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 (Academic)简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 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

CAS 具有最全面的学科连接内容合集

Over
50K
scientific journals and documents

Over
274
million substances

Over
50
languages translated

Over
109
patent offices worldwide

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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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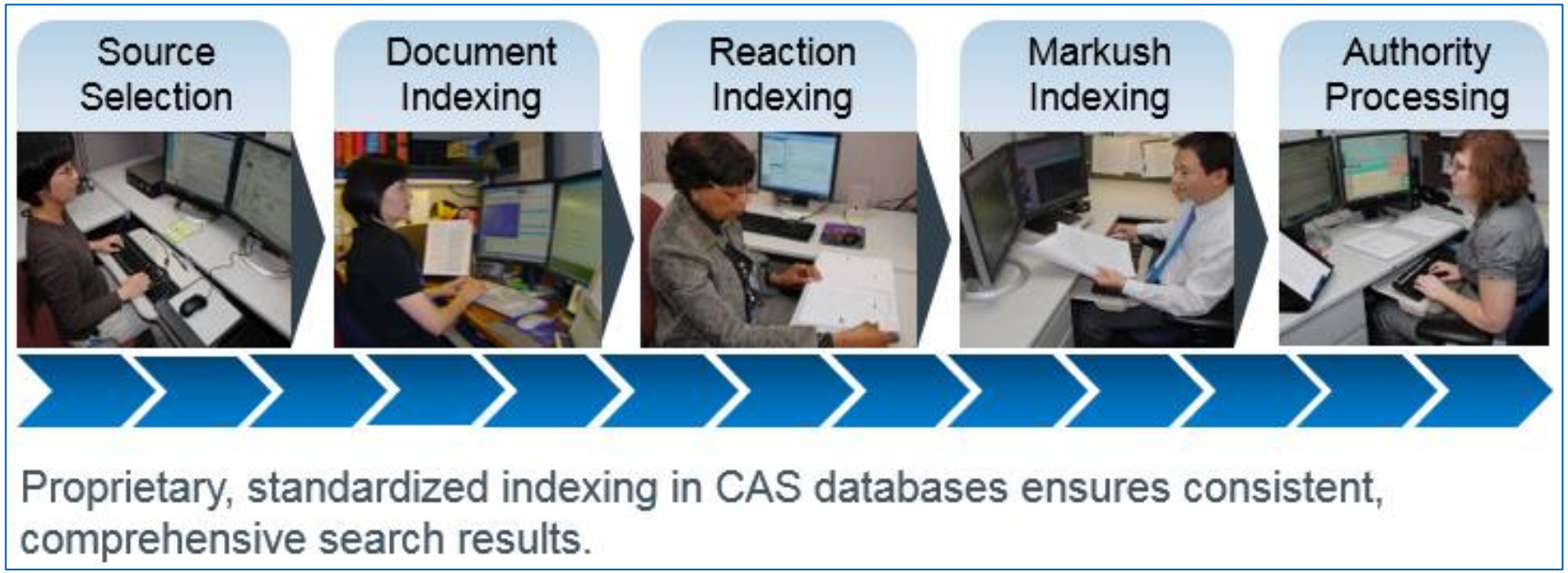
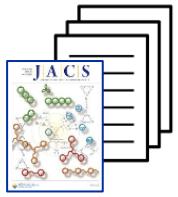
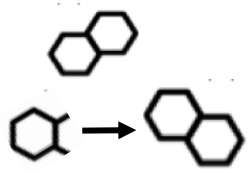
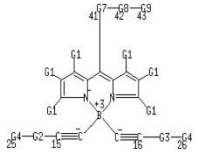
CAS 科学家的智力标引





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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CAS 解决方案与服务

Discovery

CAS SciFinder Discovery Platform™

Get discoveries to market faster and optimize margins by giving researchers the information they need

Intellectual Property

STN IP Protection Suite™

Ensure that your intellectual property is protected and find opportunities to extend into new markets

Custom Solutions

CAS Custom Services℠

Customized data, analytics and insights to maximize the value of information assets and fuel digitalization success

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CAS SciFinder Discovery Platform 解决方案

CAS SciFinder^{n} ——加速科学发现的业界领先的科学工具

业界最领先的相关性搜索引擎，提供和化学相关的各学科的文献、物质、反应和生物序列等检索内容，检索智能、高效、简单。可用于基金申请的文献准备、为新课题制定实验计划、寻求学术合作者、进行逆合成分析以及更多其他的教学和科研活动。

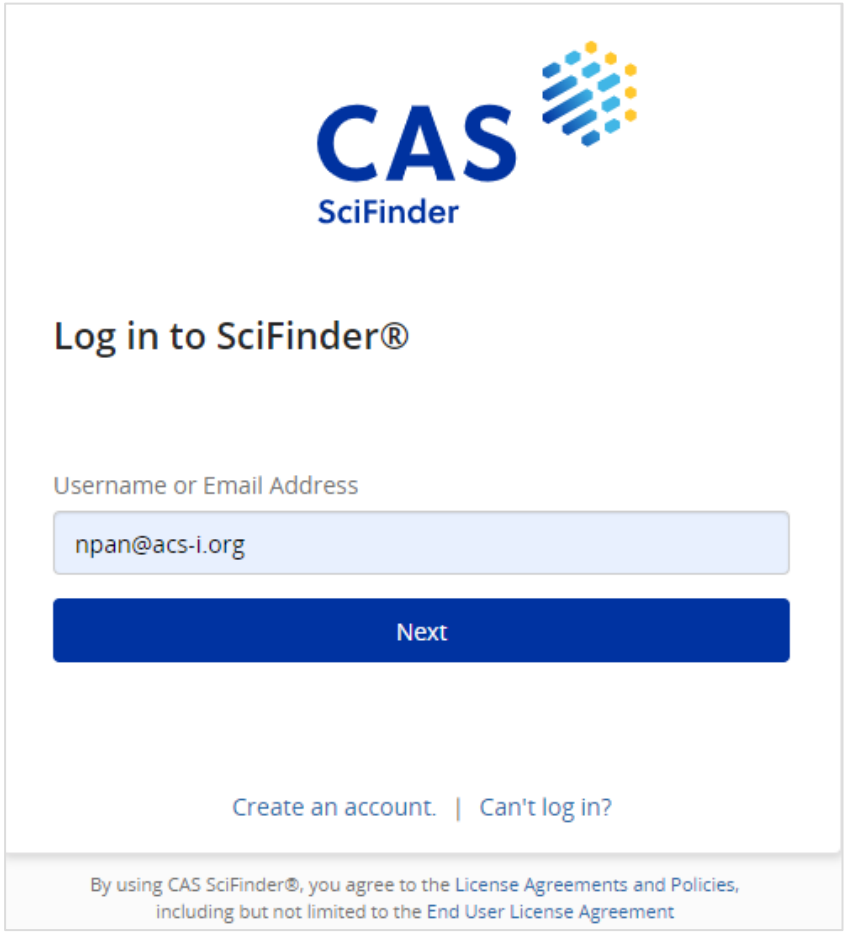
CAS Analytical Methods™ ——借助CAS科学家深度加工的科学方法，提升研究效率

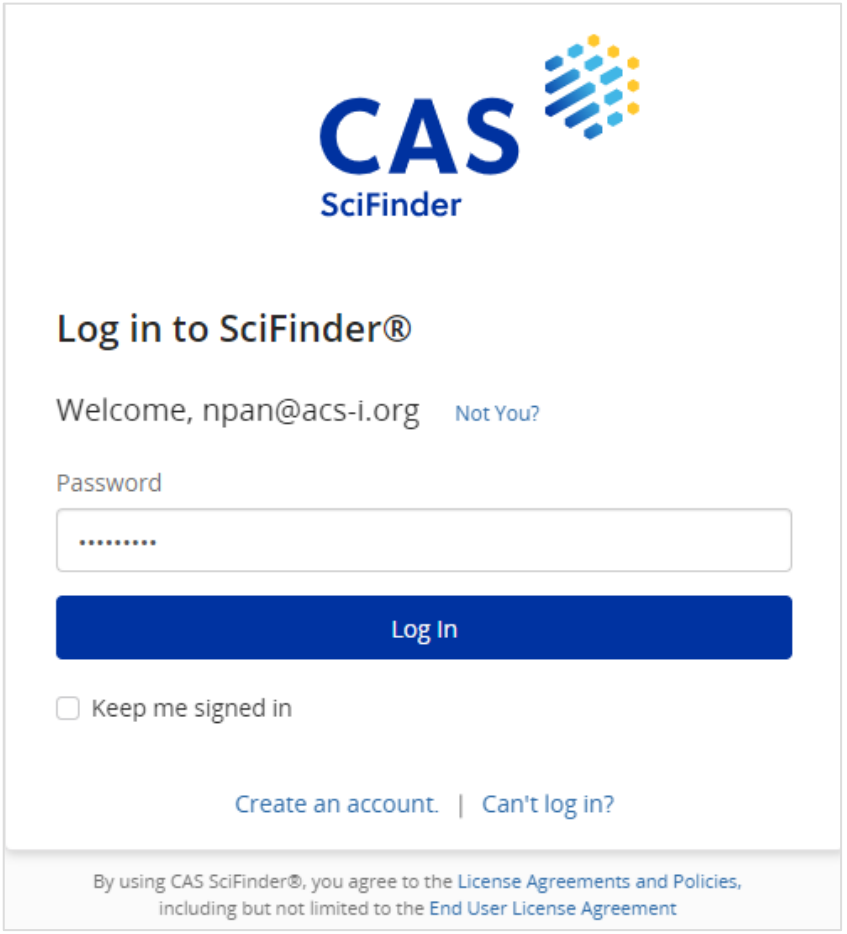
分析方法解决方案涵盖来自期刊中的化学分析方法，提供检索和对比功能，可快速获得能直接在实验室操作的分析方法。可为法医学、食品科学、农学、制药、环境等学科的教学和实验提供帮助。

CAS Formulus® ——助力开发安全、有效的产品

集成配方（制剂）数据与工作流程的解决方案，提供来自期刊、专利和产品说明中的配方详情。可检索制药、化妆品、食品、农化、油墨、涂料等众多领域中的配方，及其工艺、成分、目标成分的常见配伍成分、设计配方、和探索合规要求等。

CAS SciFinder 登录网址：https://scifinder-n.cas.org/





使用CAS SciFinder账号登录

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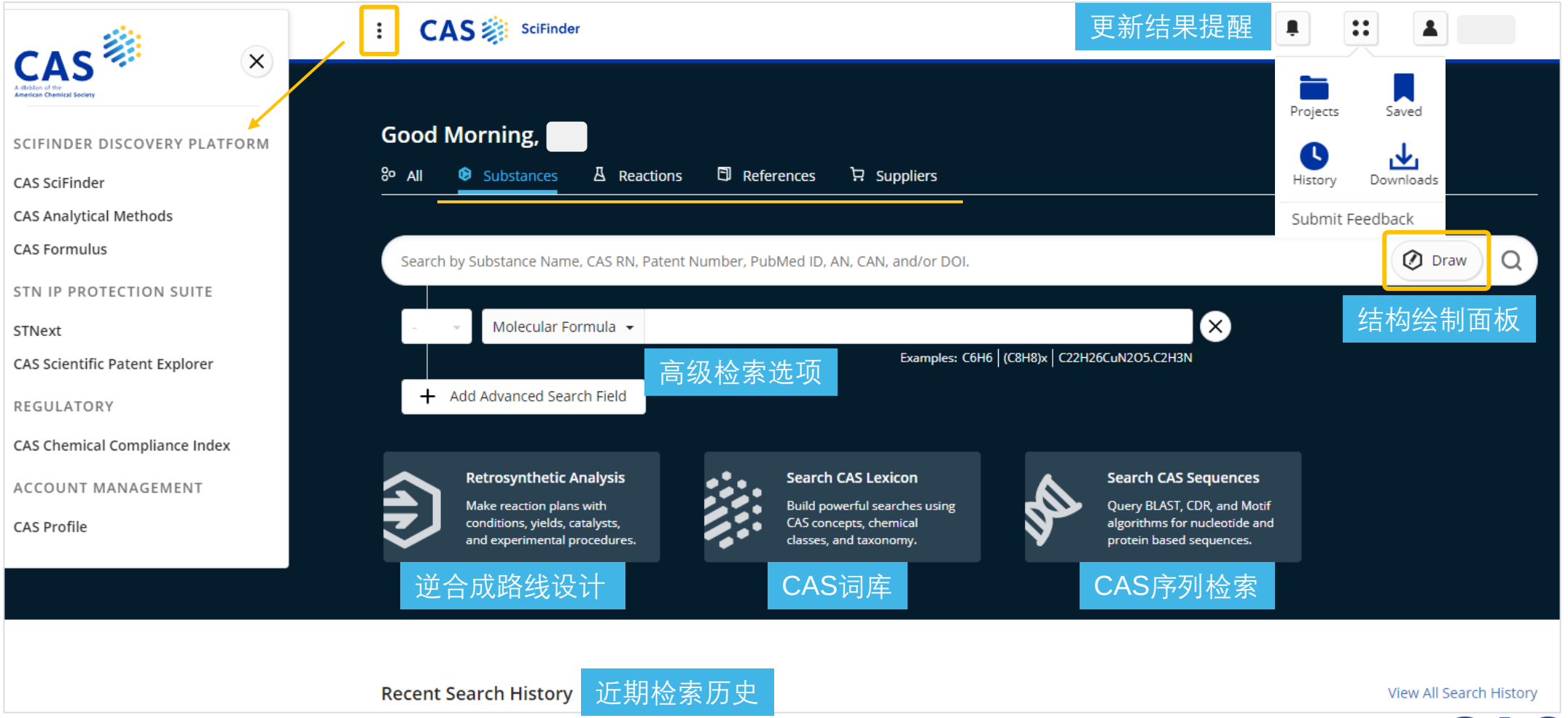
CAS SciFinder 登录主界面

丰富的CAS解决方案，灵活的检索角度



大纲

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- 常见问题Q&A

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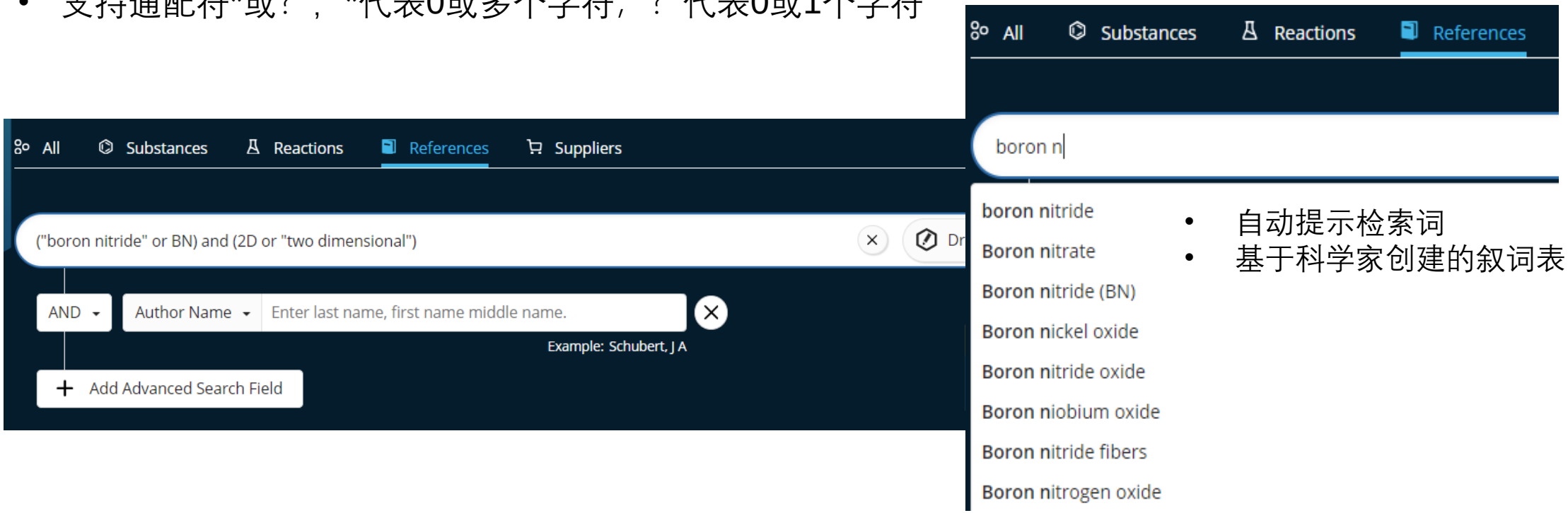
1. 如何开展文献检索?

- 主题词怎么选择？如何构建检索主题?
- 想要研究某结构相关的文献?
- 如何筛选文献？追踪最新进展?
- 如何纵览关注的研究方向?
- 专利内容繁杂，如何高效获取信息?

1.1 如何精准构建检索主题?

- 支持使用：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
- 布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not
- “ ”不允许词形变化，但可出现单数或复数；( ) 优先运算，括号中表达式还可以和其他术语交互
- 支持通配符*或？，*代表0或多个字符；？代表0或1个字符

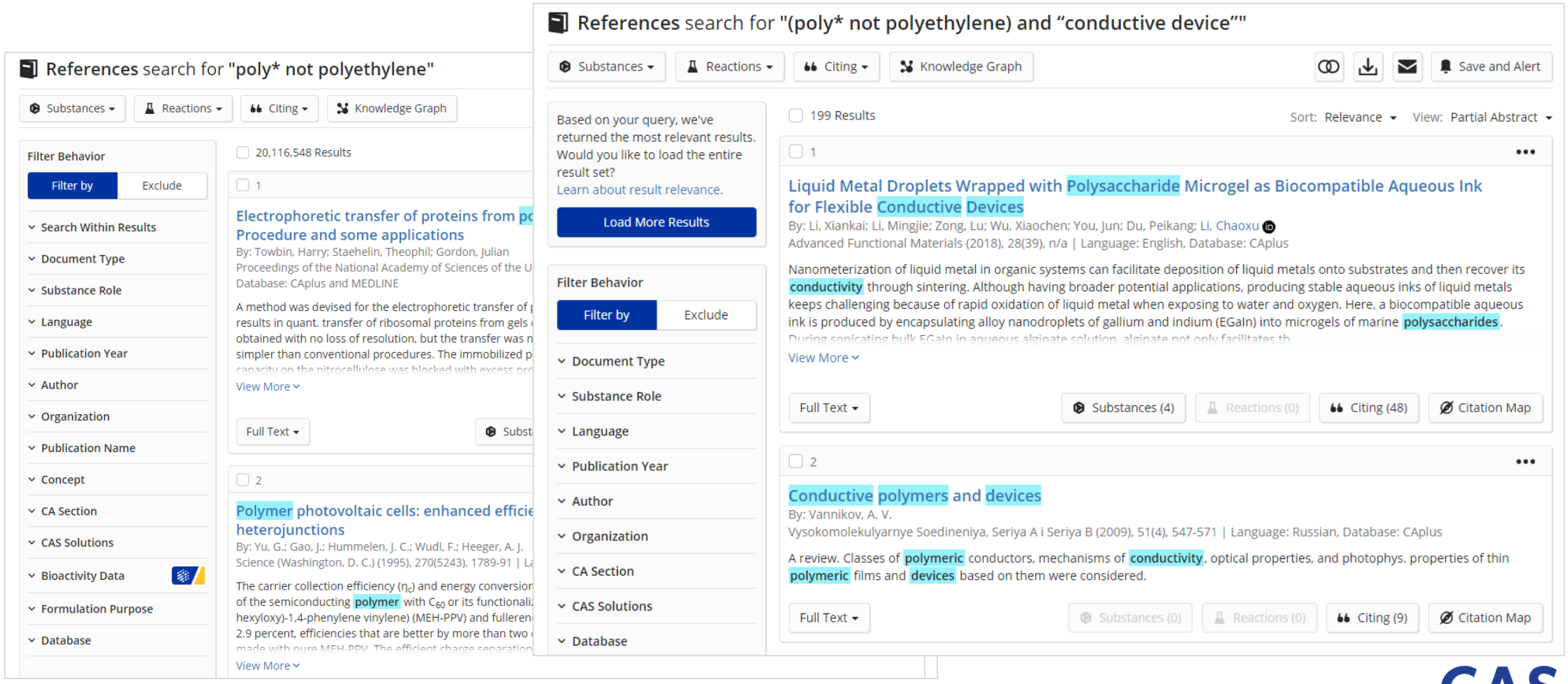


- 自动提示检索词
- 基于科学家创建的叙词表

1.1 如何精准构建检索主题?

主题词示例:

(poly* not polyethylene) and “conductive device”（聚合物但排除聚乙烯，导电装置）



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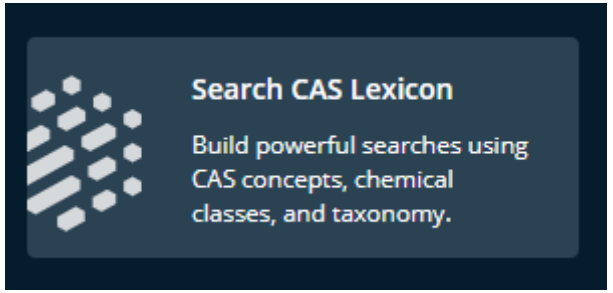
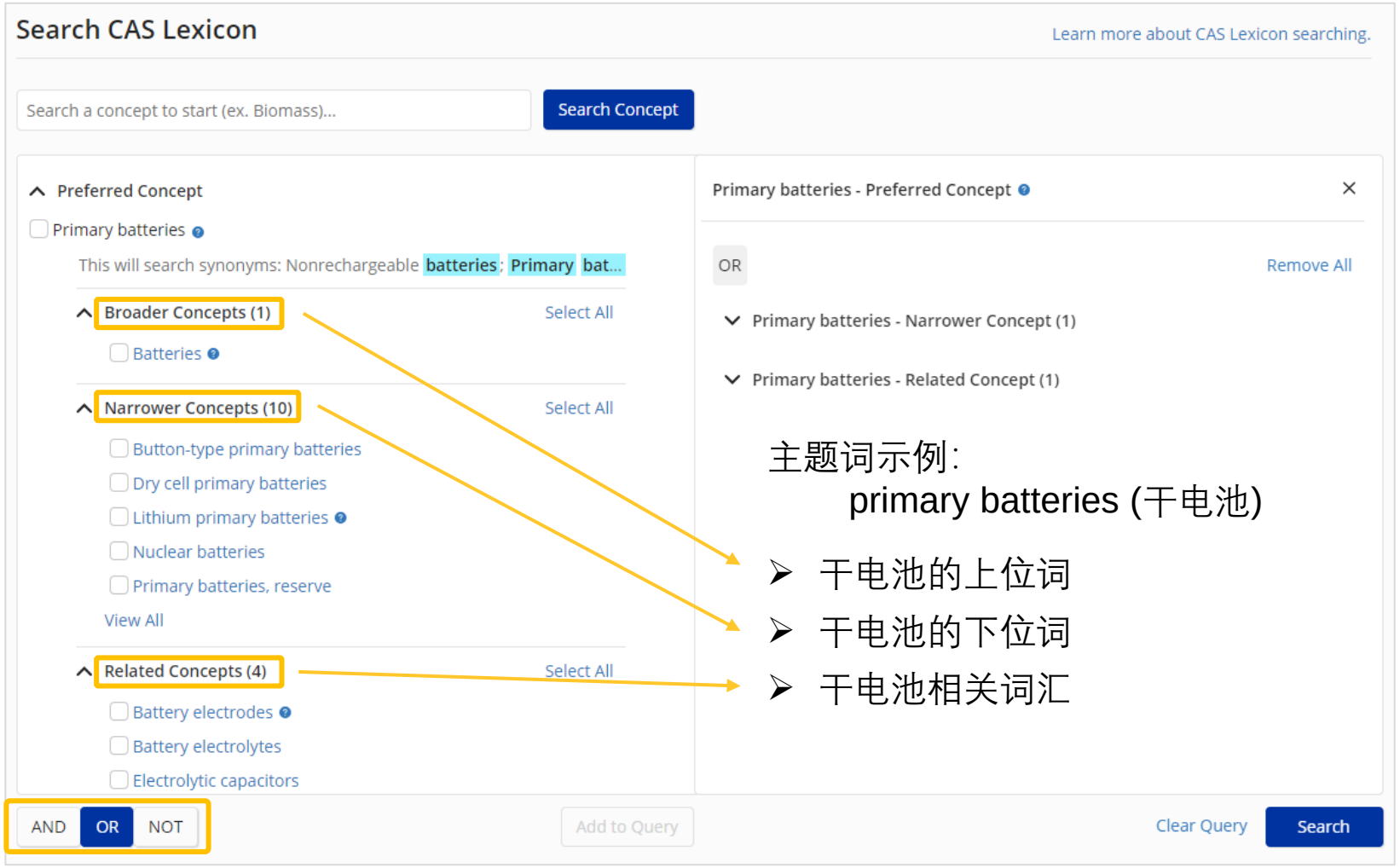
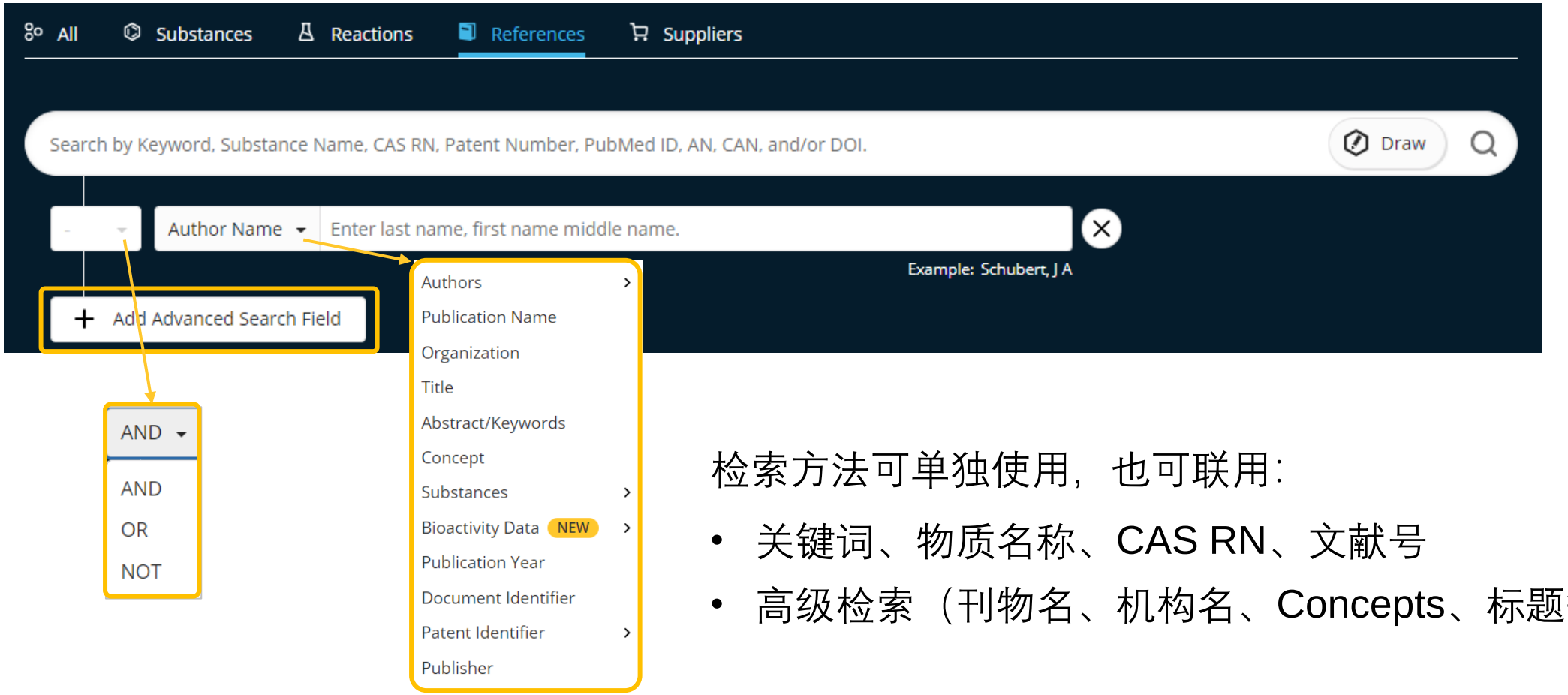
如何选择概念词？借助CAS Lexicon词库



- 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）



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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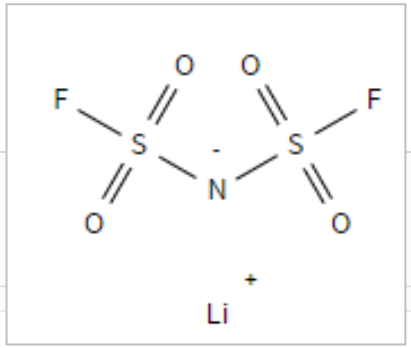
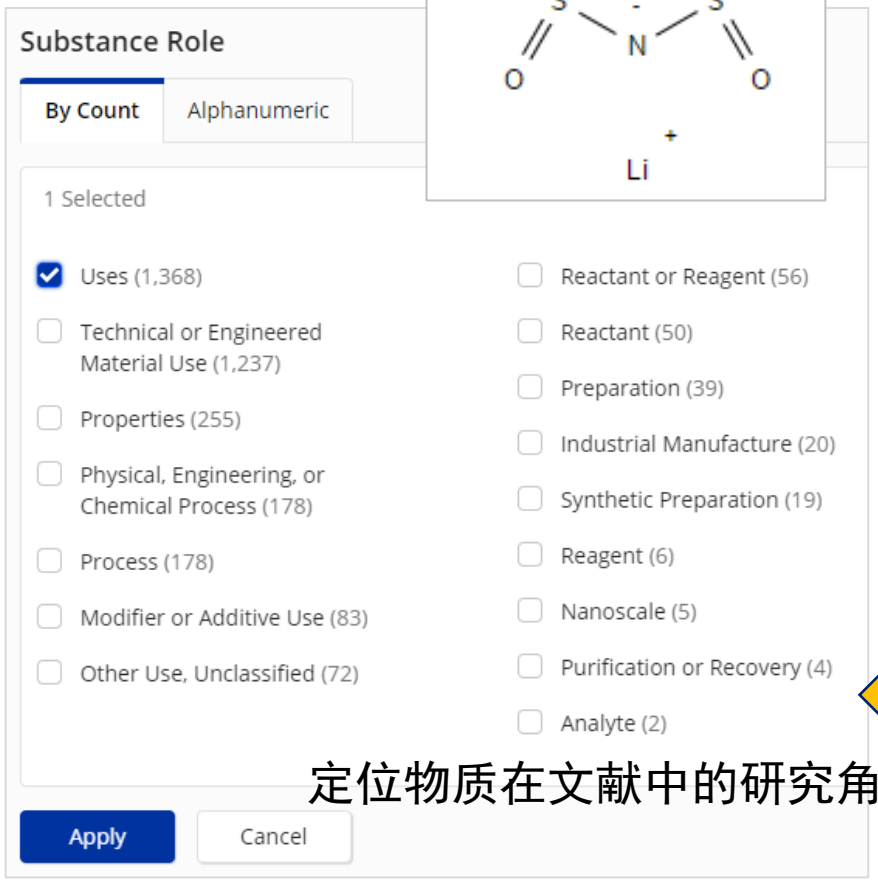
1.2 如何获得结构相关的文献?

示例：关注锂电池技术中特定的热点材料

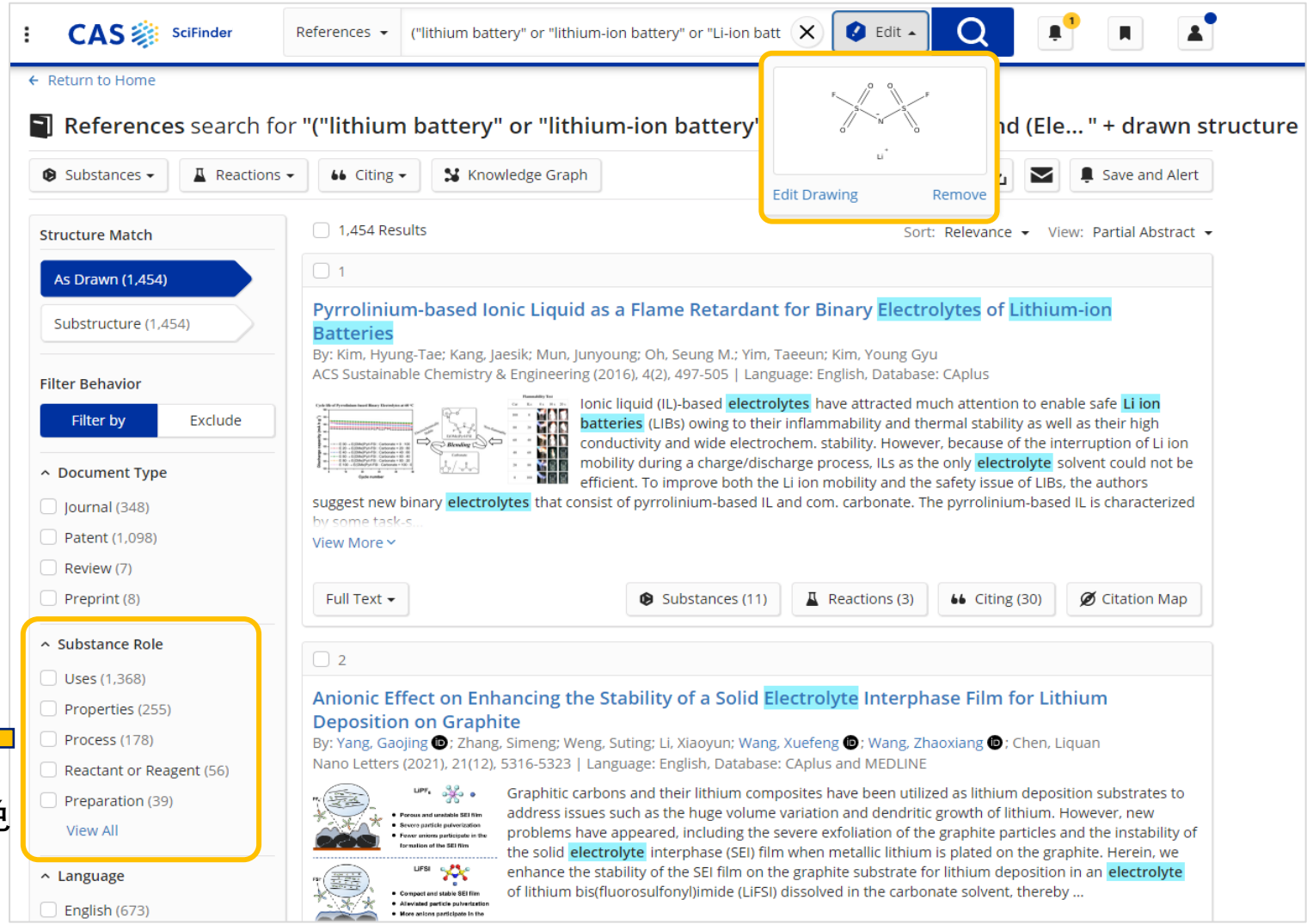
策略：从References出发，主题词+结构联用检索

文本与结构是“and”关系

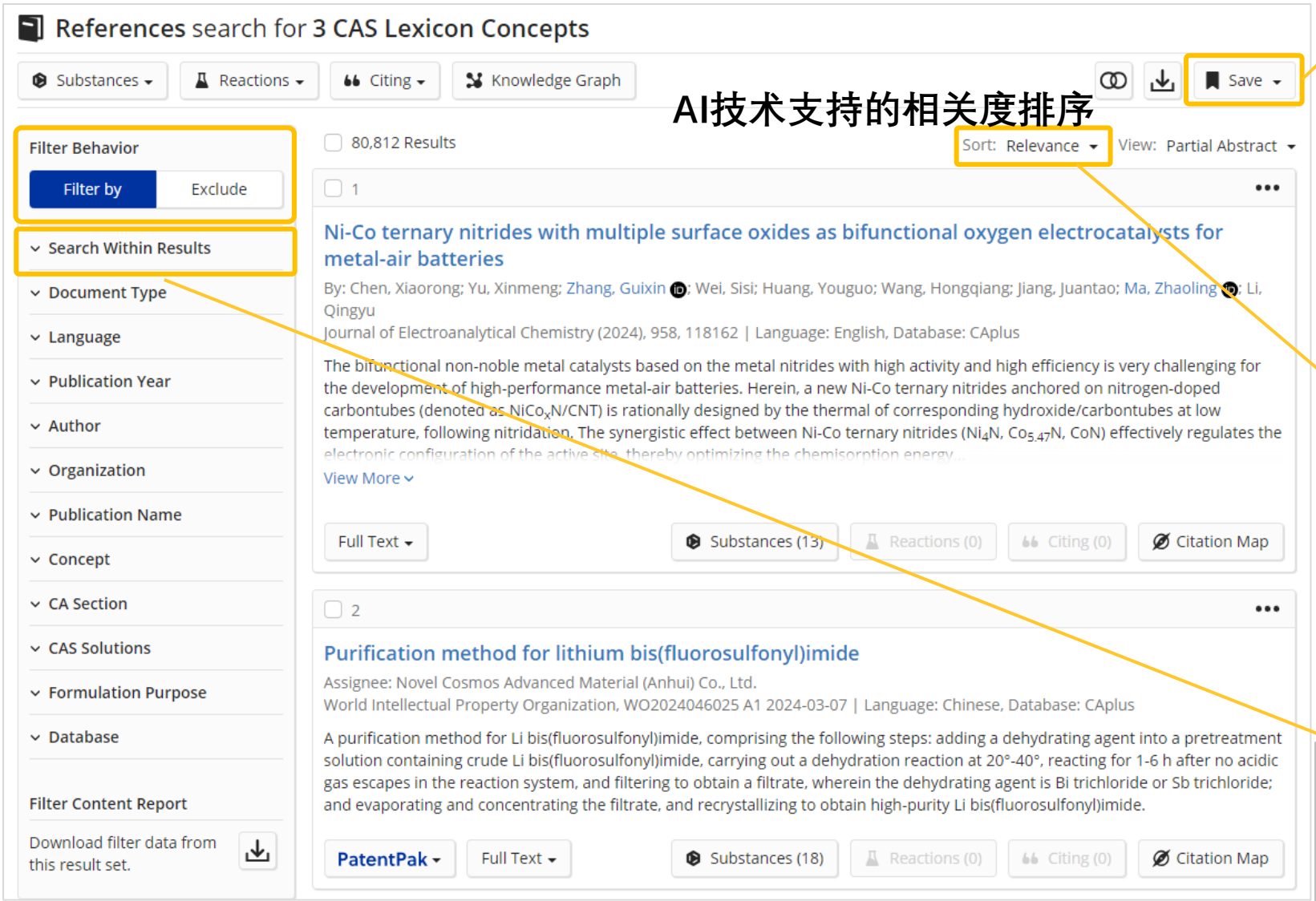


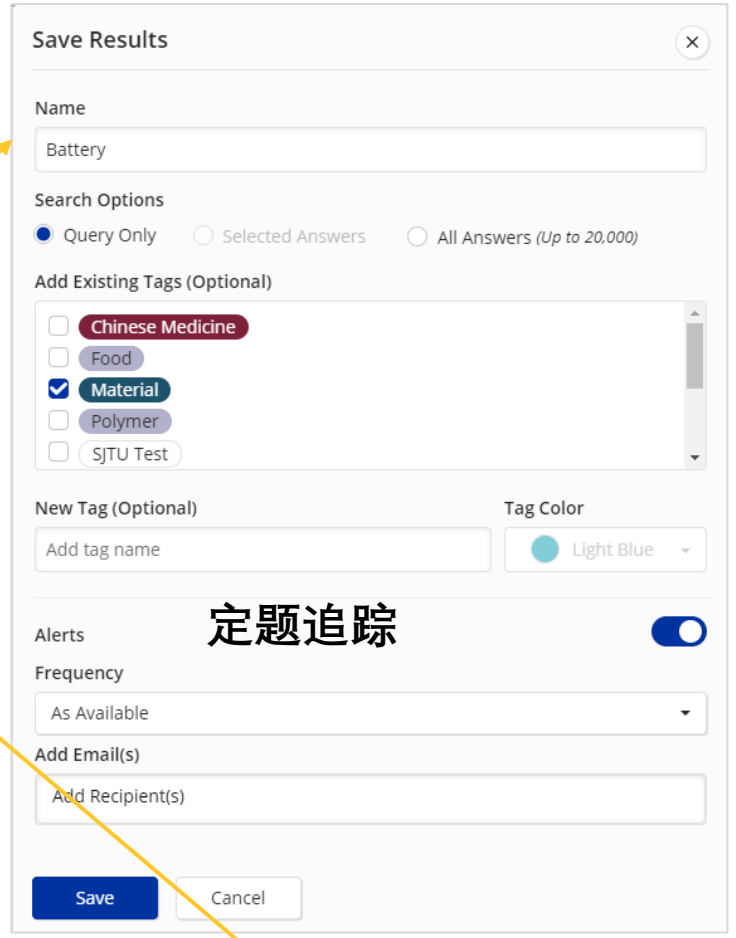


定位物质在文献中的研究角色



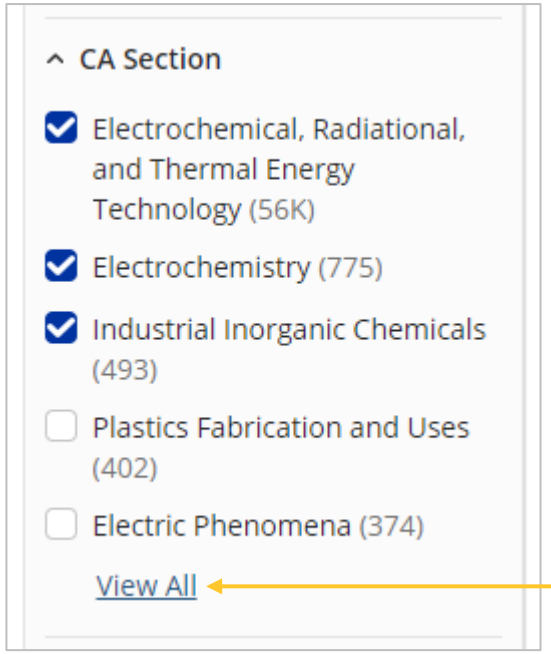
1.3 文献结果分析与筛选

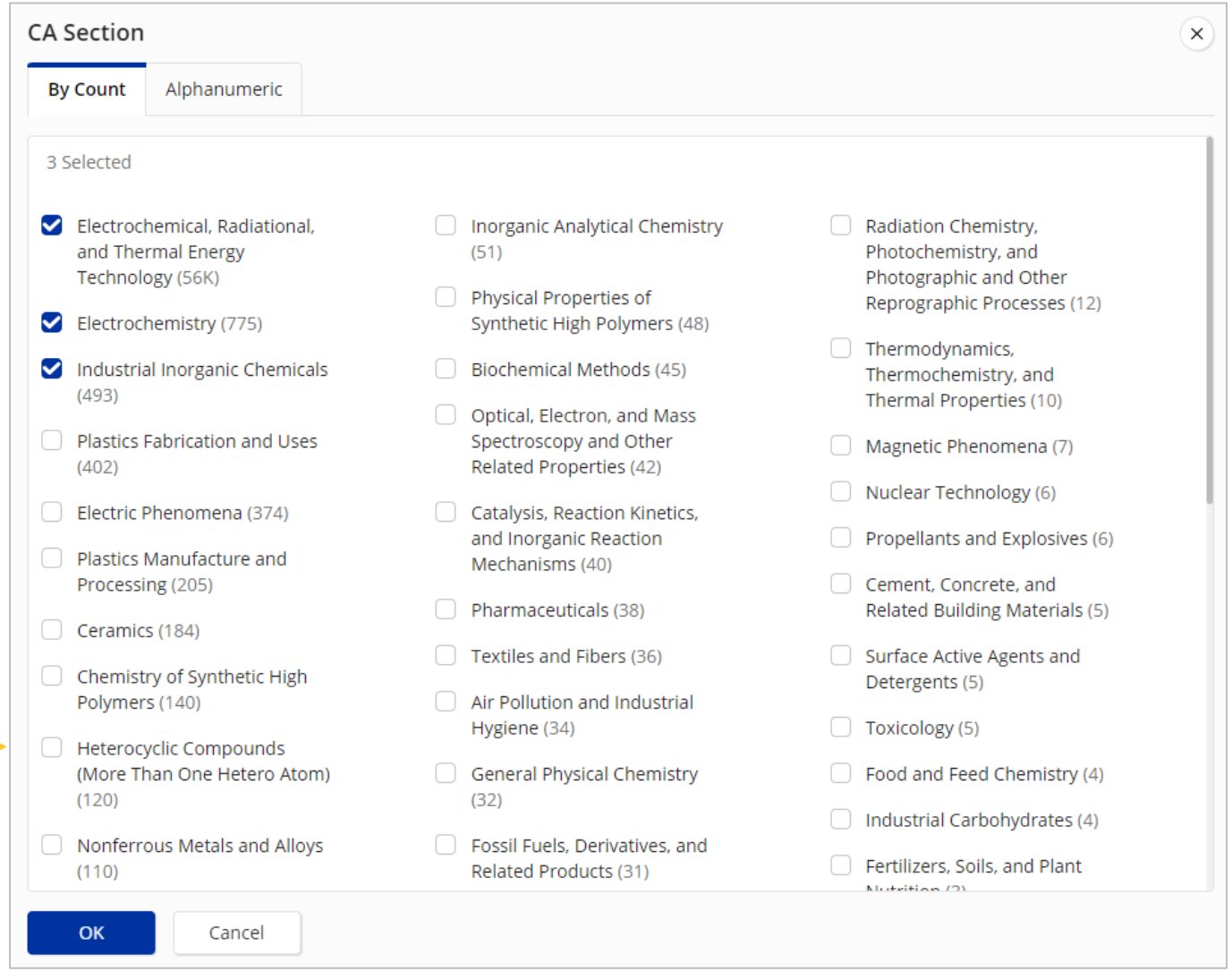




筛选工具 CA Section

纵览学科研究方向





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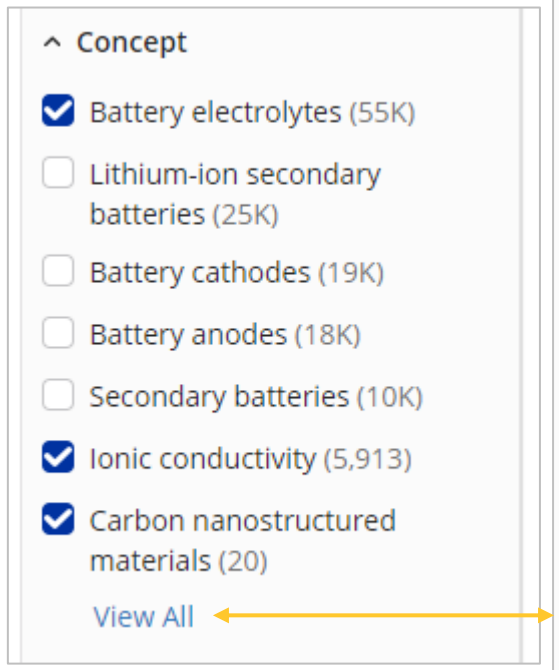
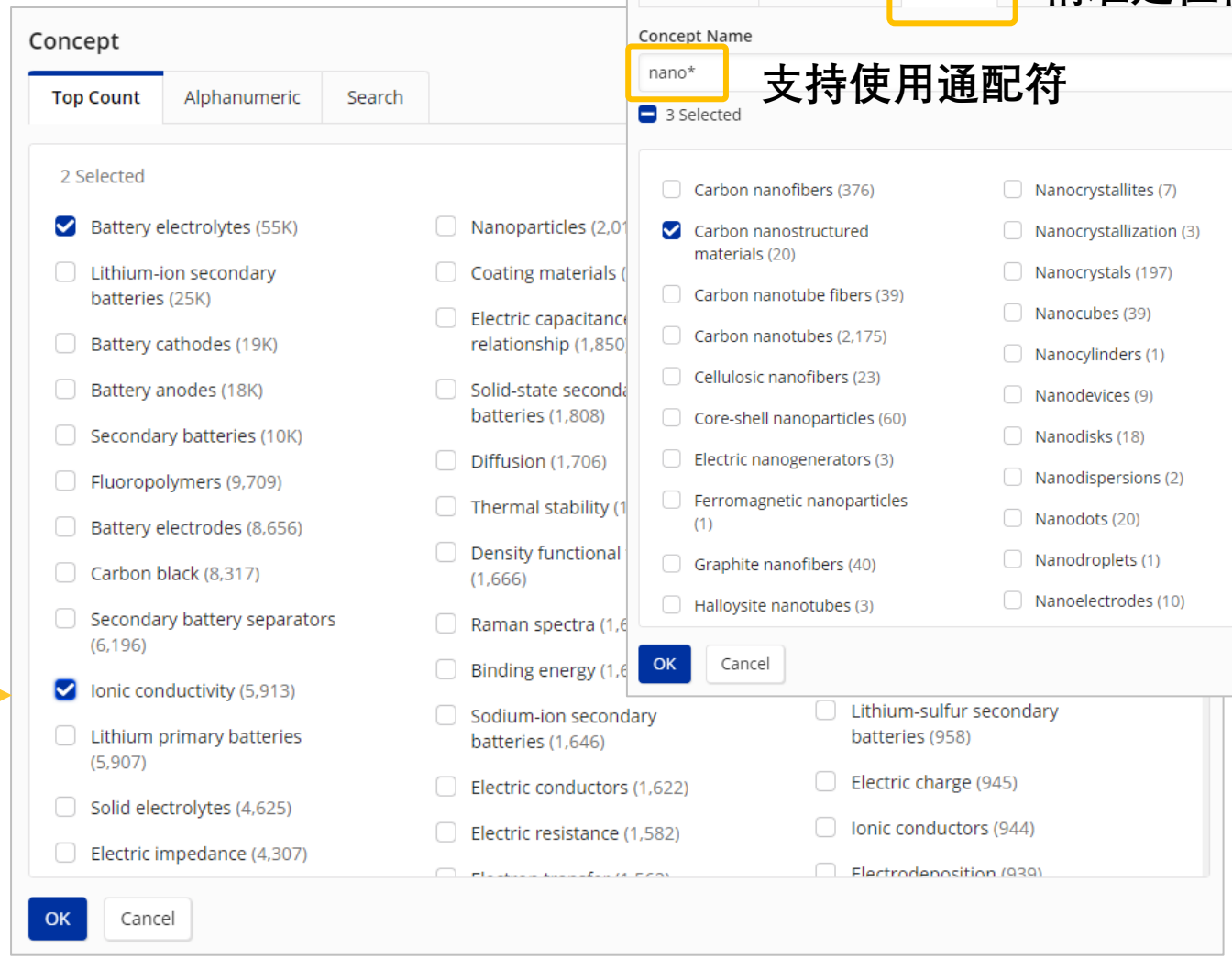
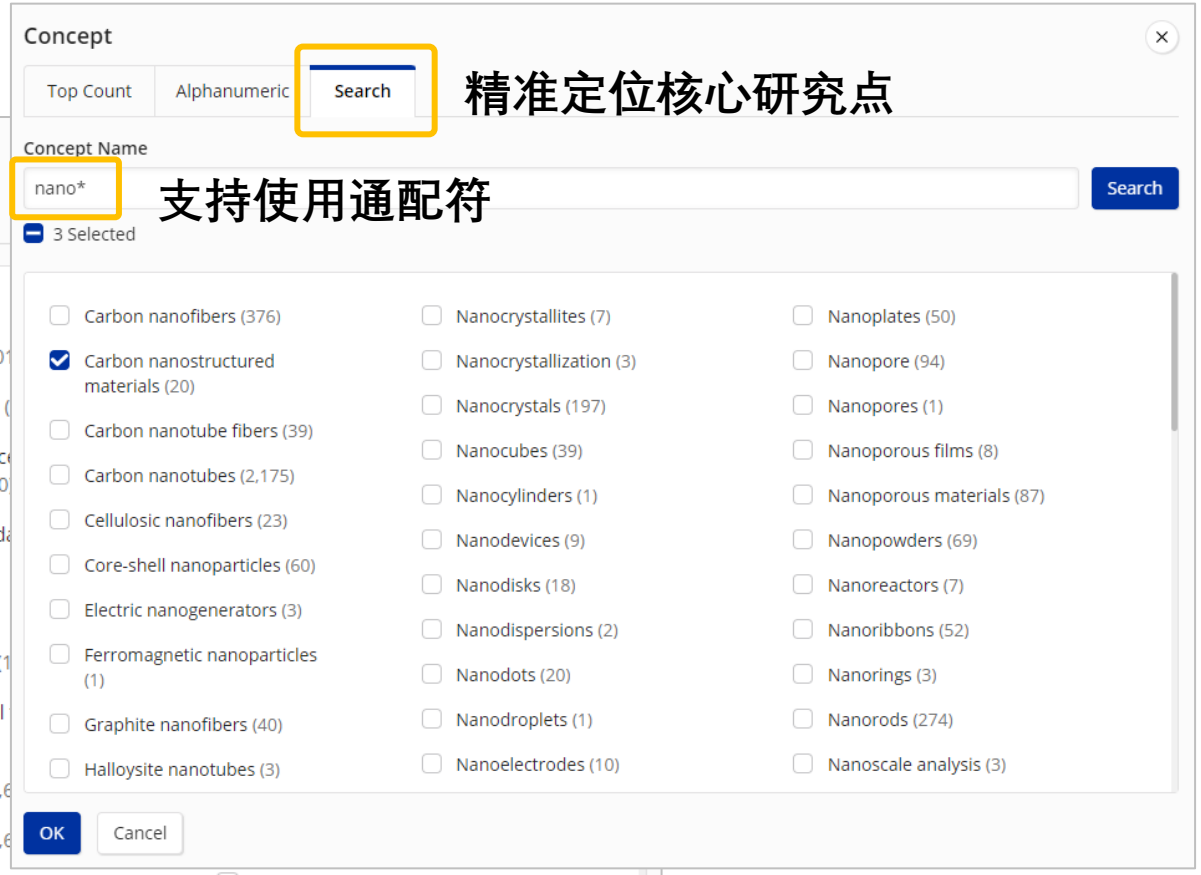
筛选工具 Concept

聚焦核心研究点







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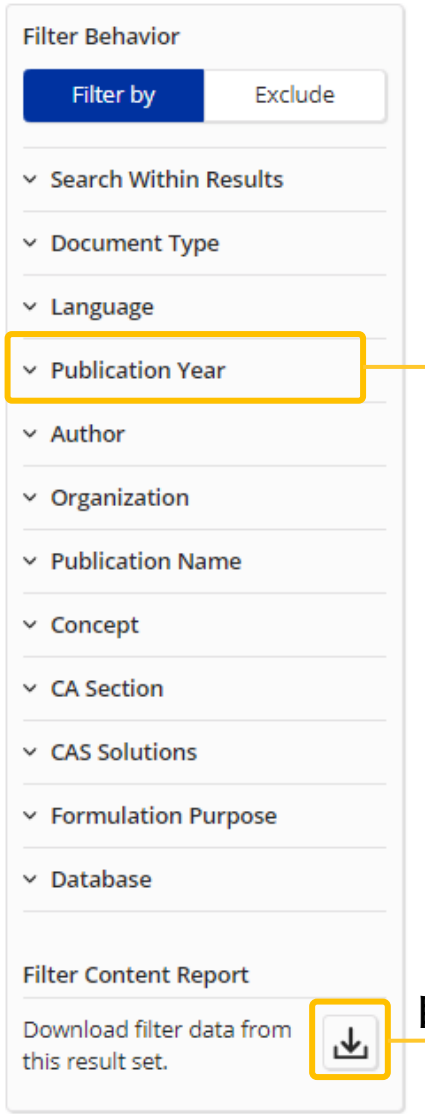
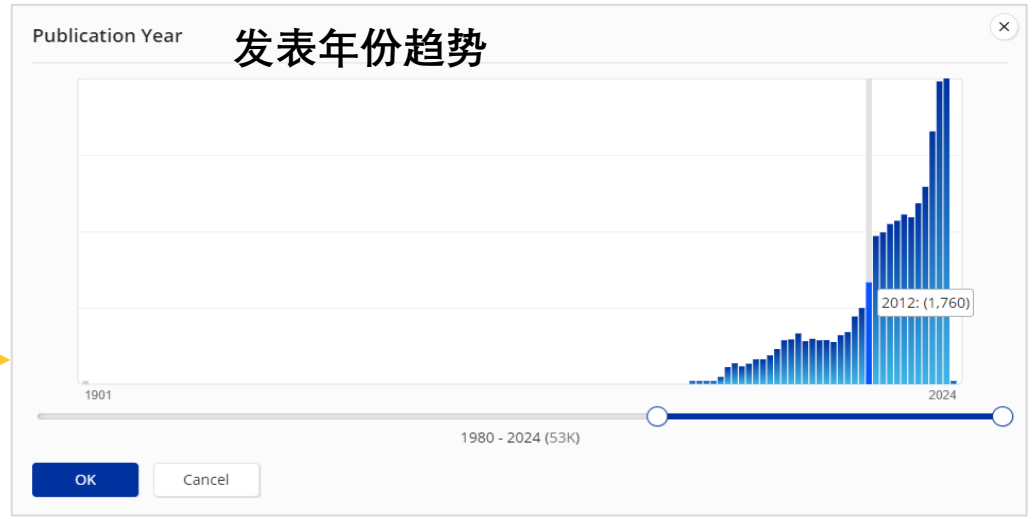
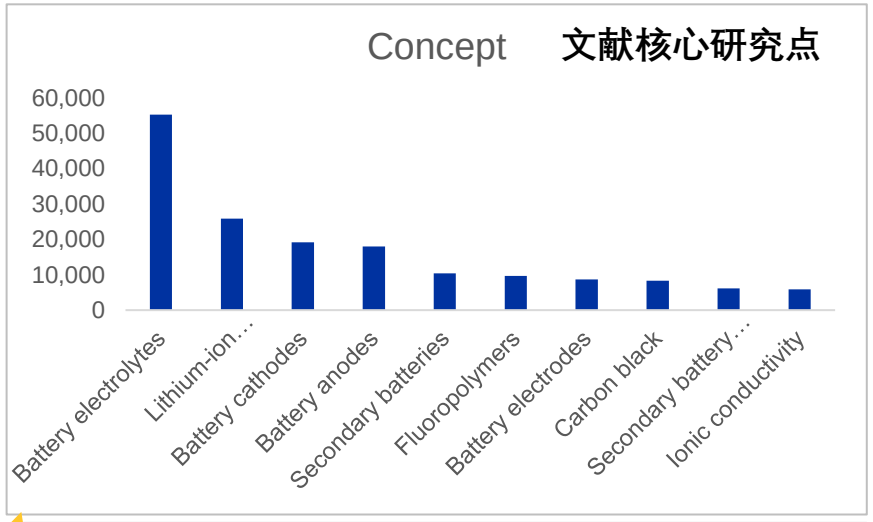
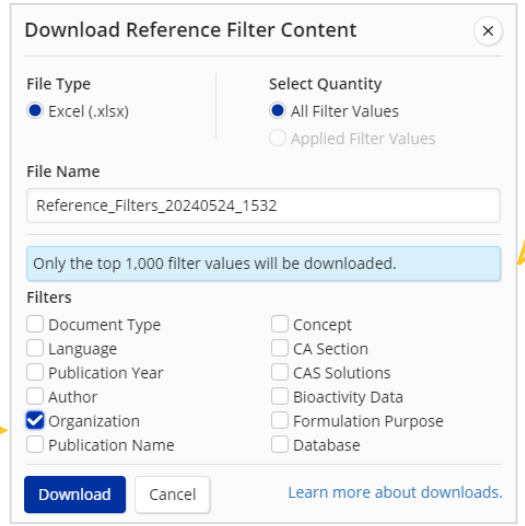
1.4 可视化分析——检索结果趋势分析

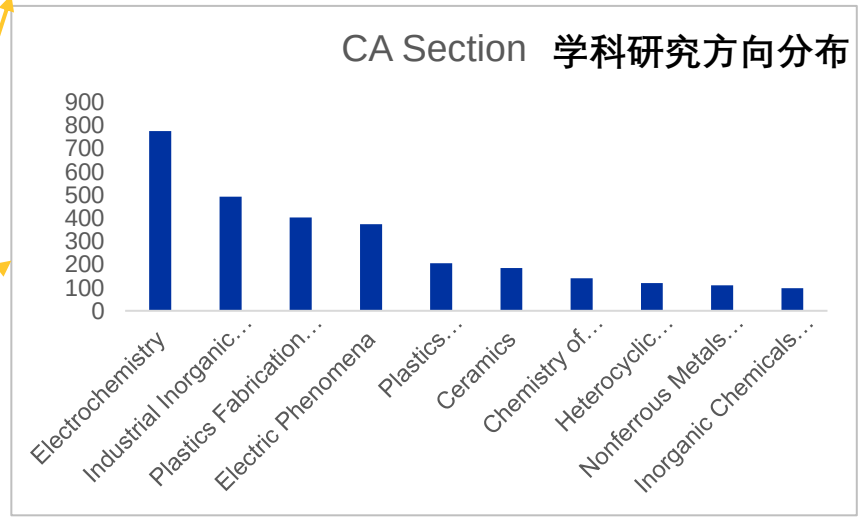






自主选择下载分析栏目





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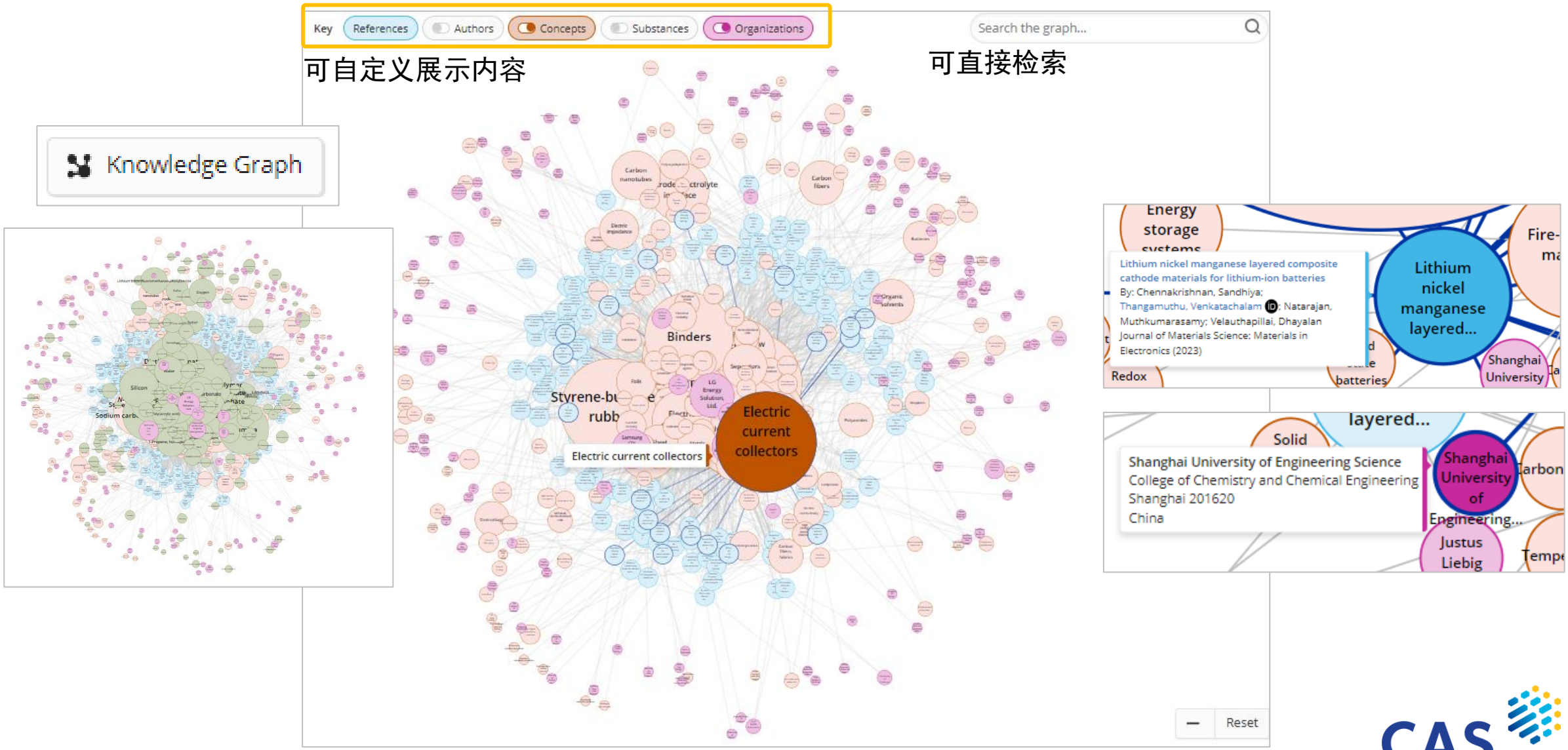
1.4 可视化分析——知识图谱



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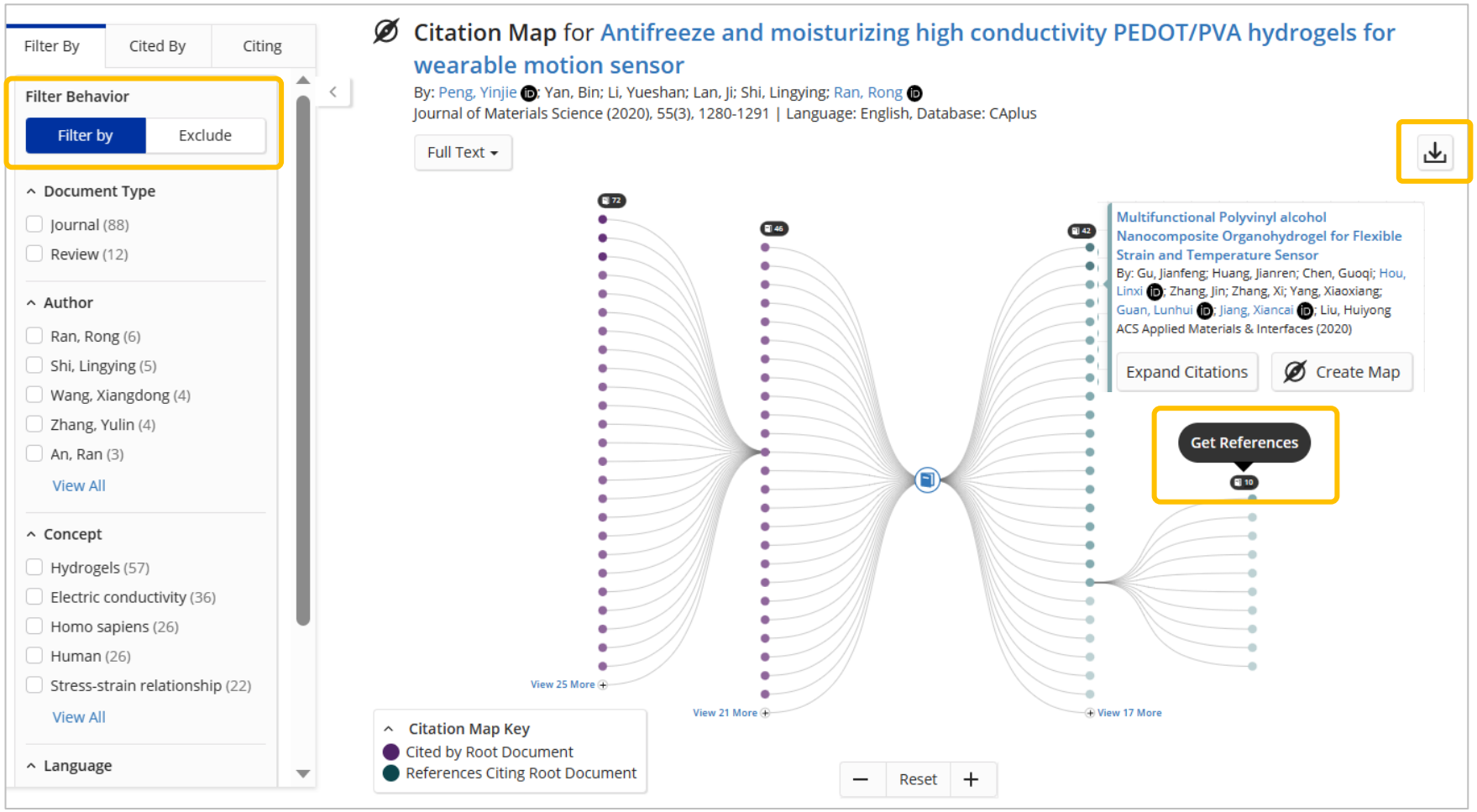
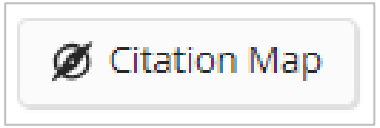
1.4 可视化分析——引文地图

便捷获得相关文献





- Cited By: 参考文献
- Citing: 引用当前文献的文献
- 通过聚类选项筛选引文
- 可下载引文地图
- 显示引文和被引文献的数量，点击可链接至对应的文献结果页面

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1.5 深入文献详情

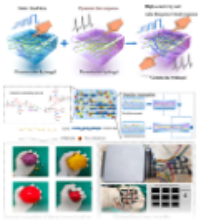
内容合集间彼此关联

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 fluori...

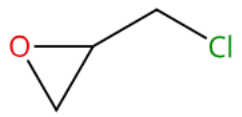
View More

Full Text

Substances (7) | Reaction (1) | Citing (9) | Citation Map

1

106-89-8



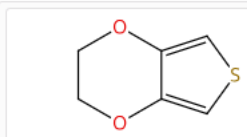
C_3H_5ClO

Epichlorohydrin

53K References | 32K Reactions | 84 Suppliers

2

126213-51-2



$(C_6H_6O_2S)_x$

Poly(3,4-ethylenedioxythiophene)

48K References | 1,505 Reactions | 7 Suppliers

3

50851-5

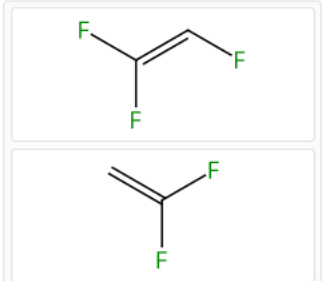
$(C_8H_8O_3S)_x$

Poly(styrenesulfonic acid)

40K References | 882 Reactions | 2 Suppliers

4

28960-88-5



$(C_2H_2F_2.C_2HF_3)_x$

Components: 2

P(VDF-TrFE)

5,483 References | 63 Reactions | 7 Suppliers

5

2839834-68-1

106602-18-0

Image Not Available

$(C_3H_5ClO.Unspecified)_x$

Components: 2

2 References | 1 Reaction | 0 Suppliers

6

106602-18-0

Image Not Available

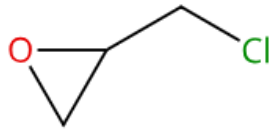
Unspecified

N-[2-Hydroxy-3-(trimethylammonium) propyl]chitosan chloride

500 References | 247 Reactions | 0 Suppliers

106602-18-0

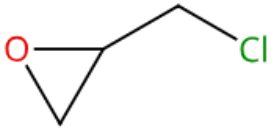
Image Not Available



Suppliers (84)

106602-18-0

Image Not Available



31-614-CAS-34510937 Steps: 1

1.1

Reagents: Poly(styrenesulfonic acid) , Poly(3,4-ethylenedioxythiophene)

Solvents: Water ; 12 h, rt

1.2

4 h, 70 °C

1.3

Reagents: Sodium hydroxide ; pH 10, 70 °C

1.4

Solvents: Dimethyl sulfoxide ; 60 min, rt; 60 min

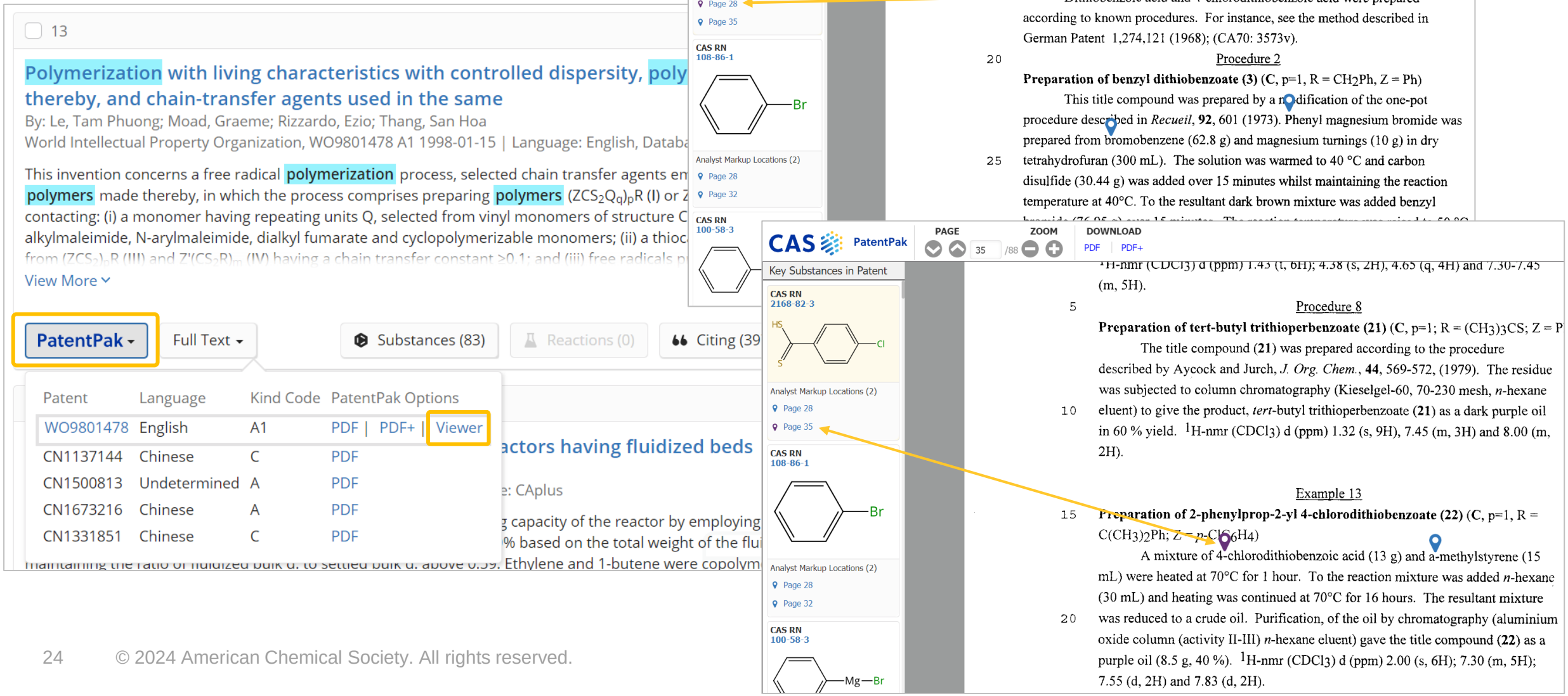
1.5

Reagents: Hydrochloric acid

Solvents: Water ; pH 7

1.5 深入文献详情

巧用CAS PatentPak浏览专利



文献检索小结

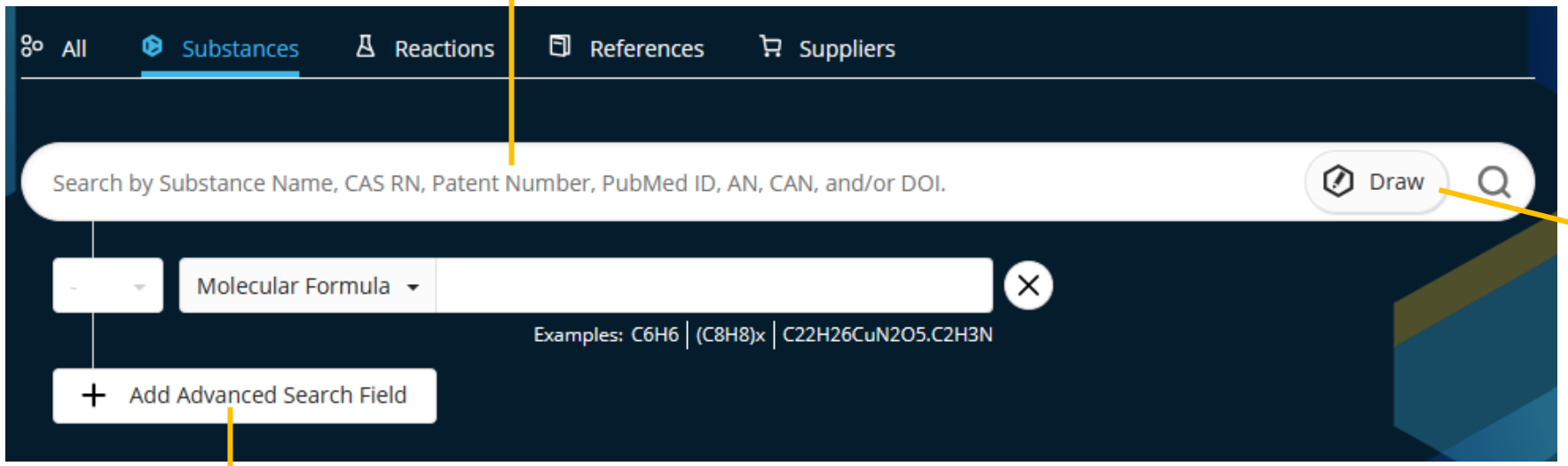
1. 检索主题的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
2. 主题词+结构联合检索，快速获得文献
3. 利用丰富的筛选工具，缩小范围，锁定目标文献
4. 检索结果趋势分析、知识图谱、引文地图
5. 文献详情，CAS PatentPak浏览专利详情

2. 如何聚焦某类物质?

- 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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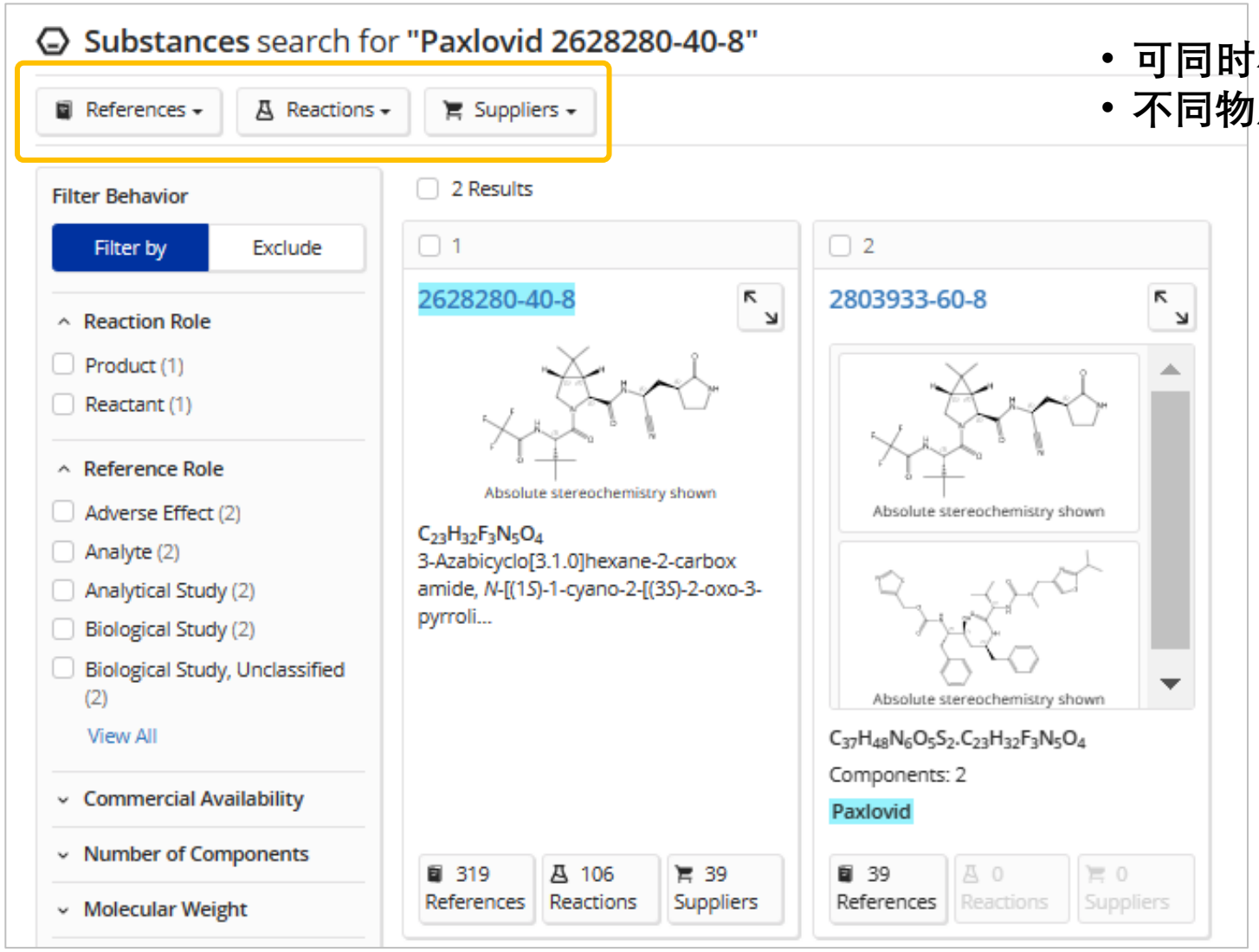
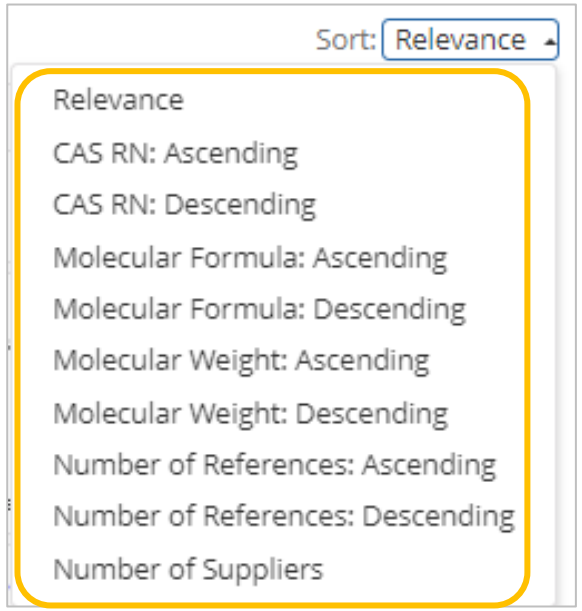
物质检索——物质标识符



- 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）



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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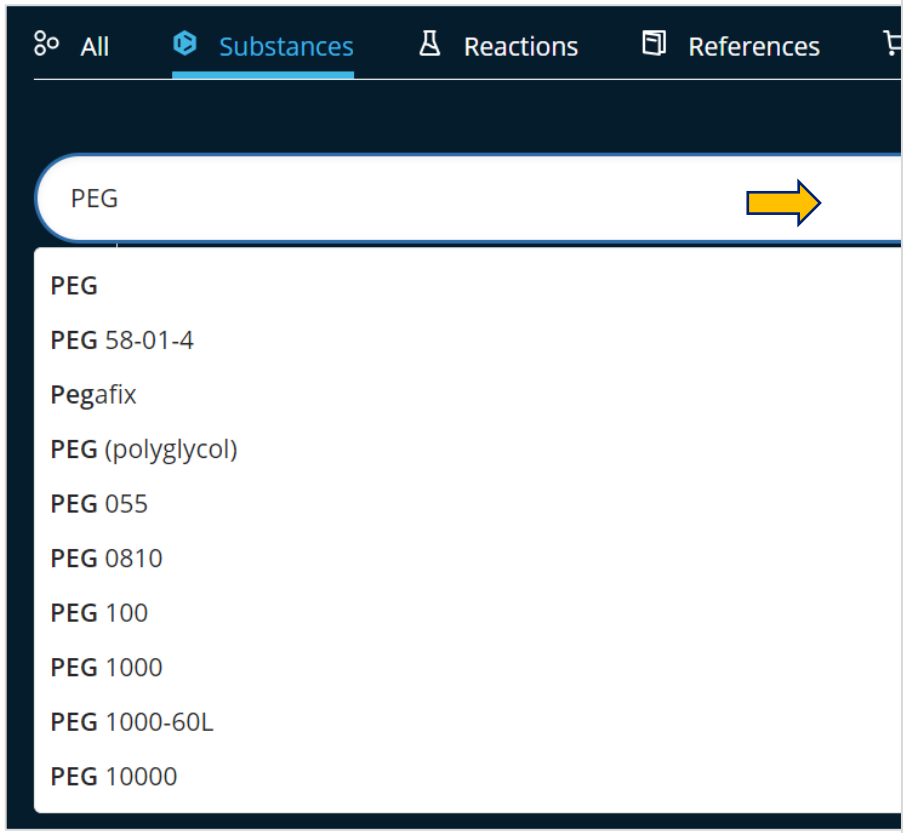
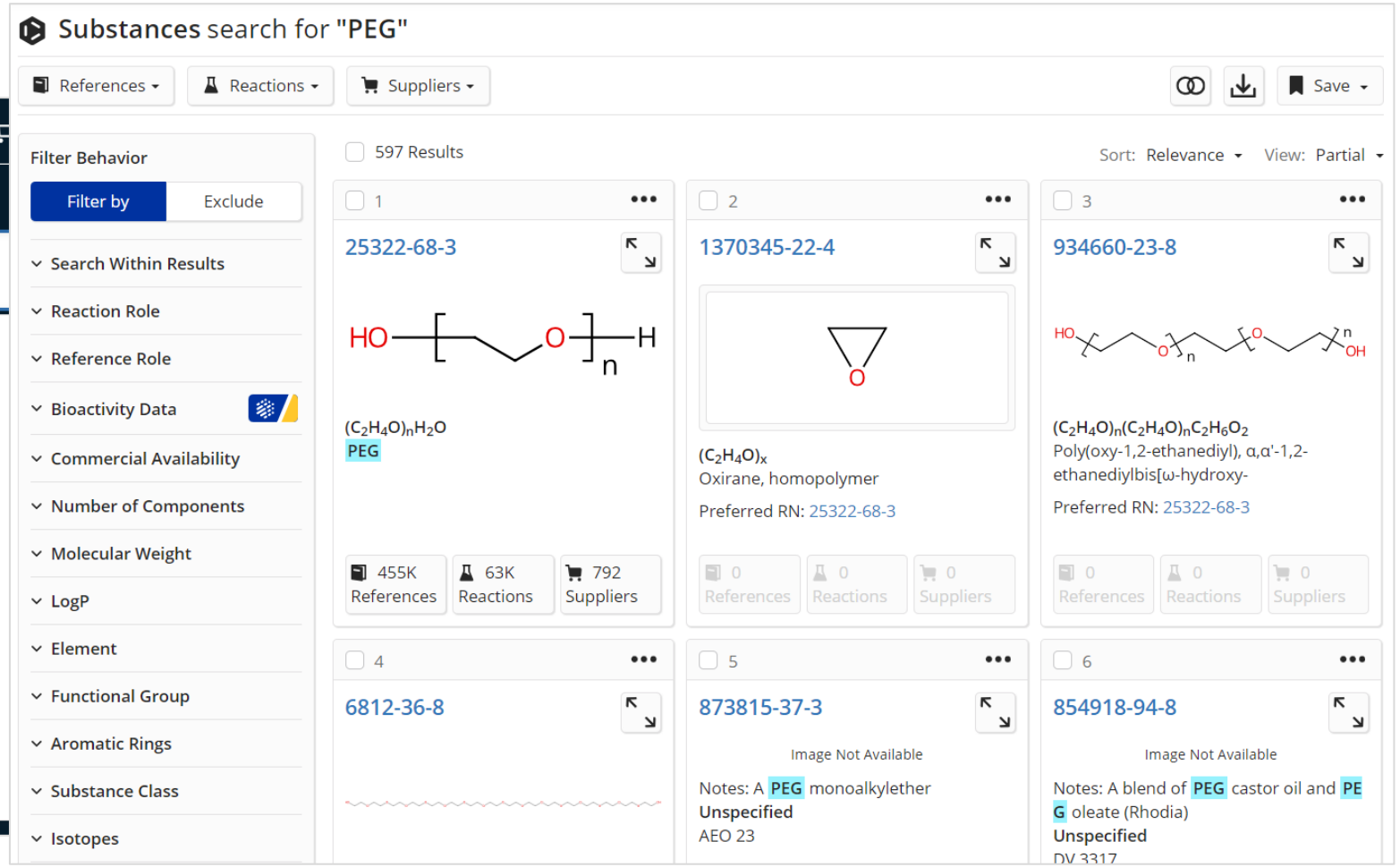
物质检索——物质标识符

示例：PEG





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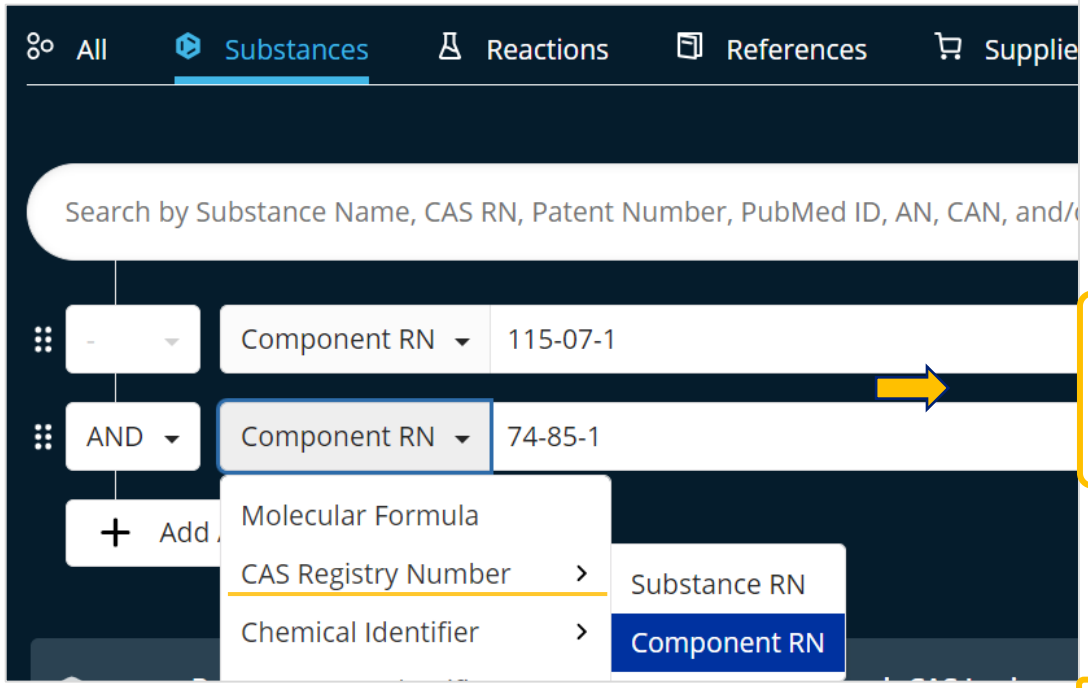
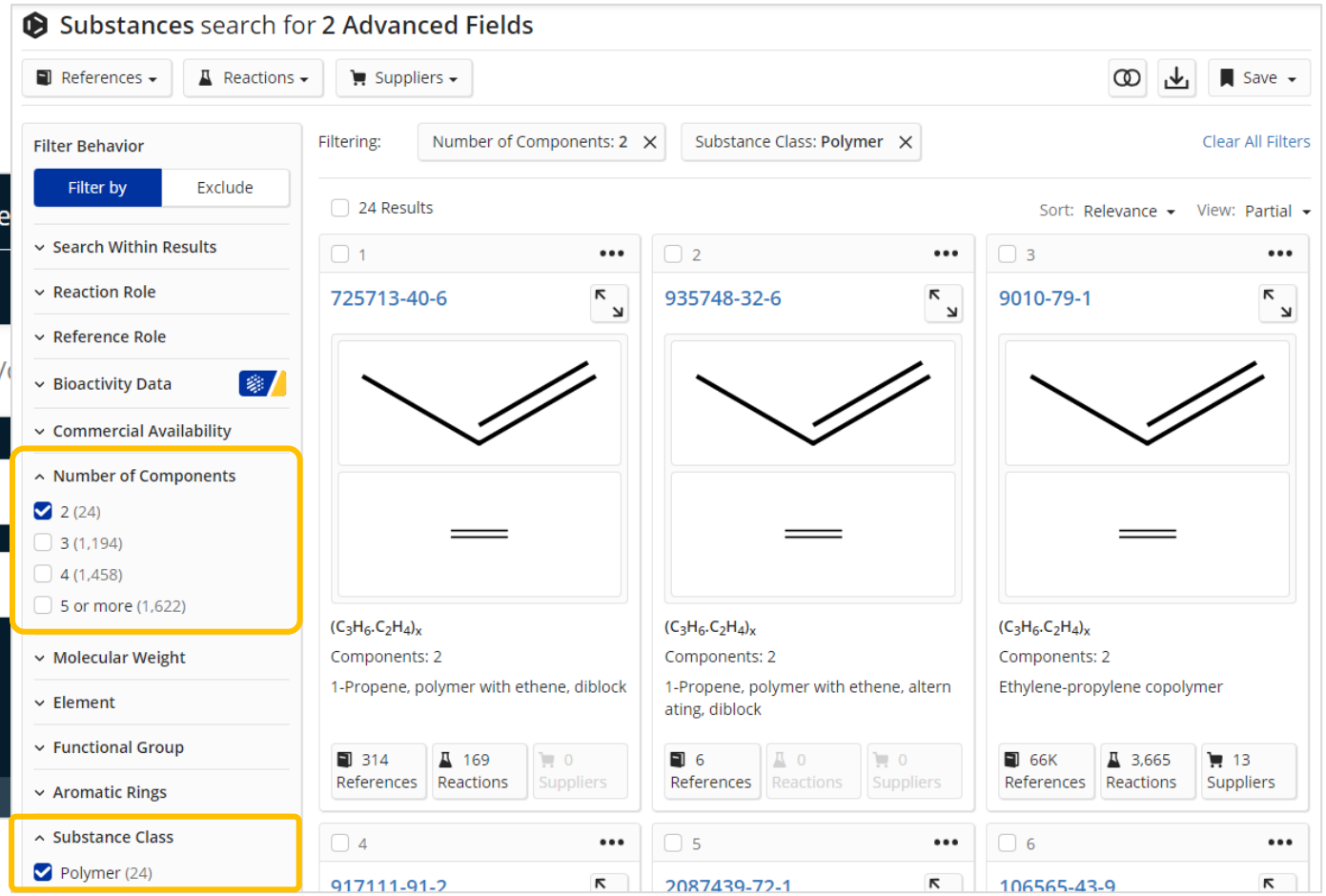
物质检索——组分的CAS登记号

示例：含有乙烯和丙烯为单体的聚合物





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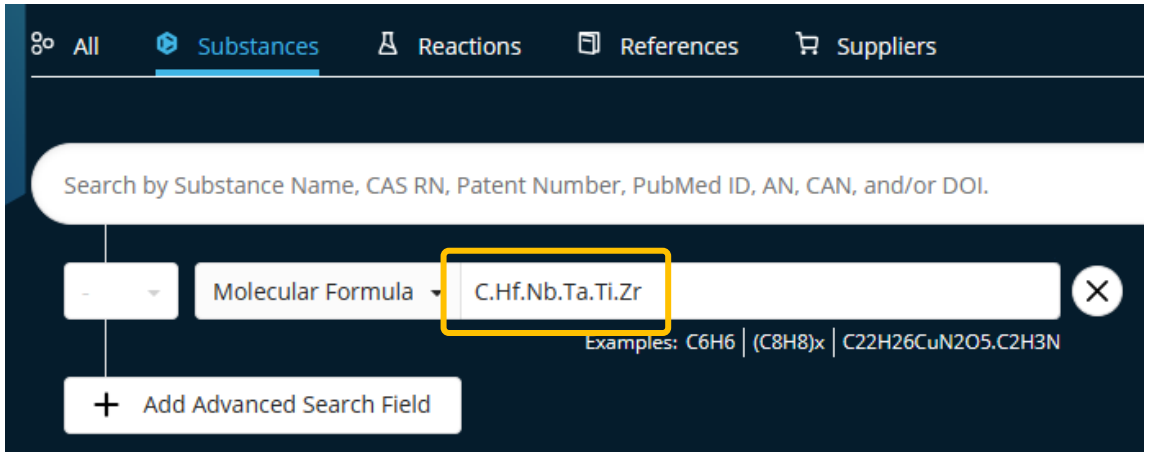
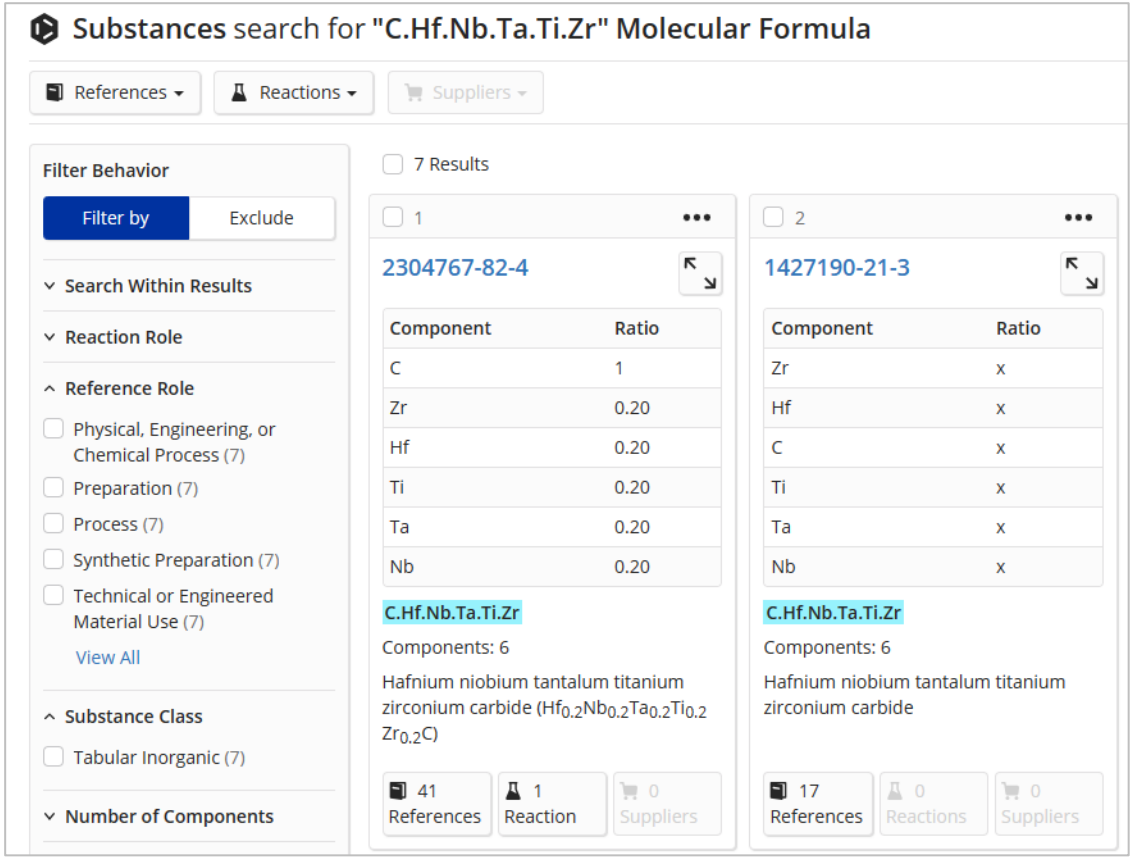
2.1 分子式检索：高效检索聚合物或无机化合物

- 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

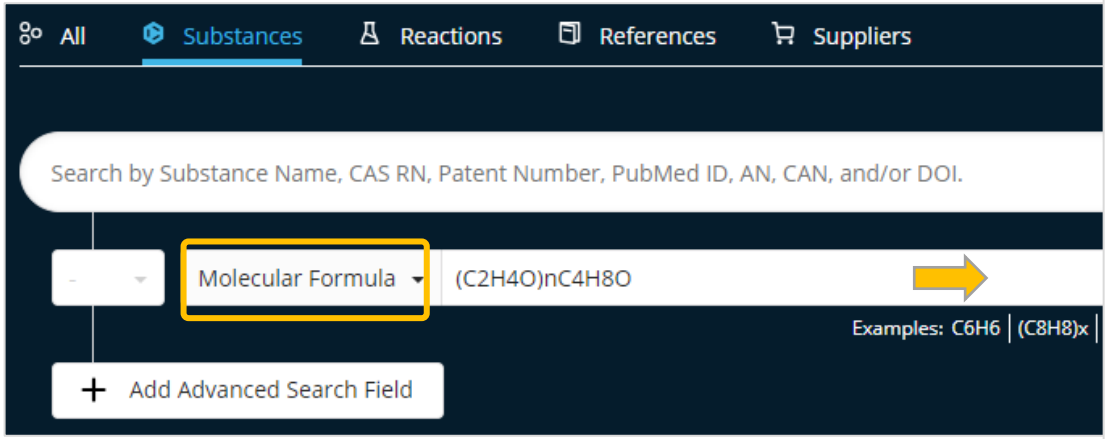


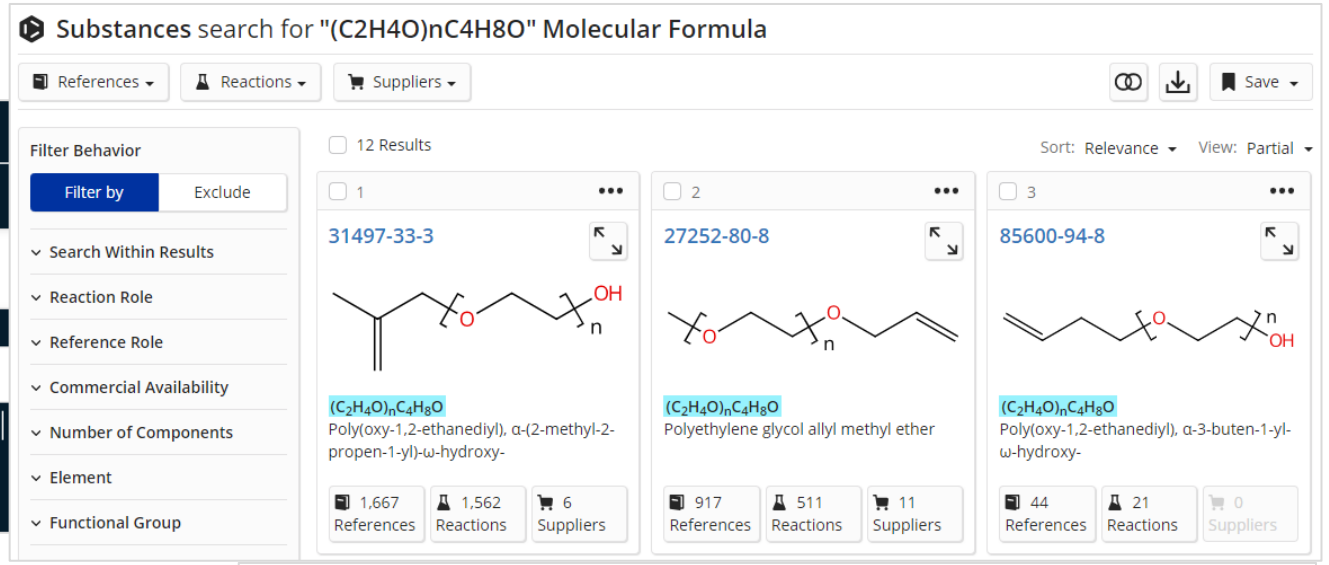
适用于分子式检索的物质类型包括：

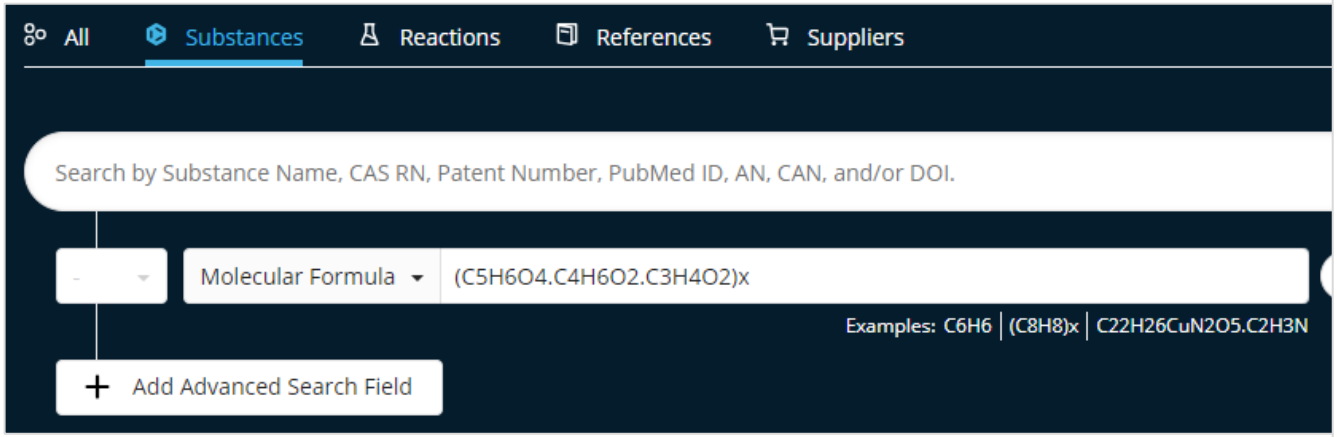
- 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
- 聚合物

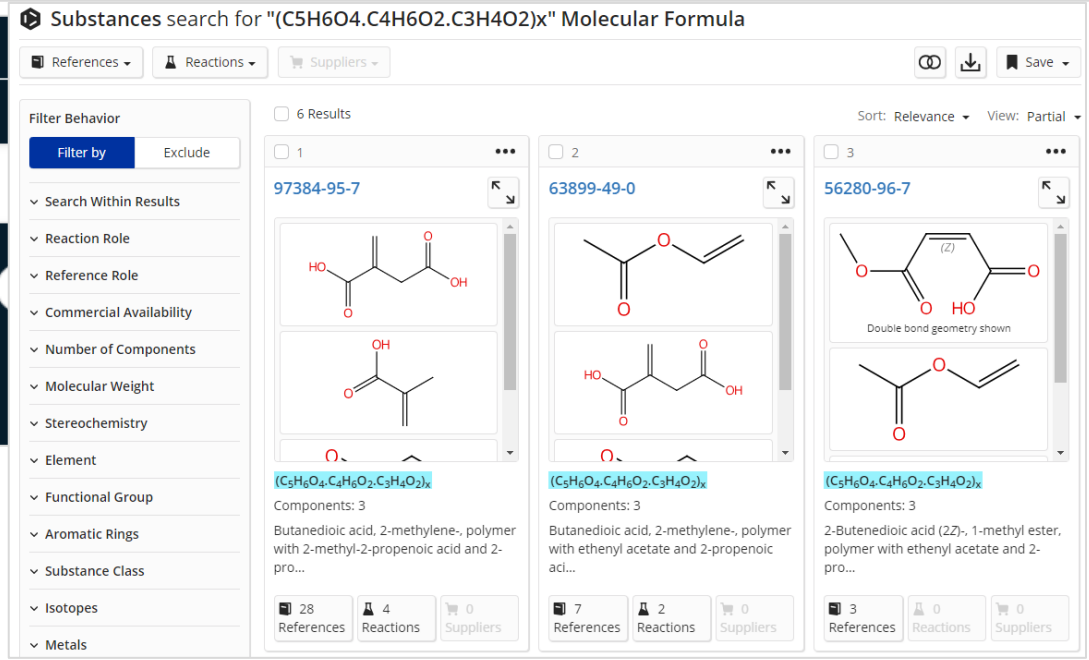


2.1 分子式检索：高效检索聚合物或无机化合物



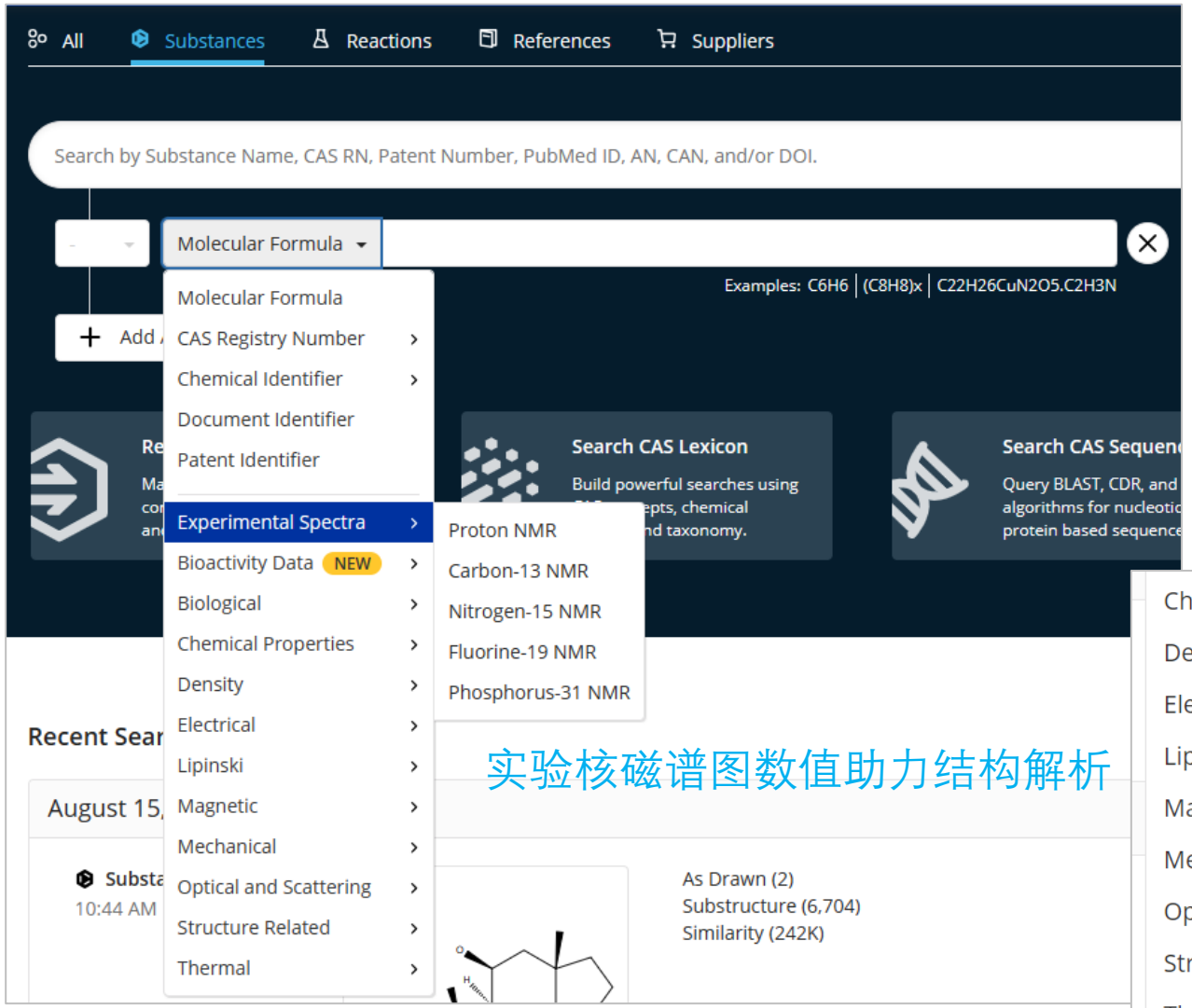




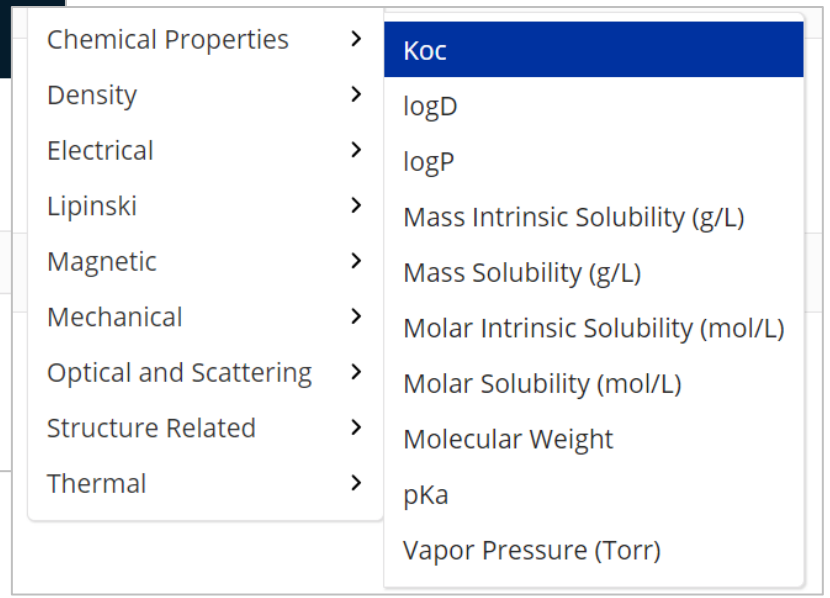


- (C2H4O)nC4H8O: 括号中是重复结构单元，括号外为n
- (C5H6O4.C4H6O2.C3H4O2)x：括号中是单体，括号外为x

2.2 属性值联用检索物质



实验核磁谱图数值助力结构解析



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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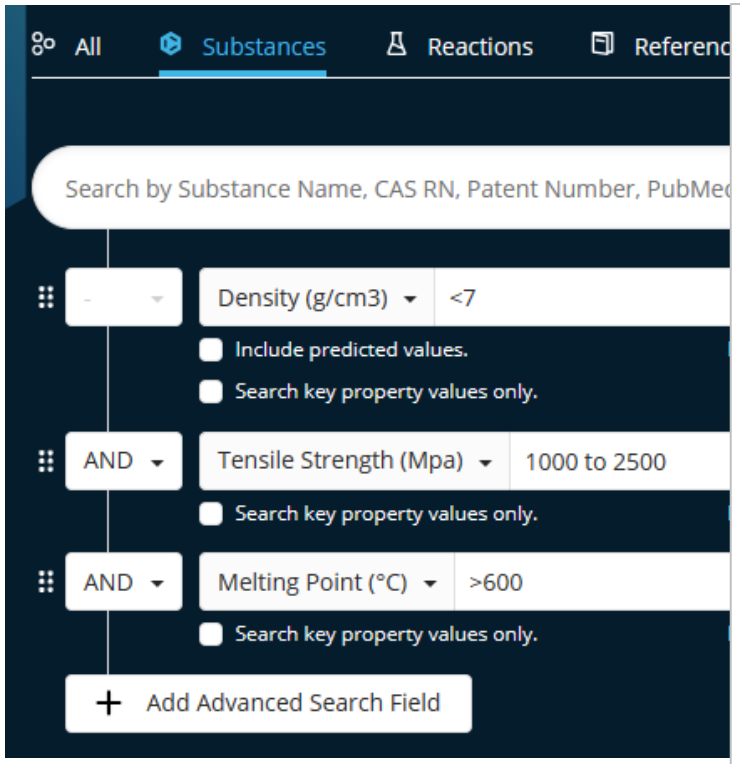
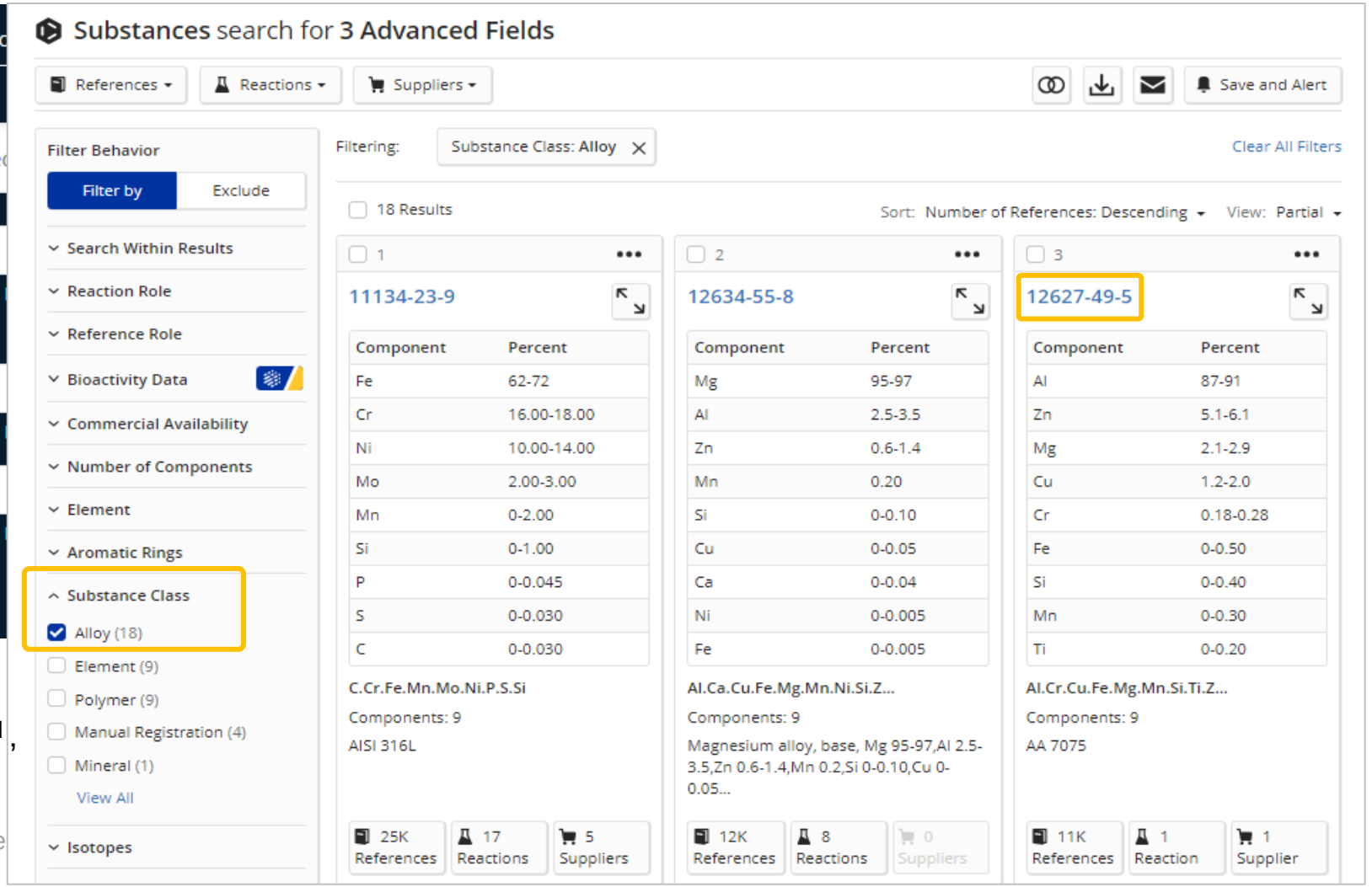
属性值联用检索物质

检索示例：

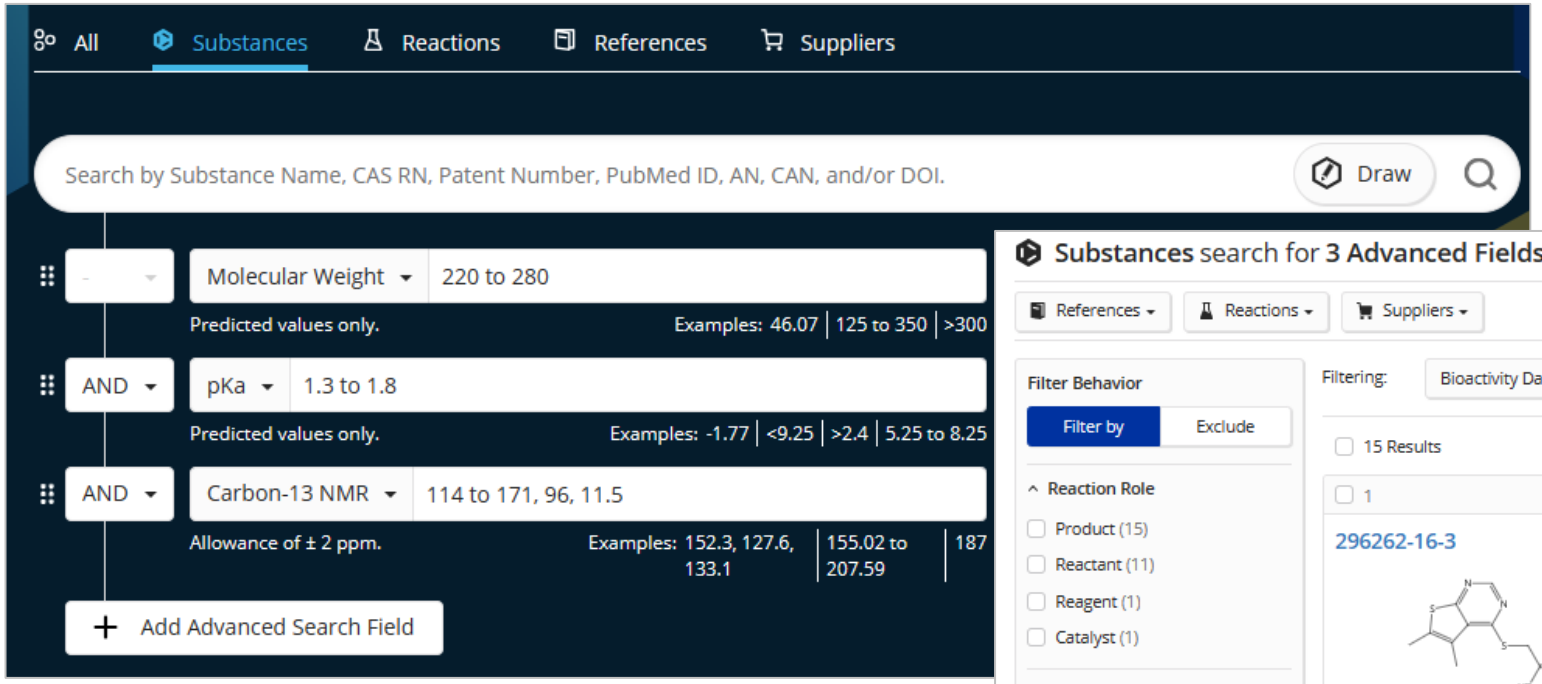
满足多属性值要求的轻质合金，密度<7g/cm3、拉伸强度>1000MPa、熔点>600℃。

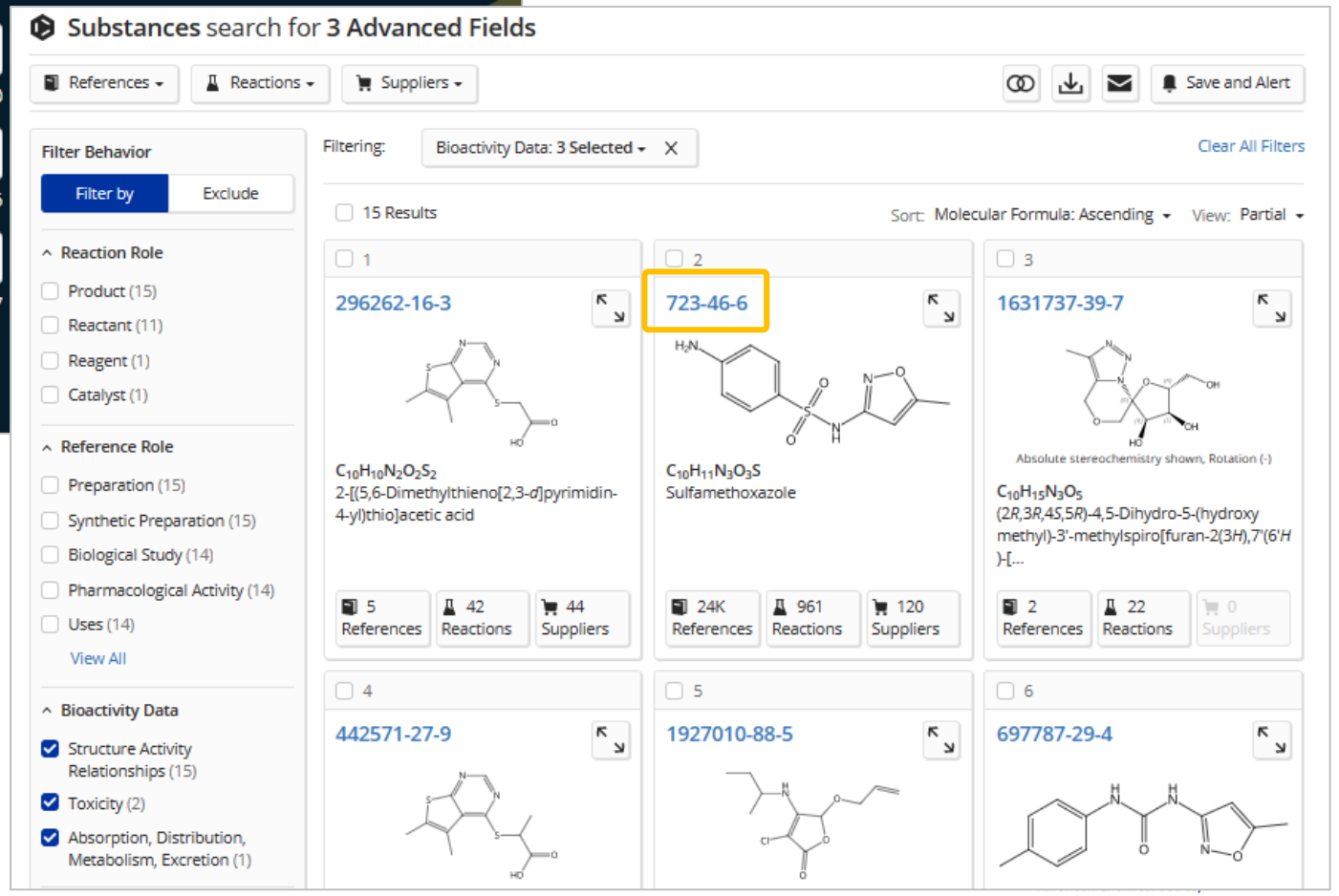


在物质类别 Substance Class 中，锁定合金 Alloy。



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

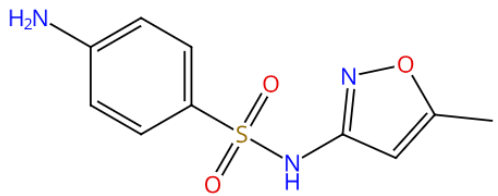
物质详情

- 折叠菜单显示物质各类信息

CAS Registry Number: 723-46-6

References (26K) | Reactions (997) | Suppliers (126) | Save

This substance contains CAS Bioactivity data, such as SAR, ADME, or Toxicity tables. Explore this information below. Learn more about CAS life sciences.

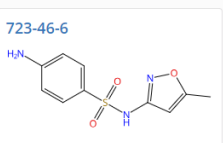


$C_{10}H_{11}N_3O_3S$

Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Poi		
Density (Ex		
pKa (Predi		
Experimen		

Carbon-13 NMR Spectrum for 723-46-6



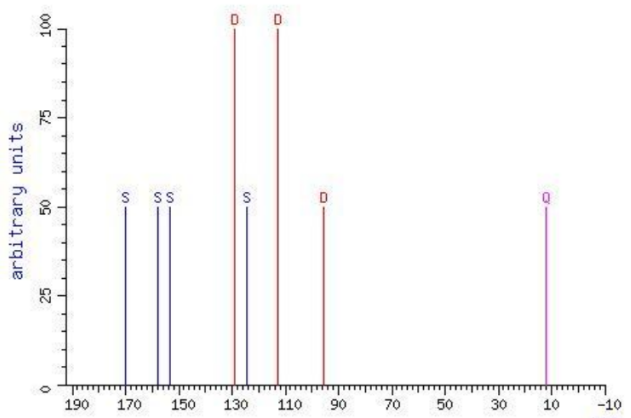
723-46-6

$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions
Solvent
DMSO-d_6 (2206-27-1)
Standard
Tetramethylsilane (75-76-3)

Spectrum Summary
Spectrum ID
CNCC-59959-233D
Spectrometer
JEOL GX-270
Source
Spectral data were obtained from John Wiley & Sons, Inc.



Other Names and Identifiers

Experimental Properties

Experimental Spectra

^{1}H NMR	^{13}C NMR	Hetero NMR	IR	Mass	Raman	UV and Visible

	Solvent	Source
View Carbon-13 NMR Spectrum	DMSO-d_6	(1) WSS
View Carbon-13 NMR Spectrum	DMSO-d_6	(2) WSS
View Carbon-13 NMR Spectrum	-	(2) WSS
View Carbon-13 NMR Spectrum	Methanol-d_4	(3) CAS
View Carbon-13 NMR Spectrum	DMSO-d_6	(4) CAS
View Carbon-13 NMR Spectrum	-	(5) BIORAD
View Carbon-13 NMR Spectrum	DMSO-d_6	(6) AIST
Carbon-13 NMR Spectrum - 1 Source	-	(7) CAS

Sources

(1) Kartashov, V. S.; Khimiko-Farmatsevticheskii Zhurnal, (1992), 26(11-12), 107-9, CAplus

(2) Fruttero, Roberta; Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999), (1988)(10), 1863-6, CAplus

(3) Ham, Won Seok; Angewandte Chemie, International Edition, (2019), 58(2), 532-536, CAplus

(4) Sunduru, Naresh; European Journal of Medicinal Chemistry, (2015), 101, 595-603, CAplus

(5) Copyright Bio-Rad Laboratories. All Rights Reserved.

(6) "Integrated Spectral Data Base System of Organic Compounds" data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan)

(7) Blasioli, Sonia; Journal of Colloid and Interface Science, (2014), 419, 148-159, CAplus

Structure Activity Relationships — CAS LIFE SCIENCES

Absorption, Distribution, Metabolism, and Excretion Data — CAS LIFE SCIENCES

Toxicity — CAS LIFE SCIENCES

Predicted Properties

Predicted Spectra

Bioactivity Indicators

Target Indicators

Regulatory Information

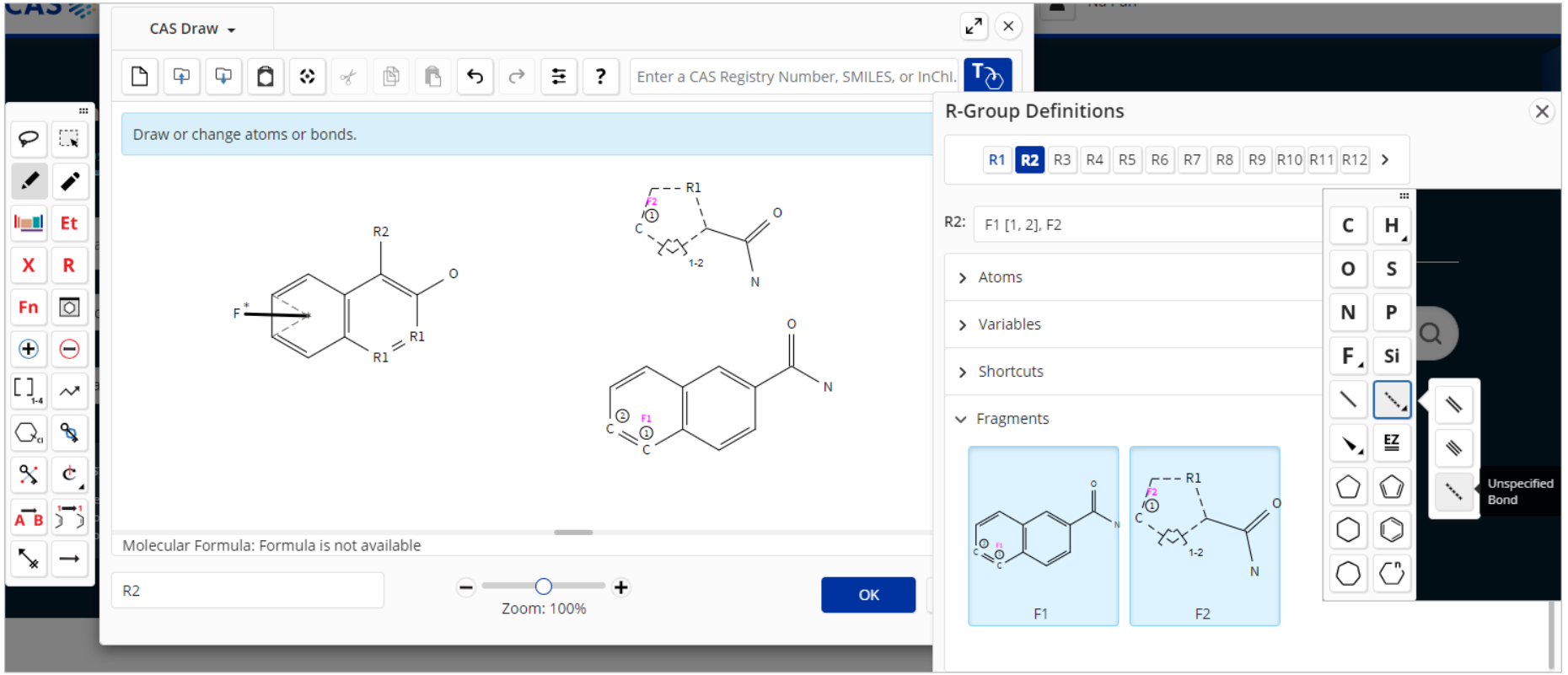
GHS Hazard Statements

Additional Details

2.3 结构检索

灵活构建通式结构，提高物质/反应信息的检索效率

- X 选择可变基团
- R 自定义R基团
- Fn 片段结构
- [ ]1-4 重复工具
- 取代位置可变
- 环锁定工具
- 原子锁定工具



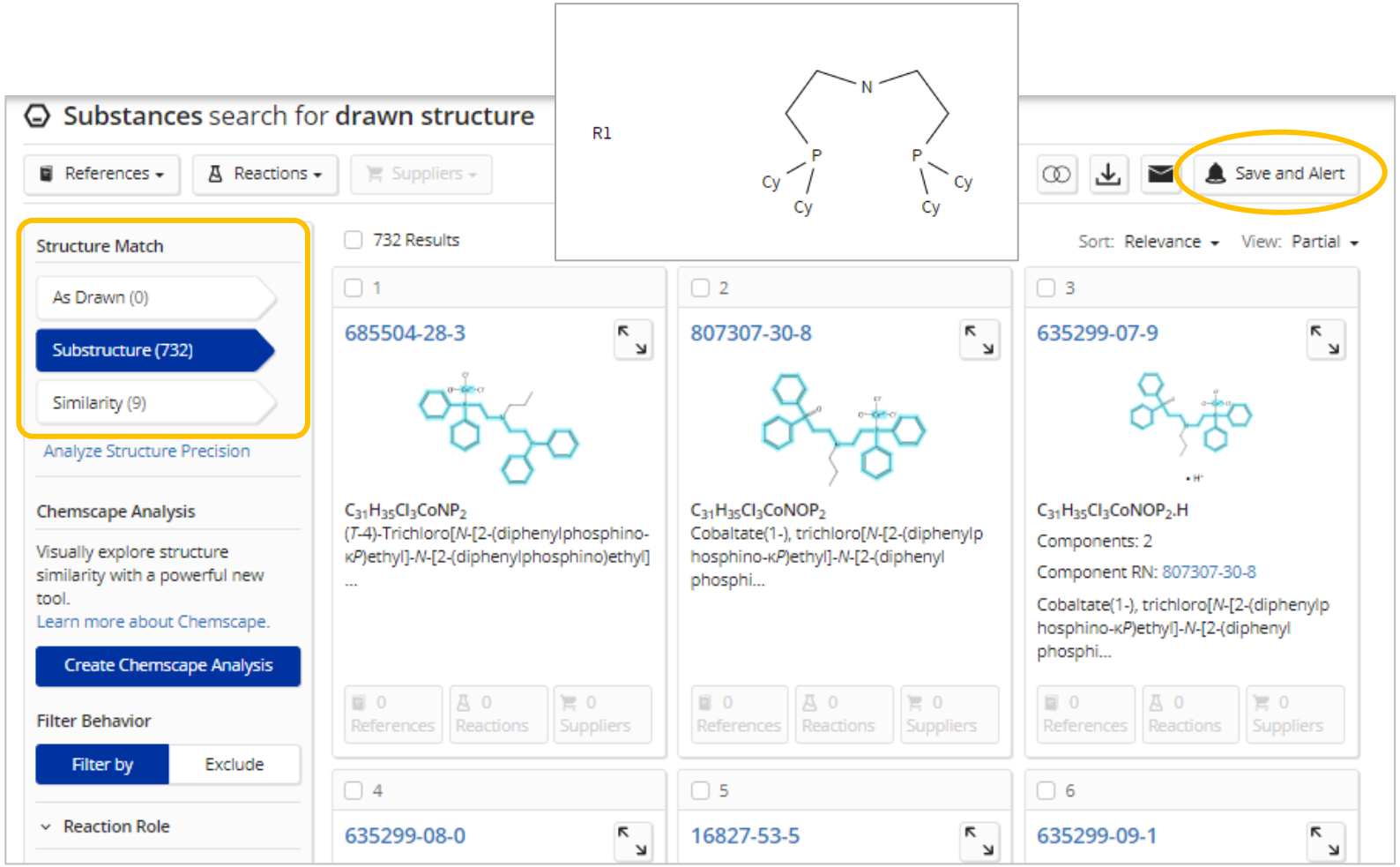
利用绘图工具自定义相似结构：

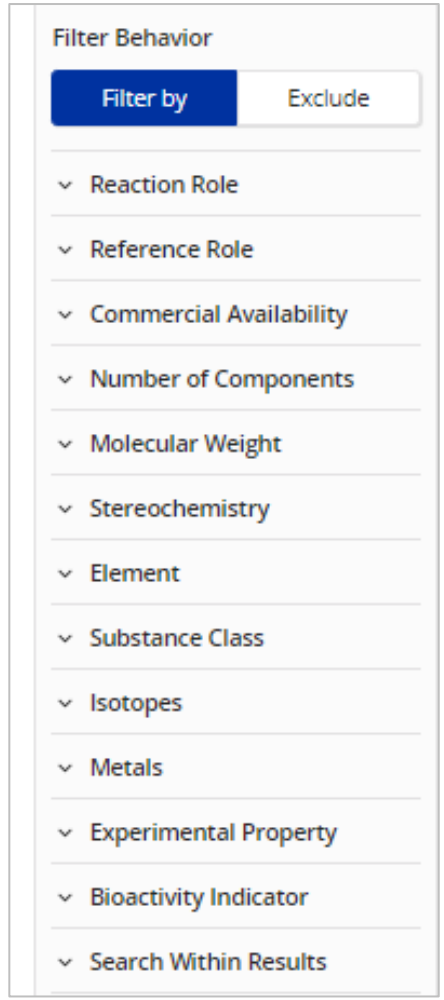
1. 化学键型键级不确定
2. 骨架结构上指定出现的原子 R
3. 环系范围的定义 [ ]1-4

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:

反应角色

文献角色

立体化学

物质类别

同位素

金属包含

实验物性数据

二次检索……

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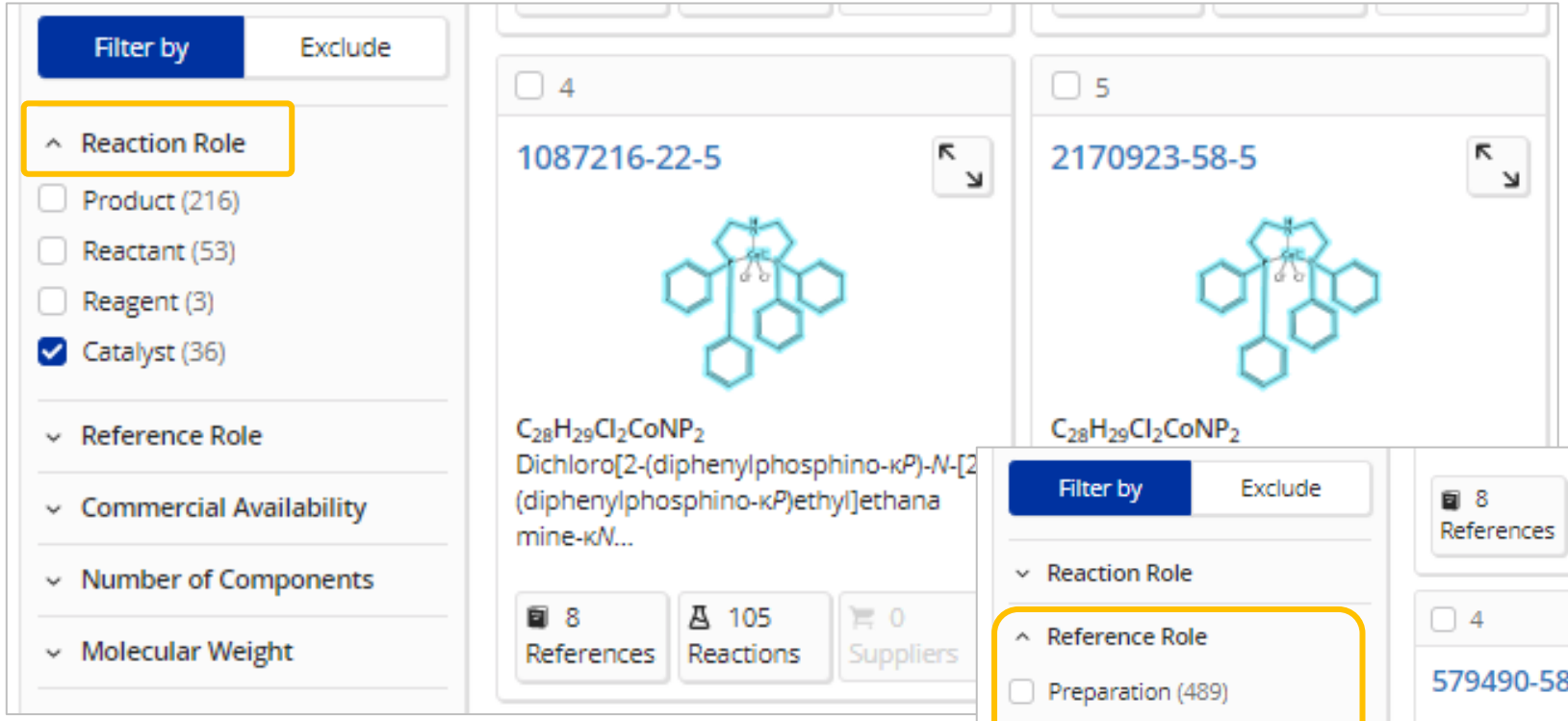
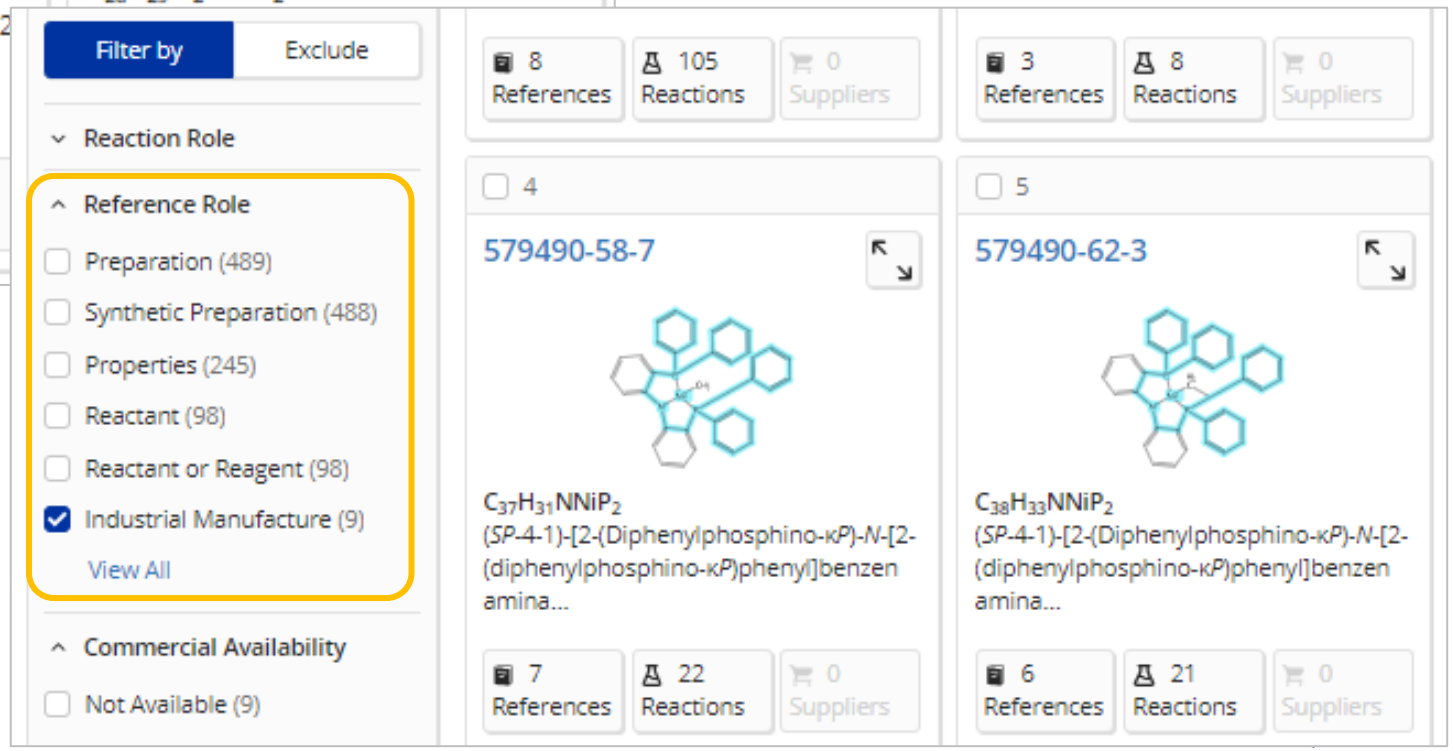
物质检索结果的筛选



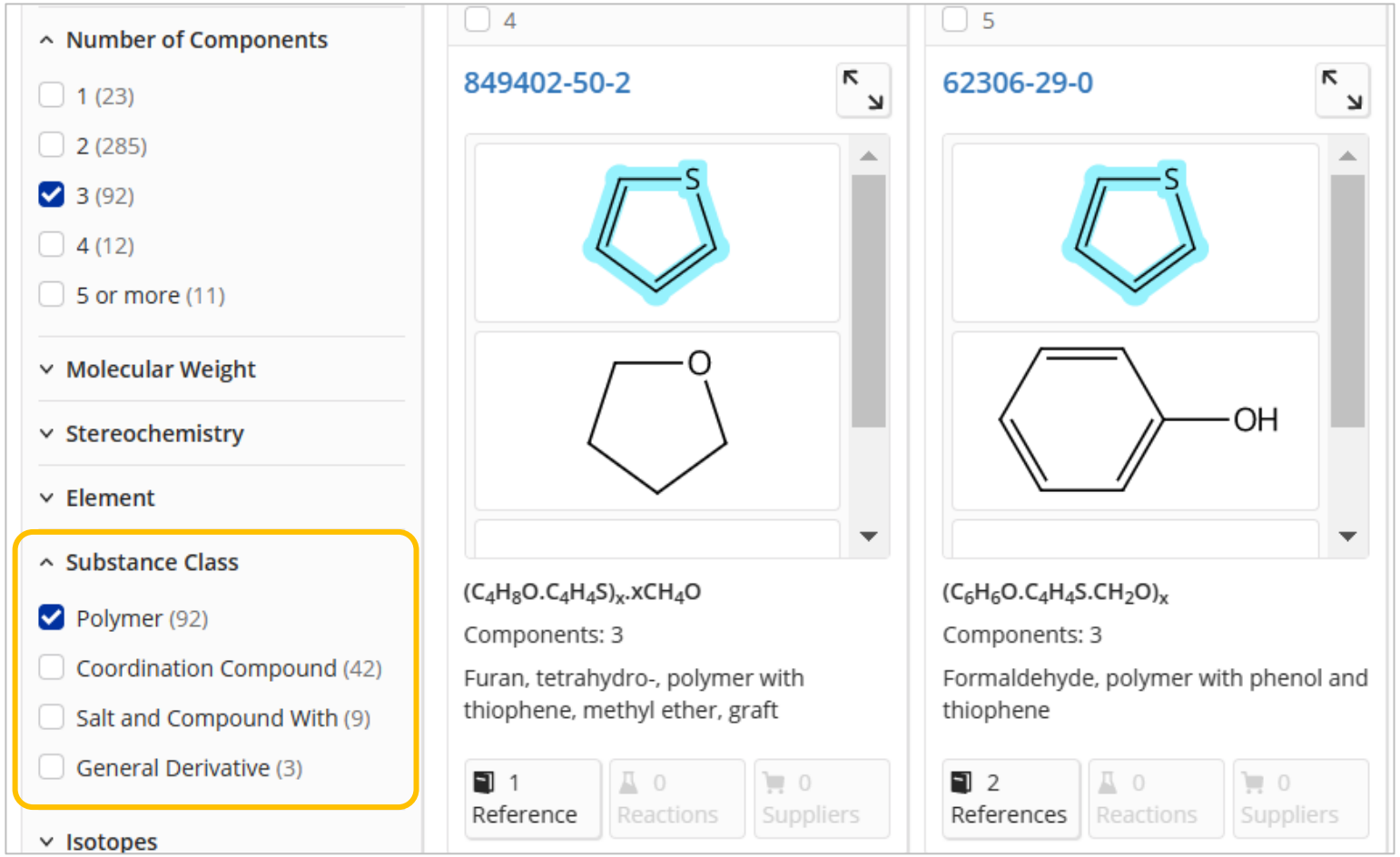
Reaction Role：
物质在反应中的角色

Reference Role：
物质在文献中的研究角色



物质检索结果的筛选

Substance Class：物质类别



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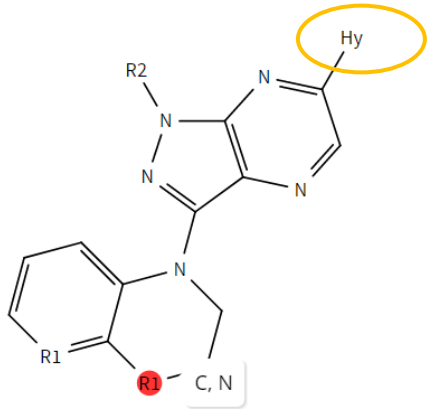
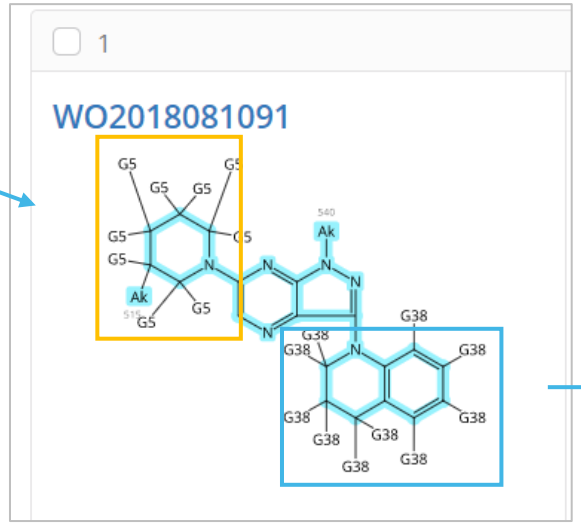
2.4 CAS Markush 检索，助力结构查新

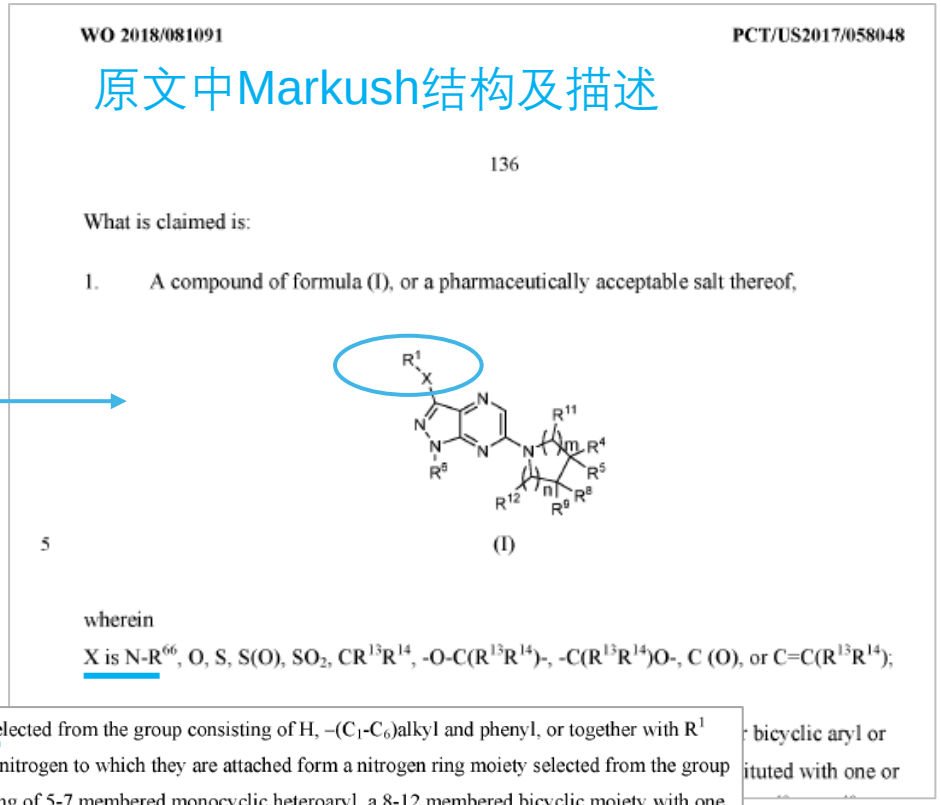
CAS科学家对文献的标引和解读





命中的Markush结构及解读

专利中的定位，专利权人、命中结构的特点等等



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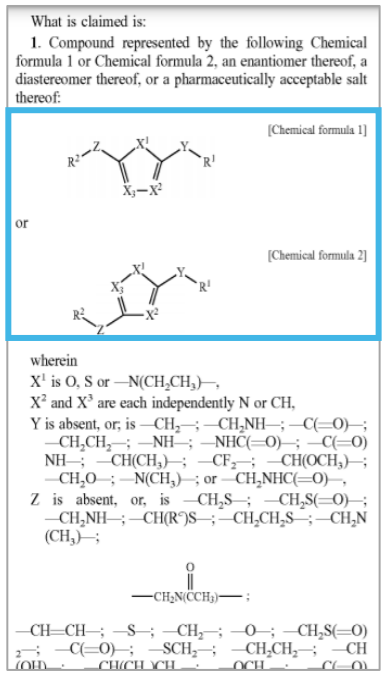
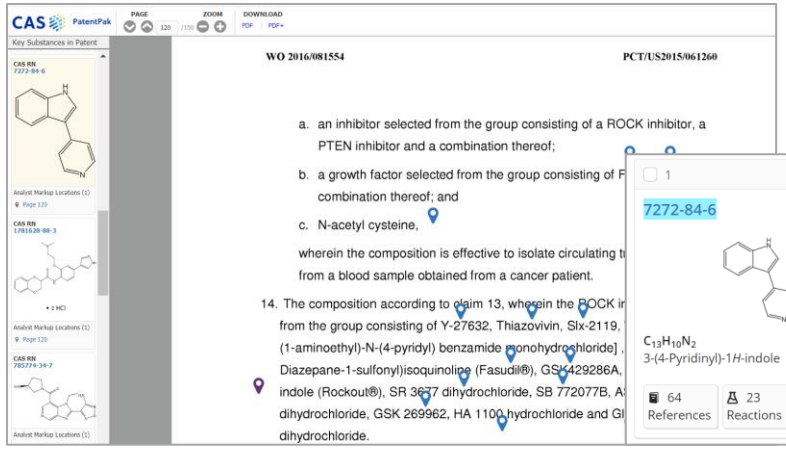
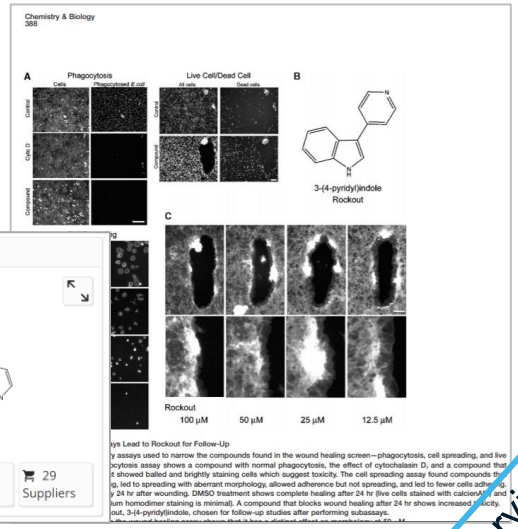
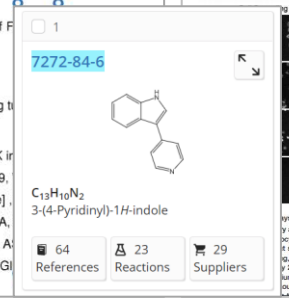
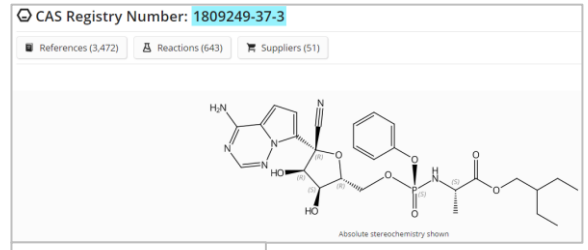
CAS 结构层面的数据集

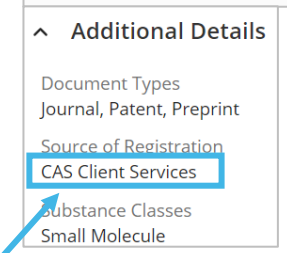


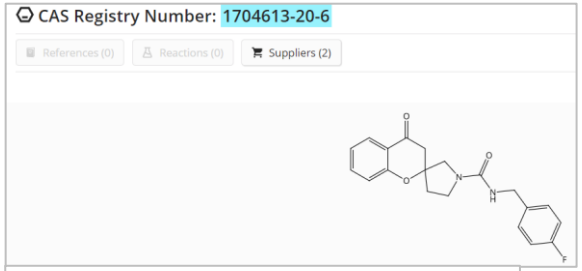


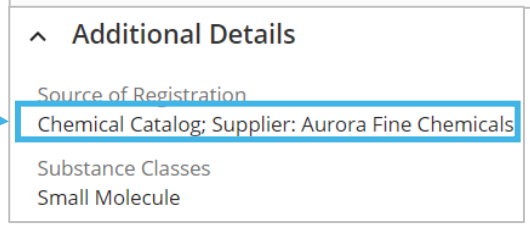






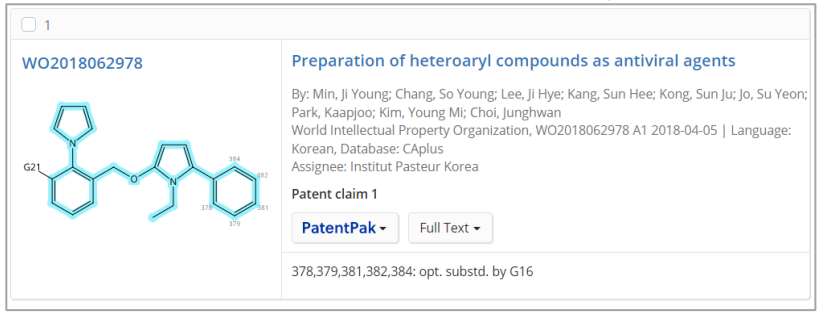






CAS Markusk

Patent



Patent

Journal

CAS REGISTRY

CAS Client Service

Chemical catalog/library

Other web sources

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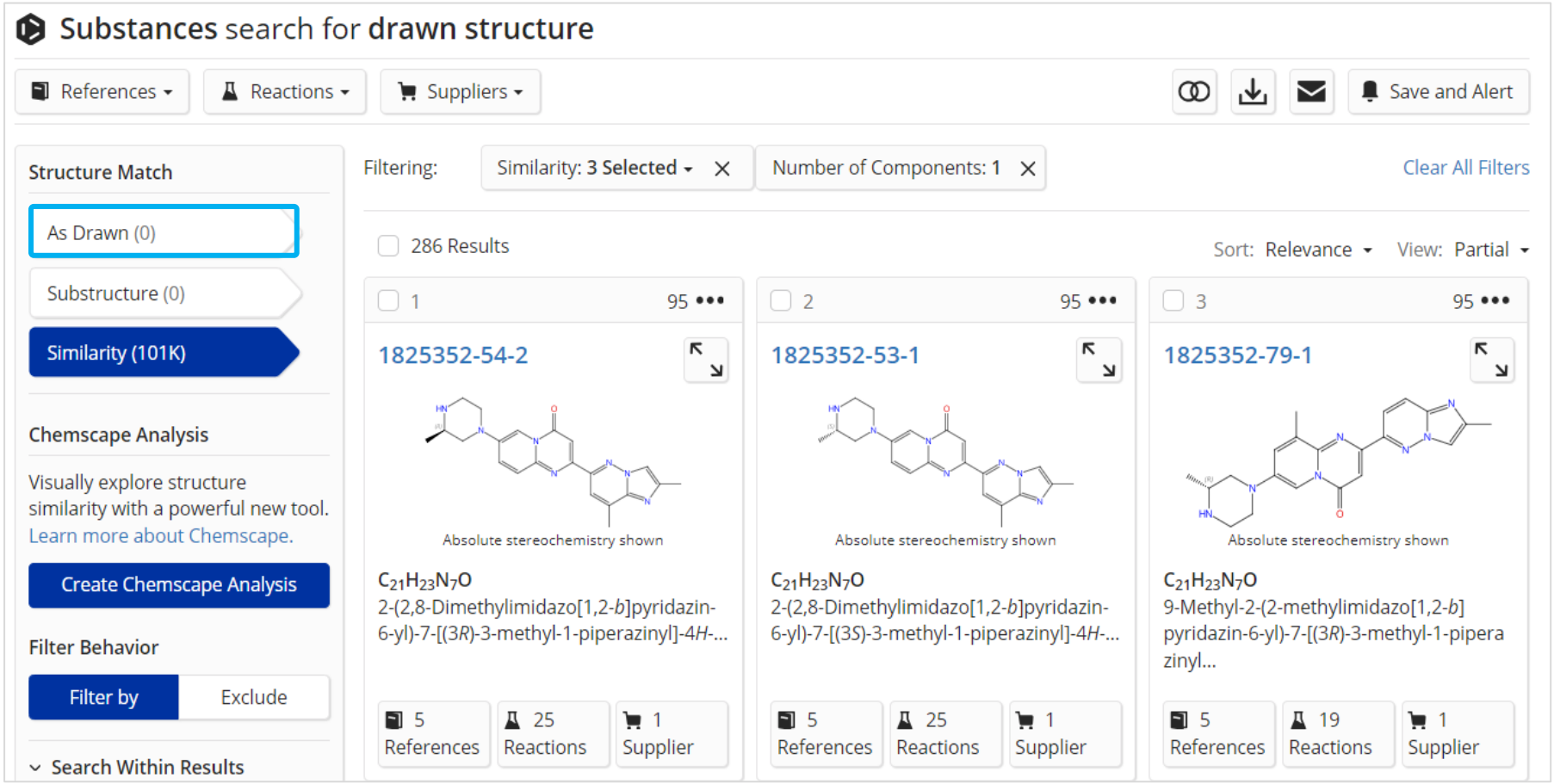
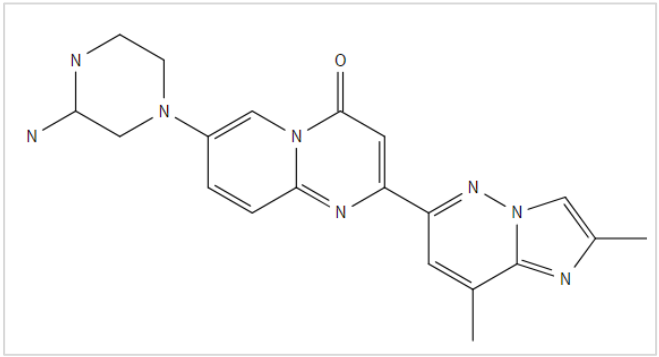
如何进行完整的分子结构检索?





CAS 物质数据集 CAS REGISTRY® 是专利审查员进行新颖性判断的重要依据，此例中的物质在 Registry 中 As Drawn 检索结果为 0，初步判断此分子比较新，同时用户可以根据必要性来选择性查看相似检索结果

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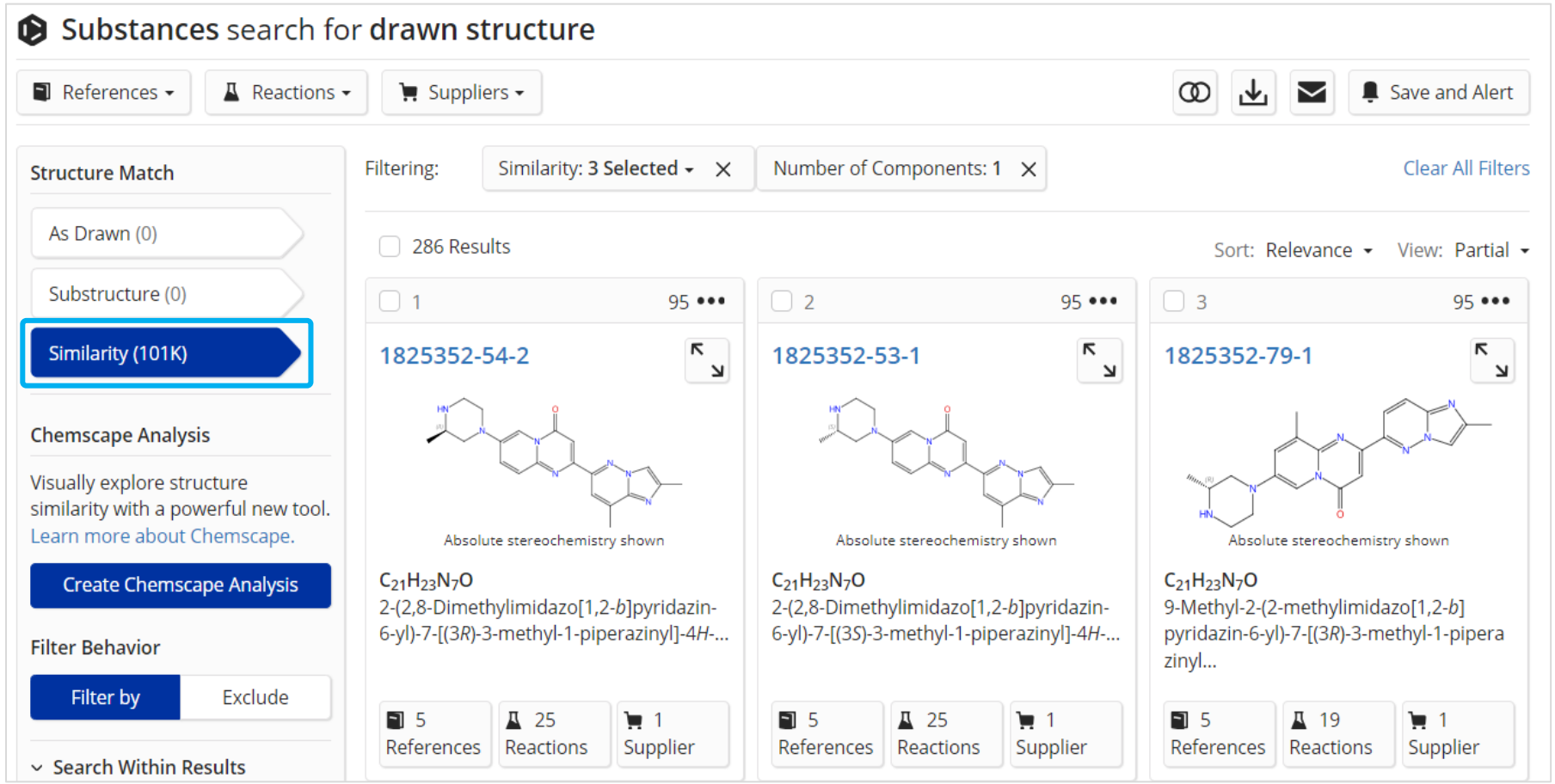
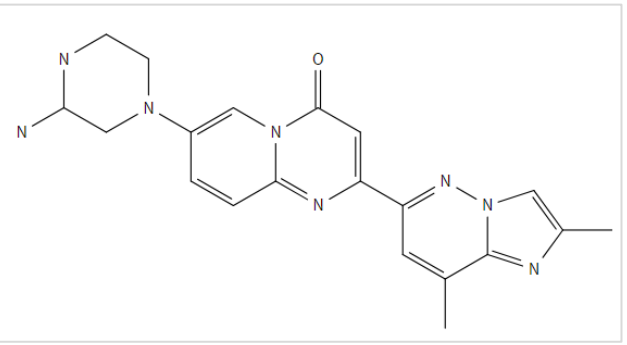
如何进行完整的分子结构检索?





查看相似结构，可参考

Similarity score

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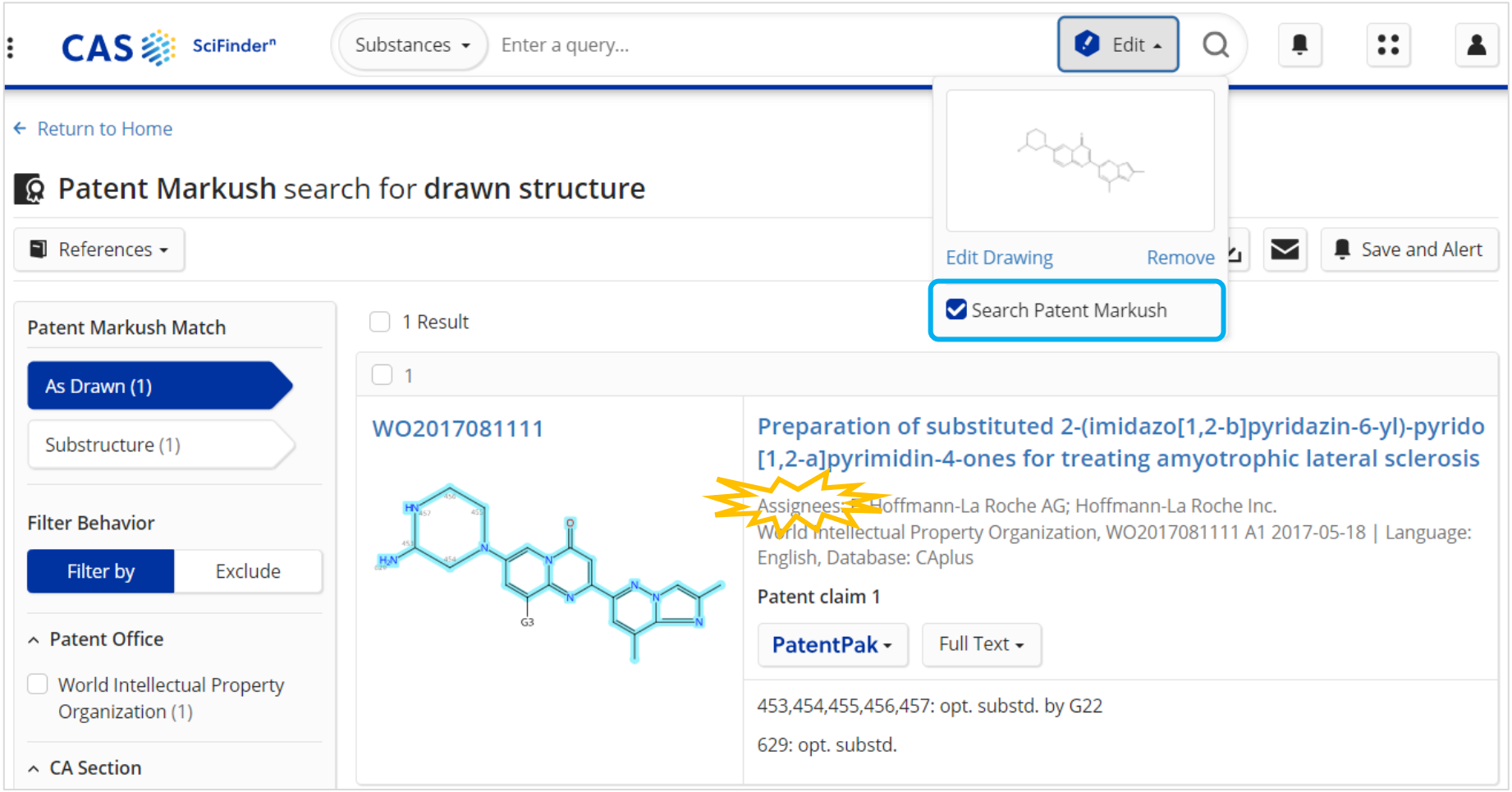
如何进行完整的分子结构检索?



- 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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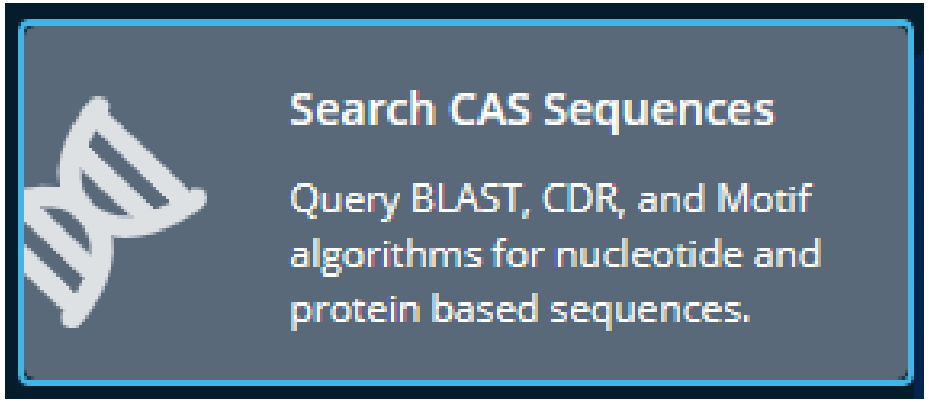
2.5 CAS SciFinder中的序列检索

- BLAST
- CDR
- Motif



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物质检索小结

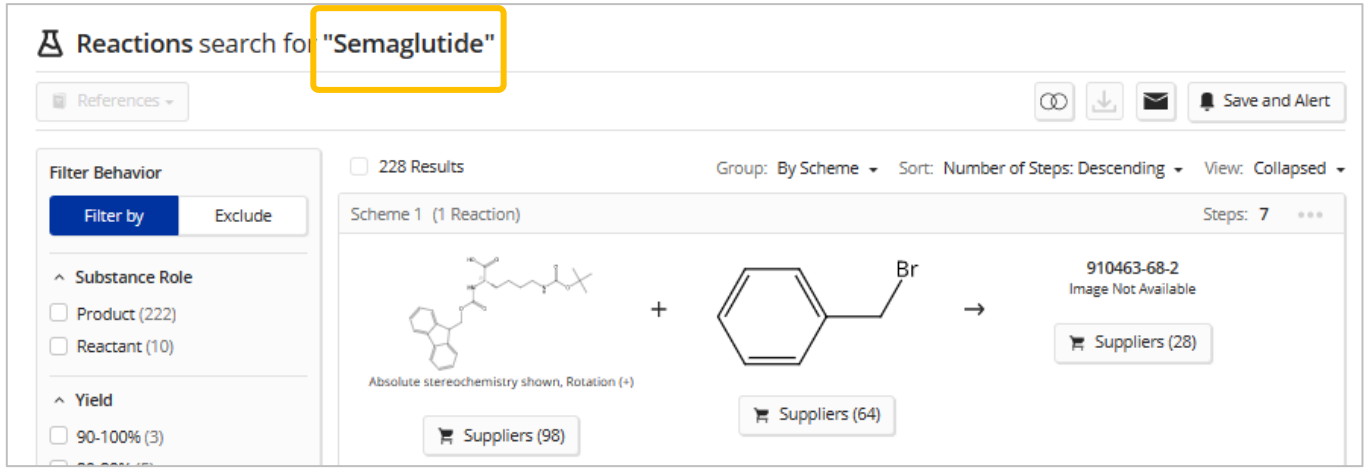
1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
3. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
4. 利用CAS Markush检索尽可能全面的获得结构的公开信息

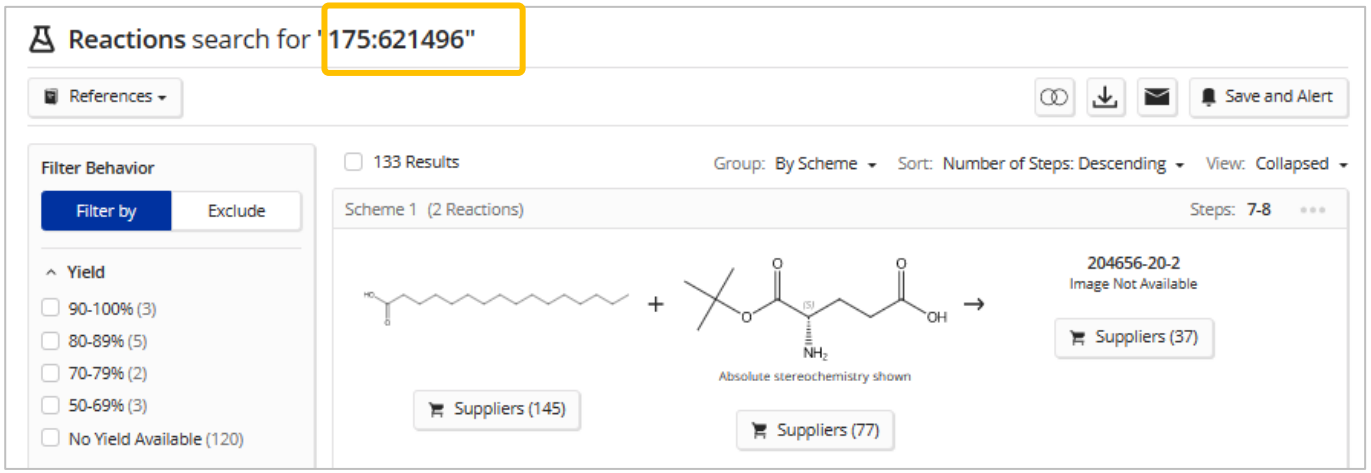
3. 如何进行反应调研?

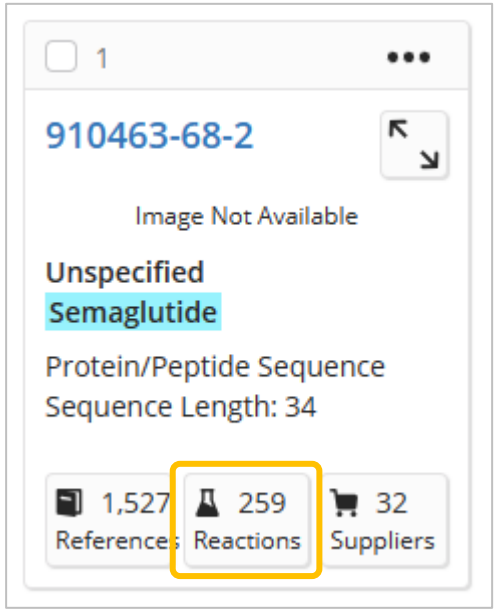
- 如何从我感兴趣的底物、产物或催化剂出发，找到关联的反应?
- 如何查找相似反应?
- 如何关注特定转化类型的反应?
- 如何在大量反应结果中，快速找到最想要的反应?
- 如何查找涉及机理研究的反应?或人名反应?
- 如何设计新化合物的逆合成路线?

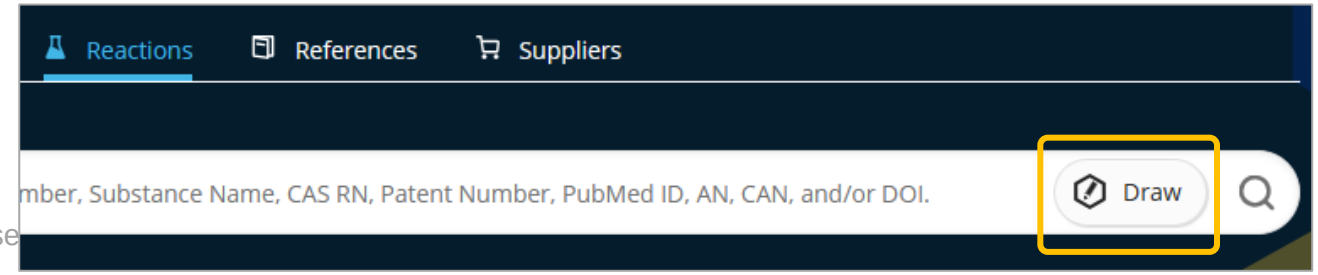
研究某类反应?

- 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

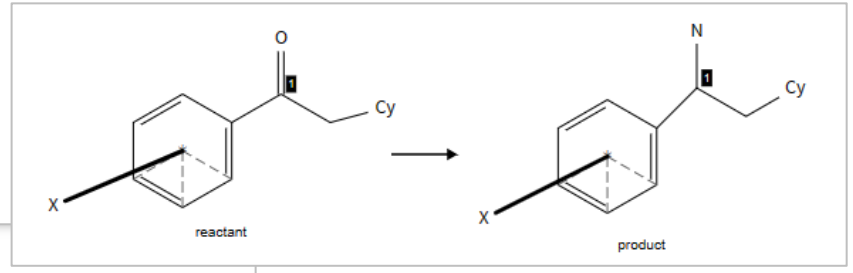








3.1 查找亚结构反应



As Drawn
亚结构反应
相似反应

Reactions search for drawn structure

References

Save and Alert

Structure Match

As Drawn (34)

Substructure (8,044)

Similarity (0)

Filtering: Reaction Mapping: Mapping Data Available

Clear All Filters

16 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 (93)

Suppliers (15)

Expand Scheme

Scheme 2 (1 Reaction)

Steps: 1 Yield: 76%

Suppliers (53)

Suppliers (3)

Filter Behavior

Filter by | Exclude

Search Within Results

Yield

80-89% (4)

70-79% (2)

50-69% (1)

No Yield Available (9)

Reaction Scale

Milligram (2)

Gram (1)

No Scale Provided (13)

Non-Participating Functional Groups

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

1.1 Reagents: *O*-Methylhydroxylamine hydrochloride
Solvents: Pyridine; rt; 1 h, 50 °C

Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

By: Heidelbaugh, Todd M.; et al

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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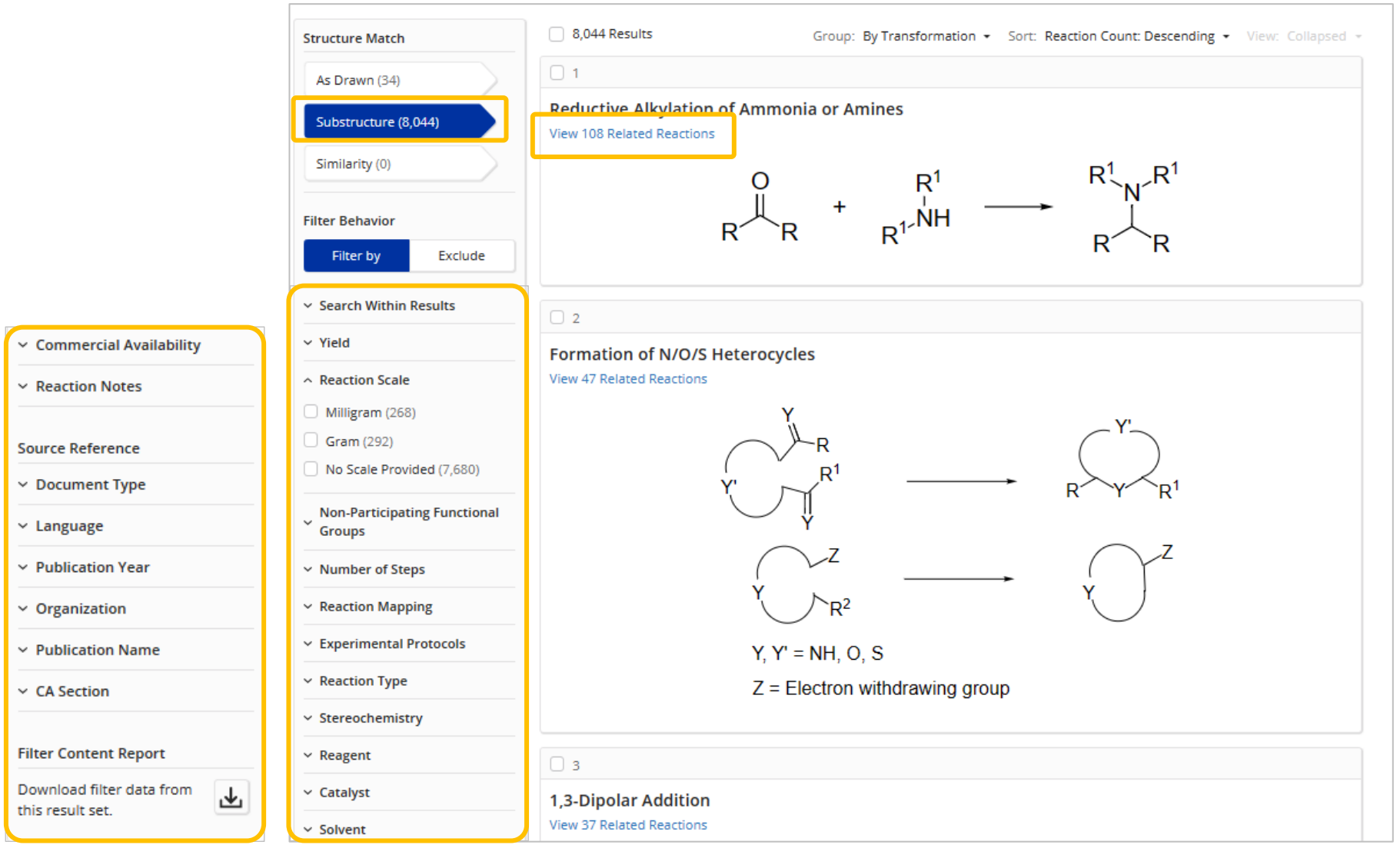
3.2 高效筛选目标反应

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

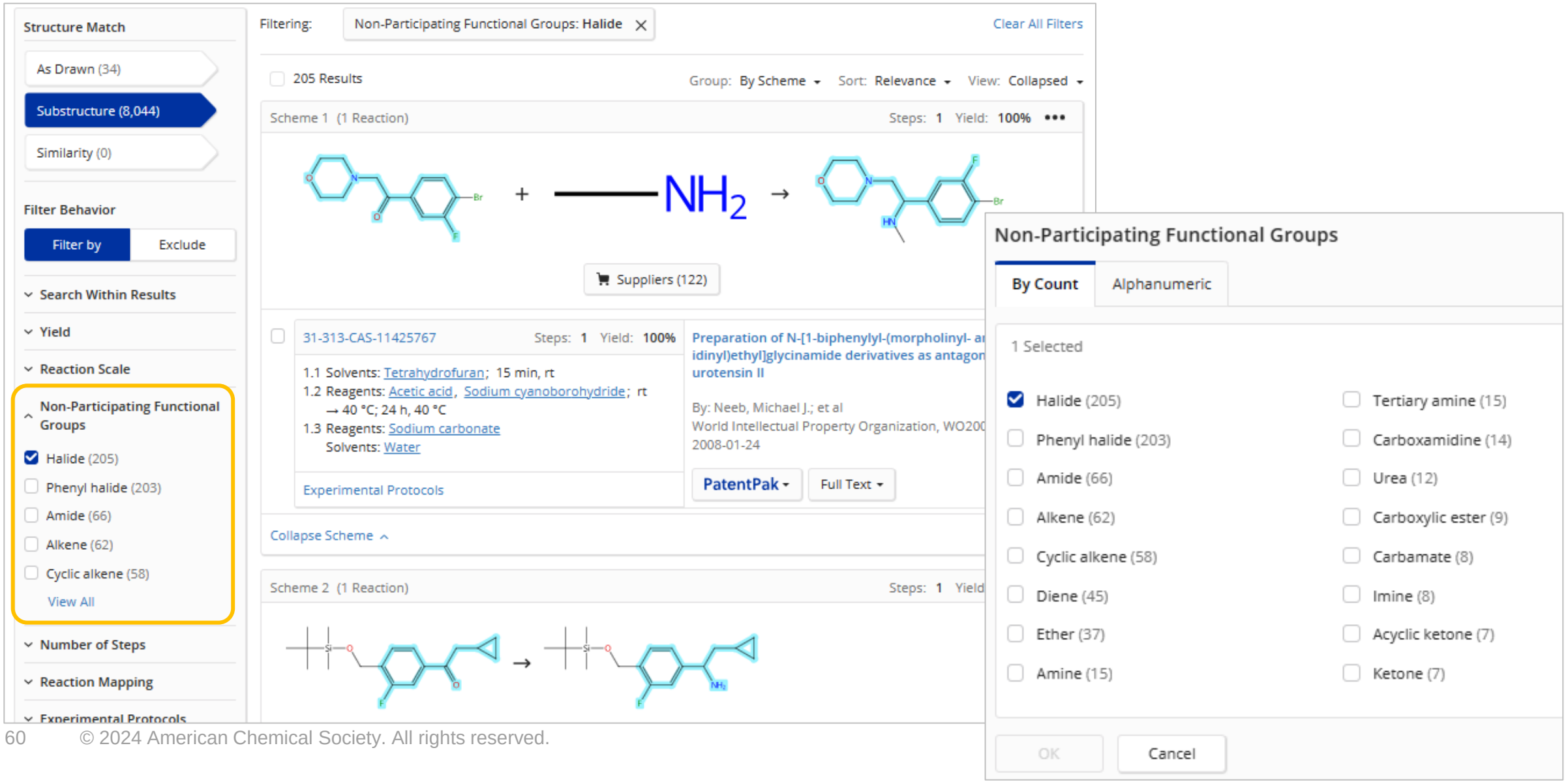
反应筛选类别：
产率、规模、步数
不参与反应的官能团
实验步骤
反应类型、立体化学
试剂、催化剂、溶剂
商品信息……

文献筛选类别：
文献类型、语言
出版年份、刊物名



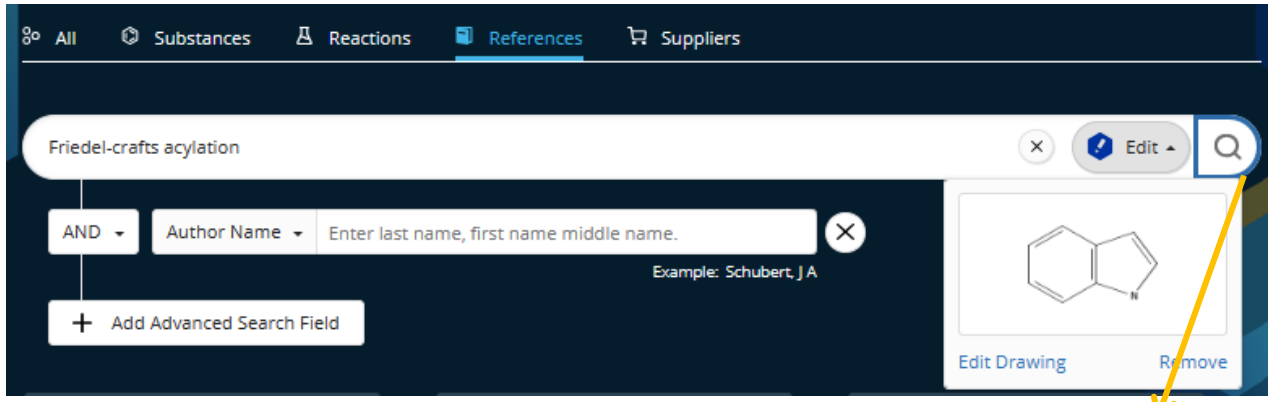
筛选工具：不参与反应官能团

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

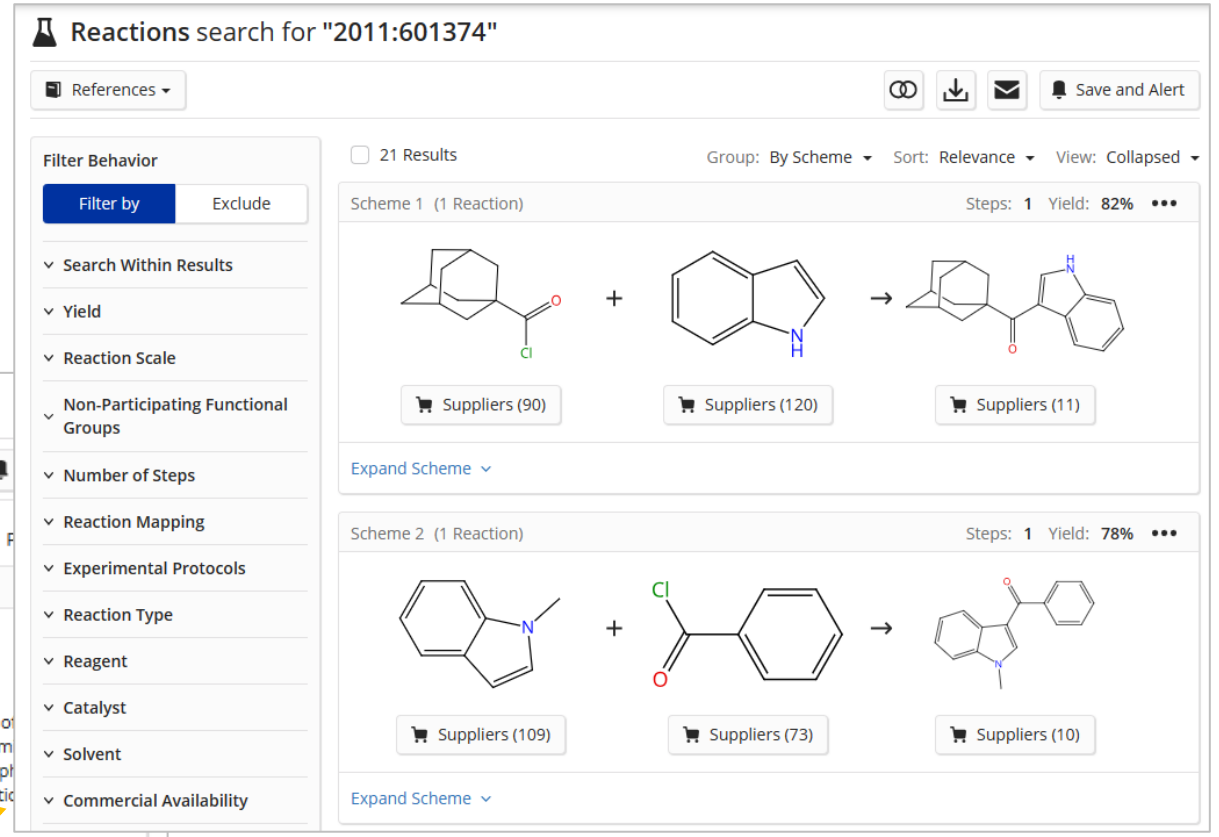


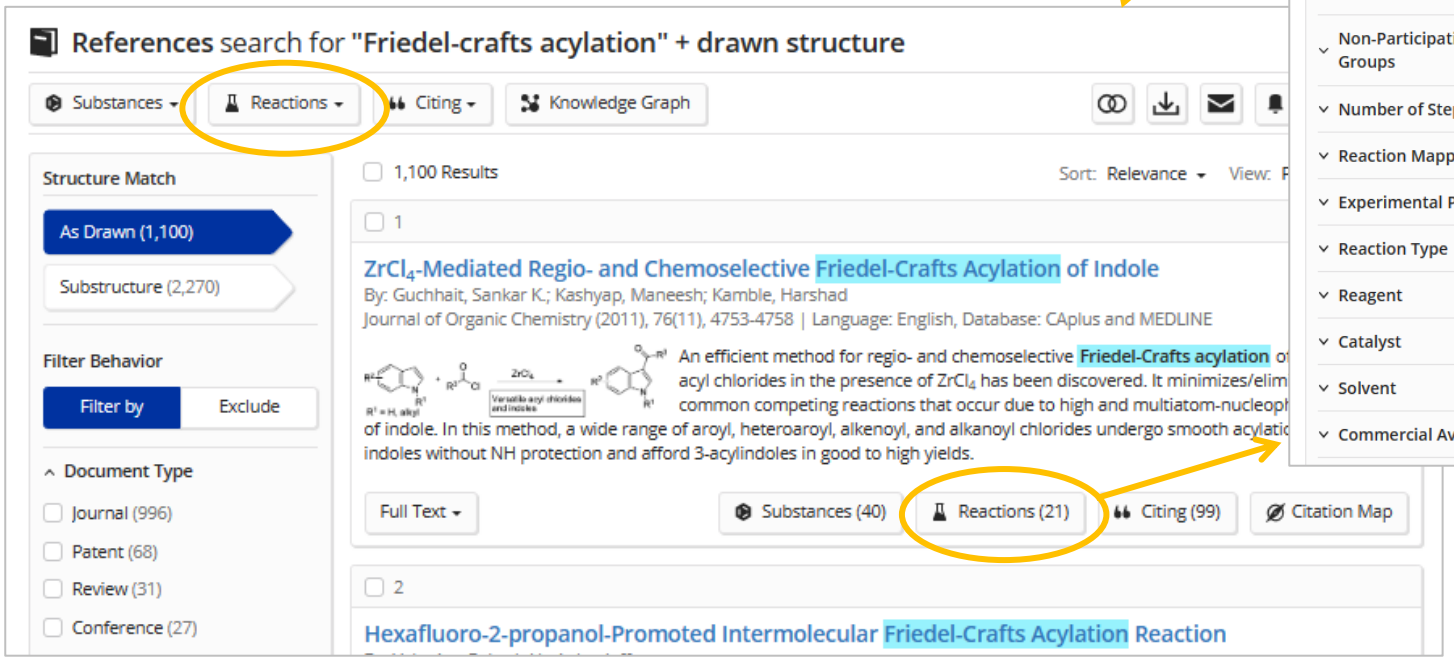
3.3 联用检索——结构与关键词

关注人名反应？



联用检索提高检索效率





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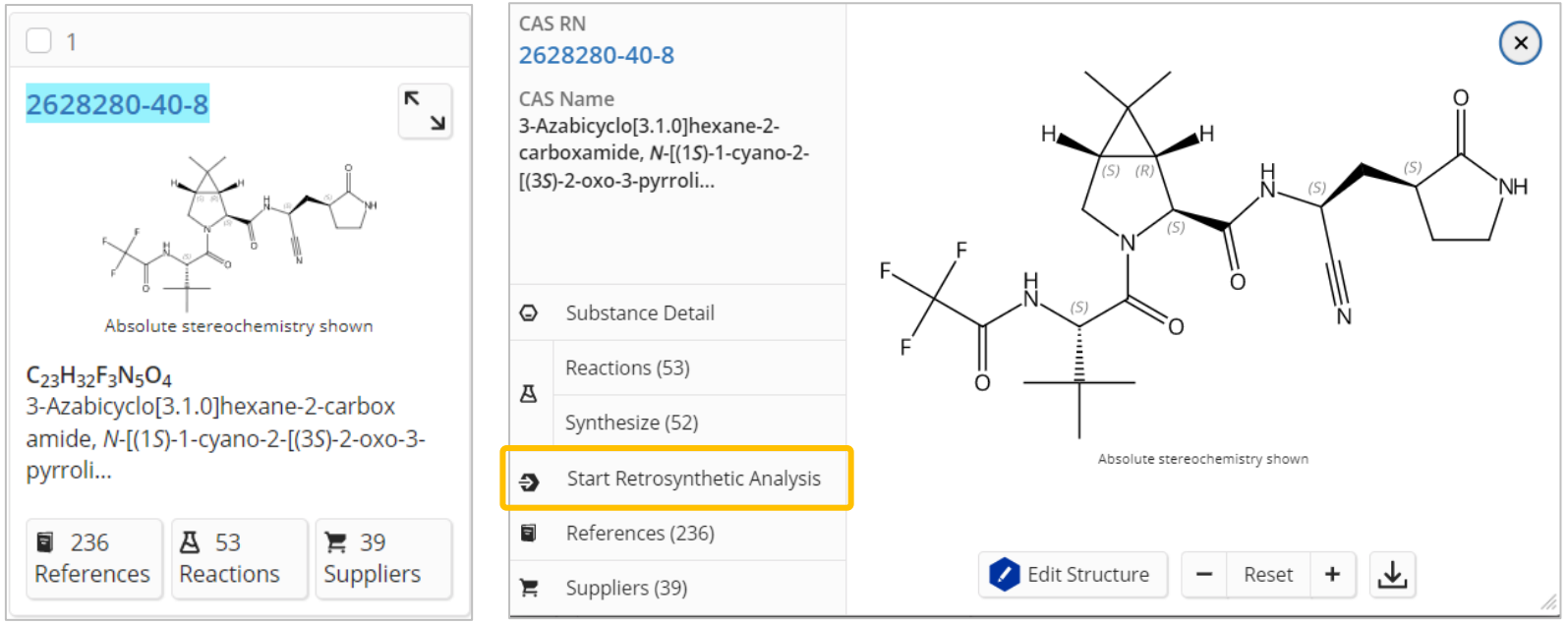
3.4 如何获得逆合成路线?

先进AI技术与CAS科学家标引的丰富反应信息相结合

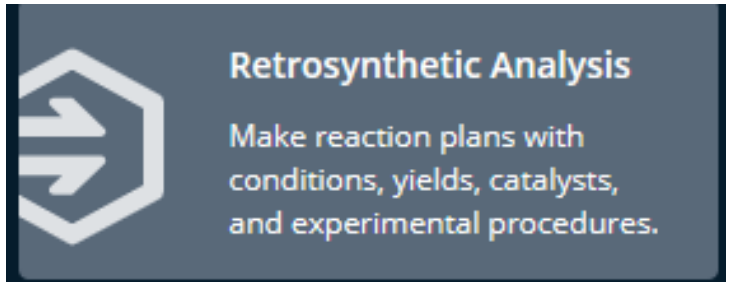
（1）已知化合物：点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis



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



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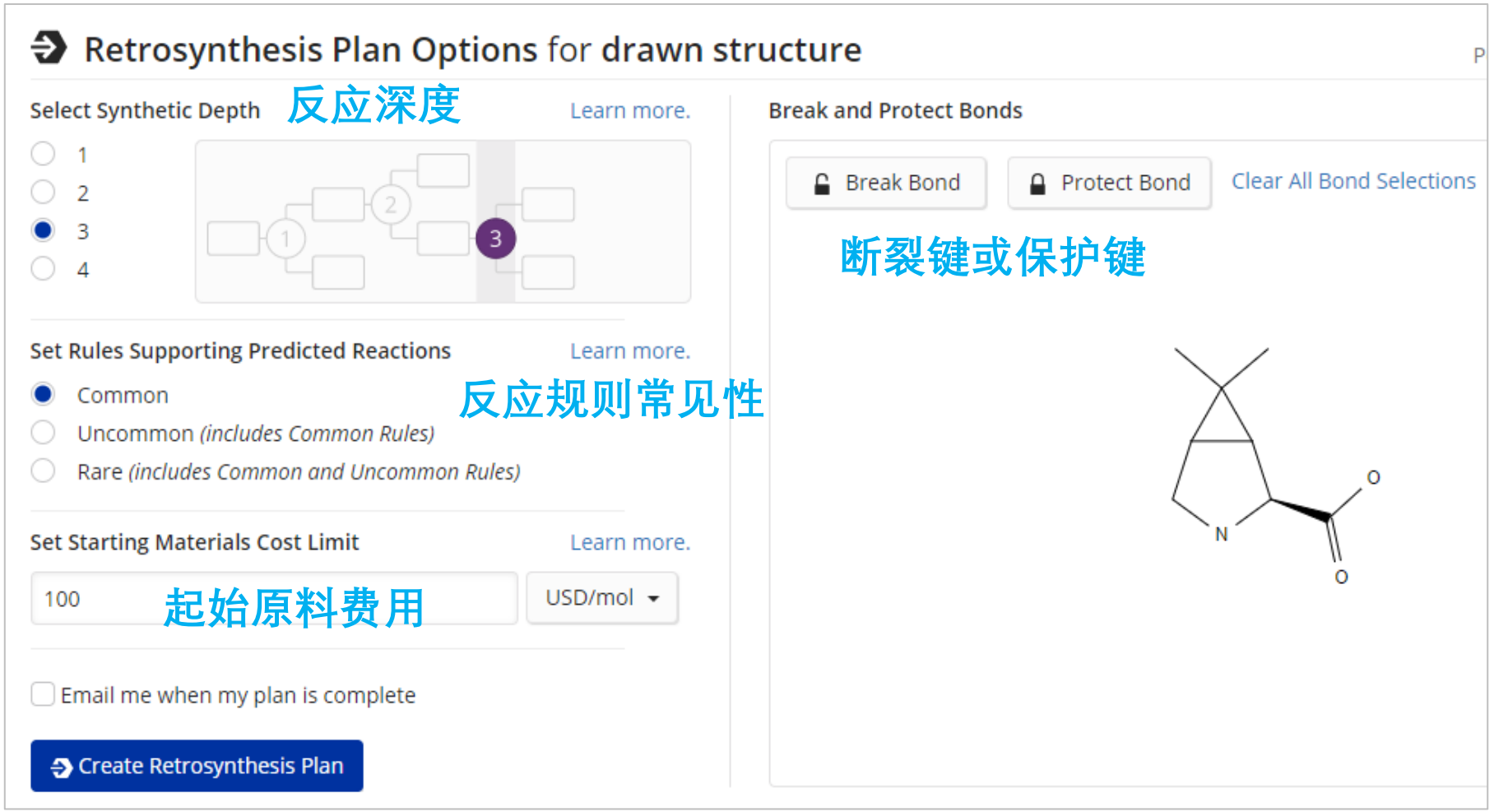
逆合成分析的预设参数



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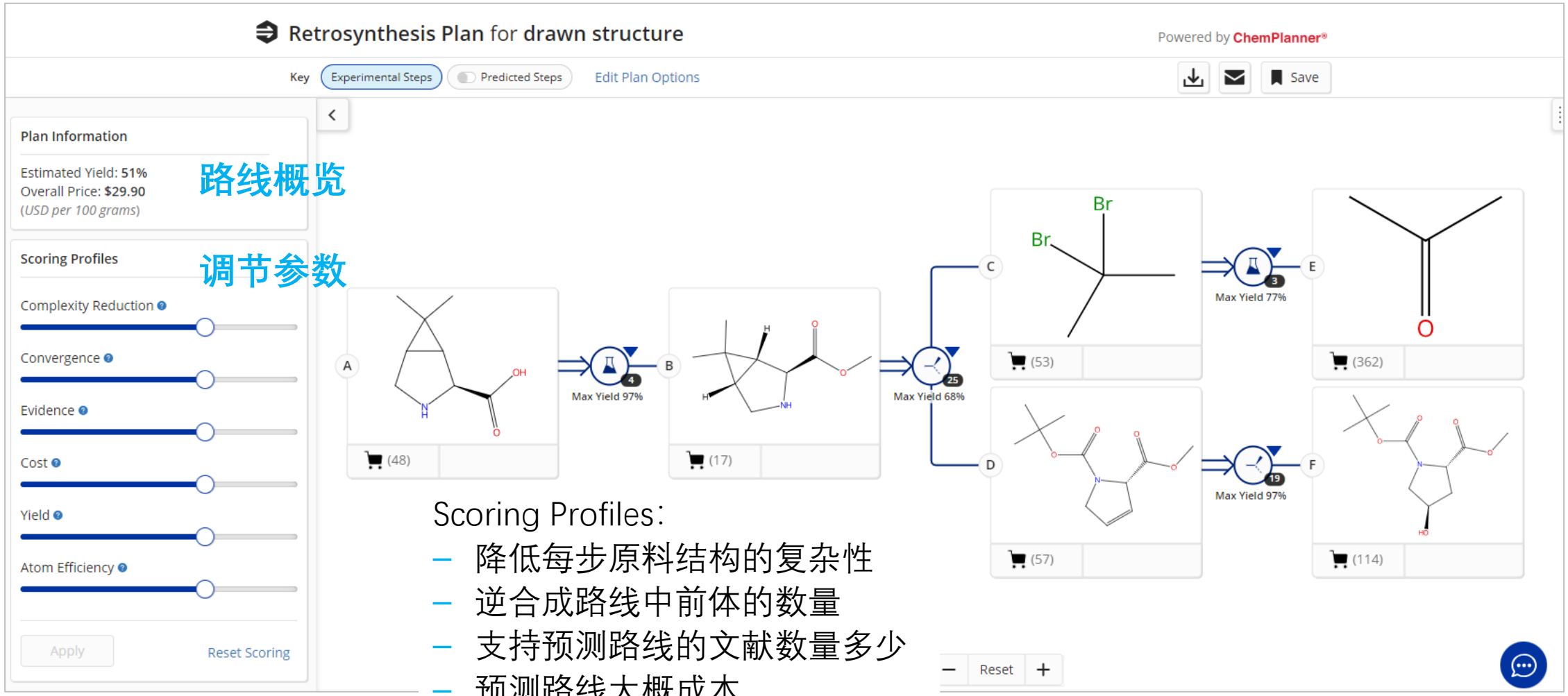
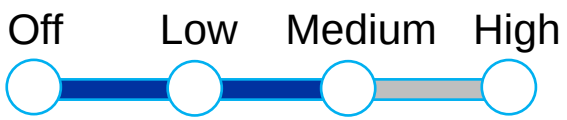
逆合成分析的调节参数



Scoring Profiles:

- 降低每步原料结构的复杂性
- 逆合成路线中前体的数量
- 支持预测路线的文献数量多少
- 预测路线大概成本
- 每步的产率
- 每步的原子转化效率



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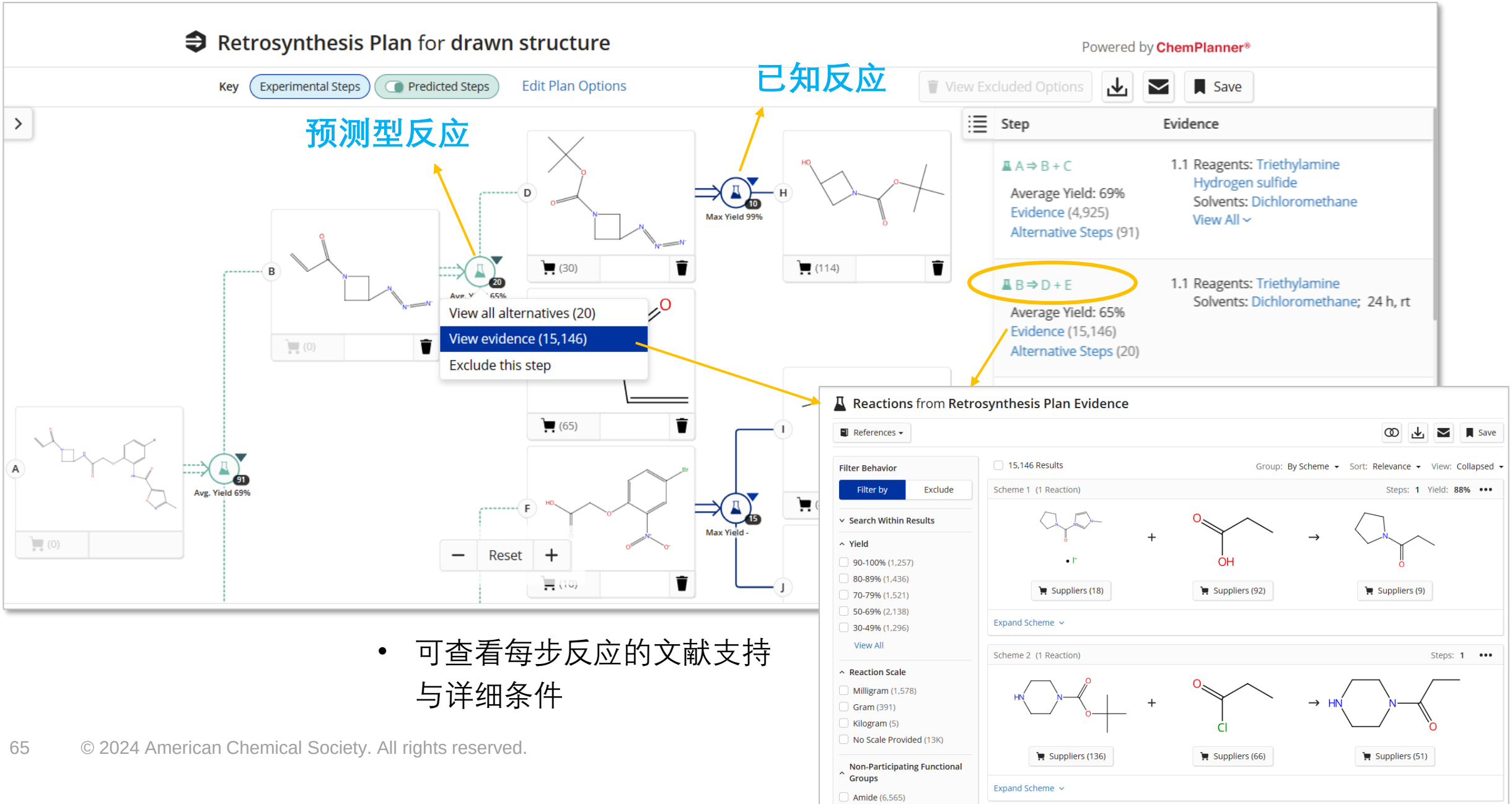
逆合成路线详情



- 可查看每步反应的文献支持与详细条件

反应检索小结

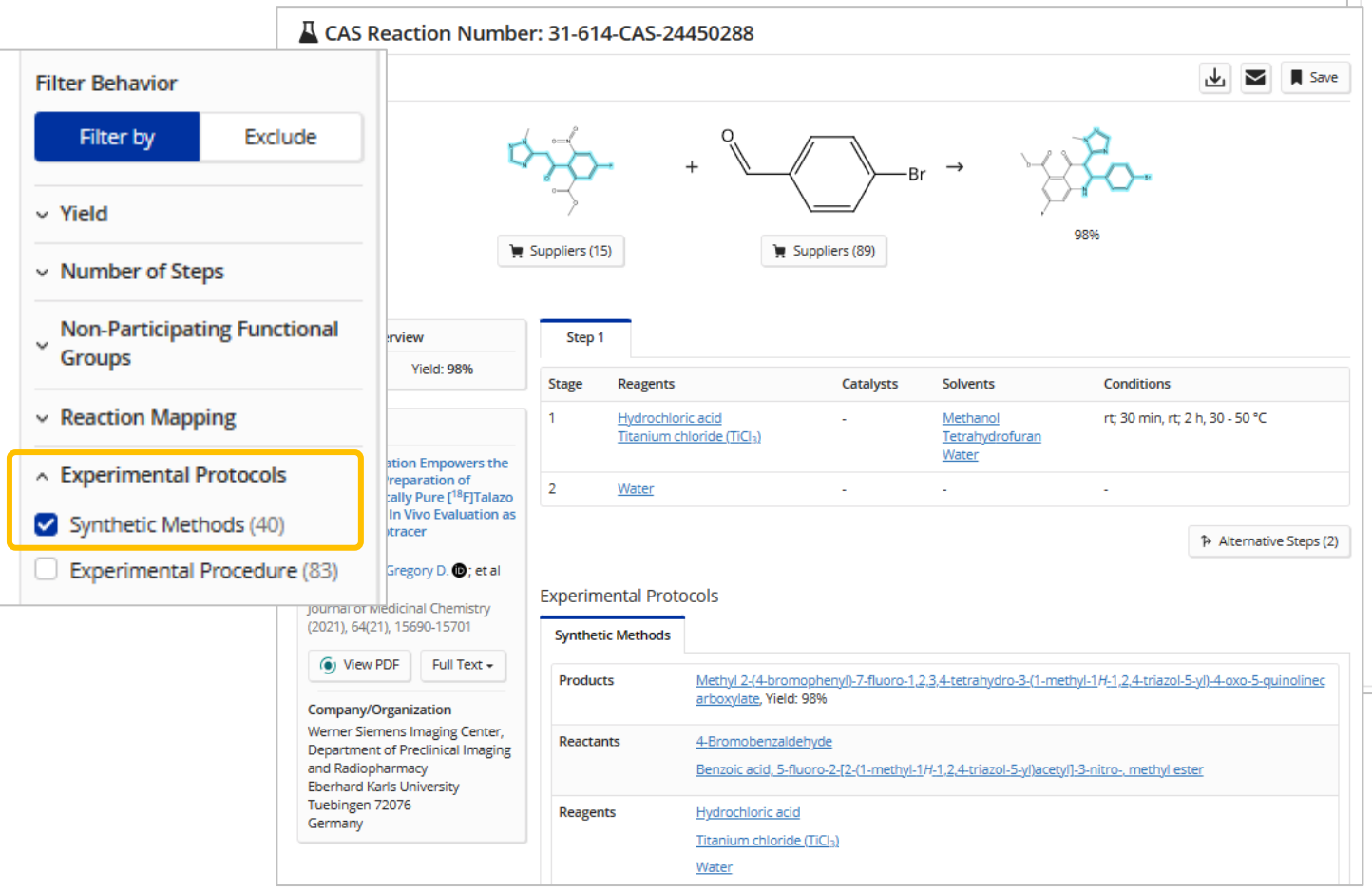
1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 关键词与反应式的联合检索
4. 获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

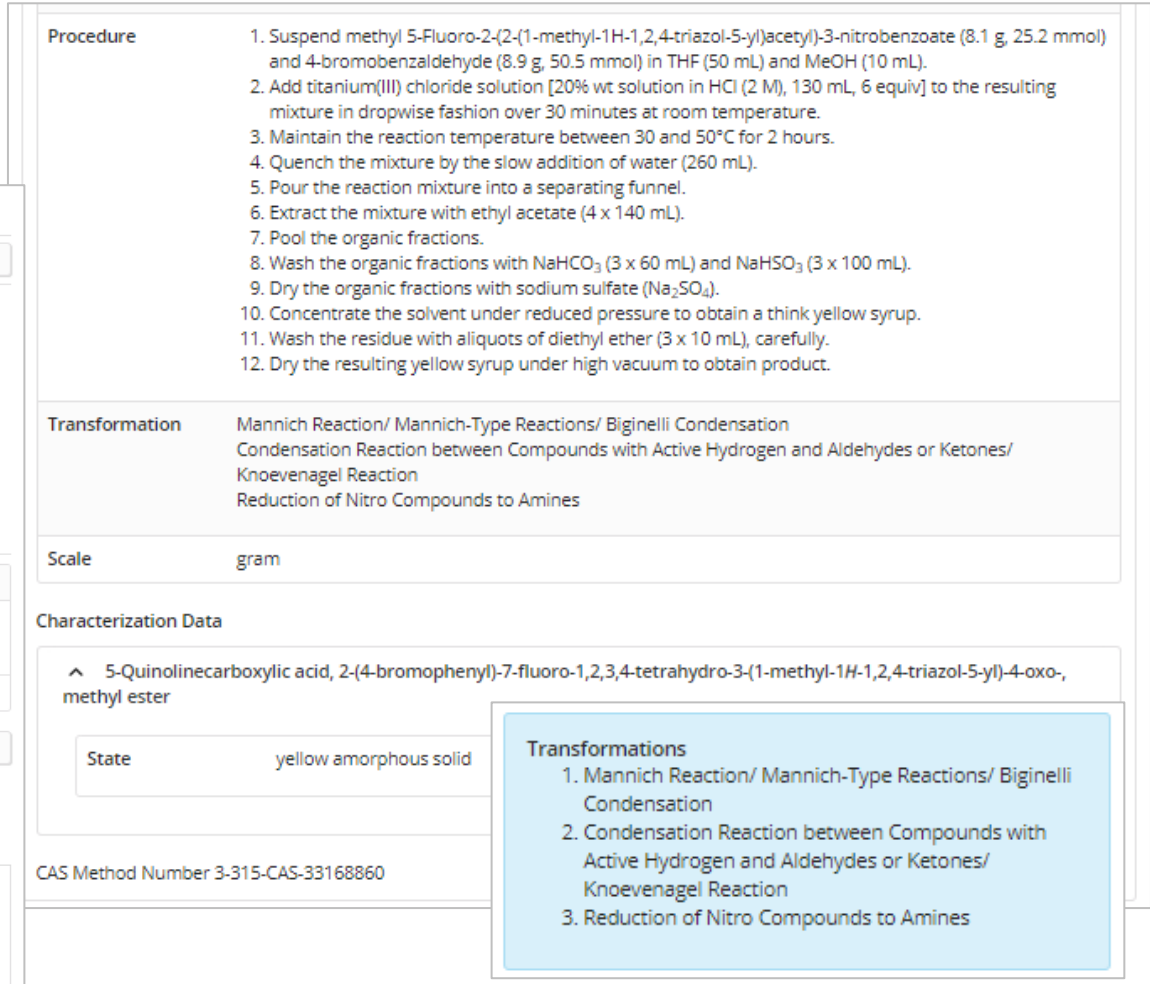
4. 具体的实验方案怎么查、怎么选?

- 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

CAS MN: 1-119-CAS-286328

Method Category: Element Detection
Technique: Electrothermal atomic absorption spectroscopy; Decomposition; Electrochemical extraction

Materials	Role	Image	CAS RN
Vanadium	analyte	View Structure	7440-62-2
Stainless steel	matrix		12597-68-1
Al_2O_3 cutting wheel	material		
SiC grinding paper	material		
0.05 µm pore size polycarbonate filter	material		
Standard calomel reference electrode	material		
Platinum ring counter electrode	material		
Hollow cathode lamps	material		
Electrodeless discharge lamp	material		
THGA graphite tubes	material		
Nitric acid	reagent	View Structure	7697-37-2
Hydrofluoric acid	reagent	View Structure	7664-39-3
Acetylacetone	reagent	View Structure	123-54-6
Chromium	reagent	View Structure	7440-47-3
Methanol	reagent	View Structure	67-56-1
Tetramethylammonium chloride	reagent	View Structure	75-57-0

实验原料

Source

Determination of alloying and impurity elements from matrix and inclusions from a process sample of a double stabilized stainless steel

Sipola, Teija; Alatarvas, Tuomas; Fabritius, Timo; Peramaki, Paavo

ISIJ International (2016), 56 (8), 1445 - 1451. Iron and Steel Institute of Japan

CODEN: IINTEY | ISSN: 09151559 | DOI: 10.2355/isijinternational.isijint-2016-071

Full Text | View in CAS SciFinder

Abstract

文献来源

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

分析仪器

Conditions

Instrument

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; injection volume: 10 µL

分析条件

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% acetylacetone

1. Perform electrolytic extraction on a BioLogic SP-150 potentiostat.
2. Use 10% acetylacetone (10 v/v% acetylacetone, 1 w/v% tetramethylammonium chloride and methanol) 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.

Decomposition of inclusions

1. Dry the polycarbonate filter containing the extracted inclusions overnight in a desiccator.
2. Place the dry filter in a PTFE container with 5 mL concentrated nitric acid and 2 mL HF and close gently.
3. Perform decomposition for 30 minutes at 120 °C (393.15 K).
4. Cool the containers to room temperature, remove the filter and dilute to the volume with water.
5. Prepare a blank sample similarly by filtering a fresh electrolyte through a polycarbonate filter.

Quantification of inclusions 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.

操作步骤

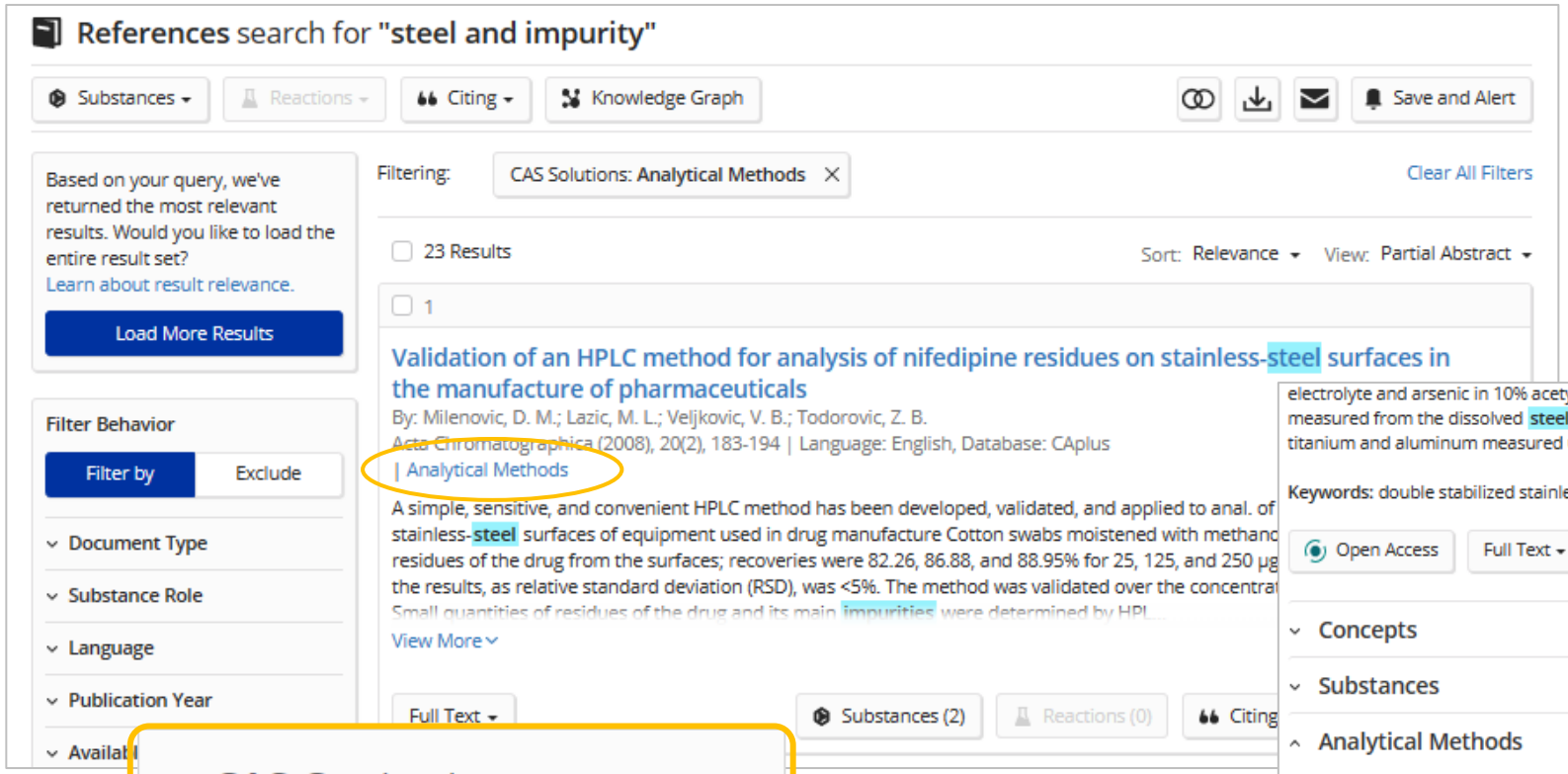
Validation

Linearity Range	0-400 µg/L
Concentration	< 1 µg

数据有效性

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



直接检索感兴趣的分析实验方法

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

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CAS Analytical Methods分析方法类别

目前涵盖13个大类，45个小类；某些子分类属于多种方法分类。

Agricultural Applications / Analysis: 除草剂分析…

Bioassays: 生物探针，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定…

Biomolecule Isolation:天然产物分离分析，蛋白质分析…

Environmental Analysis: 土壤/空气/水分析，农药残留分析…

Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析…

Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工…

Historical Analysis / Dating: 考古分析，同位素分析

Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析…

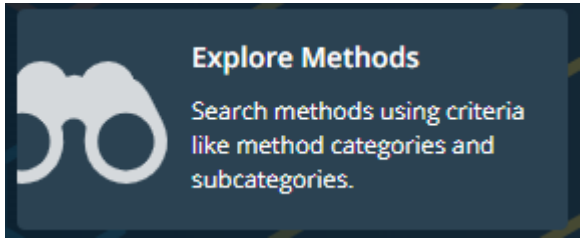
Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…

Organometallics / Inorganics: 地质分析，无机物分析，金属有机化合物分析

Pharmacology / Toxicology: 活性药物成分及代谢物，成瘾药物检测，有毒物检测…

Polymer: 塑料加工

Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析…



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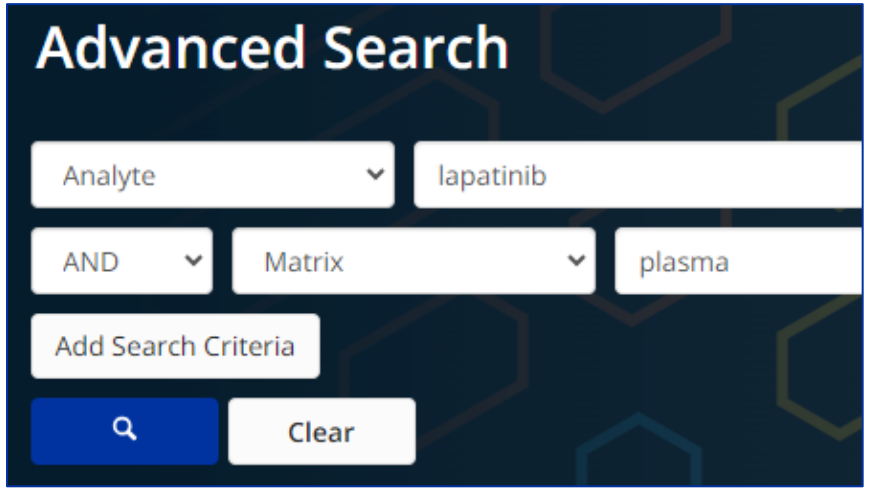
关键词检索分析方法

- **直接检索示例：**
  lapatinib 拉帕替尼

- **高级检索示例：**
  分析拉帕替尼血药浓度的方法



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检索结果分析与精炼

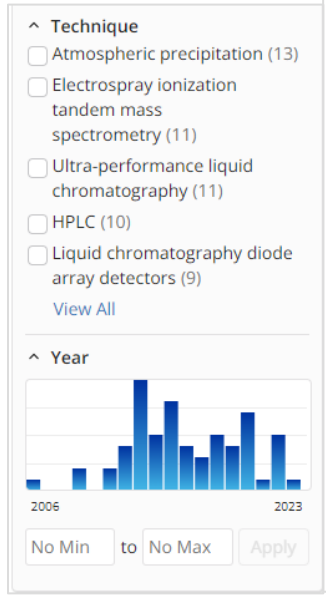
分析物

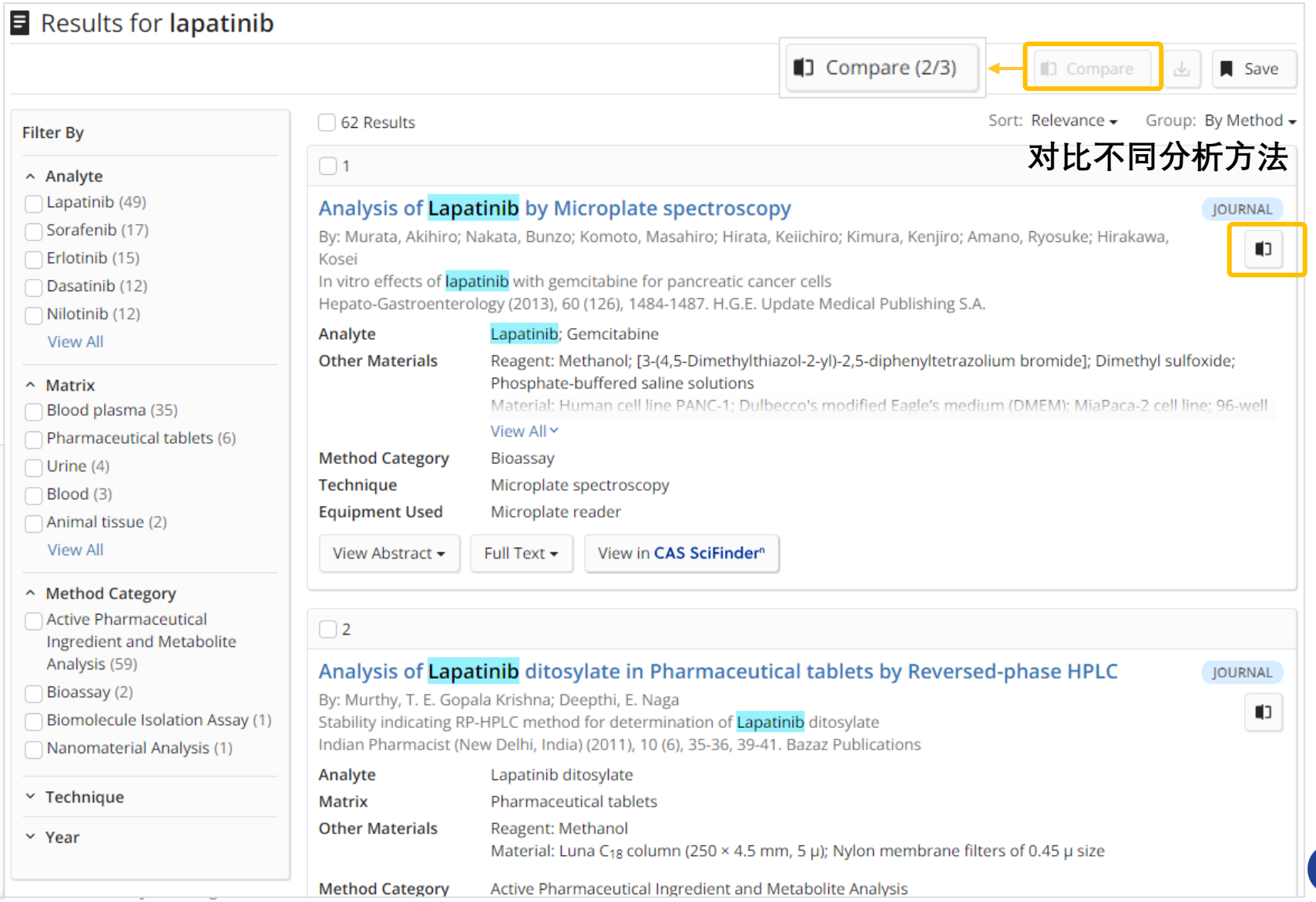
基质

方法分类

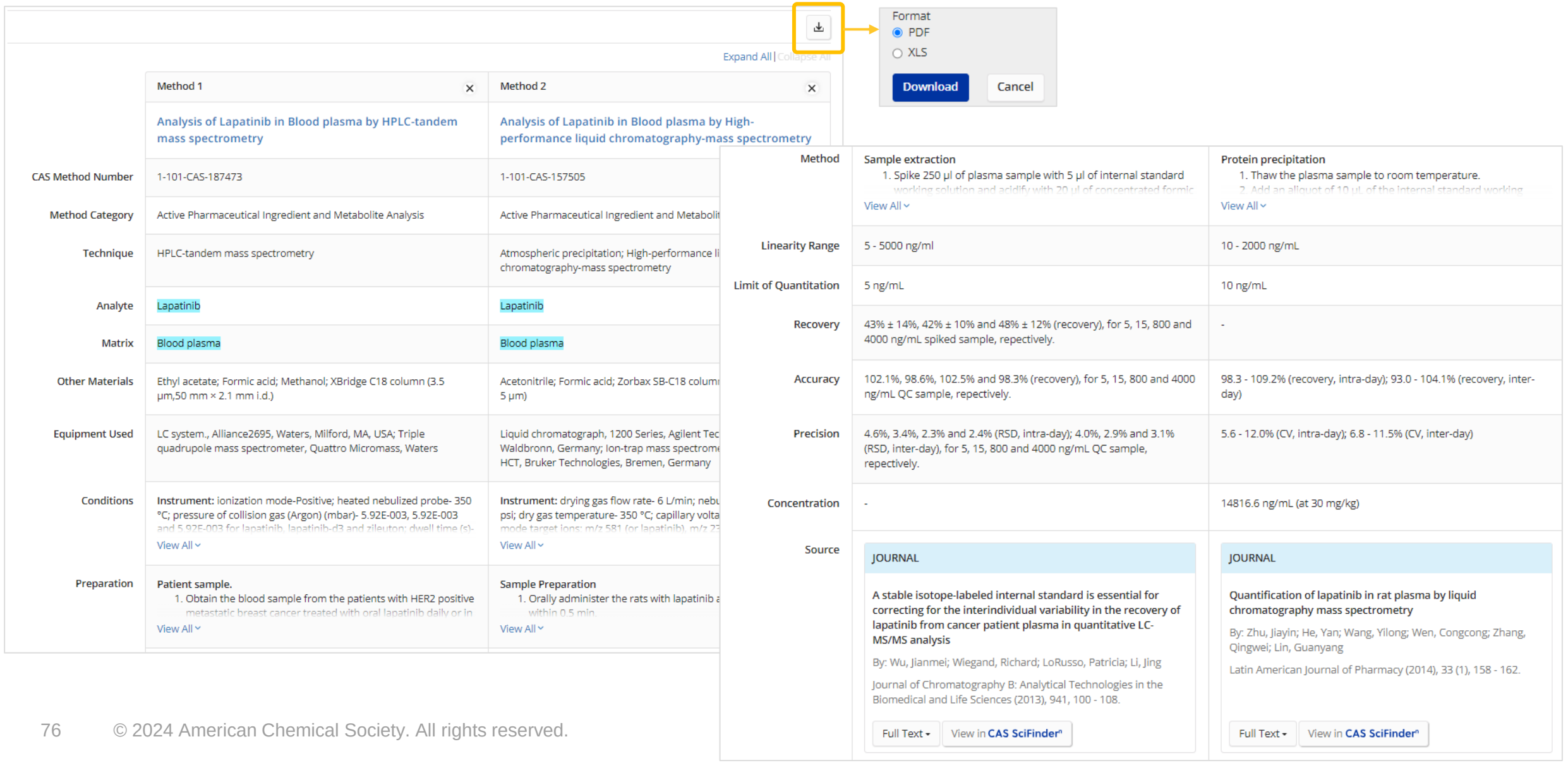
技术&仪器

年份



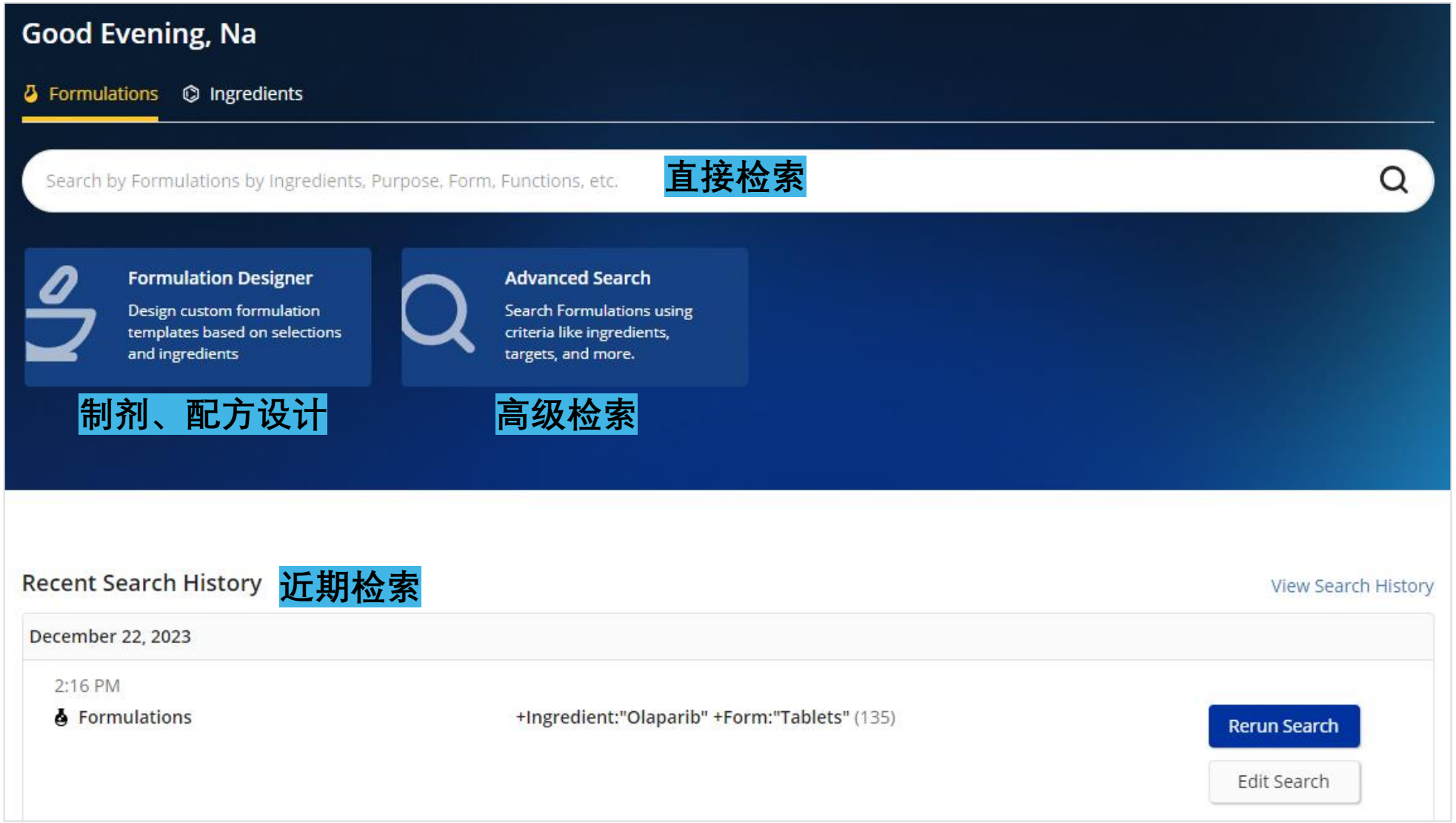


对照多个感兴趣的分析方法详情



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）进行直接检索或高级检索



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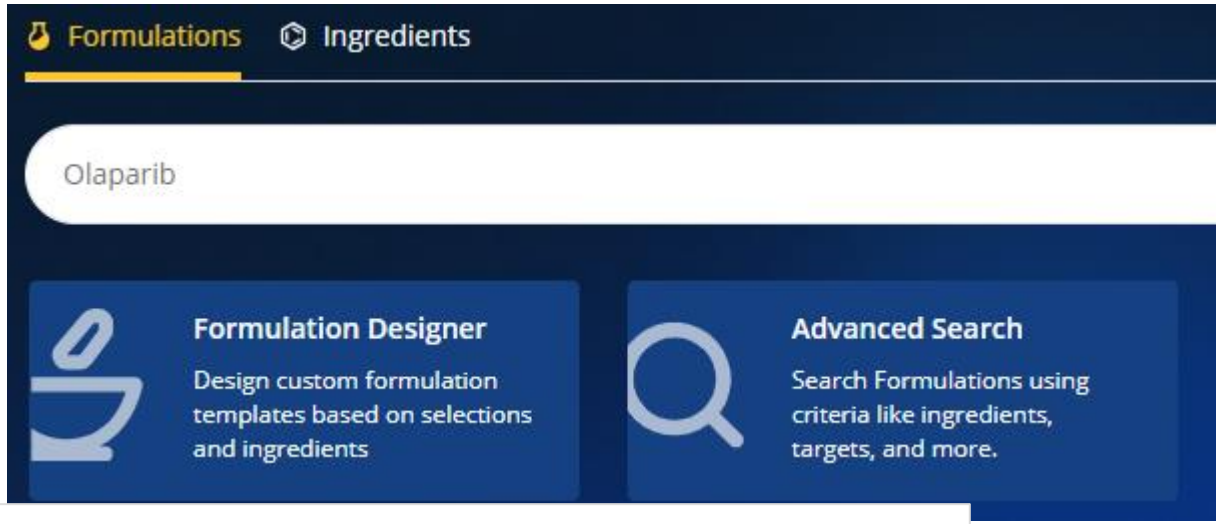
关键词检索制剂/配方

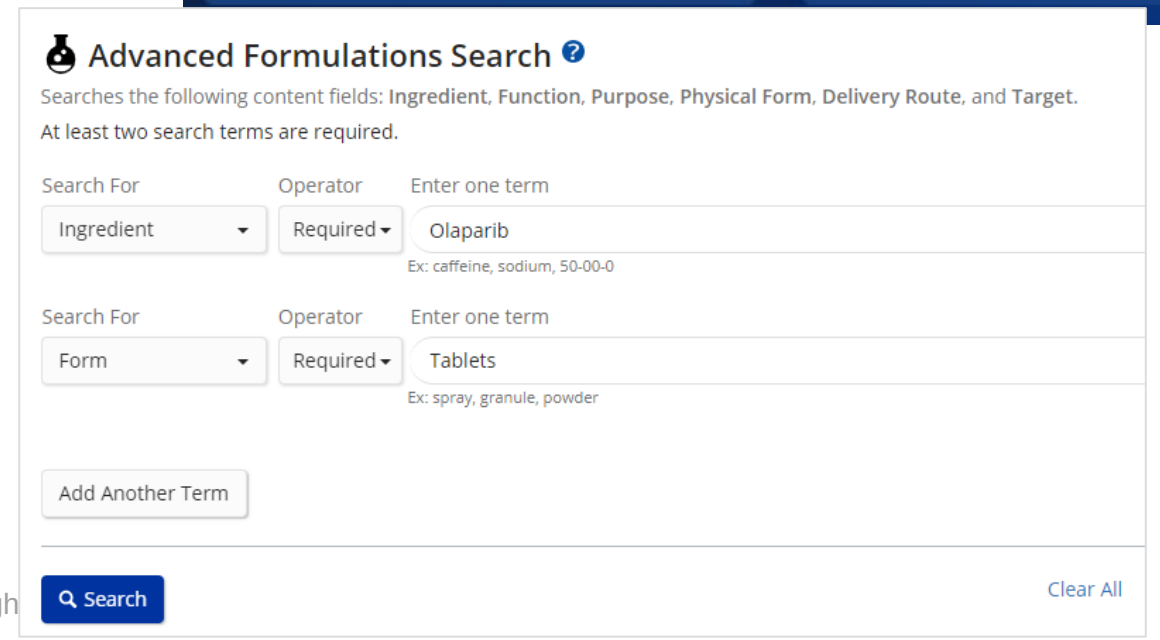
- 直接检索示例：

  Olaparib 奥拉帕尼



- 高级检索示例：

  奥拉帕尼片剂



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检索结果分析与精炼

应用领域

目的/用途

物理形态

物质状态

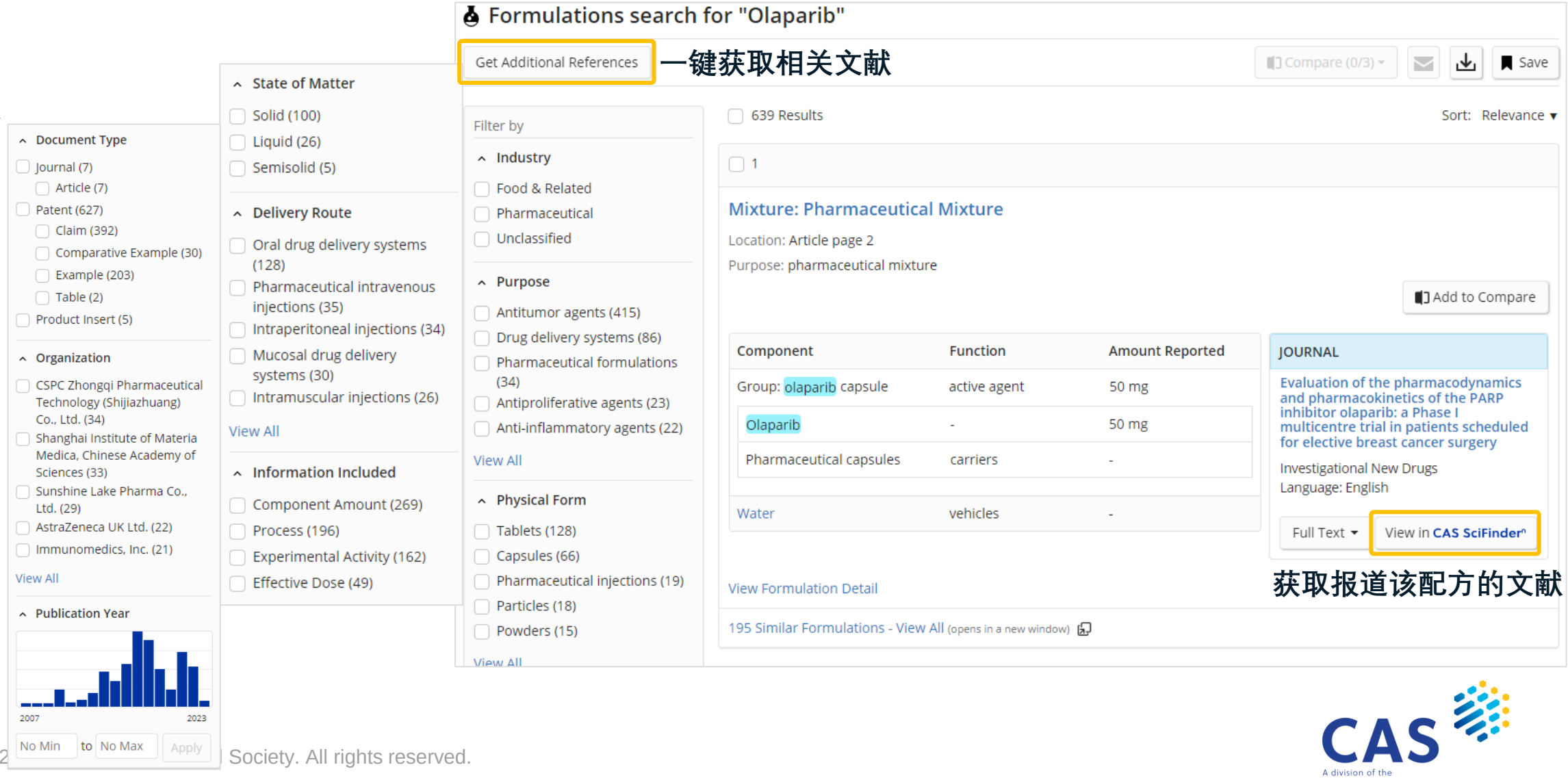
作用方式

制剂信息

文献类型

机构名

发表年份



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制剂、配方详情

Olaparib Solid Dispersion: Antitumor Agents

Save

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents	Homo sapiens, Ovary neoplasm	-	Capsules, Particles, Pharmaceutical solid dispersions, Powders	View

Predicted value

Formulation Ingredients

制剂成分、功能、用量

Component	Function	Amount Reported	Optionality
Olaparib	poly(ADP-ribose) polymerase inhibitor	200 g	Mandatory
Vinyl acetate-vinylpyrrolidone copolymer	carrier, polymeric stabilizer	800 g	Mandatory

More Formulations like this...

Lincomycin Solid Dispersion: Veterinary Drug
Purpose: Veterinary drugs
Target: Homo sapiens, Livestock, Poultry
Delivery Route: -
Physical Form: Pharmaceutical solid di...

Olaparib Dispersible Tablets: Antitumor Agents
Purpose: Antitumor agents
Target: Homo sapiens, Mammary glan...
Delivery Route: Oral drug delivery syst...
Physical Form: Pharmaceutical orally d...

Olaparib Dispersible Tablets: Antitumor Agents
Purpose: Antitumor agents
Target: Homo sapiens, Mammary glan...
Delivery Route: Oral drug delivery syst...
Physical Form: Pharmaceutical orally d...

Lincomycin Solid Dispersion: Veterinary Drug
Purpose: Veterinary drugs
Target: Homo sapiens, Livestock, Poultry
Delivery Route: -
Physical Form: Pharmaceutical solid di...

Process

工艺信息

preparation of olaparib solid dispersions and capsules. olaparib (50 g) and copolyvidone VA64 (950 g) were passed through a 60 mesh sieve, and the sieved olaparib and copolyvidone VA64 were uniformly mixed to obtain a raw material mixture (1000 g). the extrusion temperature of the twin-screw extruder was set to 150 °C. after the temperature was reached, the raw material mixture was added to the extruder, melted, extruded, and finally extruded in a strip shape to obtain a strip shape. extrudate (960 g). the above strip-like extrudate was cooled to room temperature, pulverized and passed through a 20 mesh sieve to obtain a granulated olaparib solid dispersion (960 g). the above granulated olaparib solid dispersion was placed in a hard capsule shell according to the loading amount of 50 mg of the solid dispersion per granule to obtain a corresponding capsule.

Source Patent

Olaparib solid dispersion and preparation method thereof
Assignee : Farmasino Pharmaceuticals (Jiangsu) Co., Ltd.
CN106692066
Language: Chinese
Location: Example 4

Patent PDF | View in CAS SciFinder

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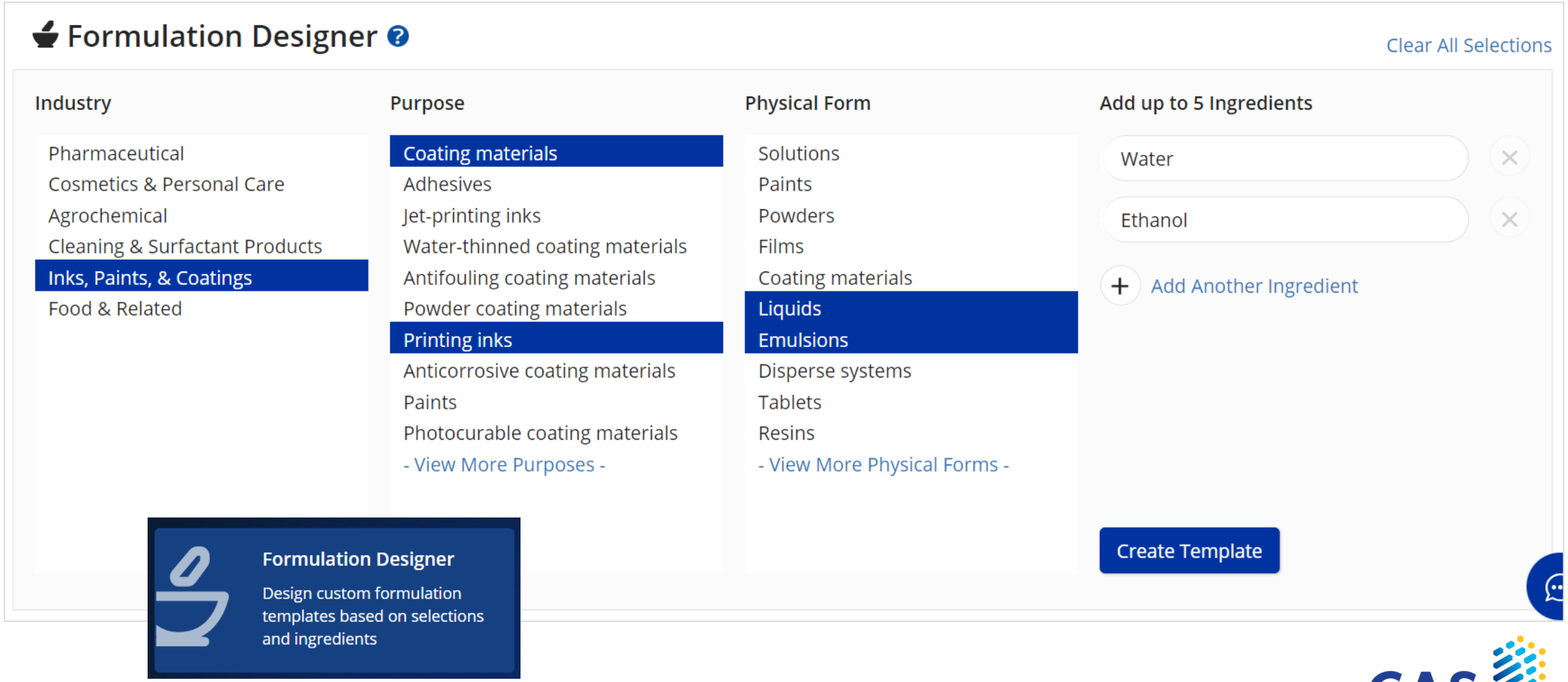
检索原料

- 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

设计配方/制剂



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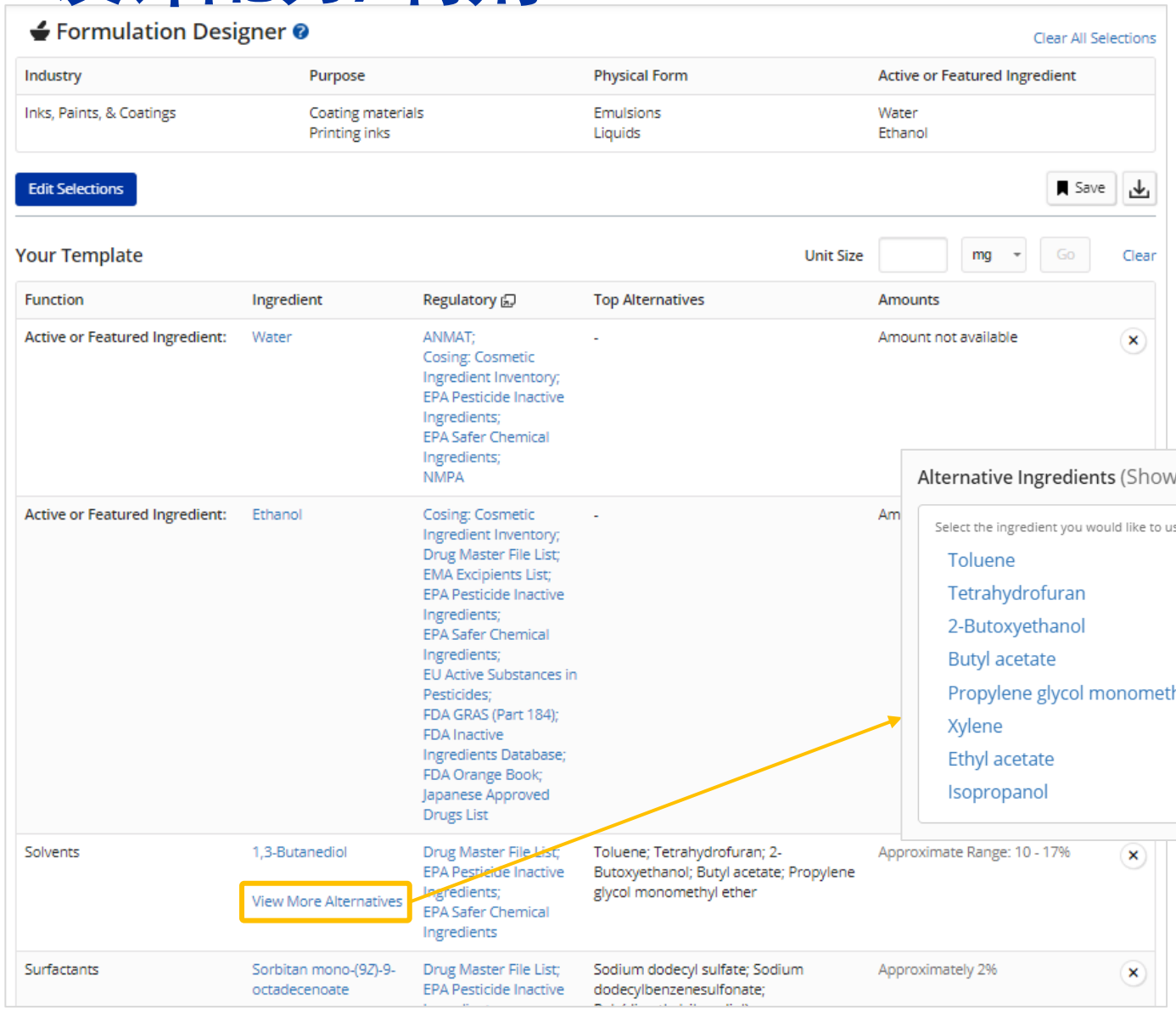
设计配方/制剂



- 原料详情
- 原料管制信息
- 可替代的原料选项

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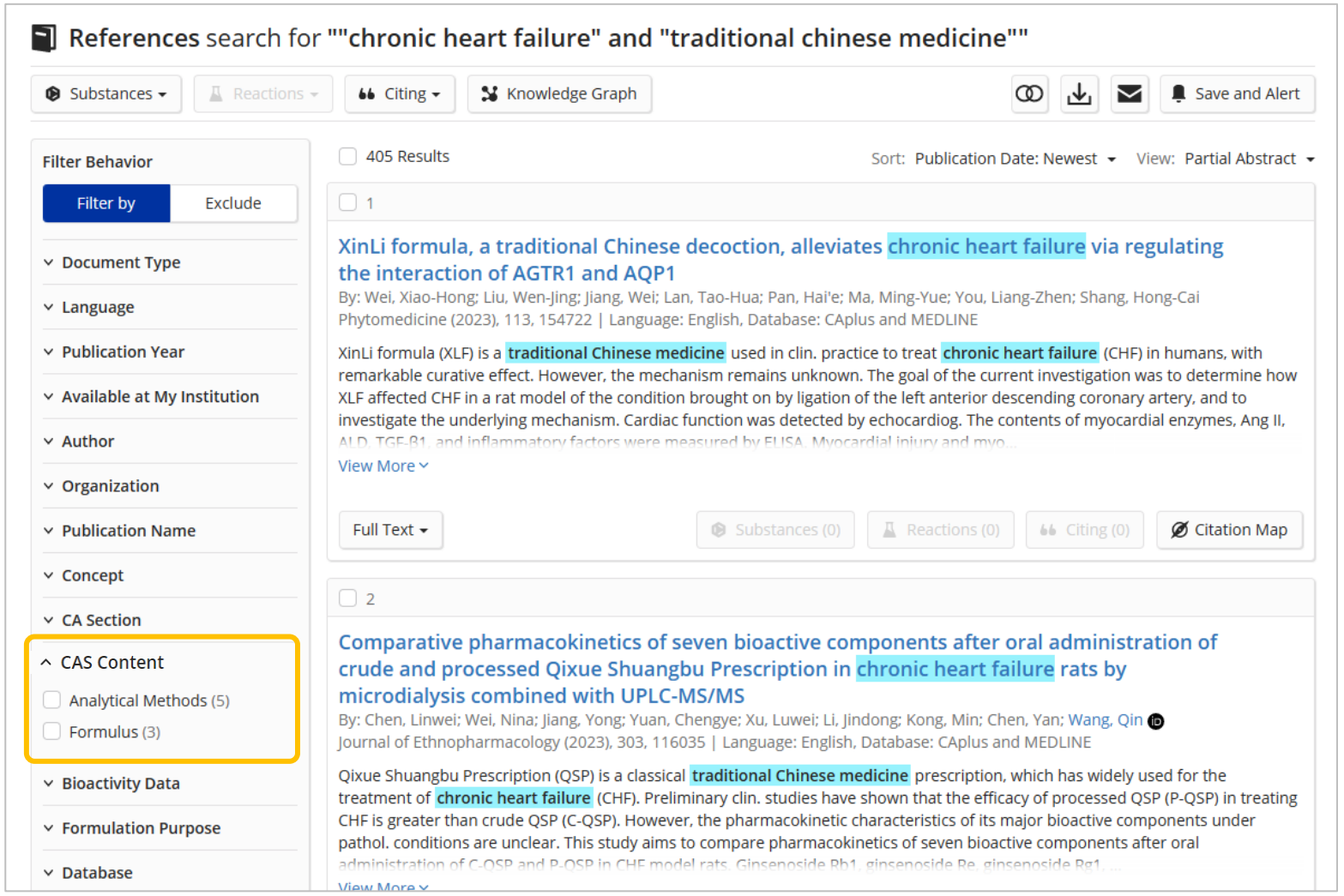
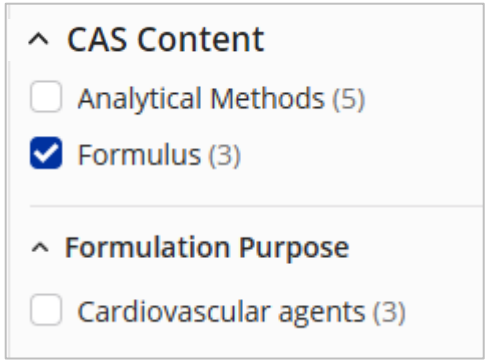
文献关联的配方/制剂

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

Application of a traditional Chinese medicine composition for preparing medicines for preve and/or treating myocardial hypertrophy

0 0 0 Citation Map

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder^n users. View content from CAS F this document. Learn more about Formulus®.

In this Reference

- IPC Data
- CAS Concepts
- Formulations

By: Zhang, Minyu; Guo, Feifei; Wu, Hongwei; Yang, Hongjun; Wei, Junying; Wu, Sha

The invention relates to the field of medicines, in particular to an application of a traditional Chinese medicine com preparation of a medicine for preventing and/or treating myocardial hypertrophy and an application to preparation preventing pressure-loaded chronic heart failure, and expands new indications of Yixinshu capsules. Curative effect mechanism for myocardial hypertrophy resistance are studied. A new thought and a new choice are provided for trea hypertrophy and malignant heart diseases caused by further development of myocardial hypertrophy.

Keywords: myocardial hypertrophy prevention traditional Chinese medicine composition

PatentPak PDF | Get Prior Art Analysis | Full Text

Publication Information • Patent

Patent Number	Publication Date	Application Number	Application Date	Kind Code
CN112190652	2021-01-08	CN2020-11207191	2020-11-03	A

Assignee	Source	Database Information	Language
Capital Medical University, China	China CODEN: CNXXEV	AN: 2021:56481 CAN: 176:120018 CAplus	Chinese

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Appli
CN112190652	Chinese	A	PDF	2021-01-08	CN2020-11207191	2020-11-03

Formulations

Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents

View CAS Formulus® Detail

Location: Claim 1, 2, 3, 4, 5, 6, 7, 8, 9
Purpose: Cardiovascular agents
Target: myocardial hypertrophy, human

Component 成分	Function 功能	Amount Reported 用量
Panax ginseng	-	175-225 wt. parts
Ophiopogon japonicus	-	175-225 wt. parts
Schisandra chinensis	-	100-150 wt. parts
Astragalus membranaceus	-	175-225 wt. parts

Additional Components Reported in Full Text

Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents

View CAS Formulus® Detail

Location: Example
Purpose: Cardiovascular agents
Target: myocardial hypertrophy, human

Component	Function	Amount Reported
Panax ginseng	-	200 wt. parts

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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**

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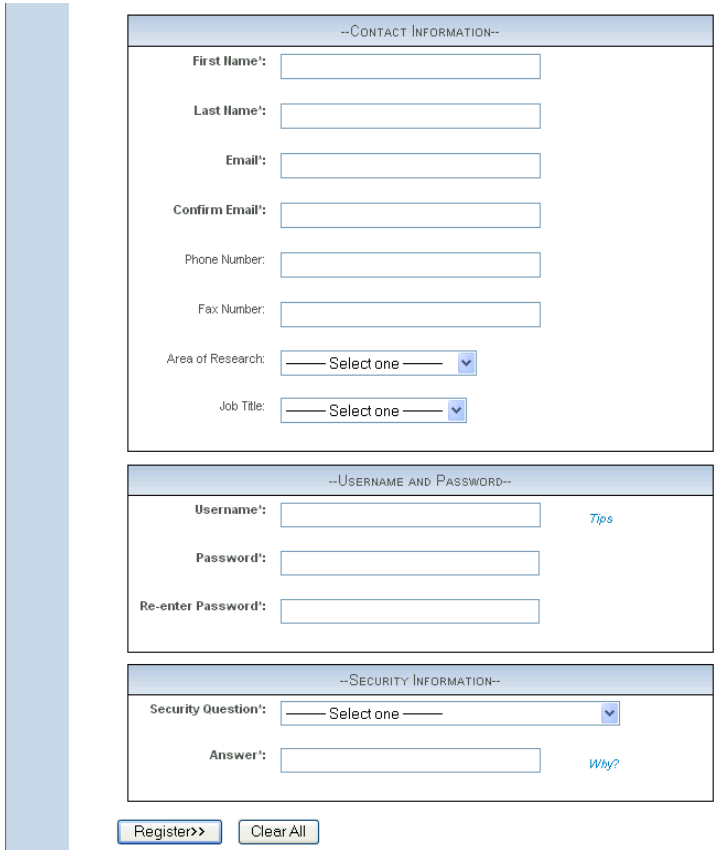
（登录图书馆网站，查看注册相关的链接和说明）



请注意：

1.必须输入真实姓名和学校邮箱。

2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- -（破折号）
- _（下划线）
- .(句点)
- @（表示“at”的符号）

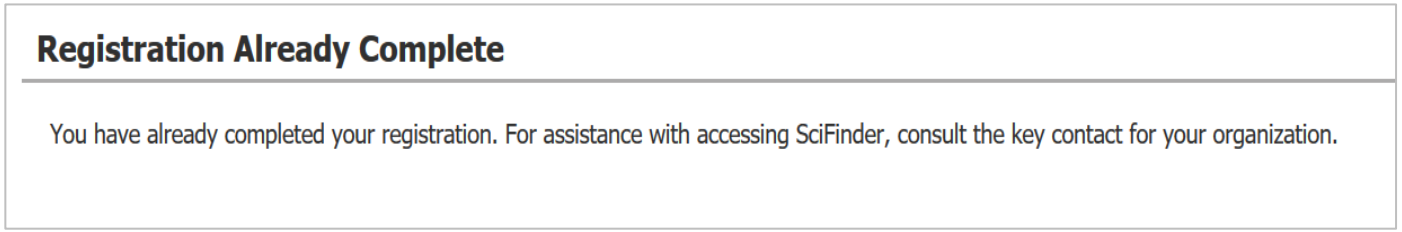
3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

例：abc@123

4.从下拉列表中选择一个密码提示问题并给出答案。

单击 Register（注册）。



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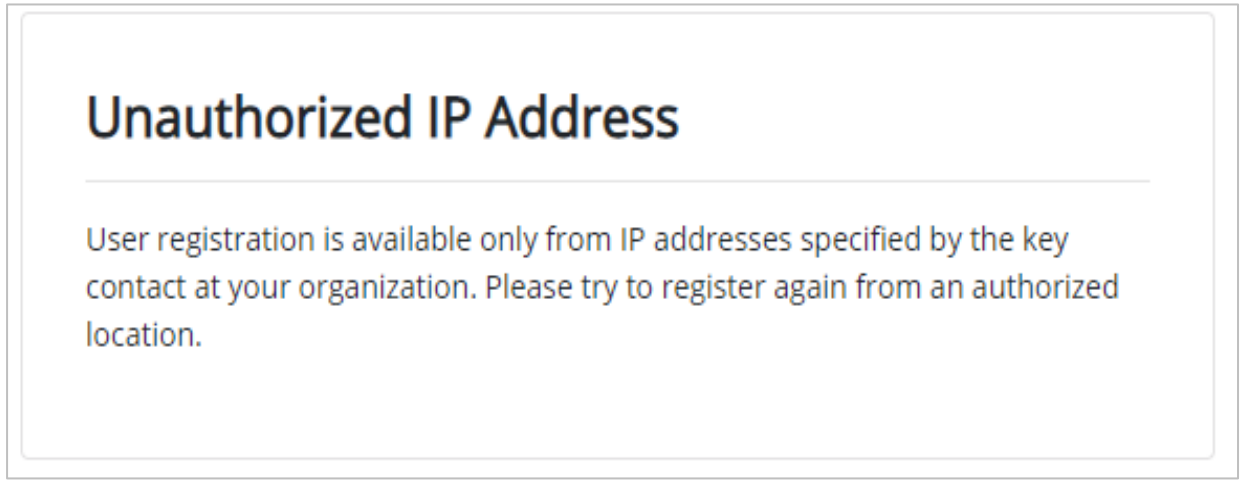
常见注册问题



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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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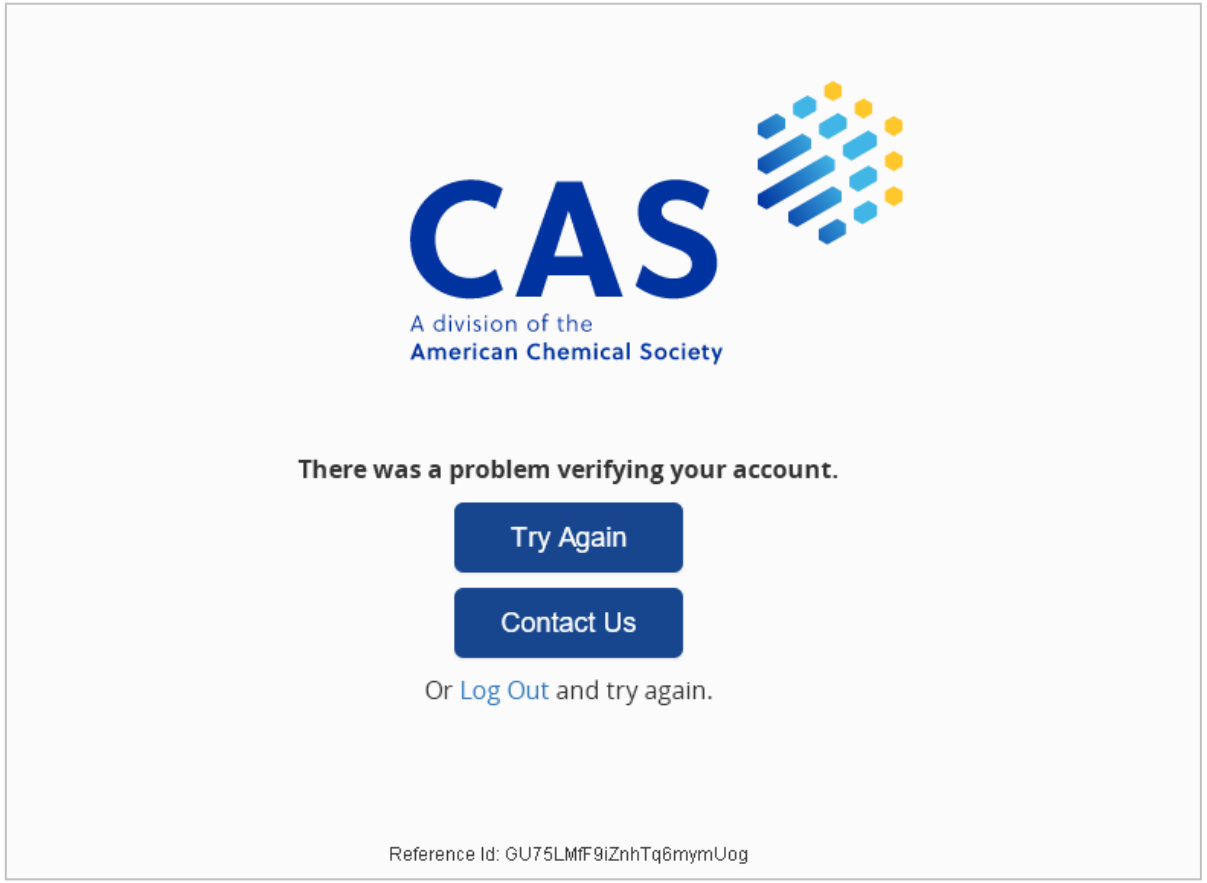

- 确认账号密码是否正确
- 如果账号密码正确，请填写问题报告后联系图书馆或china@acs-i.org

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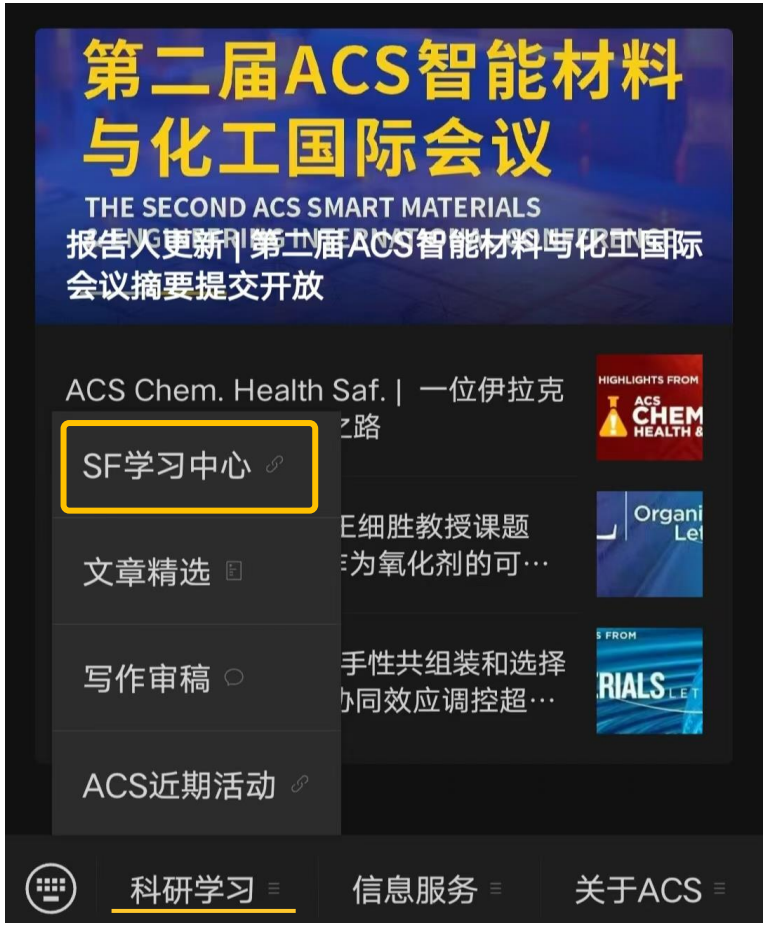

历史文章：按标签分类的检索技巧及案例等

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结合CAS信息科学家精心撰写的相关洞察报告，了解不同领域的研究进展、趋势与创新、挑战与机会，同时进行安全的专利布局和侵权风险管理，助力自信应对立项布局、研发流程和专利调研相关的信息挑战。

9月26日 | 药物立项调研策略

11月14日 | 电池及电化学能源材料

10月24日 | 聚合物的研发与应用

12月19日 | 专利查新与规避专利侵权风险

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一等奖：1名
Macbook Air®

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三等奖：10名
索尼耳机
WH-CH720N

入围奖：30名
JBL音箱

扫码参赛：

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*需要完成第一阶段且成绩不低于85分

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