CAS SciFinder$^{n}$ 论坛

# 物质信息的获取

钱欣博士
2022年3月8日



ACS International | CAS A division of the American Chemical Society

# 提纲

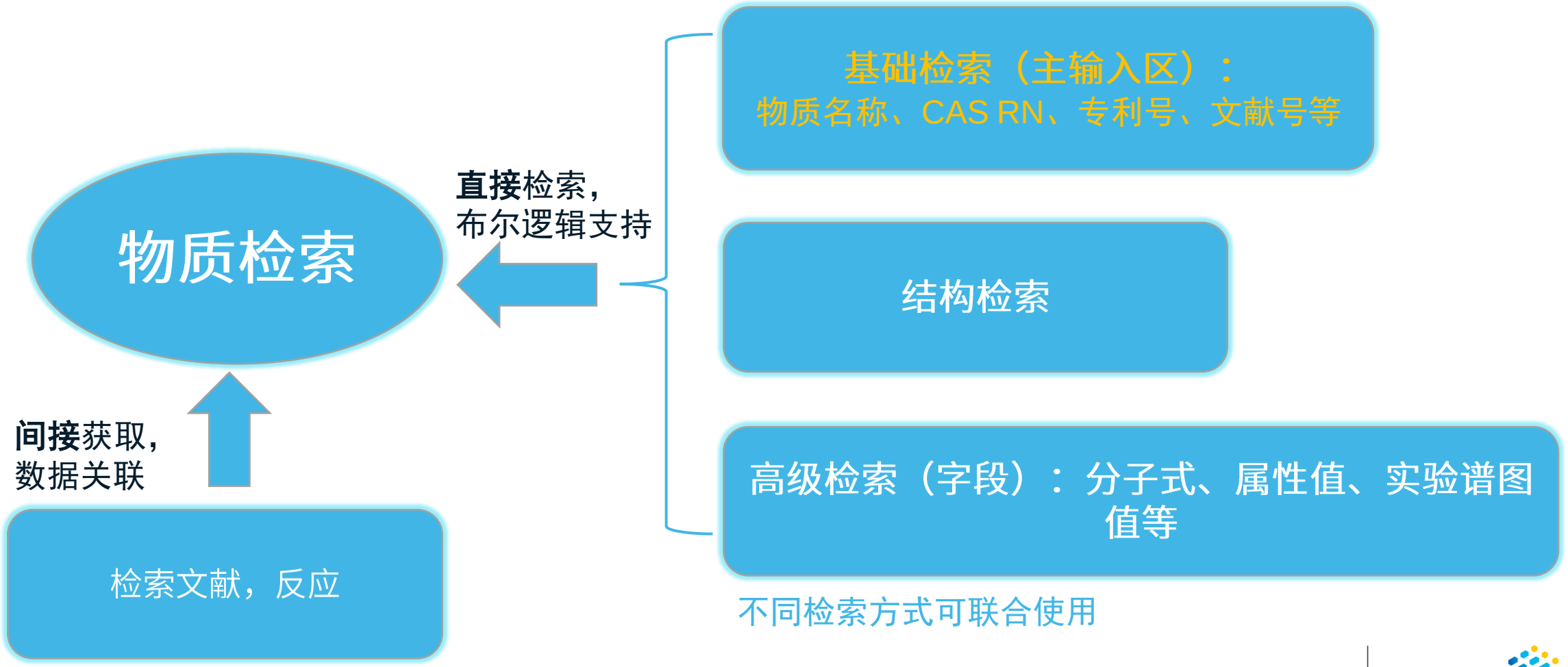
- CAS和CAS SciFinder$^n$简介
- CAS SciFinder$^n$ 物质检索方式
- 物质属性或谱图查询
- 在线演示以及Q&A

# CAS SciFinder$^{n}$中覆盖的内容合集


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

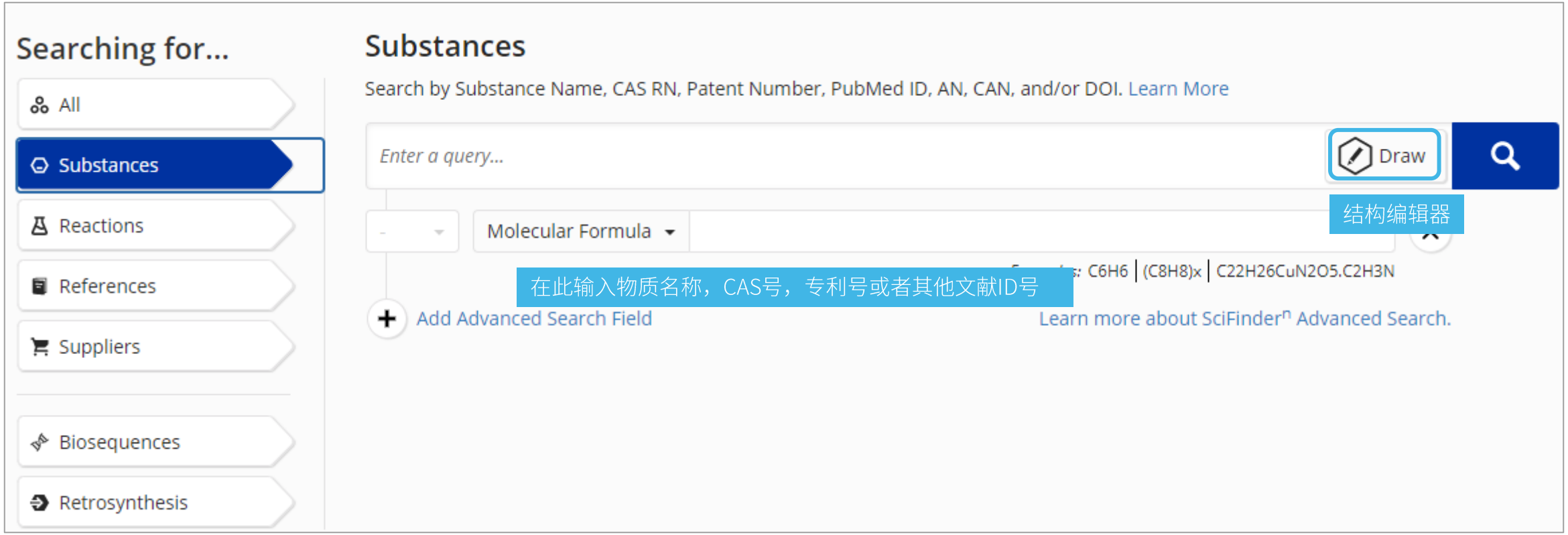
ACS International | CAS A division of the American Chemical Society

# 物质检索方法

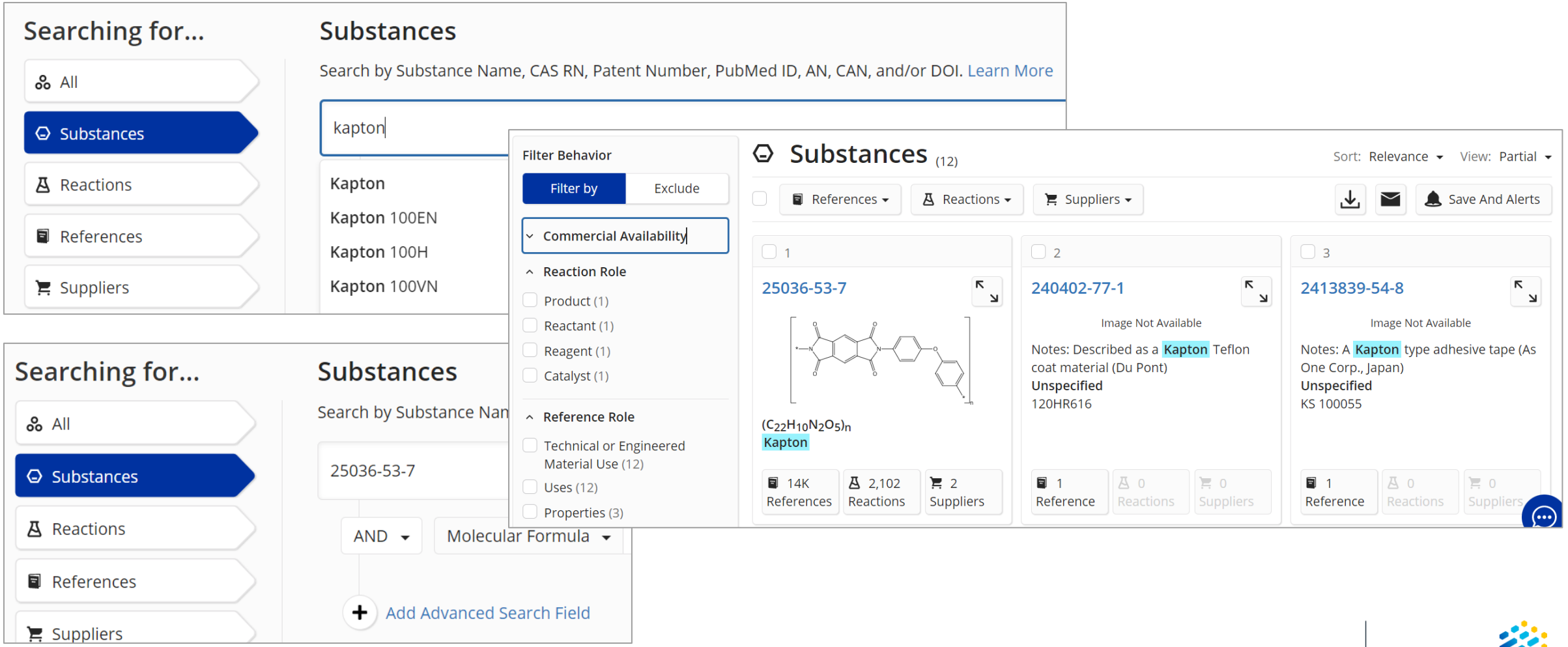



不同检索方式可联合使用

# 丰富的物质检索方式



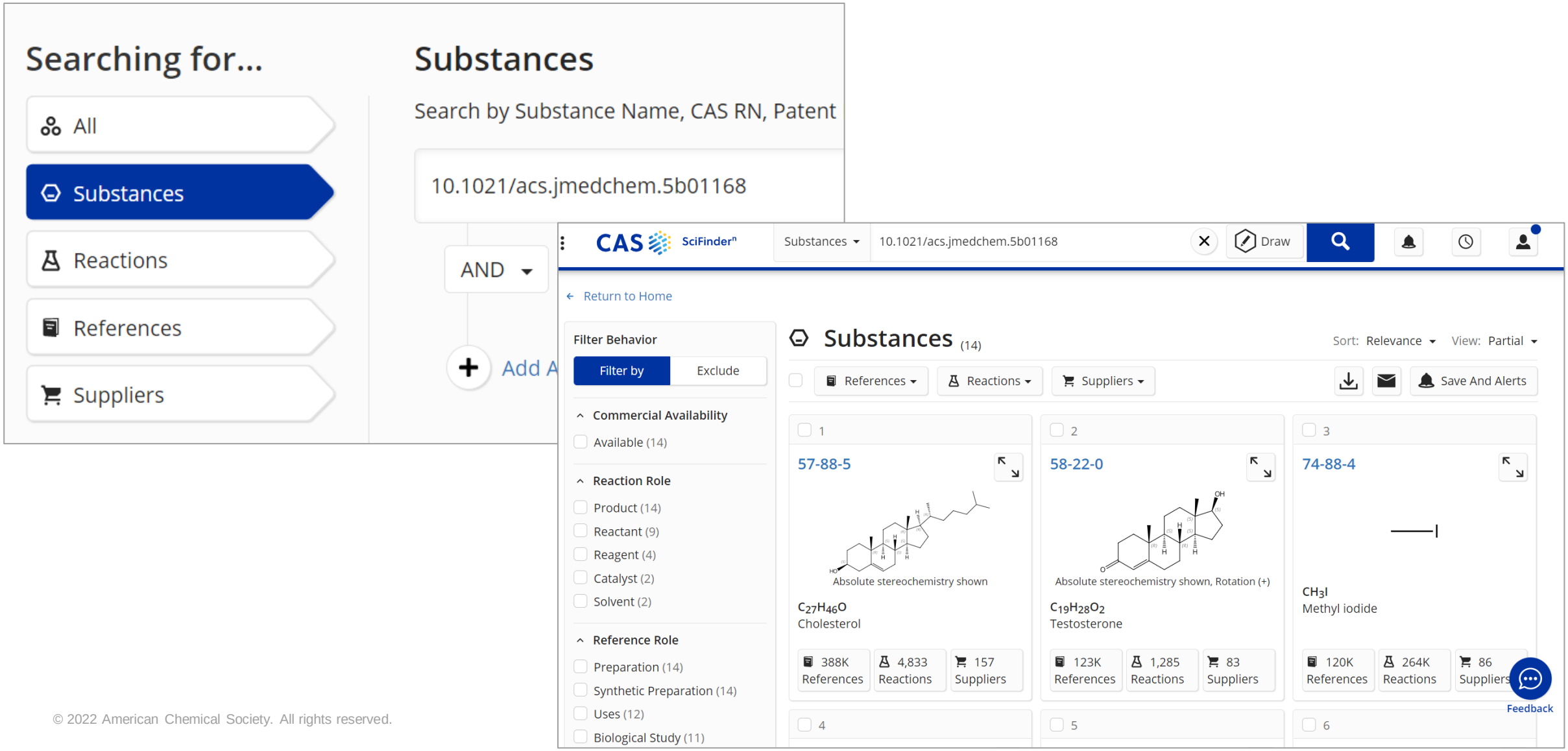
# 物质名称、CAS号检索



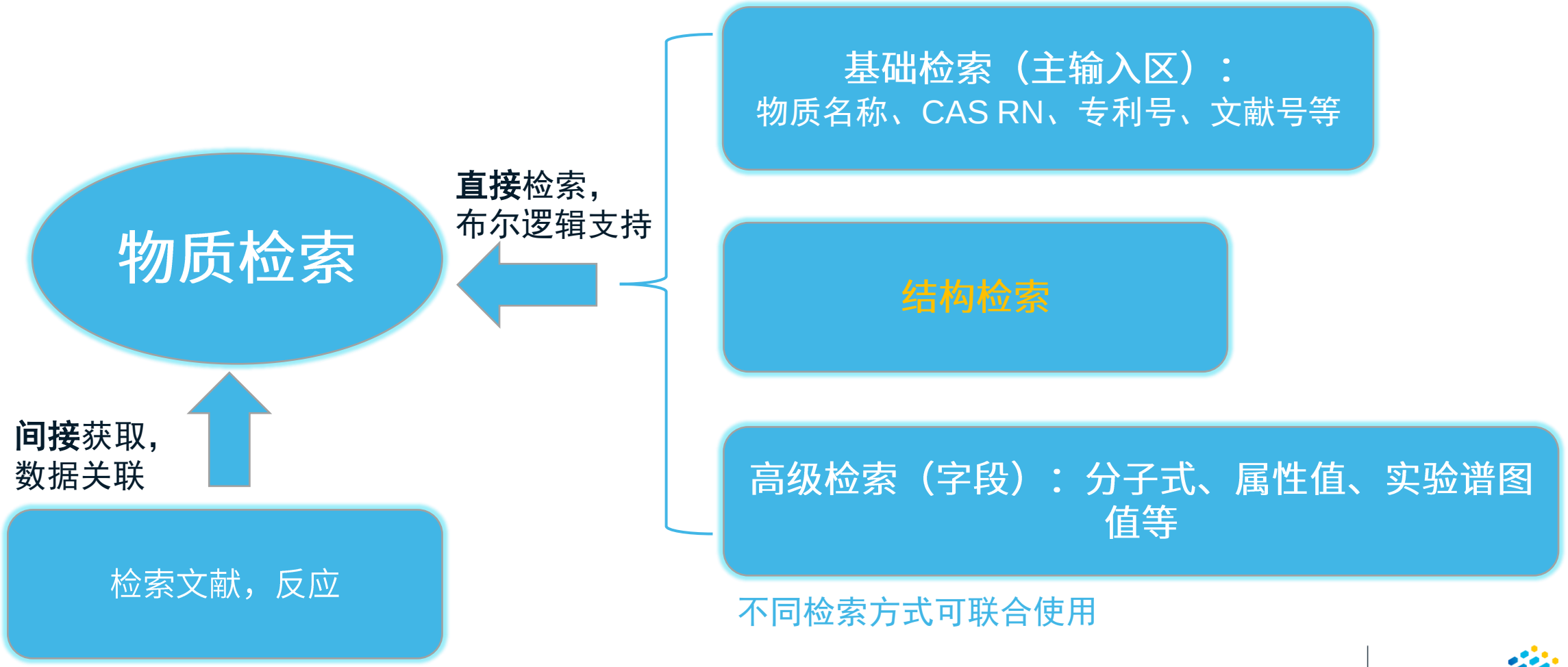

ACS International

CAS
A division of the American Chemical Society

# 由文献号或者专利号获取



# 物质检索方法




不同检索方式可联合使用

# 结构绘制面板的介绍

重要绘制工具注释

选择可变基团

自定义R基团

重复工具

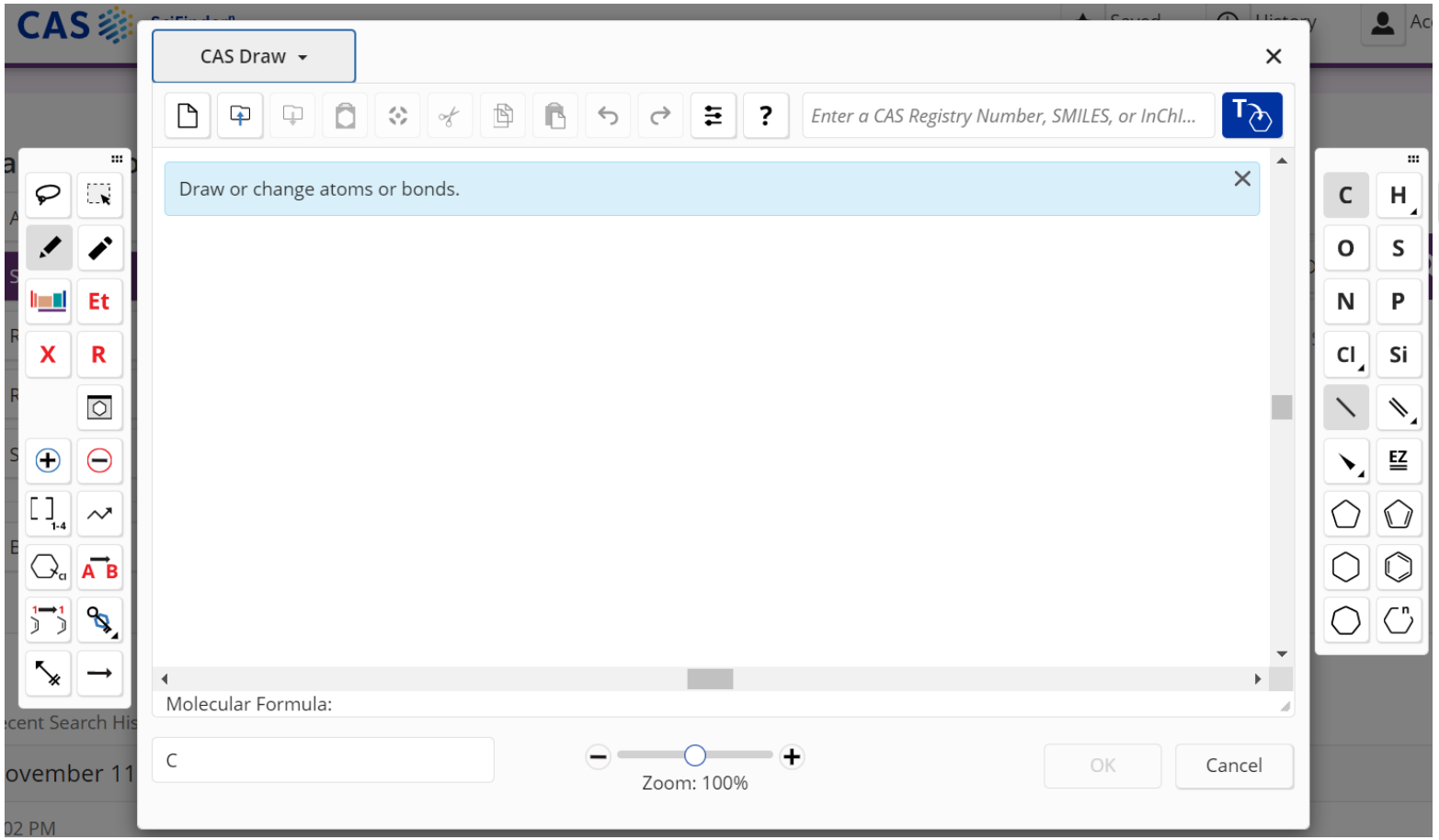
取代位置可变

锁定工具

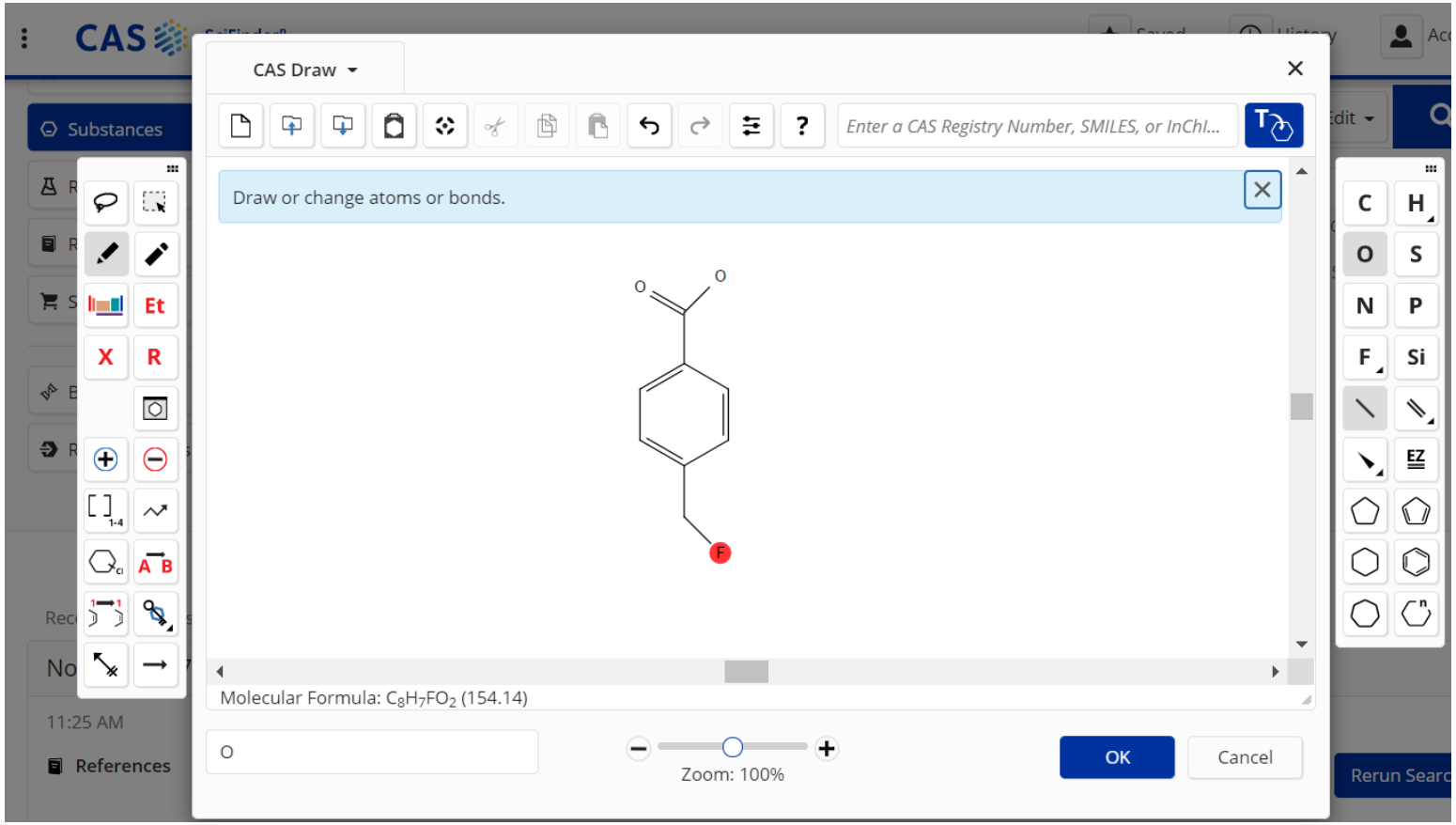
反应角色标记

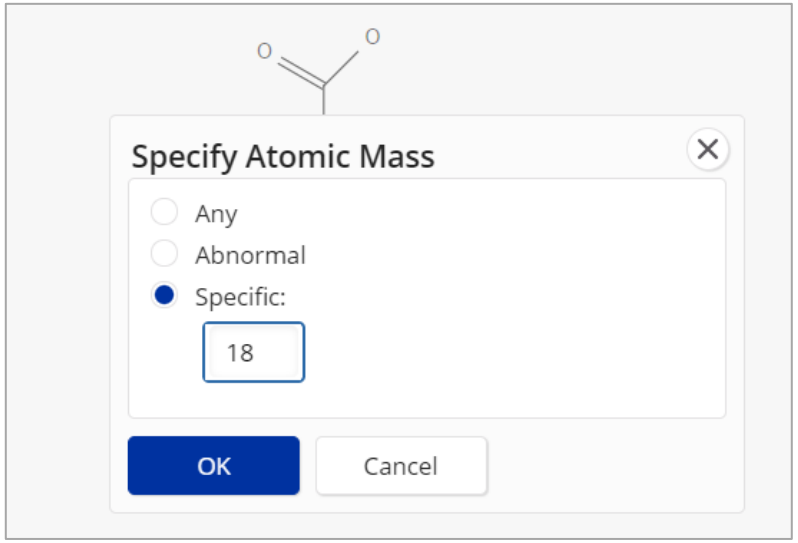
原子标记

化学键标记



# 结构绘图工具的使用：同位素原子的绘制




鼠标右键点击某原子，选中Abnormal获取其各种同位素的化合物，选择Specific可以精准输入具体的同位素质量数

# ChemDraw与SciFinder$^n$联用检索的方法

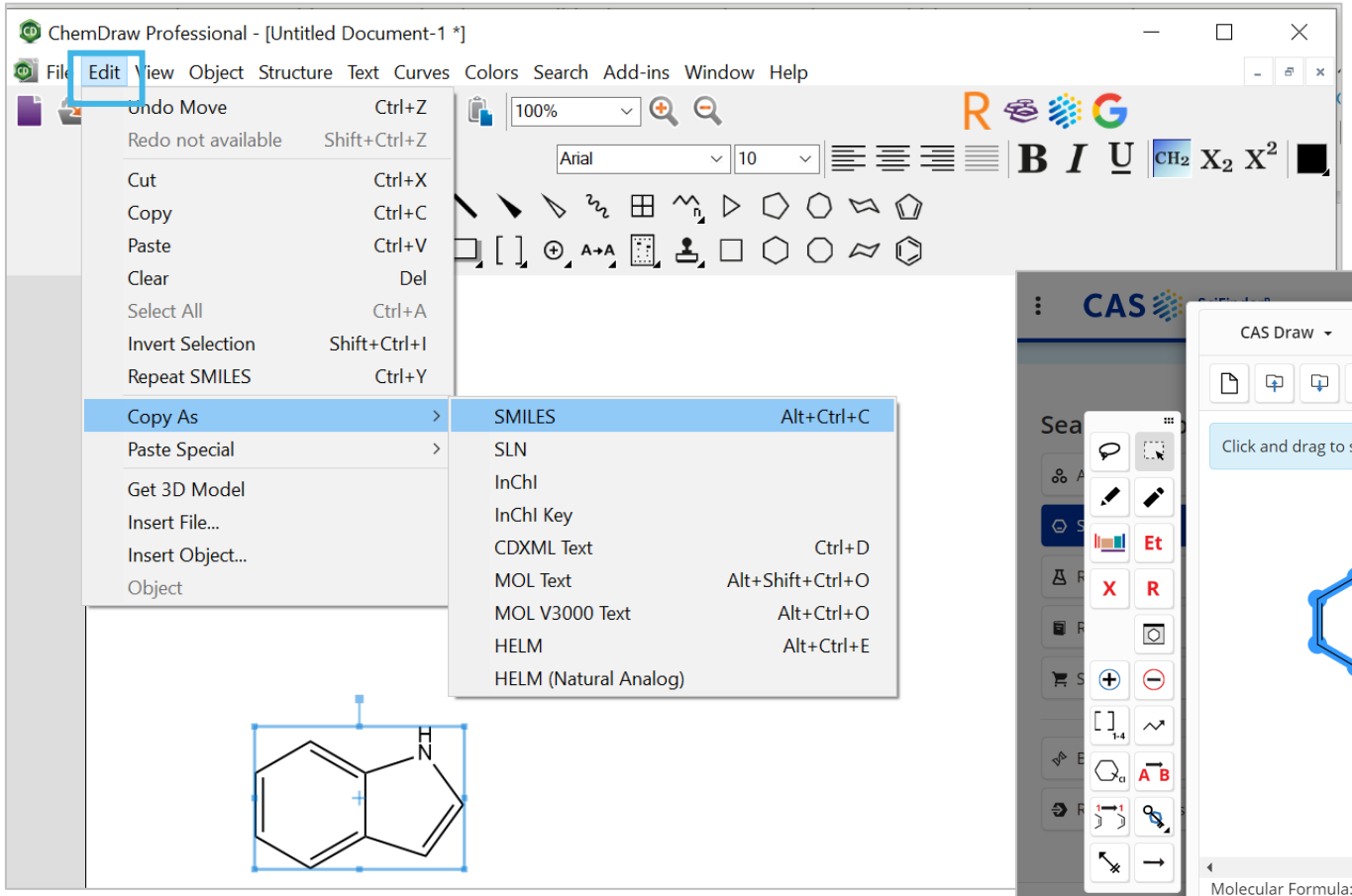
(1) 通过SMILES或InChI字符串切换

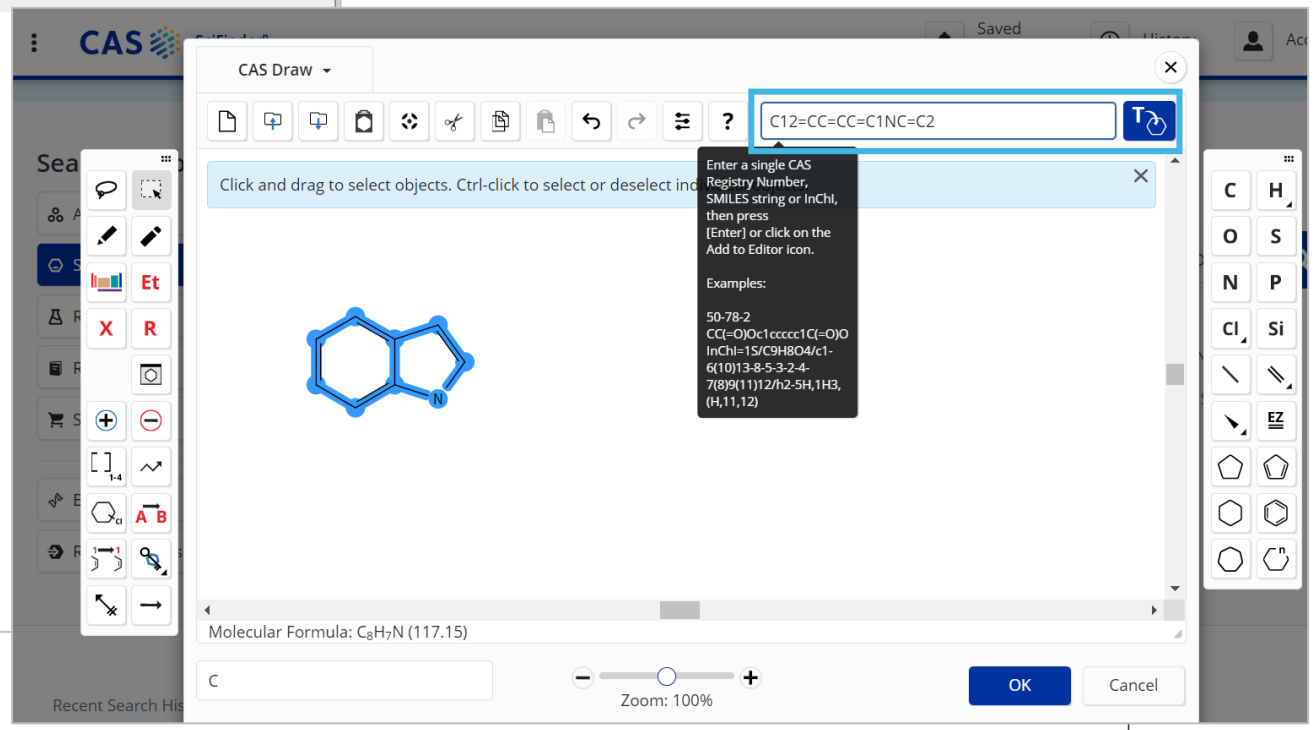
(2) 直接在ChemDraw中Add-in SciFinder$^n$（ChemDraw 18.2及以上版）

(3) 通过MDL Molfile (.mol)文件导入

# (1)通过SMILES或InChI字符串切换

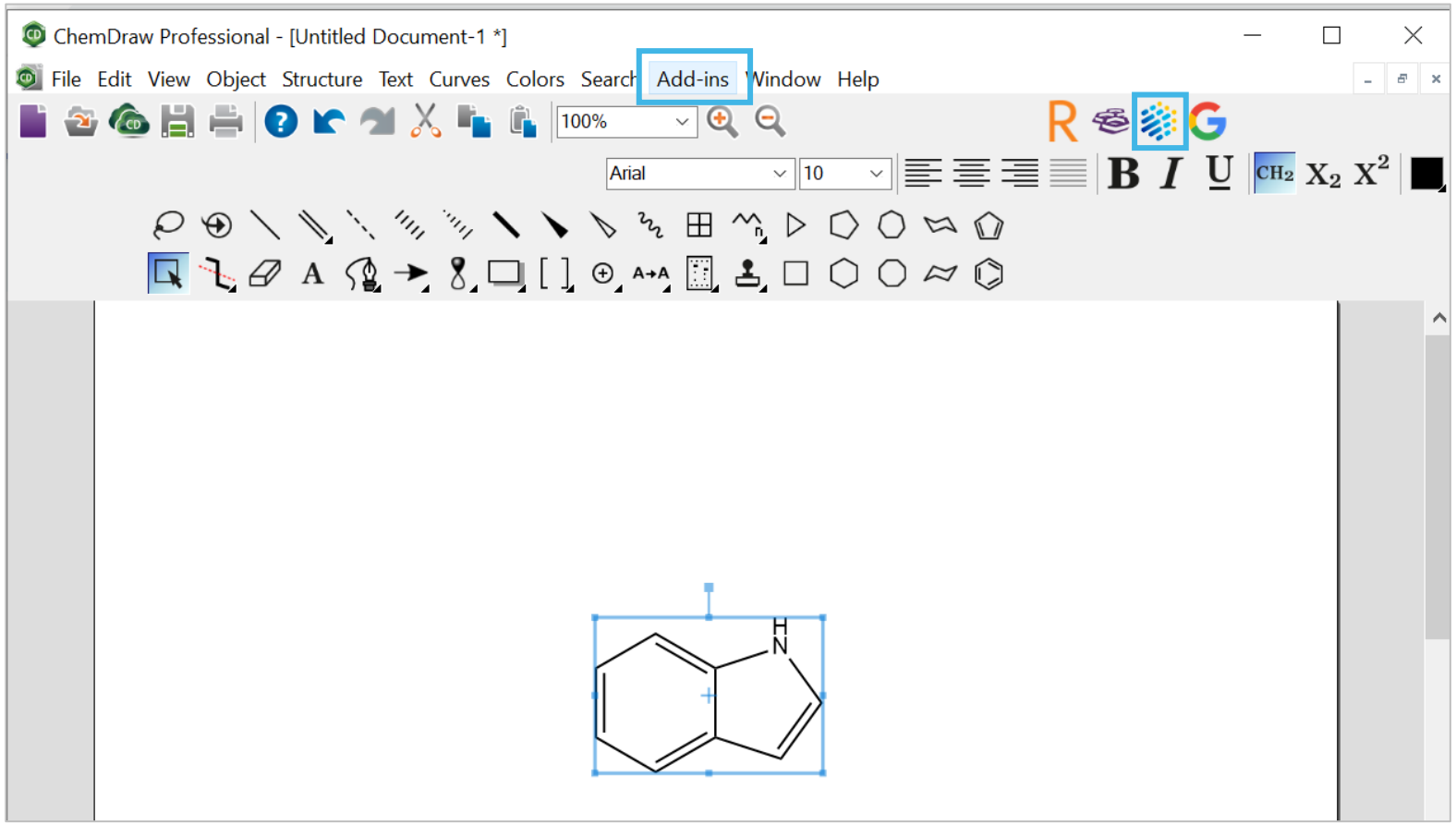
C12=CC=CC=C1NC=C2

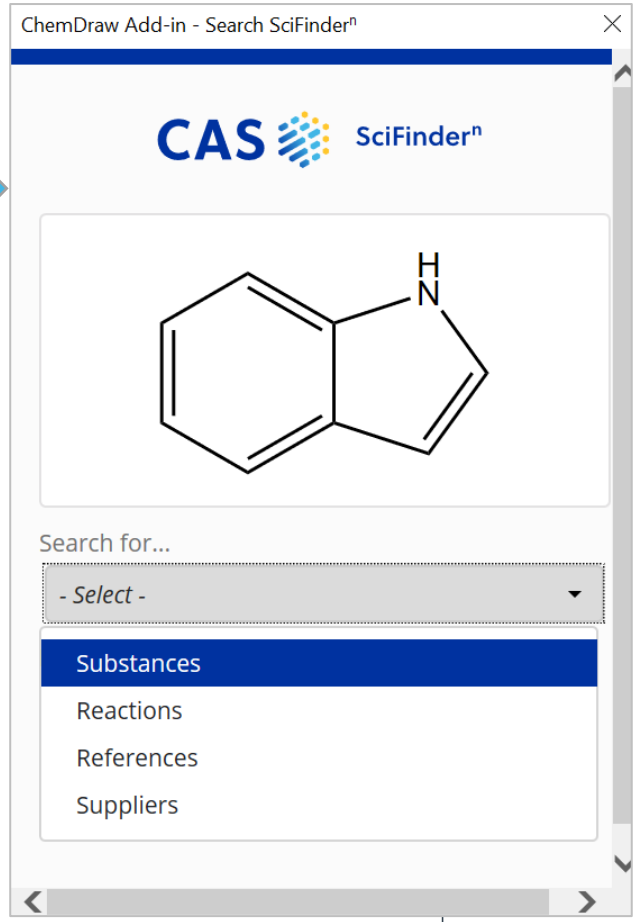


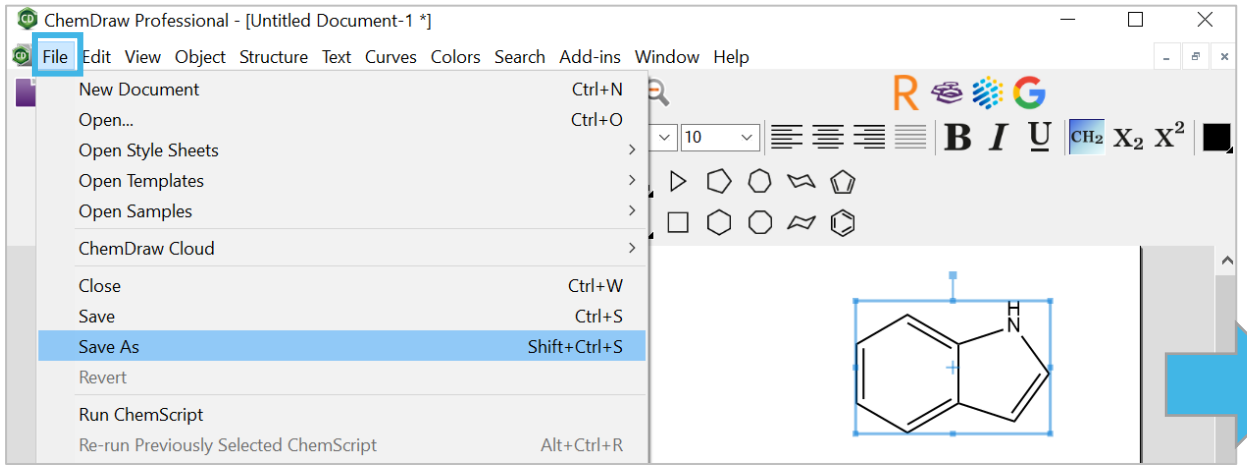
# (2)直接在ChemDraw中进入SciFinder$^n$联用检索

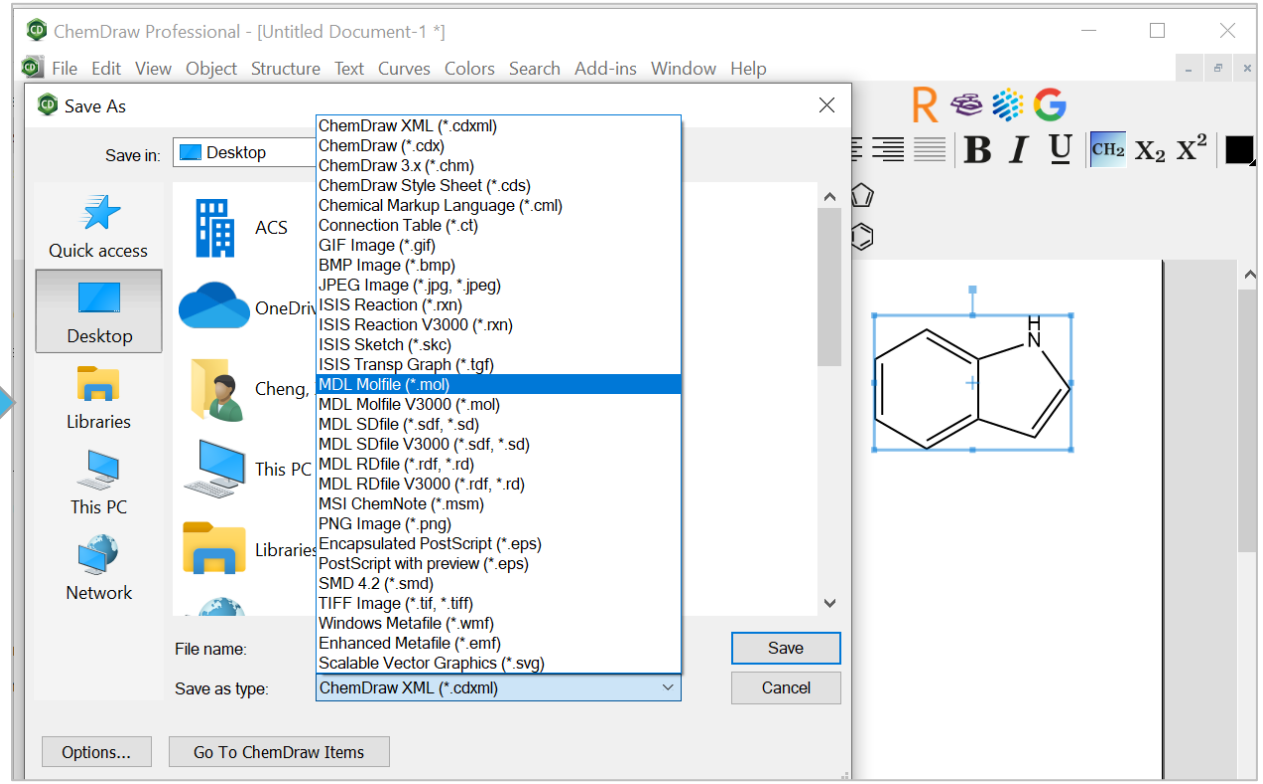
点击ChemDraw菜单Add-ins列表中Search SciFinder$^n$这项; 或点击CAS SciFinder$^n$的新Logo

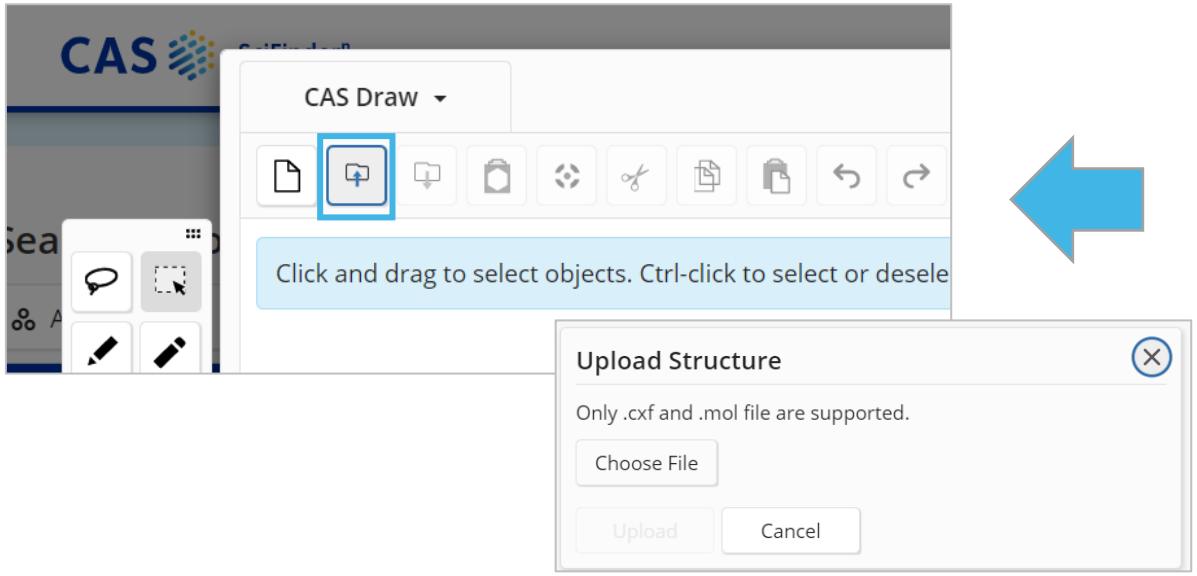


# (3) 通过MDL Molfile 文件导入



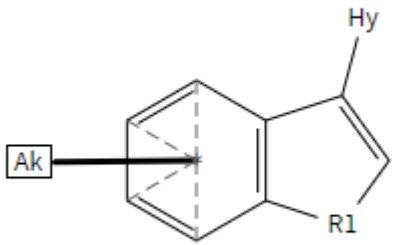






ACS International

CAS
A division of the American Chemical Society

# 结构式检索




R1 = O, N, B


获取物质结果集的文献，反应和供应商信息

同时获取三个精准度的物质检索结果

# 结构检索匹配维度

- 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，环系（如有）不能与其他的环稠合或成桥环

- Substructure：

  包括As Drawn的检索稠合或成桥环结果，另外价态未达饱和的原子可以连接氢以外的其他原子，环系（如有）可以与其他环

- Similarity：

  绘制结构中不能出现R基团、可变基团，绘制的结构必须是一个确定的结构。获得片段或整体结构与被检索结构相似的物质，母体结构可以被取代，也可以被改变

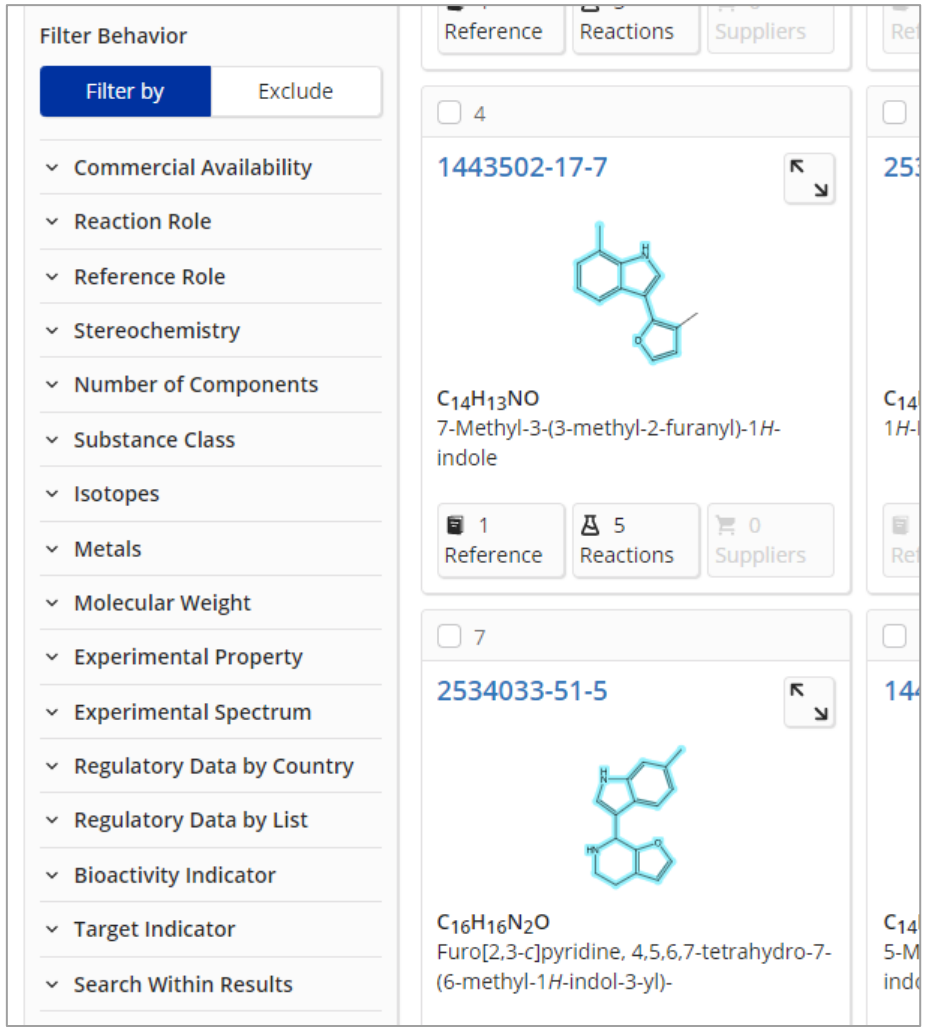
Structure Match Introduction
https://scifinder-n.cas.org/help/#t=Working_with_Search_Results%2FSubstances%2FStructure_Match.htm&rhsearch=as%20drawn



ACS International | CAS A division of the American Chemical Society

# Filter by从物质角色、属性、活性、结构等多方面对结果进行分析

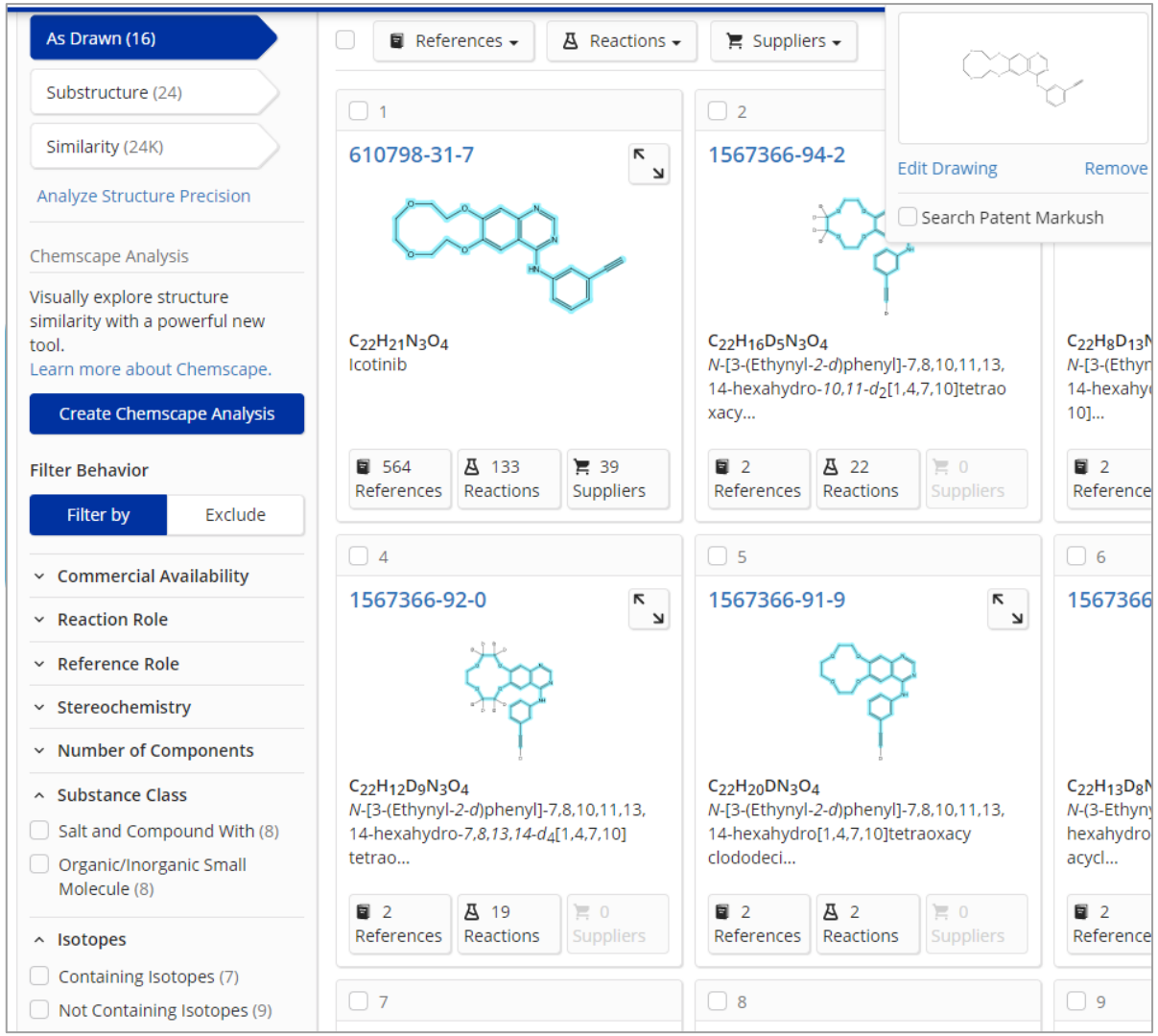
丰富直观的聚类分析，
高效直观地纵览结果，
便捷地选择或排除结果






ACS International | CAS A division of the American Chemical Society

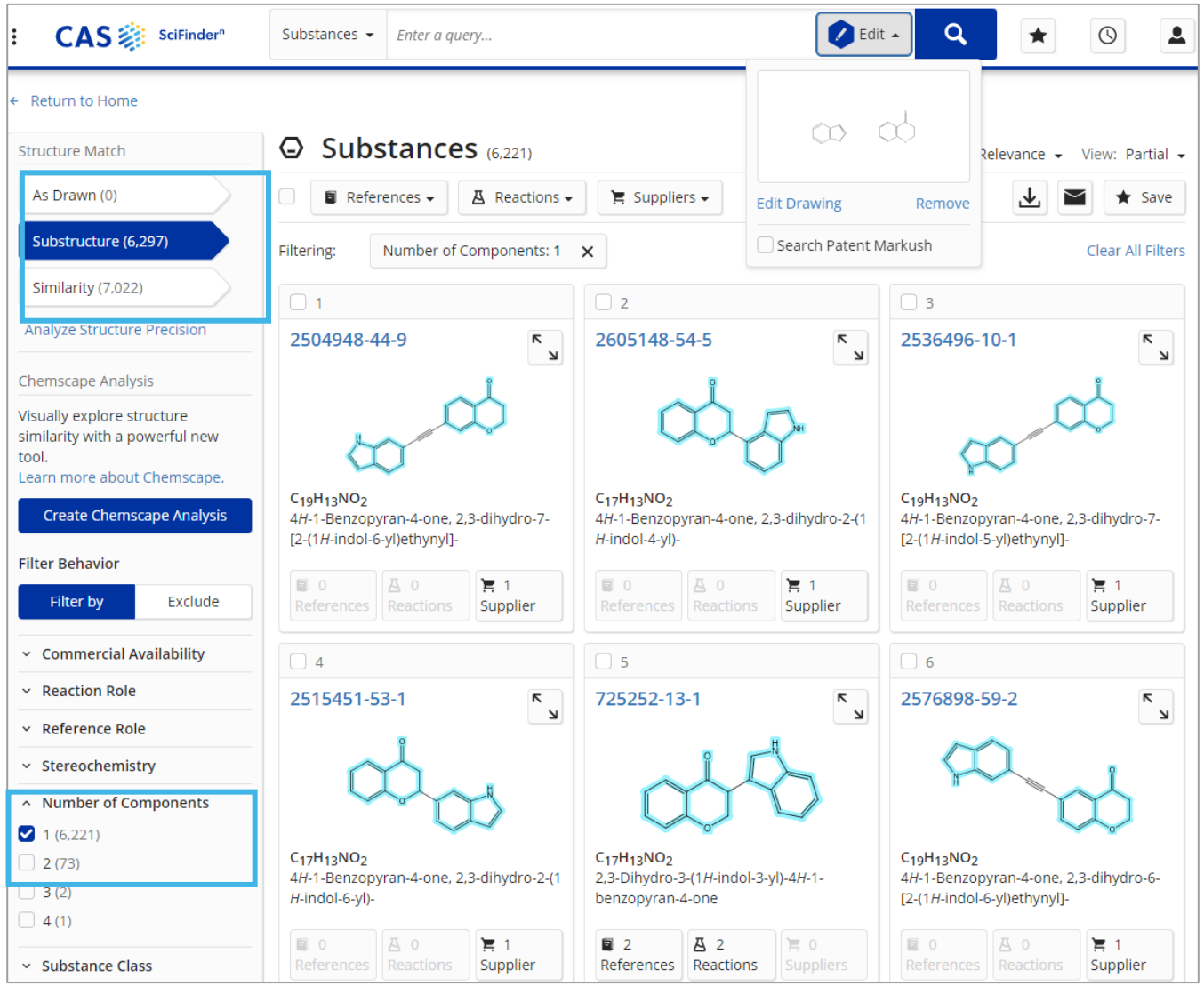
# As Draw——检索盐或者同位素标记物






ACS International | CAS A division of the American Chemical Society

# 片段结构的物质检索——亚结构

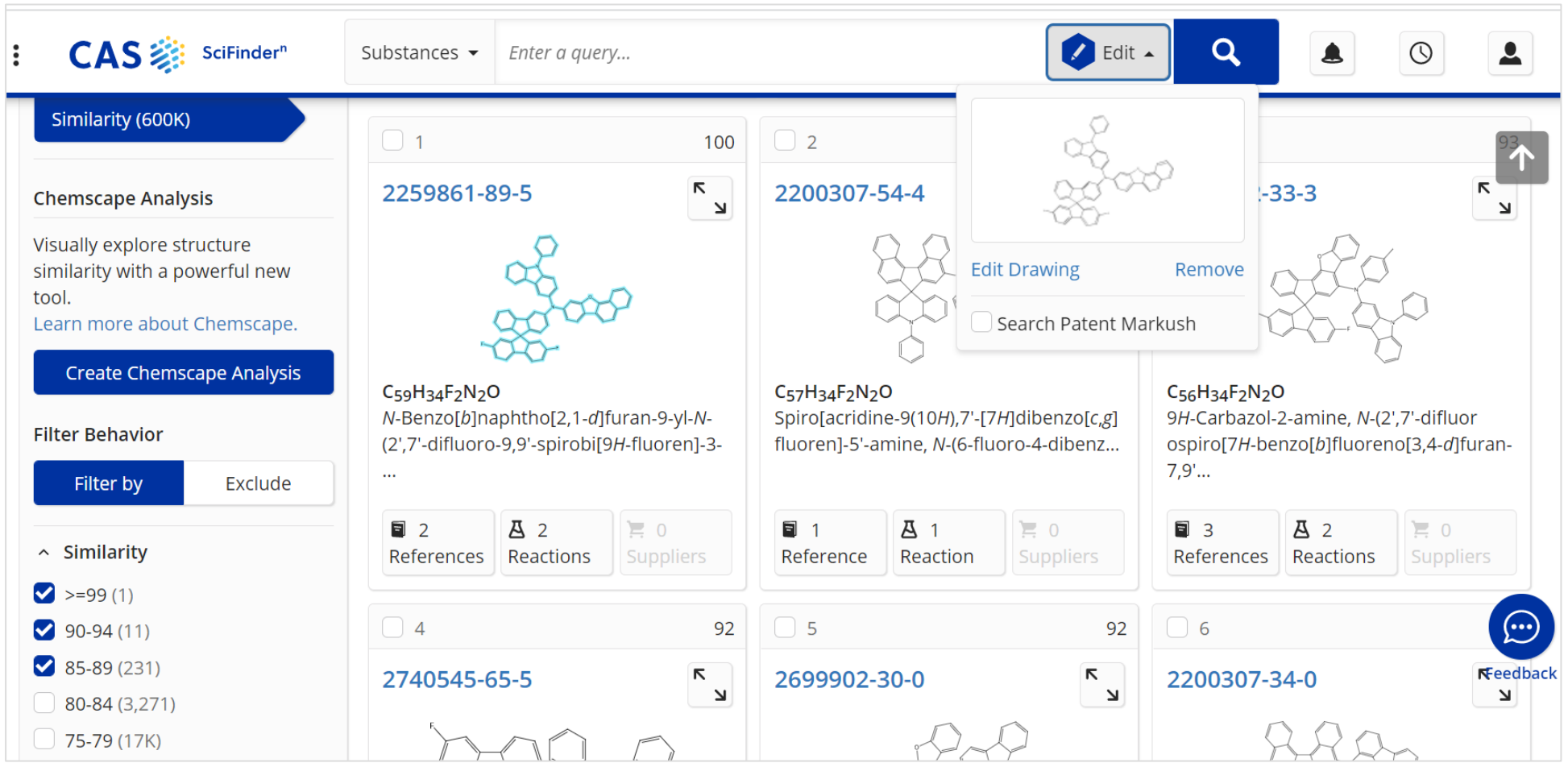




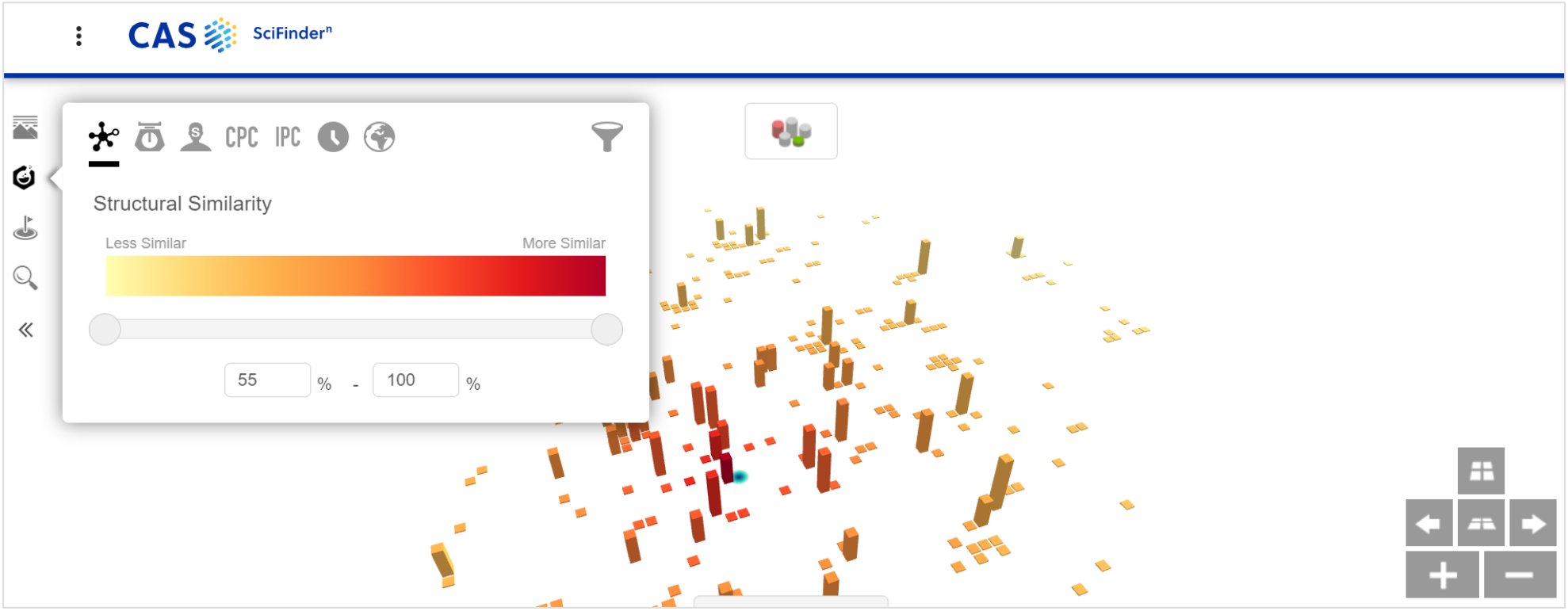

ACS International | CAS A division of the American Chemical Society

# 相似结构检索

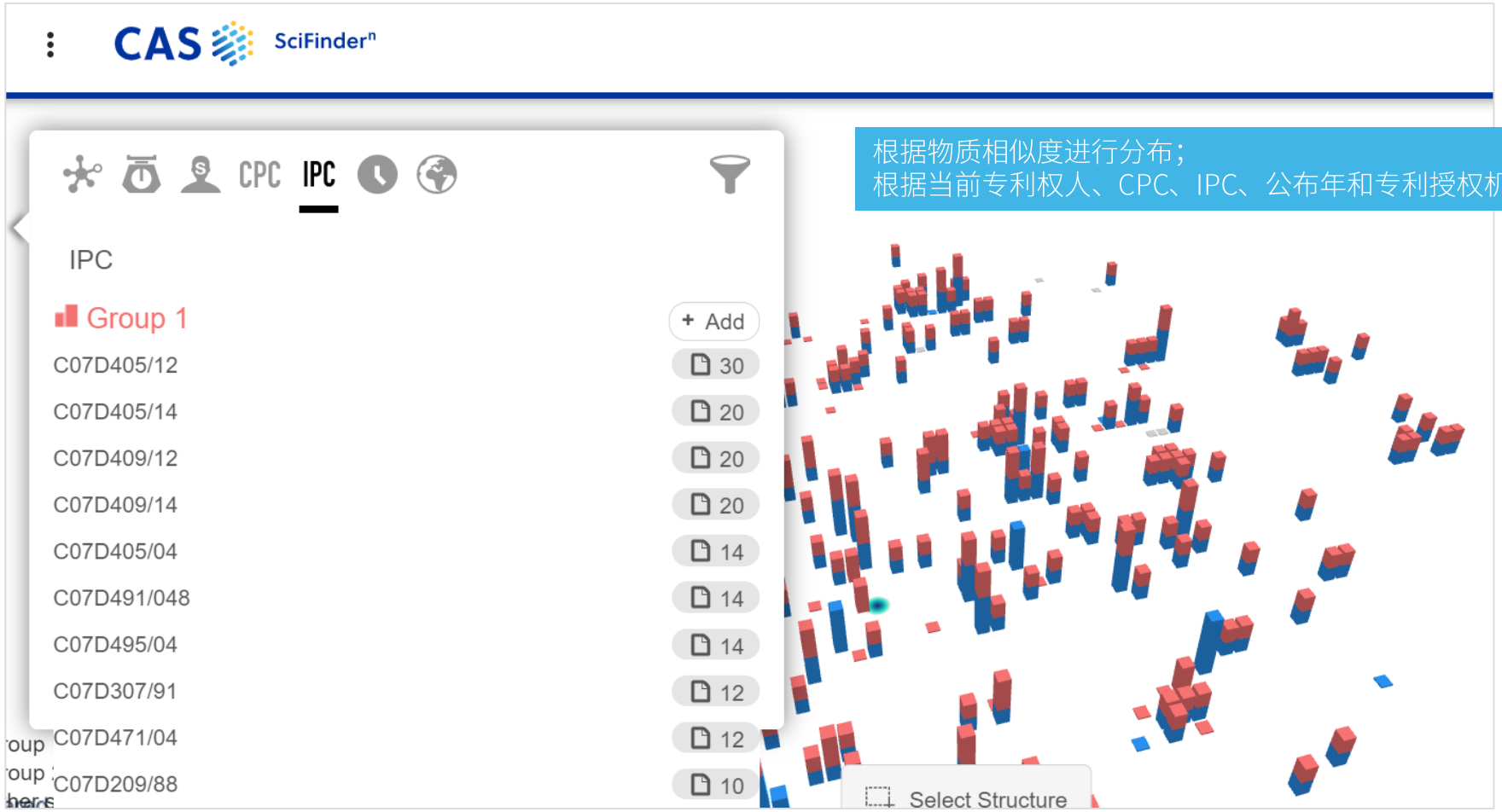
## 推荐使用确定的结构进行Similarity检索



# 对结构检索结果集进行可视化分析：发现物质研究空白及专利布局



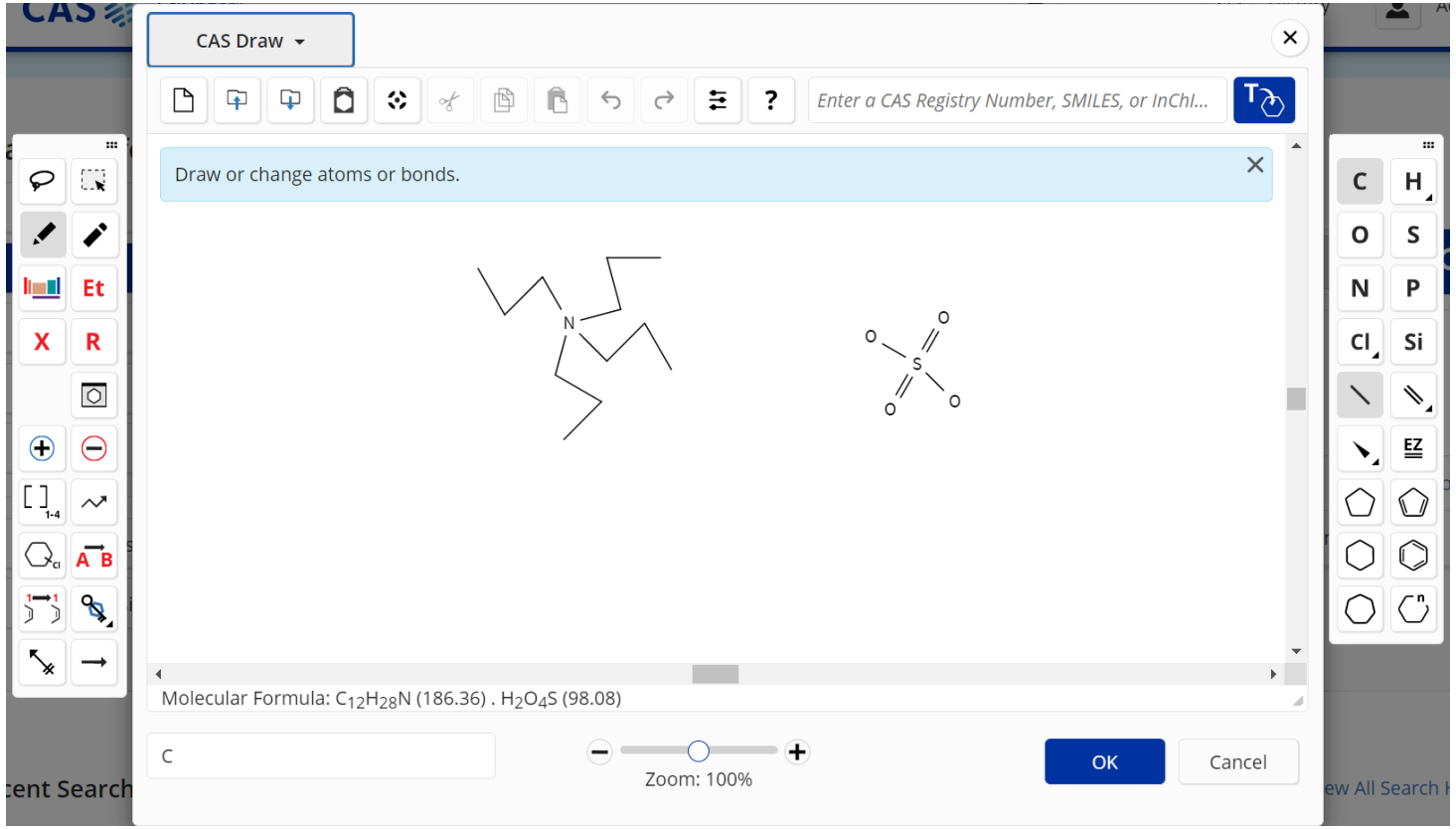
# 对结构检索结果集进行可视化分析：发现物质研究空白及专利布局



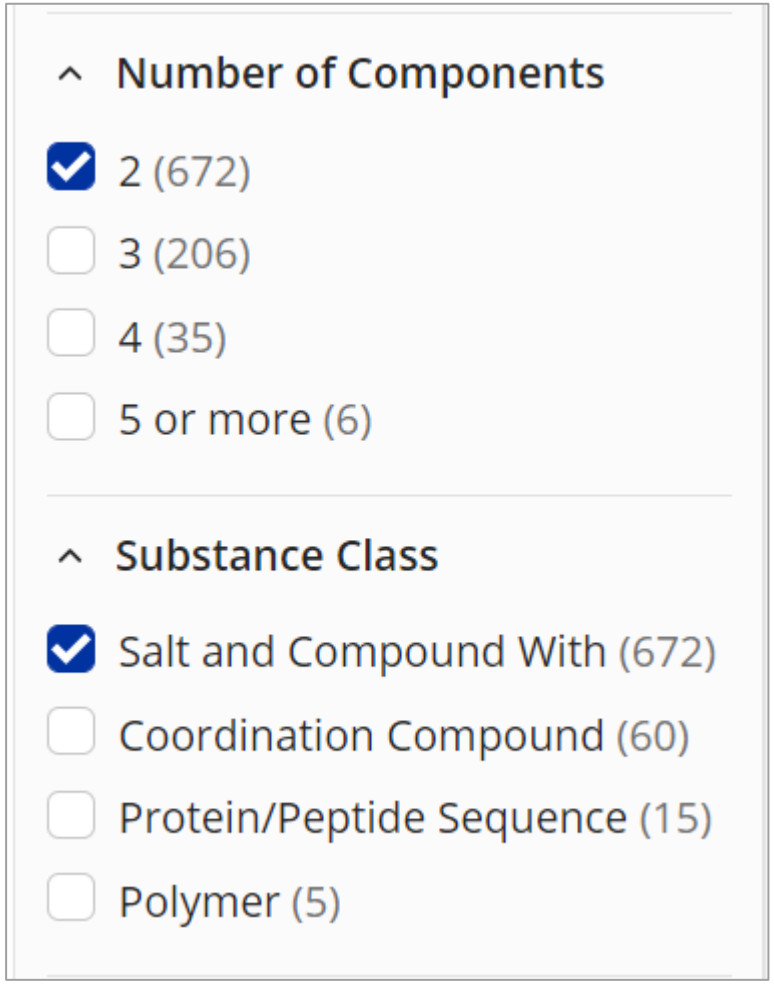

根据物质相似度进行分布；
根据当前专利权人、CPC、IPC、公布年和专利授权机构等对物质进行分组

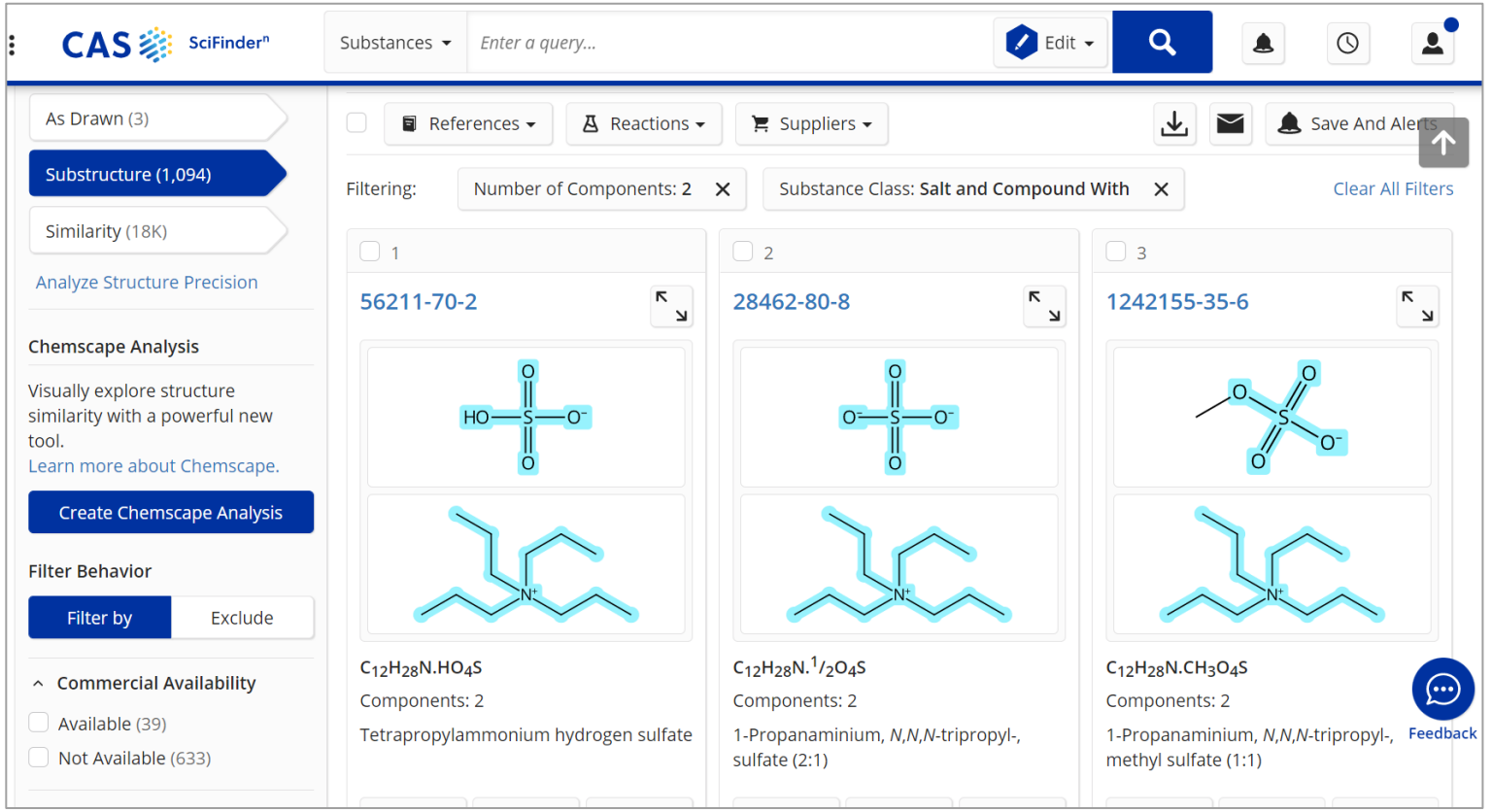
# 案例1：季铵盐的检索

方法一：绘制不同组分，忽略化合价



# 获得所需结果

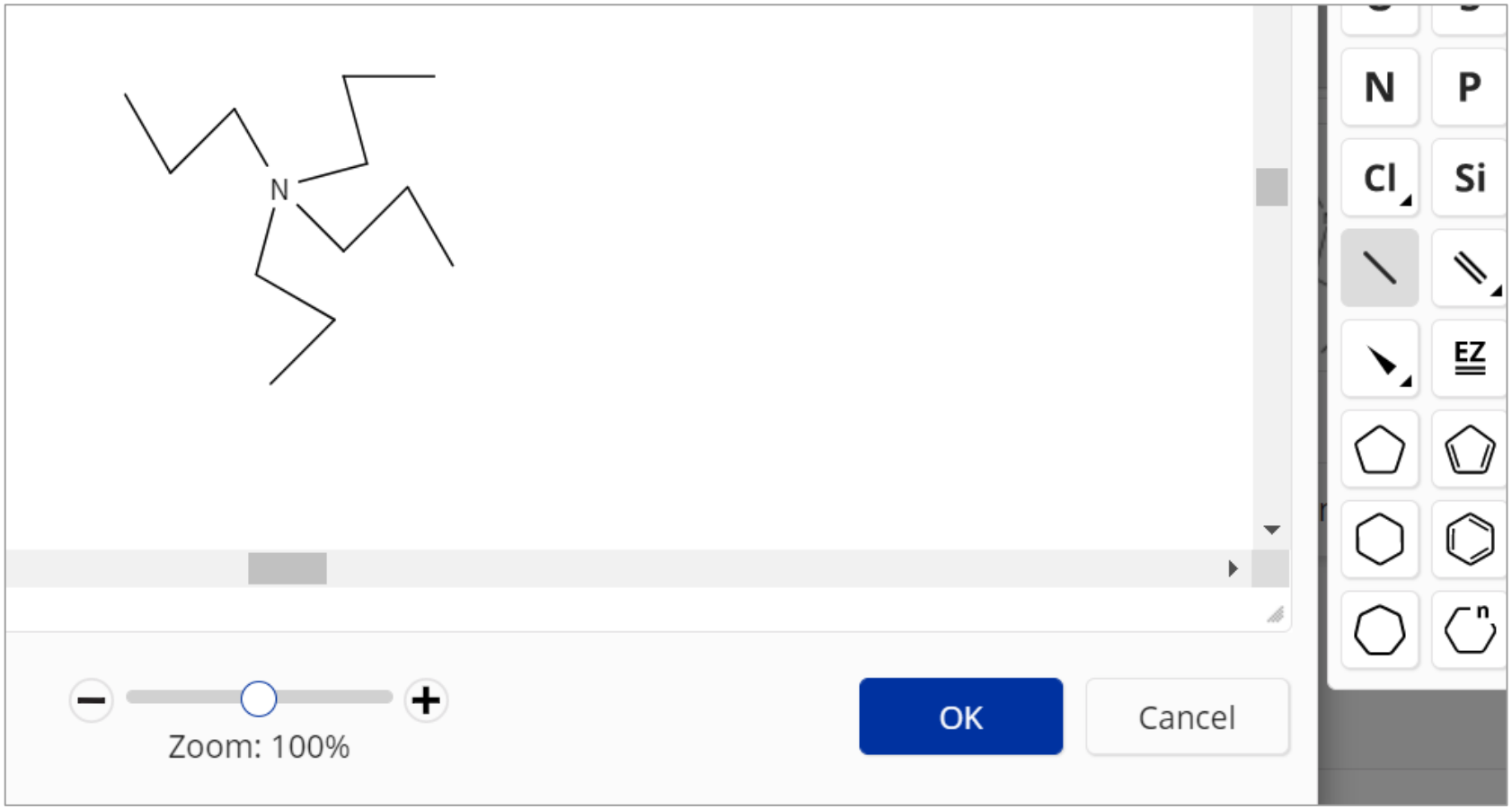


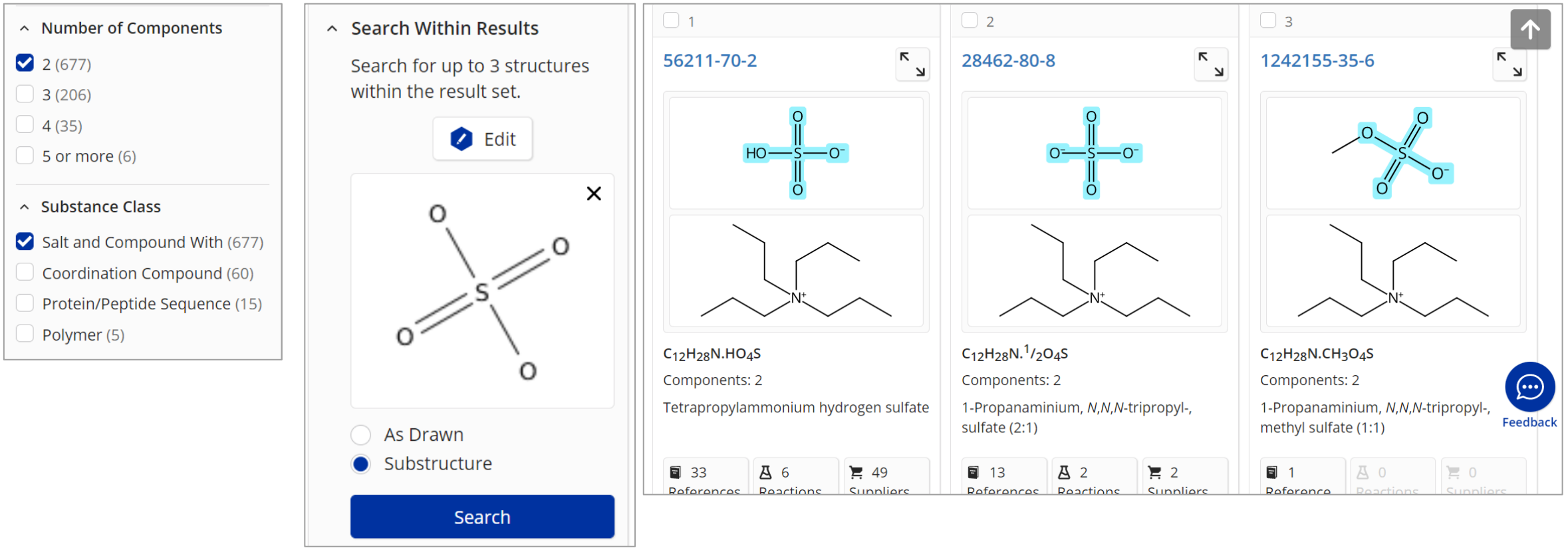



ACS International | CAS A division of the American Chemical Society

# 方法二：绘制其中一部分结构



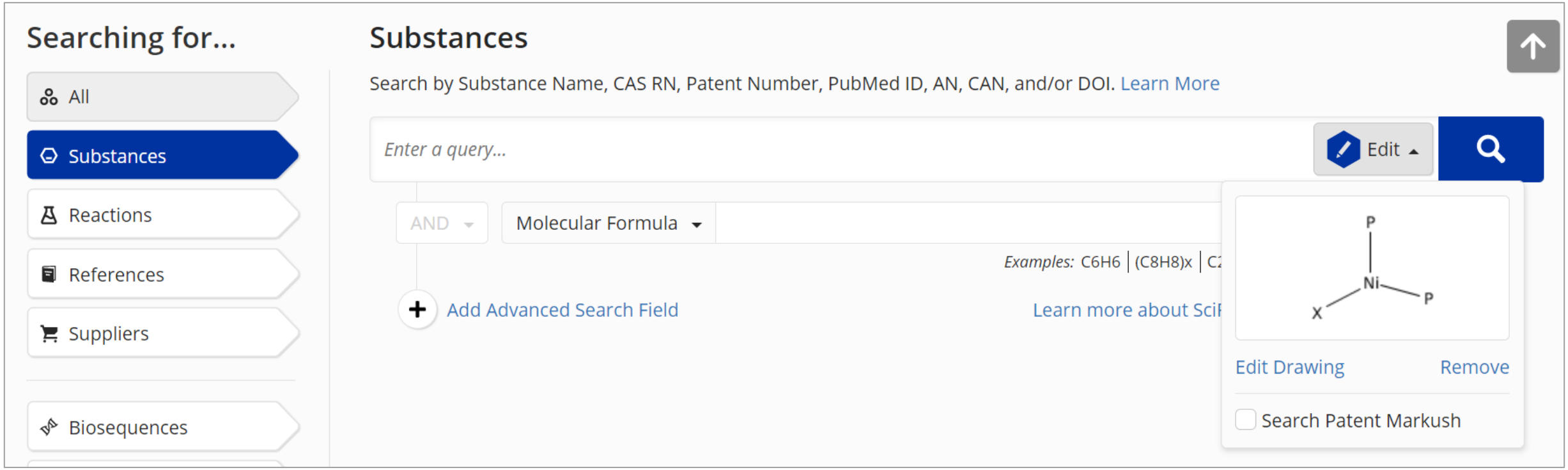
# 在结果集中通过另外组分结构筛选






ACS International | CAS A division of the American Chemical Society

# 案例2：双膦配体-镍基手性催化剂检索



# 选择物质结果集中带有立体键的结果

Properties (110)

Catalyst Use (77)

Uses (77)

View All

**Stereochemistry**

Stereo in Answer Structure (238)

No Stereo in Answer Structure (13K)

**Number of Components**

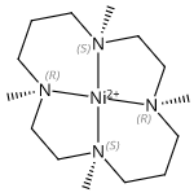
**Substance Class**

Coordination Compound (238)

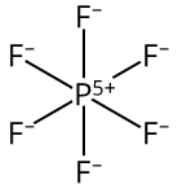
**Isotopes**

**Metals**

**Molecular Weight**



Relative stereochemistry shown

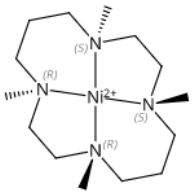


$C_{14}H_{32}N_4Ni.2F_6P$

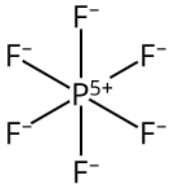
Components: 2

Nickel(2+), (1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane-κ$N^1$,κ$N^4$,κ$N^8$,...

4 References | 1 Reaction | 0 Suppliers



Relative stereochemistry shown

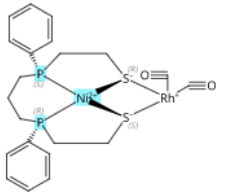


$C_{14}H_{32}N_4Ni.2F_6P$

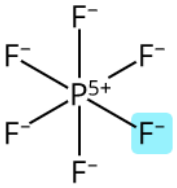
Components: 2

Nickel(2+), (1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane-κ$N^1$,κ$N^4$,κ$N^8$,...

2 References | 0 Reactions | 0 Suppliers



Relative stereochemistry shown



$C_{21}H_{24}NiO_2P_2RhS_2.F_6P$

Components: 2

1 Reference | 2 Reactions | 0 Suppliers

Feedback



ACS International | CAS A division of the American Chemical Society

# 可通过物质的Reaction role或者Reference role筛选物质

**Reaction Role**

- [ ] Product (62)
- [ ] Reactant (15)
- [x] Catalyst (57)

**Reference Role**

- [x] Catalyst Use (57)
- [ ] Uses (57)
- [ ] Preparation (49)
- [ ] Synthetic Preparation (48)
- [ ] Properties (23)

View All

4

220502-56-7

Absolute stereochemistry shown

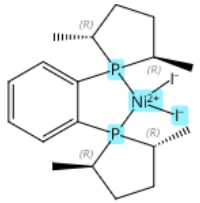
$C_{18}H_{28}I_2NiP_2$

(*SP*-4-2)-Diiodo[(2*S*,2'*S*,5*S*,5'*S*)-1,1'-(1,2-phenylene)bis[2,5-dimethylph ospholane-...

3 References | 5 Reactions | 0 Suppliers

5

332131-31-4



Absolute stereochemistry shown

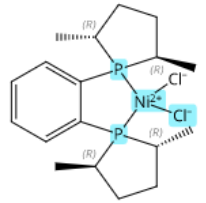
$C_{18}H_{28}I_2NiP_2$

(*SP*-4-2)-Diiodo[(2*R*,2'*R*,5*R*,5'*R*)-1,1'-(1,2-phenylene)bis[2,5-dimethylph ospholane-...

2 References | 5 Reactions | 0 Suppliers

6

332131-30-3



Absolute stereochemistry shown

$C_{18}H_{28}Cl_2NiP_2$

Nickel, dichloro[(2*R*,2'*R*,5*R*,5'*R*)-1,1'-(1,2-phenylene)bis[2,5-dimethylph ospholane...

3 References | 3 Reactions | 0 Suppliers

Feedb



ACS International | CAS A division of the American Chemical Society

# 结果符合检索需求

Scheme 1 (1 Reaction) Steps: 1 Yield: 83%


Absolute stereochemistry shown, Rotation (-)

Suppliers (2)

Reaction Summary Steps: 1 Yield: 83%

1.1 Reagents: Lithium triethylborohydride
Catalysts: (*SP*-4-2)-Diiodo[(2*R*,2'*R*,5*R*,5'*R*)-1,1'-(1,2-phenylene)bis[2,5-dimethylphospholane-...
Solvents: Toluene, Tetrahydrofuran; 72 h, -20 °C

Asymmetric
in the metal
insertion and

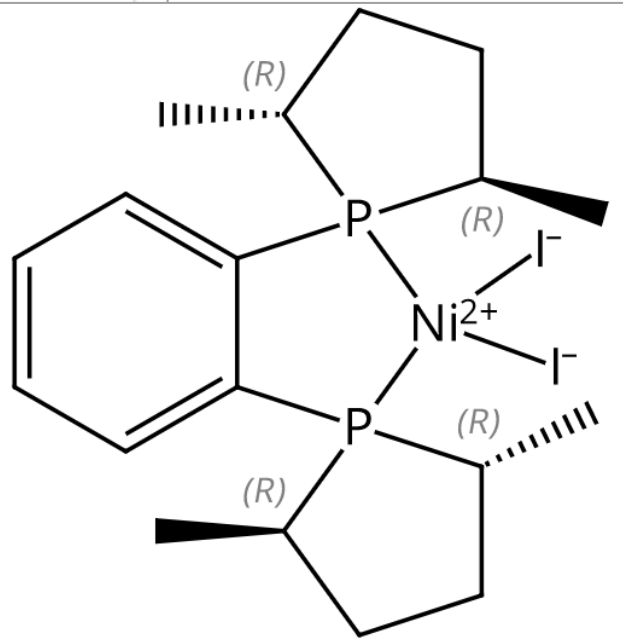
By: Flock, Sus
ARKIVOC (Ga

Full Text

CAS RN
332131-31-4

CAS Name
(*SP*-4-2)-Diiodo[(2*R*,2'*R*,5*R*,5'*R*)-1,1'-(1,2-phenylene)bis[2,5-dimethylphospholane-...

Substance Detail
Reactions (5)
Synthesize (0)
Start Retrosynthetic Analysis
References (2)
Suppliers (0)



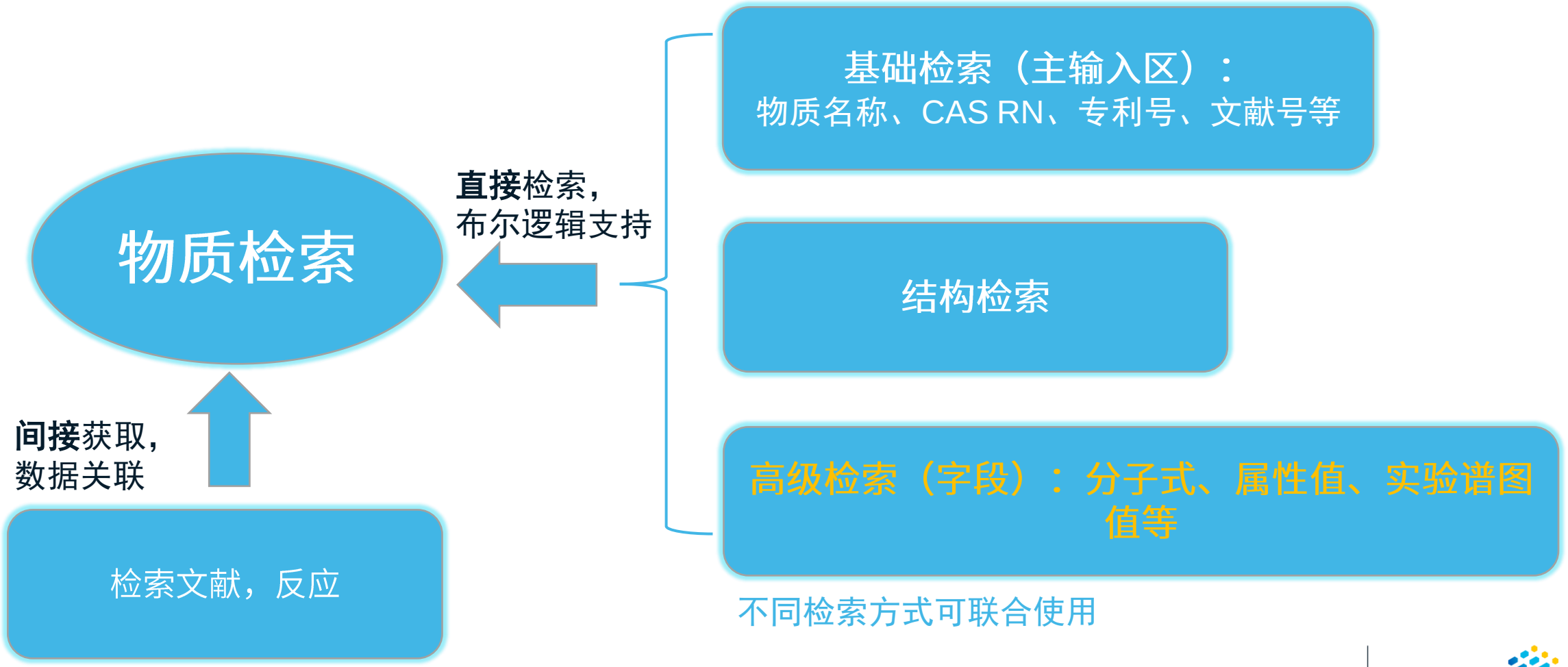

Absolute stereochemistry shown

Edit Structure − Reset +

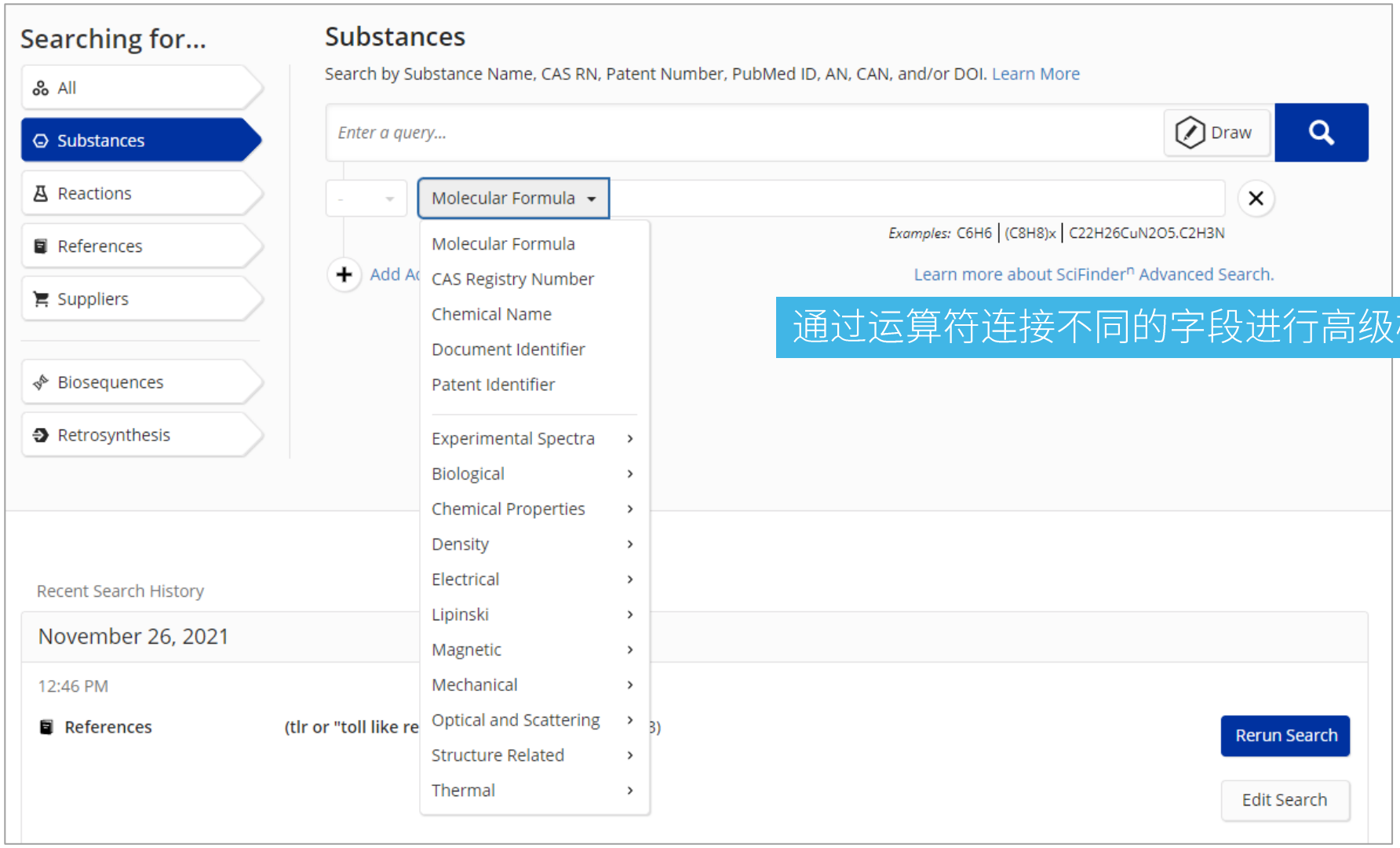


ACS International | CAS A division of the American Chemical Society

# 物质检索方法



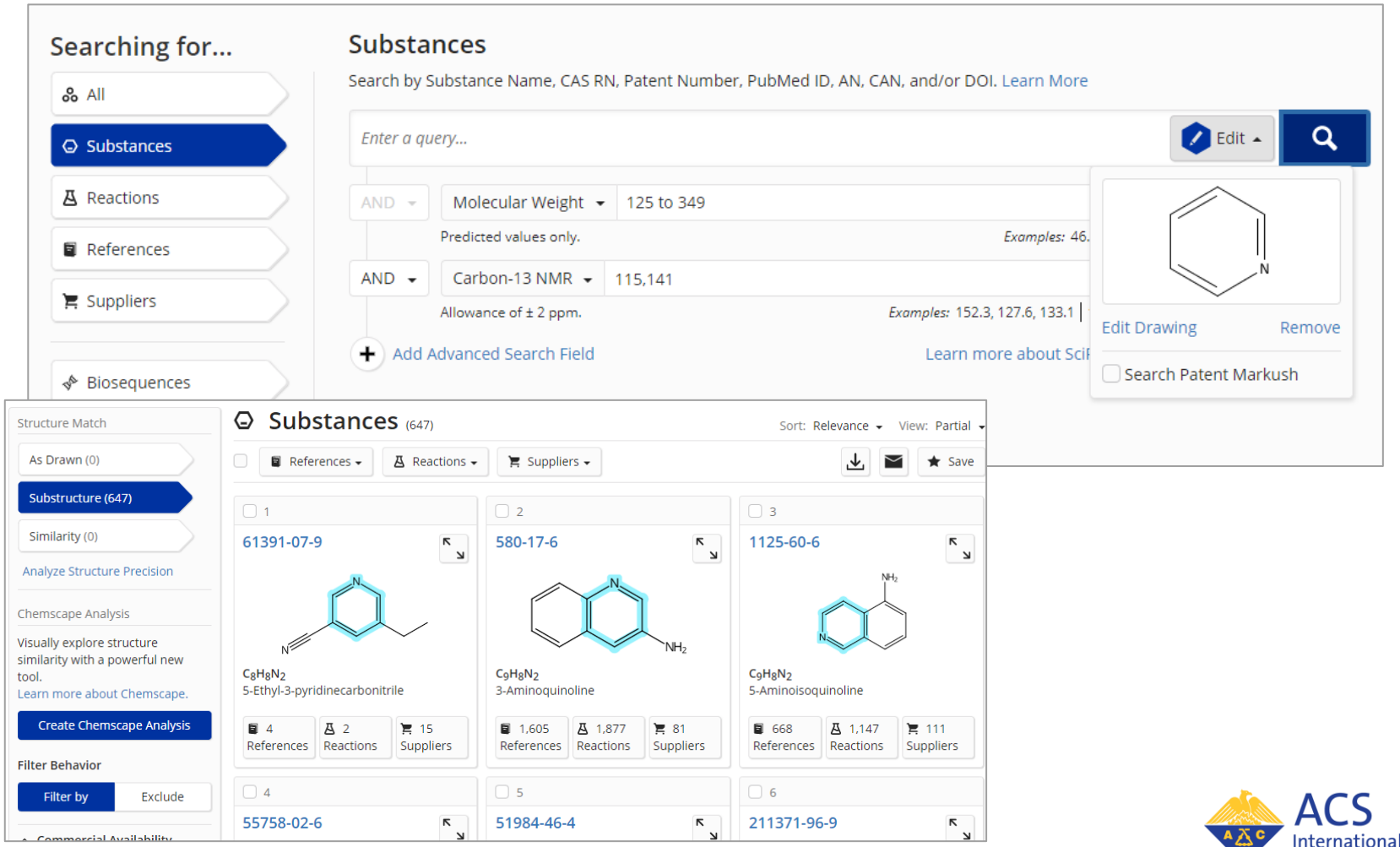
# 物质检索-高级检索




通过运算符连接不同的字段进行高级检索

# 案例1：查找符合分子量在125-350之间；核磁碳谱峰值包括115，141；包含吡啶结构的物质

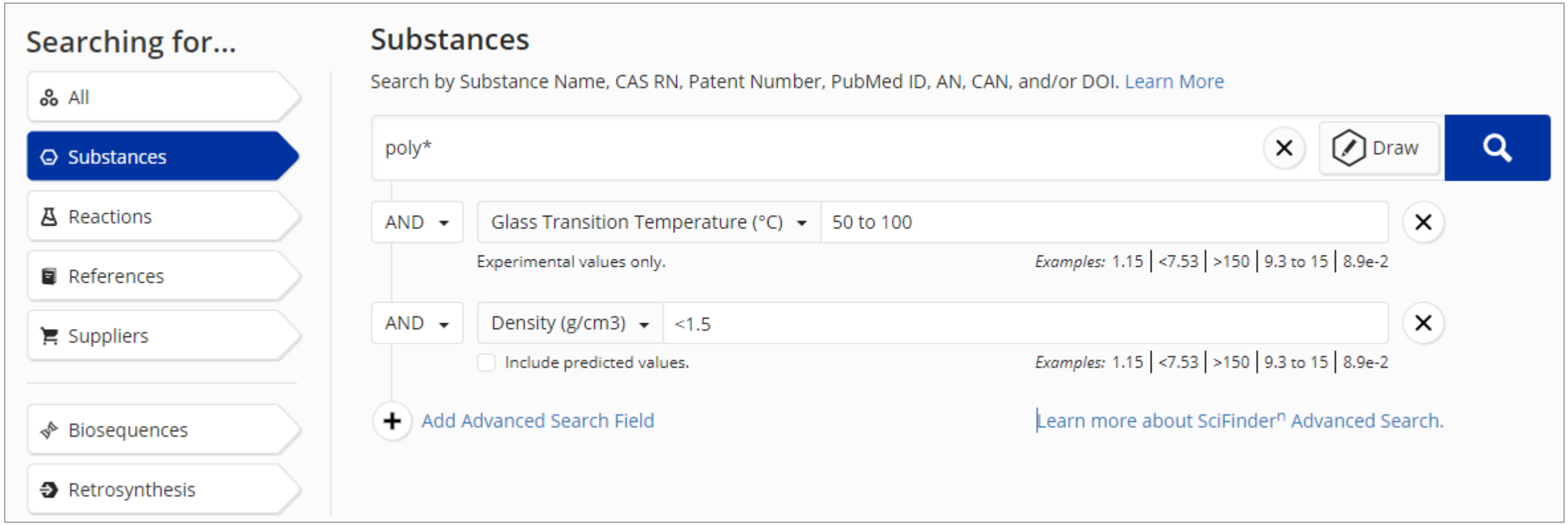
满足要求的结果



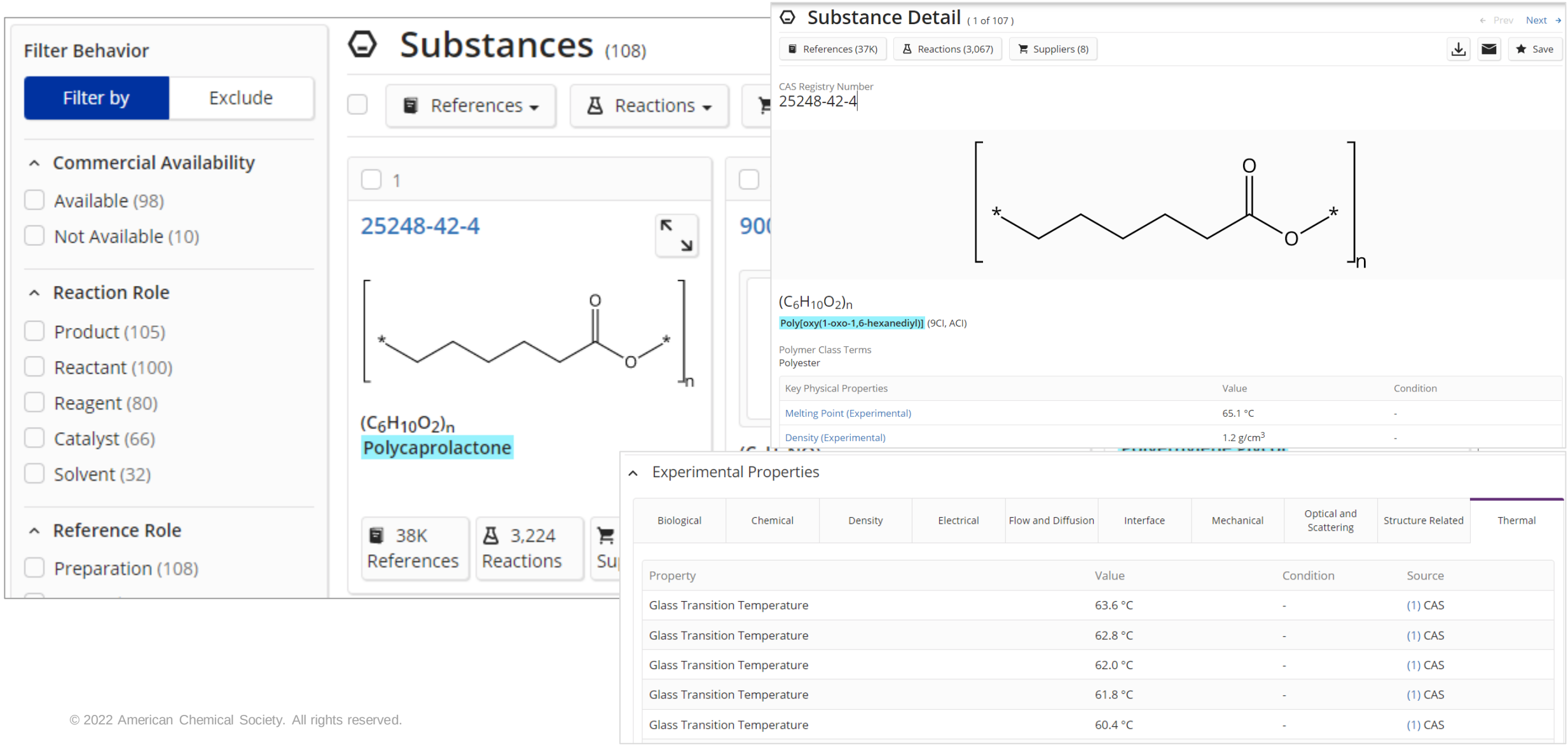



ACS International | CAS A division of the American Chemical Society

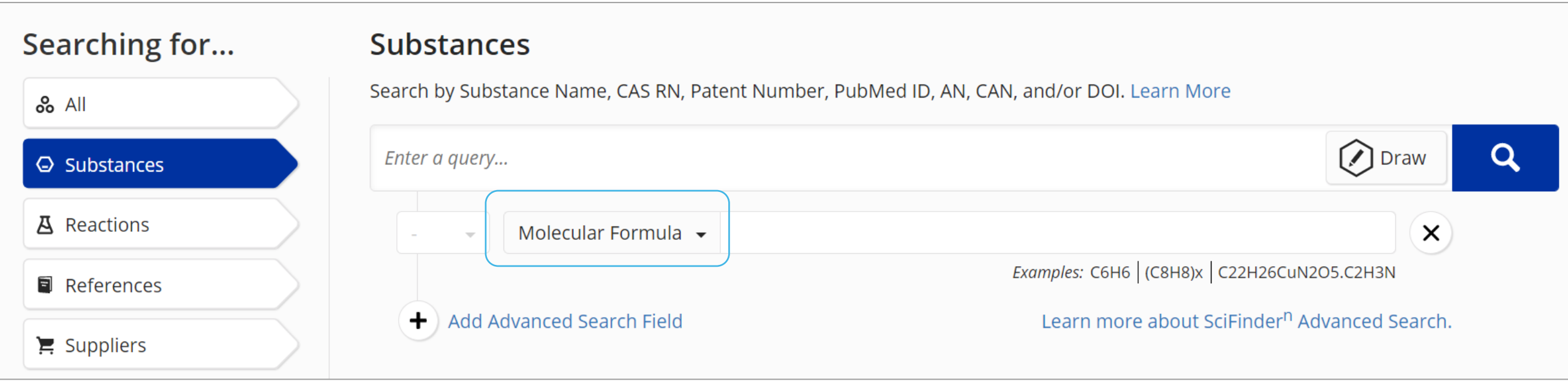
# 案例2：获取玻璃体转化温度在50-100摄氏度之间；密度小于1.5g/cm3的聚合物



# 获得的结果均满足检索需求



# 分子式检索化合物

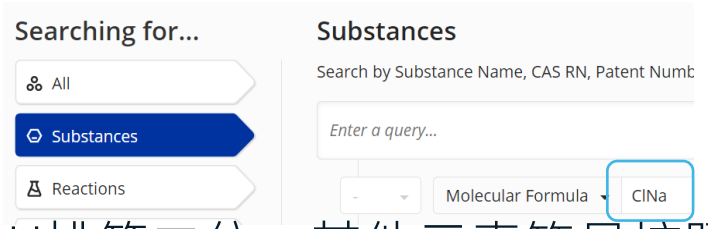



适用于分子式检索的物质类型包括：

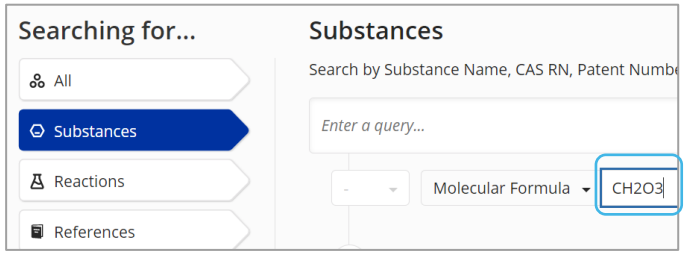
1. 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
2. 聚合物

# 分子式检索化合物检索规则

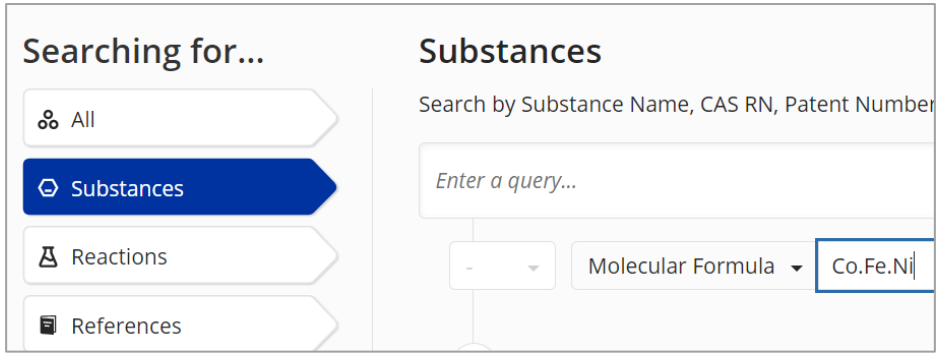
- 不含碳化合物，按照元素符号的首字母顺序进行排列，如：氯化钠NaCl




- 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，如：碳酸$H_2CO_3$




- 不同组分之间用“.”隔开，如：铁钴镍合金

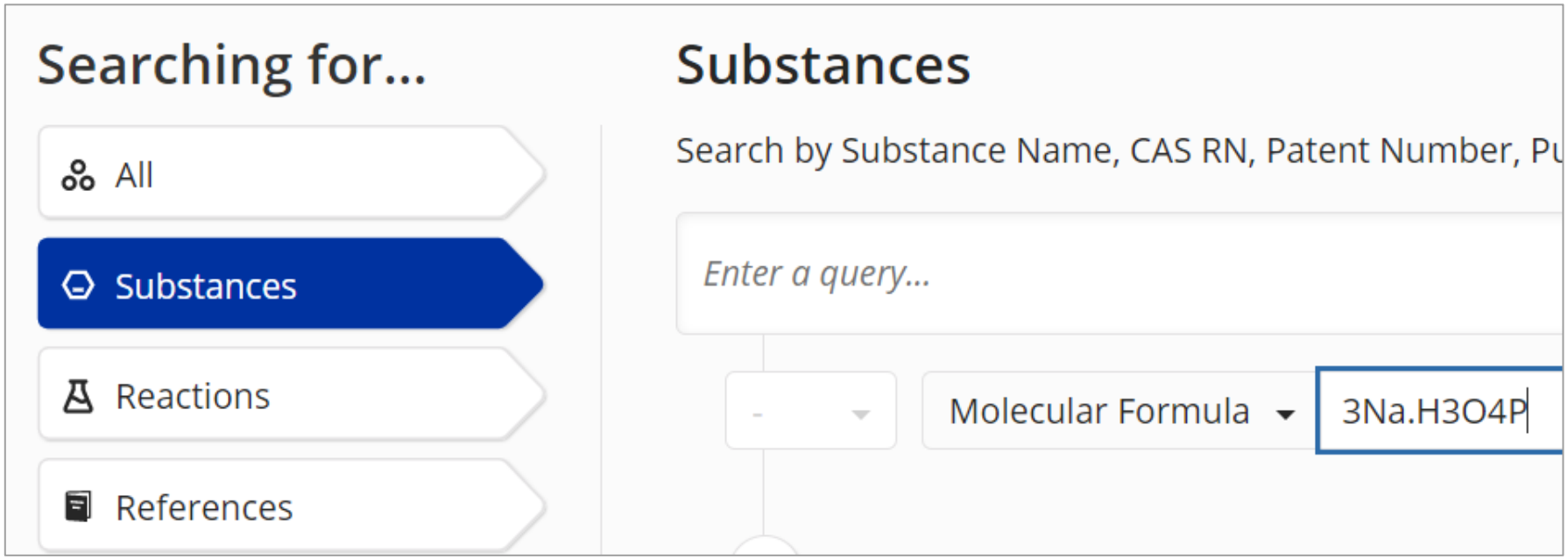




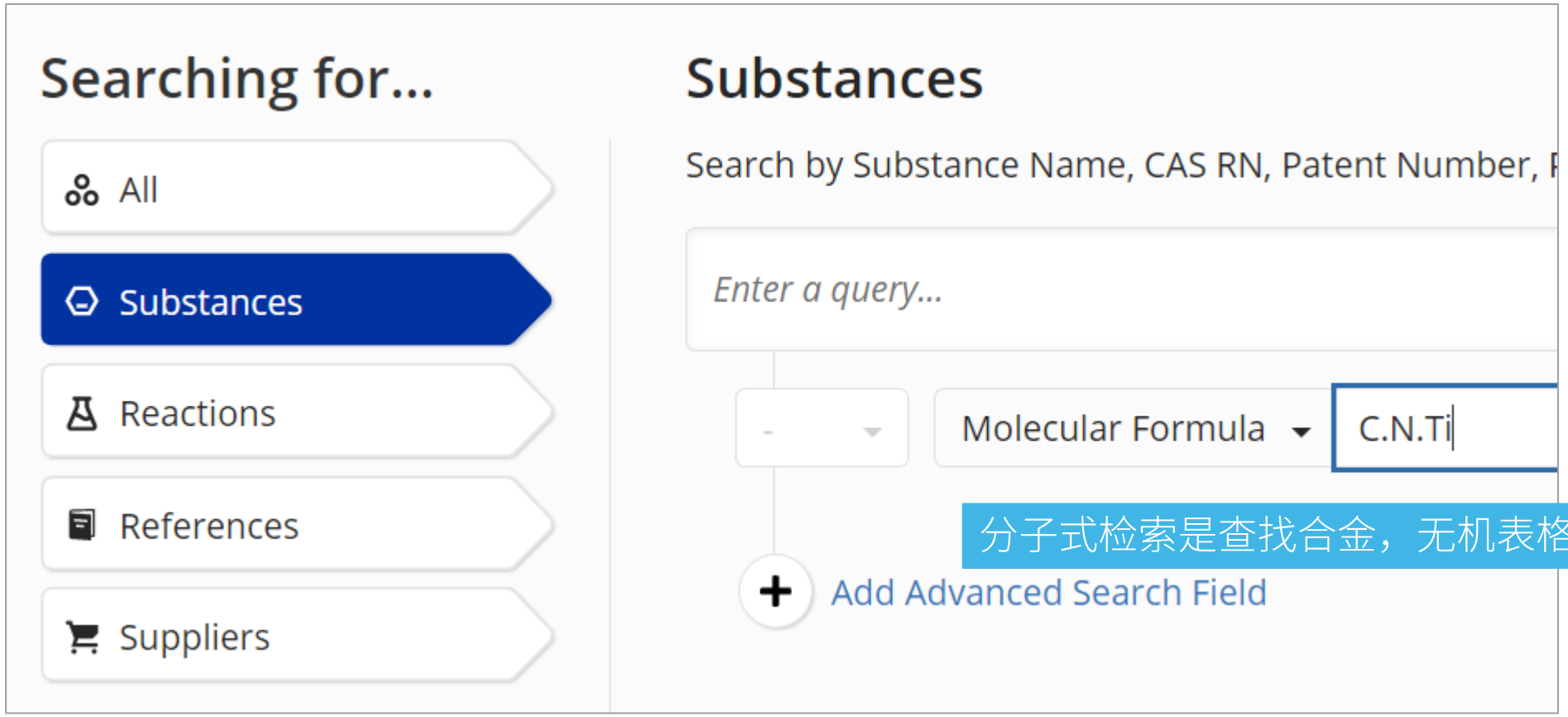

ACS International | CAS A division of the American Chemical Society

# 分子式检索化合物检索规则

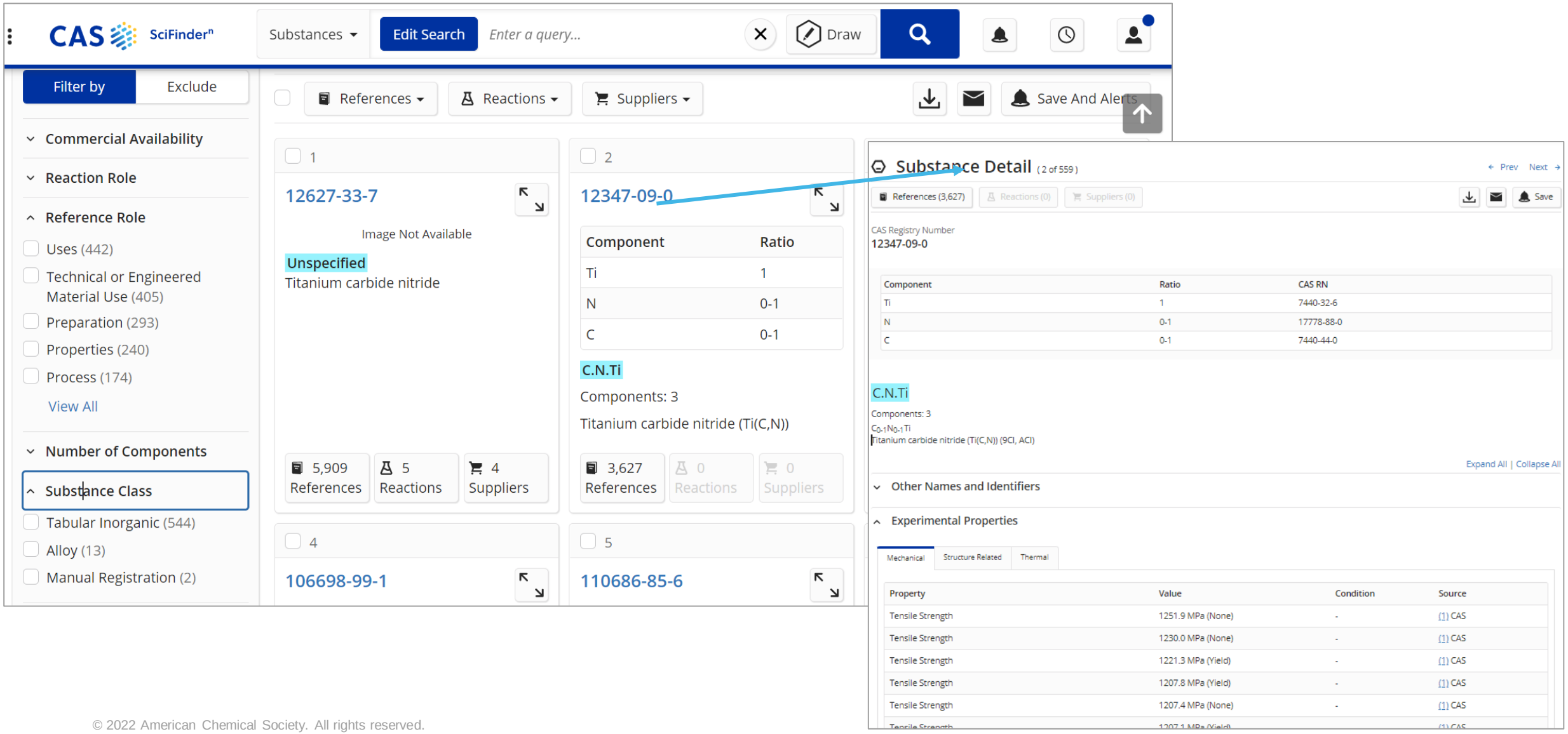
- 无机含氧酸盐，标引规则为金属离子和相应的含氧酸的混合物，即：在分子式中，需要补充和阳离子等同个数的氢原子，如：磷酸钠$Na_3PO4$



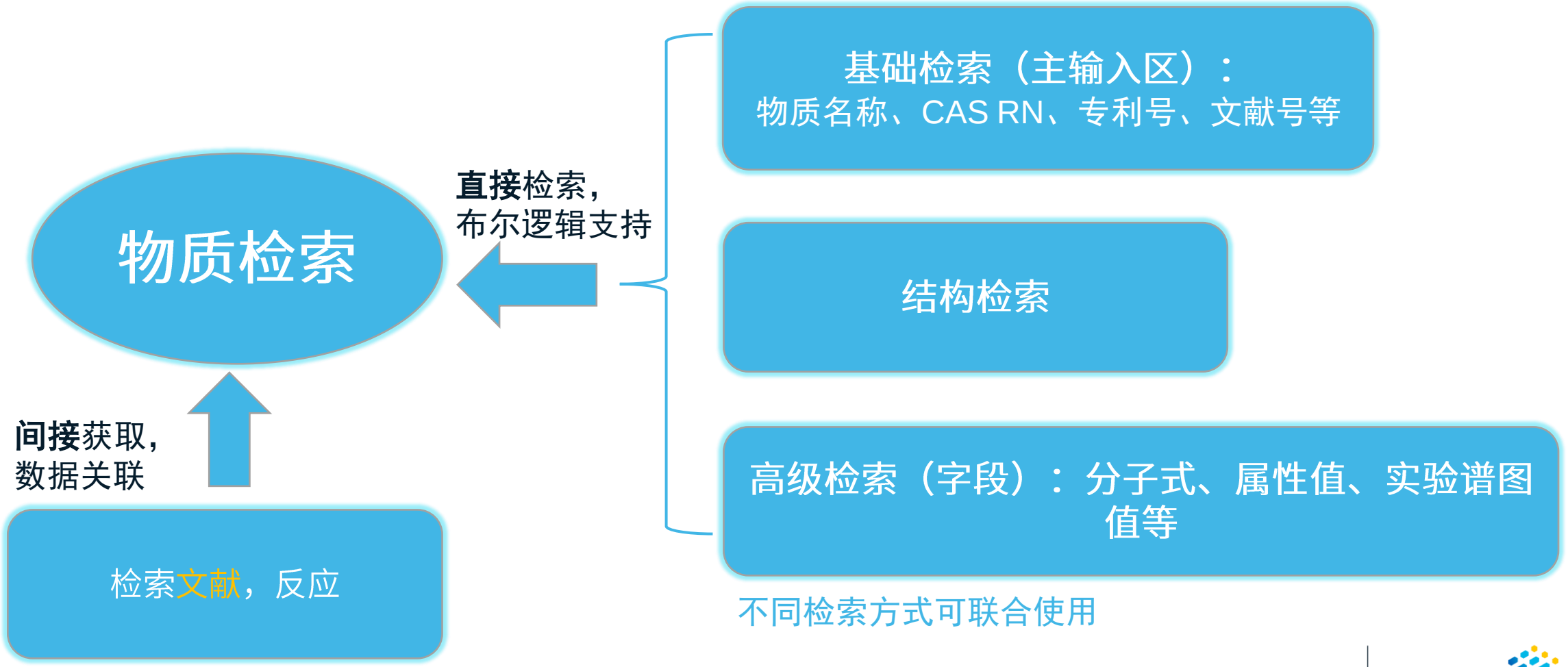
# 案例：碳氮化钛化合物检索



# 可通过物质的文献角色或者物质类别筛选结果

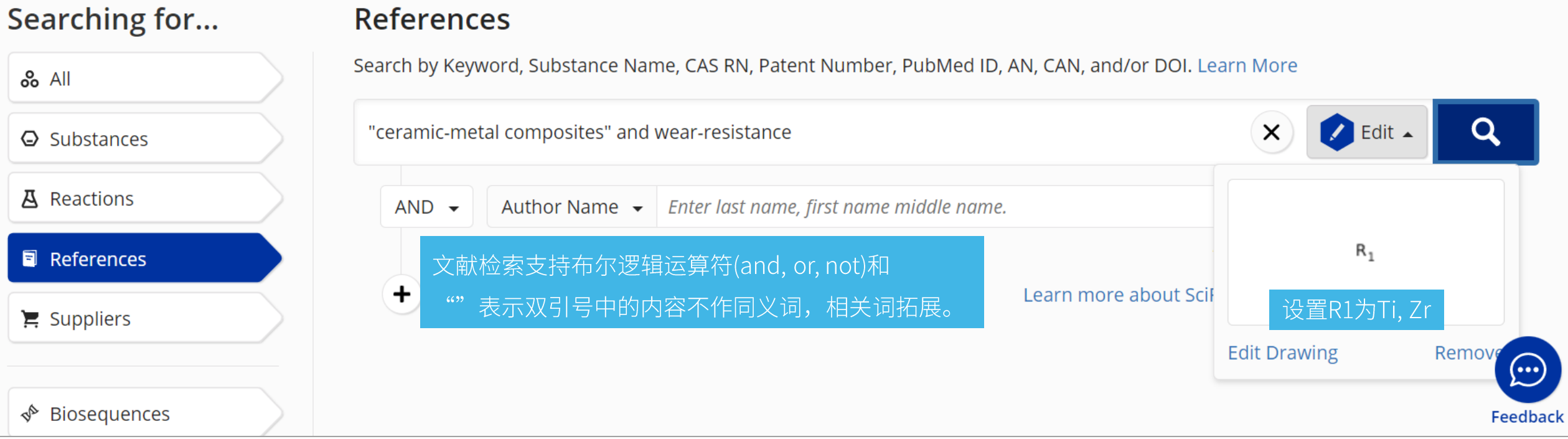


# 物质检索方法

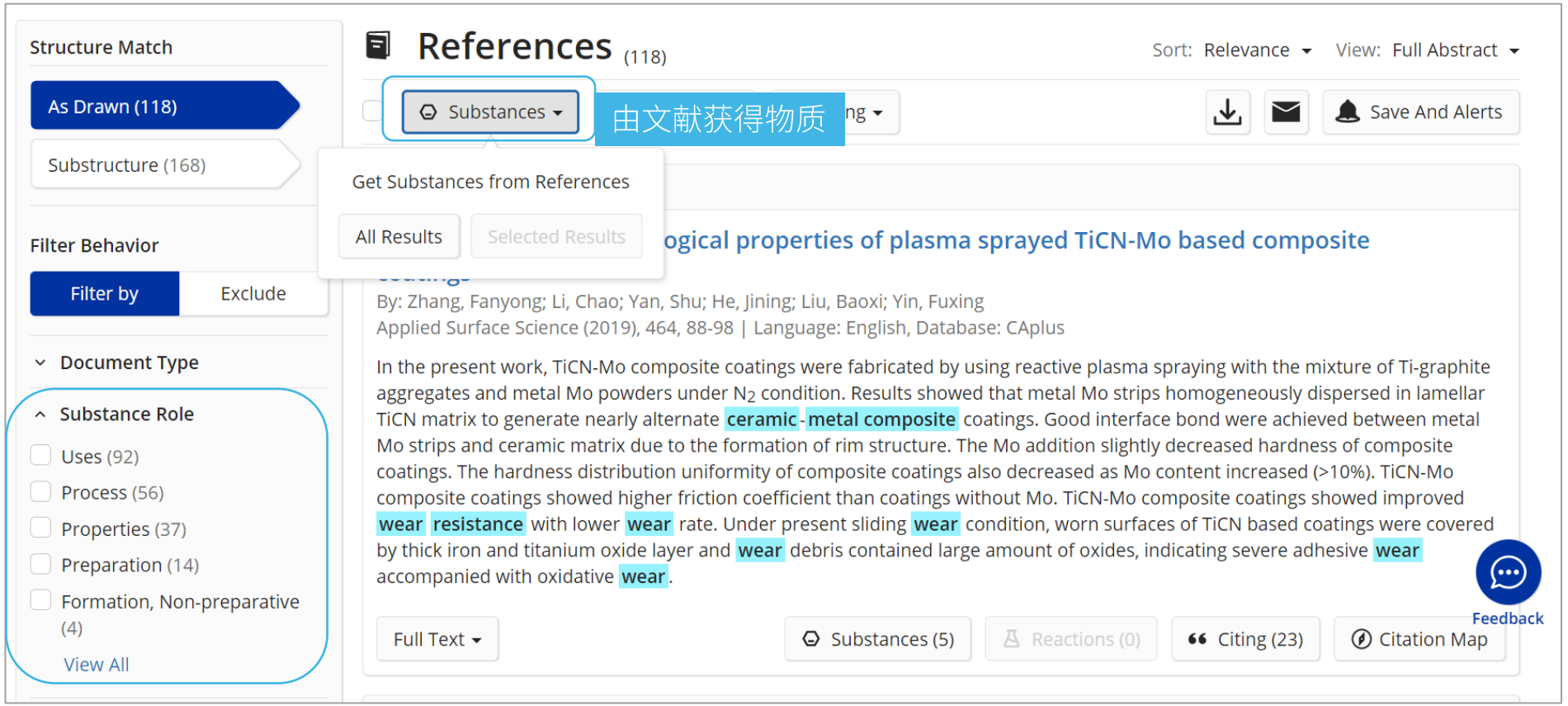



不同检索方式可联合使用

# 案例：含Ti或者Zr的耐磨陶瓷复合材料



# 可通过物质角色筛选选项快速筛选文献

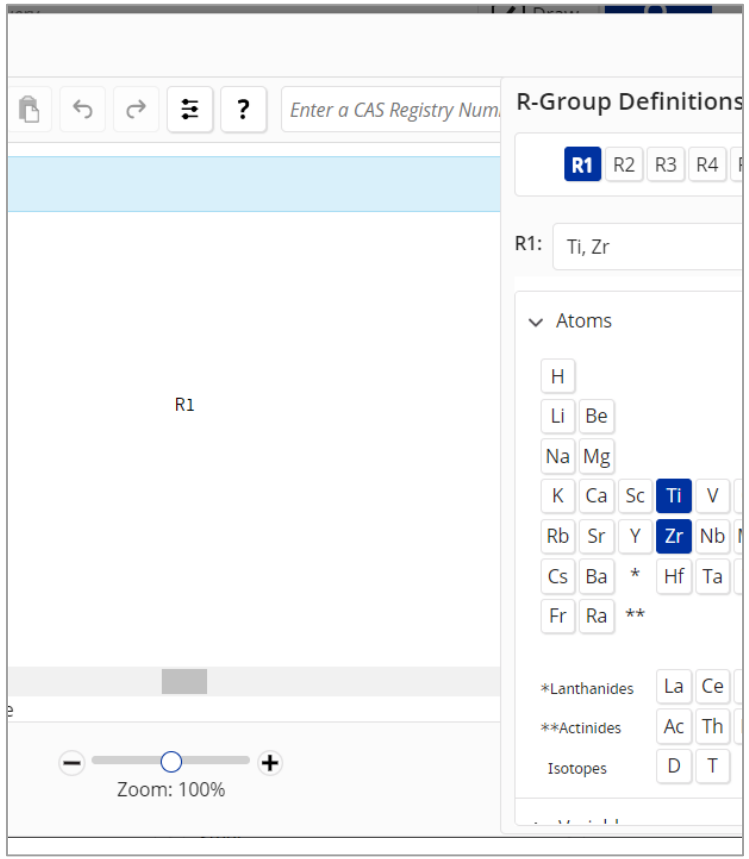


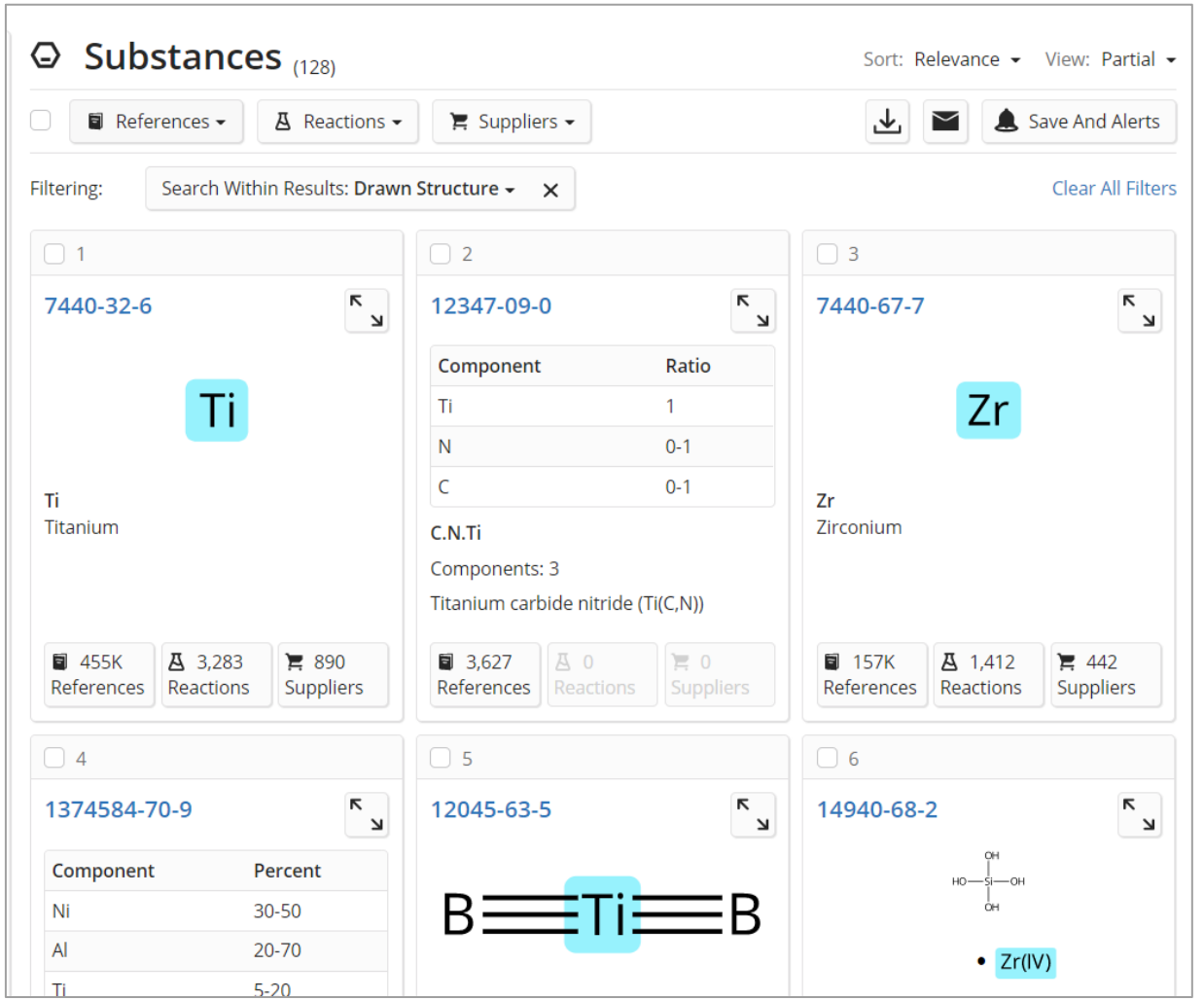

Substance role为物质在文献中的研究角色，如uses表明物质在文献中作应用研究；process作工艺研究等



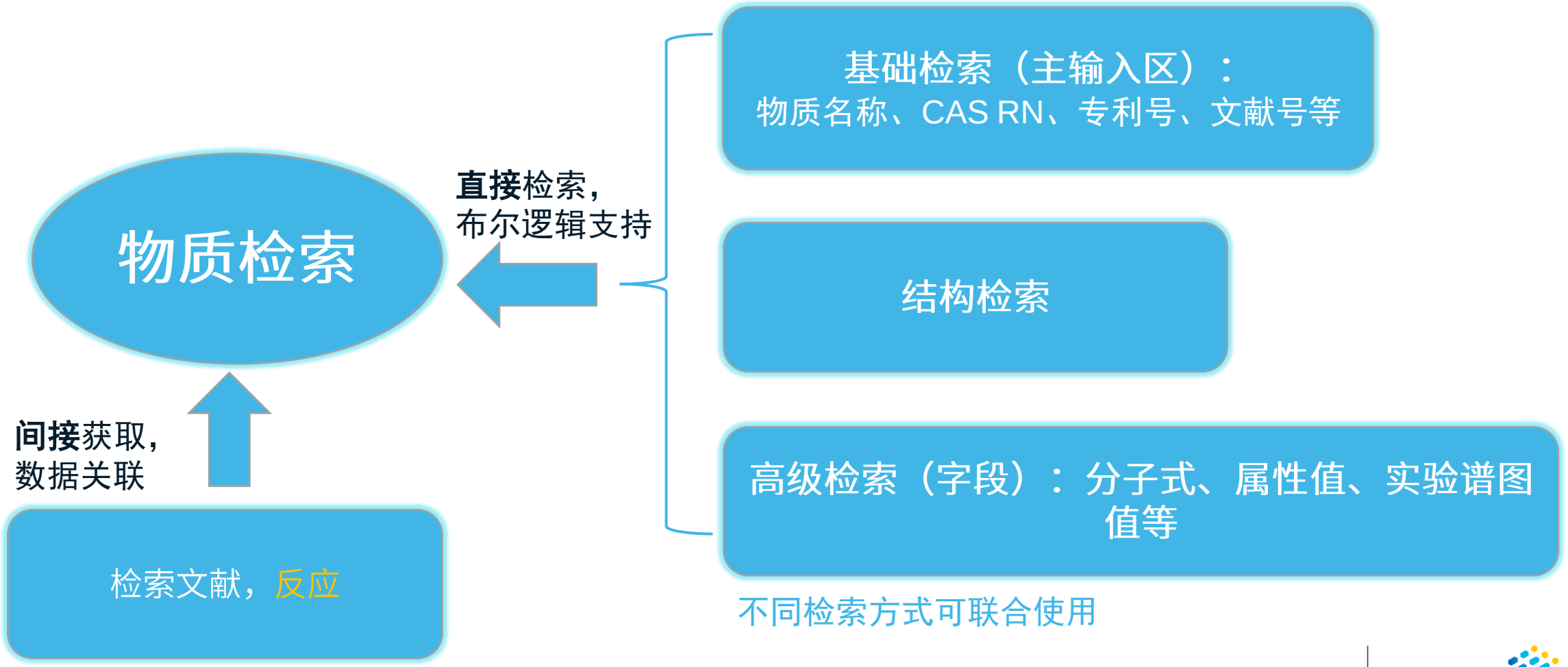
ACS International | CAS A division of the American Chemical Society

# 物质结果集中，用结构筛选出包含Ti或者Zr的结果

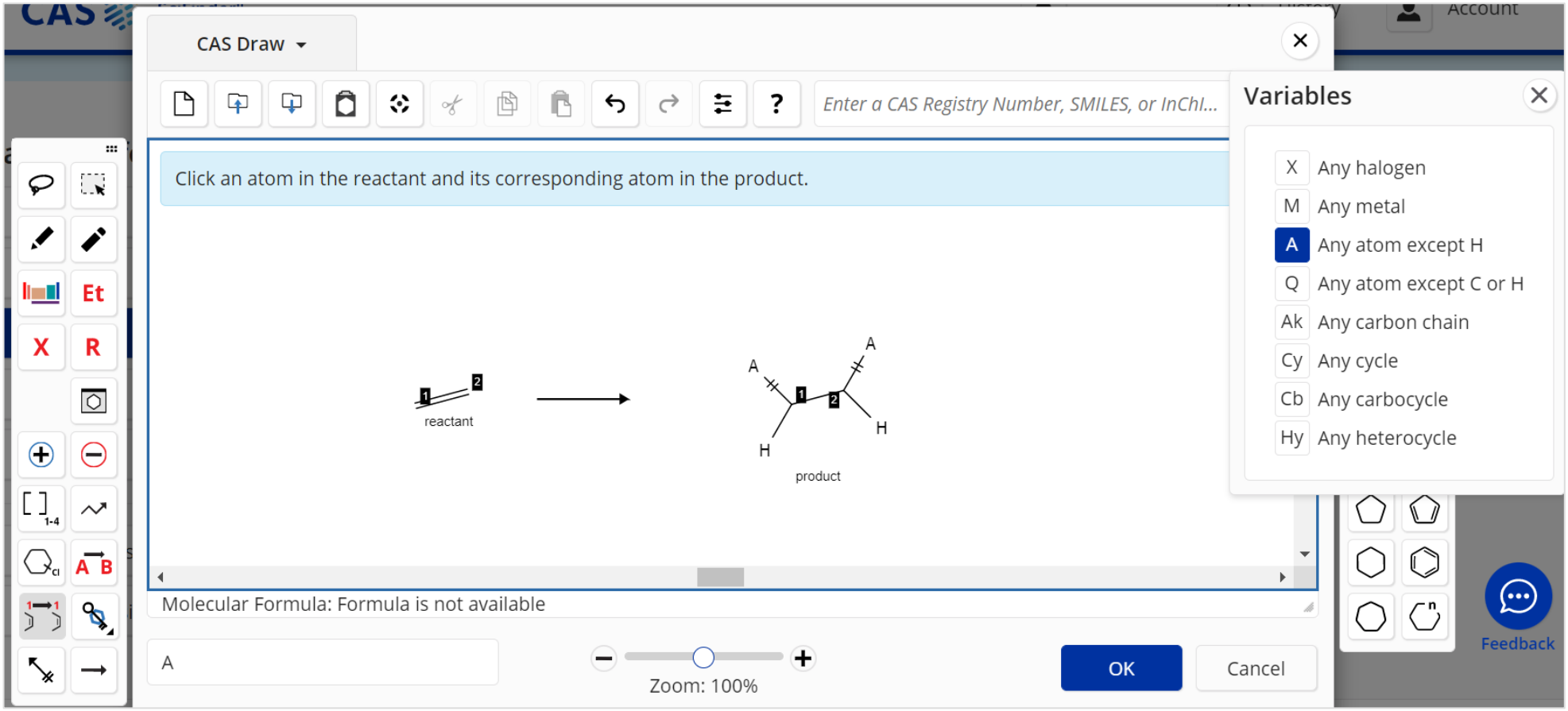


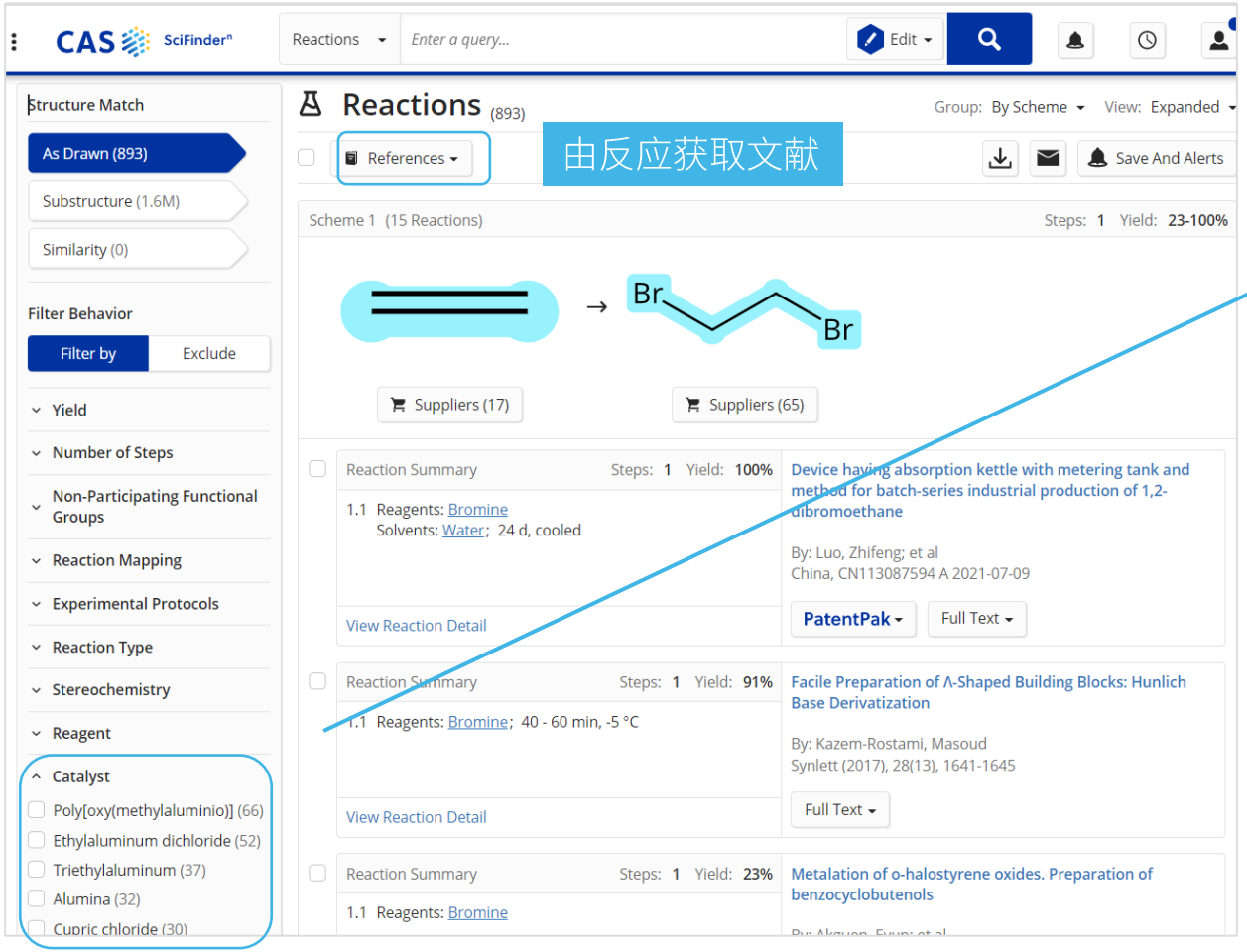
# 物质检索方法

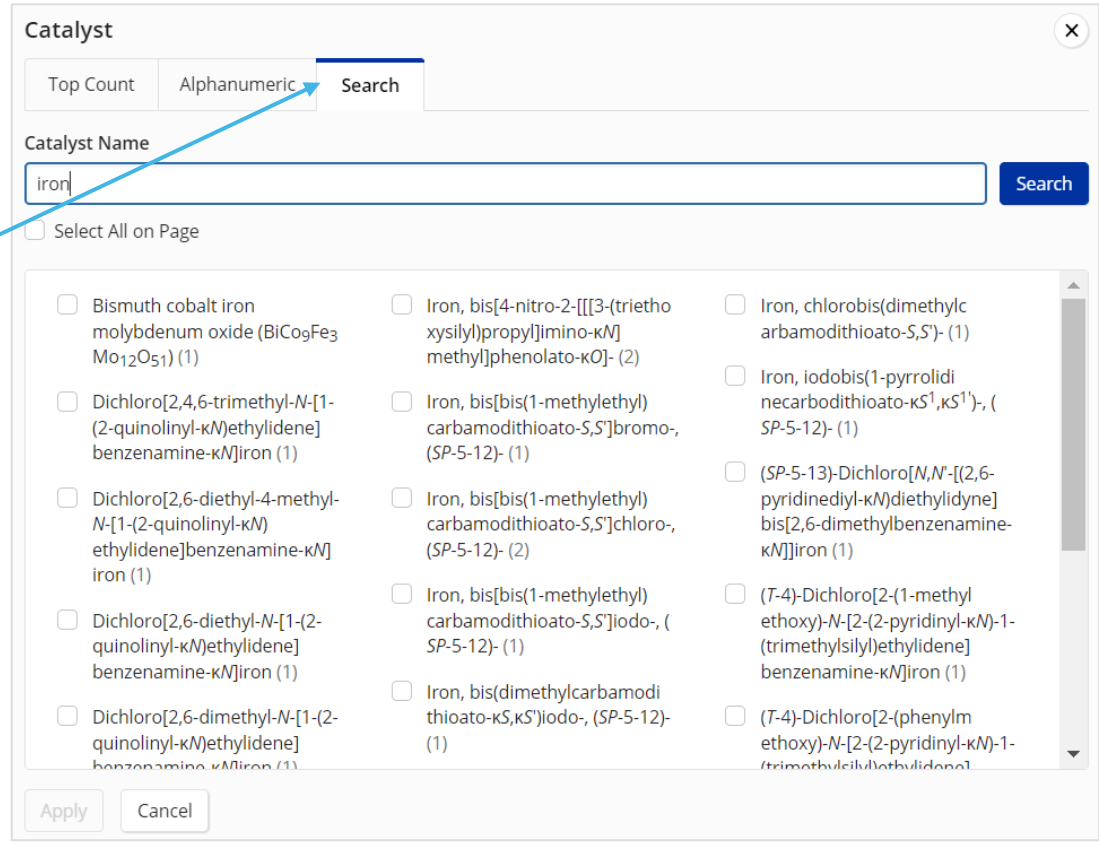


# 案例：乙烯加成反应中，铁/钴/镍基催化剂检索



# 在反应结果集中，可通过Catalyst直接查看，筛选催化剂

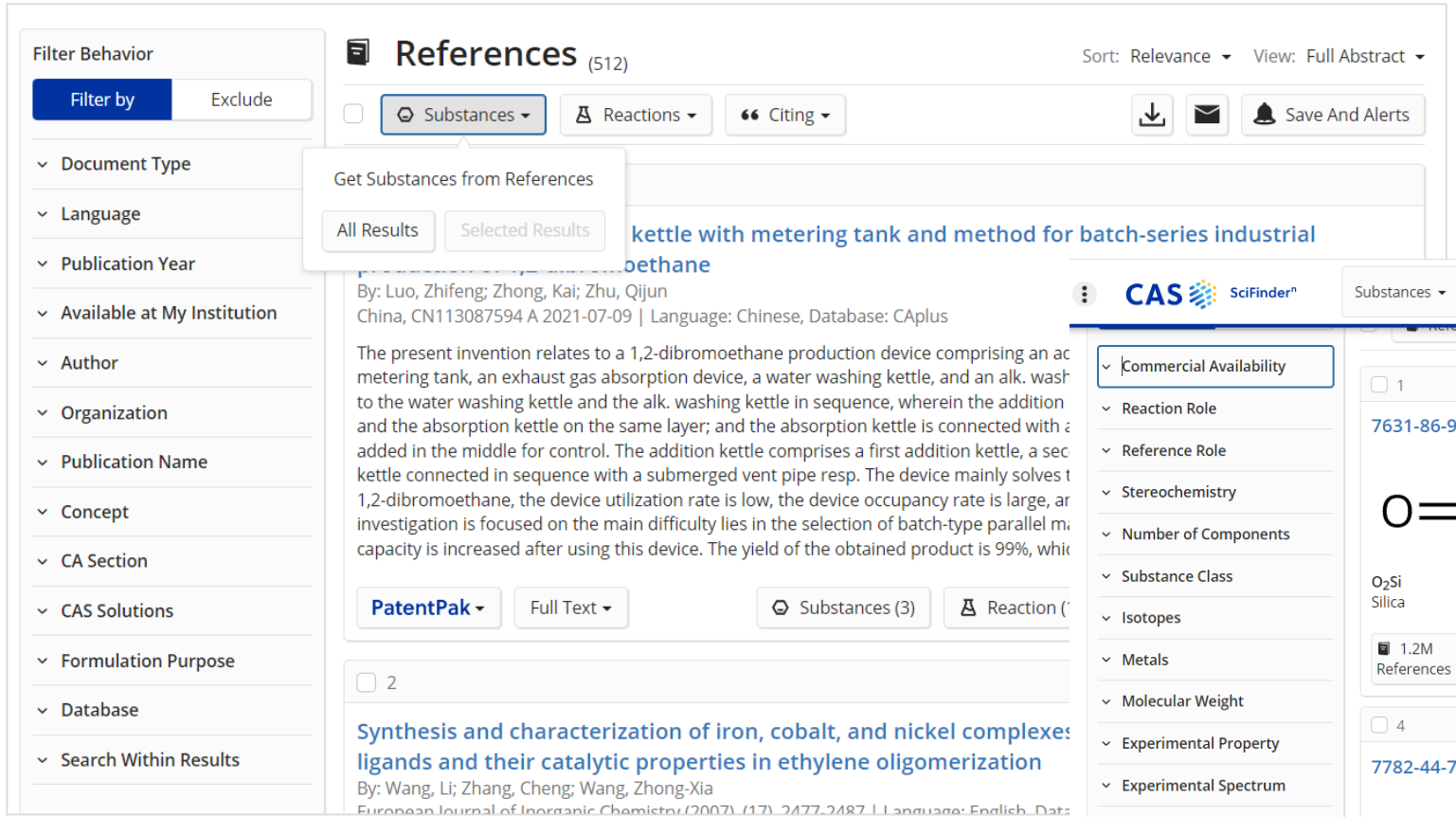


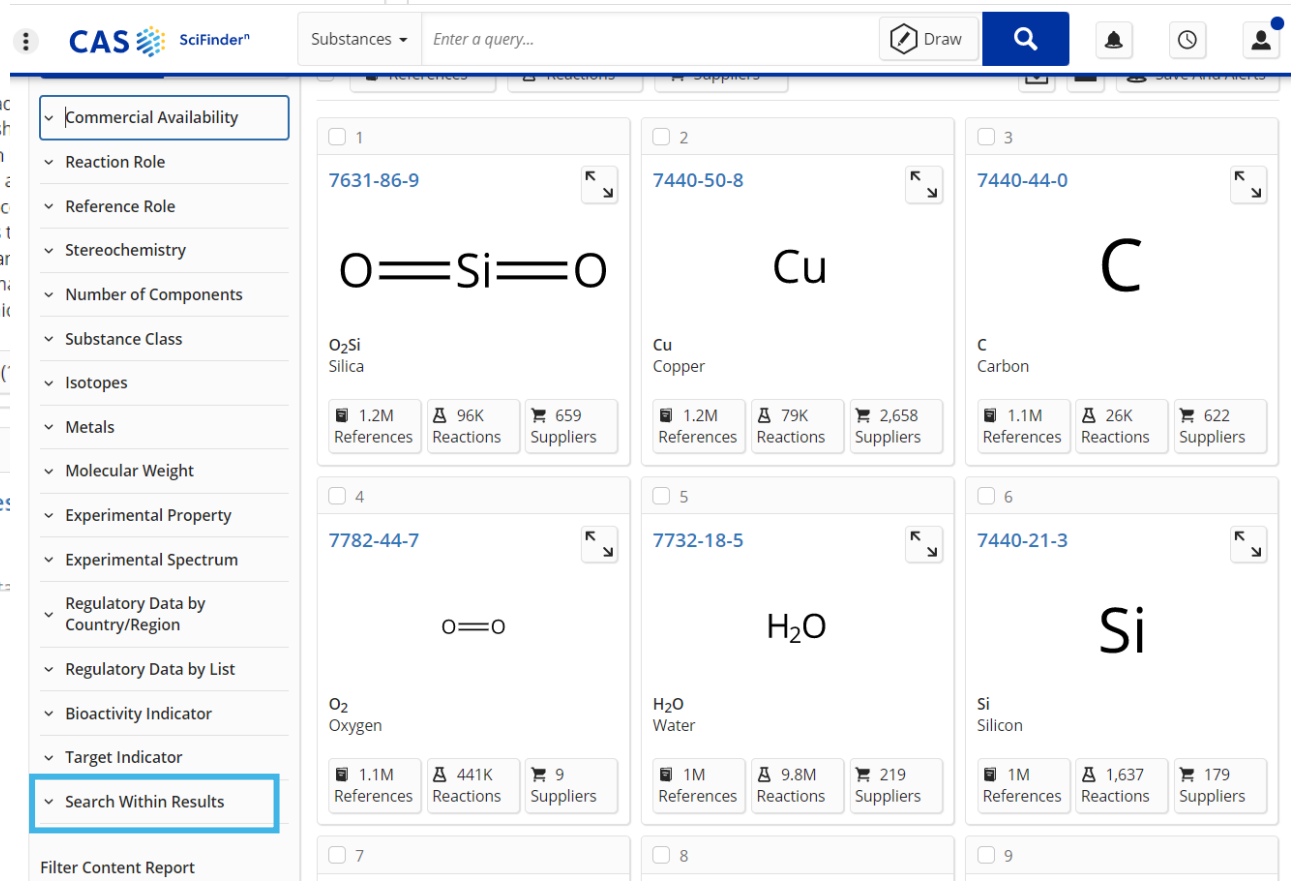





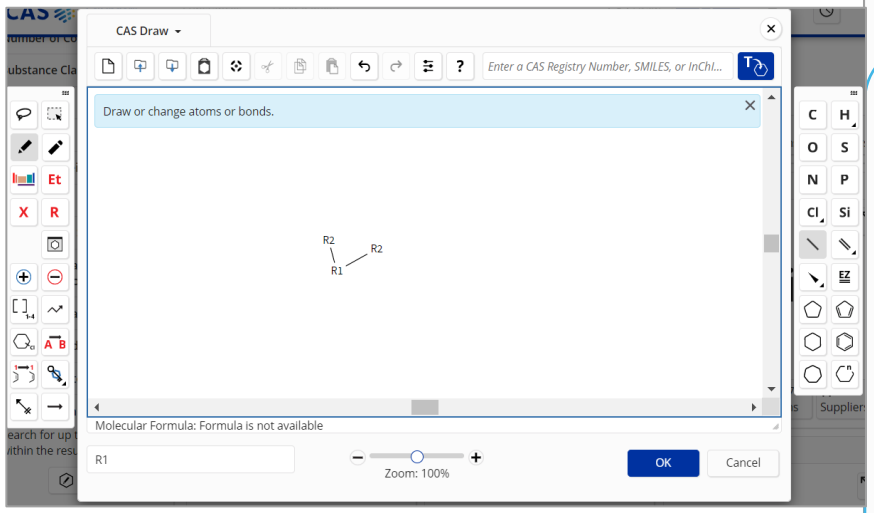

ACS International | CAS A division of the American Chemical Society

# 获得文献后，经过筛选再获取物质



# 通过结构筛选物质




R1 = Fe, Co, Ni

R2 = N, P


可以通过物质的反应角色或者文献角色筛选物质



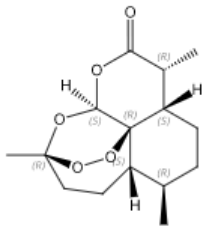
ACS International

CAS
A division of the American Chemical Society

# 物质属性或者谱图查看

1 点击物质CAS号

63968-64-9



Absolute stereochemistry shown

$C_{15}H_{22}O_5$

Qinghaosu

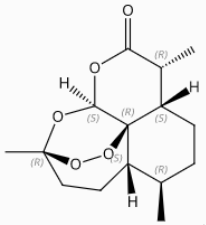
7,843 References | 2,965 Reactions | 95 Suppliers

## Substance Detail ( 1 of 1 )

References (7,843) | Reactions (2,965) | Suppliers (95)

CAS Registry Number

63968-64-9



Absolute stereochemistry shown

$C_{15}H_{22}O_5$

3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)- (9CI, ACI)

| Key Physical Properties | Value | Condition |
|---|---|---|
| Molecular Weight | 282.33 | - |
| Melting Point (Experimental) | 156-157 °C | - |
| Boiling Point (Predicted) | | |
| Density (Experimental) | | |

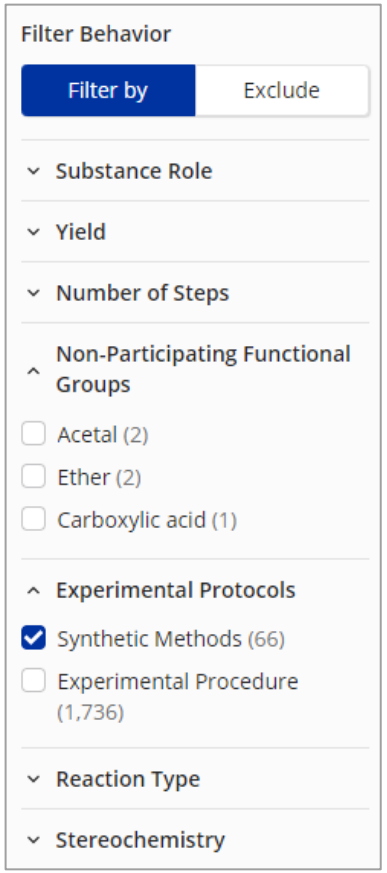
### Experimental Properties

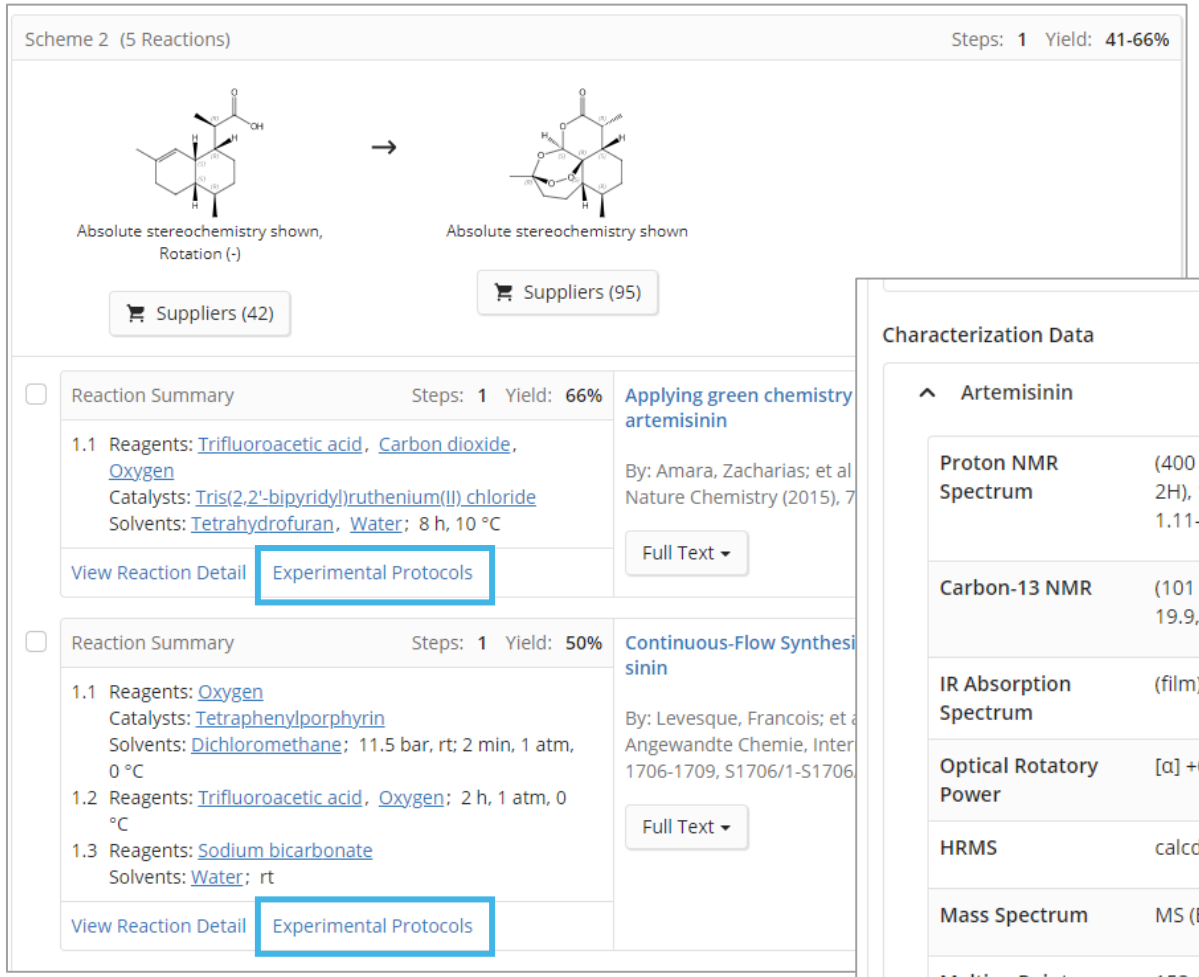
Biological | Chemical | Density | Flow and Diffusion | Lipinski | Optical and Scattering

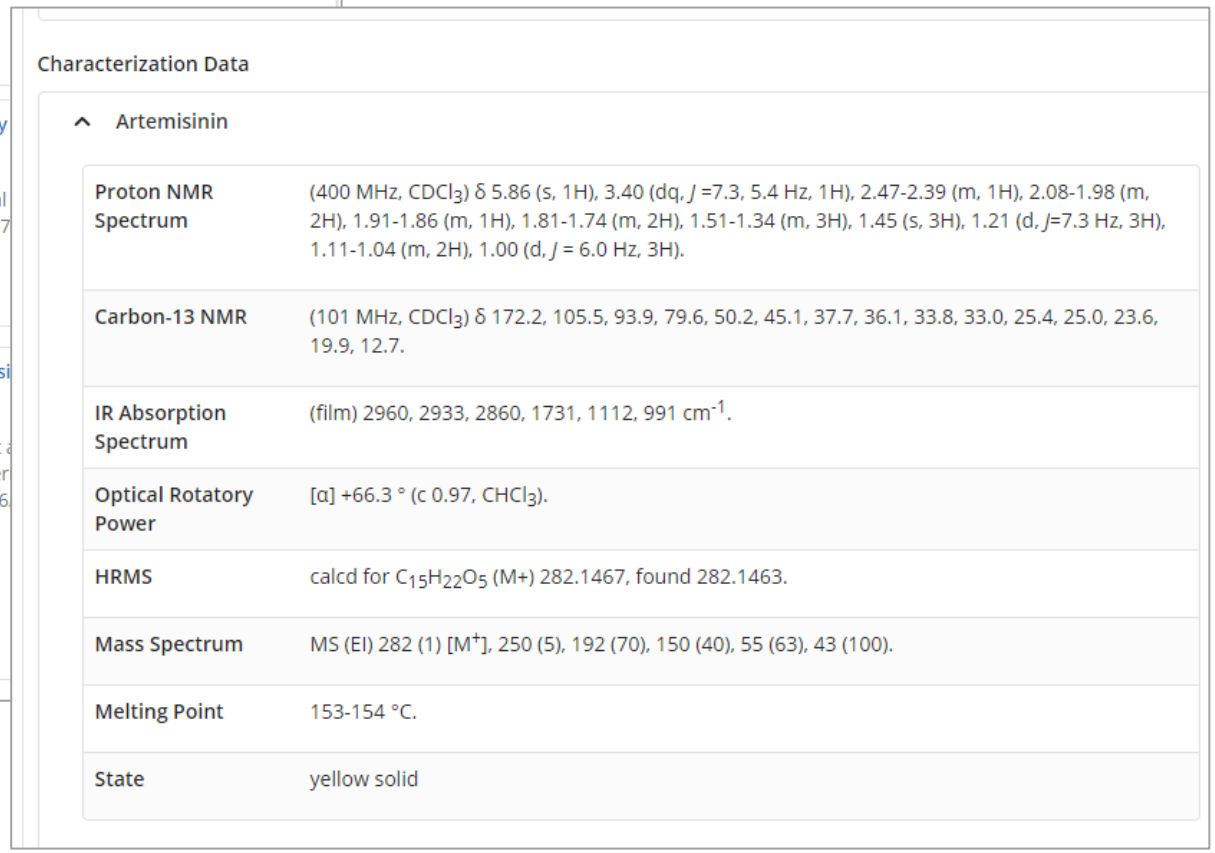
| Property | Value | Condition |
|---|---|---|
| Median Lethal Dose | 5576 mg/kg | Organism: rat; Route: oral |
| Median Lethal Dose | 5105 mg/kg | Organism: mouse; Route: o |
| Median Lethal Dose | 2800 mg/kg | Organism: mouse; Route: i |
| Median Lethal Dose | 2571 mg/kg | Organism: rat; Route: intra |
| Median Lethal Dose | 1558 mg/kg | Organism: mouse; Route: i |

- Experimental Spectra
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- Additional Details

# 在反应方法中查看



# 总结：CAS SciFinderⁿ支持多途径物质检索

- 基础检索：物质标识符；文献号
- 结构式检索：
  - 与Chemdraw联用
  - 有机化合物、盐类、金属有机化合物均支持结构式检索
- 高级检索：
  - 属性值检索：助力结构解析、快速检索功能材料
  - 分子式检索：无机盐、合金等
- 通过文献或者反应获取物质
- 点击物质CAS号，或者在反应方法中查看物质属性、谱图信息

# 学习资源

1. 关注“ACS美国化学会”微信公众号, 搜索SciFinder-n，查看检索技巧、检索视频，以及论坛回放视频

2. CAS SciFinder$^{n}$网络在线演示培训资料
https://www.cas.org/about/events/scifinder-webinars

3.CAS官网上的培训资料
https://www.cas.org/support/training/scifinder-n

4.CAS SciFinder$^{n}$ Help使用指南
https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FIntroduction_to_searching.htm

ACS International | CAS A division of the American Chemical Society