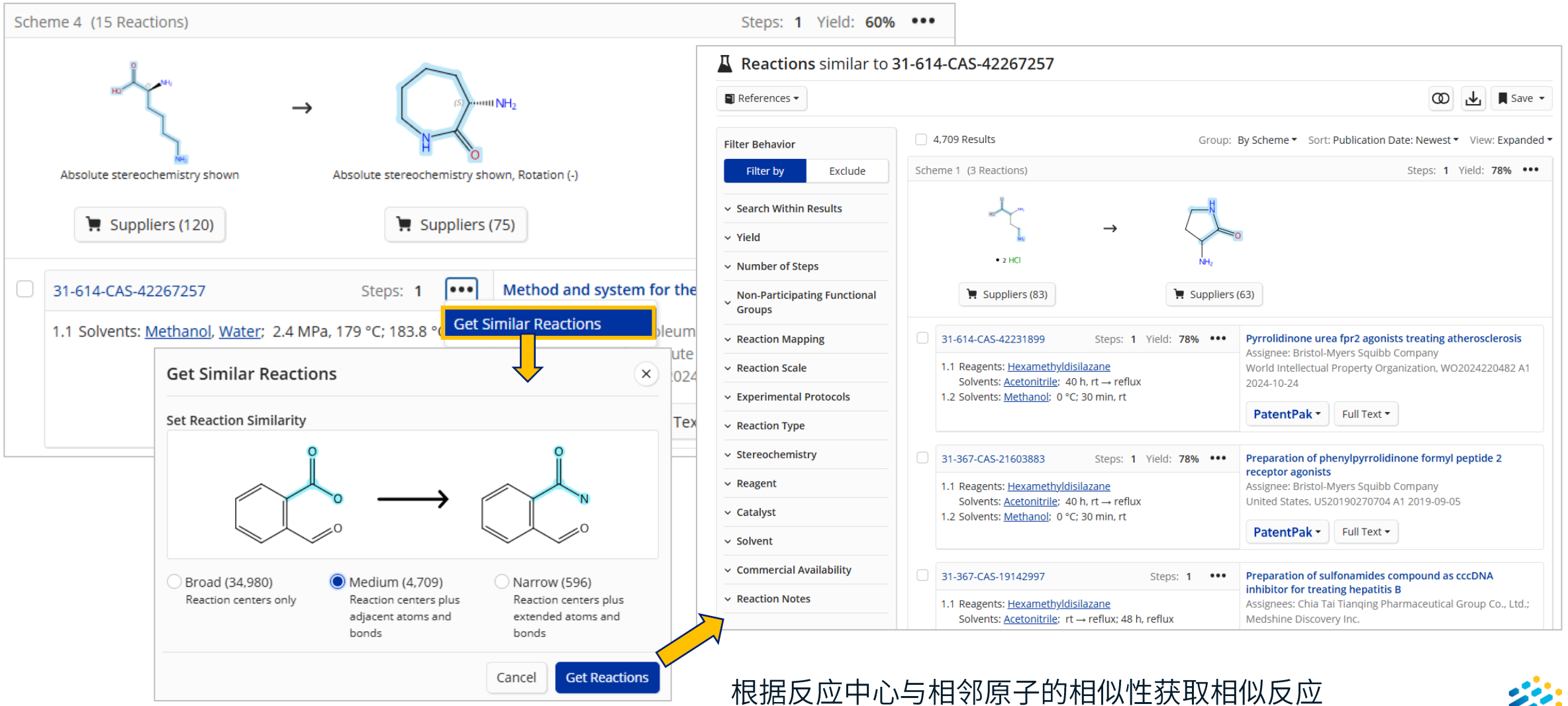
获取相似反应，拓展实验设计思路



根据反应中心与相邻原子的相似性获取相似反应

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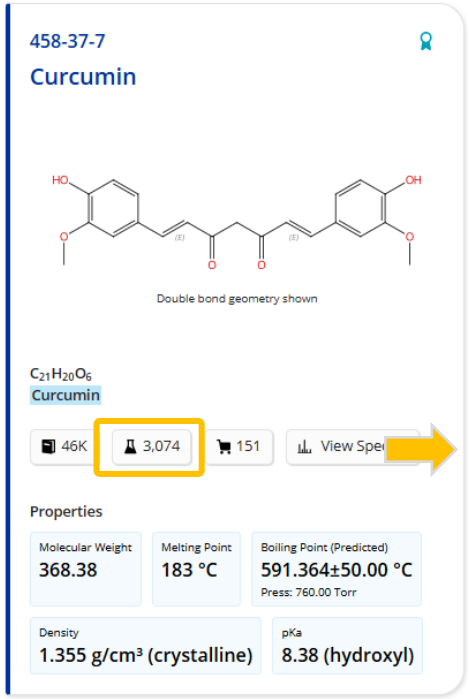
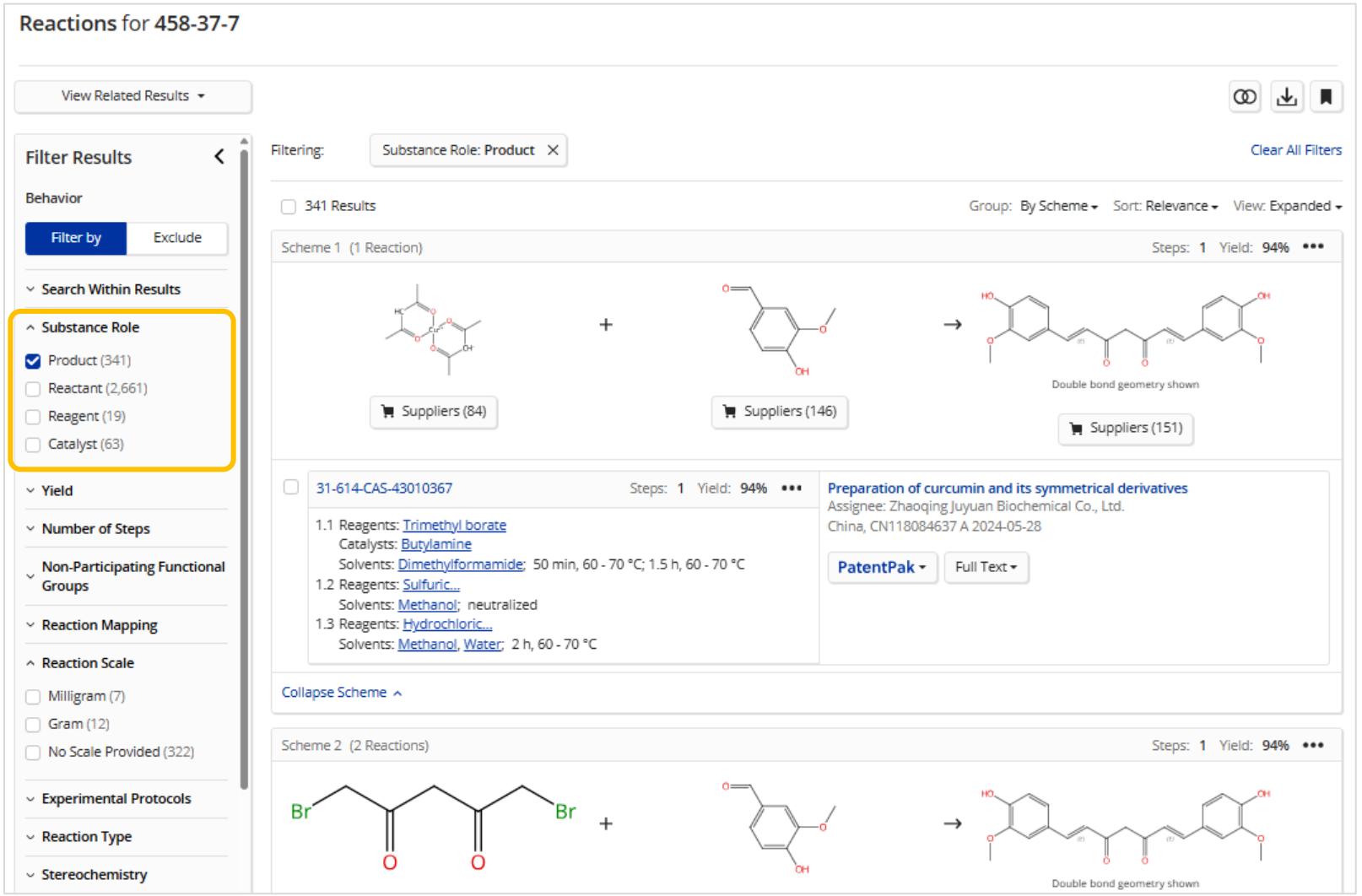
如何检索重要化合物的相关反应与合成工艺?





- 通过物质结构、名称或其他物质标识符检索物质
- 一键链接到相关反应
- 限定物质角色为产物，通过产率筛选较优的反应条件
- 可进一步筛选反应规模、实验详情等

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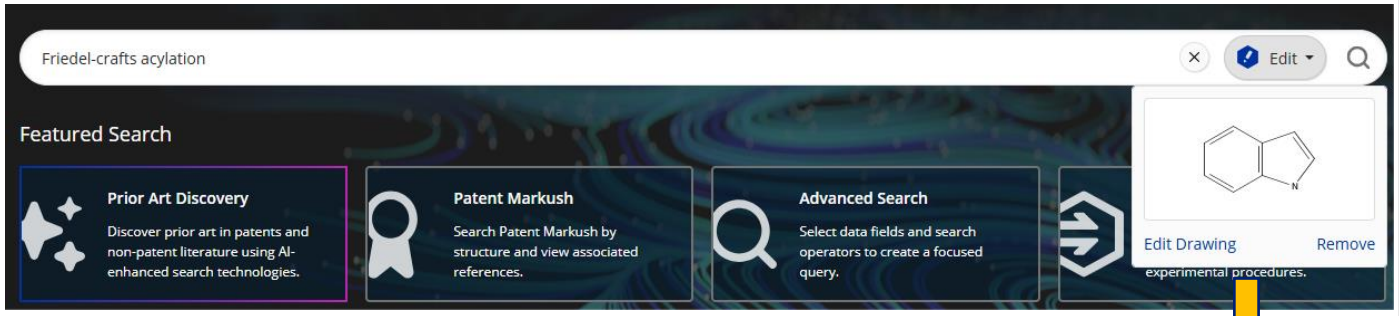
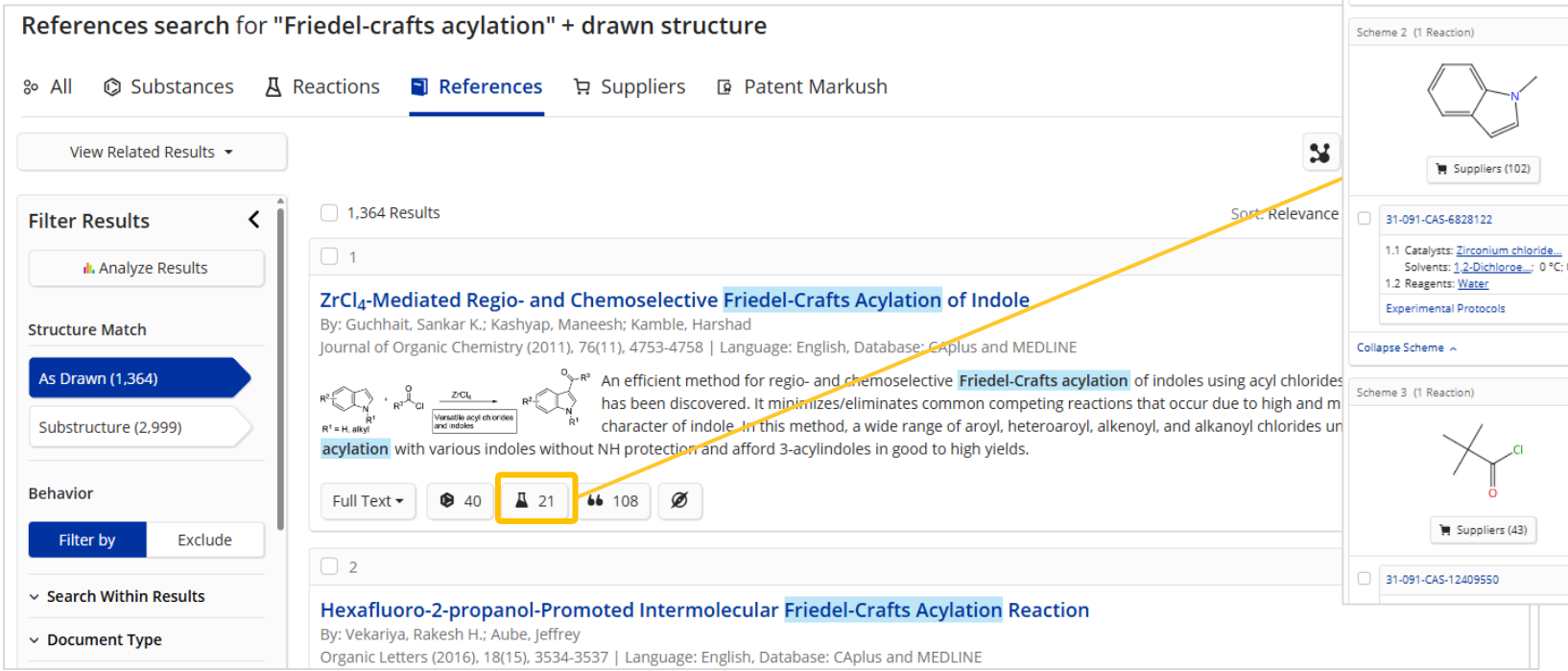
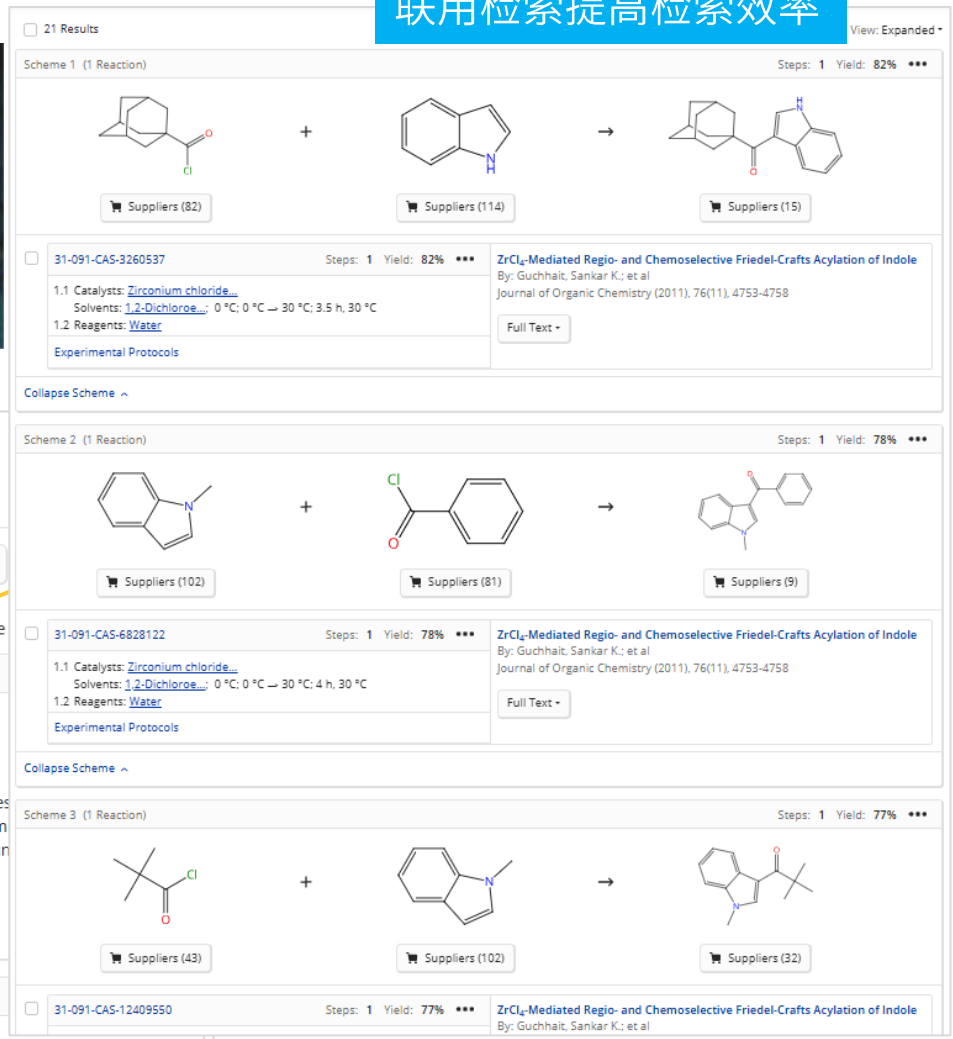
使用联用检索——结构与关键词检索反应

联用检索提高检索效率







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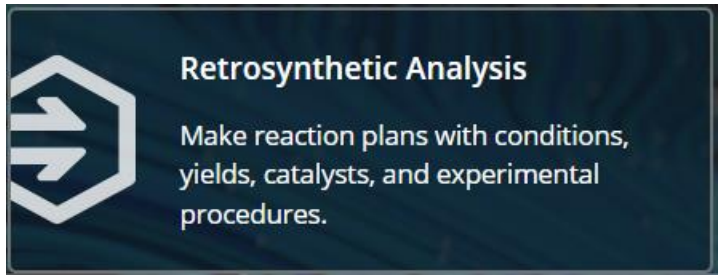
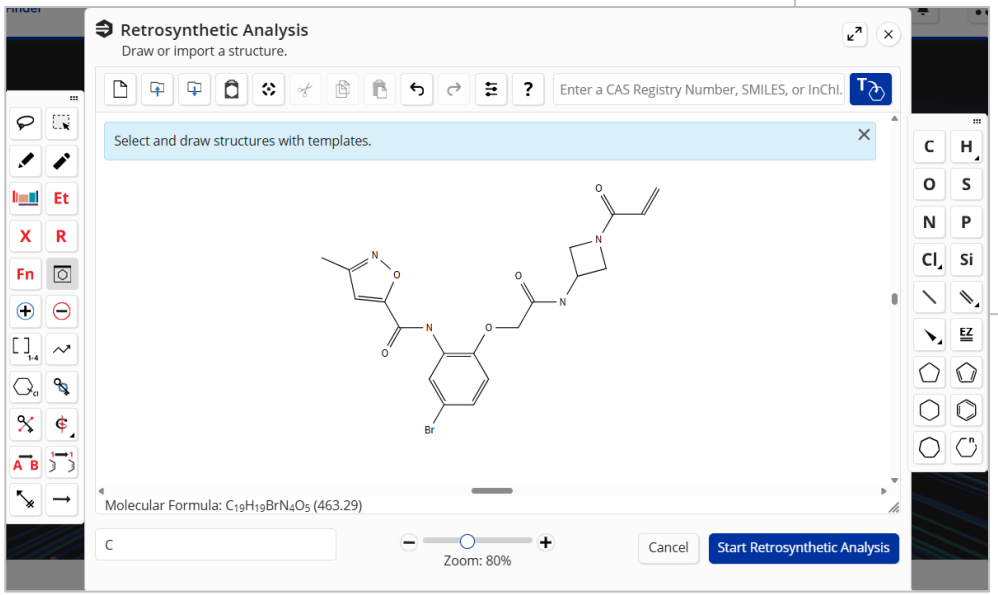
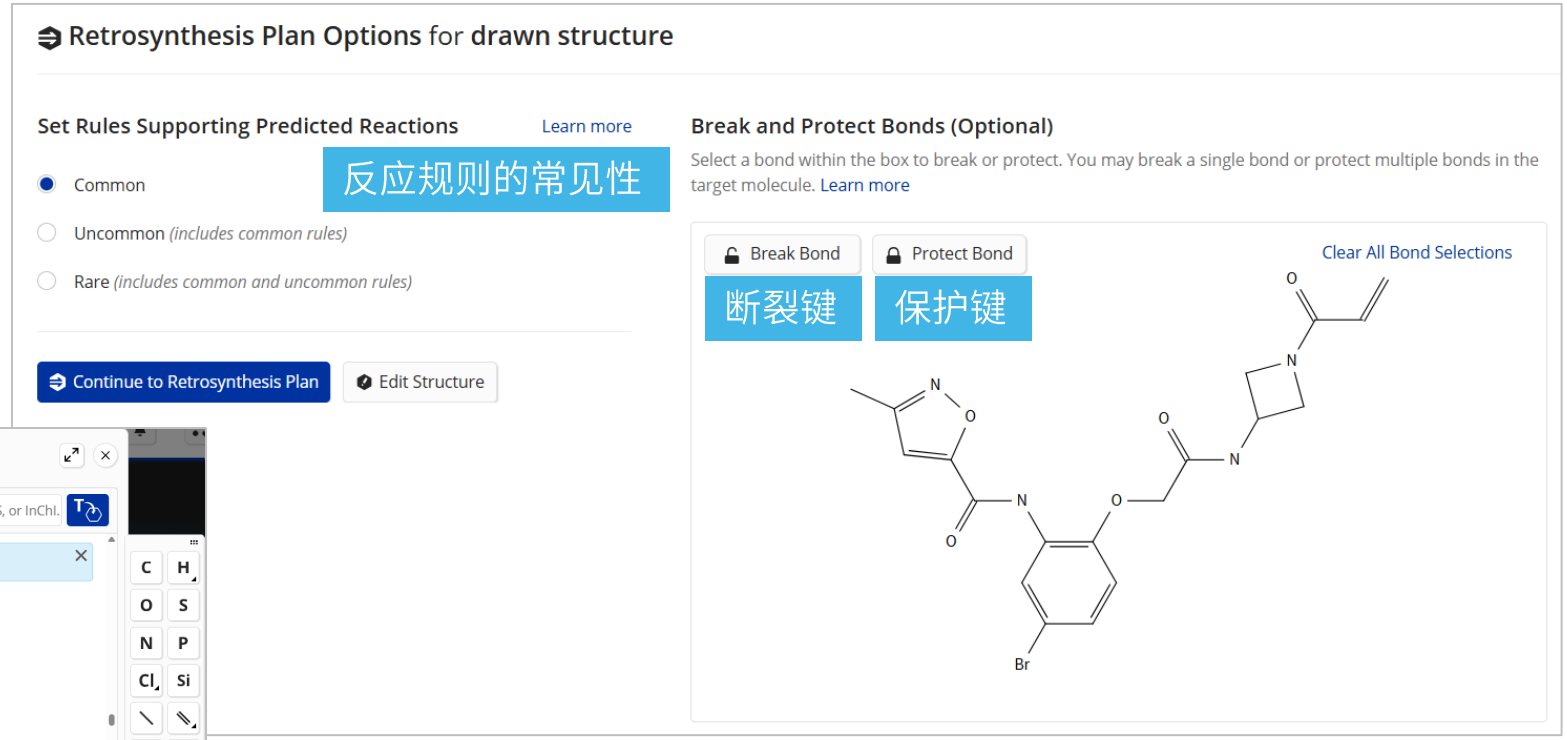
Retrosynthetic Analysis——拓展反应路线设计思路

结合先进的AI技术和CAS科学家标引的高质量反应数据，为已知或未知分子设计合成路线







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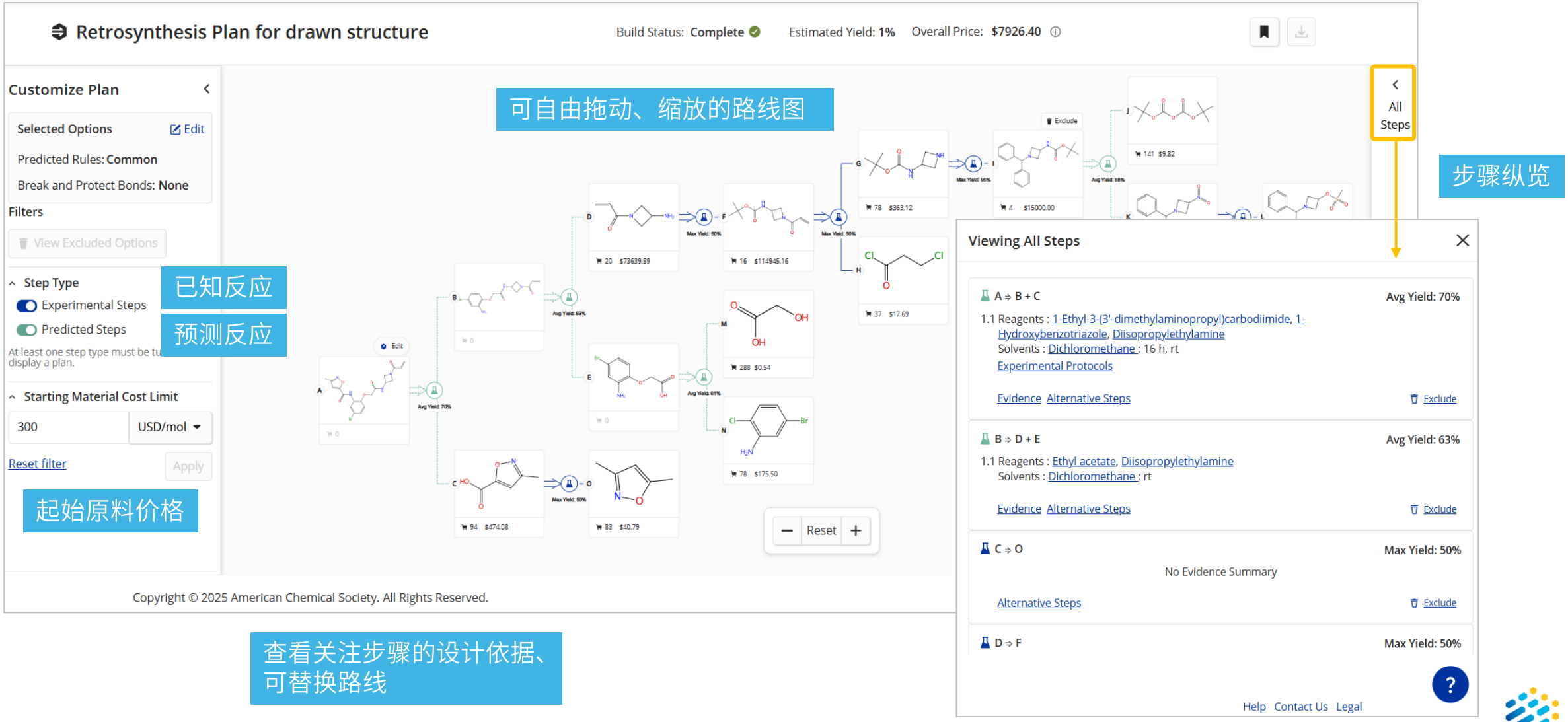
逆合成路线详情



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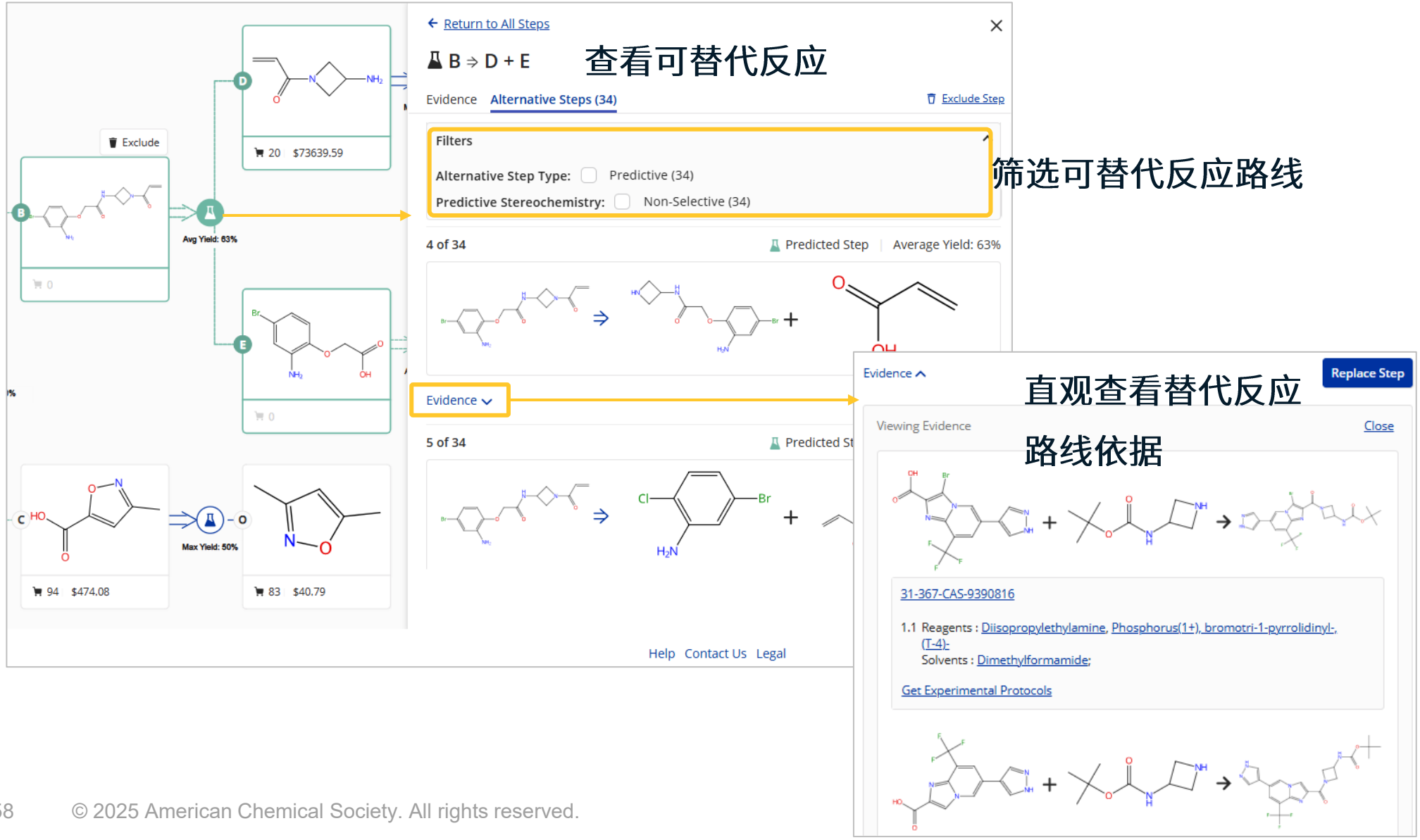
了解其他反应路线，拓宽实验设计思路



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设计该步反应的依据从何而来?

进一步明确底物/产物的结构特征

筛选最感兴趣的合成路线

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小结

1. 通过自然语言、标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 关键词与反应式的联合检索
4. 获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

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- 多角度出发检索物质结构及相关属性
- 探索实验方案以获取反应与合成相关策略
- 高效获取分析方法及配方制剂信息

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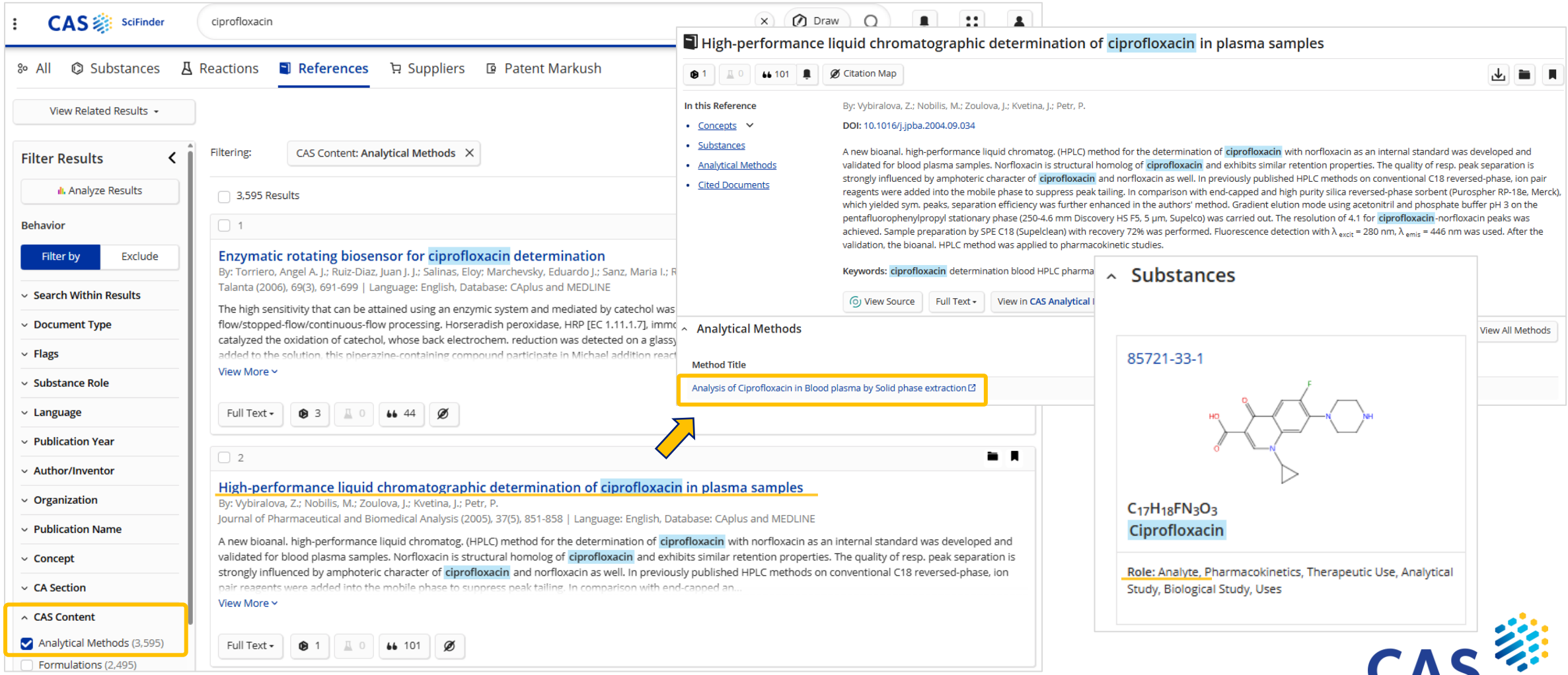
关注文献关联的分析方法?

在CAS SciFinder的文献结果集页面，点击CAS Content中的 Analytical Methods获得有具体分析实验方法的文献，从文献详情页中链接至分析实验方法



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CAS科学家增值标引的分析方法详情

Analysis of Ciprofloxacin in Blood plasma by HPLC

CAS Method Number
1-101-CAS-44938

Method Category
Active Pharmaceutical Ingredient and Metabolite Analysis

Technique
UV-visible spectroscopy; HPLC

Analyte	Matrix	Material 所用材料	Reagent	Biological Reagen
Ciprofloxacin	Blood plasma	Silanized glass tube Eppendorf tube Glass syringe ACE 5 C18 column (250 mm × 4.6 mm, 5 µm) View All	Acetonitrile Methanol Phosphate-buffered saline solutions	-

Source 文献来源

JOURNAL

A simple HPLC-UV method for the determination of ciprofloxacin in human plasma
Vella, Janis; Busuttil, Francesca; Bartolo, Nicolette Sammut; Sammut, Carmel; Ferrito, Victor; Serracino-Inglott, Anthony; Azzopardi, Lilian M.; LaFerla, Godfrey

Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2015), 989, 80 - 85. Elsevier B.V.

CODEN : JCBAAI | ISSN : 15700232 | DOI : 10.1016/j.jchromb.2015.01.006

View Abstract | Full Text

Equipment Used 所用仪器

HPLC unit, Pro Star, Varian
Online degasser
Column oven
UV-vis detector
Analytical balance, XS104, Mettler Toledo
Automated evaporation system, LV, TurboVap
Concentrator, Turbovap
Centrifuge

Conditions 实验条件

Instrument

column: reversed phase ACE 5 C18 column (250 mm × 4.6 mm, 5 µm); guard column: Agilent Pursuit 5 C18 Meta guard column (10 mm × 4.6 mm, 5 µm); injection sample loop volume: 50 µL; gradient: isocratic

detection wavelength: 277 nm

Validation 数据验证

Linearity Range	0.05 - 8 µg/mL
Limit of Detection	0.01 µg/mL
Limit of Quantitation	0.05 µg/mL
Recovery	97.50, 96.75, 95.50, 93.25, 100.00% in 3.90, 3.87, 3.82, 3.73, 4.00 µg/mL calculated quantity
Accuracy	96.1117, 99.0000, 90.0000% in 6, 2, 0.5 µg/mL spiked
Precision	1.1268, 2.3273, 1.688, 3.8570, 8.8059, 0.0455, 13.0820% (RSD, intraday); 0.9989, 4.7934, 2.0837, 4.1180, 4.4613, 6.0831, 12.0374% (RSD, interday) in 8, 6, 4, 2, 0.5, 0.1, 0.05 µg/mL added
Retention Time	3.26 min

Instructions 操作步骤

Preparation of the mobile phase

1. Prepare 0.02 M phosphate buffer at pH 2.7 using disodium hydrogen phosphate and orthophosphoric acid.
2. Elute together with acetonitrile to dilute mobile phase of buffer and acetonitrile 77:23 (v/v).
3. Keep reagents in amber glass bottles.

Plasma sample preparation using silanized tubes

1. Transfer spiked 400 mL of plasma with ciprofloxacin to 1.5 mL Eppendorf tubes.
2. Add 30 mL of internal standard (IS, sulfadimidine sodium) working solution in water (100 g/mL) to each tube.
3. Add 1 drop of 10 M phosphate buffer (pH 2.7).
4. Vortex mix for 3 min.
5. Add 500 mL of ice cold acetonitrile using a glass syringe.
6. Vortex mix the tubes for 5 min.
7. Centrifuge the samples at 3500 × g for 5 min.
8. Pour the supernatant into 8 mL silanized glass tubes.
9. Place the silanized tubes in a Turbovap concentrator with the water bath set at 50 °C for 20 min.
10. Reconstitute the dried residue with 100 µL mobile phase.
11. Vortex mix for 3 min.
12. Re-centrifuge at 15000 rpm for 3 min.
13. Inject 50 mL of the clear supernatant into the HPLC unit.

Standard solution preparation

1. Prepare 1 mg/mL ciprofloxacin stock solution in methanol.
2. Obtain working solutions from the stock solution by dilution with mobile phase.
3. Store at 4 °C.

HPLC-UV analysis

1. Perform HPLC-UV analysis using Varian Pro Star HPLC unit consisting of an online degasser, column oven and UV-vis detector.
2. Carry out separation on a reversed phase ACE 5 C18 column (250 mm × 4.6 mm, 5 µm; Advances chromatography Technologies, Aberdeen, Scotland) protected by Agilent Pursuit 5 C18 Meta guard column (10 mm × 4.6 mm, 5 µm; Agilent Technologies, Amstelveen, Netherlands).
3. Maintain column and injection temperature at 25 °C.
4. Program the system isocratically.
5. Set the flow rate at 1.5 mL/min.
6. Inject fixed sample through a loop having a volume of 50 µL.
7. Perform detection at 277 nm.

- CAS科学家增值标引的分析实验详情
- 无需购买、浏览全文，高效获取所需实验信息

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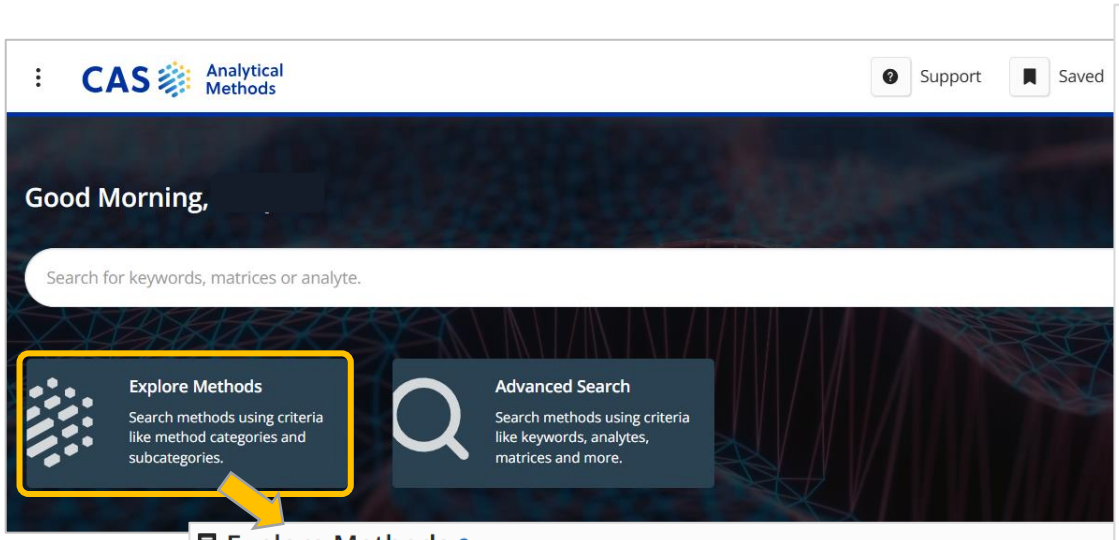
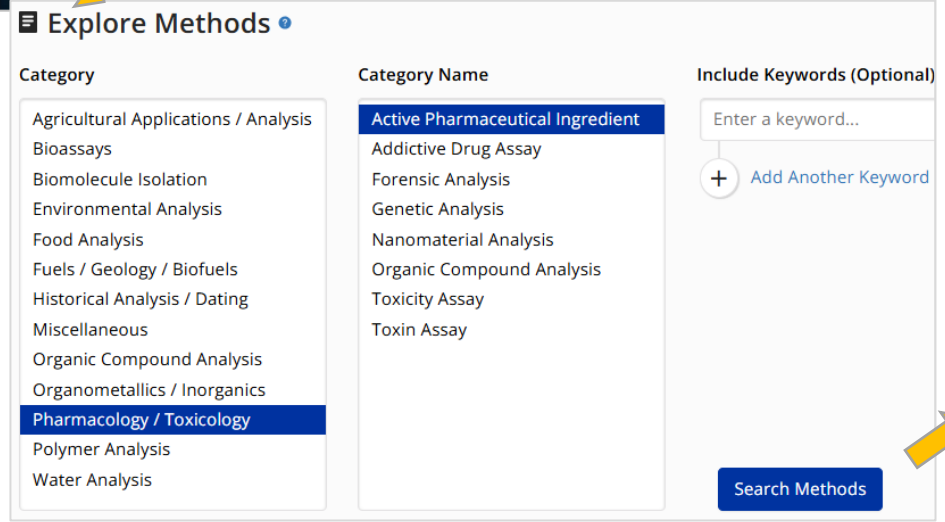
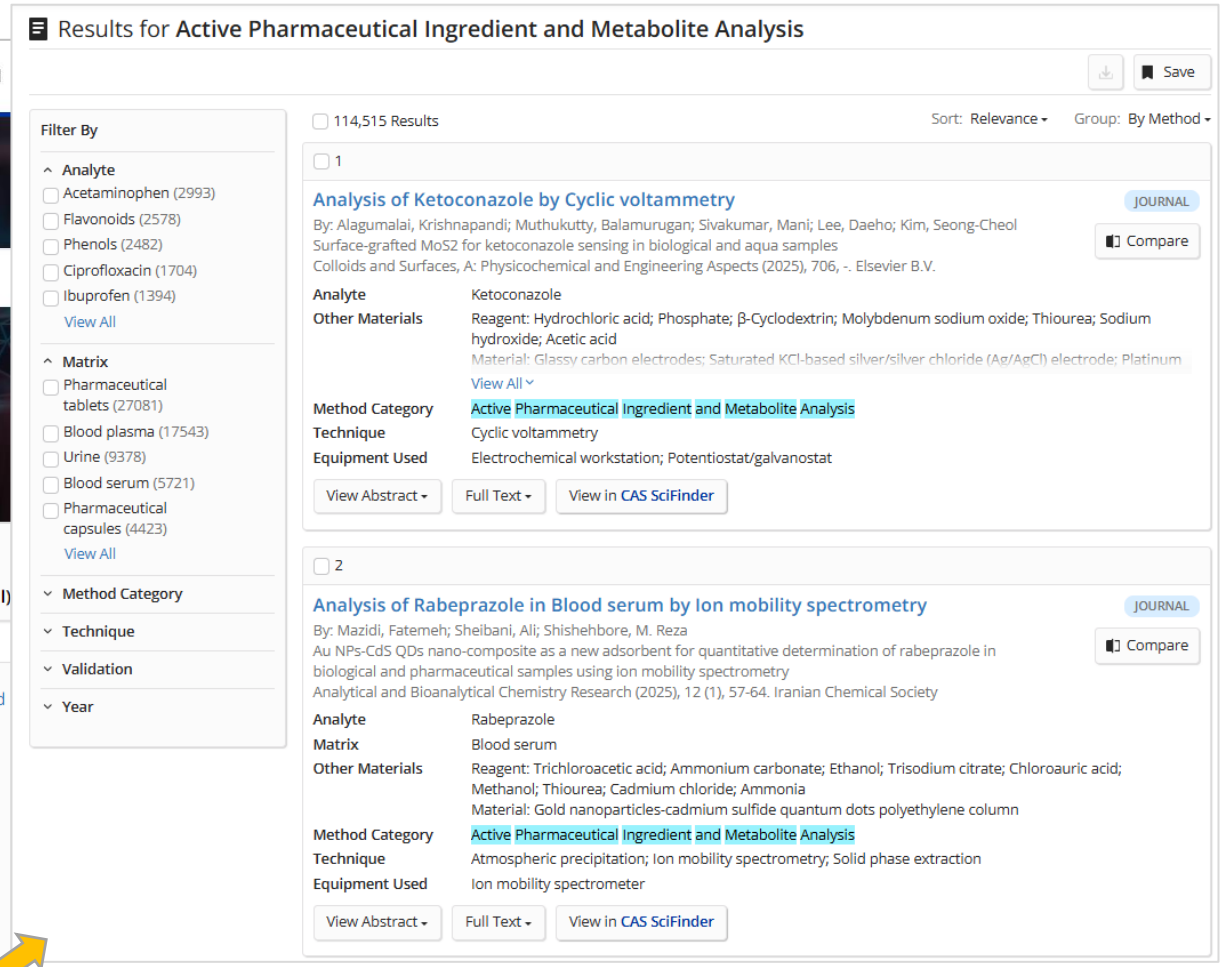
通过CAS Analytical Methods获取分析方法详情

方法(2)：登录https://methods.cas.org，主题检索或分类浏览







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分析方法检索结果的分析与精炼

分析物

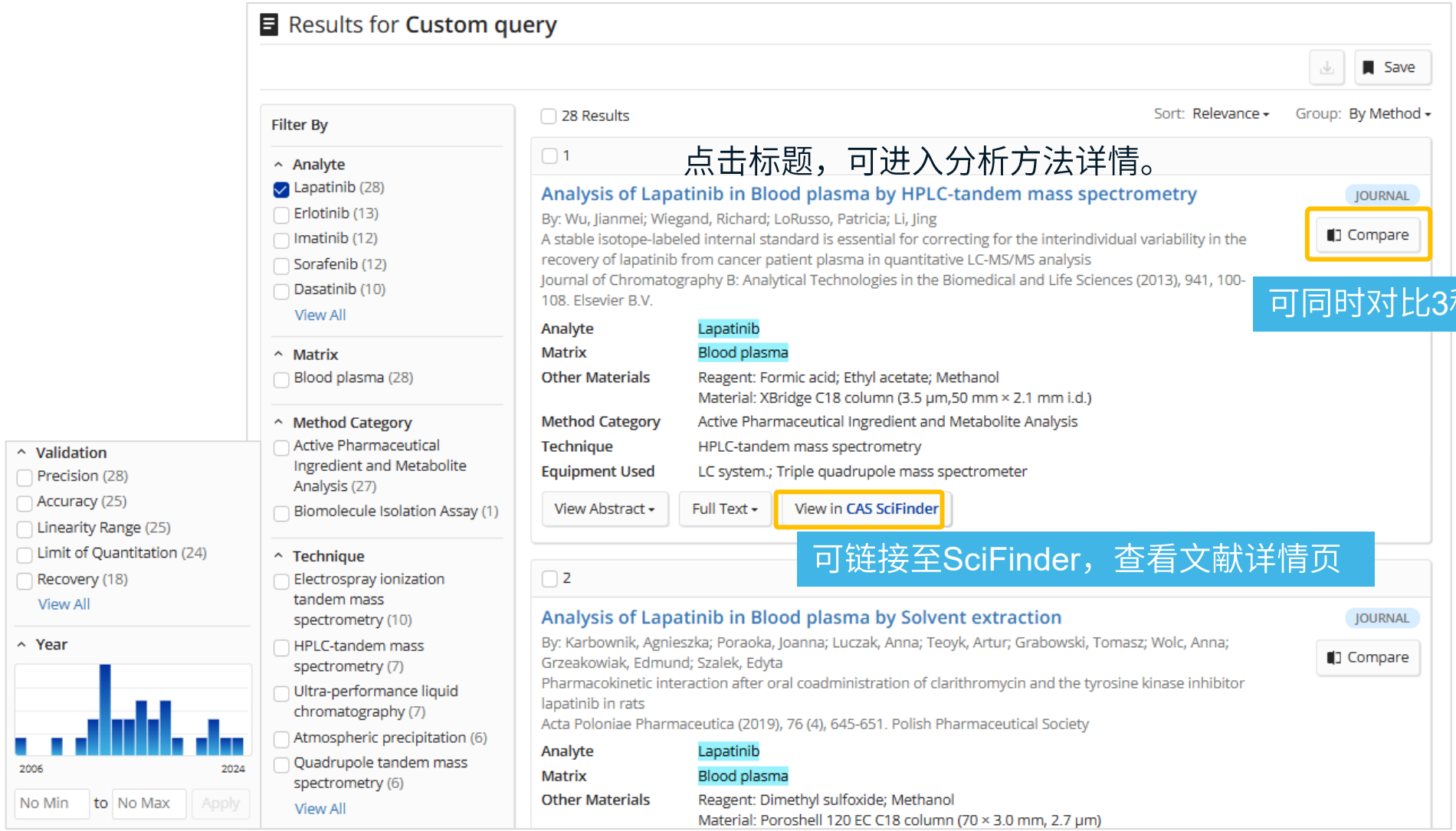
基质

方法分类

技术&仪器

实验验证

年份



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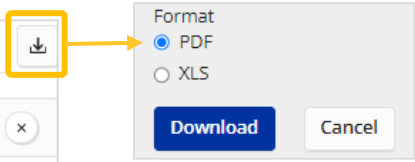
对照多个感兴趣的分析方法详情



	Method 1	Method 2
	Analysis of Lapatinib in Blood plasma by HPLC-tandem mass spectrometry	Analysis of Lapatinib in Blood plasma by Atmospheric precipitation
CAS Method Number	1-101-CAS-187473	1-101-CAS-43
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharm
Technique	HPLC-tandem mass spectrometry	HPLC-tandem spectrometry
Analyte	Lapatinib	Lapatinib
Matrix	Blood plasma	Blood plasma
Other Materials	Formic acid; Methanol; Ethyl acetate; XBridge C18 column (3.5 µm,50 mm × 2.1 mm i.d.)	Acetonitrile; A precipitation Security guar
Equipment Used	LC system., Alliance2695, Waters, Milford, MA, USA; Triple quadrupole mass spectrometer, Quattro Micromass, Waters	HPLC system, Shimadzu, Ky Kyoto, Japan; Sciex, Ontaric
Conditions	**Instrument:** ionization mode-Positive; heated nebulized probe- 350 °C; pressure of collision gas (Argon) (mbar)- 5.92E-003, 5.92E-003 and 5.92E-003 for lapatinib, lapatinib-d3 and zileuton; dwell time (s)- 0.5, 0.5 and 0.5, for lapatinib, lapatinib-d3 and zileuton; cone voltage (V)- 60, 60 and 22 for lapatinib, lapatinib-d3 and zileuton; collision energy (eV)- 34, 34 and 12, for lapatinib, lapatinib-d3 and zileuton; transition- 581.4>364.96, 584.1>366 and 237.43>161.09, for lapatinib, lapatinib-d3 and zileuton.**Chromatographic:** XBridge C18 column (3.5 µm,50 mm × 2.1 mm i.d.); internal standard- lapatinib-d3; temperature- 30 °C; mobile phase- methanol and 0.45% formic acid in water (50:50, v/v); isocratically; flow rate- 0.2 ml/min.	**Instrument:** (and security g 10 mM ammo acetonitrile; (supply 2: 80 a V; source gas declustering potential: 102 V and collision energy: 50 V for both lapatinib and internal standard
Linearity Range	5 - 5000 ng/ml	2.50 - 1000 ng/mL
Limit of Quantitation	5 ng/mL	2.50 ng/mL (LLOQ)
Recovery	43% ± 14%, 42% ± 10% and 48% ± 12% (recovery), for 5, 15, 800 and 4000 ng/mL spiked sample, repectively.	81, 87 and 87% in 5.00, 100 and 800 ng/mL spiked concentrations, respectively
Accuracy	102.1%, 98.6%, 102.5% and 98.3% (recovery), for 5, 15, 800 and 4000 ng/mL QC sample, repectively.	107% (inter-assay) in 2.50 ng/mL concentration
Precision	4.6%, 3.4%, 2.3% and 2.4% (RSD, intra-day); 4.0%, 2.9% and 3.1% (RSD, inter-day), for 5, 15, 800 and 4000 ng/mL QC sample, repectively.	3.03% (RSD, inter-assay) in 2.50 ng/mL concentration
Source	JOURNAL A stable isotope-labeled internal standard is essential for correcting for the interindividual variability in the recovery of lapatinib from cancer patient plasma in quantitative LC-MS/MS analysis By: Wu, Jianmei; Wiegand, Richard; LoRusso, Patricia; Li, Jing Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 941, 100 - 108. Full Text	JOURNAL A sensitive LC-MS-MS assay for the determination of lapatinib in human plasma in subjects with end-stage renal disease receiving hemodialysis By: Kocan, Geralyn P.; Huang, Mike; Li, Fumin; Pai, Sudhakar Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2018), 1097-1098, 74 - 82. Full Text

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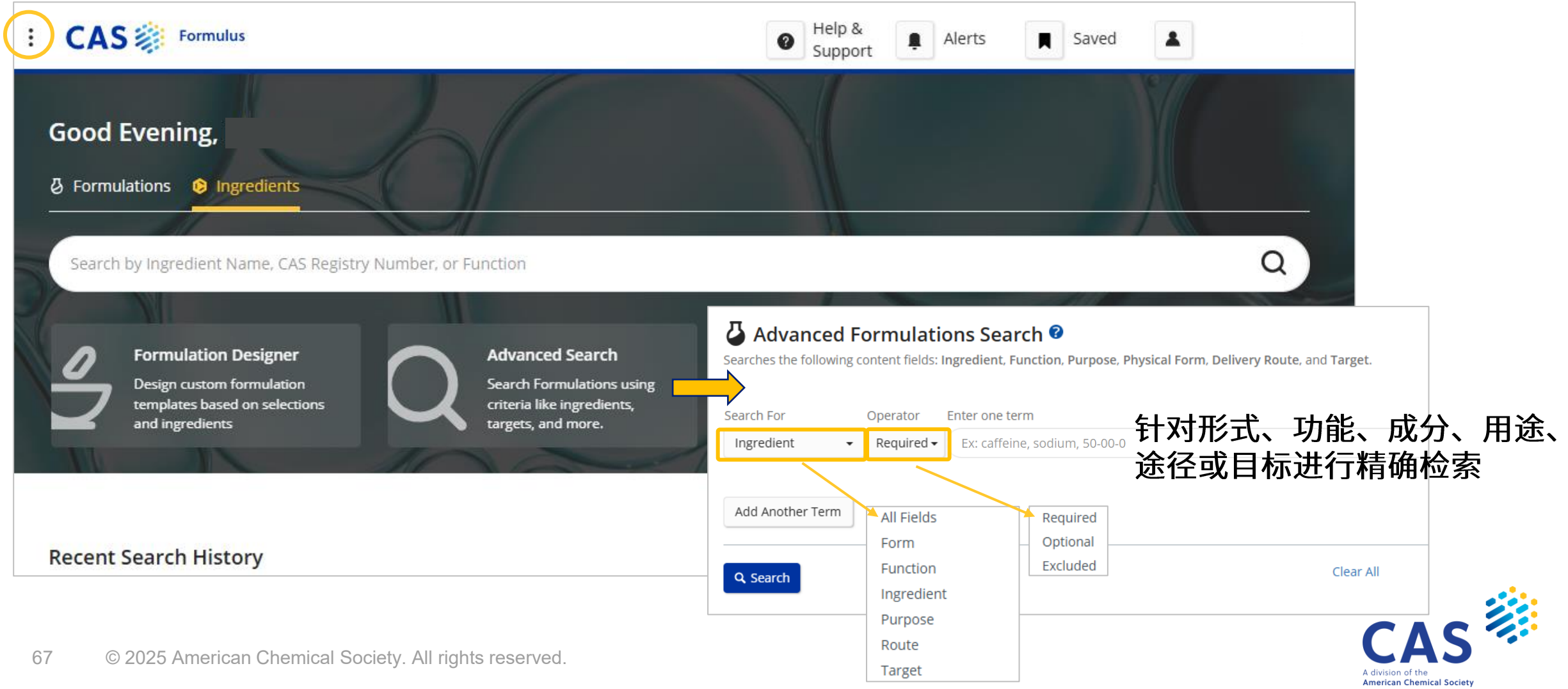
研究课题在产品中的应用？配方/制剂的检索与设计

- 访问网址：https://formulus.cas.org/



针对形式、功能、成分、用途、途径或目标进行精确检索

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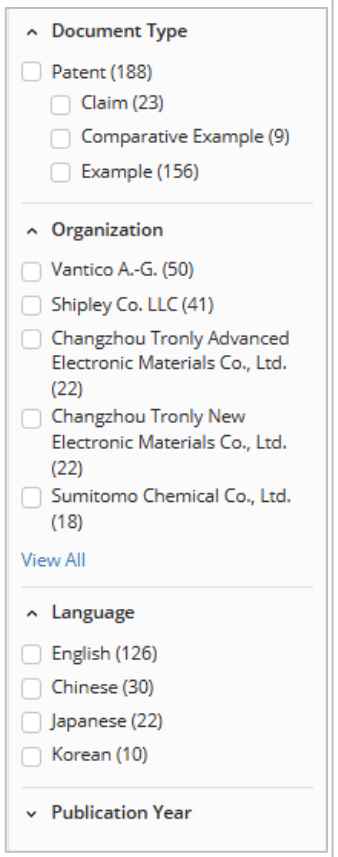
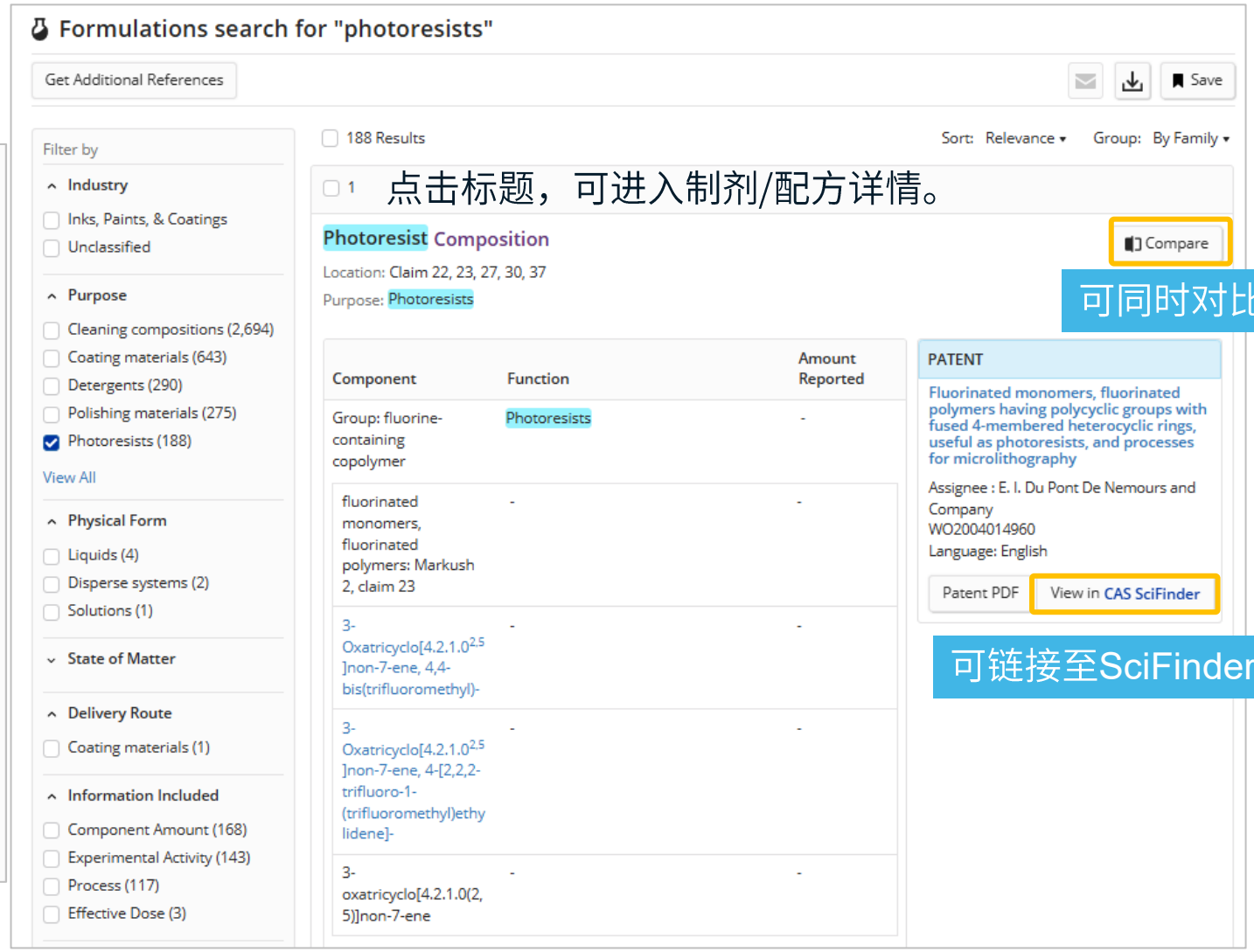
多角度筛选精炼配方检索结果

领域
用途
物理形态
物质状态
递送途径
所含信息
文献类型
机构/组织
语言
发表年份





可同时对比3种制剂/配方

可链接至SciFinder，查看文献详情页

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制剂/配方详情页

Positive Photosensitive Anionic Electrodeposition Coating Composition: Electrodeposition Coating Agents

配方用途

Purpose	Target	Delivery Route	Physical Form	Source
electrodeposition coating agents	Printed circuit boards	-	Solutions	View

Formulation Ingredients

配方成分

Expand All Gr

Component	Function	Amount Reporte
Group: vinyl copolymer	-	122 wt. parts
4,4'-[1-[4-[1-(4-Hydroxyphenyl)-1-methylethyl]phenyl]ethylidene]bis[phenol]	-	15 wt. parts
1,2-Naphthoquinonediazide-5-sulfonic acid	-	-
Water	-	418.5 wt. parts
Water	-	444.4 wt. parts

Source Patent

文献来源

Photosensitive anionic electro-deposition coating compositions for positive-working photoresists with good storage stability and high sensitivity

Assignee : Honey Kasei Co., Ltd.
JP4302178
Language: Japanese
Location: Example 1, Table 1

Patent PDF | View in CAS SciFinder

Feedback

Process

preparation of positive photosensitive anionic electrodeposition coating composition: mix vinyl copolymer (place 10.0 parts of isopropanol and 10.0 parts of butyl cellosolve in a 3-liter four-necked flask equipped with a stirrer, a reflux condenser and a nitrogen inlet tube, and heat to 90 °C. separately, 16.0 parts of isopropanol, 6 parts of acrylic acid, 1 part of 2-hydroxyethyl acrylate, 14 parts of 2-ethylhexyl acrylate, 10 parts of ethyl acrylate, 34 parts of n-butyl acrylate, 35 parts of methyl methacrylate, 1 part of mercaptoacetic acid, charge 2 parts of azobisisobutyronitrile into the dropping funnel and drop into the flask over 120 minutes, add 2 parts of isopropanol and 0.2 parts of azobisisobutyronitrile three times every 30 minutes, and the continue reaction at 90° C. for 90 minutes at temperature was below 50 °C and add 2.3 parts of dimethylaminoethanol, stir) and 4,4'-[1-[4-[1-(4-hydroxyphenyl)-1-methylethyl]phenyl]ethylidene]bisphenol with 6-diazo-5,6-dihydro-5-oxonaphthalene-1-sulfonic acid, and add deionized water while stirring, continue to effect phase inversion emulsification and electrolysis (stock solution), add water and stock solution was added while stirring to obtain an electrodeposition solution.

Experimental Activity

详细、直观的工艺步骤与实验数据

Descriptor	Notes	s
developability	the exposed printed circuit board was immersed in a 0.5% sodium metasilicate aqueous solution at 32 °C for 2 minutes to confirm whether development was possible.	Yes
etching solution resistance	after the developed printed circuit board was immersed in an etching solution of ferric chloride at 40 °C for 5 minutes, the electrodeposition coating film was checked for cracks and creases.	good
	the composition was allowed to stand for 24 hours, and the presence or absence of sediments deposited on the bottom of the container was confirmed.	No sedimentation
	-	10 μM

Feedback

无需阅读原文
即可获取配方详情

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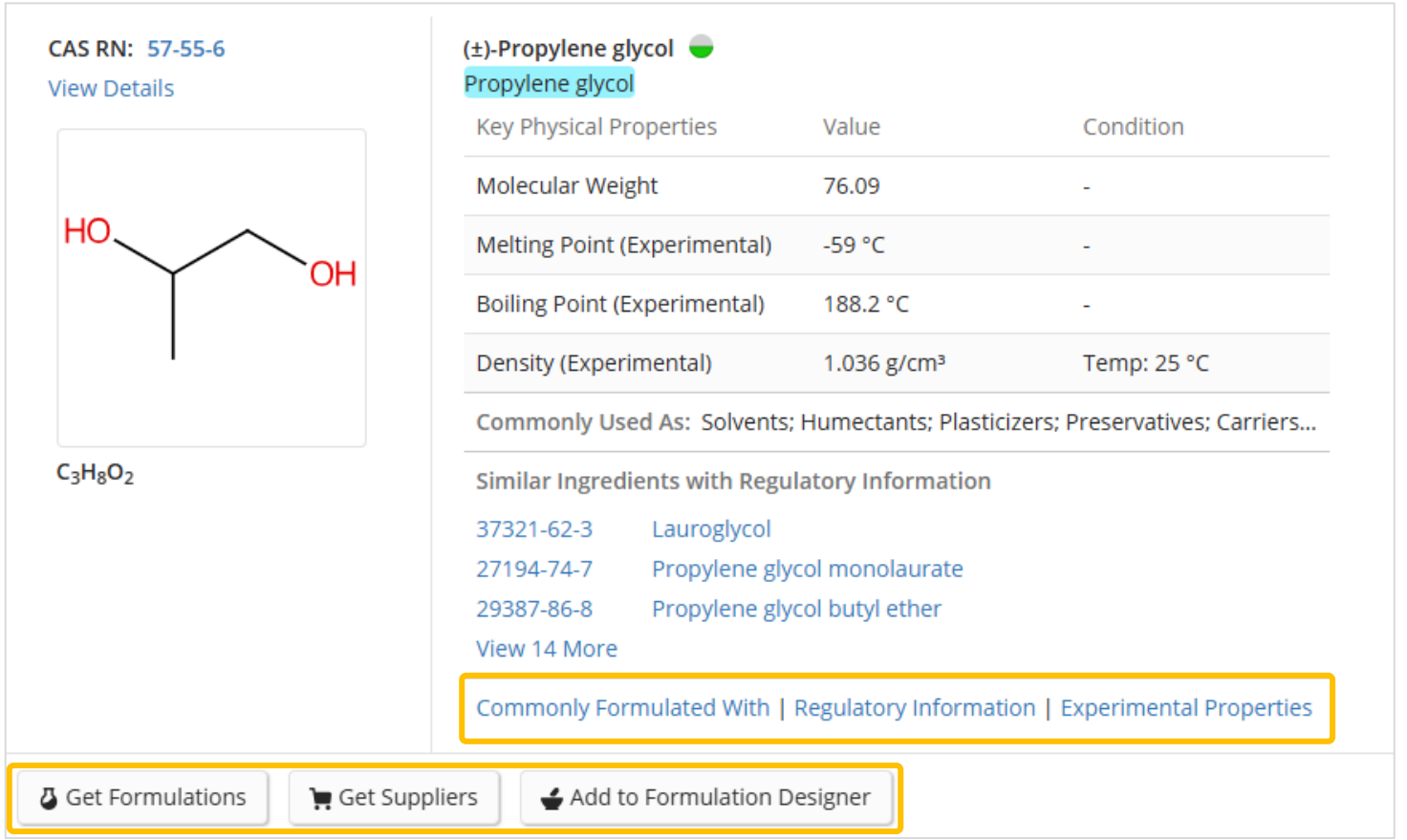
制剂、配方主要成分检索

- 制剂或配方中，与该原料同时使用的其它配伍成分
- 管控信息及清单
- 实验属性



- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至设计工具 Formulation Designer

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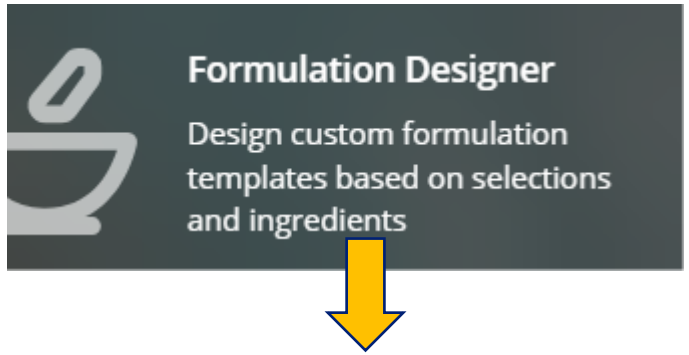
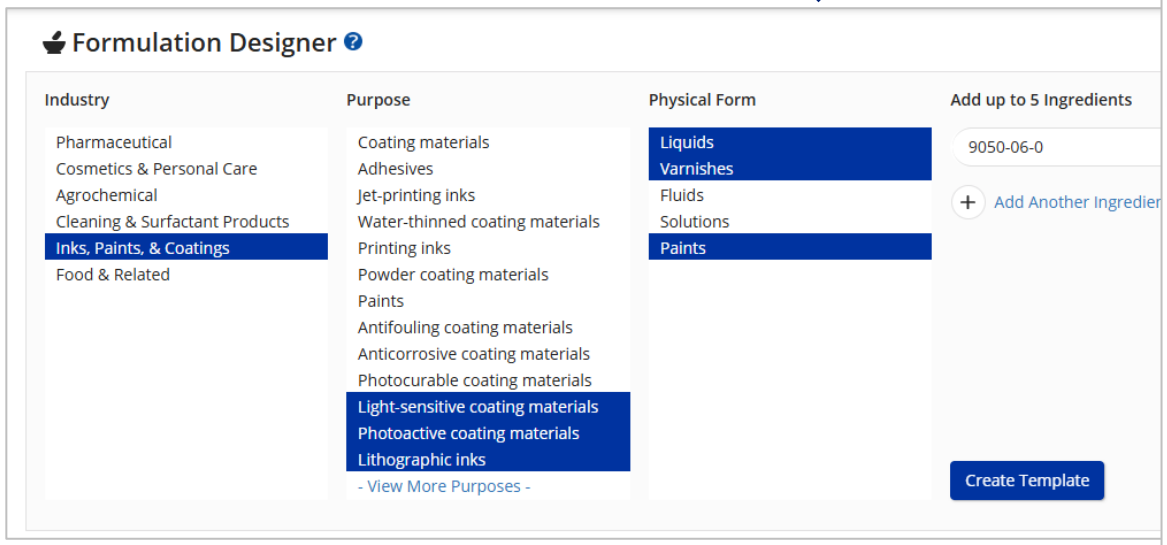
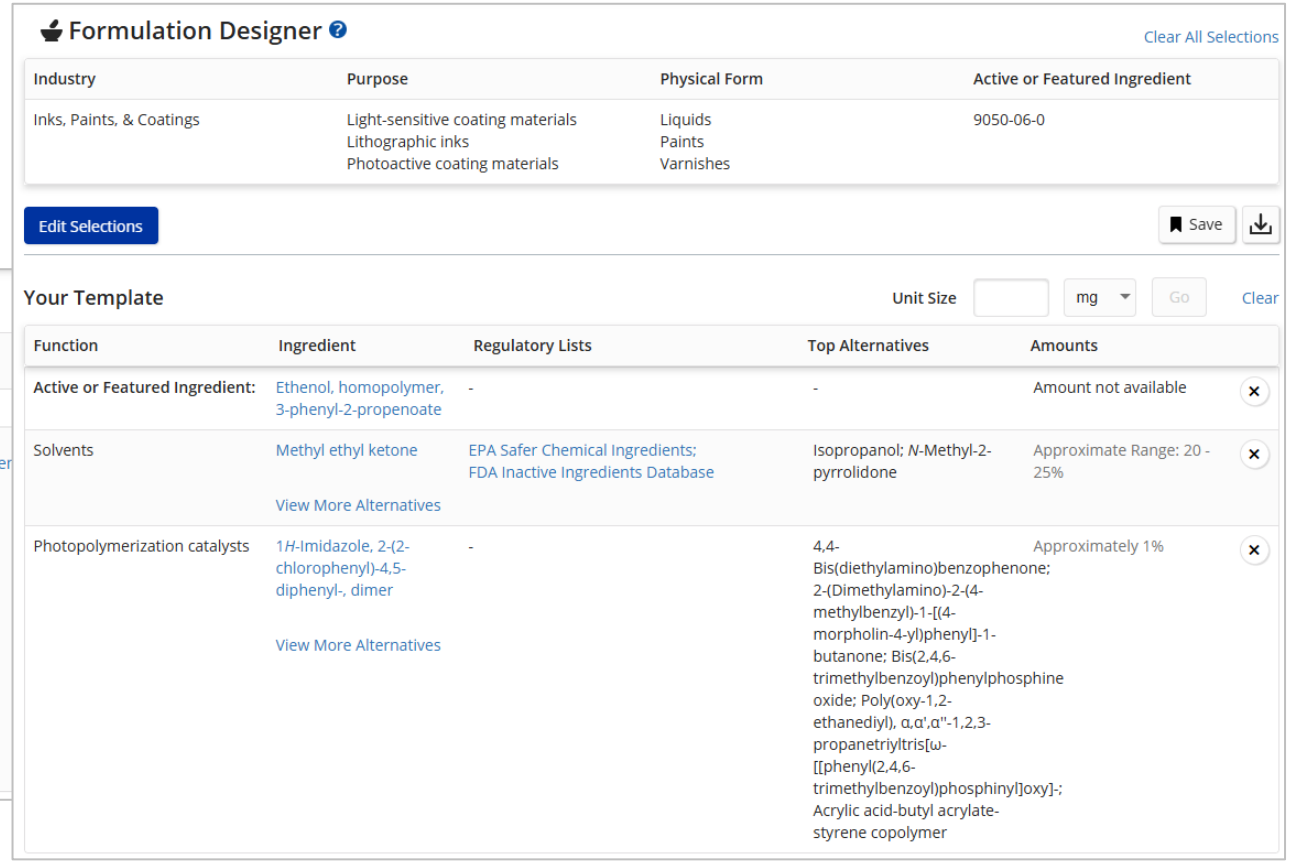
Formulation Designer辅助设计制剂、配方

启发制剂配方设计







基于期刊、专利和产品说明书中标引的制剂、配方数据，获得见解。

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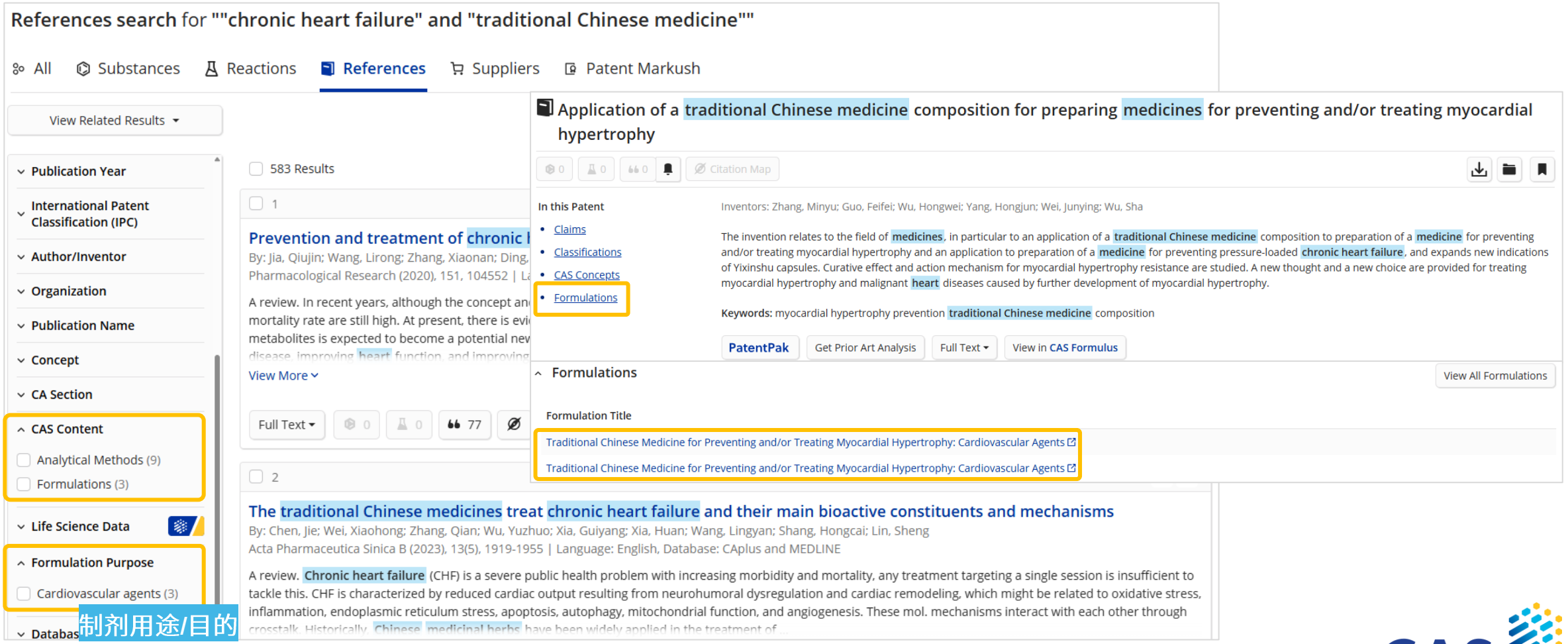
文献关联的配方/制剂

在CAS SciFinder的文献结果集页面，点击CAS Content中的 Formulation 获得有具体配方或制剂信息的文献，从文献详情页中链接获取



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小结

1. 利用CAS Analytical Methods进行主题检索或分类浏览获得分析方法，或通过文献查看关联的分析实验及数据详情
2. 利用CAS Formulus检索原料、配方/制剂，或通过文献结果集获得关联的配方/制剂信息；利用配方设计工具启发产品配方的开发

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总结

- CAS 内容合集来源于化学并超越于化学，支持多学科、跨学科研发创新
- 全面覆盖的内容确保不遗漏任何重要的信息
- CAS 科学家人工智慧与先进专有技术结合标引的数据，能够揭示隐藏在数据间的隐秘关联
- 强大的功能确保降低文献检索和分析的时间，将更多宝贵的时间应用于创新工作中，提升科研创新效率

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CAS SciFinder 检索浏览器推荐

浏览器推荐：

- Windows（7，8.1，10)：Chrome 60及更高版本，Firefox 55及更高版本，Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13)：Safari 9.3及更高版本，Chrome 60及更高版本，Firefox 55及更高版本，Firefox 52 (ESR)
- **不建议使用360浏览器，相关功能或插件会被自动拦截**

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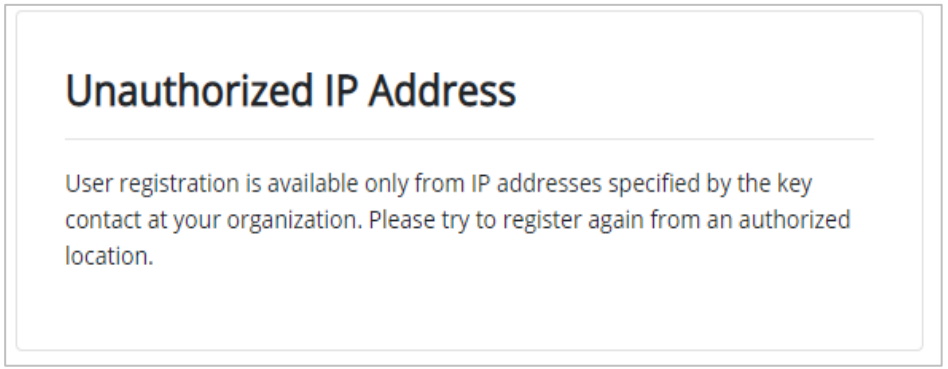
常见问题



- 检查注册链接是否正确
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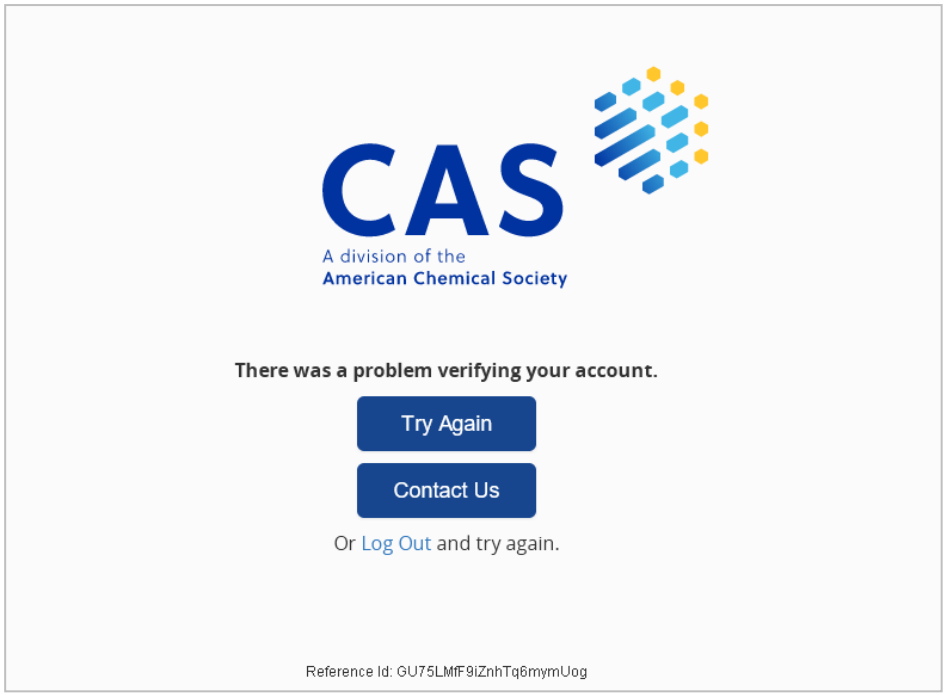

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使用注意事项

- 一人注册一个帐号
- 实名注册，请提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（https://www.cas.org/legal/infopolicy）
- 不得账号分享
- 不得将账号用于非学术研究

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CAS SCIFINDER DISCOVERY PLATFORM

2025 秋季专题论坛直播时间表

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演讲人：杜德鑫 博士

10 月 23 日 | 最新进展及在知识产权工作流程中的应用

演讲人：钱欣 博士

11 月 13 日 | 助力生物医药研发创新与可持续发展

演讲人：陈开乾 博士

12 月 18 日 | 独特数据与AI技术结合赋能研发突破

演讲人：钱欣 博士

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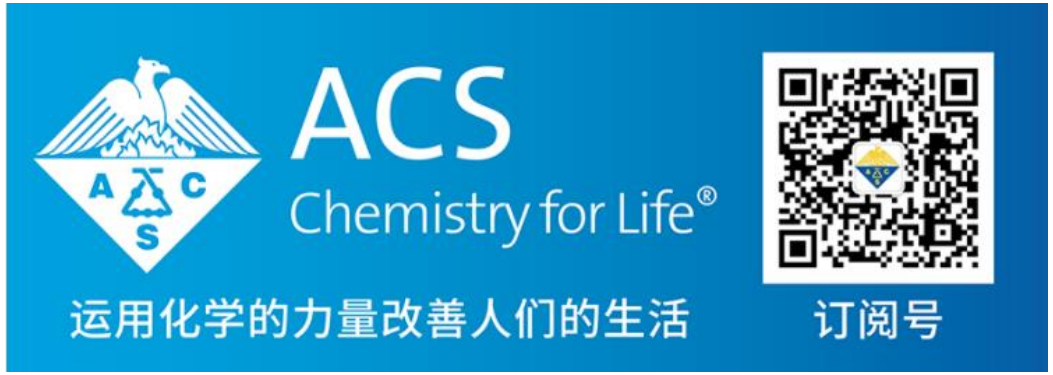

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Between problems and progress are connections that matter

谢谢！

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