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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 (Academic)简介
- 科研信息的高效查阅
  - 如何拓展文献调研?
  - 如何调研某类物质?
  - 如何调研反应信息?
  - 怎么查、怎么选具体的实验方案?
- 常见问题Q&A

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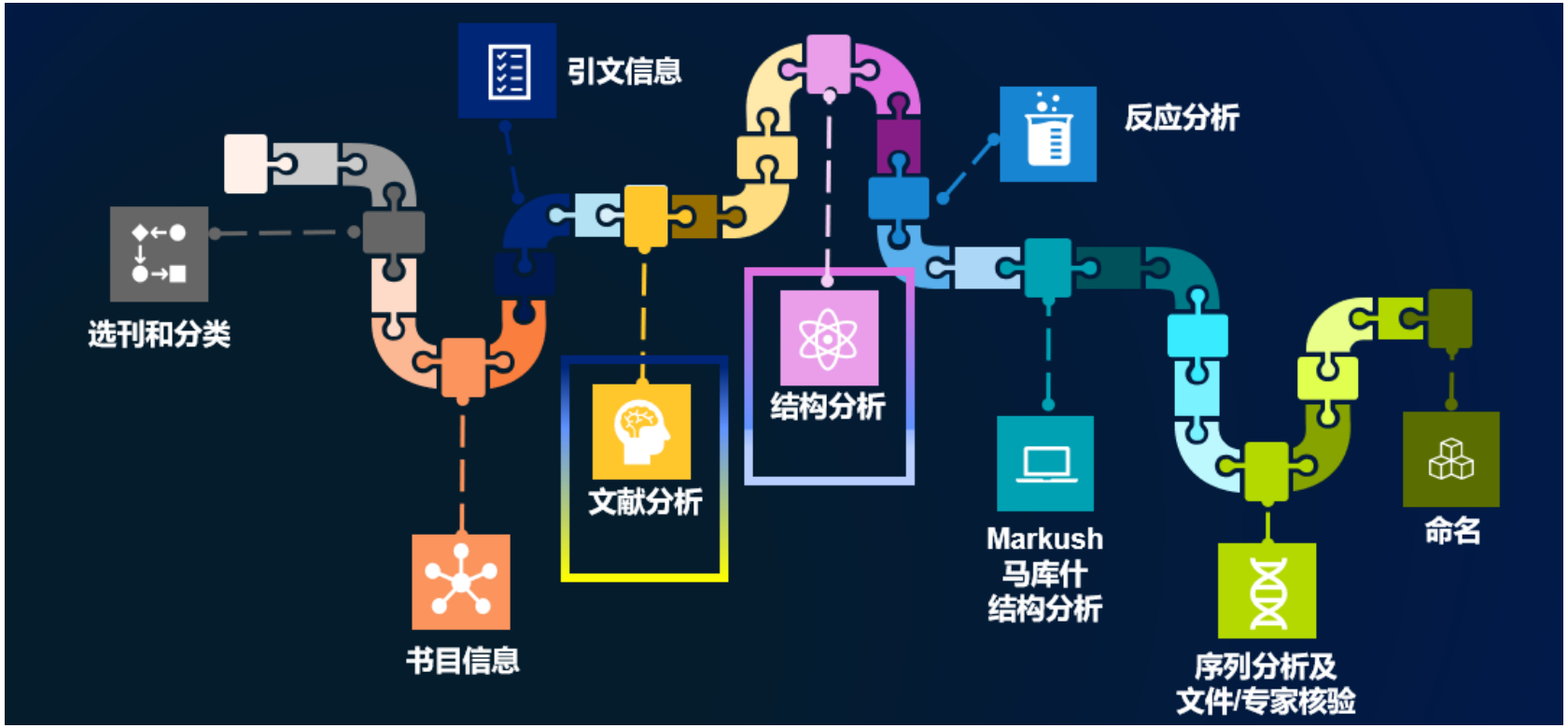

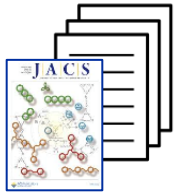

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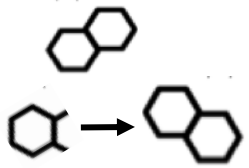

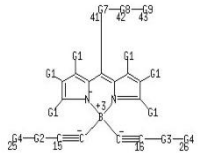

Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17β)-

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CAS科学家增值的文献研究

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Journal of Medicinal Chemistry
Article
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Structure-Based Design of Novel Class II c-Met Inhibitors: 2. SAR and Kinase Selectivity Profiles of the Pyrazolone Series

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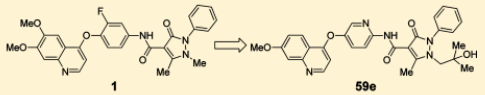
Supporting Information



ABSTRACT: As part of our effort toward developing an effective therapeutic agent for c-Met-dependent tumors, a pyrazolone-based class II c-Met inhibitor, *N*-(4-((6,7-dimethoxyquinolin-4-yl)oxy)-3-fluorophenyl)-1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazole-4-carboxamide (**1**), was identified. Knowledge of the binding mode of this molecule in both c-Met and VEGFR-2 proteins led to a novel strategy for designing more selective analogues of **1**. Along with detailed SAR information, we demonstrate that the low kinase selectivity associated with class II c-Met inhibitors can be improved significantly. This work resulted in the discovery of potent c-Met inhibitors with improved selectivity profiles over VEGFR-2 and IGF-1R that could serve as useful tools to probe the relationship between kinase selectivity and in vivo efficacy in tumor xenograft models. Compound **59e** (AMG 458) was ultimately advanced into preclinical safety studies.

INTRODUCTION

The receptor tyrosine kinase (RTK) c-Met is mainly expressed by epithelial cells. Activation of c-Met is regulated by its ligand, hepatocyte growth factor (HGF), also known as scatter factor (SF).[1] Upon binding of HGF at the extracellular domain, c-Met receptor undergoes dimerization that results in transphosphorylation of the intracellular tyrosine residues (Y1234, Y1235) within the catalytic site.[2] Further phosphorylation of residues Y1349 and Y1356 mobilizes the intracellular C-terminal docking domain that recruits and subsequently activates a wide range of downstream signaling molecules (e.g., Grb2, Gab1, PI3K, Akt, Ras, Erk, and STAT3) that modulate the survival, proliferation, migration, and invasion of cells. As such, normal HGF/c-Met signaling plays an important role during embryogenesis and tissue injury repair.[3] On the other hand, dysregulation of this pathway (through, e.g., either overexpression of HGF/c-Met or activating mutation of *MET* gene) can render many cellular processes unchecked and promote tumorigenesis. It has been established that aberrant signaling of the HGF/c-Met pathway correlates with aggressive tumor growth and poor prognosis in cancer patients.[4] Different approaches to inhibition of the HGF/c-Met pathway in cancer cells have been documented.[5] These include antagonistic ligands to c-Met, antibodies against either HGF or c-Met, and small molecule kinase inhibitors targeting the intracellular kinase domain. Numerous c-Met kinase inhibitors have been reported in the literature.[6] These inhibitors can be categorized into either class I or class II based on their binding mode in the c-Met kinase domain (vide infra). While class I molecules tend to be very selective for c-Met, thus far, a majority of the class II molecules are multikinase inhibitors. Improving the selectivity of class II c-Met inhibitors has been a significant challenge. In fact, until recently, no selective class II c-Met inhibitors have been reported and little is known as to whether the kinase selectivity profiles of class II c-Met inhibitors can be improved. Schroeder et al. reported the design of a pyridone-based c-Met inhibitor that was selective over a number of kinases, including IGF-1R.[7] The selectivity over VEGFR-2 was modest (46-fold). We postulated that knowledge from kinase structural analysis

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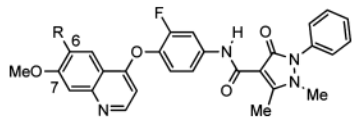
Table 1. Modification of the Quinoline Ring[a]



compd	R	c-Met K_i	VEGFR-2 K_i	VEGFR-2 fold	IGF-1R K_i	IGF-1R fold	PC3 IC_{50}
1	OMe	1	7.8	8	32.1	32	20.2
11a	Br	5.1	78.9	16	149	29	652
11b	Me	3.4	–	–	146	43	461
11c	Et	2.4	38	16	70.2	29	534
11d	H	1.1	23.7	22	178	162	37.1

[a] K_i (nM): inhibitory constant for the phosphorylation of gastrin by c-Met, VEGFR-2, or IGF-1R. Fold: ratio of K_i(kinase)/K_i(c-Met). PC3 IC_{50} (nM): inhibitory concentration for HGF-mediated c-Met phosphorylation in PC3 cells. Both K_i and IC_{50} values are reported as an average for $n > 2$. See Supporting Information for standard deviations.

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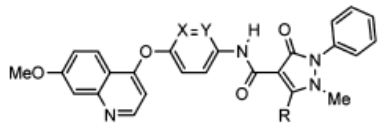
Table 3. Effects of C5-Substituents on Selectivity Profiles[a]



compd	R	X	Y	c-Met K_i	VEGFR-2 K_i	VEGFR-2 Fold	IGF-1R K_i	IGF-1R Fold	PC3 IC_{50}
11d	CH_3-	CF	CH	1.1	23.7	22	178	162	37.1
22a	CH_3-	CH	N	1.2	42	35	618	515	83
26b	NH_2CH_2-	CF	CH	1.4	541	378	928	649	42
26a	$BocNHCH_2$-	CF	CH	29	1240	43	>6600	>230	–
26c	$Et(Me)NCH_2$-	CF	CH	2.3	903	386	744	317	76.7
26d		CF	CH	1.5	1310	879	1800	1206	83.9

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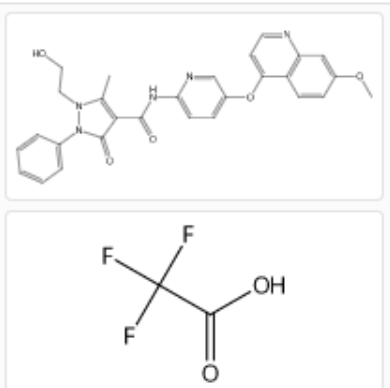
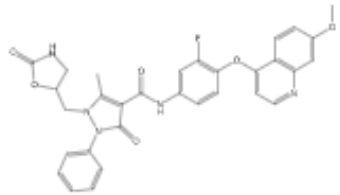


$C_{28}H_{25}N_5O_5.xC_2HF_3O_2$
1*H*-Pyrazole-4-carboxamide, 2,3-dihydro-1-(2-hydroxyethyl)-*N*-[5-[(7-methoxy-4-qui...

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

1361236-60-3



$C_{31}H_{26}FN_5O_6$
N-[3-Fluoro-4-[(7-methoxy-4-quinolinyl)oxy]phenyl]-2,3-dihydro-5-methyl-3-oxo-1-...

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

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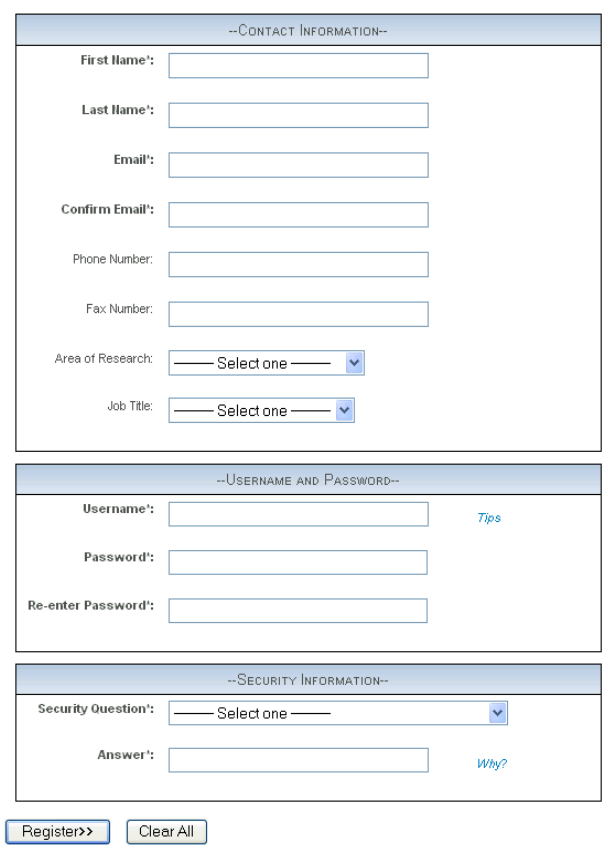

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- _（下划线）
- .(句点)
- @（表示“at”的符号）

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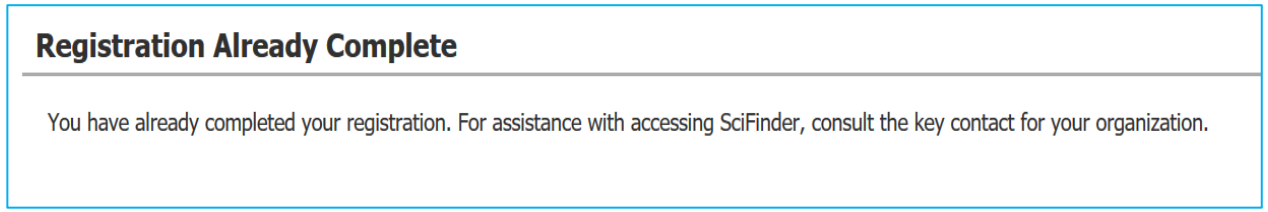

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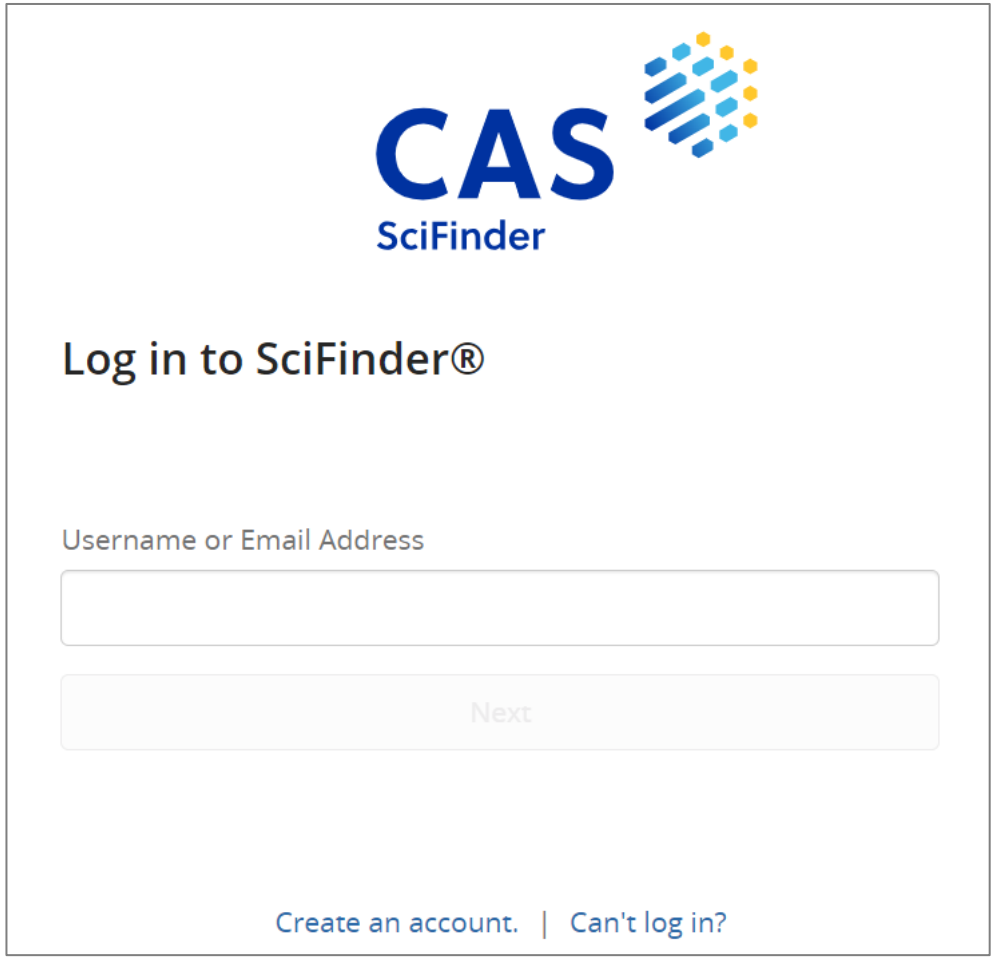

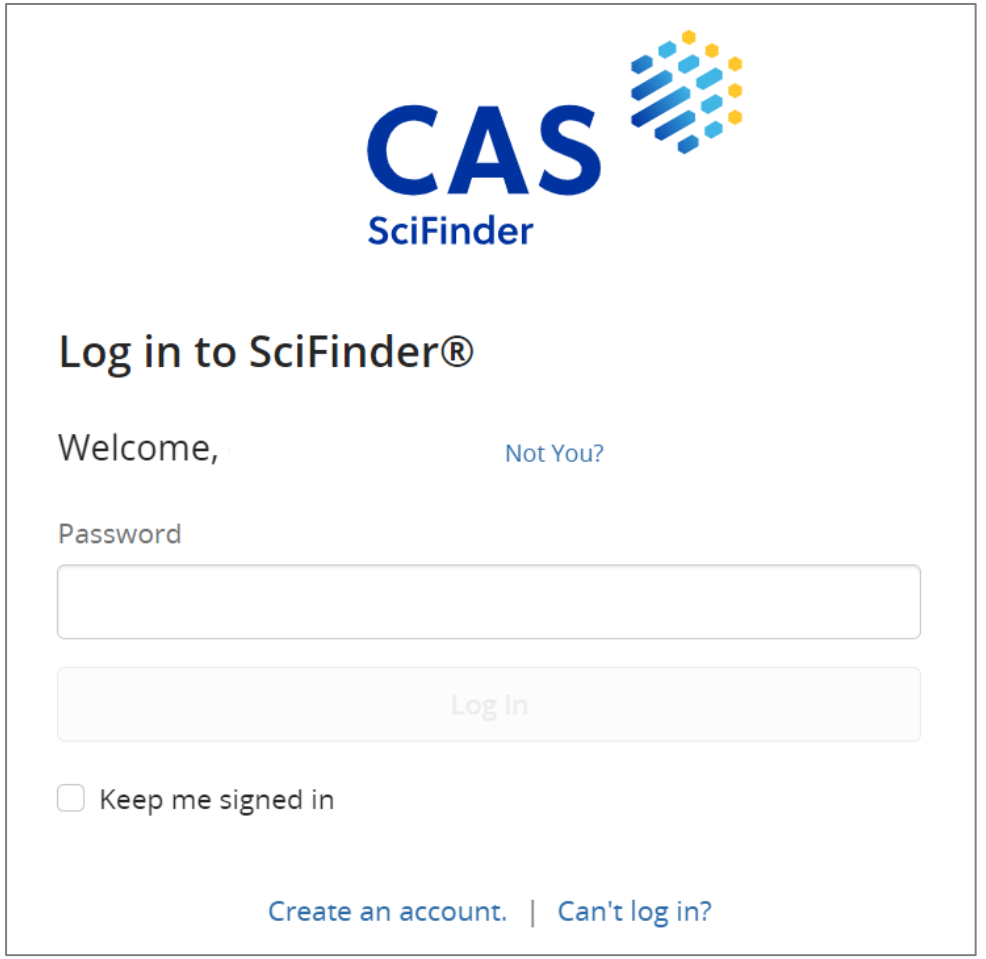

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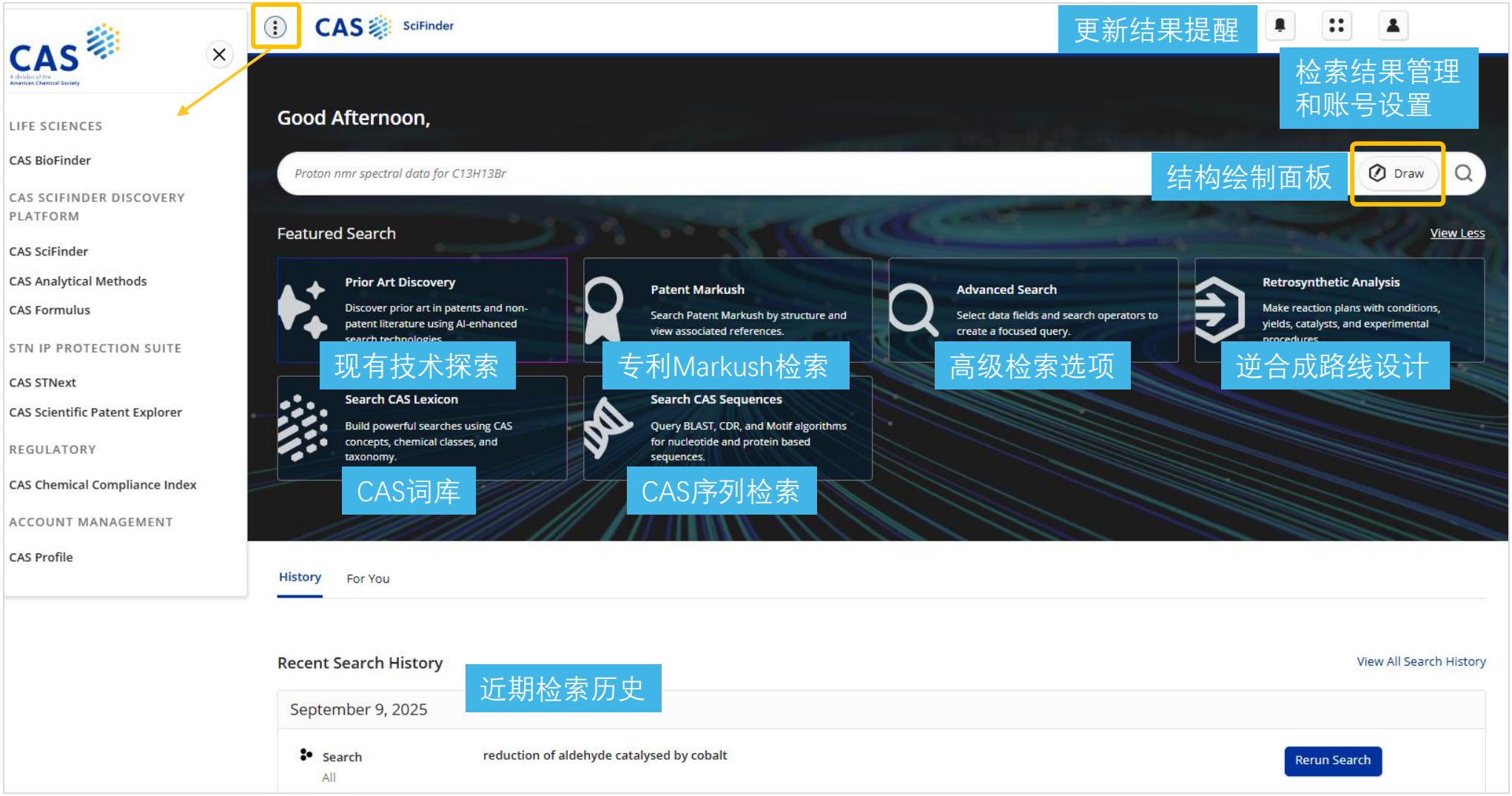

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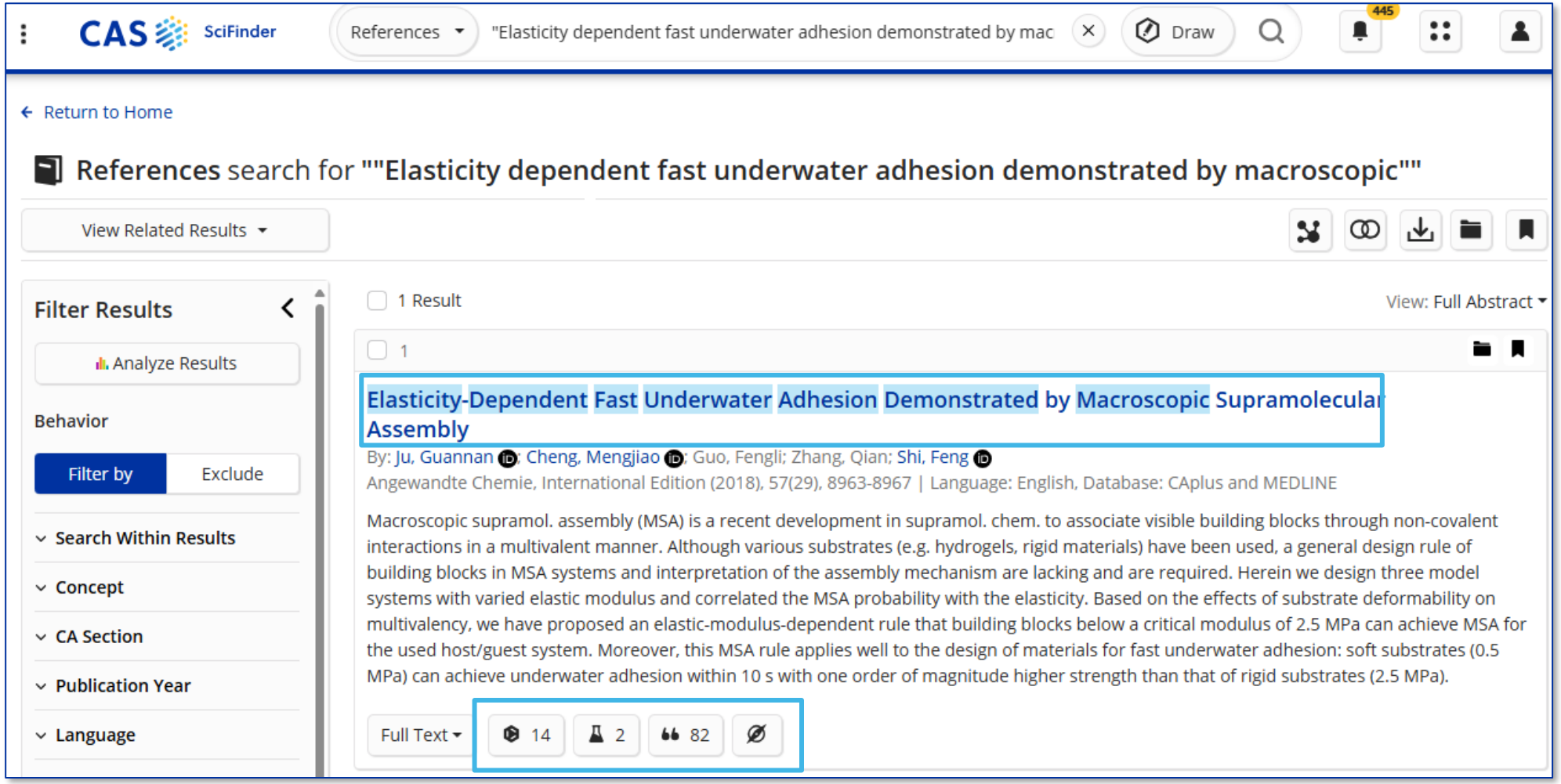

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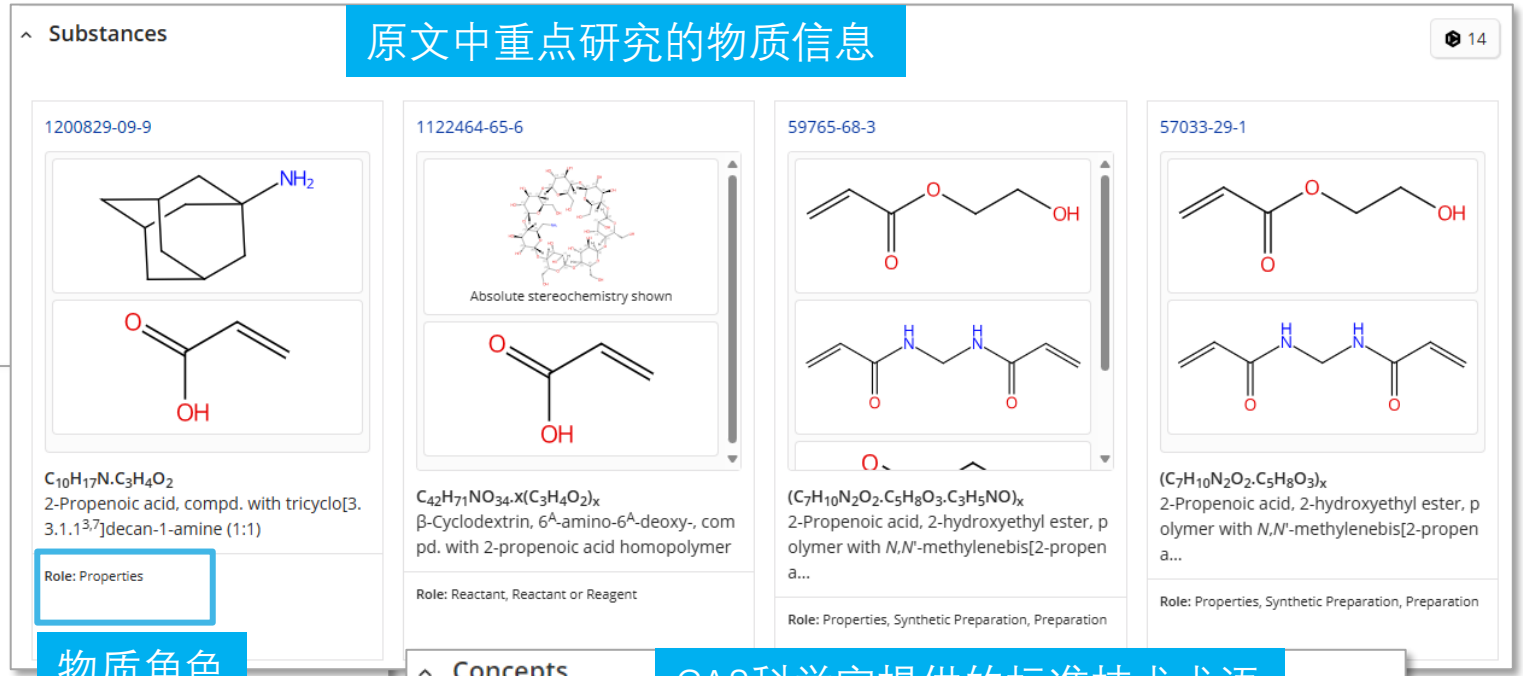

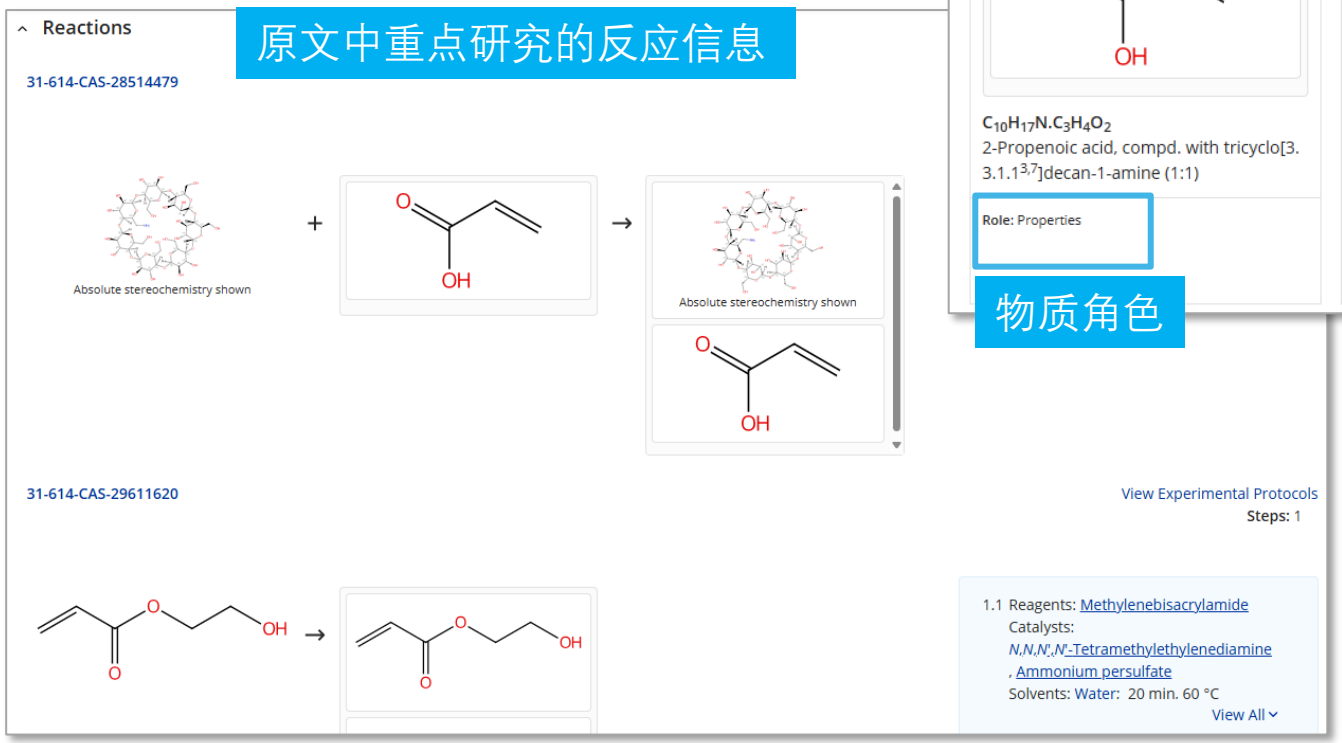

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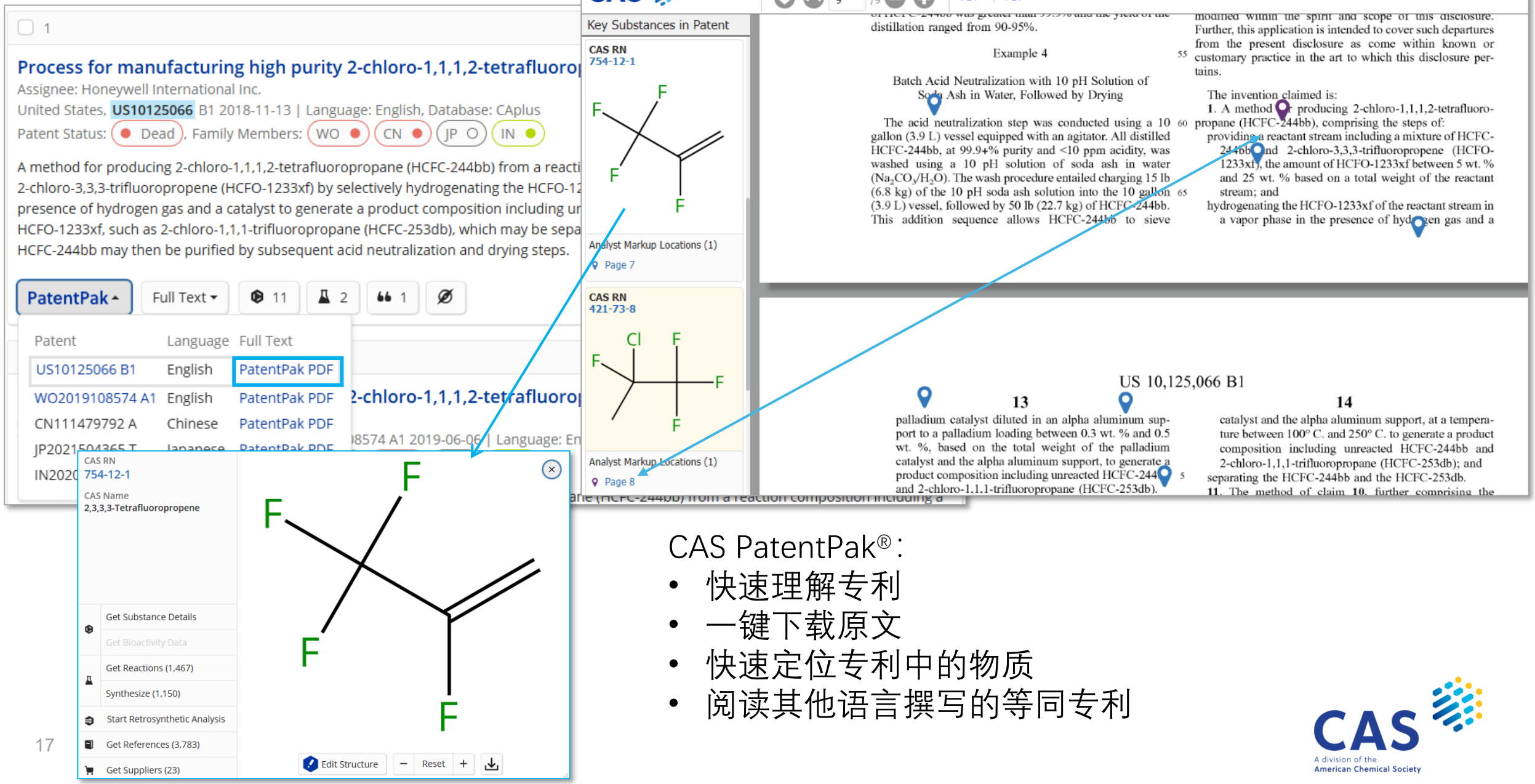

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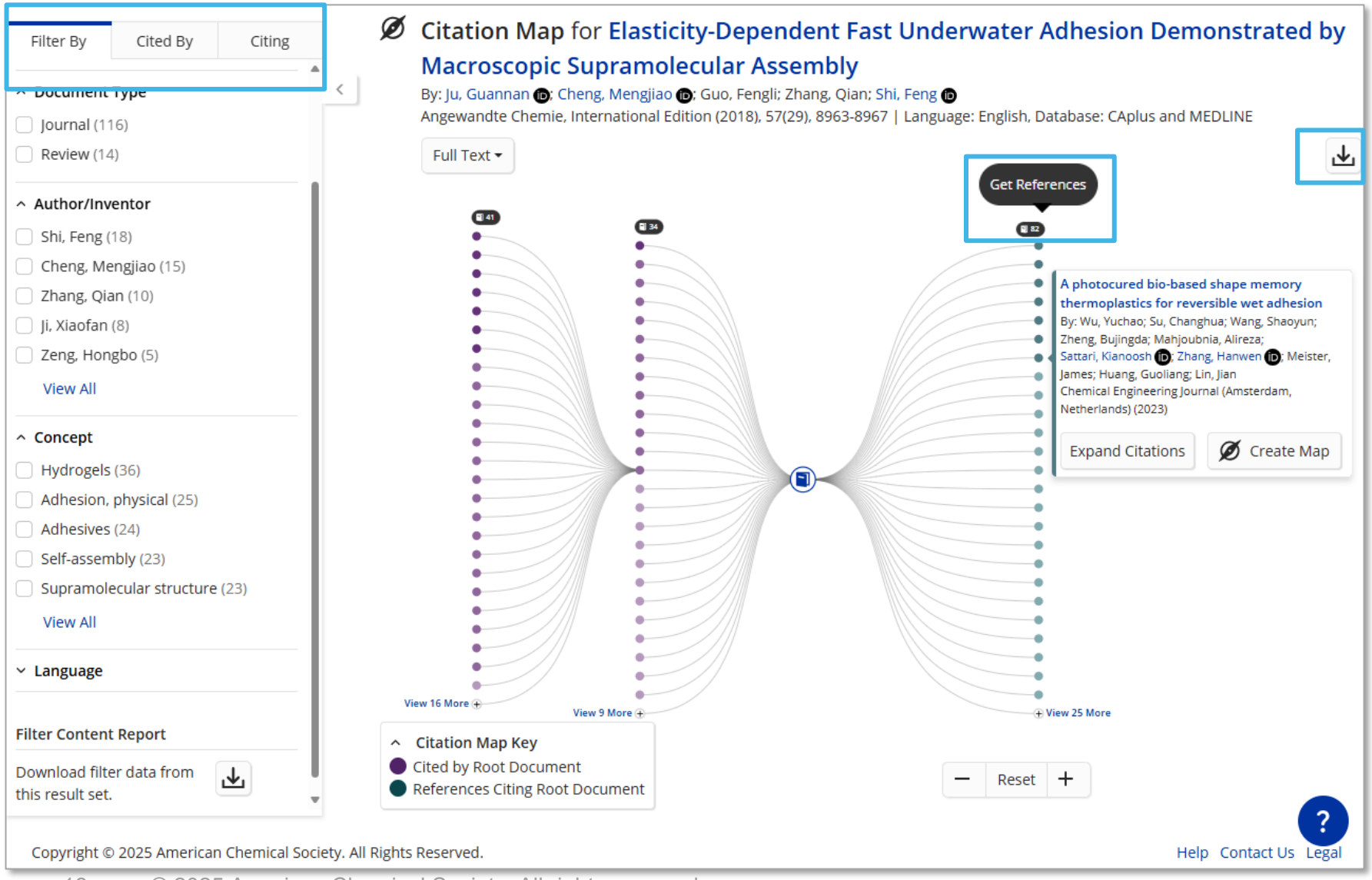

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1.2 如何选择概念词？借助CAS Lexicon词库

- 在CAS词库层级中浏览CAS标引的概念词（Concepts）和物质
- 建立用于检索文献的检索式（最多可用1000个词）

在CAS Lexicon词库层级中选择适合的主题词：

- Preferred Concept
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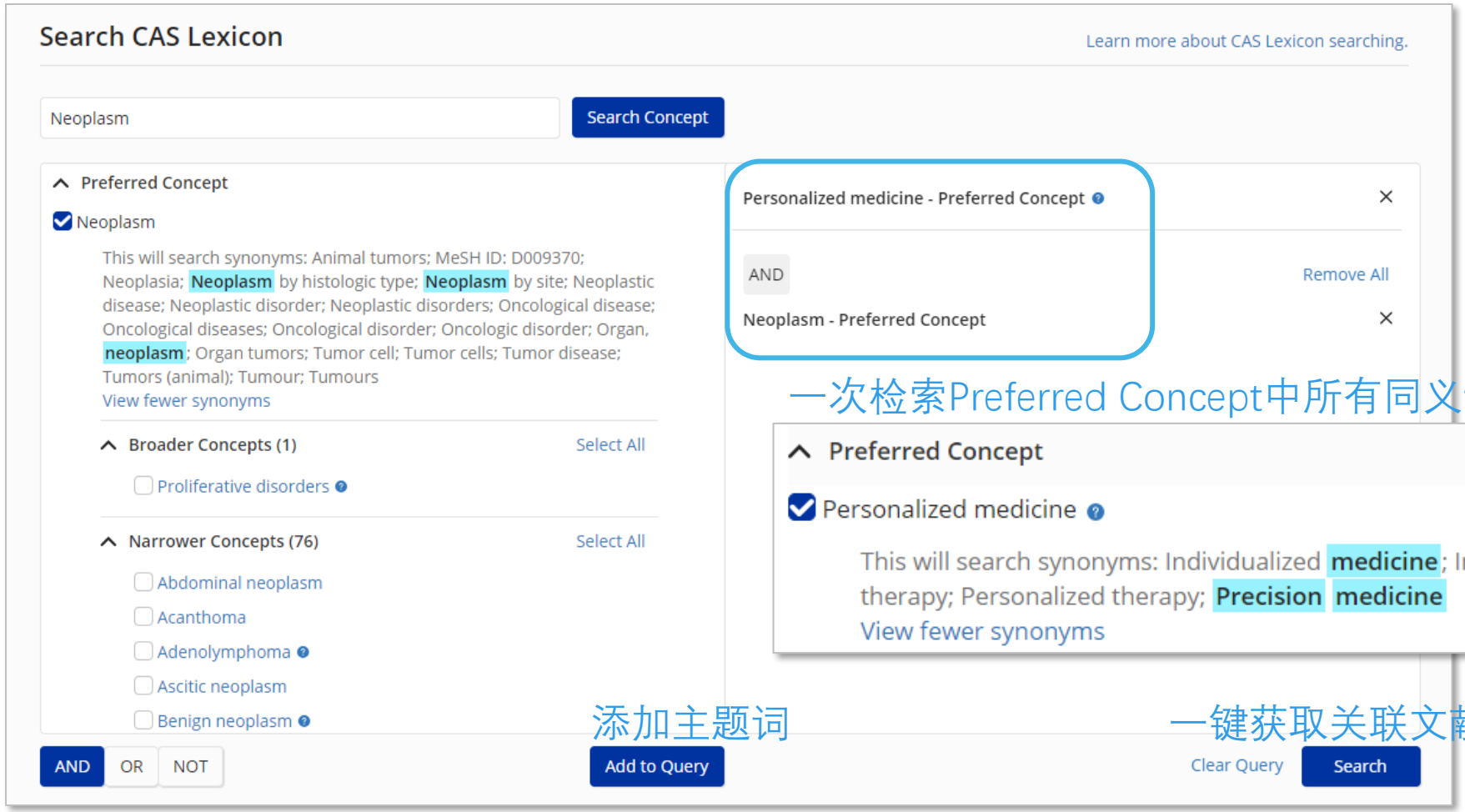
- Narrower Concepts
- Related Concepts



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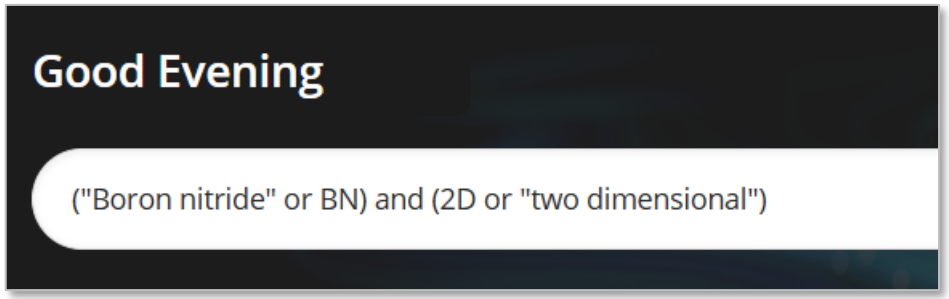
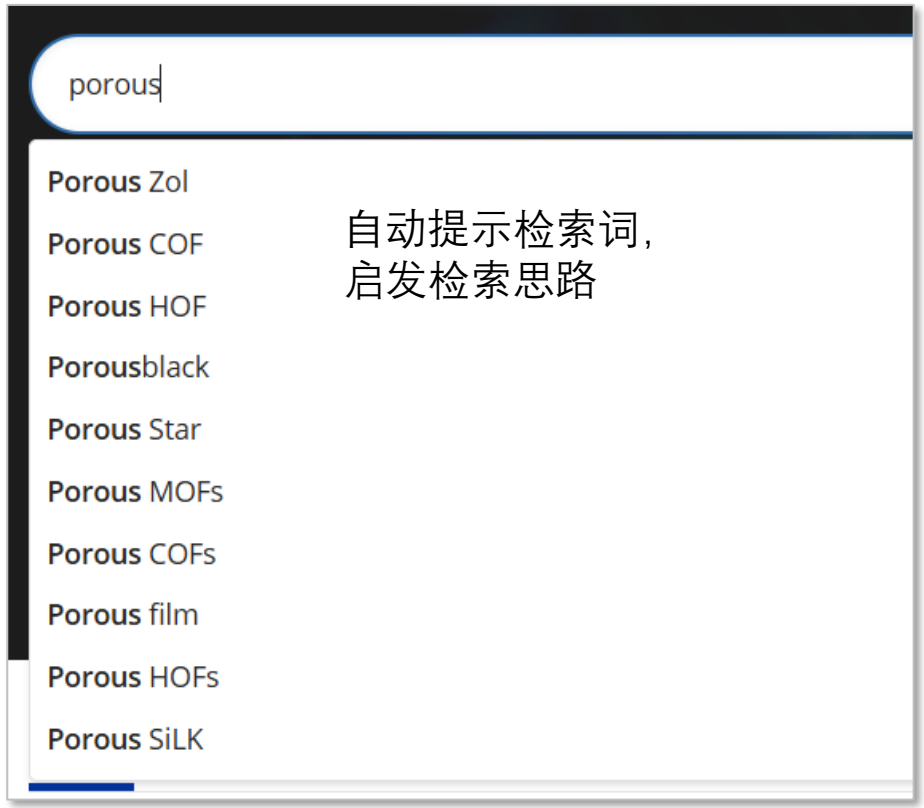
- 支持通配符*或？，如 poly*可代表polymer, polymerization, polyethylene等（* 代表0或多个字符；？代表0或1个字符）





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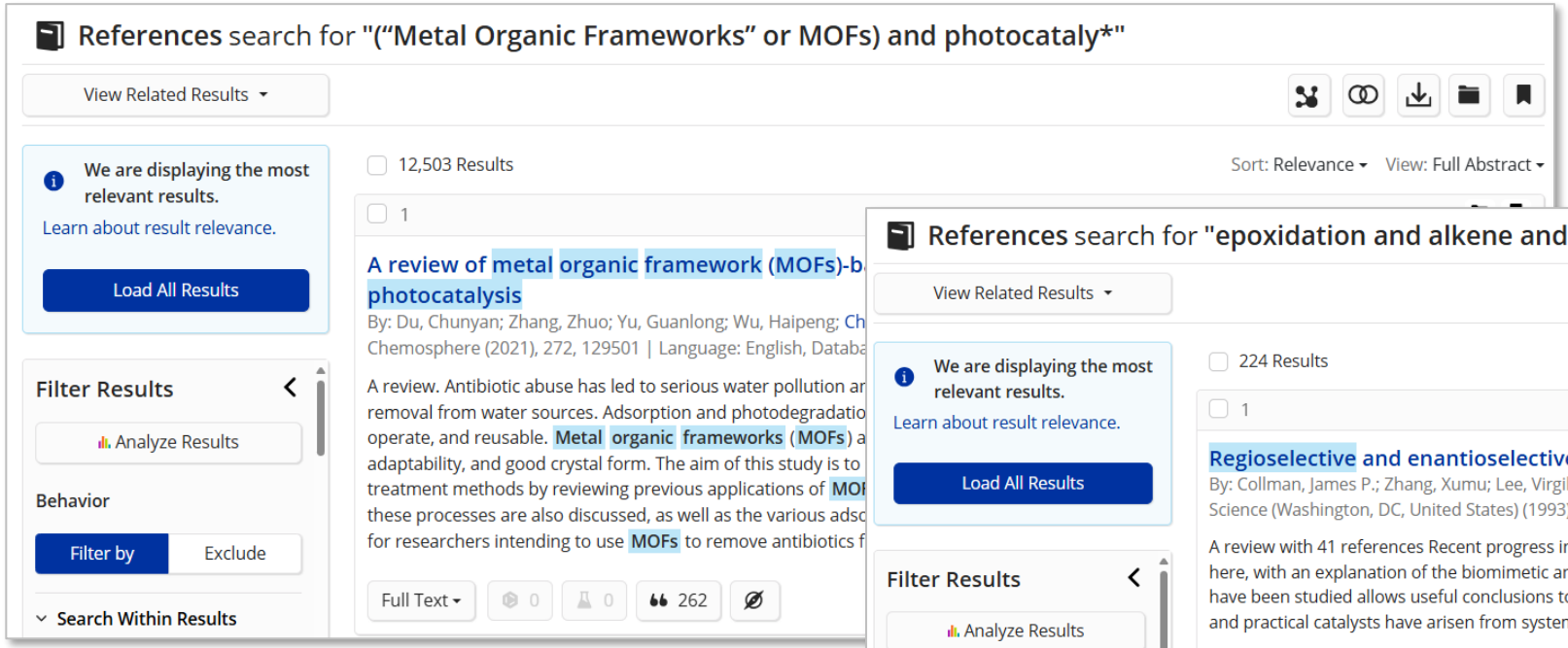
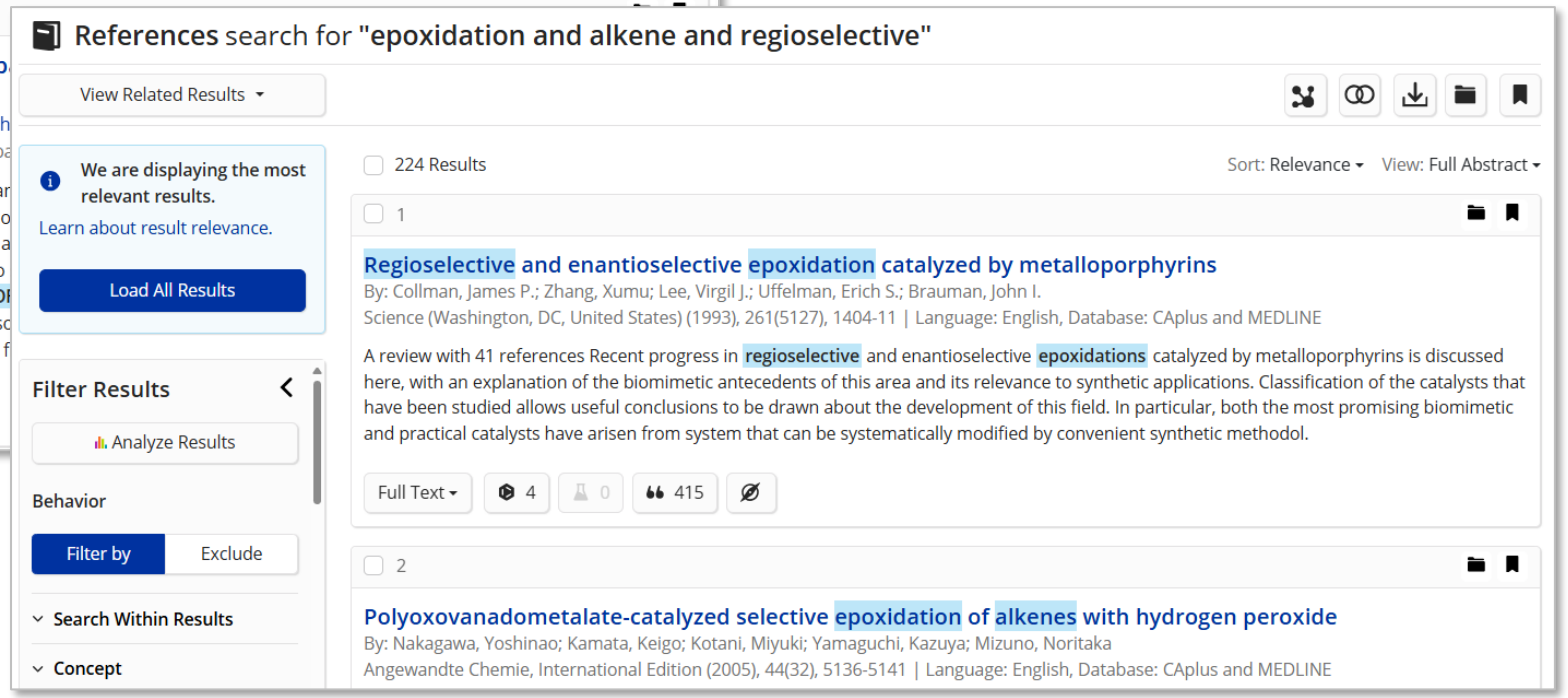


epoxidation and alkene and regioselective
检索：烯烃、选择性和环氧化



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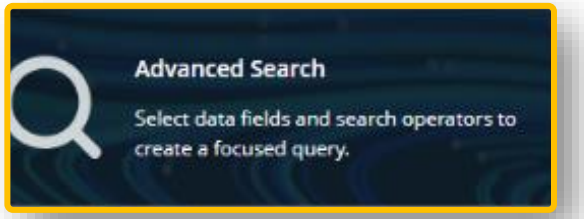
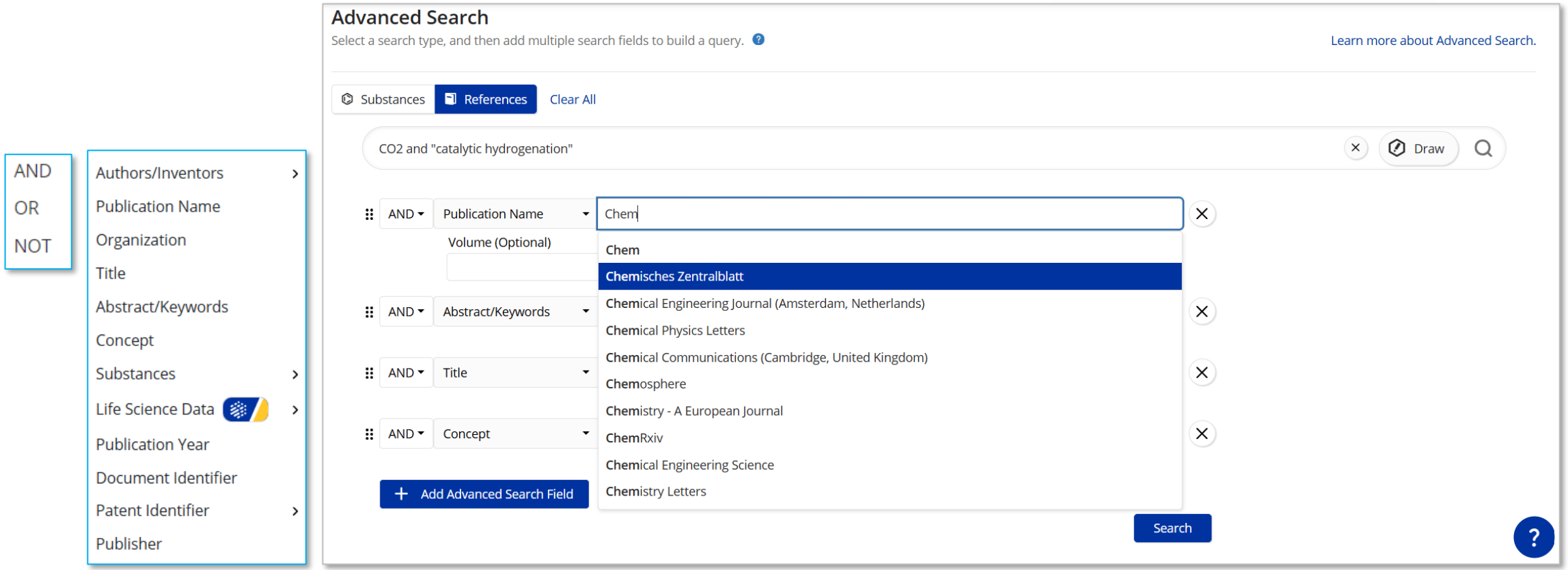
自定义组合检索

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）；
- 结构检索（包括物质结构和反应式）





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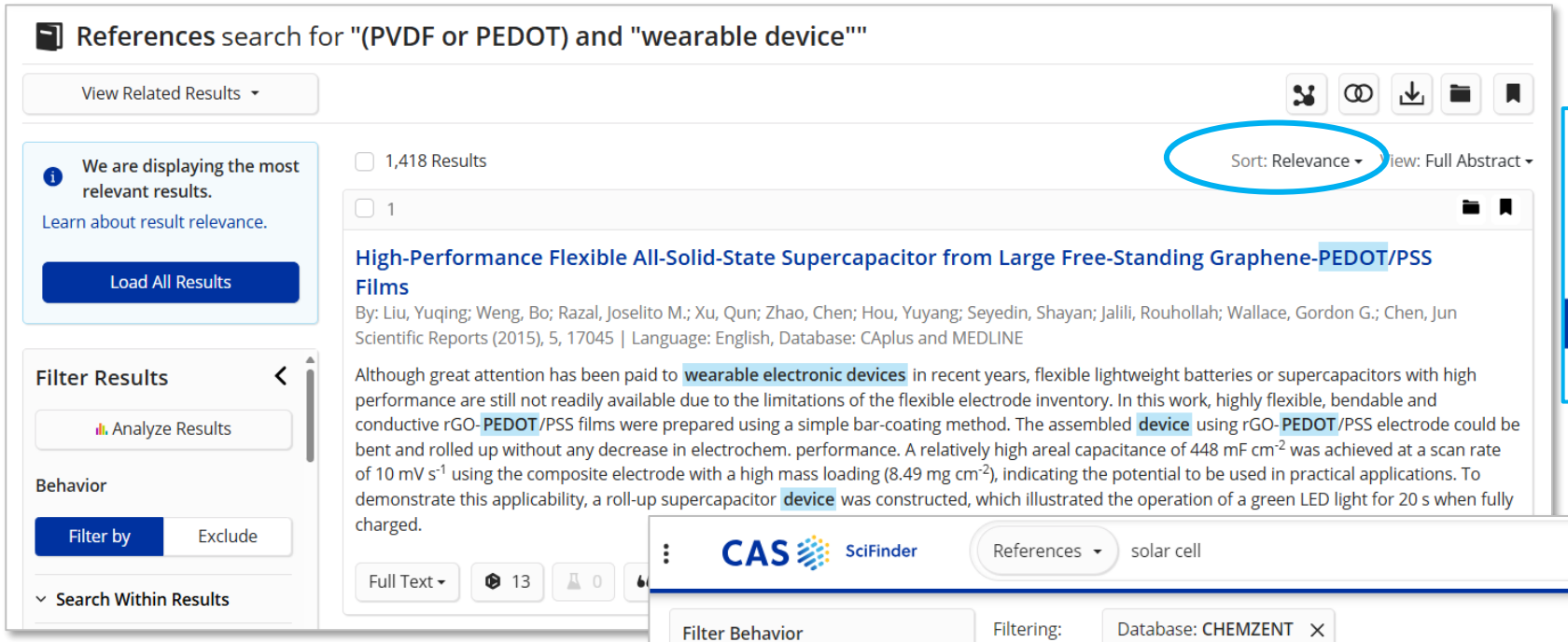
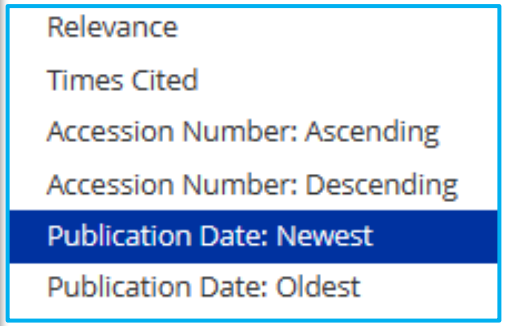
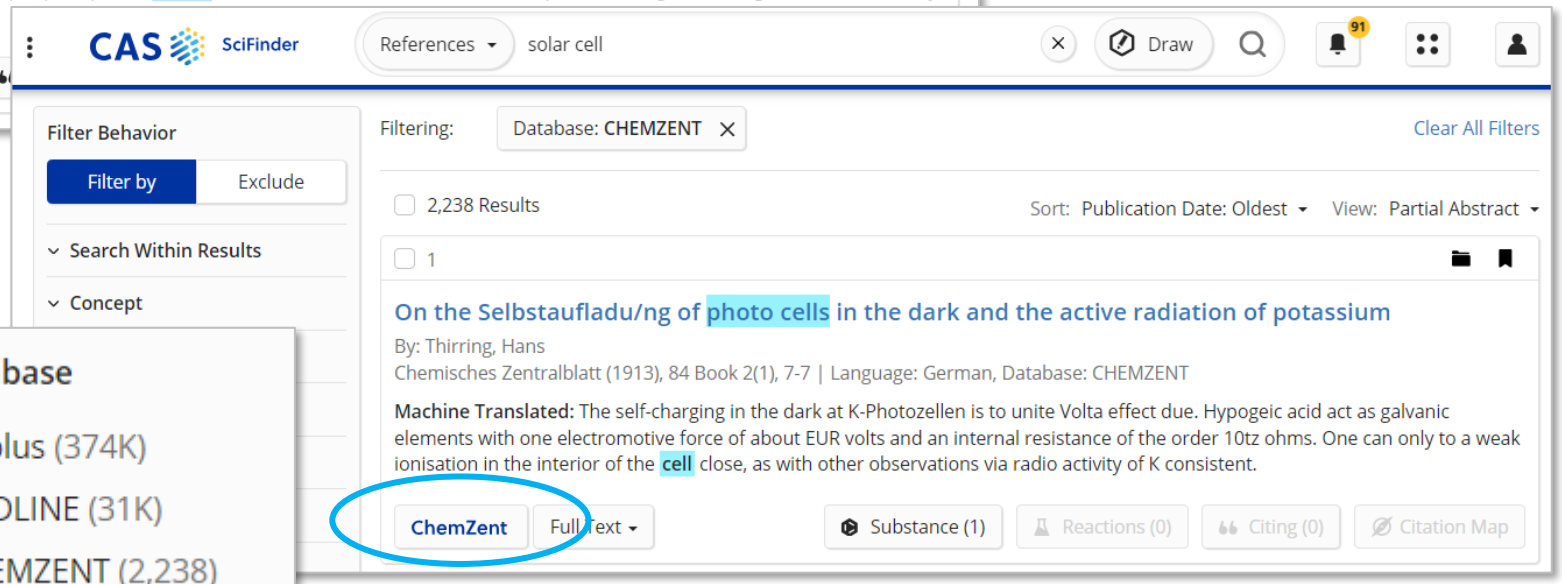
1.3 文献结果：最新 & 引用最多 & 早期科学研究





排序方式：
相关性
引用次数
收录号
发表时间



- ChemZent®：最早期的化学文摘——德国化学文摘的英文版，唯一提供可用英文获取德国化学文摘的解决方案，将化学研究相关文献回溯至十九世纪初。

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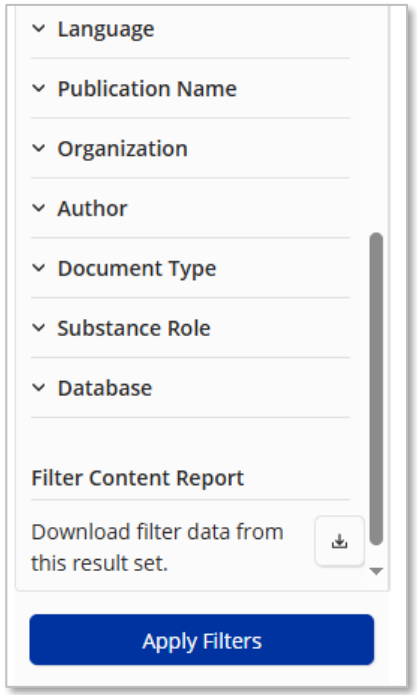
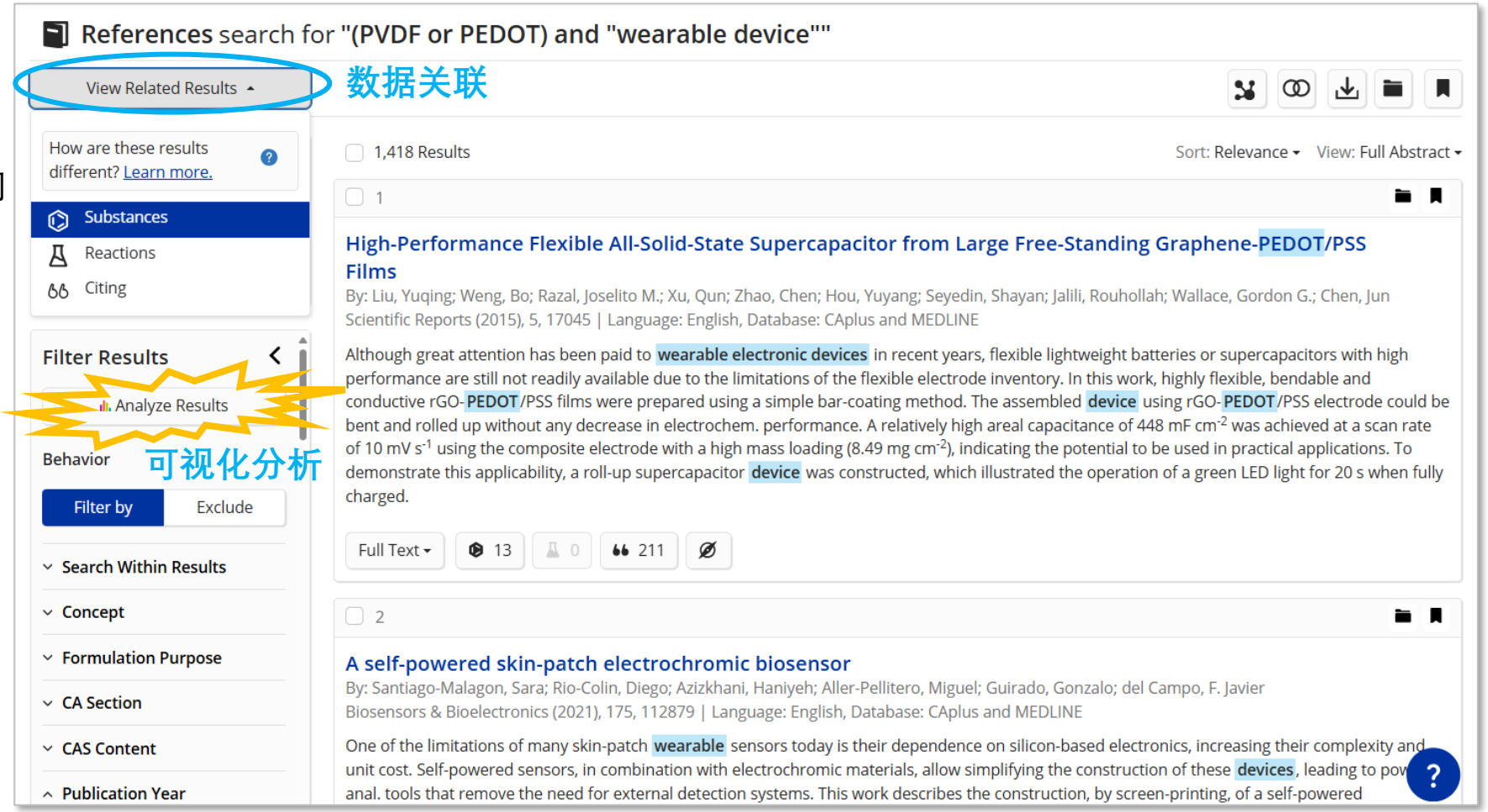
筛选目标文献

文献类型、语言、作者
发表机构、发表年份
CAS标引的技术术语
CAS标引的学科研究方向
二次检索
下载数据分析报告
…





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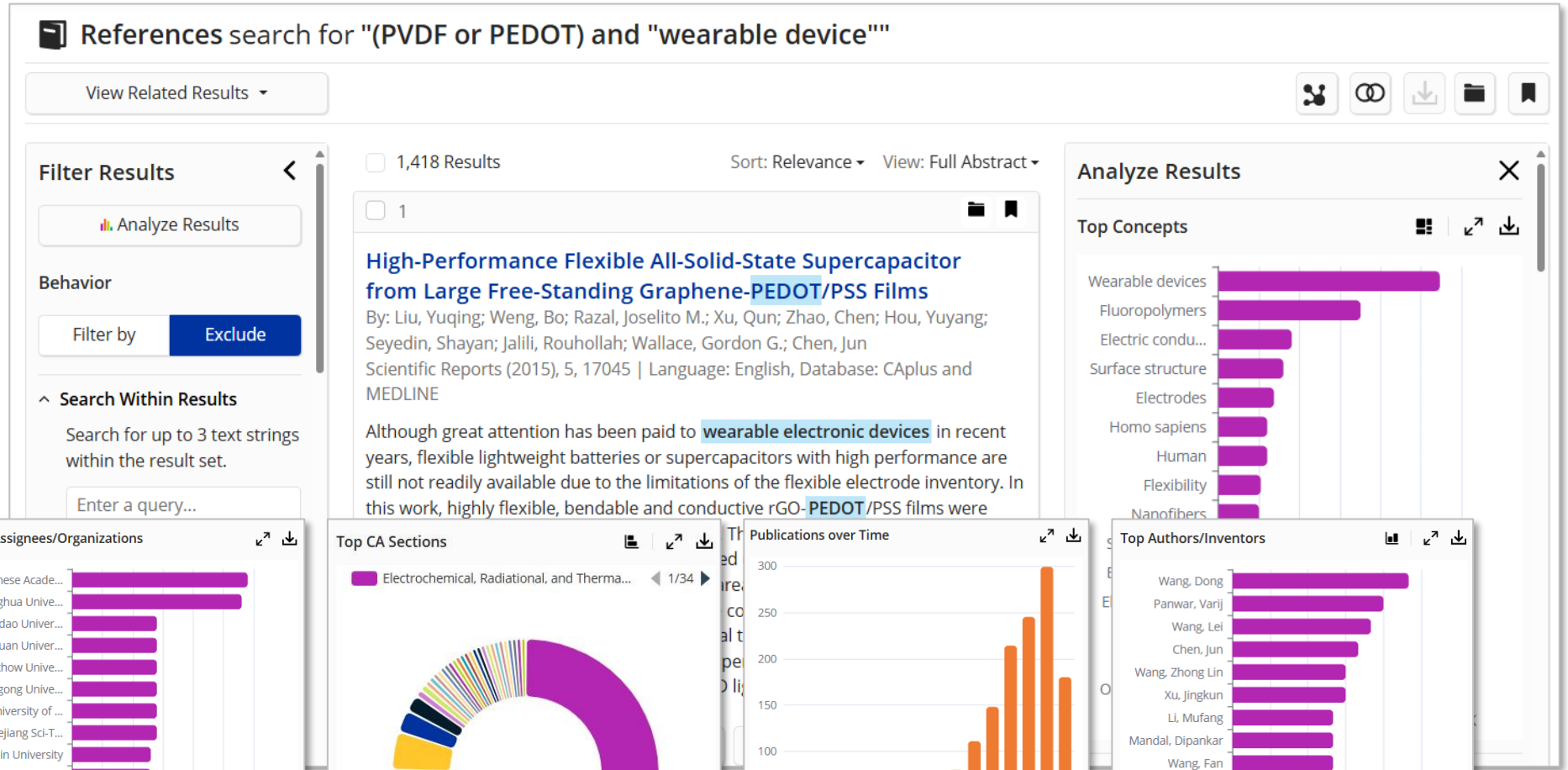
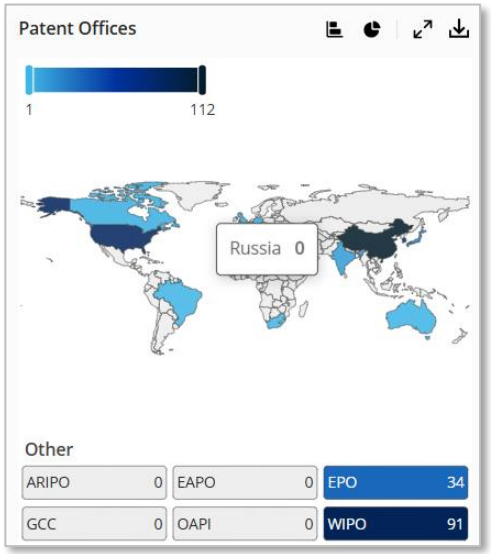
可视化的结果筛选和分析





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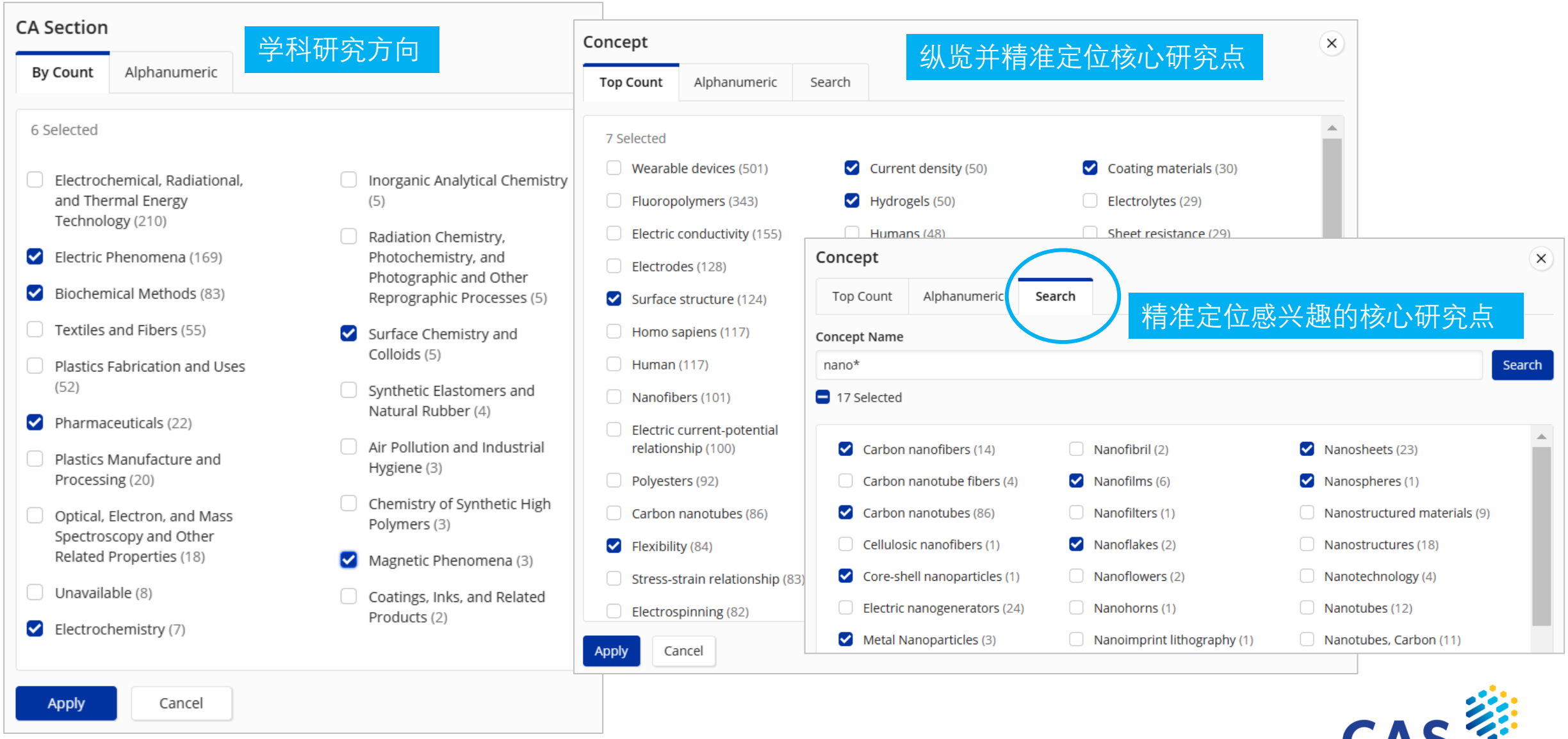
筛选工具 CAS Section & Concept



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筛选工具Search within results

合并、交集和去重

References search for "(PVDF or PEDOT) and "wearable device""

View Related Results

Filter Results

Analyze Results

Behavior

Filter by | Exclude

Search Within Results

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

Enter a query...

Search

Searching for... Clear All

dop*

Concept

CA Section

CAS Content

Filtering: Concept: Hydrogels

Excluding: Search Within Results: dop*

Clear All Filters

104 Results

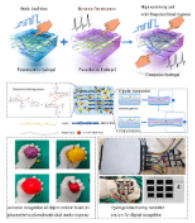
Sort: Relevance View: Full Abstract

1

Enhancing Strain-Sensing Properties of the Conductive Hydrogel by Introducing PVDF-TrFE

By: Hu, Zhirui; Li, Jie; Wei, Xiaotong; Wang, Chen; Cao, Yang; Gao, Zhiqiang; Han, Jing; Li, Yingchun

ACS Applied Materials & Interfaces (2022), 14(40), 45853-45868 | Language: English, Database: CAplus and MEDLINE



Conductive hydrogels have attracted attention because of their wide application in wearable devices. However, it is still a challenge to achieve conductive hydrogels with high sensitivity and wide frequency band response for smart wearable strain sensors. Here, we report a composite hydrogel with piezoresistive and piezoelec. sensing for flexible strain sensors. The composite hydrogel consists of cross-linked chitosan quaternary ammonium salt (CHACC) as the hydrogel matrix, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT: PSS) as the conductive filler, and poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) as the piezoelec. filler. A one-pot thermoforming and solution exchange method was used to synthesize the CHACC/PEDOT: PSS/PVDF-TrFE hydrogel. The hydrogel-based strain sensor exhibits high sensitivity (GF: 19.3), fast response (response time: 63.2 ms), and wide frequency range (response frequency: 5-25 Hz), while maintaining excellent mech. properties (elongation at break up to 293%). It can be concluded that enhanced strain-sensing properties of the hydrogel are contributed to both greater change in the relative resistance under stress and wider response to dynamic and static stimulus by adding PVDF-TrFE. This has a broad application in monitoring human motion, detecting subtle movements, and identifying object contours and a hydrogel-based array sensor. This work provides an insight into the design of composite hydrogels based on piezoelec. and piezoresistive sensing with applications for wearable sensors.

Full Text 7 1 40

定题追踪

Save Results

Name

Wearable device

Search Options

Query Only | Selected Answers | All Answers (Up to 20,000)

Add Existing Tags (Optional)

Aero

Alloys

Archaeology

Biotech

catalyst

New Tag (Optional)

Add tag name

Tag Color

Light Blue

Alerts

Frequency

As Available

Add Email(s)

china@acs-i.org ***@gmail.com

Save Cancel

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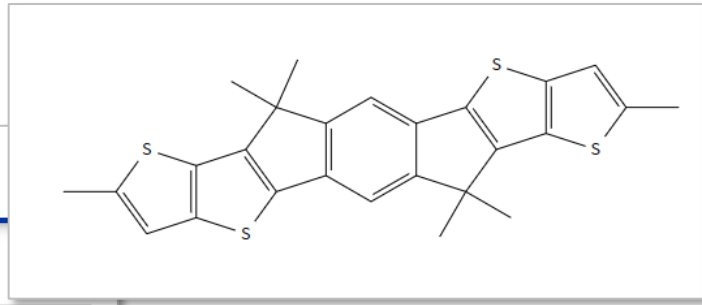
1.4 如何获得结构相关的文献?

策略：从Reference出发，主题词+结构联合检索



CAS SciFinder | References | Organic photovoltaic cell | Edit | 445

References search for "Organic photovoltaic cell" + drawn structure

Edit Drawing | Remove

View Related Results | Clear All Filters

Structure Match

As Drawn (0)

Substructure (1,303)

Behavior

Filter by | Exclude

Filtering: Substance Role: 2 Selected

172 Results

1

Preparation of hepta-fused heterocyclic organic compounds and

Assignee: Guangzhou Chasing Light Technology Co., Ltd.

China, CN120230120 A 2025-07-01 | Language: Chinese, Database: CAplus

Patent Status: Alive

...ates to preparation of hepta-fused heterocyclic organic comp...pound of general formula (I) prepared The inventive compou...vice, greatly improving the photoelec. conversion efficiency of...

Text | 68 | 49 | 0

...one-ring lock structure-based dimeric non-fulle...rial

Search Within Results

Concept

CA Section

Publication Year

Language

English (136)

Chinese (25)

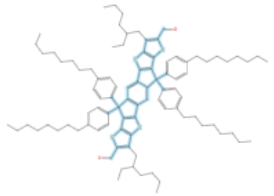
Substance Role

- Uses (1,203)
- Properties (712)
- Preparation (180)
- Process (170)
- Synthetic Preparation (167)
- Nanoscale (5)

View All

Substances

3092821-78-5

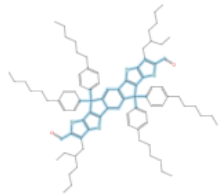


$C_{94}H_{122}O_2S_4$

PatentPak

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

3092821-75-2



$C_{86}H_{106}O_2S_4$

PatentPak

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

定位物质在文献中的研究角色

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文献检索小结

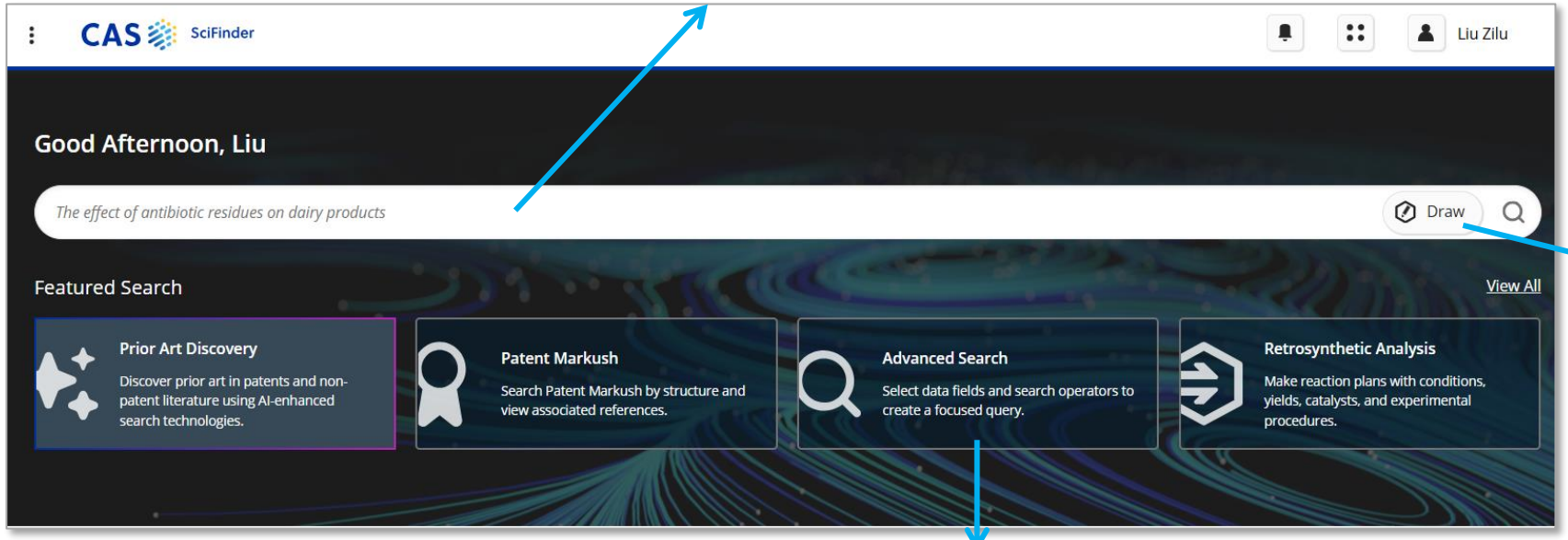
1. 利用引文地图拓展文献检索
2. 检索词的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
3. 利用丰富的筛选工具，快速获得目标文献
4. 主题词+结构联合检索快速获得文献

2.如何调研某类物质?

- 快速检索聚合物或无机化合物?
- 利用谱图数值确认产物或杂质?从属性值出发，调研某类材料?
- 检索完整分子结构?通式结构?或含有某些片段的物质?
- 如何确认结构新颖性?
- 如何查找相似的序列?

研究某种/某类物质?

- 通过物质标识符、文献标识符检索物质



- 使用结构绘制面板进行结构检索
- 高级检索

- 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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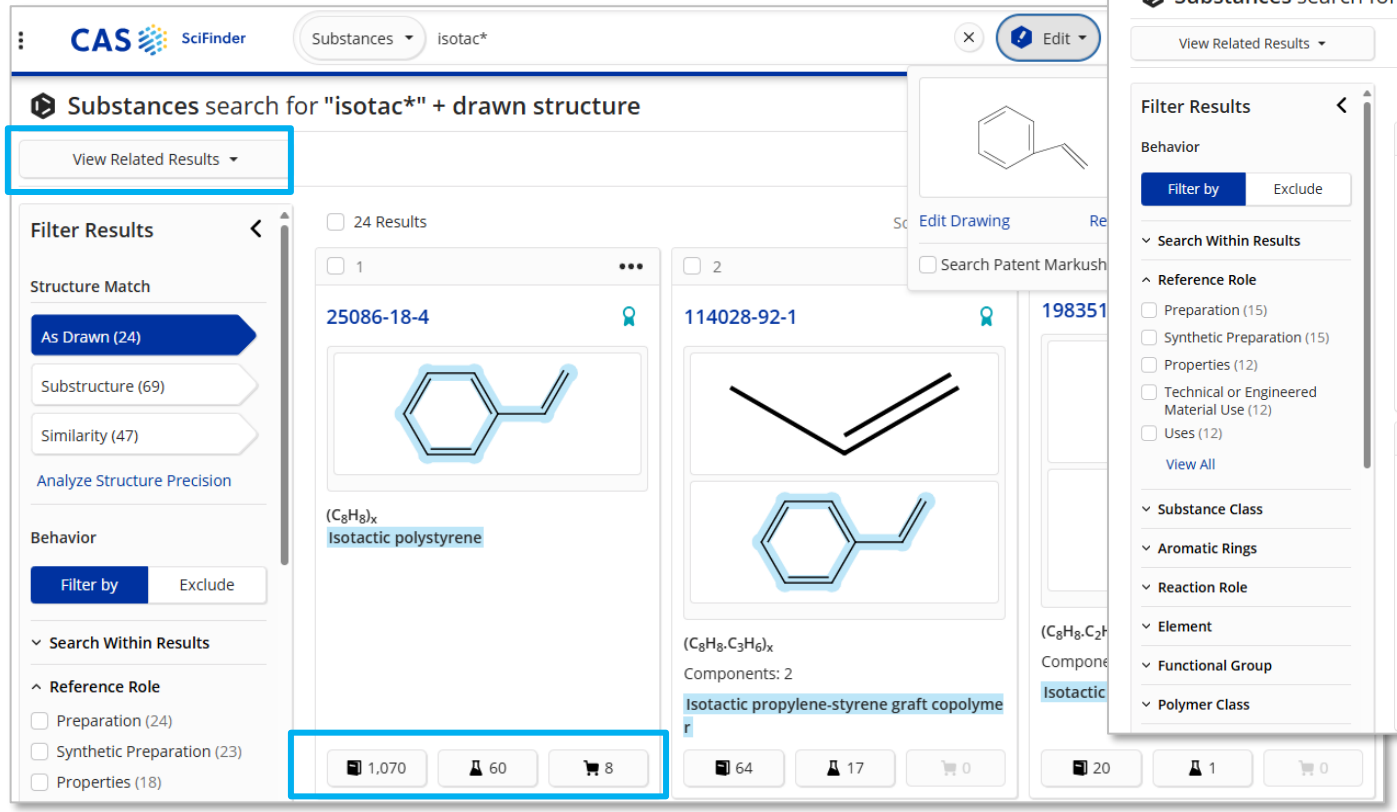
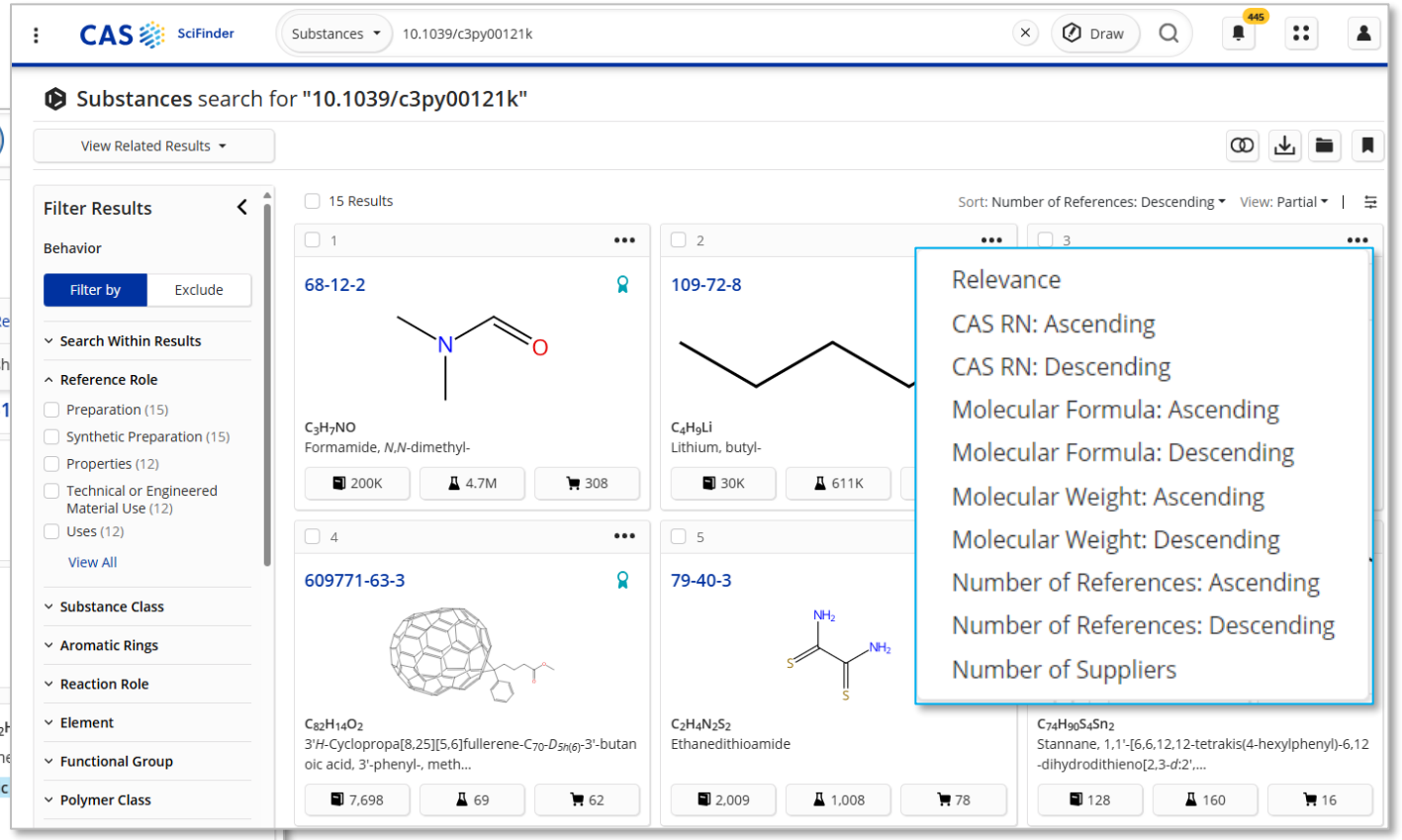
物质检索—物质/文献标识符

- 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）



- 迅速获得关注文献中的物质信息



物质排序：相关度、CAS RN、分子式、分子量、文献量、供应商数量

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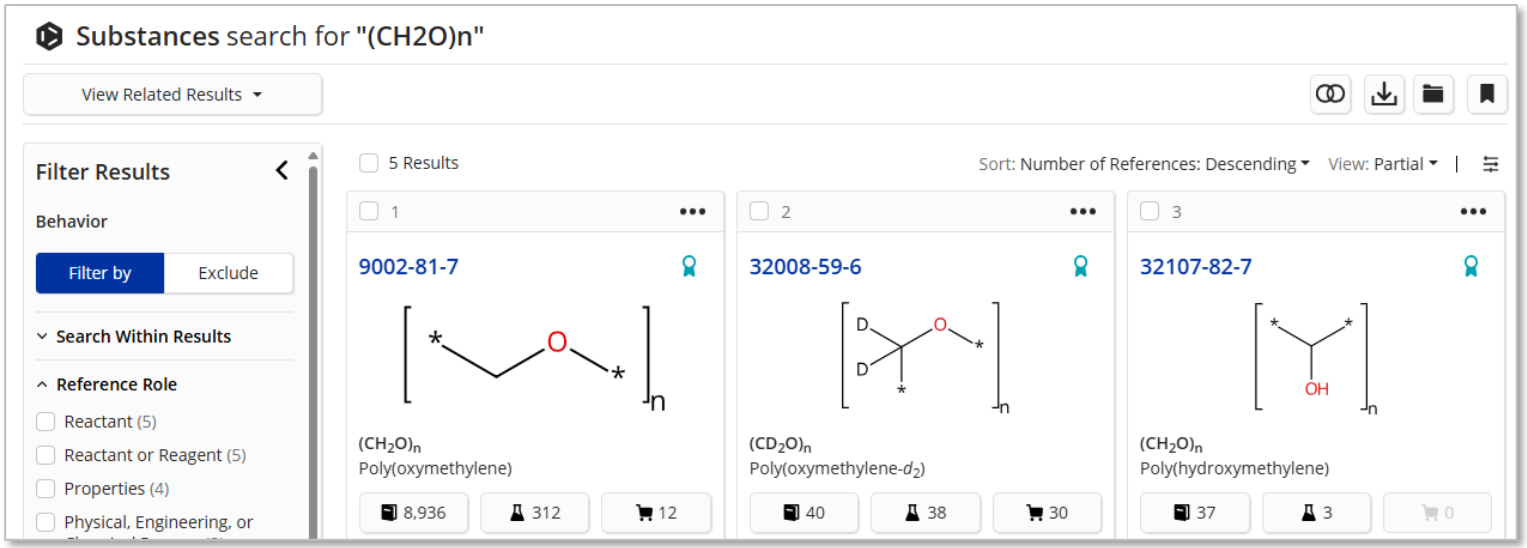
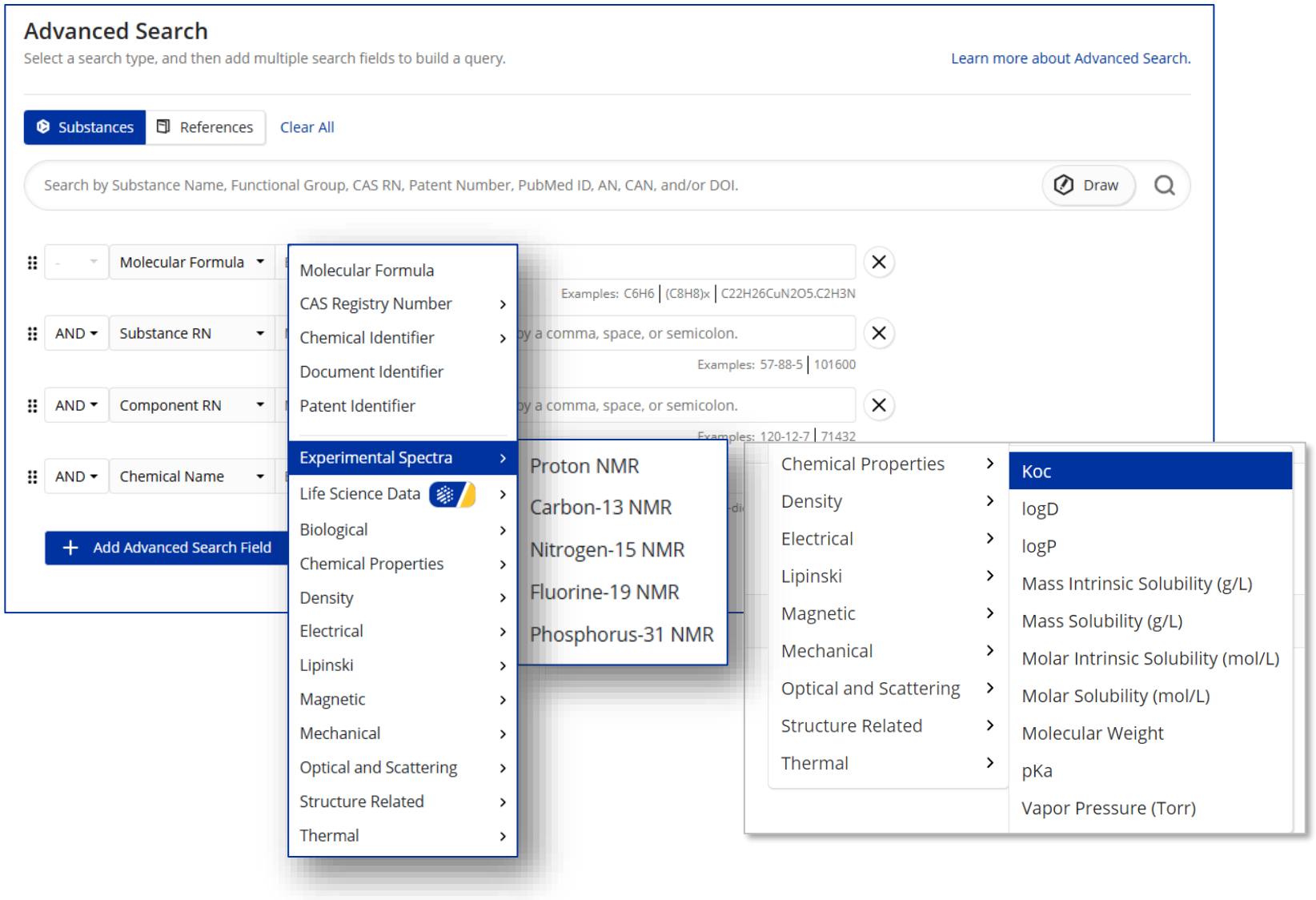
2.1 分子式检索：高效检索聚合物或无机化合物

- 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



(C2H4O)nH2O: 括号中是重复结构单元，括号外为n
(C2H6O2)x: 括号中是单体，括号外为x

2.2 属性值、谱图数值联用检索物质



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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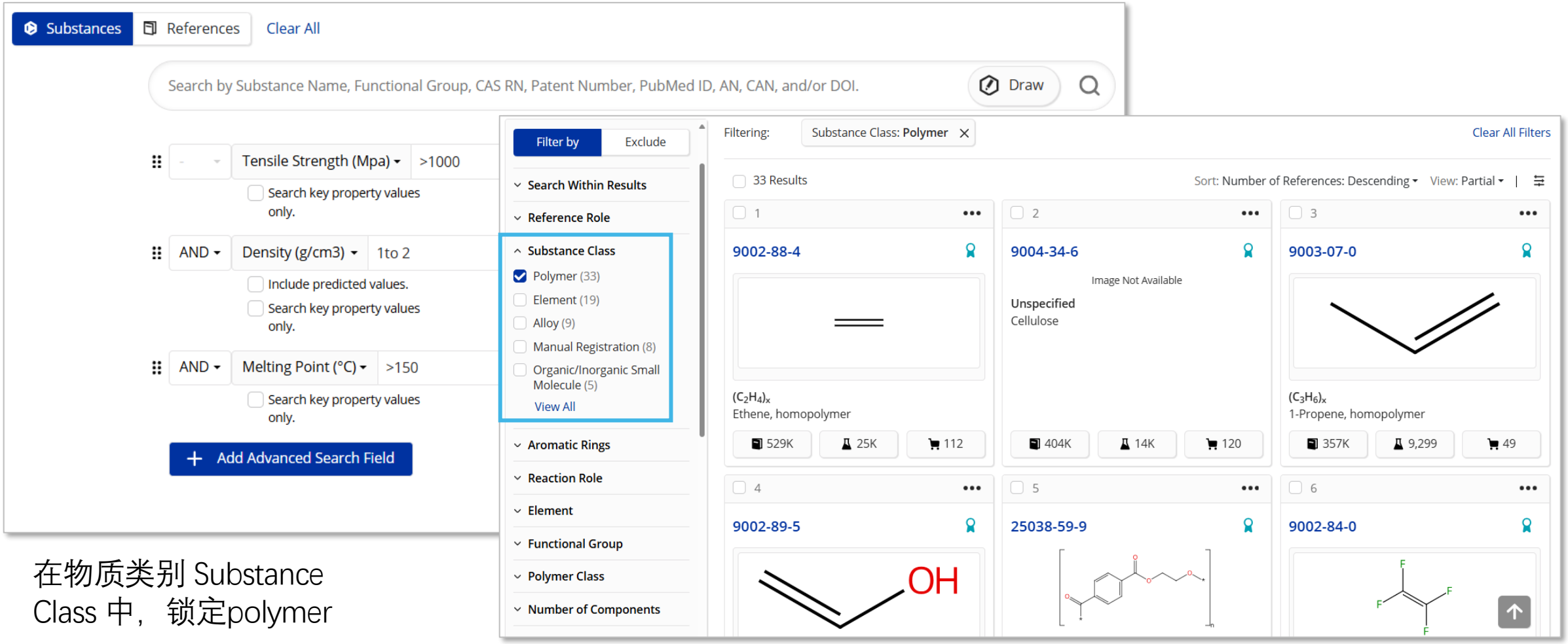
属性值联用检索物质

例如检索满足多属性值要求的聚合物：密度1-2g/cm^3、拉伸强度>1000 MPa、熔点>150℃



在物质类别 Substance Class 中，锁定polymer

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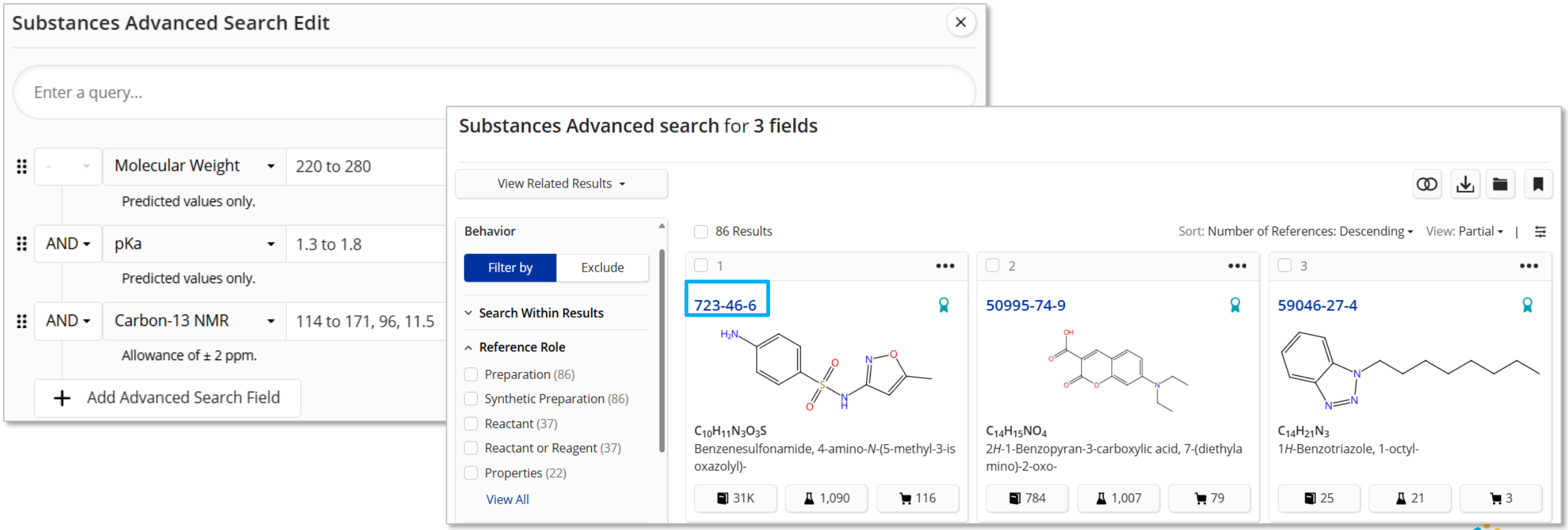
属性值、谱图数值联用检索物质

- 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

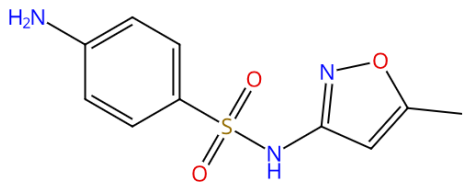


物质详情

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



$C_{10}H_{11}N_3O_3S$

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

Properties
Molecular Weight
Melting Point (Experimental)
Boiling Point (Predicted)
Density (Experimental)
pKa (Experimental)

Experimental Properties | Spectra

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
Patent Number: CN120305271
Publication Date: 2025-07-15

View All Pate

Condition
-
-
Press: 760.00 Torr
-

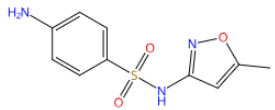
- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Pharmacological Data
- ADME
- Toxicity
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements
- Additional Details

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

723-46-6



$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

Working Frequency
400 MHz

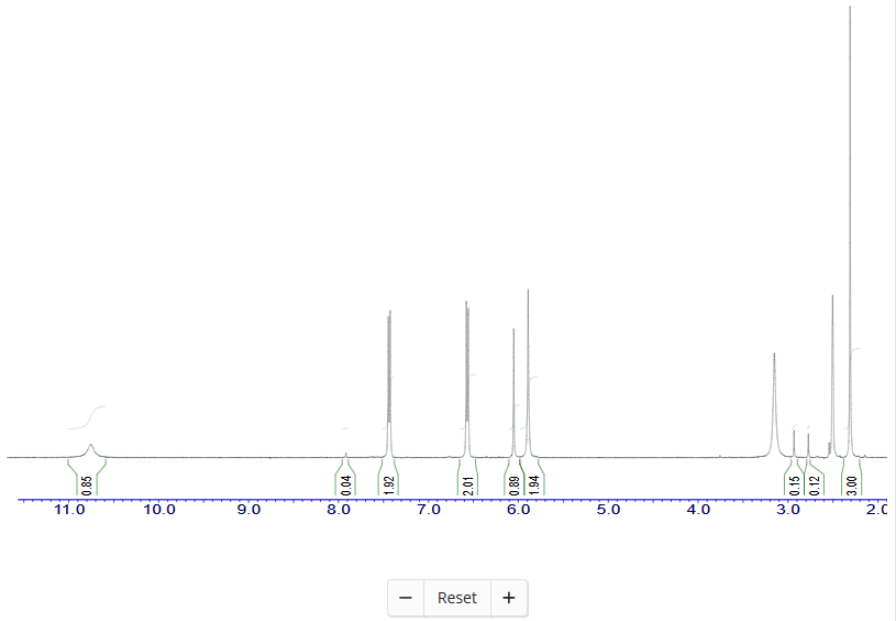
Solvent
Dimethyl sulfoxide (67-68-5)
Carbon tetrachloride (56-23-5)

Temperature
20 °C

Spectrum Summary

Spectrum ID
F0175-0013

Source
Spectral data were obtained from Life Chemicals



- 折叠菜单显示物质各类信息

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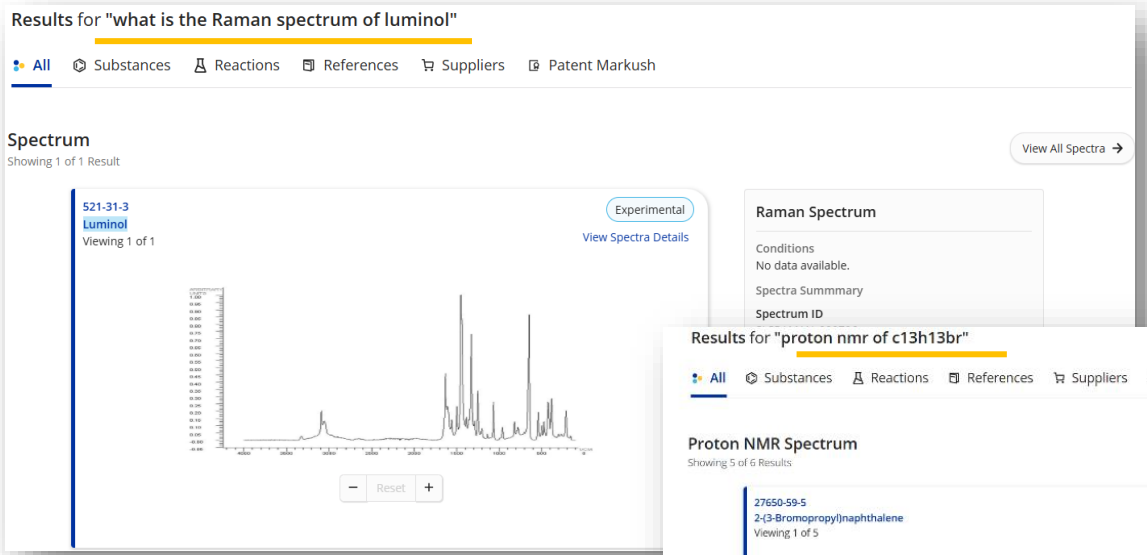
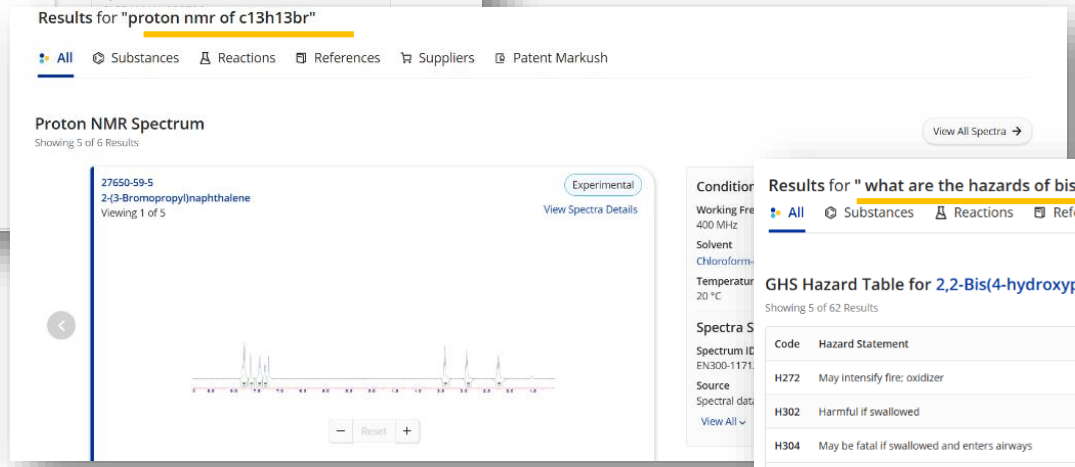
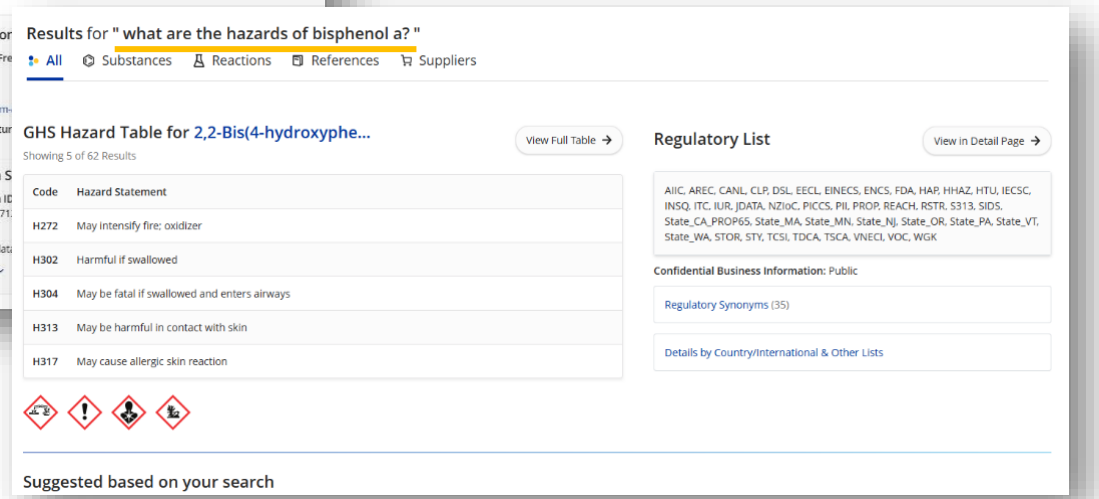
扩展问答类型，快速聚焦物质谱图和安全信息



自然语言直接查阅Raman谱图



自然语言直接查阅NMR谱图



自然语言直接查阅物质安全信息

CAS
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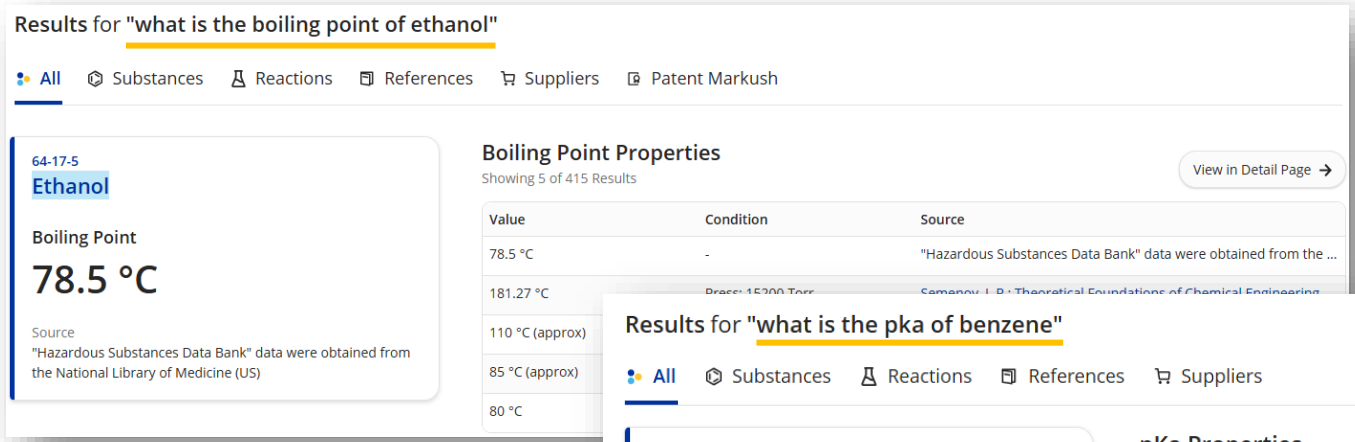
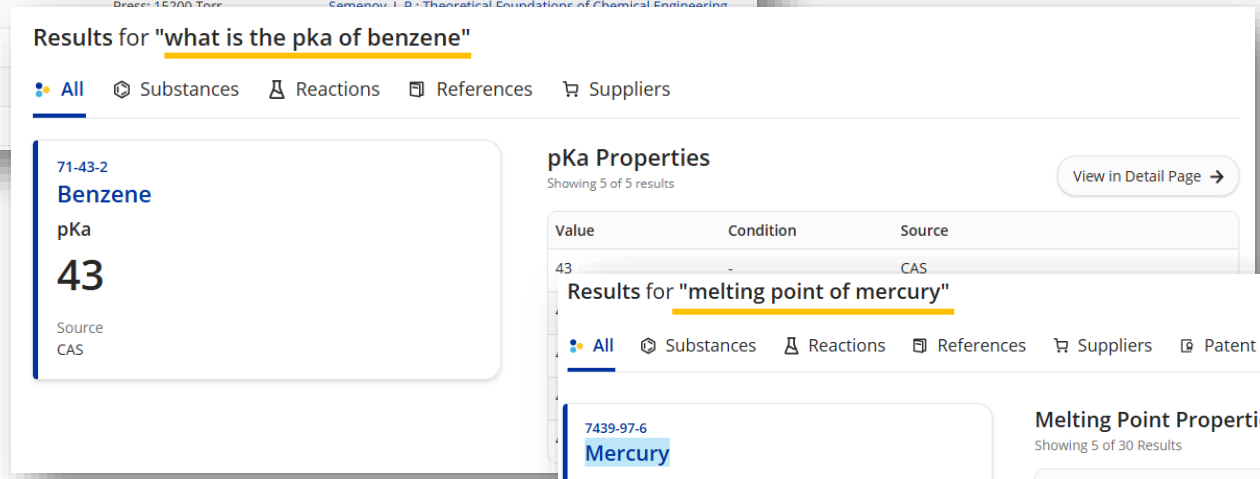
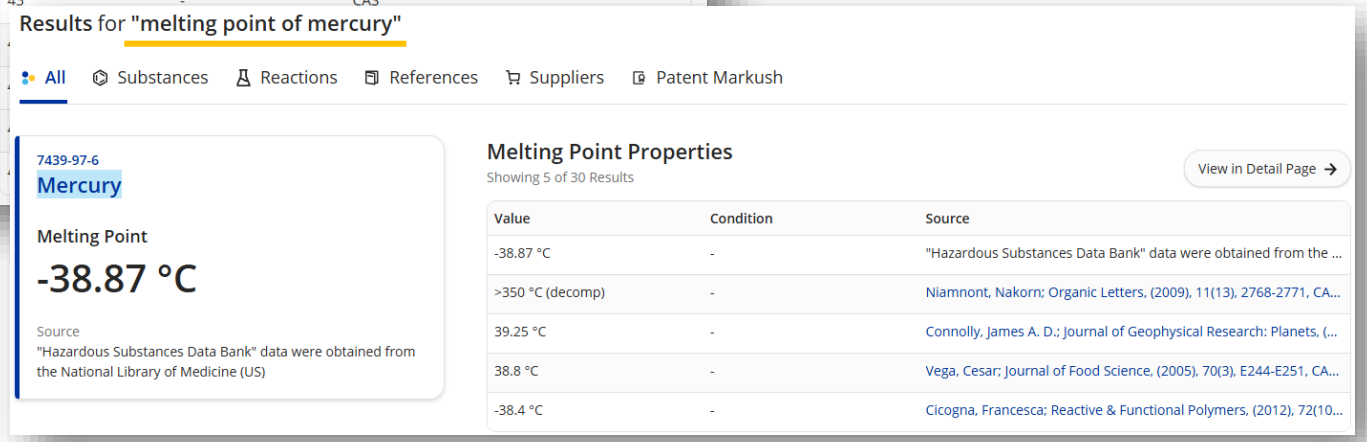
支持自然语言直接检索物质理化性质，直观高效



自然语言直接查阅物质沸点



自然语言直接查阅pKa值



自然语言直接查阅熔点

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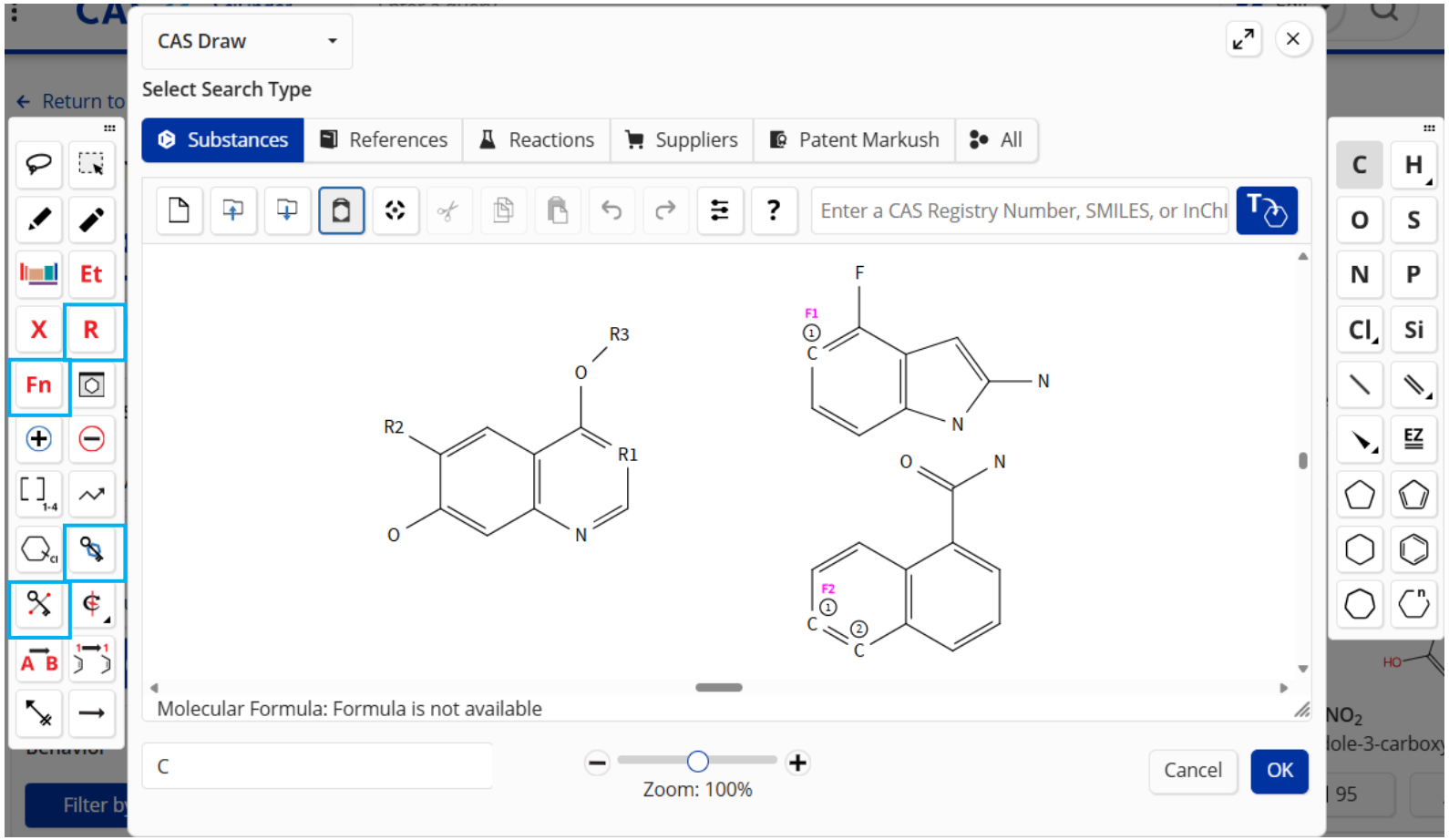
2.4结构检索



氢同位素：氕、氘和氚

双键、三键和不确定化学键

R 自定义 R 基团

R基团可设置为原子、可变基团、常用官能团，也可以是自定义的片段结构

Fn 片段结构标记

定义R基团中特定的片段结构，且一个片段可设置多个连结位点

环锁定工具

锁定的环无法成为更大环系的组成部分，锁定的链键无法成为环上的键

原子锁定工具

被锁定的原子或官能团不发生非氢取代

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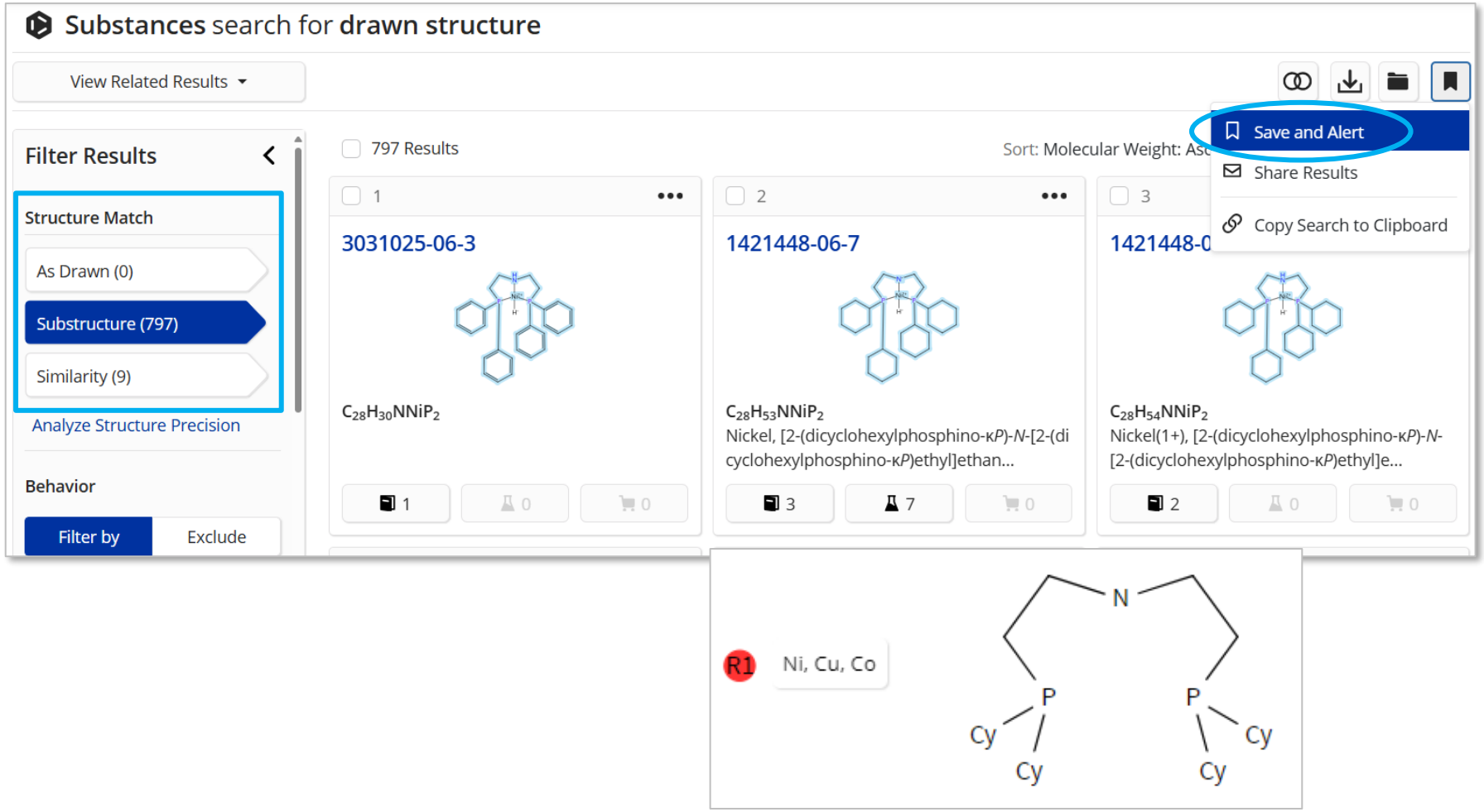
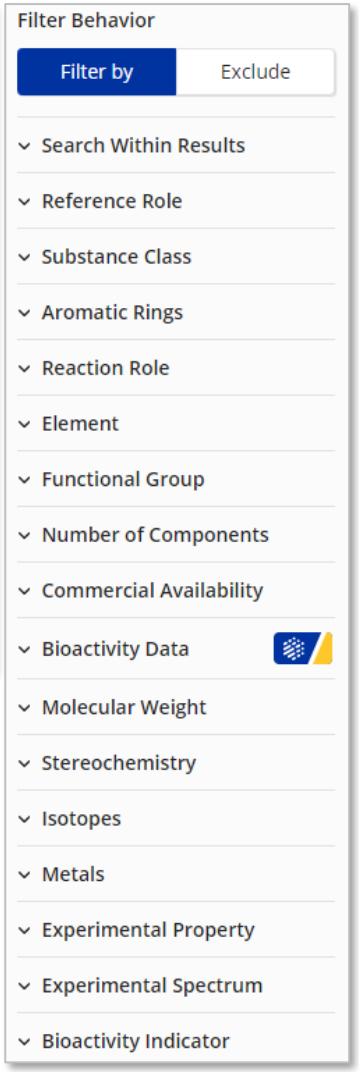
结构检索

例：已知结构片段的物质检索

结构检索时，无需分步进行，一次检索即可得到As Drawn, Substructure和Similarity结果





物质筛选类别：

二次检索（结构）

文献角色

物质类别

芳环数

反应角色

元素

官能团

生物活性数据

分子量

立体化学

同位素

金属包含

实验物性数据

……

结构检索

结构检索类别:

- As Drawn

  绘制结构中可出现R基团、可变基团；绘制结构中价态未达饱和的原子只能接氢；如有环系，不与其他环稠合或成桥环

- Substructure 亚结构

  包括As Drawn检索结果；价态未达饱和的原子可以连接氢以外的其他原子；如有环系，可形成其他环

- Similarity 相似结构

  获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

  注：如果关注相似结构检索结果，请不要绘制通式结构

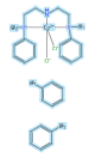
物质检索结果的筛选

Reference Role：物质在文献中的研究角色

Reference Role
- Preparation (515)
- Synthetic Preparation (513)
- Properties (297)
- Uses (138)
- Catalyst Use (123)
- Reactant (104)
- Reactant or Reagent (104)
- Process (36)
- Physical, Engineering, or Chemical Process (35)
- Substance Claimed (15)
- Technical or Engineered Material Use (12)
- Industrial Manufacture (10)
- Formation, Non-preparative (6)
- Biological Study (4)
- Pharmacological Activity (4)

View All

1 — 1087216-22-5

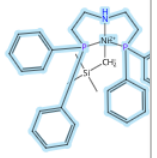


$C_{28}H_{29}Cl_2CoNP_2$

Cobalt, dichloro[2-(diphenylphosphino-κ*P*)-*N*-[2-(diphenylphosphino-κ*P*)ethyl]ethan...

10 | 106 | 0

2 — 2924724-62-7



$C_{32}H_{40}NNiP_2Si$

1 | 1

4 — 579490-58-

Substance Class：物质类别

Substance Class
- Polymer (138)
- Mixture (27)
- Coordination Compound (6)
- General Derivative (2)
- Salt and Compound With (2)

Aromatic Rings

Reaction Role

Element

Functional Group

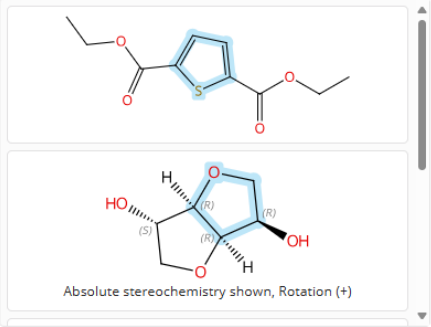
Polymer Class

Number of Components
- 1 (233)
- 2 (494)
- 3 (189)
- 4 (138)
- 5 or more (480)

Filtering: Substance Class: Polymer ✕ | Number of Components: 4 ✕

138 Results

2757996-73-7



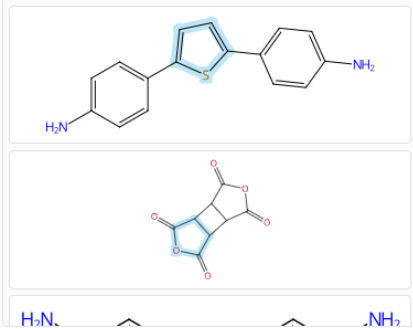
$(C_{10}H_{12}O_4S.C_8H_{14}O_4.C_6H_{10}O...$

Components: 4

D-Glucitol, 1,4:3,6-dianhydro-, polymer with 1,4-diethyl butanedioate, 2,5-dieth...

1 | 1 | 0

2226925-66-0



$(C_{16}H_{14}N_2S.C_{13}H_{14}N_2.C_{10}H_2...$

Components: 4

1*H*,3*H*-Benzo[1,2-*c*:4,5-*c*']difuran-1,3,5,7-tetrone, polymer with 4,4'-methylenebis...

1 | 0 | 0

Reaction Role：物质在反应中的角色

Reaction Role
- Product (234)
- Reactant (58)
- Reagent (3)
- Catalyst (38)

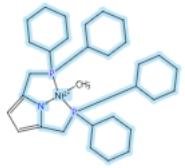
Element

Functional Group

Number of Components

Commercial Availability

4 — 1449235-31-7

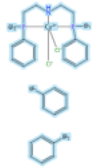


$C_{31}H_{53}NNiP_2$

Nickel, [2,5-bis[(dicyclohexylphosphino-κ*P*)methyl]-1*H*-pyrrolato-κ*N*]methyl-, (*SP*-...

2 | 4 | 0

1087216-22-5



$C_{28}H_{29}Cl_2CoNP_2$

Cobalt, dichloro[2-(diphenylphosphino-κ*P*)-*N*-[2-(diphenylphosphino-κ*P*)ethyl]ethan...

10 | 106 | 0

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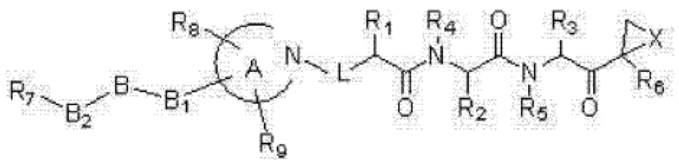
2.5 CAS Markush检索，助力结构查新

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

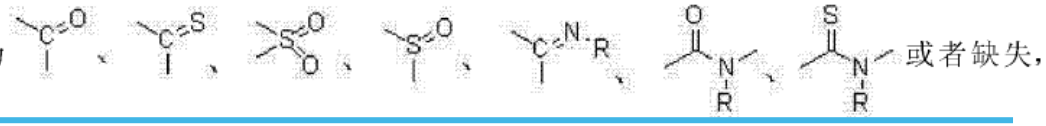
其中：

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 RN

预测性物质[Prophetic Substance]：

- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，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 Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

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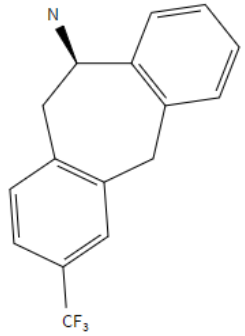
CAS Markush检索

第一步：物质结构检索

- As drawn结果为0
- Substructure结果为2
- Similarity相似度最高85-89%



为了尽可能完整地获得公开的结构信息，需要同时进行Substance和Markush结构检索；根据需要，可进行文献检索补充

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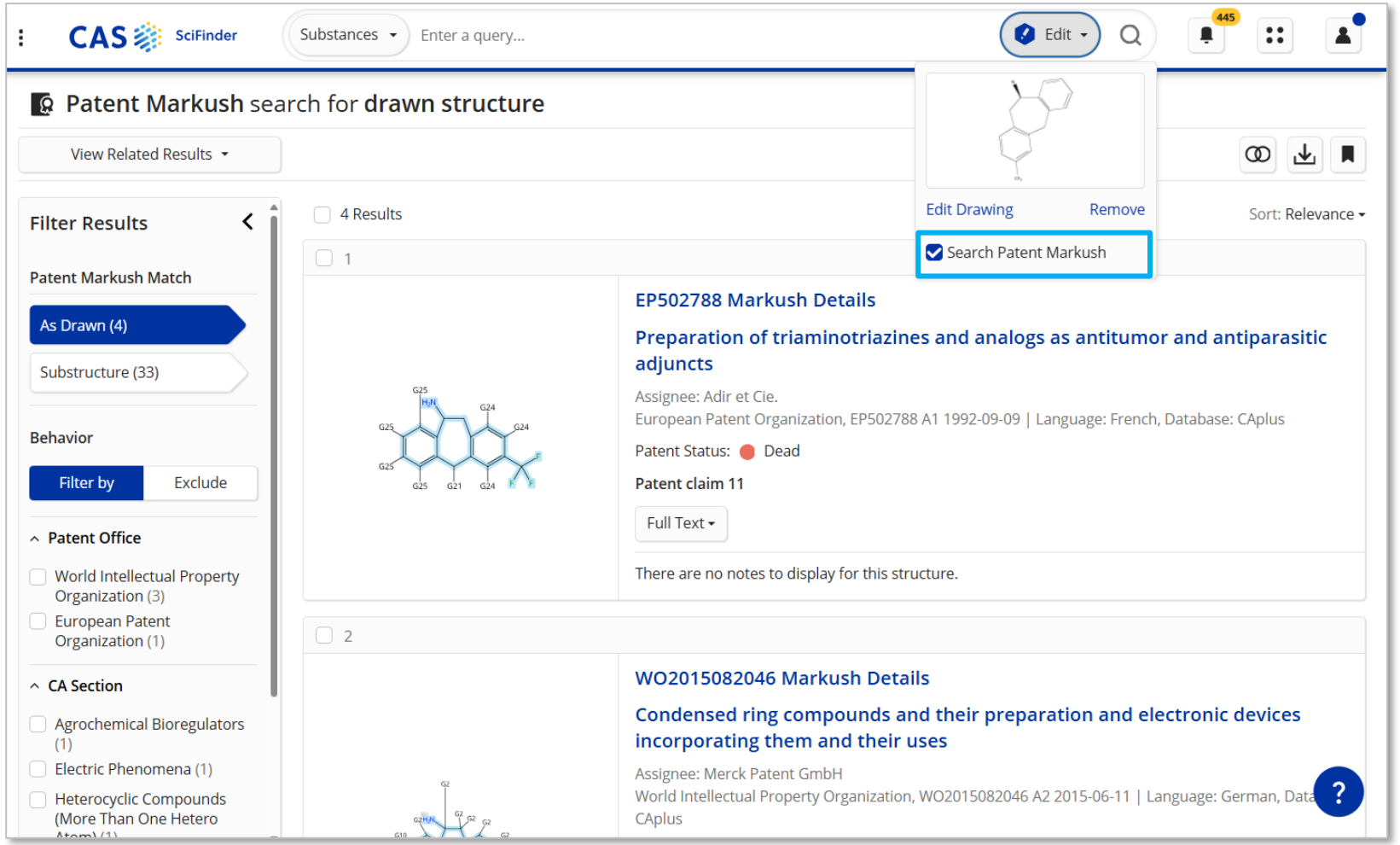
CAS Markush检索

第二步：Markush结构检索
获得四项专利文献

- 直观呈现检索结构与专利原文中Markush匹配部分的结构；
- 标引其在专利中出现的位置；
- 详细的结构取代信息描述



物质检索小结

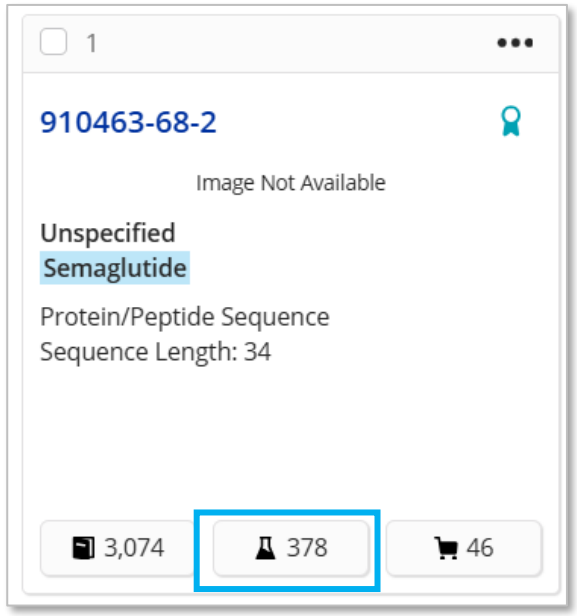
1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
3. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
4. 利用CAS Markush检索尽可能全面的获得结构的公开信息，根据需要可进行文献检索补充

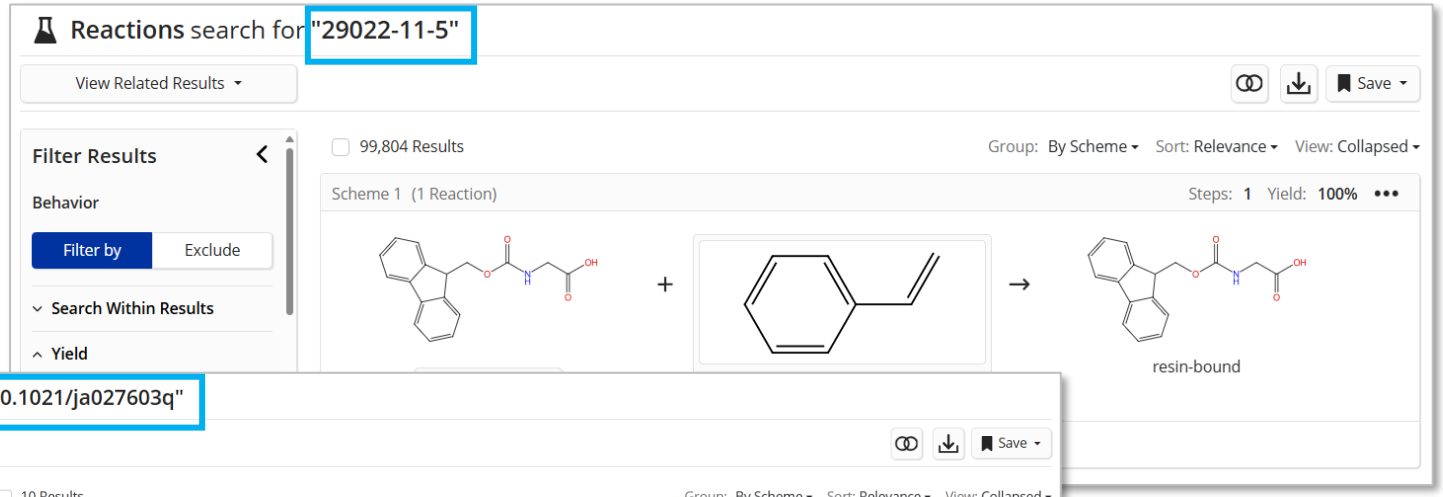
3.如何进行反应调研?

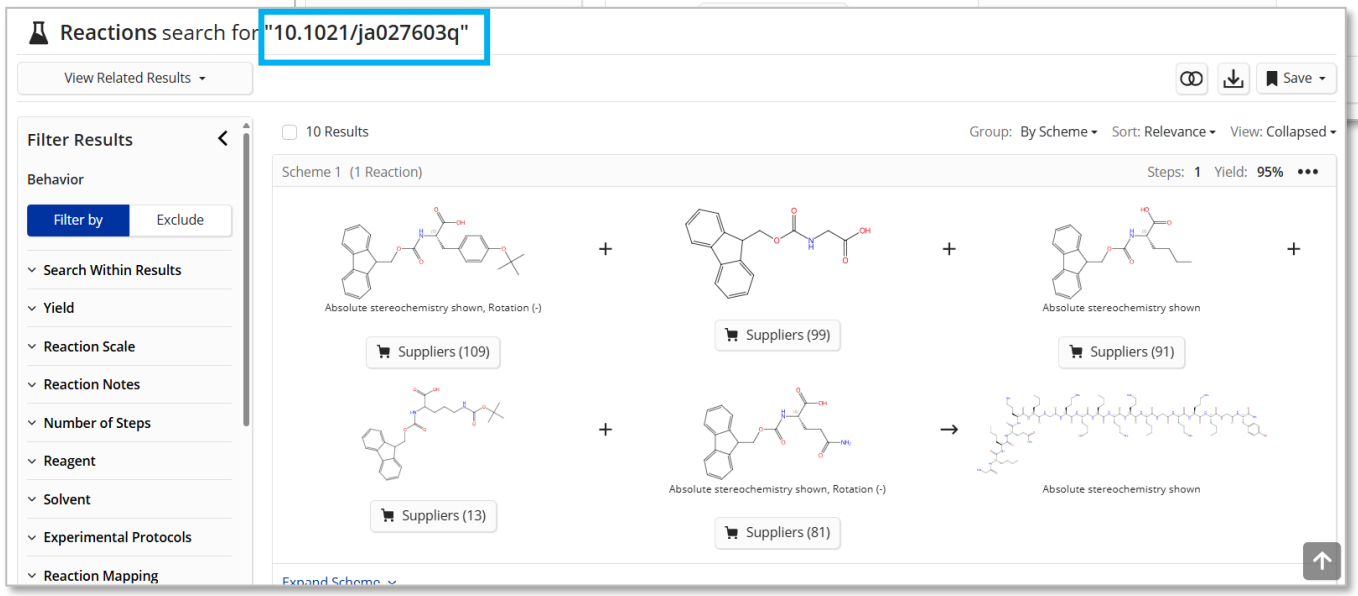
- 如何从我感兴趣的底物、产物或催化剂出发，找到关联的反应?
- 如何查找相似反应?
- 如何关注特定转化类型的反应?
- 如何在大量反应结果中，快速找到最想要的反应?
- 如何查找涉及机理研究的反应？或人名反应?
- 如何设计新化合物的逆合成路线?

研究某种/某类反应?

- 反应检索方法
  - 物质或文献标识符
  - 结构式
  - 关键词与结构联用
  - 文本







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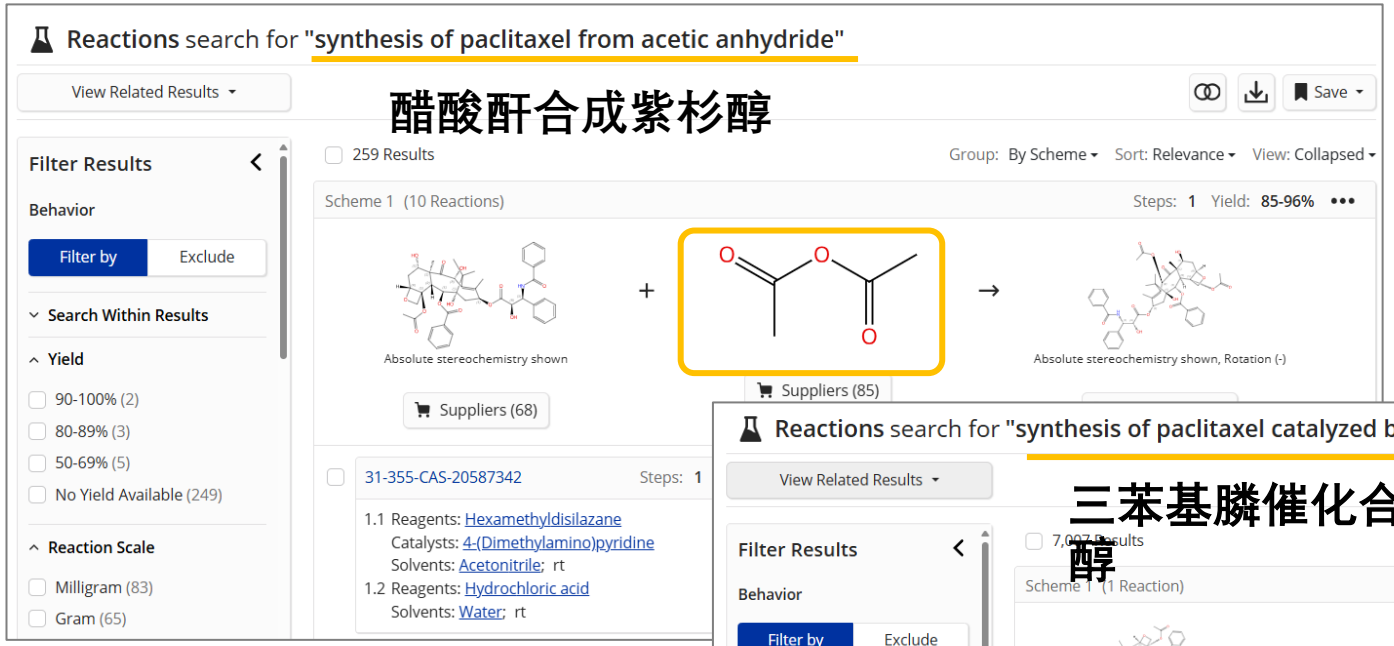
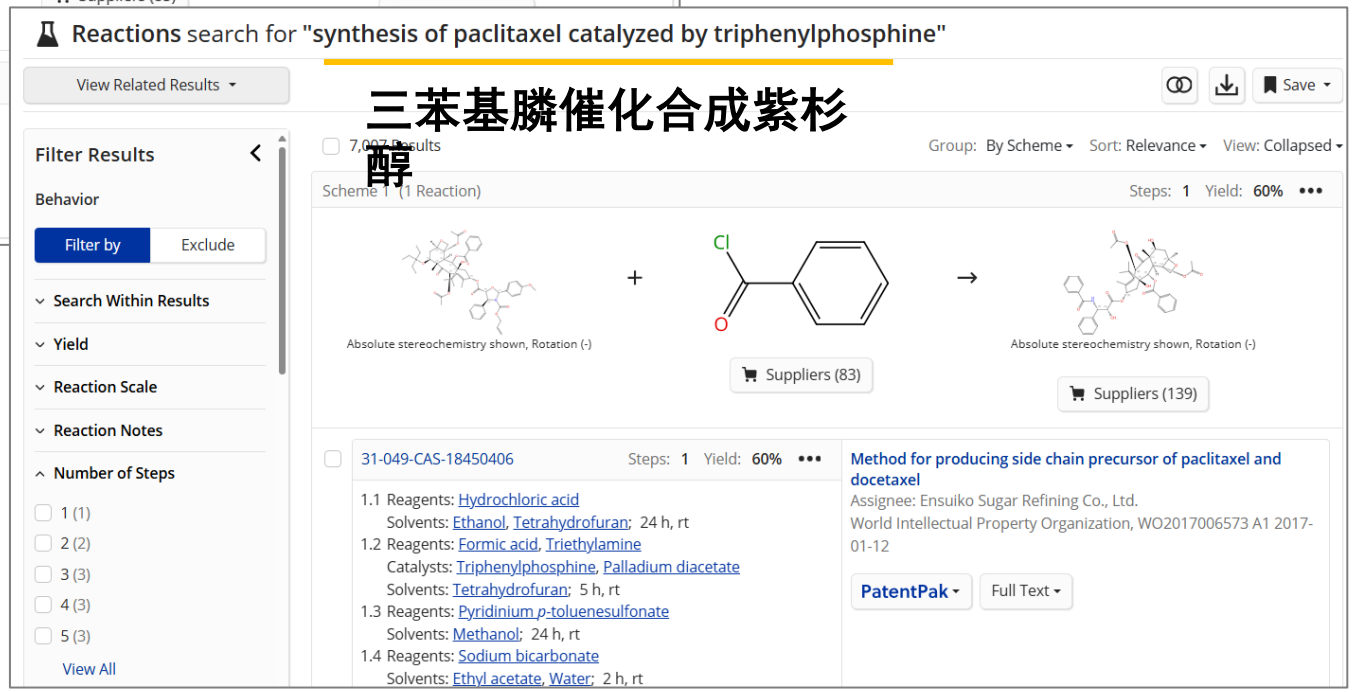
利用自然语言检索反应

支持反应转化类型名称、物质类别、物质官能团和反应参与角色（包括溶剂、试剂和催化剂）





- “**of**”连接特定关键词指定反应产物，如synthesis（合成），preparation（制备）和 manufacture（生产）。
- “**from**”连接物质指定反应物或试剂
- “**catalyzed by**”连接物质指定催化剂

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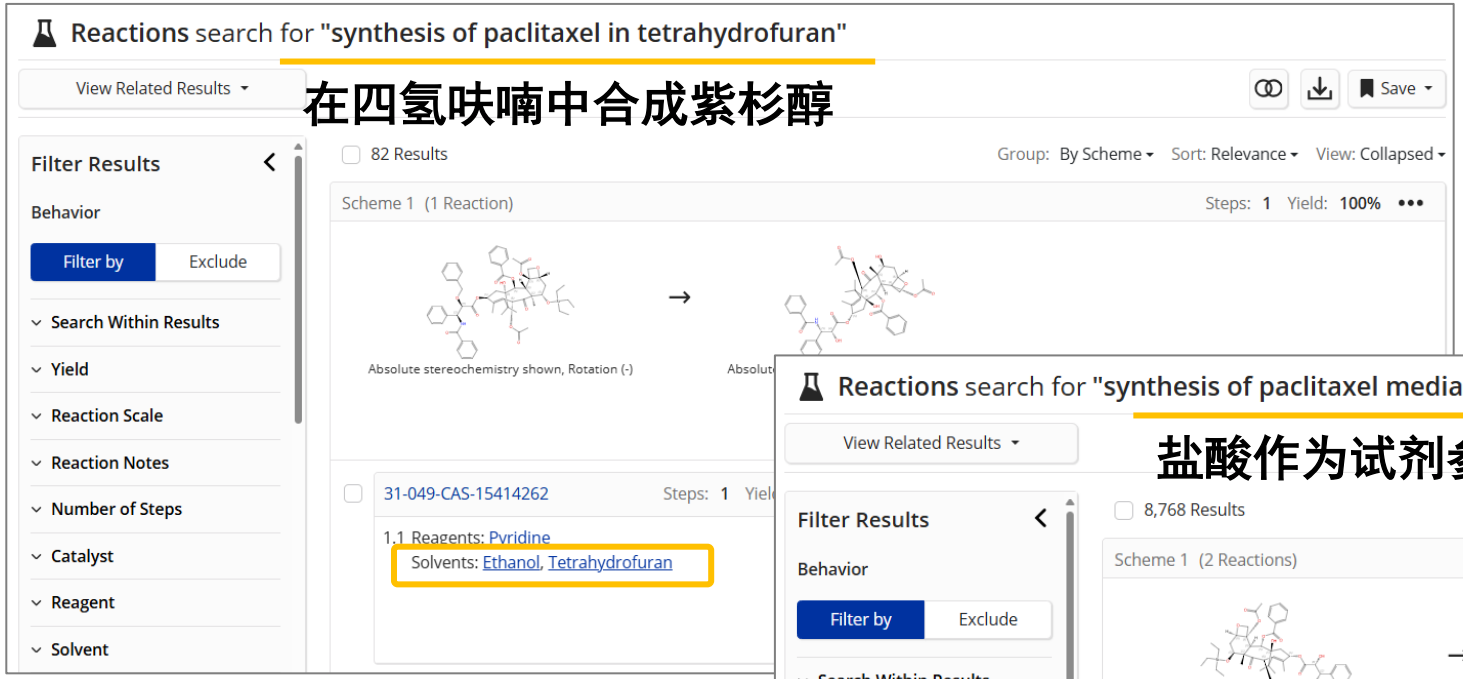
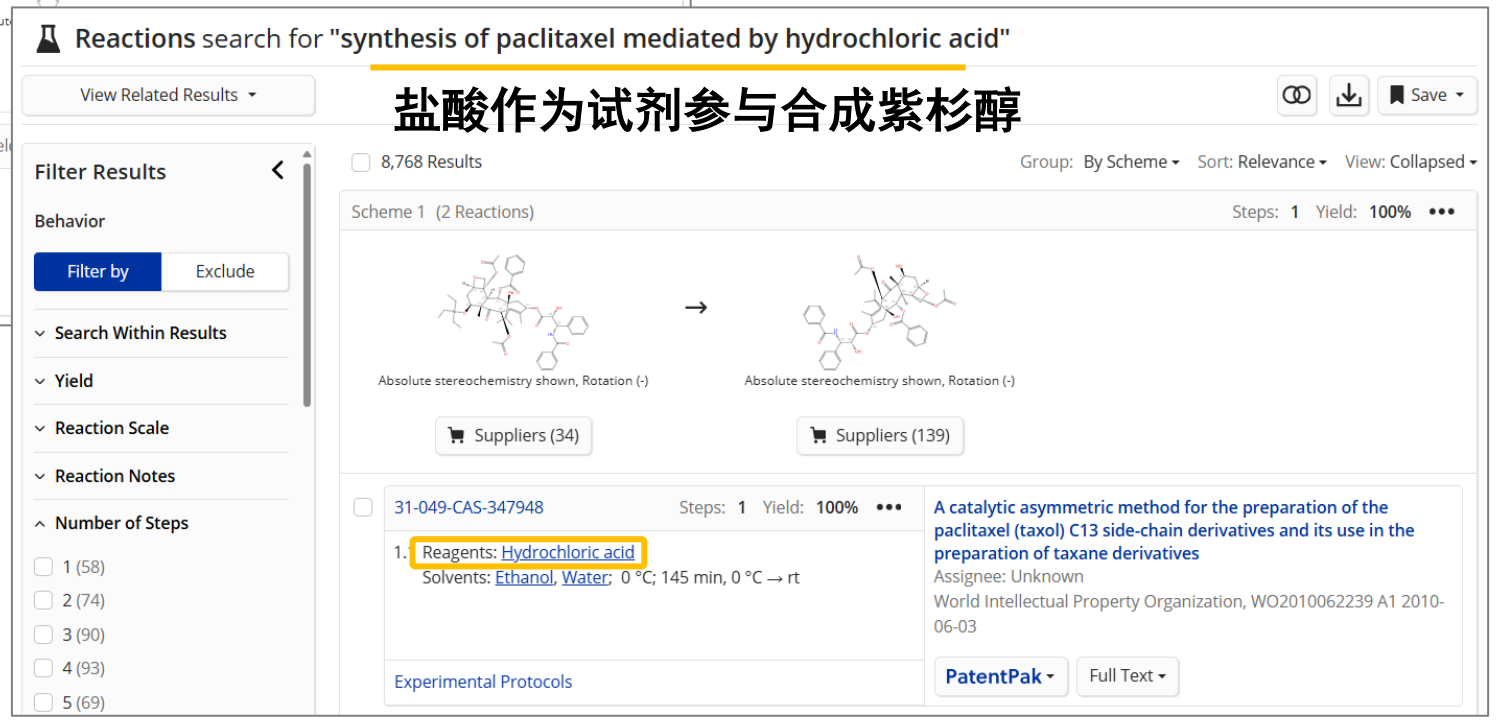
自然语言检索反应



在四氢呋喃中合成紫杉醇

“in”连接物质指定溶剂

“mediated by”连接物质指定试剂



盐酸作为试剂参与合成紫杉醇

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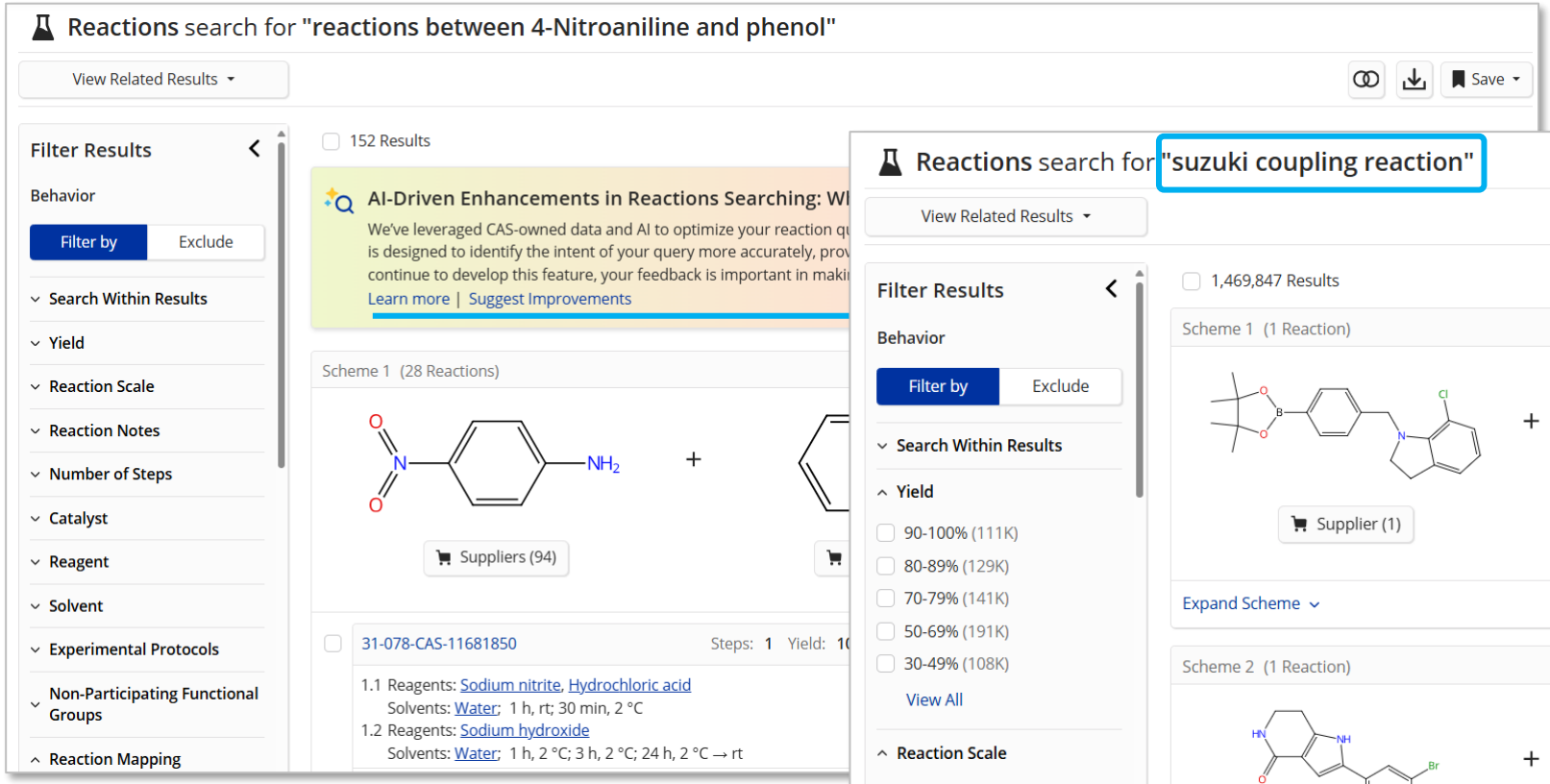
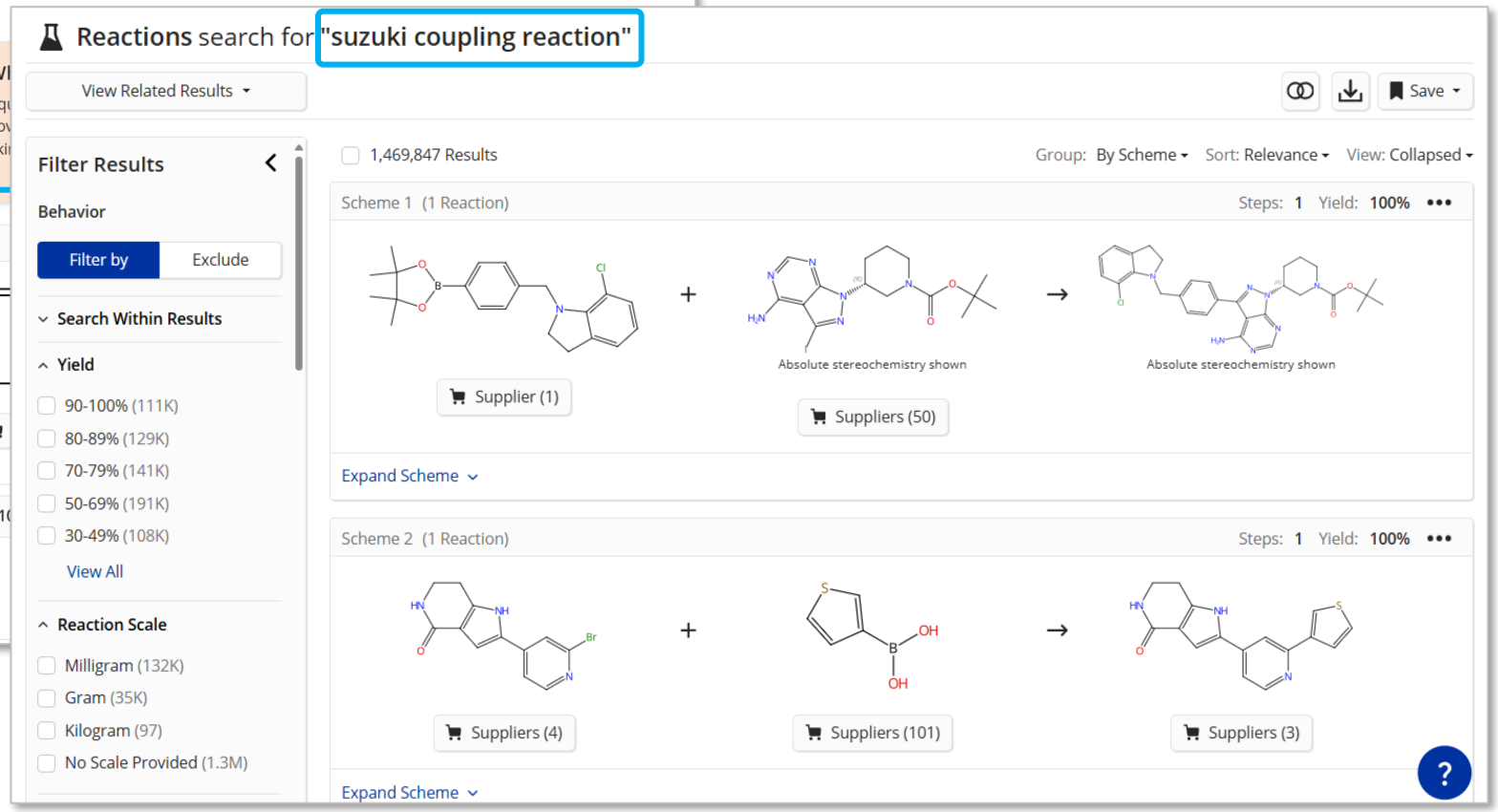
AI识别检索意向，提供最相关反应检索结果





文献检索时识别反应检索意向，
便捷获取目标反应信息

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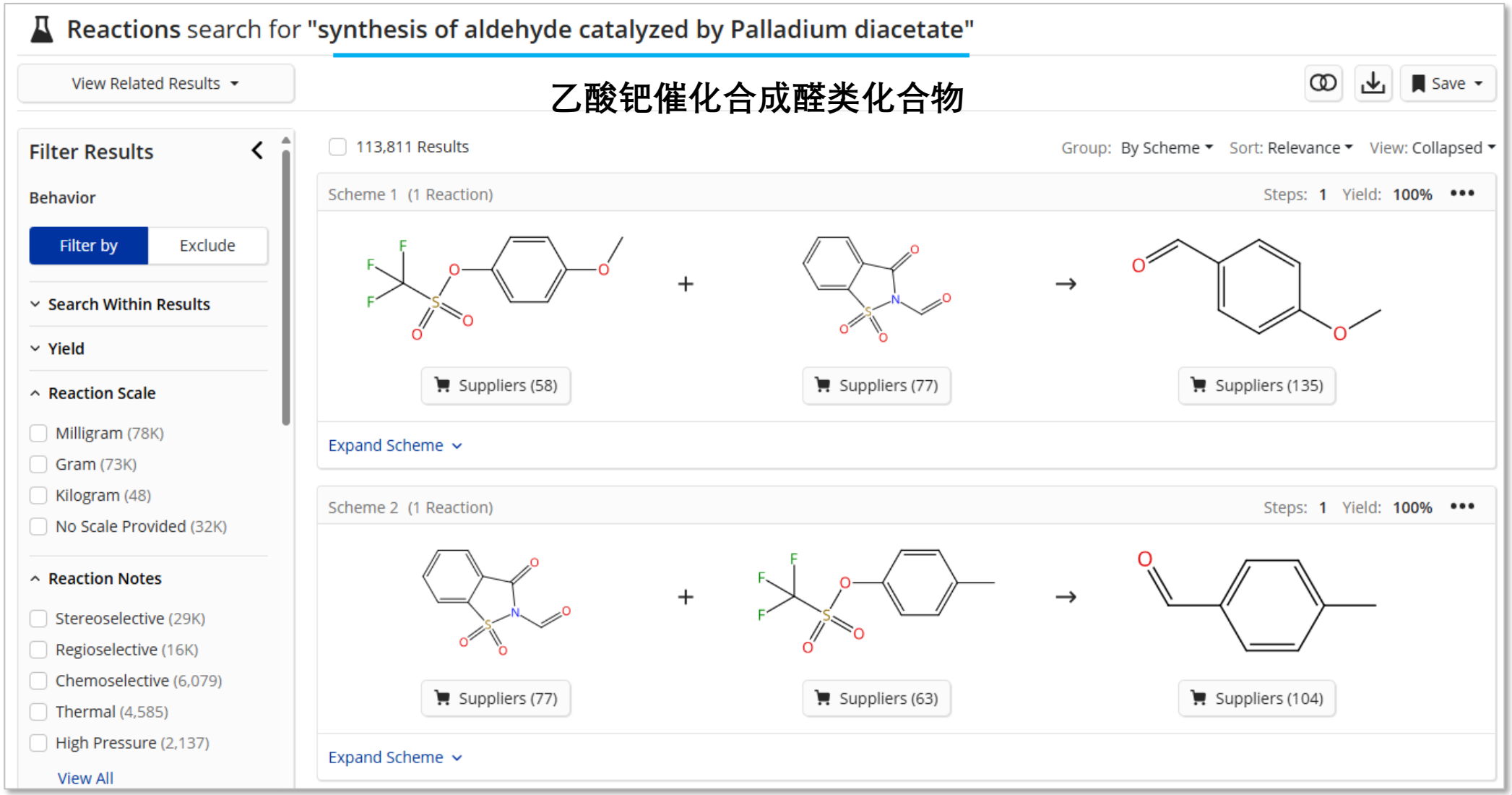
不止具体反应，还可便捷检索某一类反应



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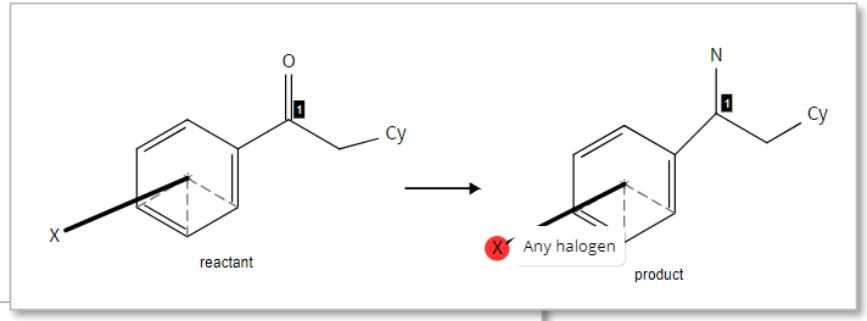
3.2 查找亚结构反应或相似反应



As Drawn
亚结构反应
相似反应

Reactions search for drawn structure

View Related Results

Save

Filter Results

Structure Match

As Drawn (34)

Substructure (8,806)

Similarity (0)

Behavior

Filter by | Exclude

Search Within Results

Yield

80-89% (4)

70-79% (2)

50-69% (1)

No Yield Available (27)

34 Results

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

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)

Suppliers (79)

Suppliers (13)

Expand Scheme

Scheme 2 (1 Reaction)

Steps: 1 Yield: 76%

Suppliers (45)

Suppliers (3)

反应分组:
按反应式
按文献
按转化类型

反应排序:
相关度
公布时间
产率
步数

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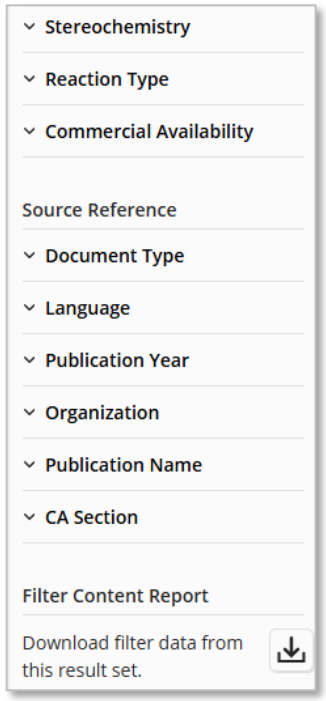
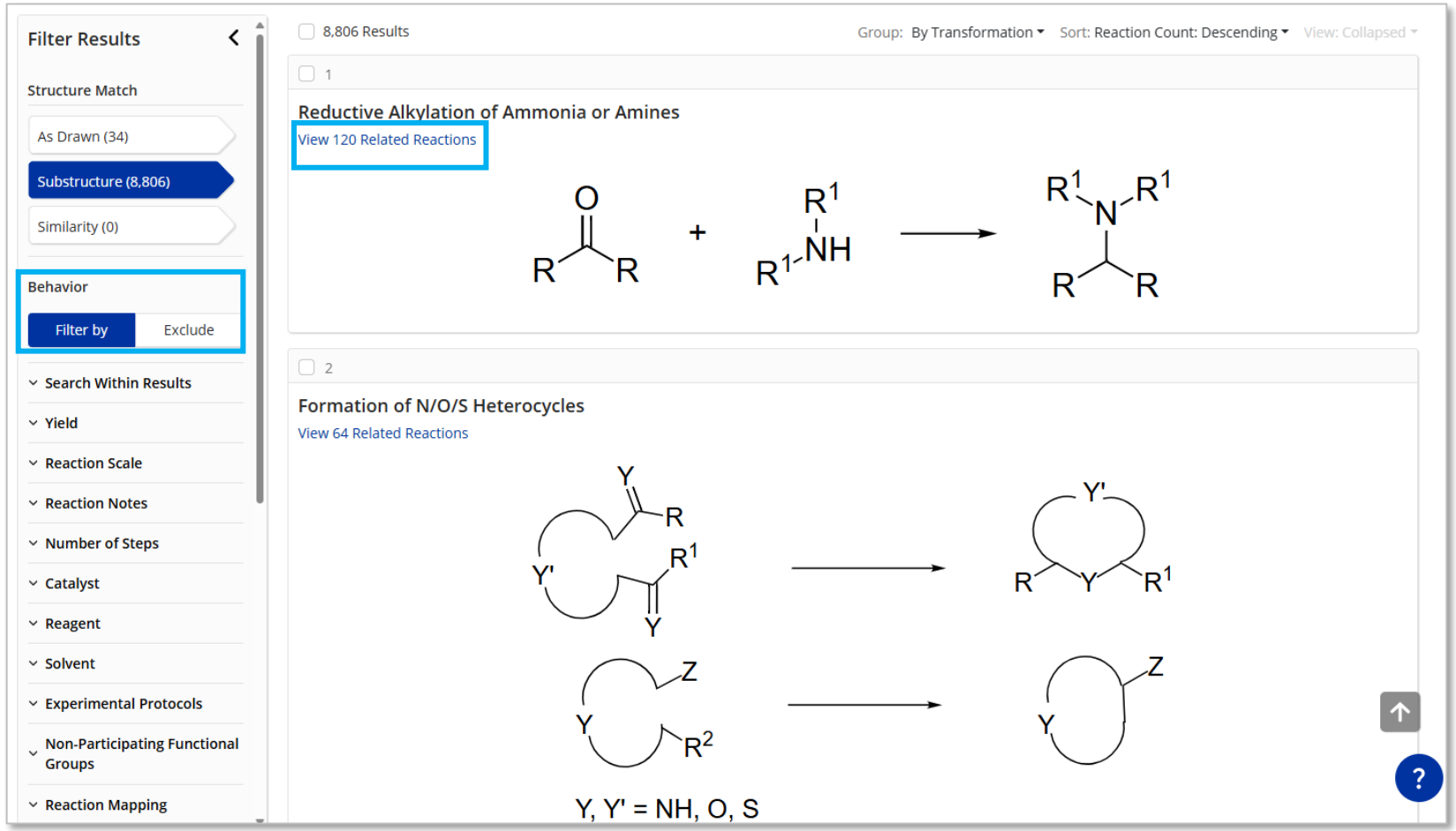
3.3 高效筛选目标反应

反应筛选类别:
产率、规模、步数、不参与反应的官能团、实验步骤、反应类型、立体化学、试剂、催化剂、溶剂、商品信息等

文献筛选类别:
文献类型、语言、出版年份、刊物名等



折叠菜单：相同反应类型的反应在同一菜单里，方便阅读和筛选



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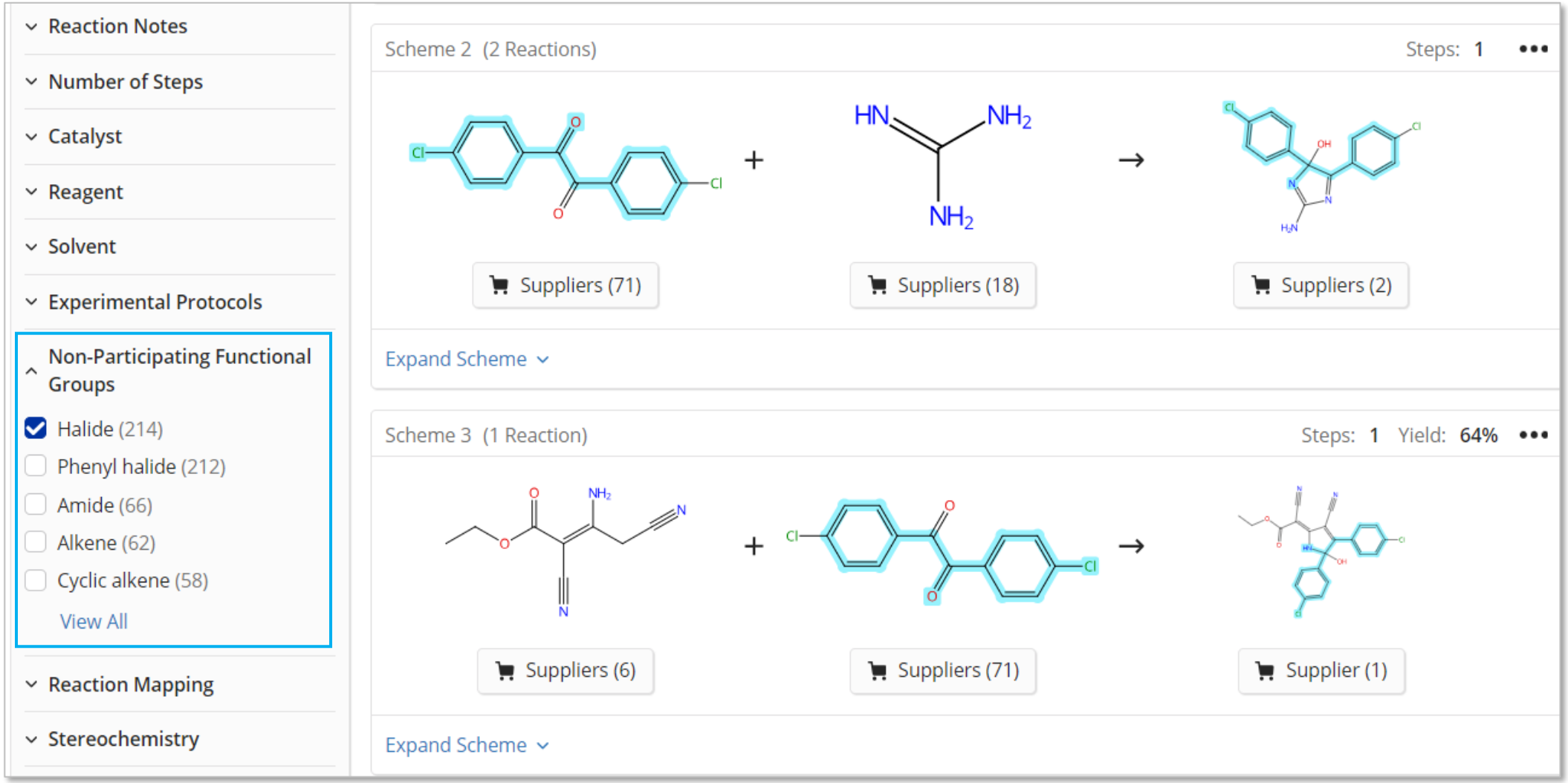
筛选工具：不参与反应官能团

不参与反应官能团：出现在反应前后，但未发生变化的官能团



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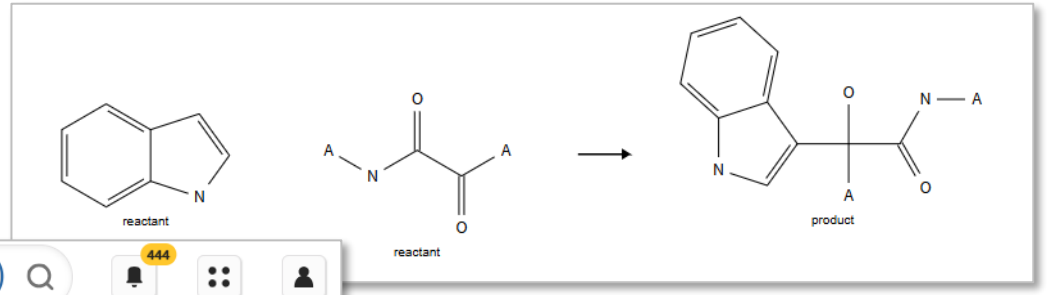
3.4 联用检索——结构与关键词

关注反应的机理研究？　联用检索提高检索效率



CAS SciFinder　References　Reaction mechanism　Edit　444

References search for "Reaction mechanism" + drawn structure

View Related Results

Filter Results

Analyze Results

Structure Match

As Drawn (0)

Substructure (6)

Behavior

Filter by　Exclude

Search Within Results

Concept

CA Section

Publication Year

Language

Publication Name

Organization

6 Results

1

Friedel-Crafts Hydroxyalkylation of Indoles with α-Keto Amides using Reusa
in Water

By: Muthukumar, Alagesan; Sekar, Govindasamy

Journal of Organic Chemistry (2018), 83(16), 8827-8839 | Language: English, Database: CAplus and M

In the presence of K_3PO_4 and tetrabutylammonium bromide
underwent green Friedel-Crafts hydroxyalkylation reactions
PhCOCONHPh to give α-aryl-α-hydroxyindoleacetamides suc
the method relies on reaction at the solid-liquid interface. T
studied; ^{1}H NMR experiments indicated that the reaction p

Full Text　82　65　25

2

Experimental and computational investigation of the α-amylase catalyzed Friedel-Crafts reaction of isatin to access symmetrical and unsymmetrical 3,3',3''-trisindoles

By: Kamboj, Priya; Mohapatra, Abinash; Mandal, Debasish; Tyagi, Vikas

65 Results　Group: By Scheme　Sort: Relevance　View: Collapsed

Scheme 1 (1 Reaction)　Steps: 1　Yield: 97%

Suppliers (2)　Suppliers (117)

Expand Scheme

Scheme 2 (1 Reaction)　Steps: 1　Yield: 96%

Suppliers (6)　Suppliers (117)

Expand Scheme

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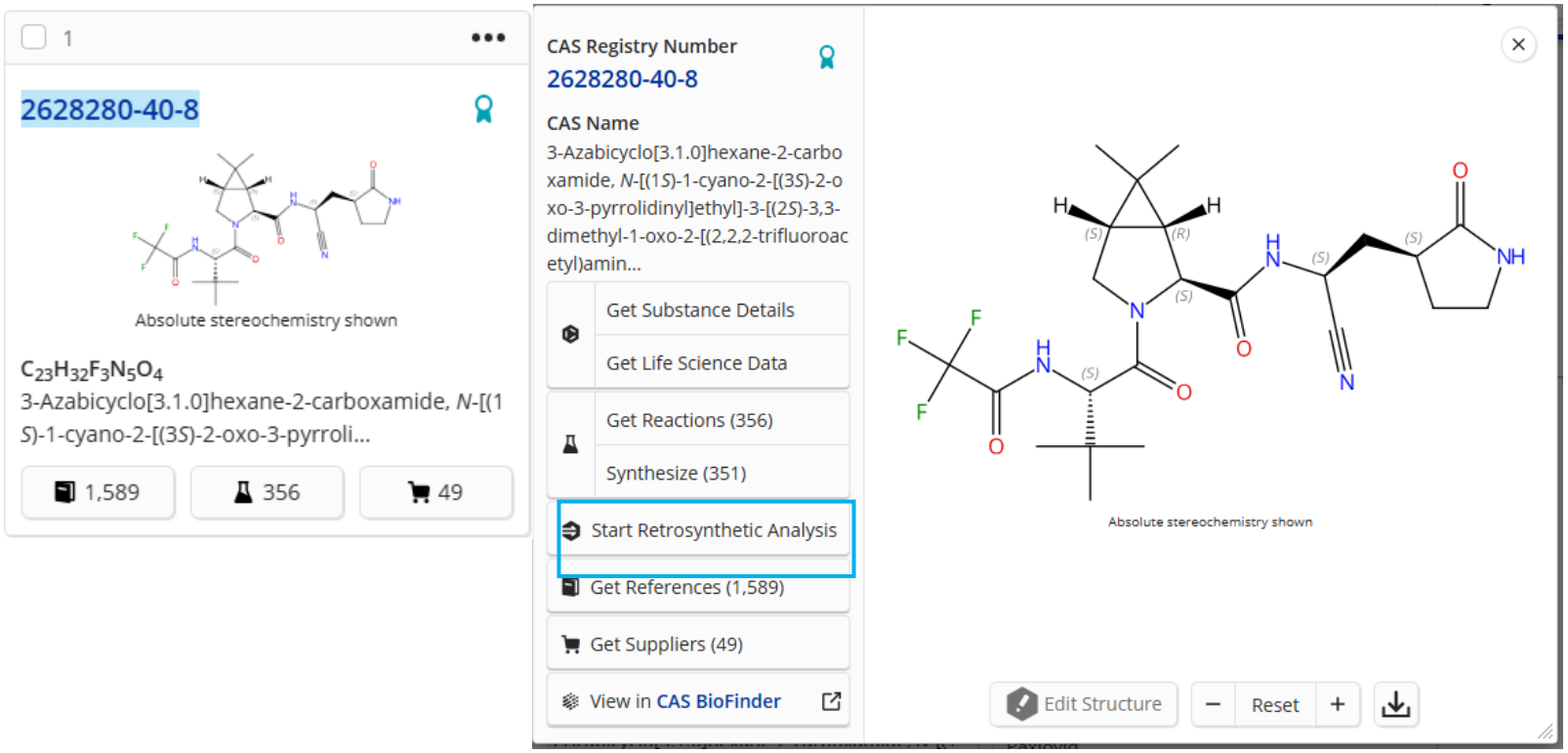
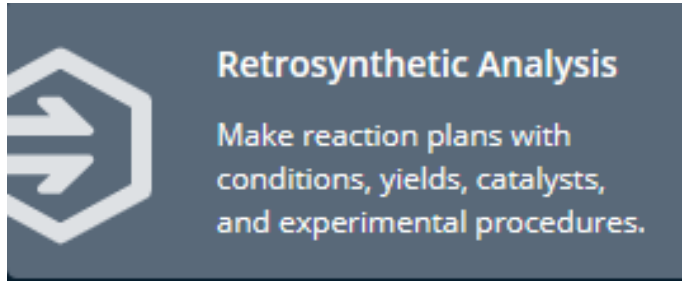
3.5 如何获得逆合成路线?

（1）已知化合物：点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis



CAS Retrosynthesis Tool:

- 逆合成反应路线设计功能
- 启发合成实验设计思路
- 高效获取逆合成反应路线



（2）已知/未知化合物：点击Retrosynthesis检索项，打开绘图板，绘制目标化合物，获得实验路线

预设参数

Retrosynthesis Plan Options for drawn structure

Set Rules Supporting Predicted Reactions

Learn more

- (●) Common — 反应规则常见性
- ( ) Uncommon *(includes common rules)*
- ( ) Rare *(includes common and uncommon rules)*

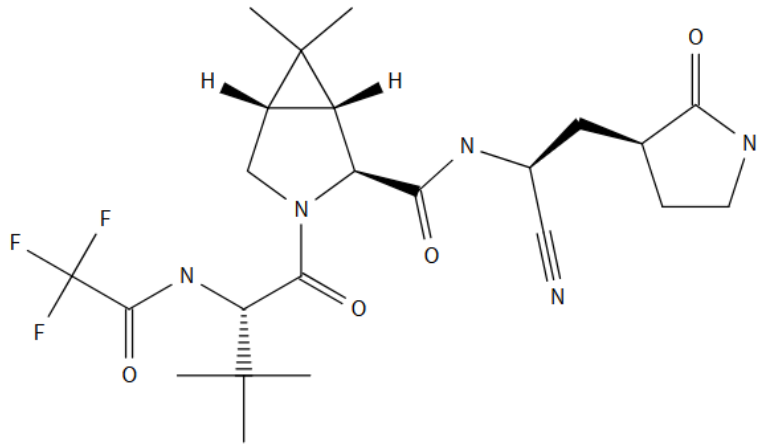
Continue to Retrosynthesis Plan | Edit Structure

Break and Protect Bonds (Optional)

断裂键或保护键

Select a bond within the box to break or protect. You may break a single bond or protect multiple bonds in the target molecule. Learn more

Break Bond | Protect Bond | Clear All Bond Selections



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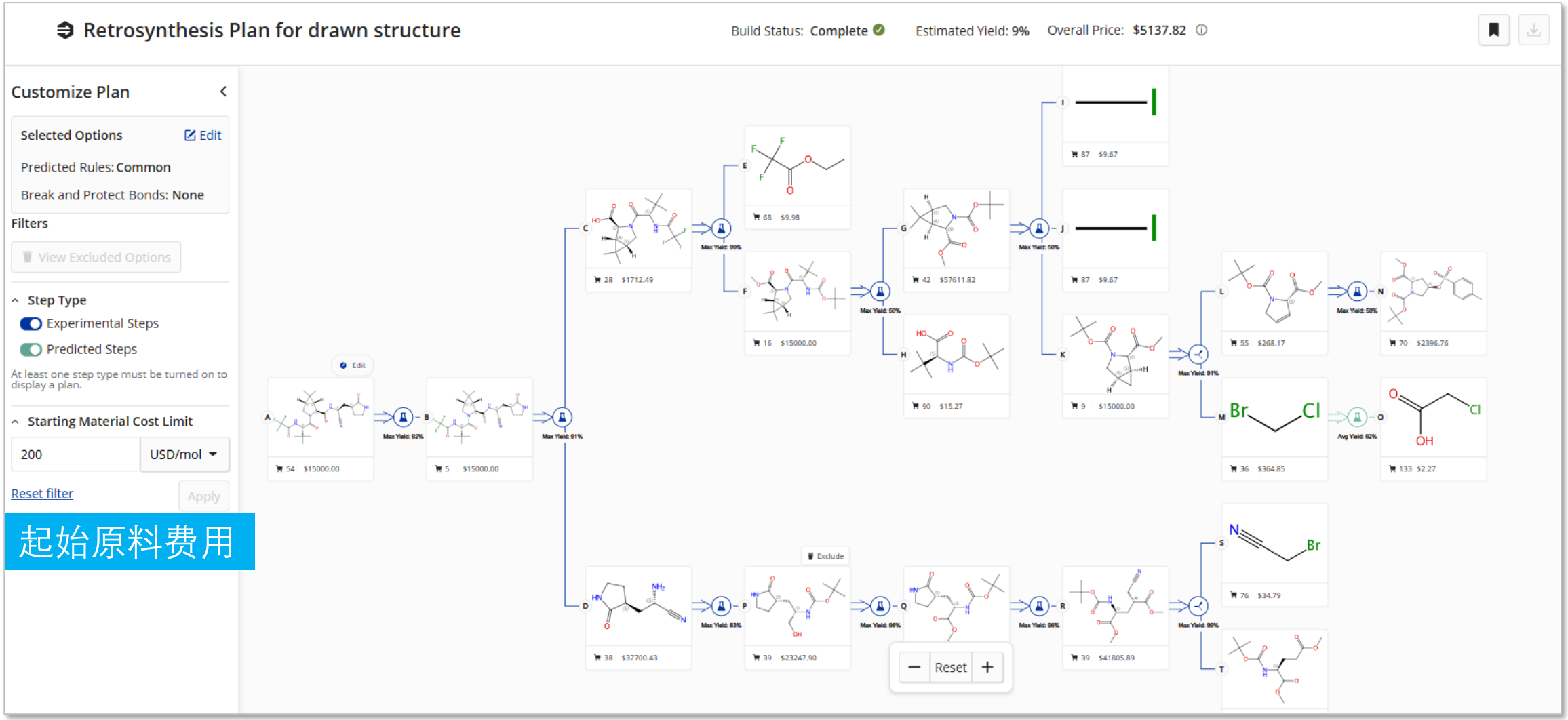
逆合成路线详情



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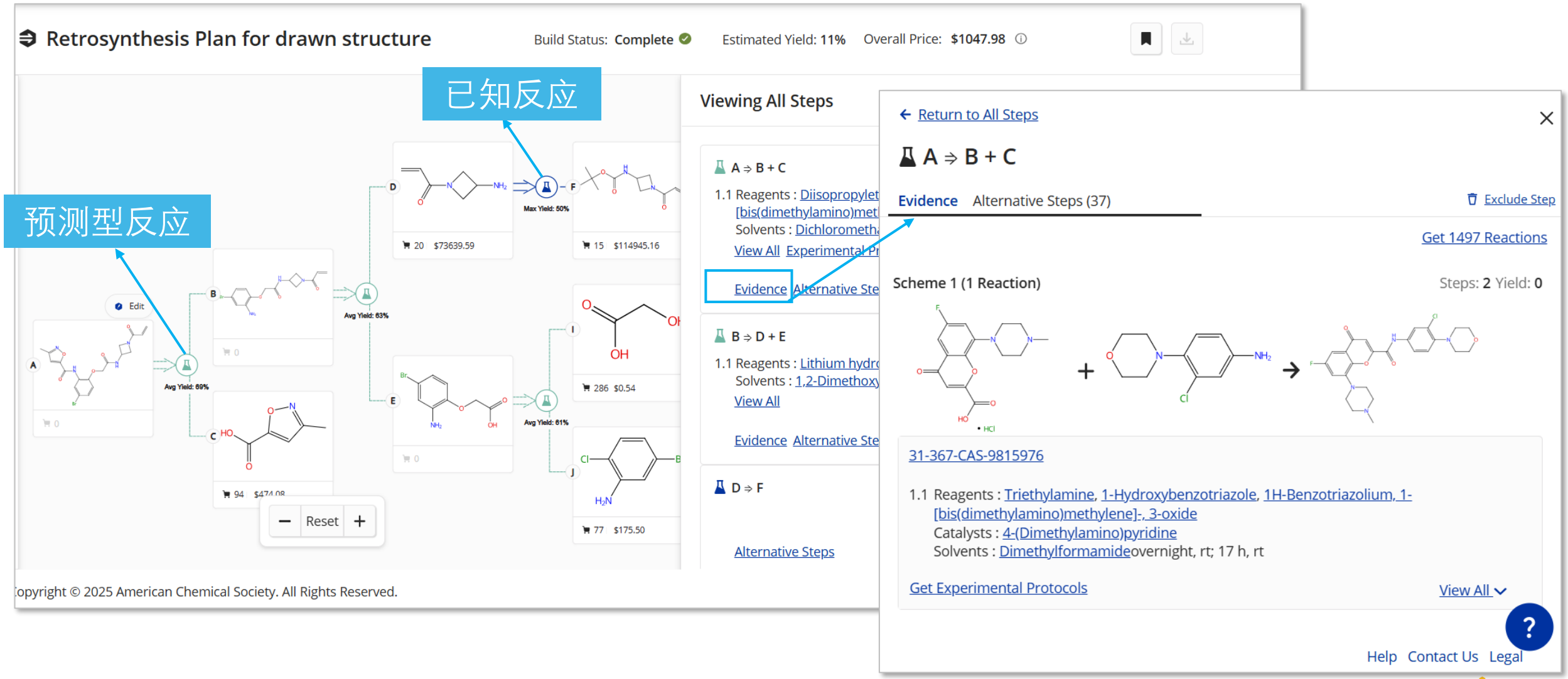
逆合成路线详情



- 可查看每步反应的文献支持与详细条件

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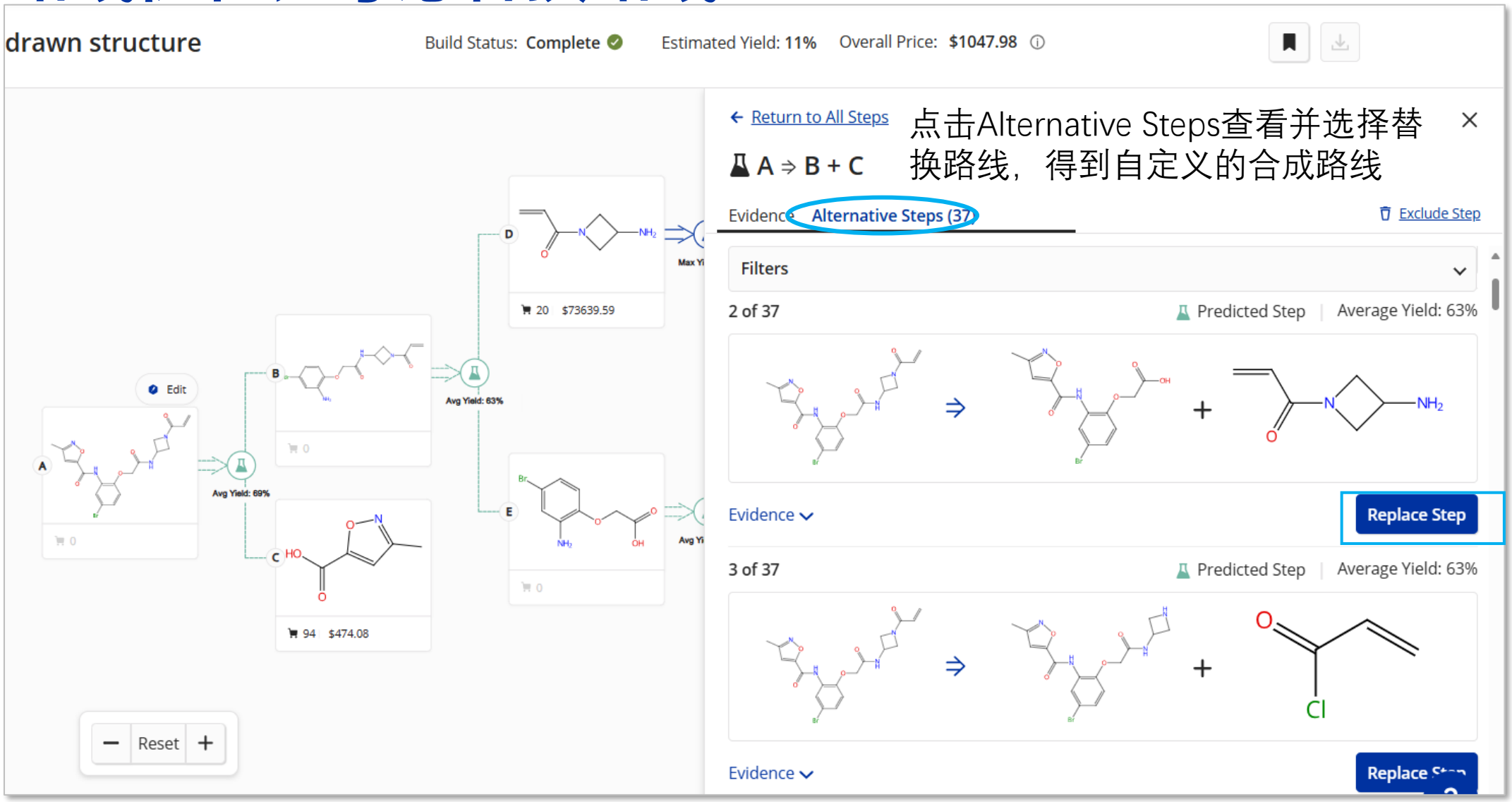
路线优化，考虑替换路线?



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反应检索小结

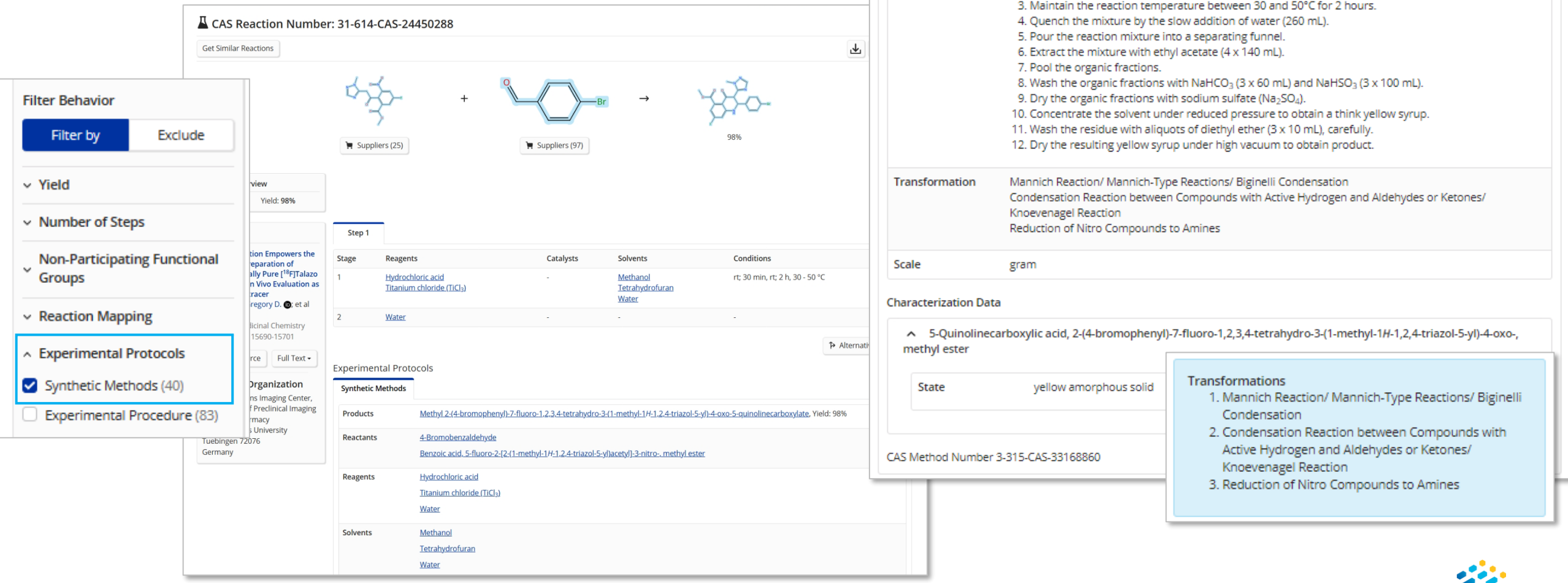
1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 关键词与反应式的联合检索
4. 获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

4. 具体的实验方案怎么查、怎么选?

- 如何获取获得具体的实验操作和表征数据等信息?
- 能一键获取从原文中提取的分析操作和数据详情吗?
- 如何对多种分析方法进行充分评估?
- 我研究的物质有什么具体的配方应用?
- 专利配方的组成和制备工艺是什么? 如何进行实验评估?

4.1 直观的合成实验详情 Synthetic Methods™

- CAS科学家标引的合成详情
- 节省阅读全文的时间，高效获得所需的合成实验信息



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4.2 CAS分析实验方法详情

- CAS科学家标引的分析实验详情
- 无需下载全文，高效获得所需的分析实验信息

Analysis of Vanadium in Stainless steel by Electrochemical extraction

Save

CAS Method Number
1-119-CAS-292609

Method Category
Element Detection

Technique
Electrothermal atomic absorption spectroscopy; Electrochemical extraction

实验原料

Analyte	Matrix	Material
Vanadium	Stainless steel	Al_2O_3 cutting wheel SiC grinding paper 0.05 µm pore size polycarbonate filter Standard calomel referen View All

分析仪器

Equipment Used

Cutting machine, Secotom-10, Struers

Ultrasonic cleaning unit, P 30 H, Elmasonic

Grinding machine, Labopol-6, Struers

Potentiostat, SP-150, BioLogic

Vacuum pump, BUSCHI

Graphite furnace atomic absorption spectrometer, AAnalyst 600, PerkinElmer

Autosampler, AS-800, PerkinElmer

操作步骤

Instructions

Preparation of stainless steel process samples

1. Cut stainless steel pieces from a corner piece of different slabs using a Struers Secotom-10 cutting machine with an Al_2O_3 cutting wheel.
2. Grind and polish the steel samples using a Struers Labopol-6 grinding machine with SiC grinding paper to a size of approximately 15 x 10 x 5 mm.
3. Clean the sample from grinding paper traces using an Elmasonic P 30 H ultrasonic cleaning unit (frequency 37 kHz, room temperature).
4. Clean all glassware in an acid bath, rinse with ultrapure water and methanol sequentially.

Electrolytic extraction of stainless steel using 10% HCl

1. Perform electrolytic extraction on a BioLogic SP-150 potentiostat.
2. Use 10% HCl (10 v/v% HCl, 1 w/v% tartaric acid and methanol) (~200 mL) as the electrolyte.
3. Use the sample as the working electrode and set the potential to 0.150 V vs. the standard calomel electrode (SCE).
4. Suspend the sample in the electrolyte in a platinum basket and use a platinum ring as a counter electrode.
5. Filter the electrolyte through a 0.05 µm pore size polycarbonate filter with the help of a BUSCHI vacuum pump.
6. Expose the sample to ultrasound in methanol and filter the methanol with the electrolyte.
7. Dry and weigh the steel sample.
8. Dilute the filtered electrolyte to the volume with water in a volumetric flask and subject to analysis.
9. Prepare a blank sample by filtering the blank electrolyte through a polycarbonate filter.

Quantification using graphite furnace atomic absorption spectrometry (GFAAS) with Cr as a matrix modifier

1. Perform GFAAS on a PerkinElmer AAnalyst 600 graphite furnace atomic absorption spectrometer equipped with an AS-800 autosampler and PerkinElmer THGA graphite tubes (standard platform B0504033).
2. Use a hollow cathode lamp (HCL) as the radiation source.
3. Use the following furnace program: ramp for 10 s to 110 °C, hold for 30 s; ramp for 10 s to 140 °C, hold for 30 s; ramp for 10 s to 1300 °C, hold for 20 s; perform atomization at 2400 °C for 6 s; ramp for 1 s to 2500 °C and hold for 5 s.
4. Set the instrument parameters as follows: internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm.
5. Add 0.05 µg Cr as a matrix modifier.
6. Inject 10 µL of the sample and perform measurements.

数据有效性

Validation

Linearity Range	0-400 µg/L
Recovery	0.03 wt% (0.05 wt% reference value, sample data)

分析条件

Conditions

Instrument

Internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; slit width: 0.7 nm; wavelength: 318.4 nm; injection volume: 10 µL

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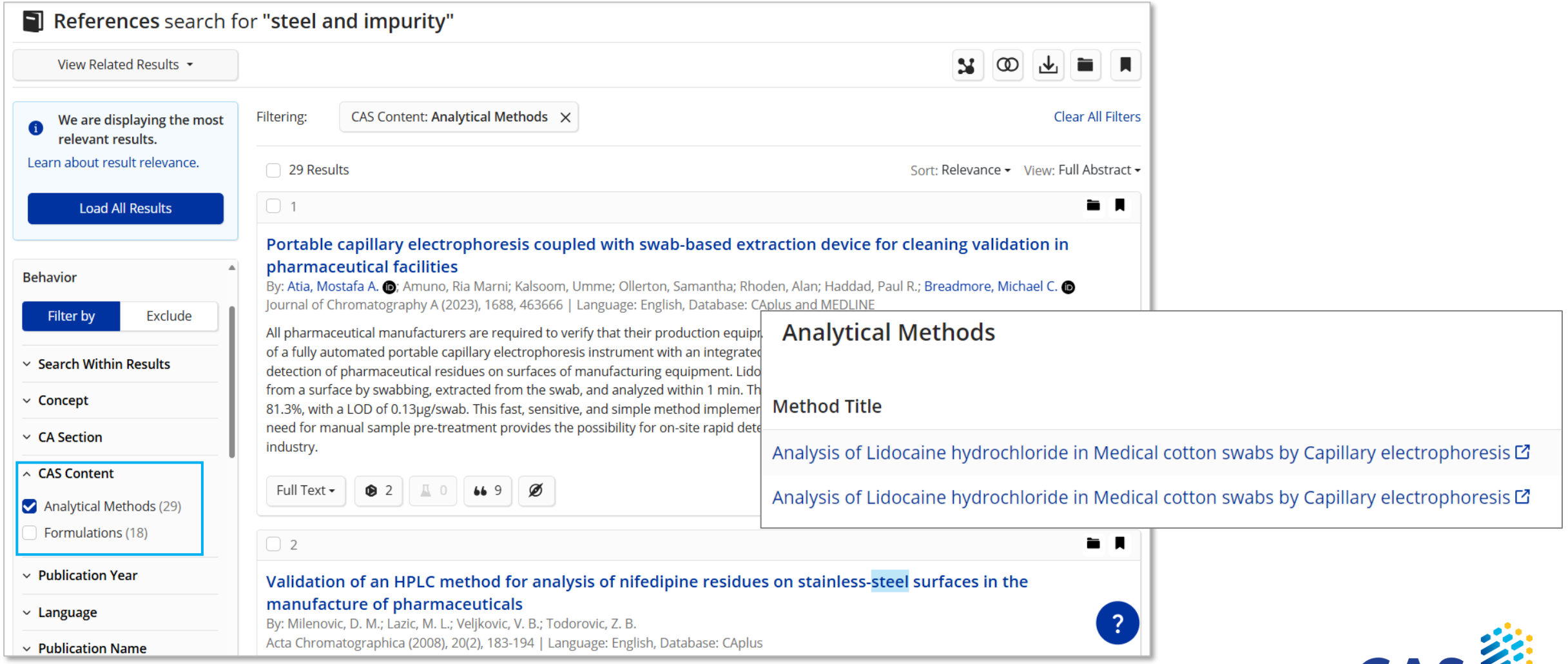
关注文献关联的分析方法?

方法 (1)：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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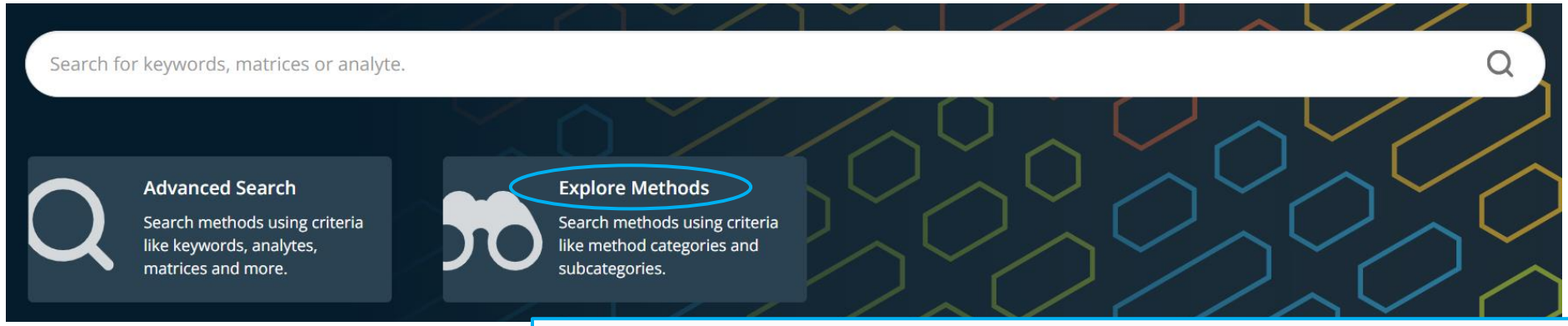
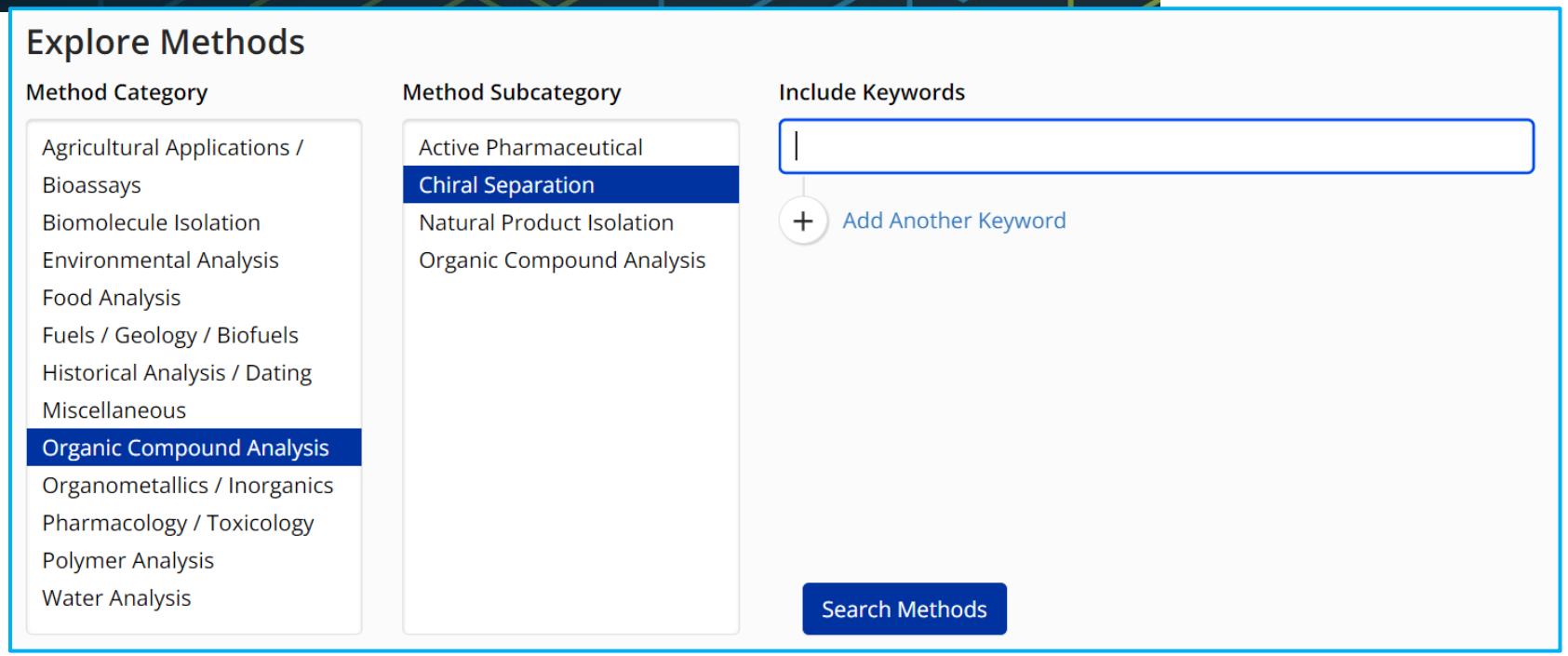
直接检索感兴趣的分析实验方法

方法(1)：登录https://methods.cas.org，主题检索或分类浏览



方法分类: 13大类，45小类

农业应用、生物鉴定、生物分子分离、环境、食品、考古、有机物、药学、毒理学等



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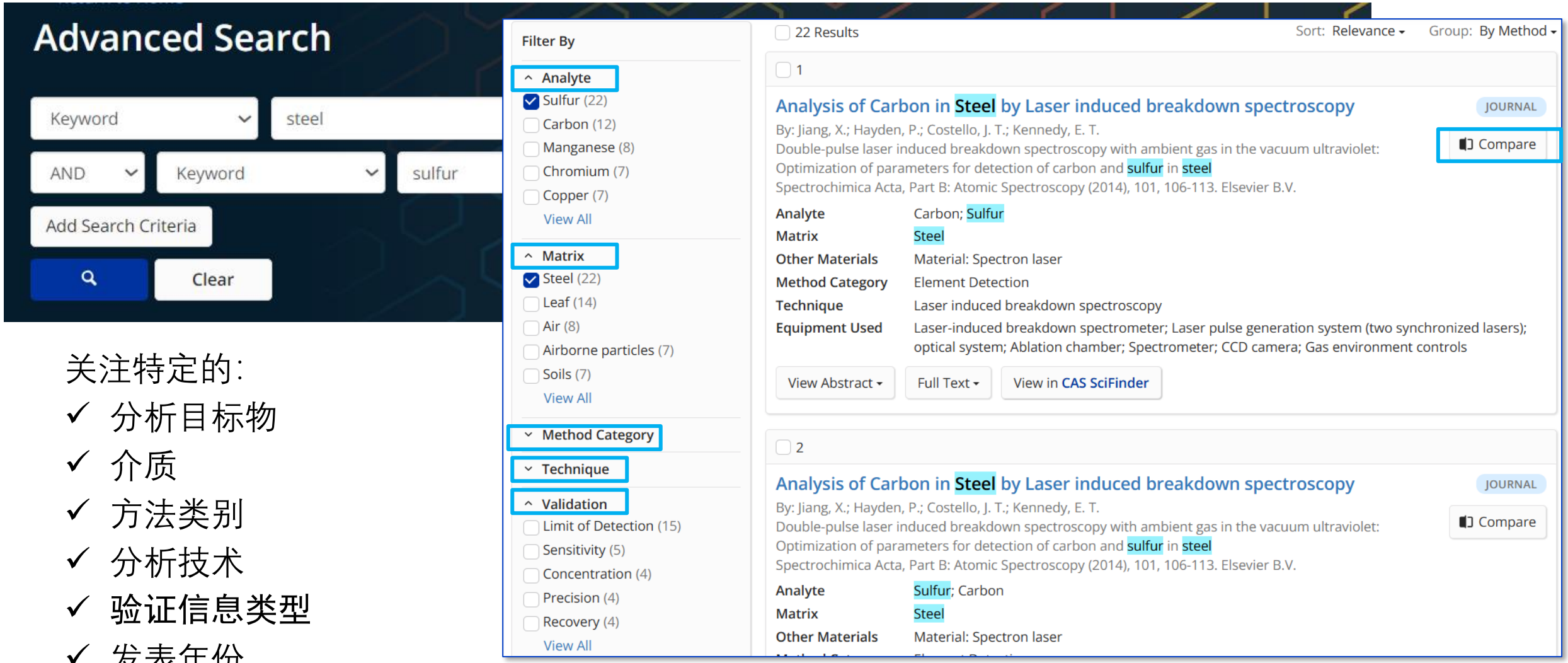
如何选择合适的分析方法?



关注特定的:

- ✓ 分析目标物
- ✓ 介质
- ✓ 方法类别
- ✓ 分析技术
- ✓ 验证信息类型
- ✓ 发表年份

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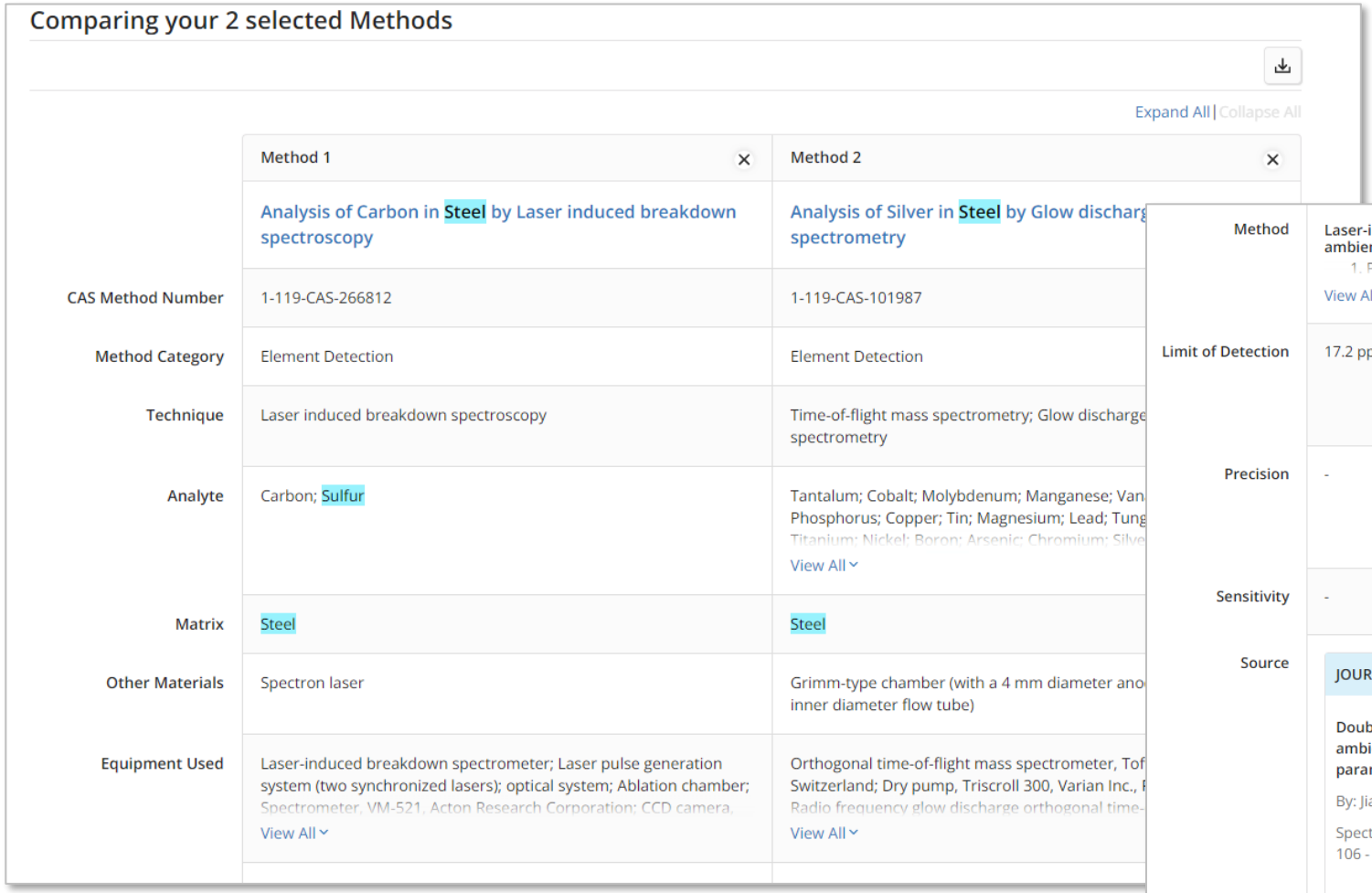
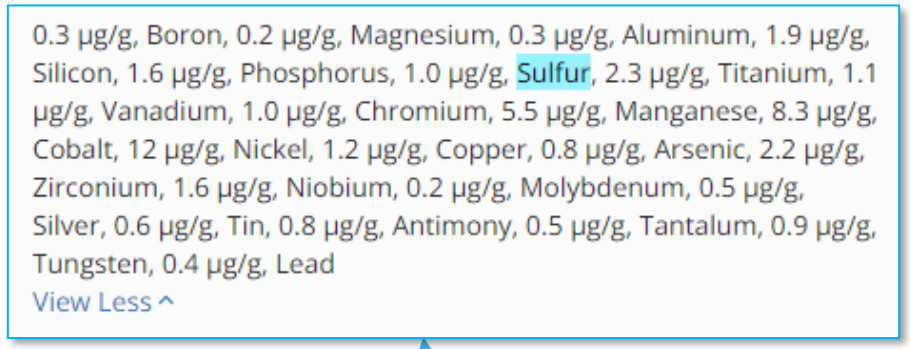
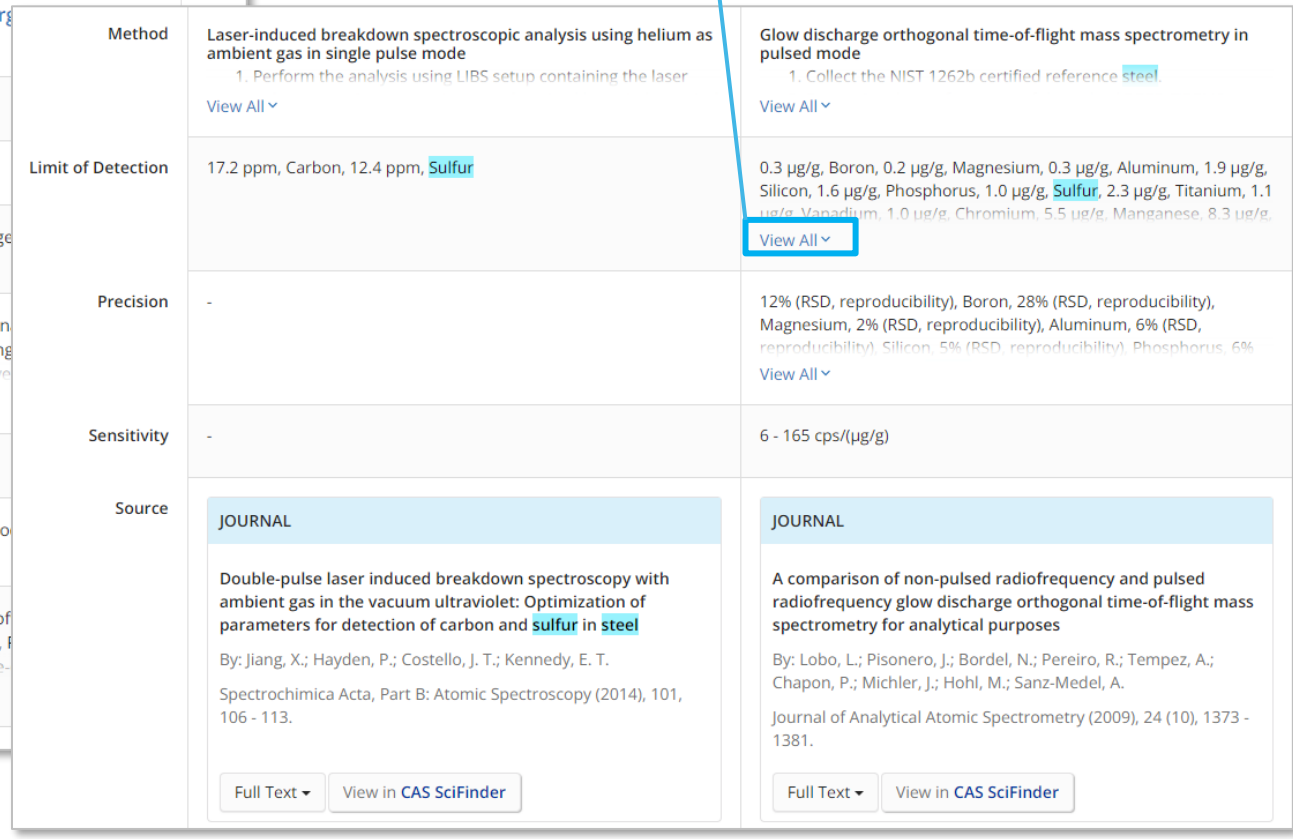
如何选择合适的分析方法?







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4.3 研究课题在产品中的应用？配方/制剂的检索与设计

方法（1）： 登录CAS Formulus主页（https://formulus.cas.org）输入检索式

- 制药、化妆品、食品、农化、油墨、涂料等多领域中的配方
- 工艺、成分、目标成分的常见配伍成分、设计配方、探索合规要求等

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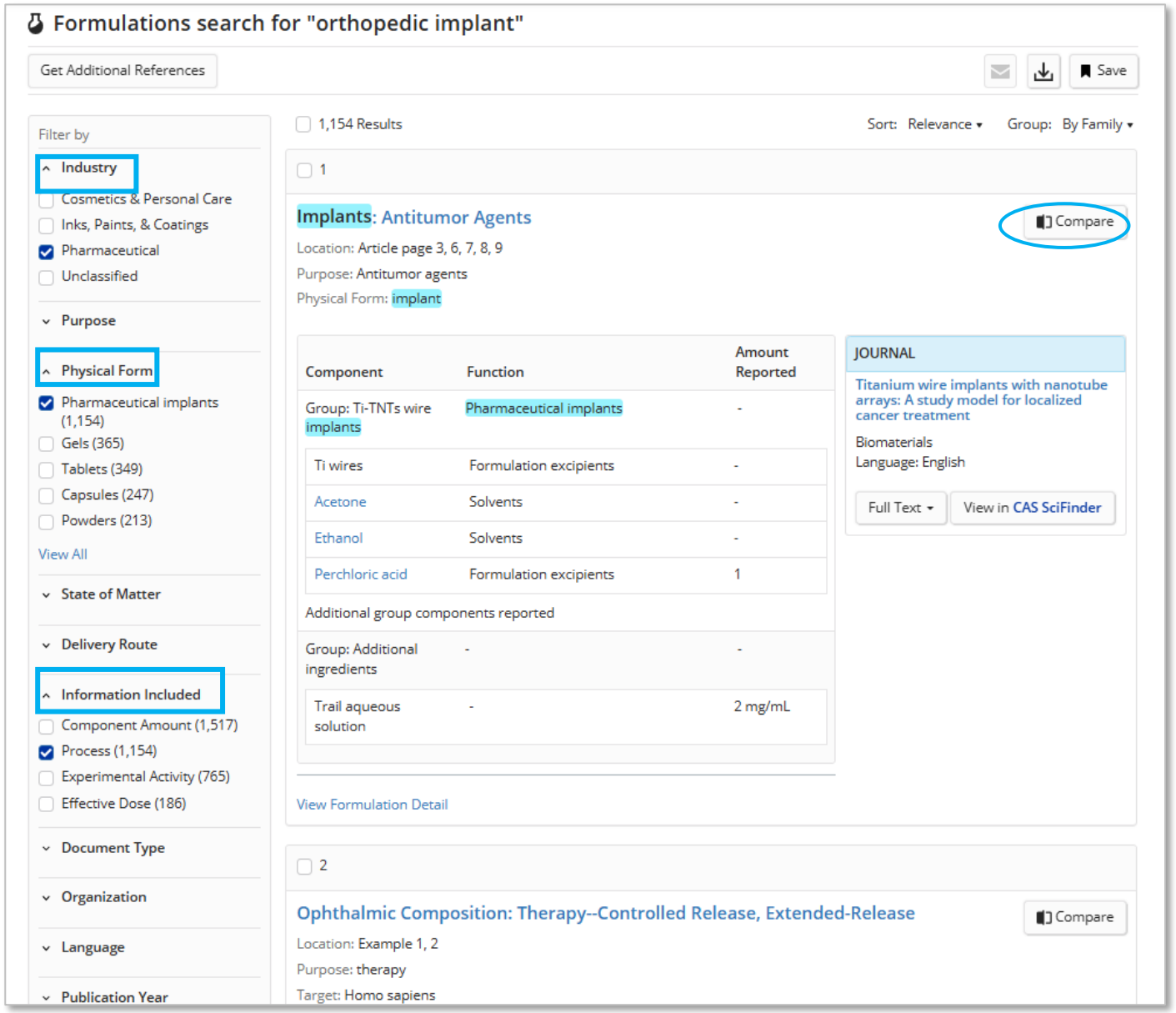
配方/制剂结果集

- 利用聚类项精简结果：

行业、配方/制剂用途、物理形式、物质状态、递送方式、涵盖信息、文献类型、发表机构、发表年份

- 可查看制剂或配方成分，功能及用量
- 可查看原料详情
- 支持对比选中的制剂或配方
- 支持查看或下载专利全文
- 可查看制剂或配方详情



一次最多可以比较三种不同制剂或配方的信息详情

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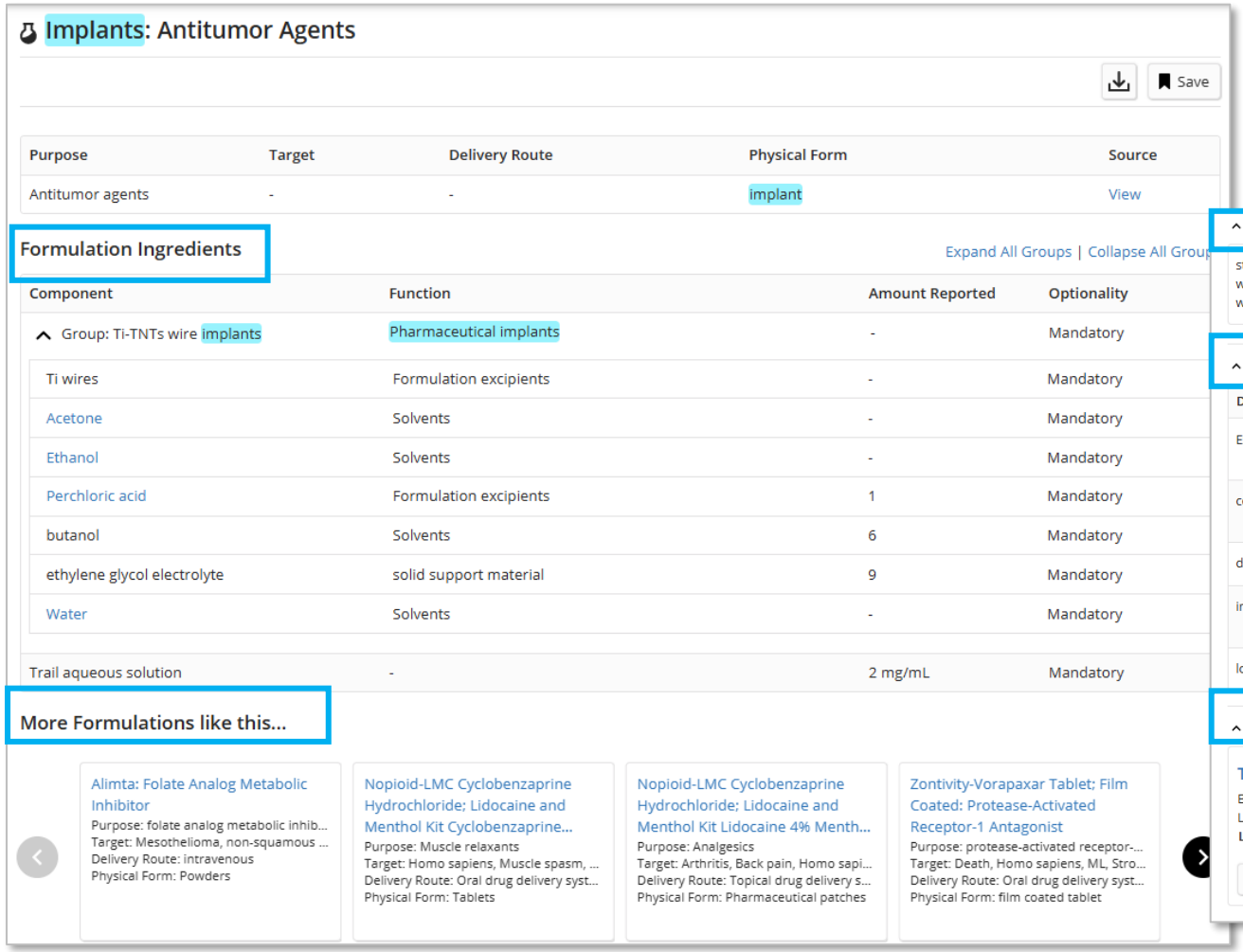
配方/制剂的制备？实验评估？

- 制剂或配方原料
- 相似的制剂或配方
- 制备工艺
- 制剂或配方实验评估
- 专利来源



Implants: Antitumor Agents

Save

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents	-	-	implant	View

Formulation Ingredients

Expand All Groups | Collapse All Group

Component	Function	Amount Reported	Optionality
Group: Ti-TNTs wire implants	Pharmaceutical implants	-	Mandatory
Ti wires	Formulation excipients	-	Mandatory
Acetone	Solvents	-	Mandatory
Ethanol	Solvents	-	Mandatory
Perchloric acid	Formulation excipients	1	Mandatory
butanol	Solvents	6	Mandatory
ethylene glycol electrolyte	solid support material	9	Mandatory
Water	Solvents	-	Mandatory
Trail aqueous solution	-	2 mg/mL	Mandatory

More Formulations like this...

Alimta: Folate Analog Metabolic Inhibitor
Purpose: folate analog metabolic inhib...
Target: Mesothelioma, non-squamous ...
Delivery Route: intravenous
Physical Form: Powders

Nopioid-LMC Cyclobenzaprine Hydrochloride; Lidocaine and Menthol Kit Cyclobenzaprine...
Purpose: Muscle relaxants
Target: Homo sapiens, Muscle spasm, ...
Delivery Route: Oral drug delivery syst...
Physical Form: Tablets

Nopioid-LMC Cyclobenzaprine Hydrochloride; Lidocaine and Menthol Kit Lidocaine 4% Menth...
Purpose: Analgesics
Target: Arthritis, Back pain, Homo sapi...
Delivery Route: Topical drug delivery s...
Physical Form: Pharmaceutical patches

Zontivity-Vorapaxar Tablet; Film Coated: Protease-Activated Receptor-1 Antagonist
Purpose: protease-activated receptor-...
Target: Death, Homo sapiens, ML, Stro...
Delivery Route: Oral drug delivery syst...
Physical Form: film coated tablet

Process

stage 1: Ti-TNTs wire implants were loaded overnight with 2 mg/mL Trail aqueous solution for in-vitro, ex-vivo and in-vivo studies. prior to loading, implants were cleaned with ethanol, dried under sterile conditions and placed in a 30 mL drops of Trail solutions placed on a parafilm strip. after overnight drug loading, implants were dabbed with a soft tissue and dried and placed in PBS solution to monitor drug release profile at 37 °C, over a range of selected time points.

Experimental Activity

Descriptor	Notes	Details
Ex-vivo study	-	no caspase-3 activity was observed for PBS-TNTs samples
cell death	-	highest cell death was observed in Trail-TNTs
drug release	-	45 %
in-vitro cytotoxicity	-	luciferase activity confirmed 100% cell death in Trail-TNTs
loading amount	-	12.63 µg

Source Journal

Titanium wire implants with nanotube arrays: A study model for localized cancer treatment
Biomaterials
Language: English
Location: Article page 3, 6, 7, 8, 9

Full Text | View in CAS SciFinder

Feedback

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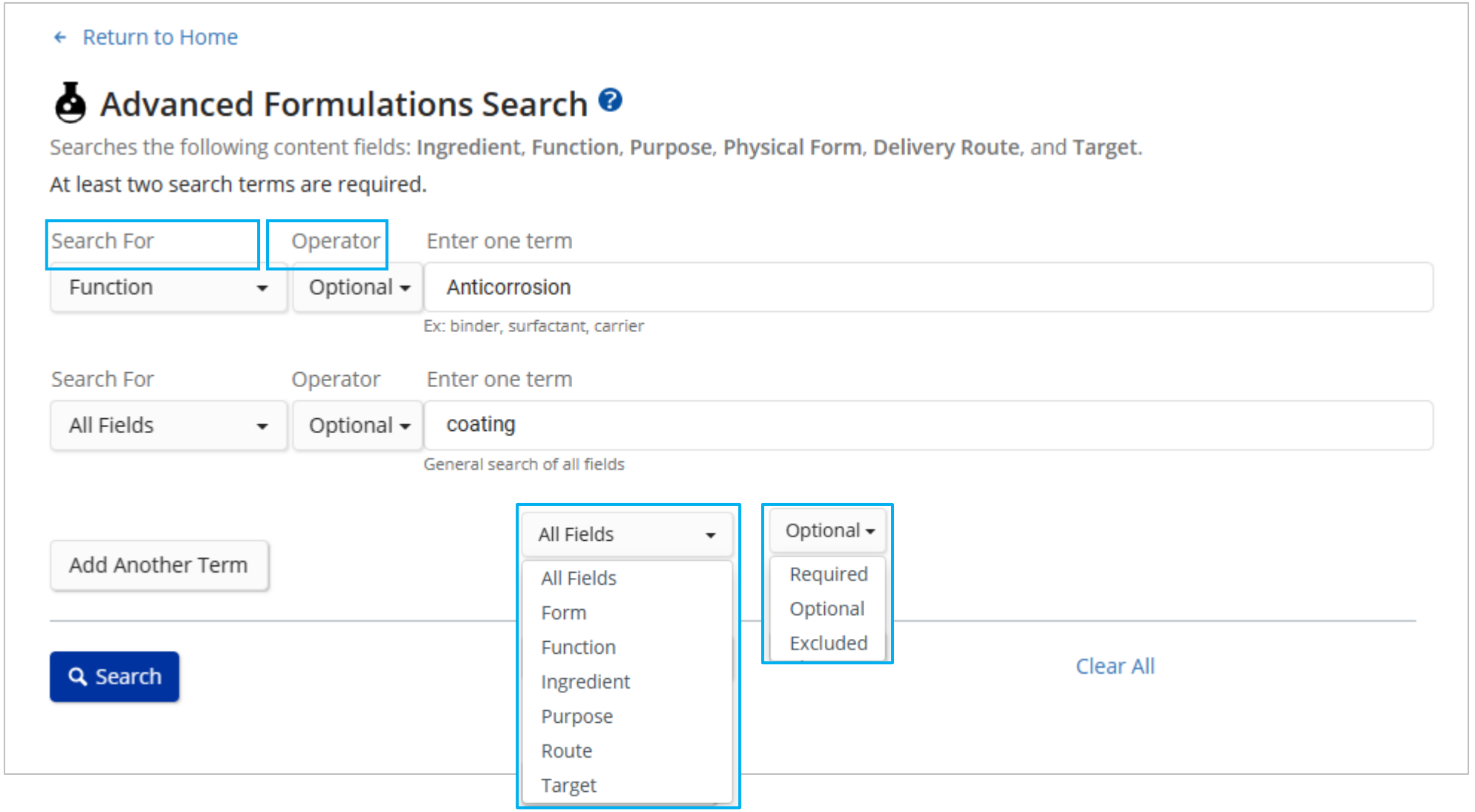
高级检索



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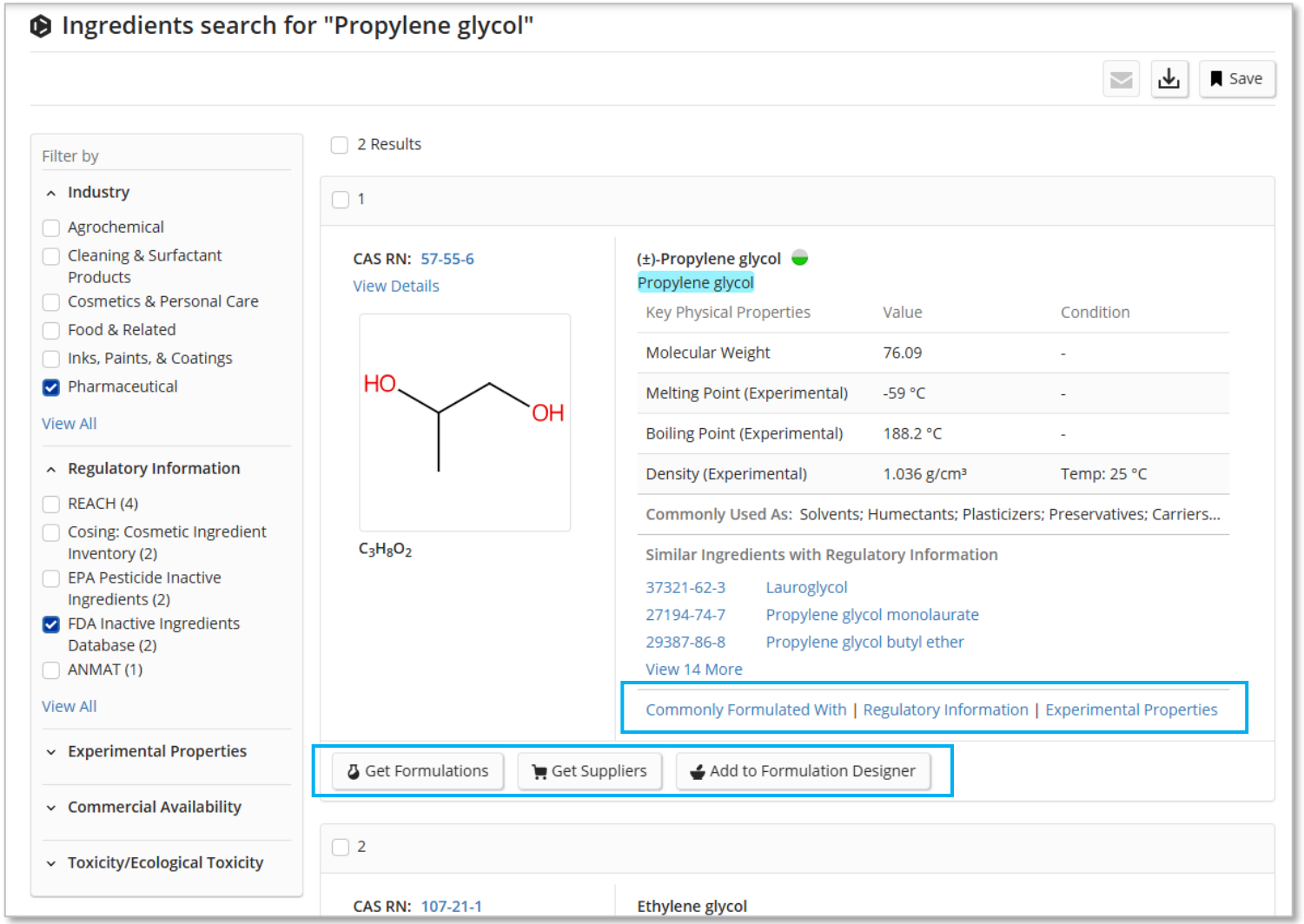
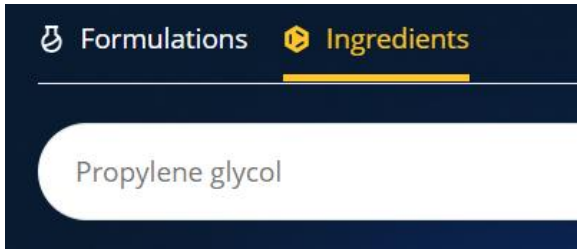
检索原料





- 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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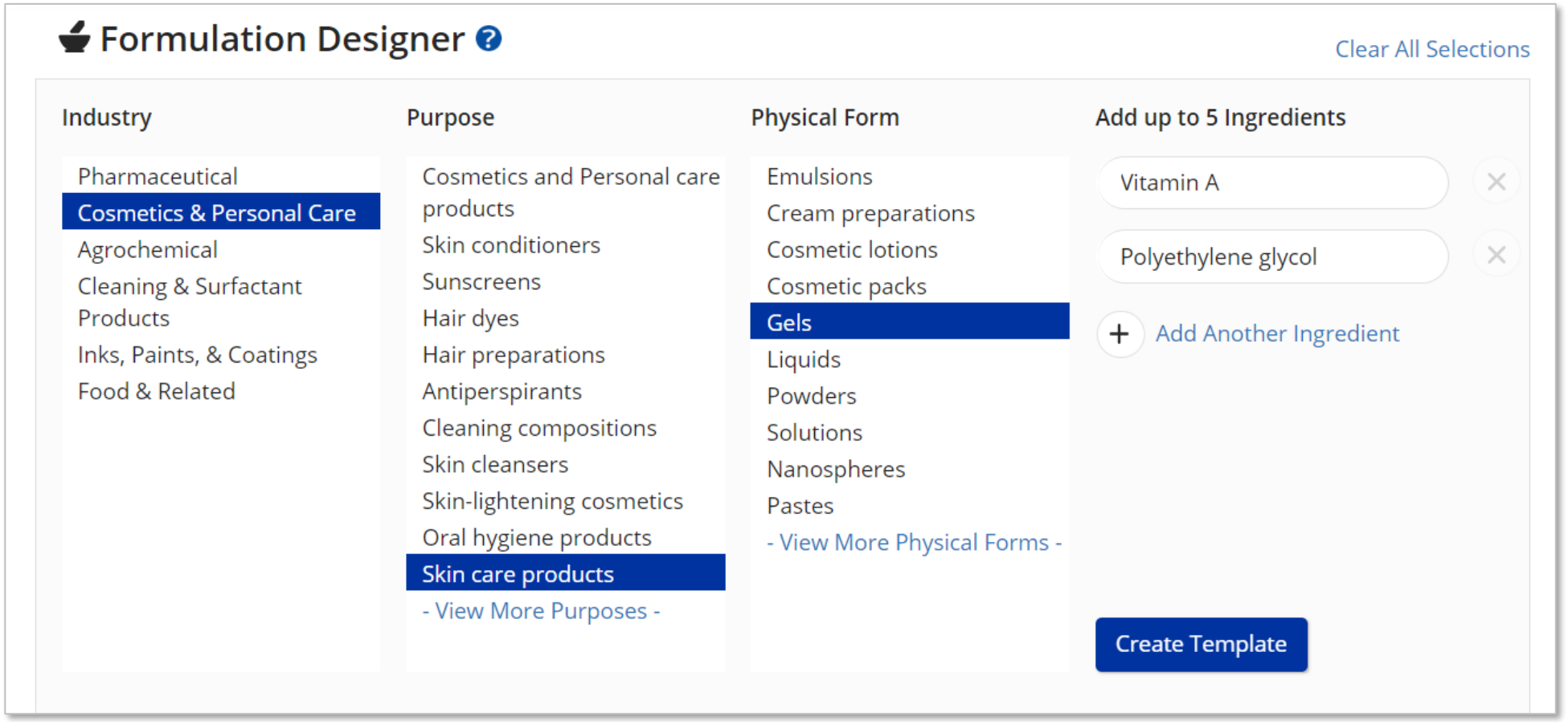
设计配方/制剂



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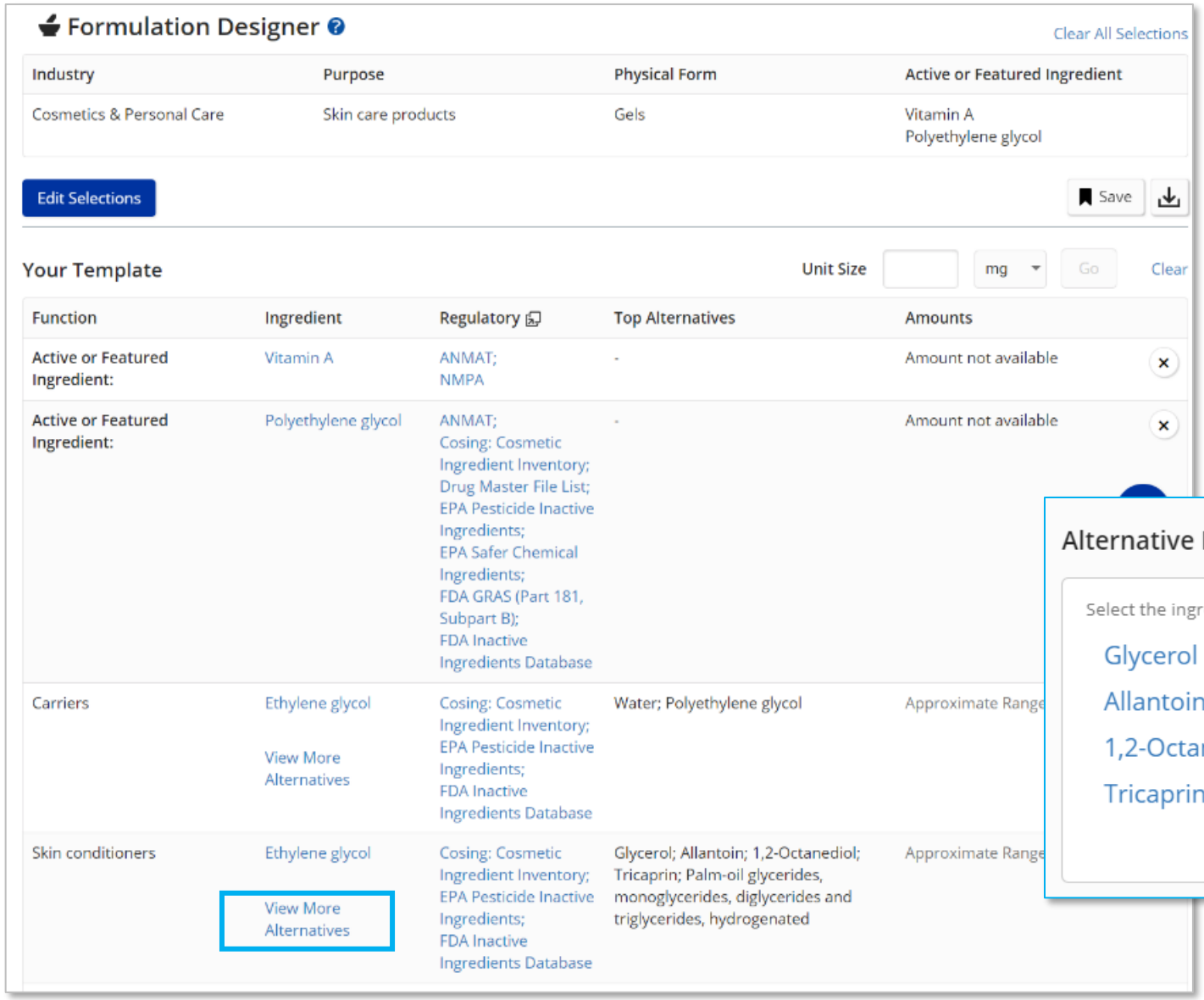
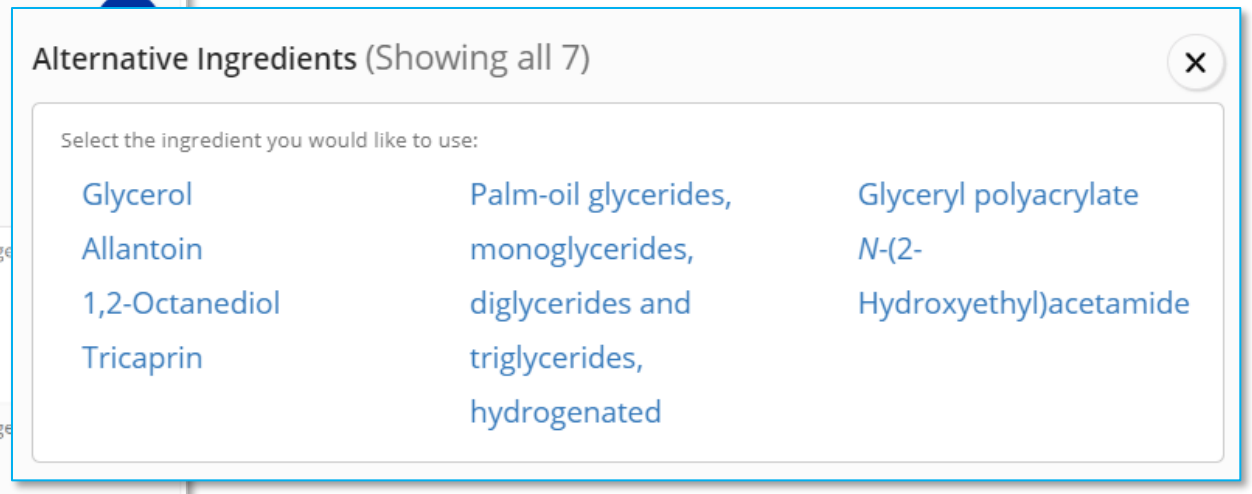
设计配方/制剂





- 原料详情
- 原料管制信息
- 可替代的原料选项

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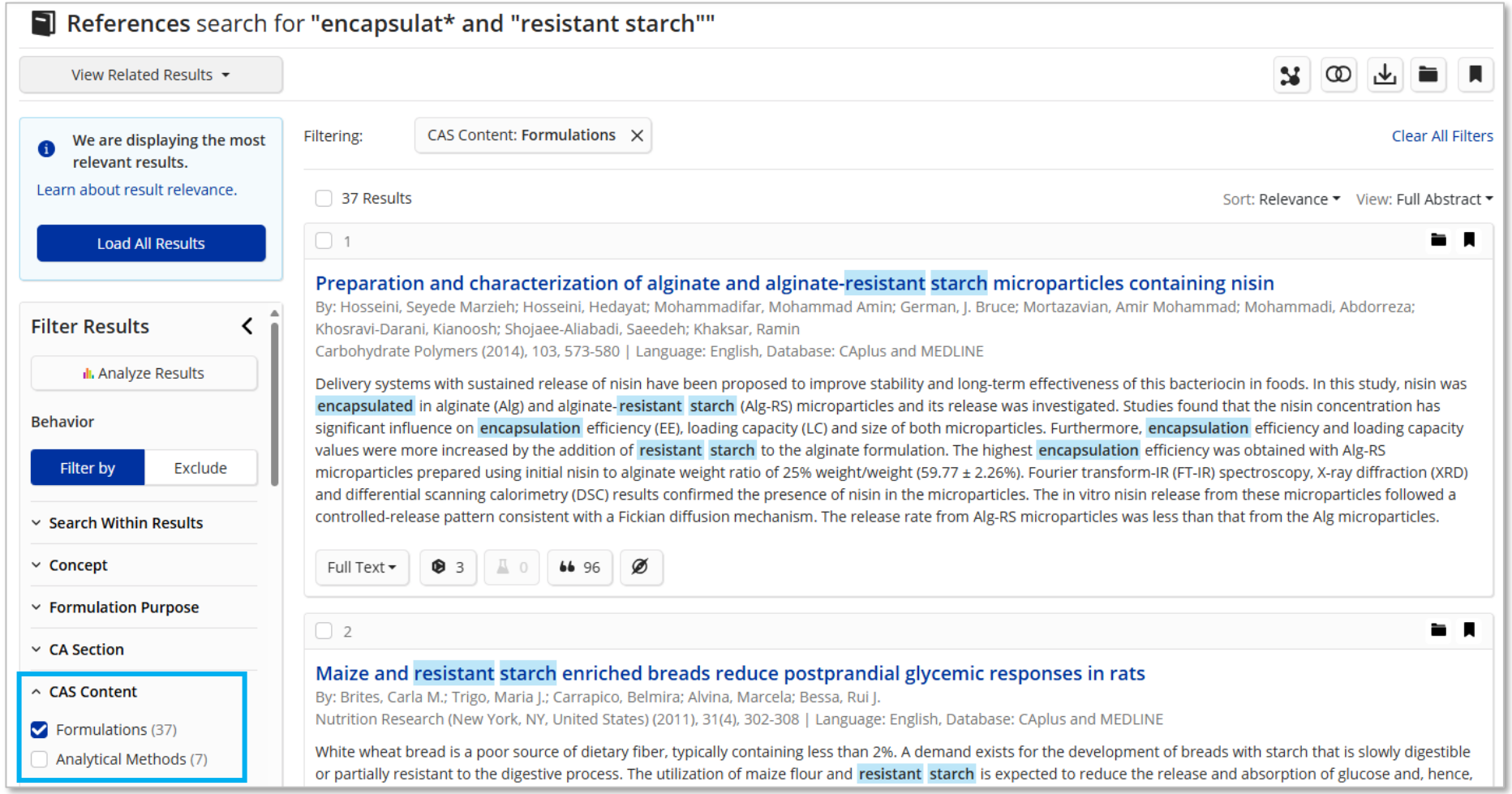
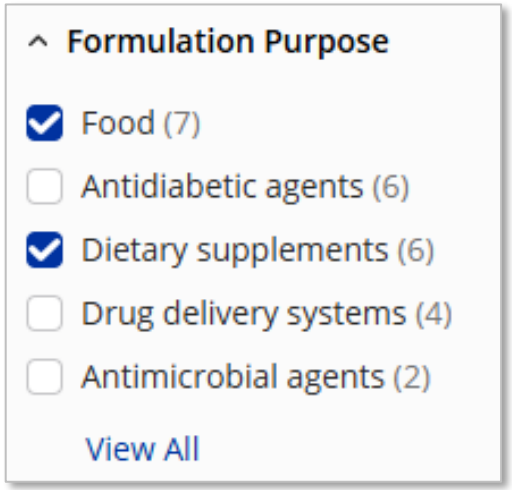
文献关联的配方/制剂

方法（2）：在CAS SciFinder的文献结果集页面，点击CAS Content中的 Formulations 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



定位配方或制剂的功能目标



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文献关联的配方/制剂

Resistant Starch Film-Coated Microparticles for an Oral Colon-Specific Polypeptide Delivery System and Its Release Behaviors

3 | 0 | 55 | Citation Map

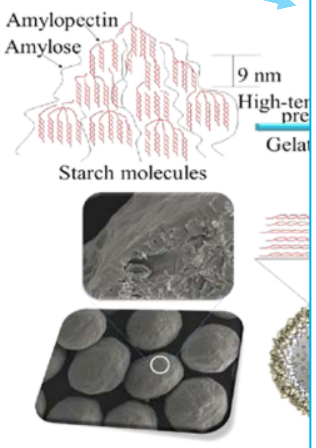
In this Reference

- Concepts
- Substances
- Formulations
- Cited Documents

By: Situ, Wenbei; Chen, Ling; Wang, Xueyu; Li, Xiaoxi

DOI: 10.1021/jf500472b

For the delivery of bioactive components to the colon, an oral colon-specific controlled release system coated with a resistant starch-based film through aqueous dispersion coating process was developed. Starch was modified by a high-temperature-pressure reaction, enzymic debranching, and retrogradation, resulting in a dramatic increase in the resistibility against enzymic digestion (meaning the formation of resistant starch, specifically RS3). This increase could be associated with an increase in the relative crystallinity, a greater amount of starch mol. aggregation structure, and the formation of a compact mass fractal structure, resulting from the treatment. The microparticles coated with this RS3 film showed an excellent controlled release property. In streptozotocin (STZ)-induced type II diabetic rats, the RS3 film-coated insulin-loaded microparticles exhibited the ability to steadily decrease the plasma gluc
with different insulin dosages after oral administration; no glycopenia c
system has been demonstrated for the accurate delivery of bioactive p



Formation of the RS3 film

Keywords: starch film coated microparticle colon polypeptide delivery i

View Source | Full Text | View in CAS Formulus

Formulations

Formulation Title
Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems
Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems
Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems or Antidiabetic Agents--Controlled Release Drug Delivery Systems
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Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

实验方案检索小结

1. 利用Synthetic Methods™查看文献中合成方法详情
2. 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
3. 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

大纲

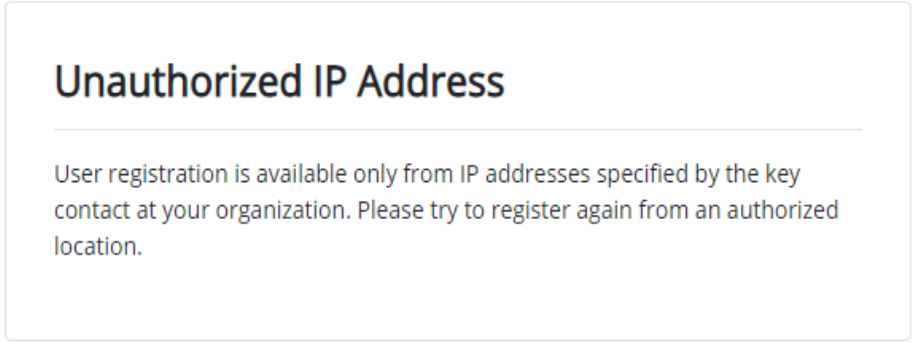
- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
- 常见问题Q&A

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**

常见登录问题



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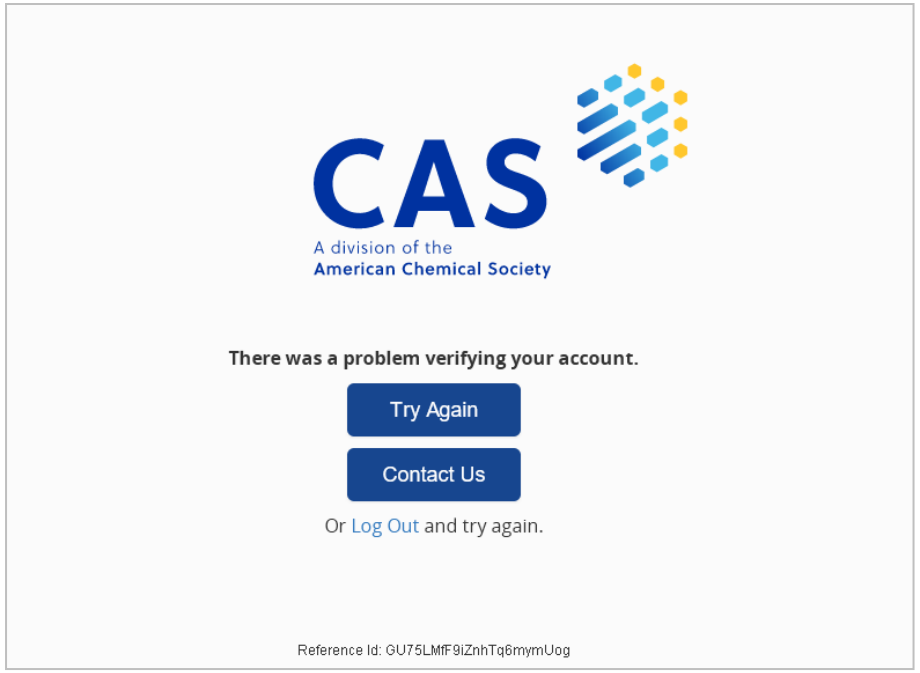
- 如果链接正确，且在校园内，请联系图书馆或china@acs-i.org



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学习资源

微信公众号：ACS美国化学会

线上学习短视频：

CAS SciFinder 学习中心

内容包括：基础演示短视频，专题培训录屏、综合应用案例等

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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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THANK YOU!

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