CAS SCIFINDER-N

高效获取科技信息

刘子露
ZLiu@acs-i.org
美国化学文摘社(CAS)北京代表处

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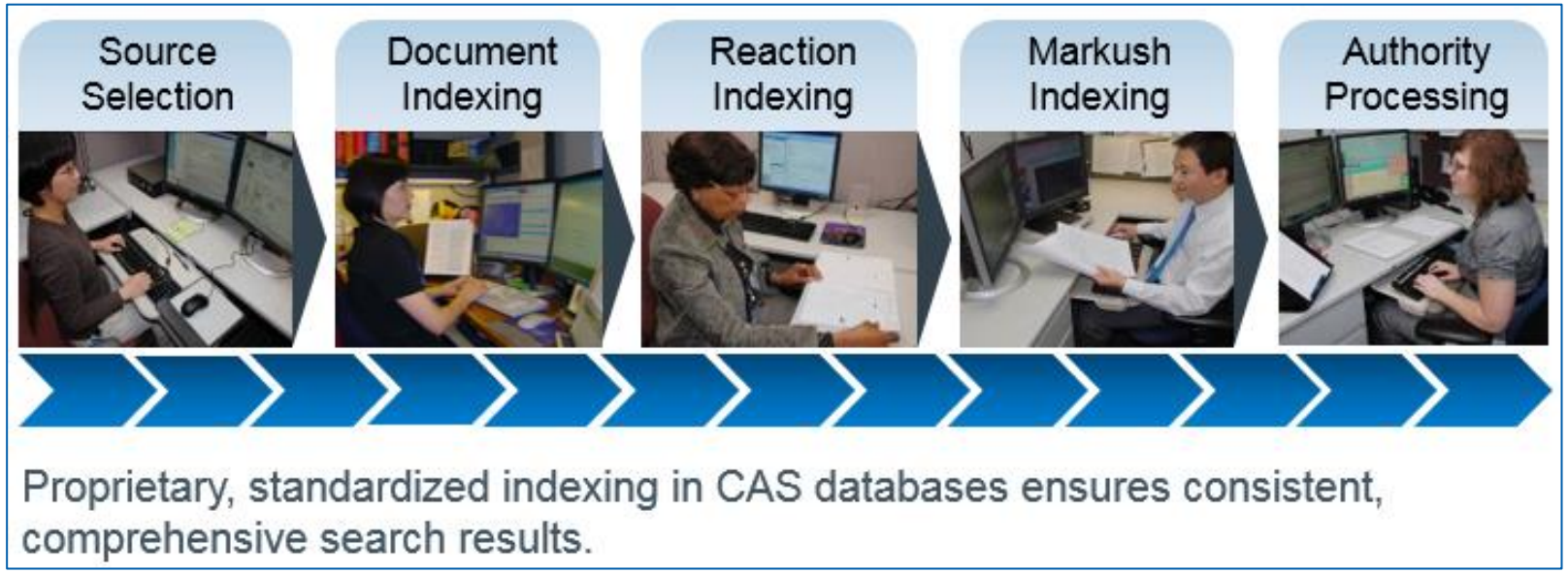
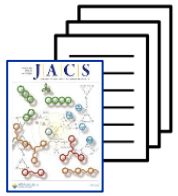
大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 常见检索方式
  - 文献检索
  - 物质检索 (CAS Markush*)
  - 反应检索
  - 逆合成反应路线设计 (CAS Retrosynthesis*)
  - 序列检索*
- 常见问题及解答

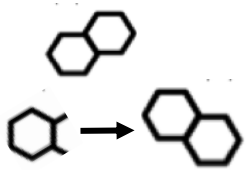
CAS科学家的智力标引

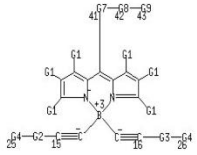


Data pre-repository



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 具有最全面的学科连接内容合集

Over
55K
scientific journals and documents

Over
274
million substances

Over
50
languages translated

Over
64
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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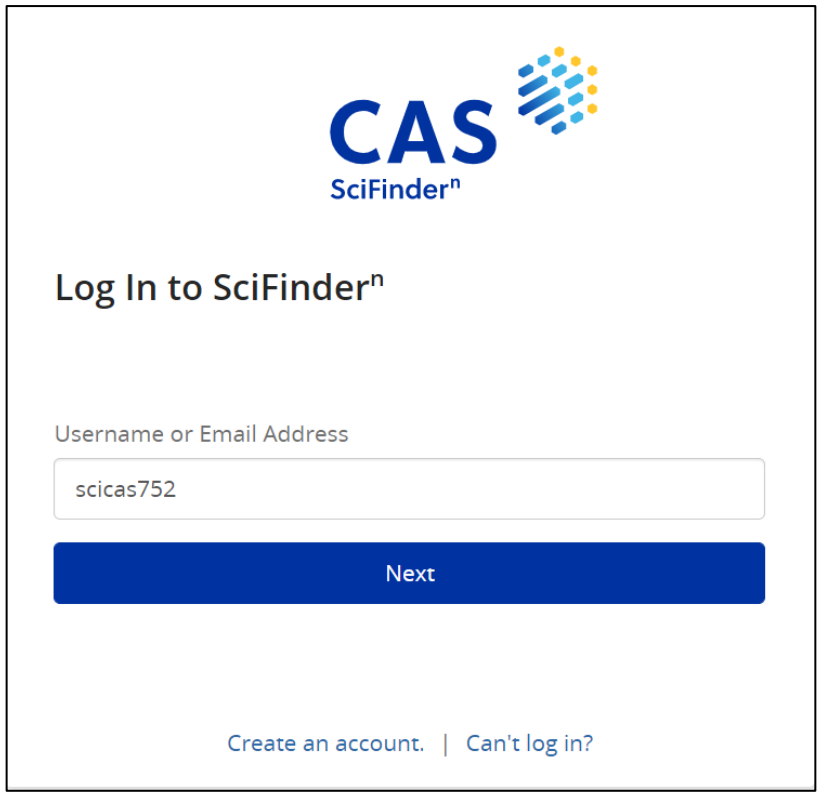
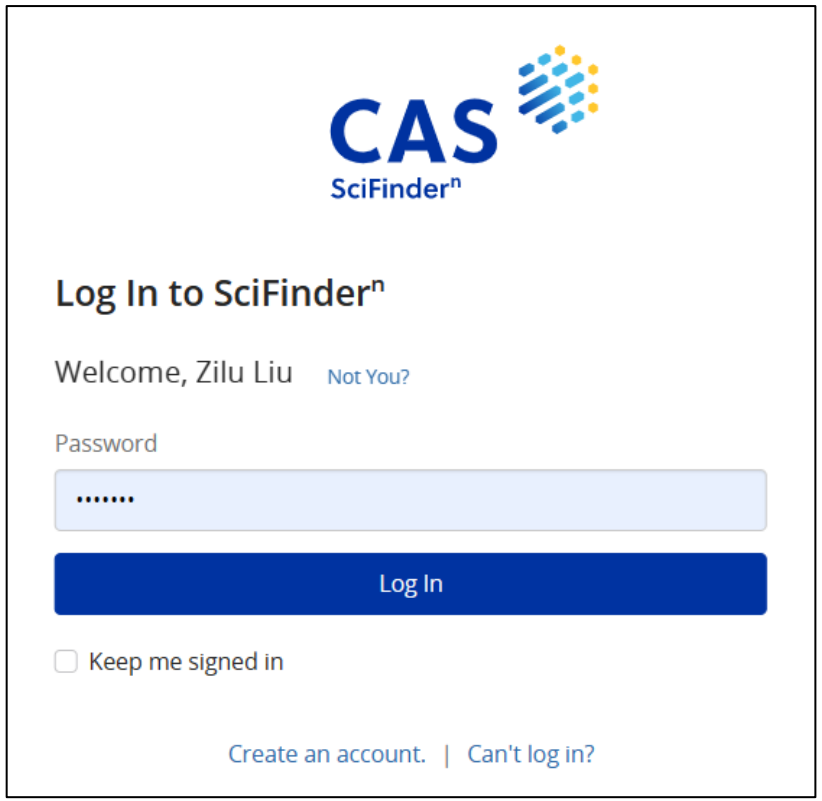
CAS SciFinder^{n}登录网址: https://SciFinder-n.cas.org





使用CAS SciFinder账号登录

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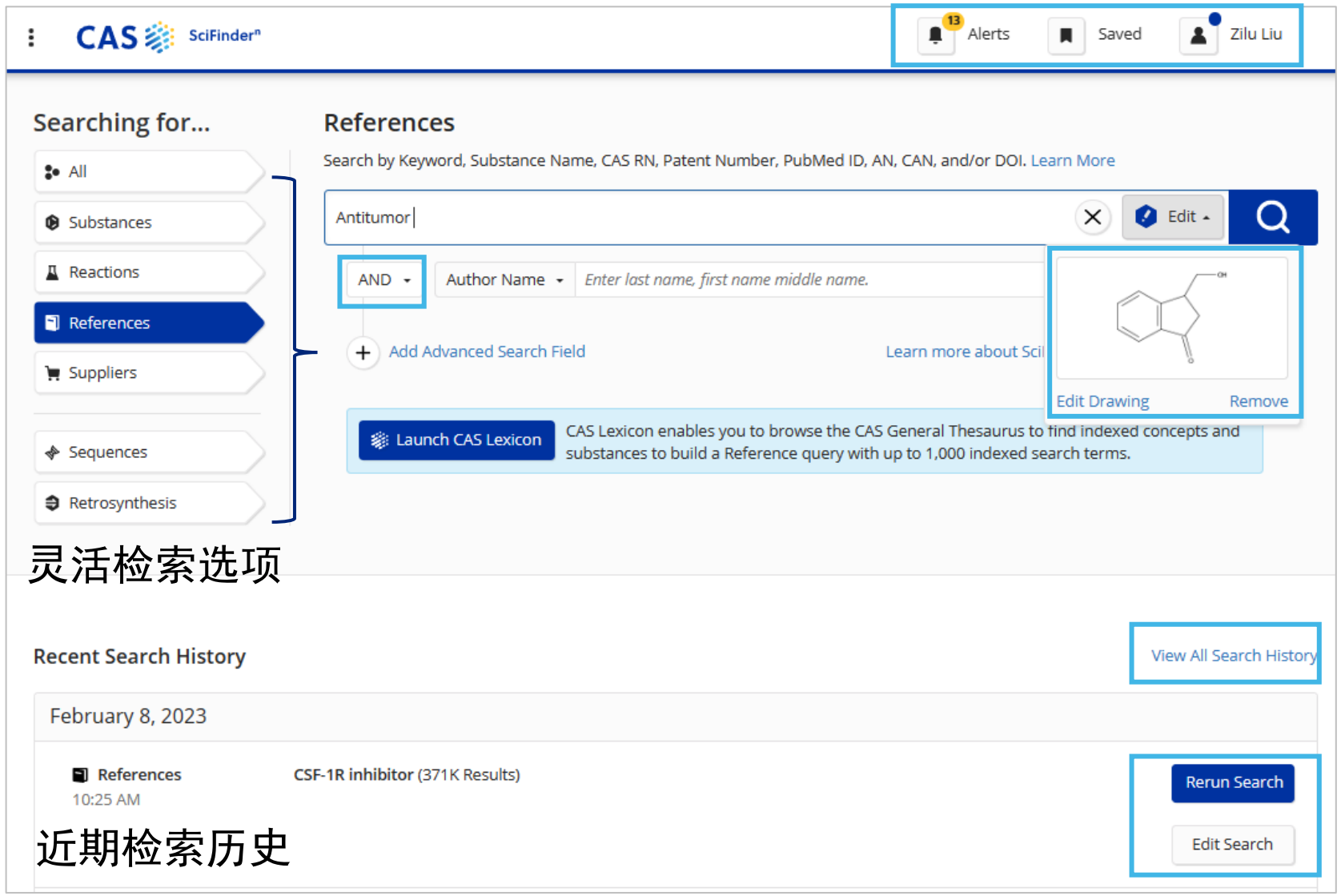
CAS SciFinder^{n}主界面



灵活检索选项

近期检索历史

提醒更新的结果
已保存的检索和结果集
账户信息

检索项逻辑关系
文本与结构检索便捷联用

查看全部检索历史

重新运行检索式
修改检索式

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大纲

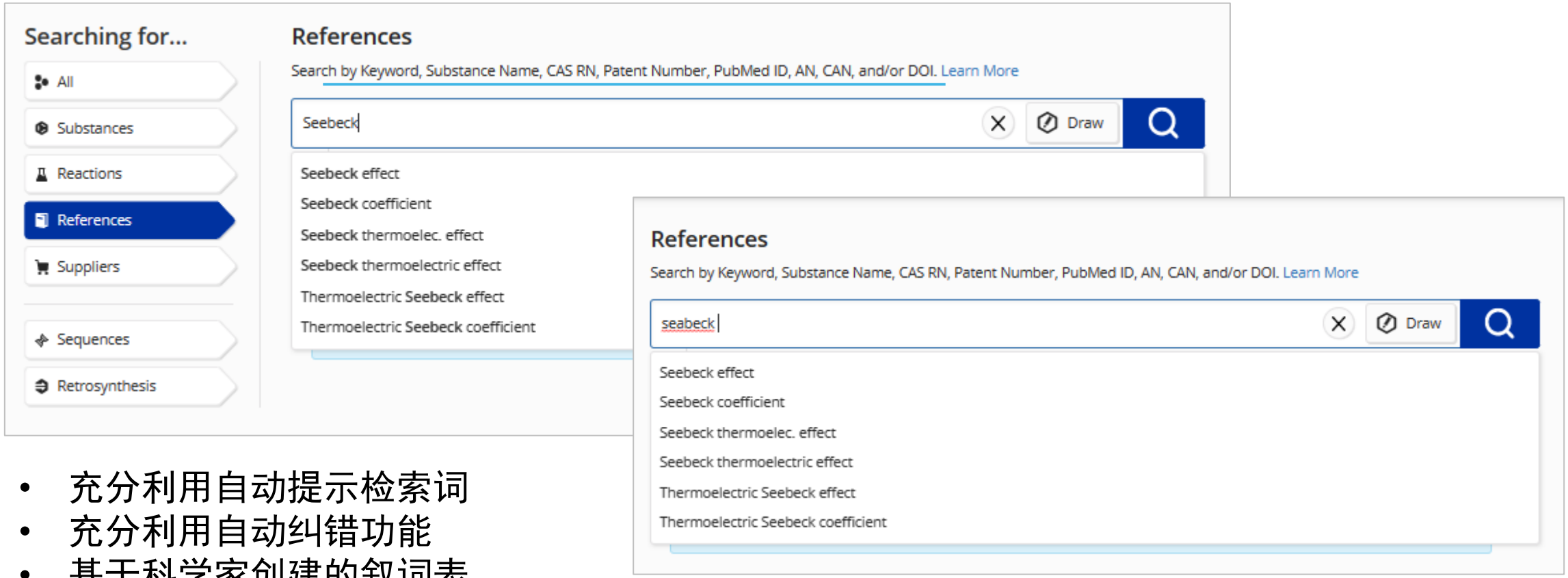
- CAS及CAS SciFinder^{n}简介
- 常见检索方式
  - 文献检索
  - 物质检索 (CAS Markush*)
  - 反应检索
  - 逆合成反应路线设计 (CAS Retrosynthesis*)
  - 生物序列检索*
- 常见问题及解答

文献检索

- 文献检索方法
  - 主题词的构建技巧
  - 利用高级检索项自定义组合检索
  - 间接检索：从物质、反应获得文献
- 检索策略推荐
  - 关注某特定领域的文献：主题检索
  - 关注物质有关的文献：先获得物质，再获得文献或文本+结构联合检索
  - 关注某科研人员的文献：作者名检索
  - 关注某机构科研进展：机构名检索

主题词检索

支持使用：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI



- 充分利用自动提示检索词
- 充分利用自动纠错功能
- 基于科学家创建的叙词表

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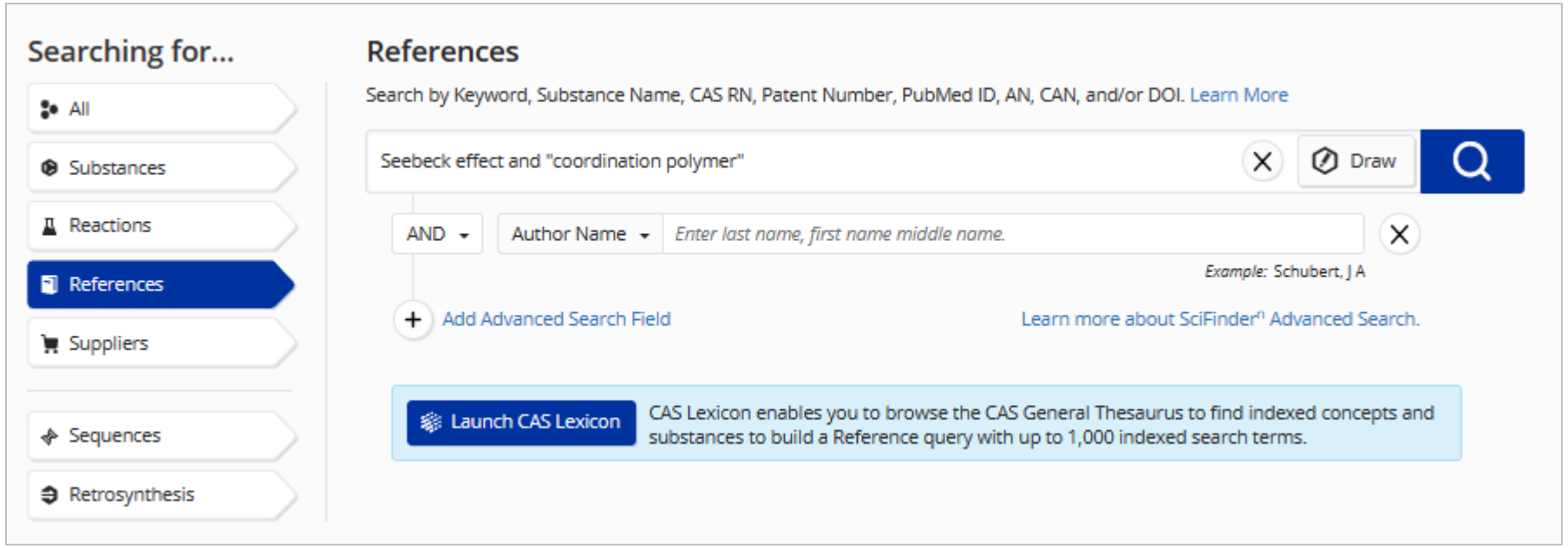
使用布尔逻辑运算符，精准构建检索主题

- 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？，如 petro*可代表petrol, petroleum, petrochemical等（*代表0或多个字符；？代表0或1个字符）



CAS SciFinder-n Help

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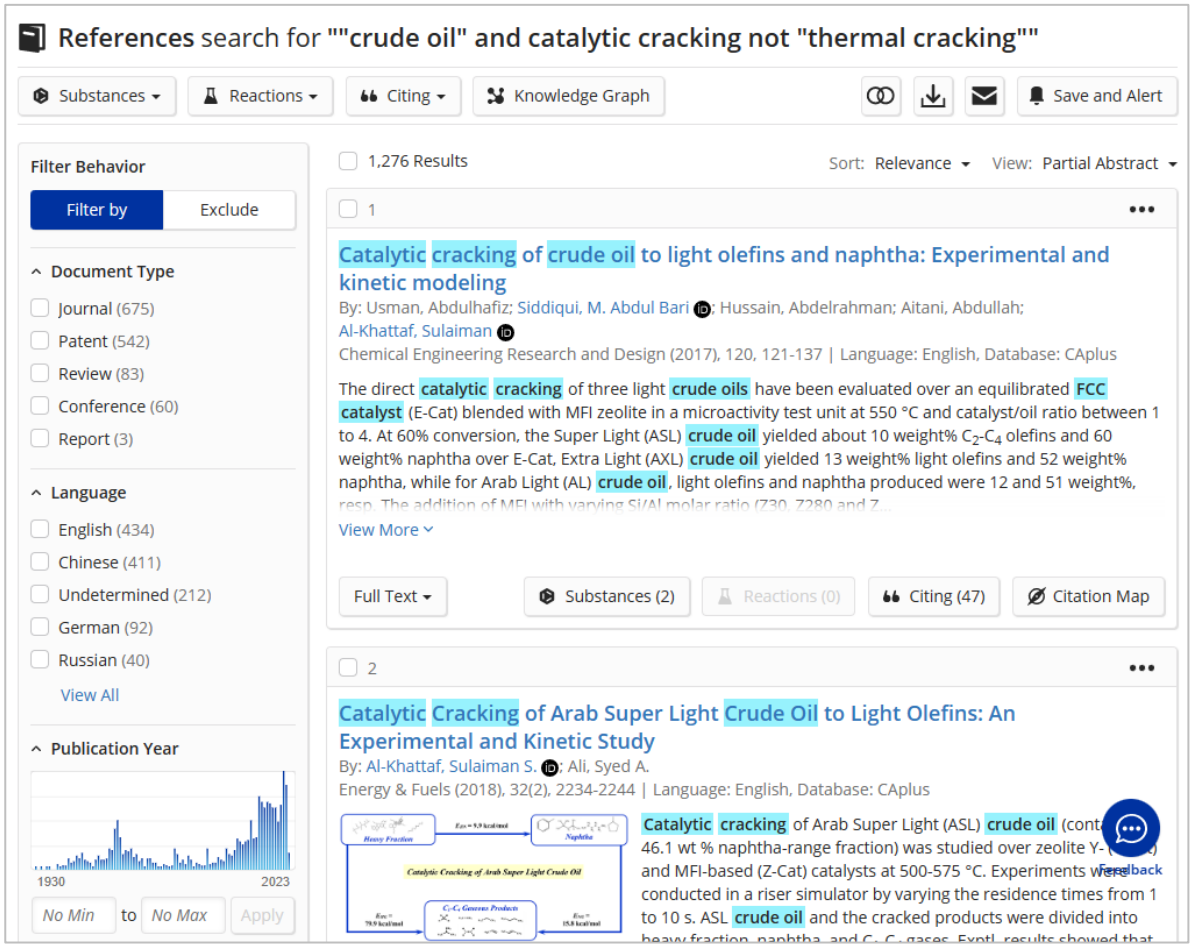
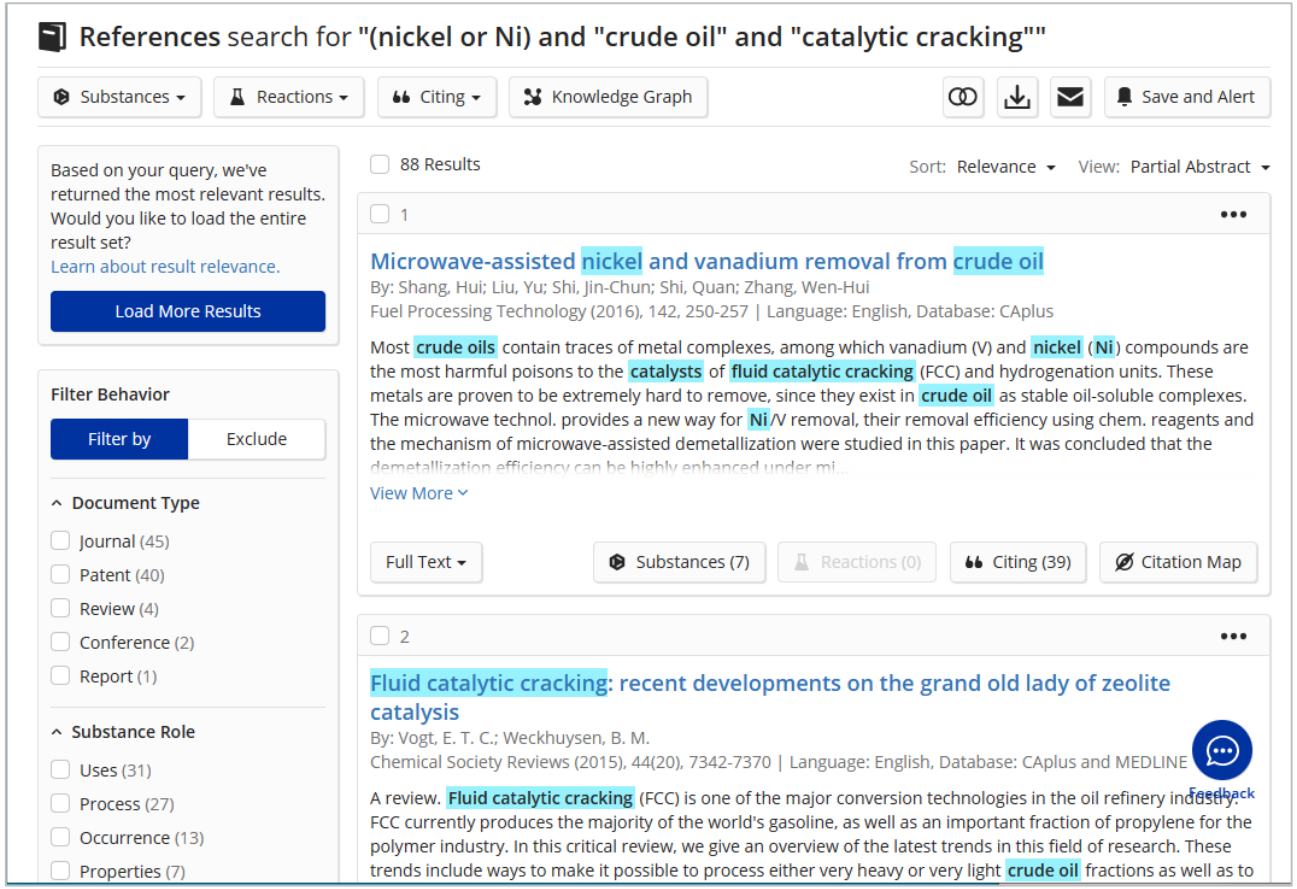
使用布尔逻辑运算符，精准构建检索主题

“crude oil” and “catalytic cracking” not “thermal cracking”
检索：原油裂解，排除热解



(Nickel or Ni) and "crude oil" and "catalytic cracking“
检索：与镍、及原油裂解相关



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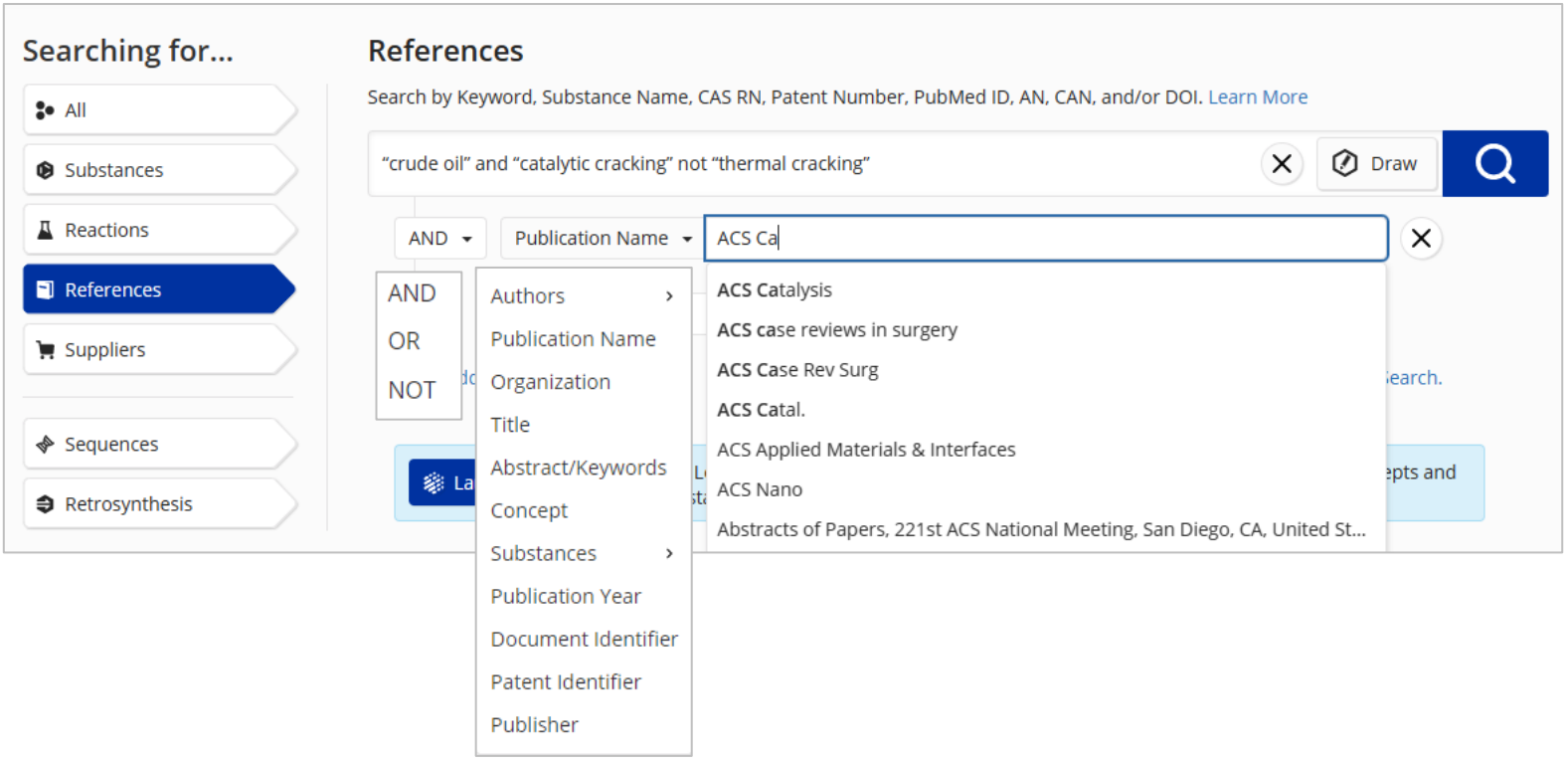
高级检索—高效实现多项自定义组合检索



文本检索：
关键词、物质名称、CAS RN、DOI等

高级检索：
作者名、期刊名、机构名、题目、摘要、概念词、物质标识符、出版商

结构检索

* 检索方法可单独使用，也可联用

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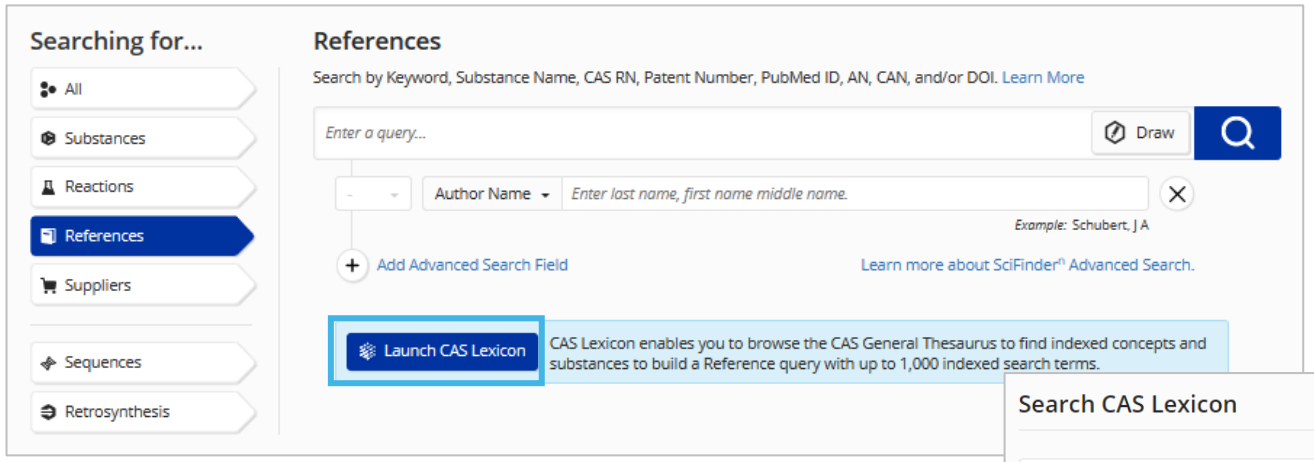
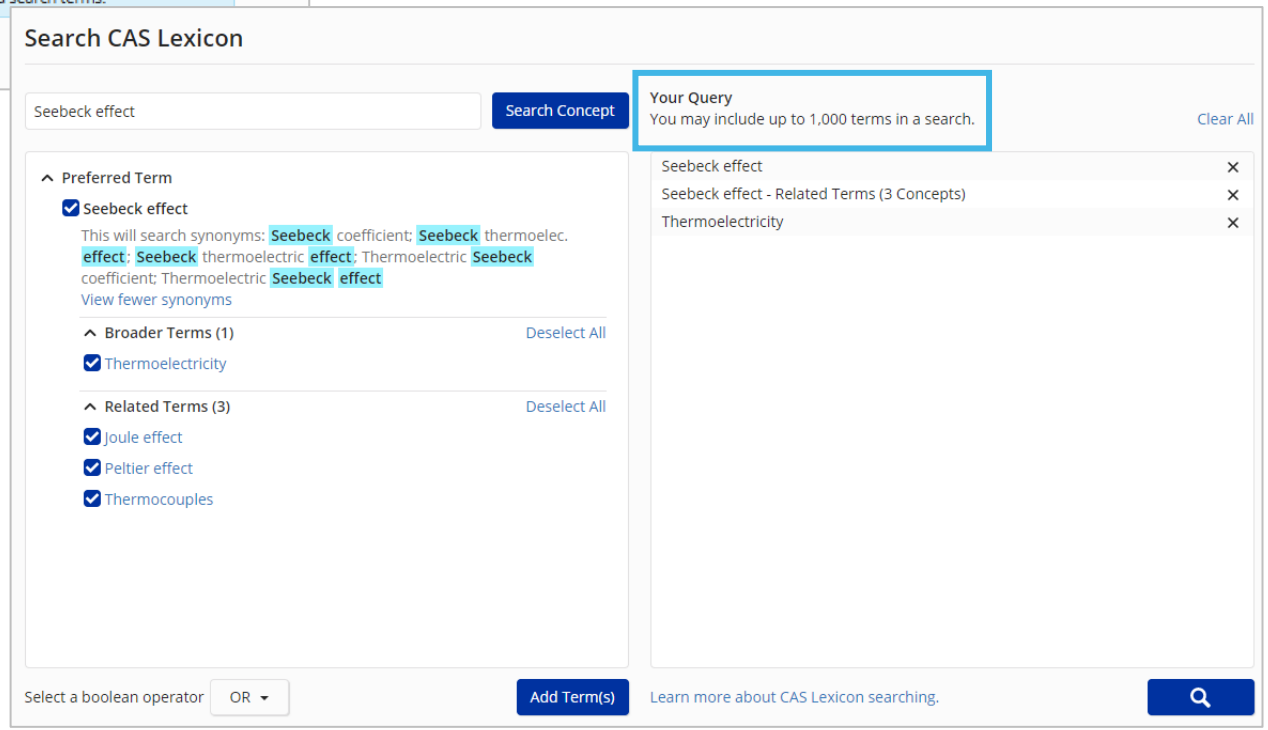
CAS Lexicon—利用词库选词启发检索



- 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 Term
- Broader Terms
- Narrower Terms
- Related Terms

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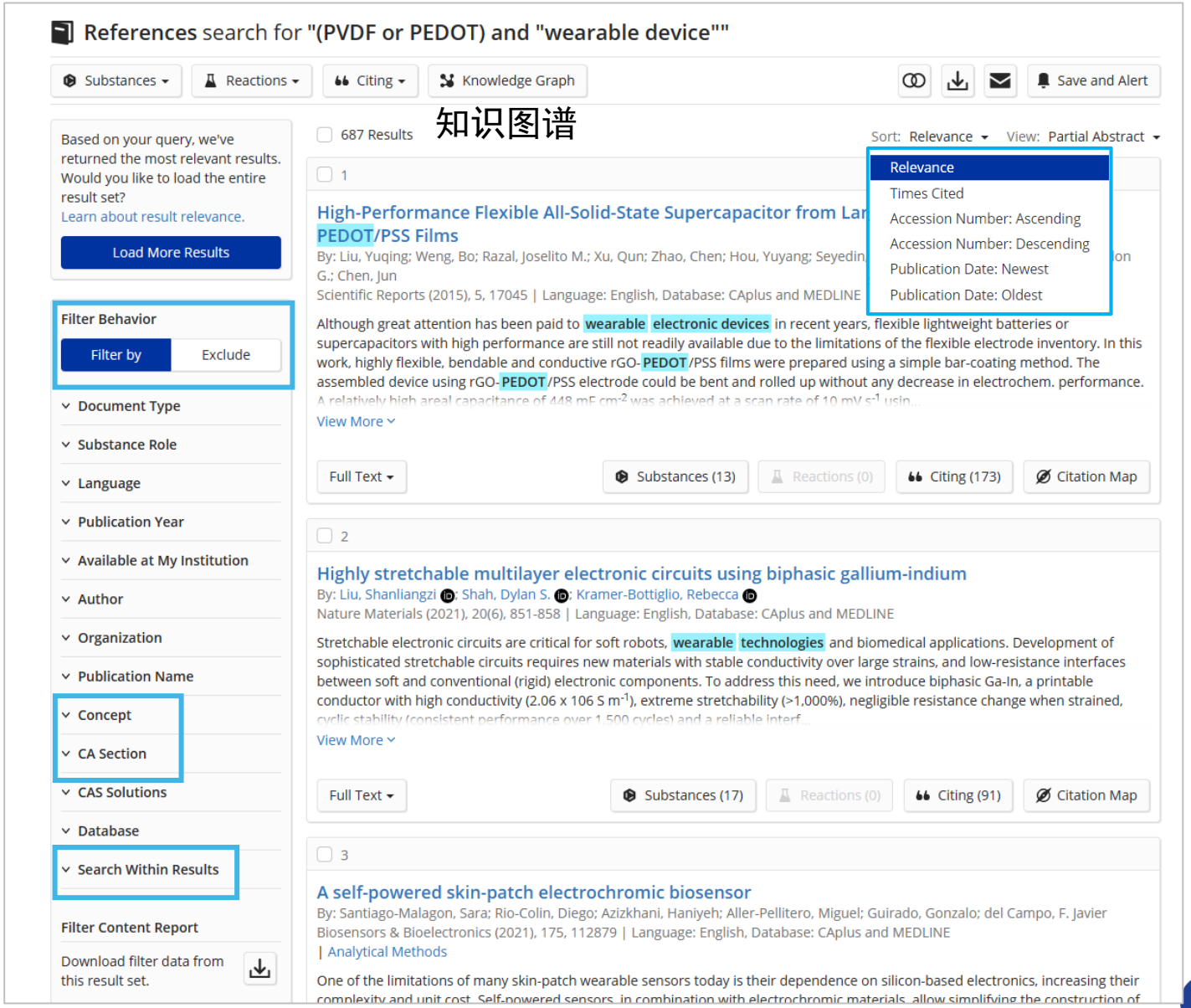
文献结果集—排序与筛选

- 聚类筛选项一目了然
- 直接勾选高效定位所需信息
- 无需逐步二次检索和限定



排序方式：
相关性
引用次数
收录号
发表时间

文献类型

文献语言

研究发展趋势

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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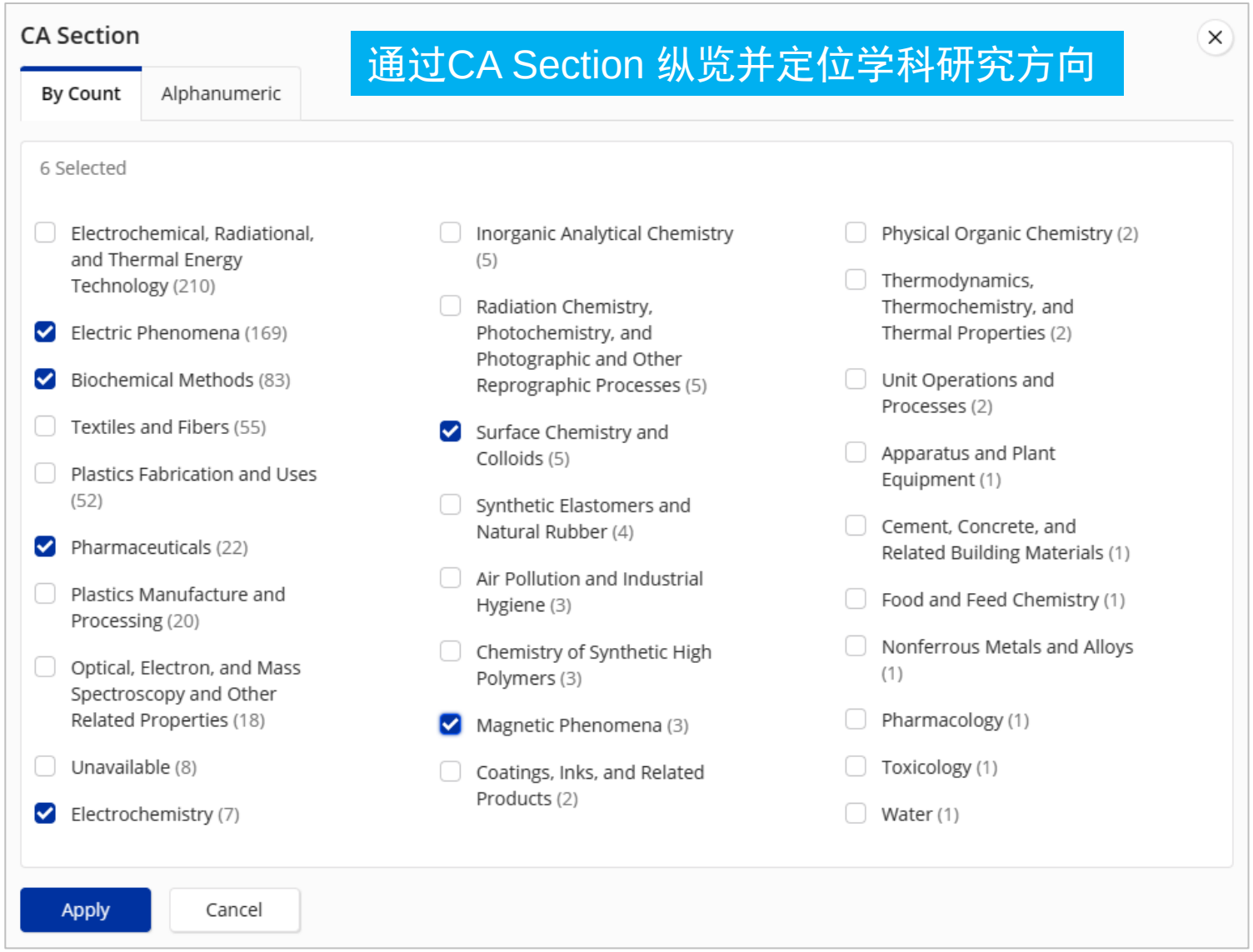
CAS标引的学科研究方向



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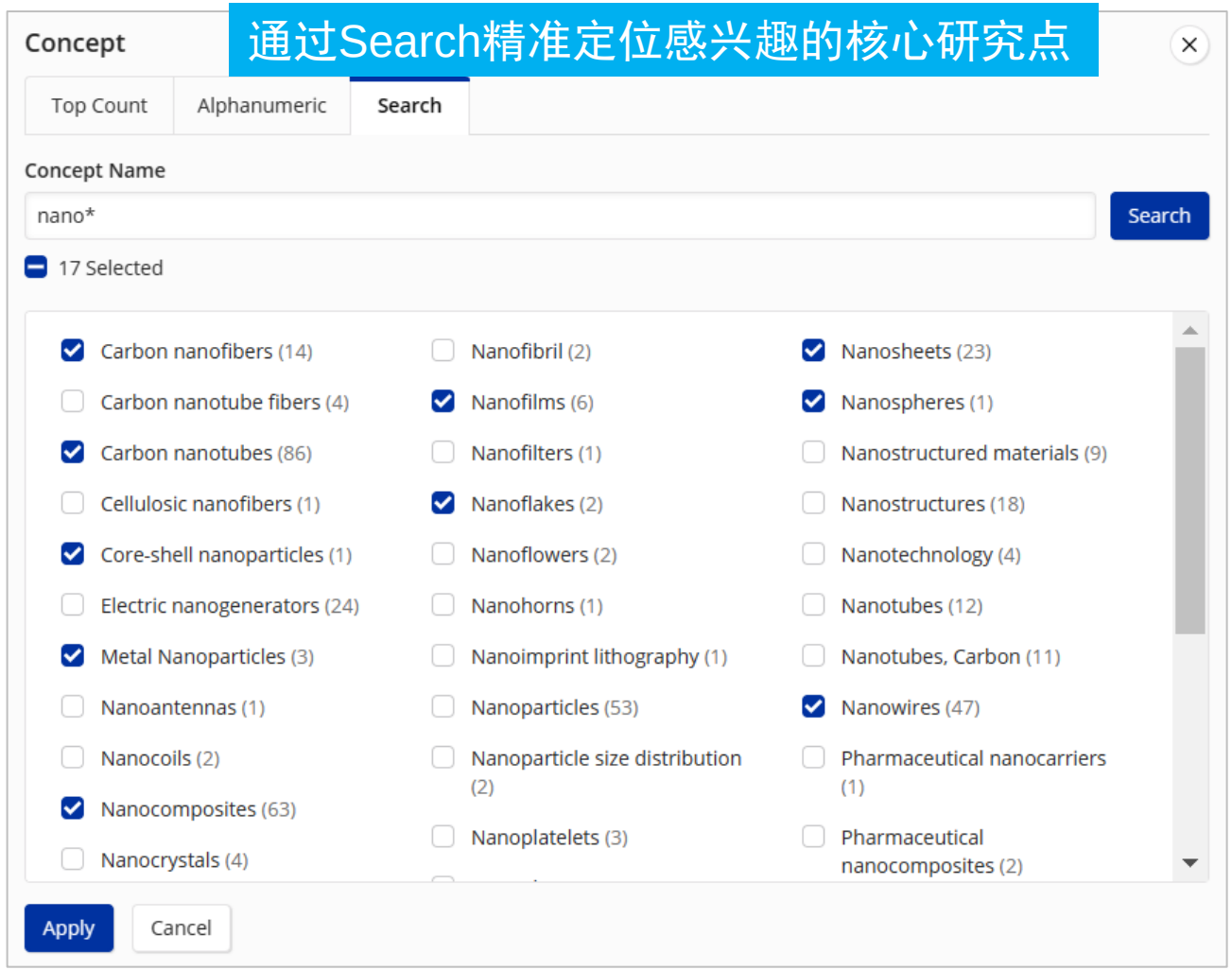
文献结果集—聚类筛选Concept



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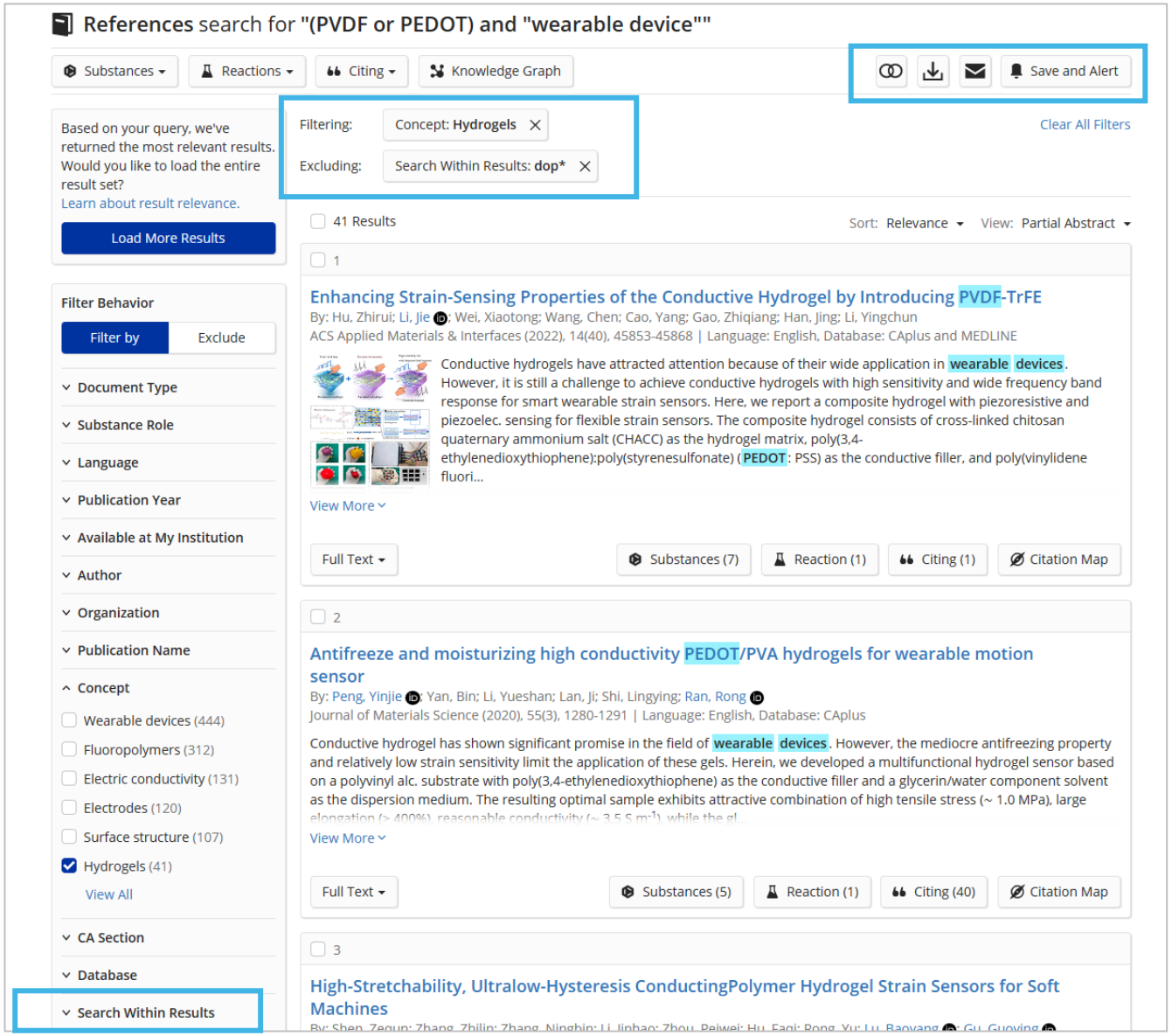
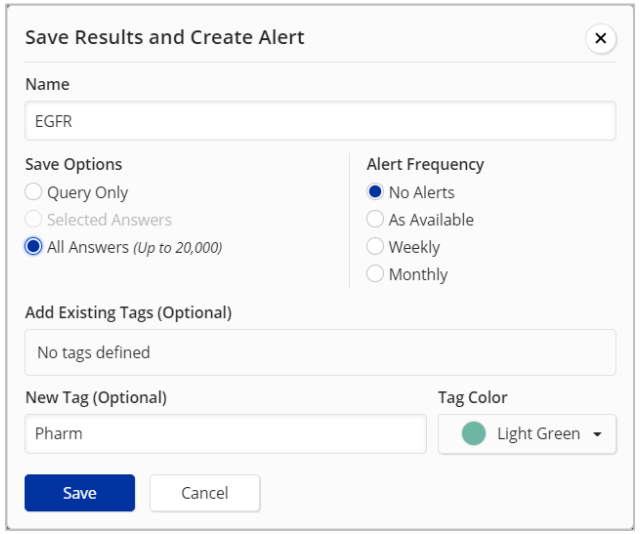
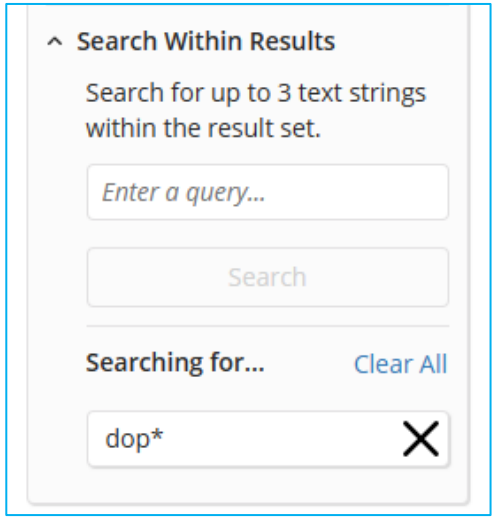
文献结果集—保存及下载







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可存为格式：

- ris
- PDF
- Rtf
- Excel
- TXT

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文献详情

文献详情界面包括：标题、摘要、重要的技术术语、引文地图、文献中重要的物质、反应、参考文献、原文链接

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

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

JOURNAL

Source
ACS Applied Materials & Interfaces
Volume: 14
Issue: 40
Pages: 45853-45868
Journal; Article
2022
DOI:
10.1021/acsami.2c13074

CODEN: AAMICK
E-ISSN: 1944-8252
ISSN-L: 1944-8244

Database Information
AN: 2022:2510278
CAN: 180:208379
PubMed ID: 36170495
CAplus and MEDLINE

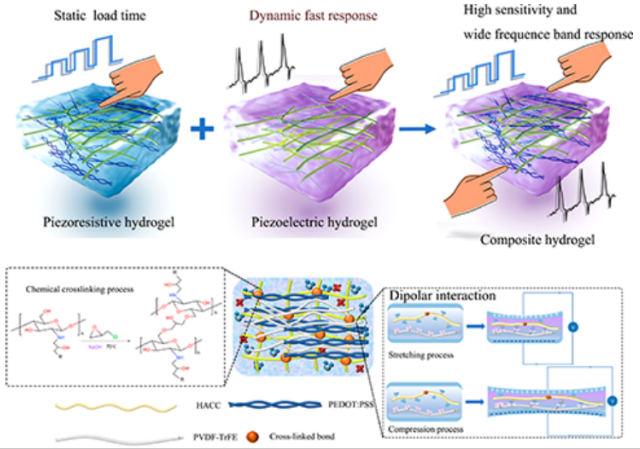
Company/Organization
School of Materials Science and Engineering
North University of China
Taiyuan 030051
China

Publisher
American Chemical Society

Language
English

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

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.



Keywords: conductive hydrogel wearable strain piezoelec sensor; composite hydrogels; fast response; high sensitivity; piezoresistive and piezoelectric sensation; wearable sensors

View Source | Full Text

Expand All | Collapse All

- Concepts
- Substances
- Cited Documents

Concepts

CAS科学家提供的标准技术术语

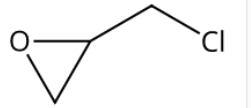
Electric resistance	Polythiophenes Role: Properties; Technical or Engineered Material Use
Elongation at break	Strain sensors
Hydrogels	Stress-strain relationship
Open circuit potential	Tensile strength
Piezoelectric sensors	Wearable devices

Substances

原文中重点研究的物质信息

Substances (7)

2839834-68-1
106602-18-0
Image Not Available



$(C_3H_5ClO.Unspecified)_x$

Role: Properties, Synthetic Preparation, Preparation

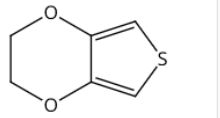
物质角色

1219717-04-0
Image Not Available

Unspecified
Clevios PH 750

Role: Properties, Technical or Engineered Material Use, Uses

126213-51-2



$(C_6H_6O_2S)_x$
Poly(3,4-ethylenedioxythiophene)

Role: Properties, Technical or Engineered Material Use, Uses

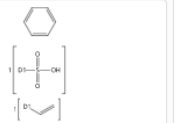
Notes: polystyrenesulfonate-doped

106602-18-0
Image Not Available

Unspecified
N-[2-Hydroxy-3-(trimethyl ammonium)propyl]chitosan chloride

Role: Reactant, Reactant or Reagent

50851-57-5

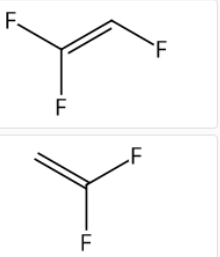


$(C_8H_8O_3S)_x$
Poly(styrenesulfonic acid)

Role: Properties, Technical or Engineered Material Use, Uses

Notes: PEDOT dopant

28960-88-5



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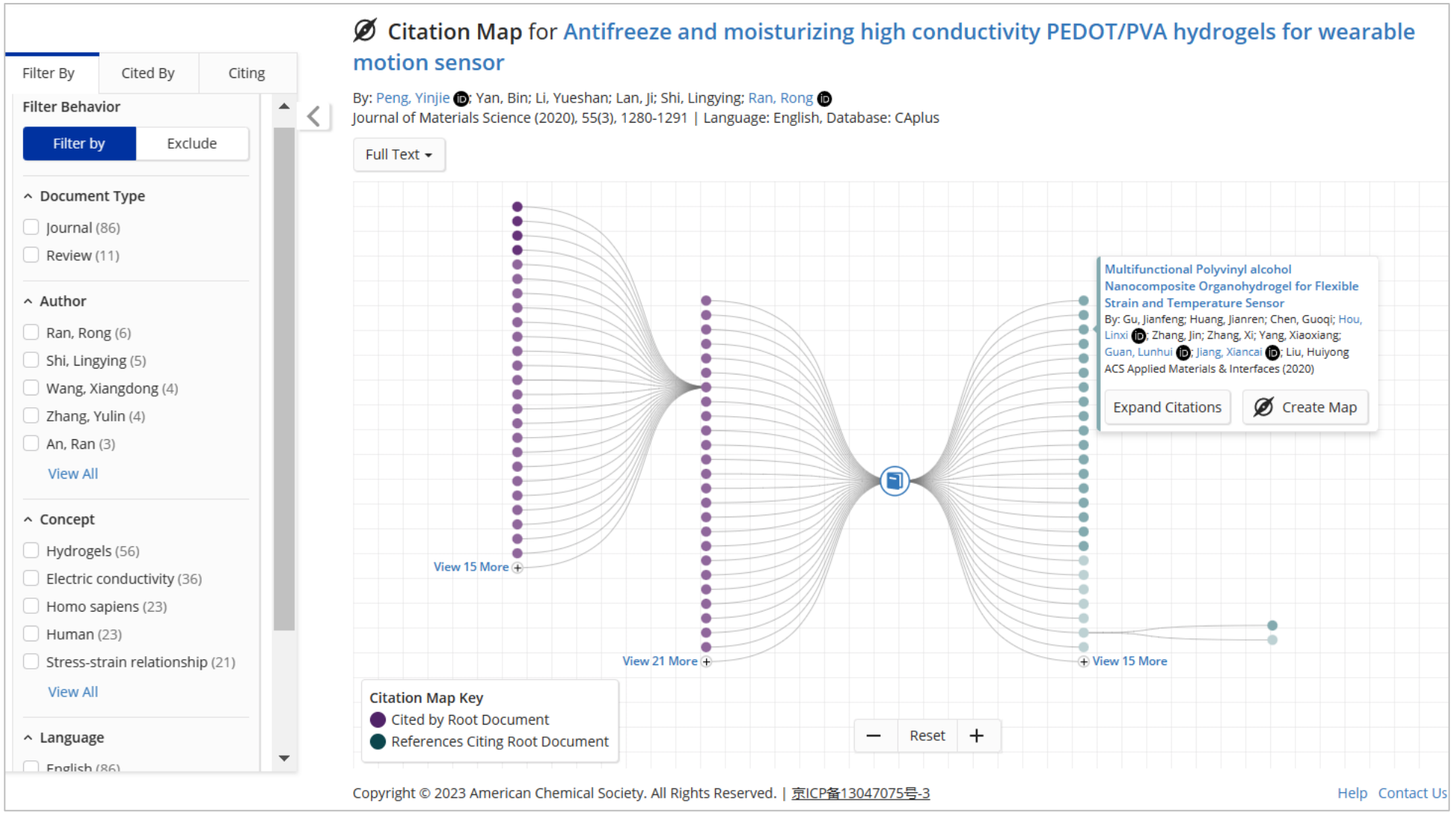
文献详情—引文地图



引文地图：

- 获取前向引文
- 获取后向引文
- 可通过聚类选项筛选引文

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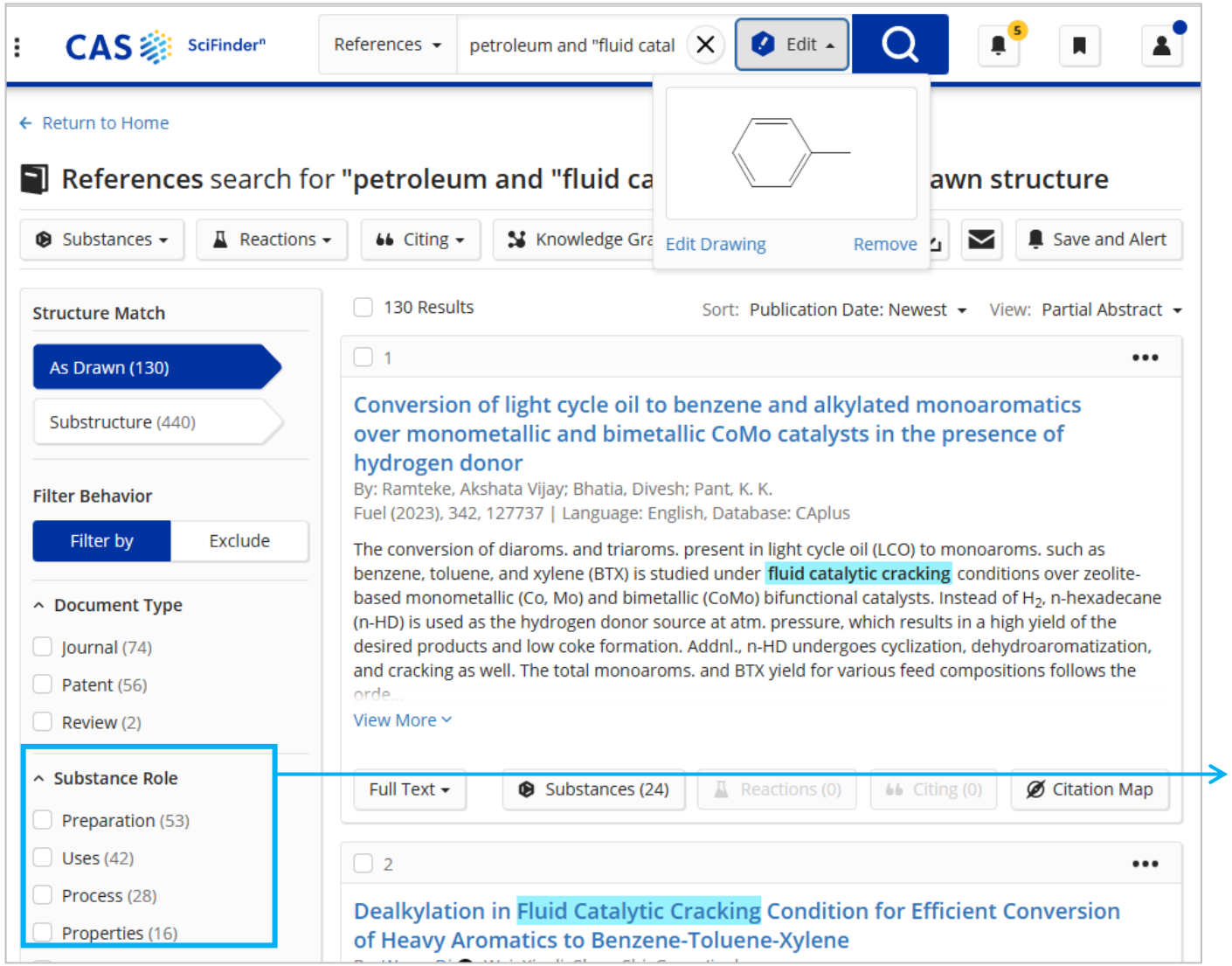
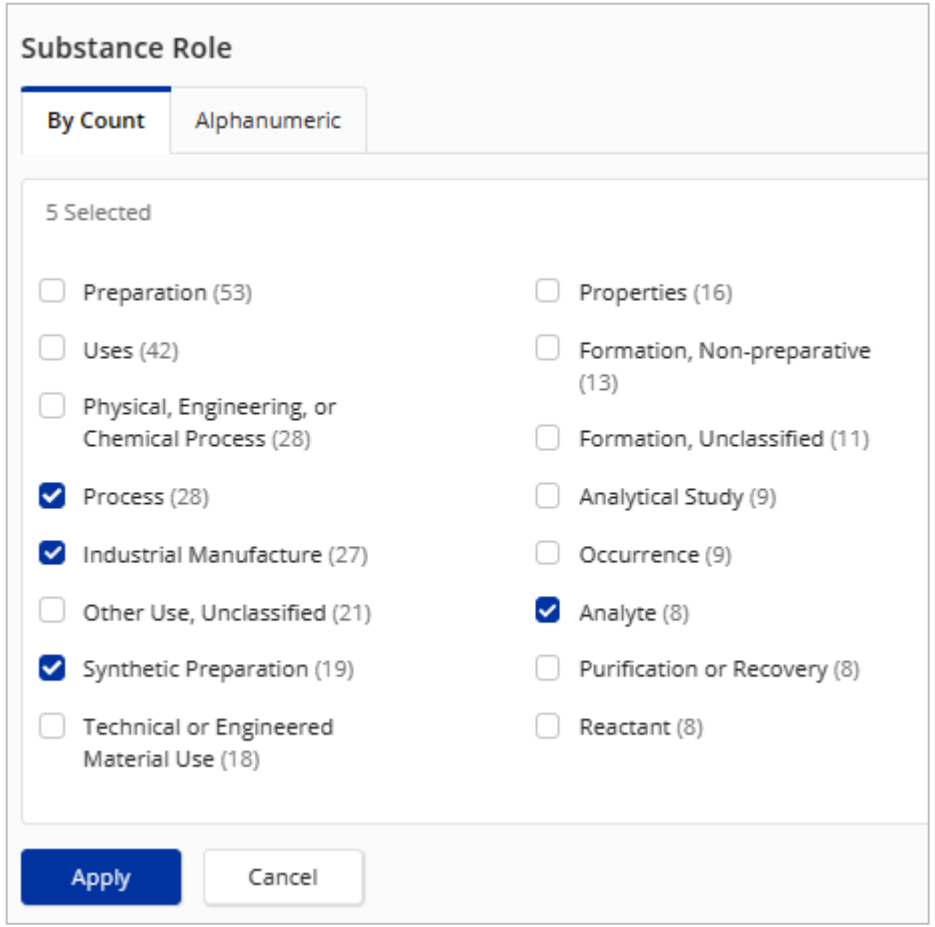
文献检索—主题词+结构联合检索



物质在文献中的研究角色



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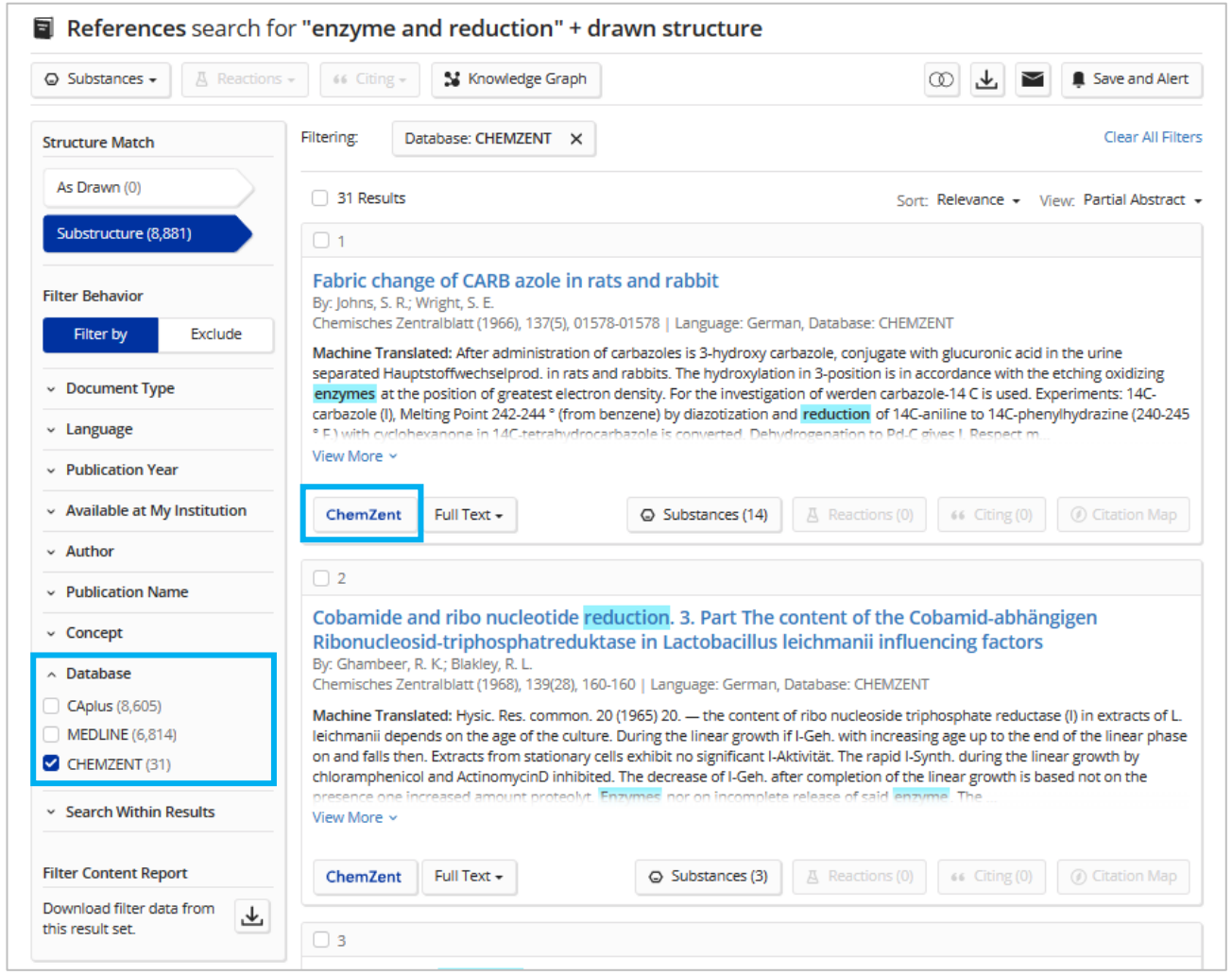
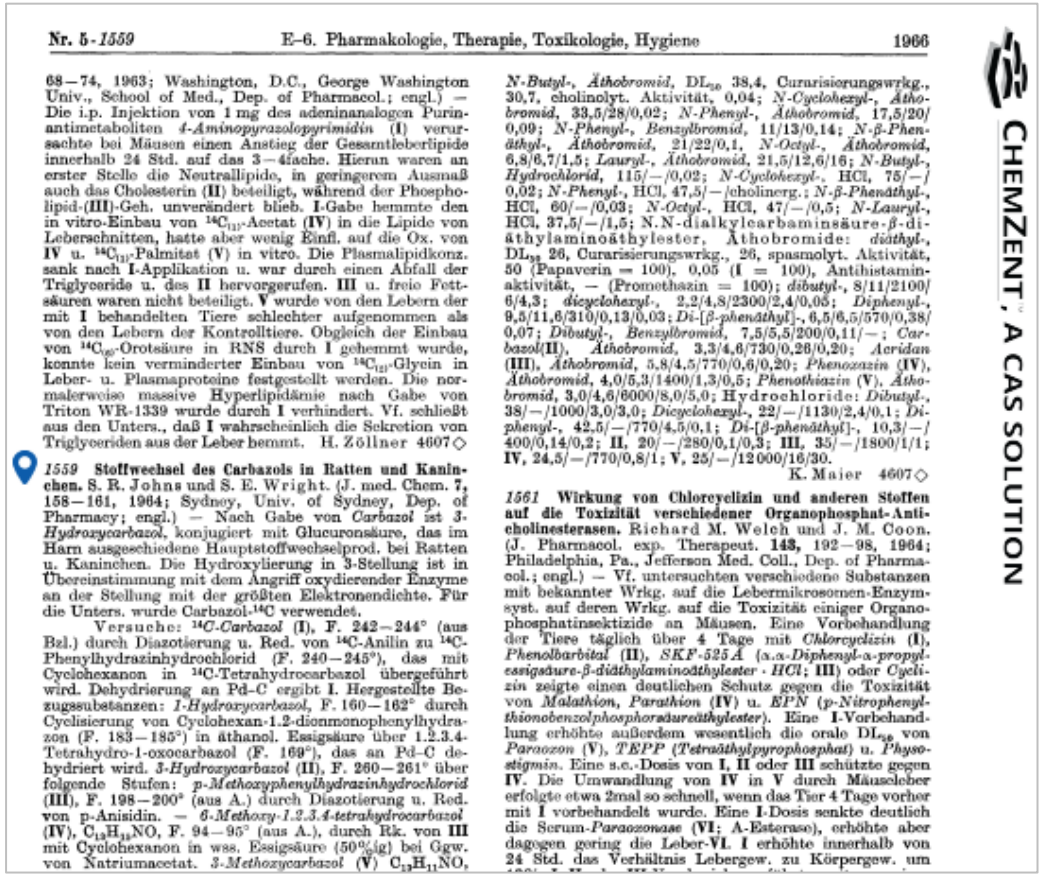
查看Chemzent 来源的文献

- ChemZent是最古老的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
- 化学研究相关文献可回溯至1830年, 可用于追溯化学科学起源时期的研究，丰富化学历史知识





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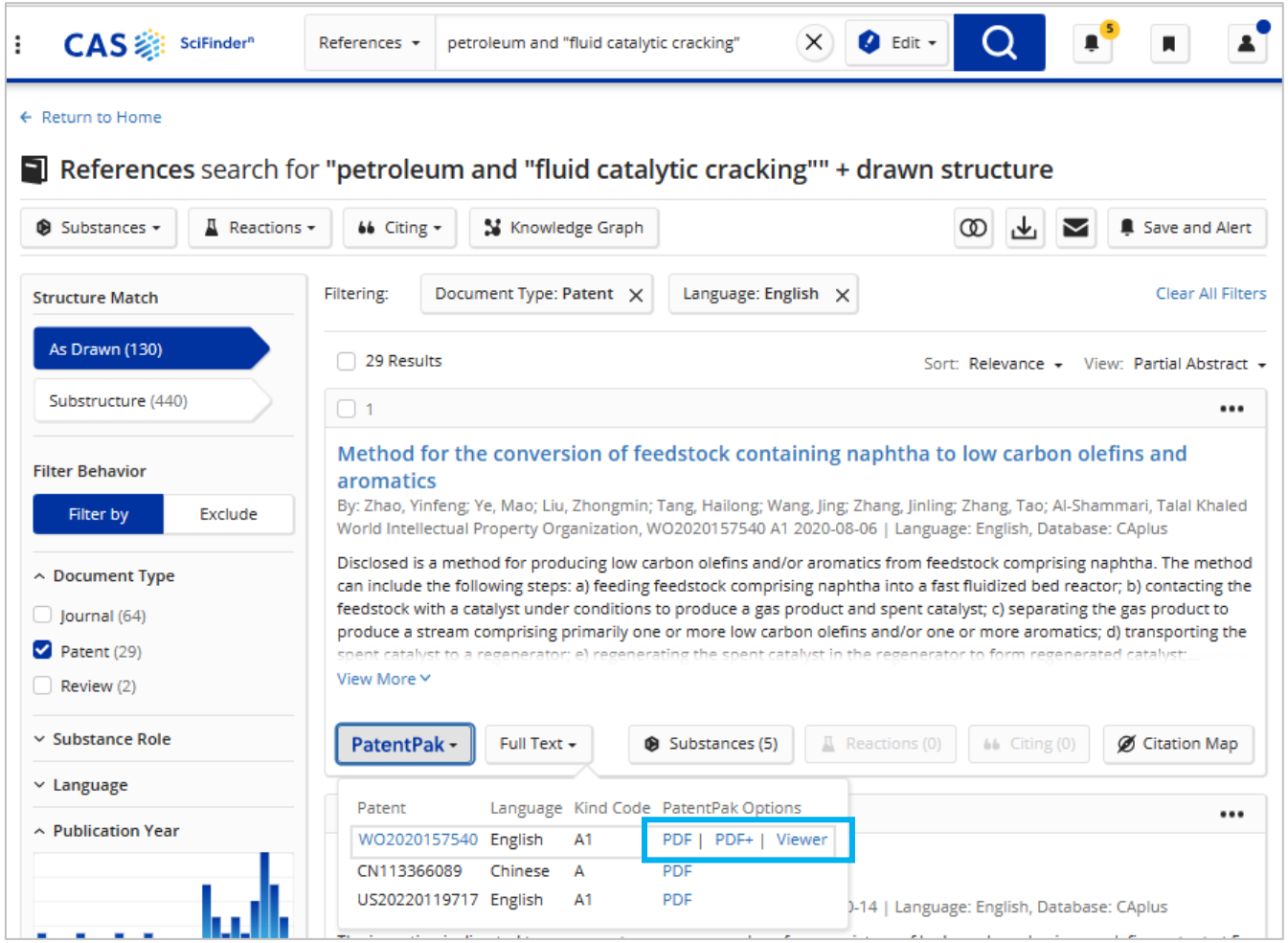
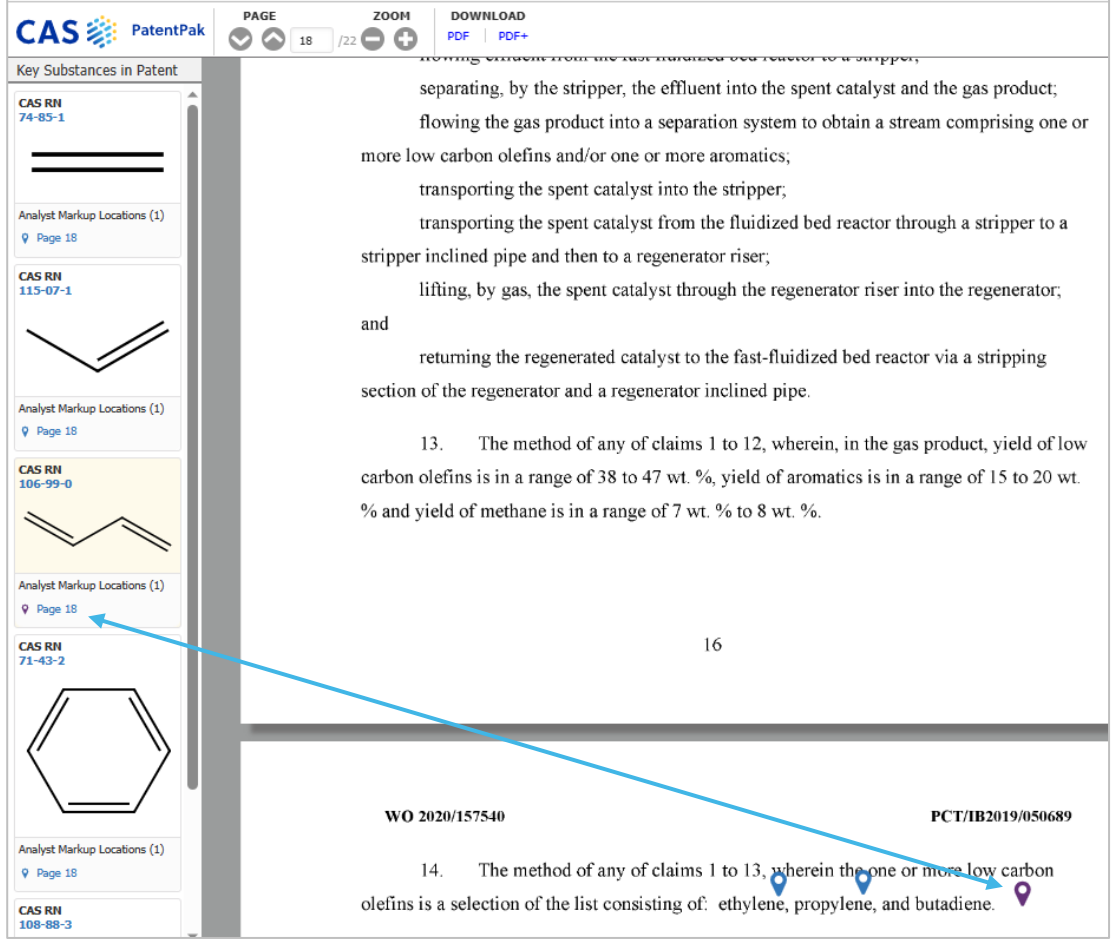
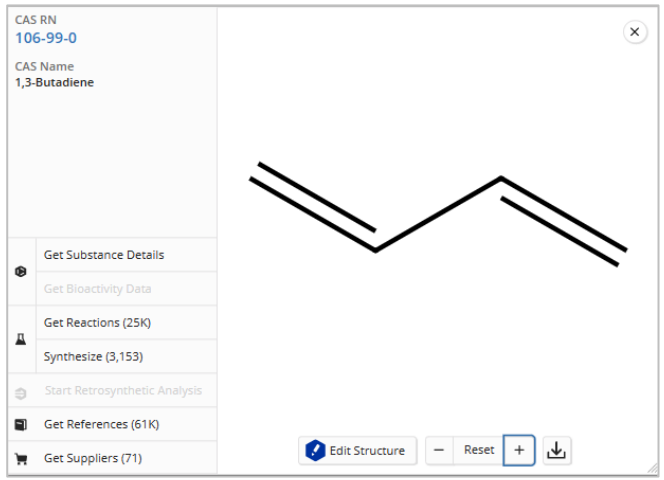
专利文献详情

PatentPak：

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







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文献检索小结

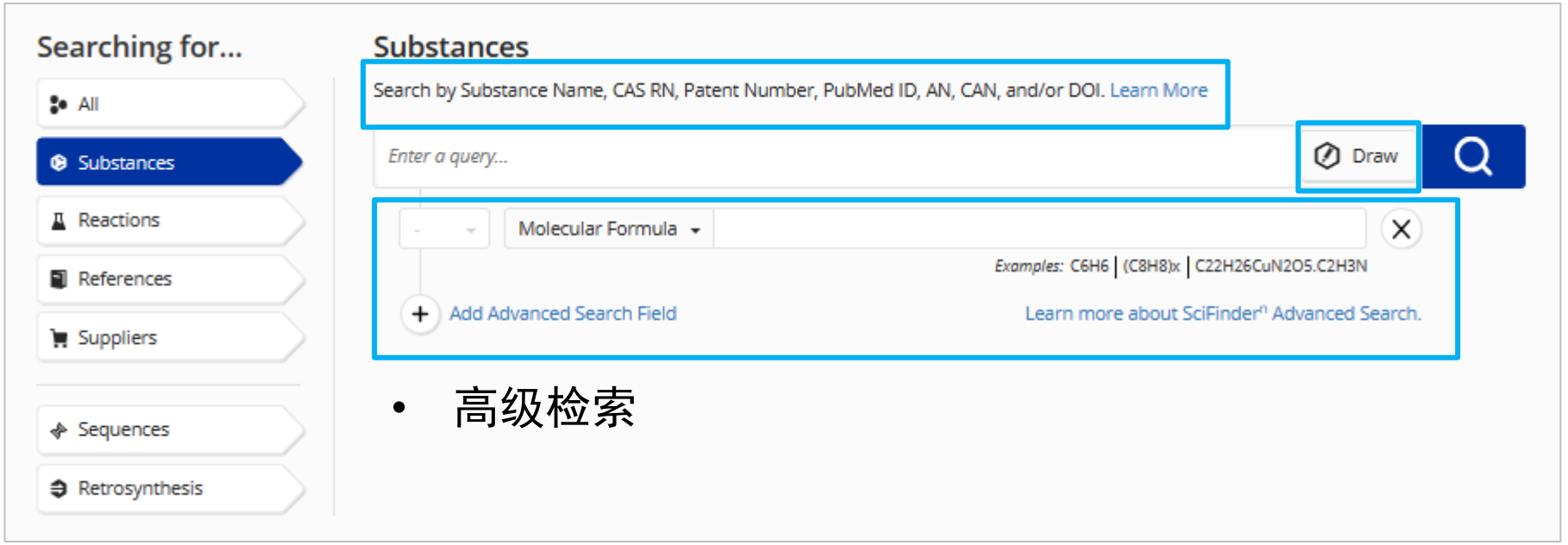
1. 检索词的构建：使用布尔逻辑算符及通配符连接主题词，利用CAS Lexicon精准选词
2. 利用高级检索选项进行自定义组合检索
3. 通过聚类筛选工具快速获得目标文献
4. 利用引文地图拓展检索
5. 主题词+结构联合检索快速获得文献
6. 使用PatentPak高效阅读专利

物质检索

- 物质检索方法
  - 物质标识符、文献标识符检索
  - 分子式、物性参数、谱图数据检索
  - 结构式检索
- 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

物质检索

- 通过物质标识符、文献标识符检索物质



- 高级检索

- 使用结构绘制面板进行结构检索

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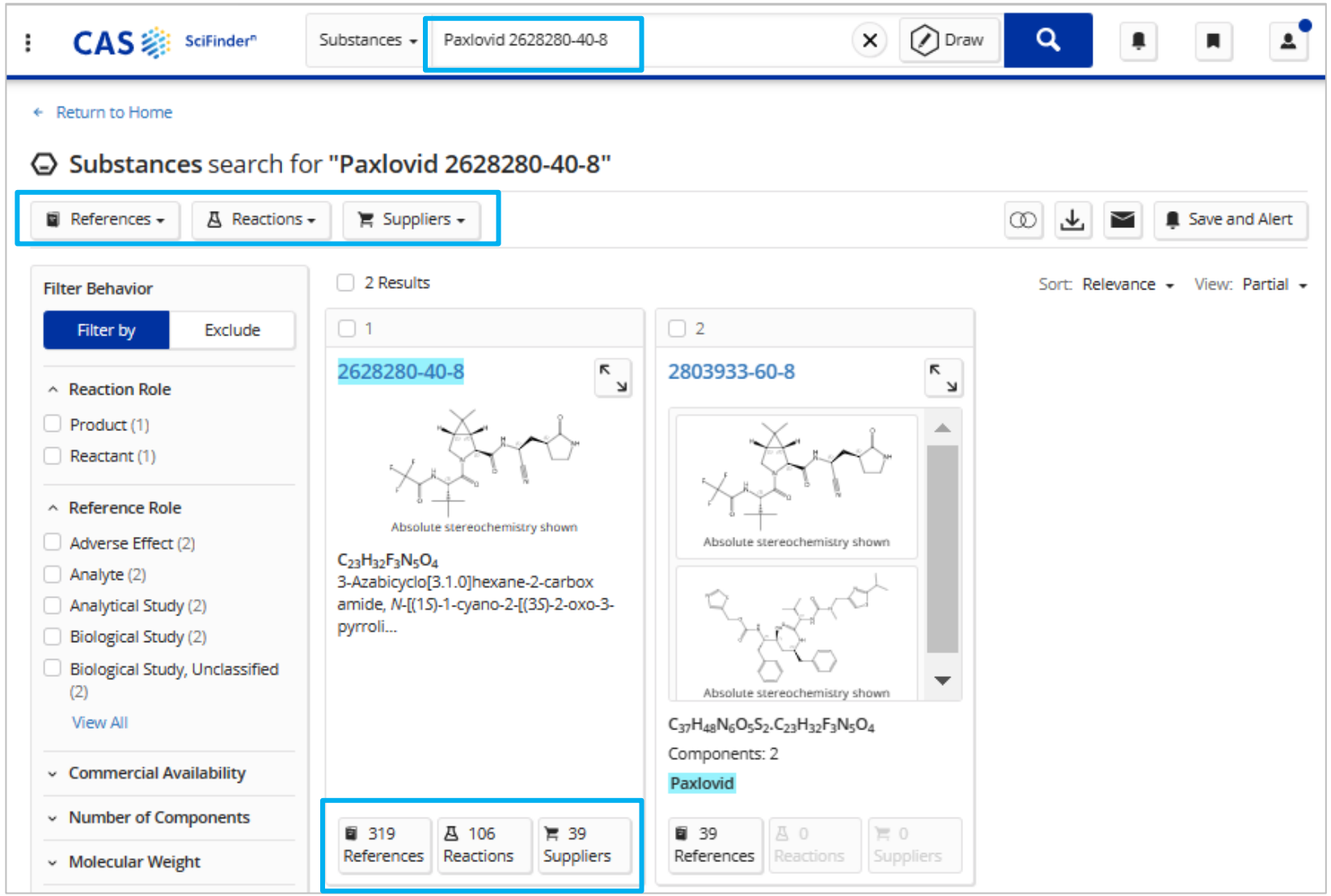
物质检索—物质名称、CAS RN、代码



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

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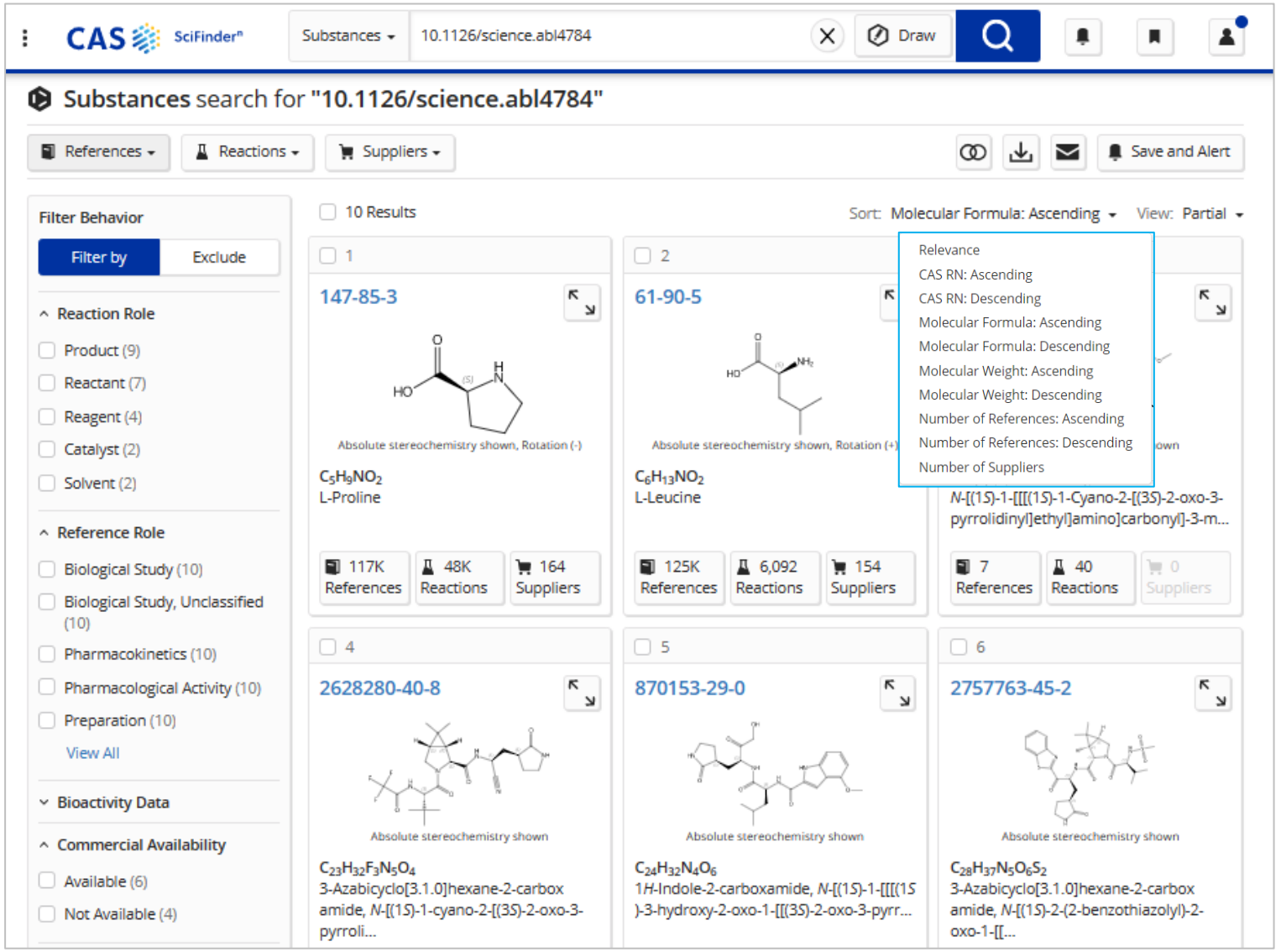
物质检索—文献标识符及结果集排序



使用文献标识符，迅速获得关注文献中的物质信息

不同物质排序：

- 相关度
- CAS RN
- 分子式
- 分子量
- 文献量
- 供应商数量

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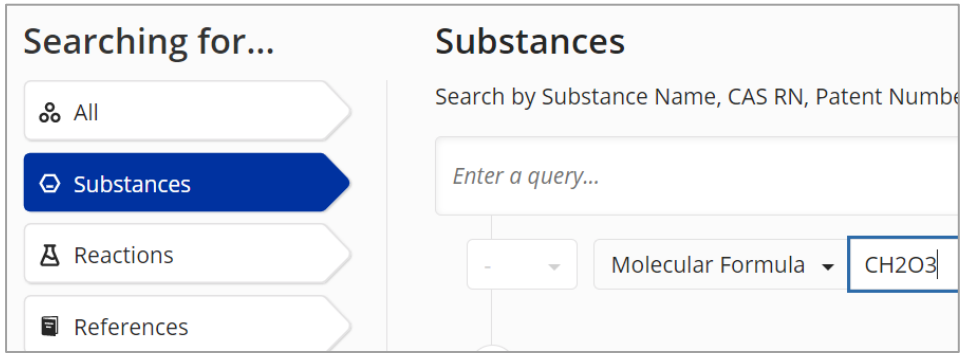
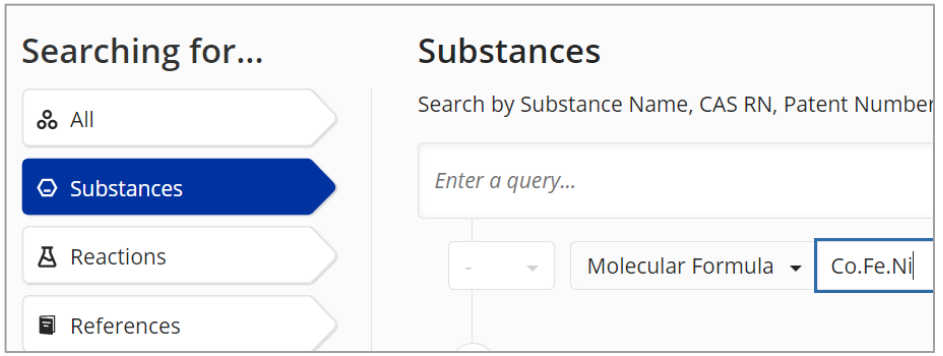
物质检索—分子式

- 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：铁钴镍合金　Co.Fe.Ni
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性　Na2SO4：H2O4S.2Na





适用于分子式检索的物质类型包括：

- 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
- 聚合物

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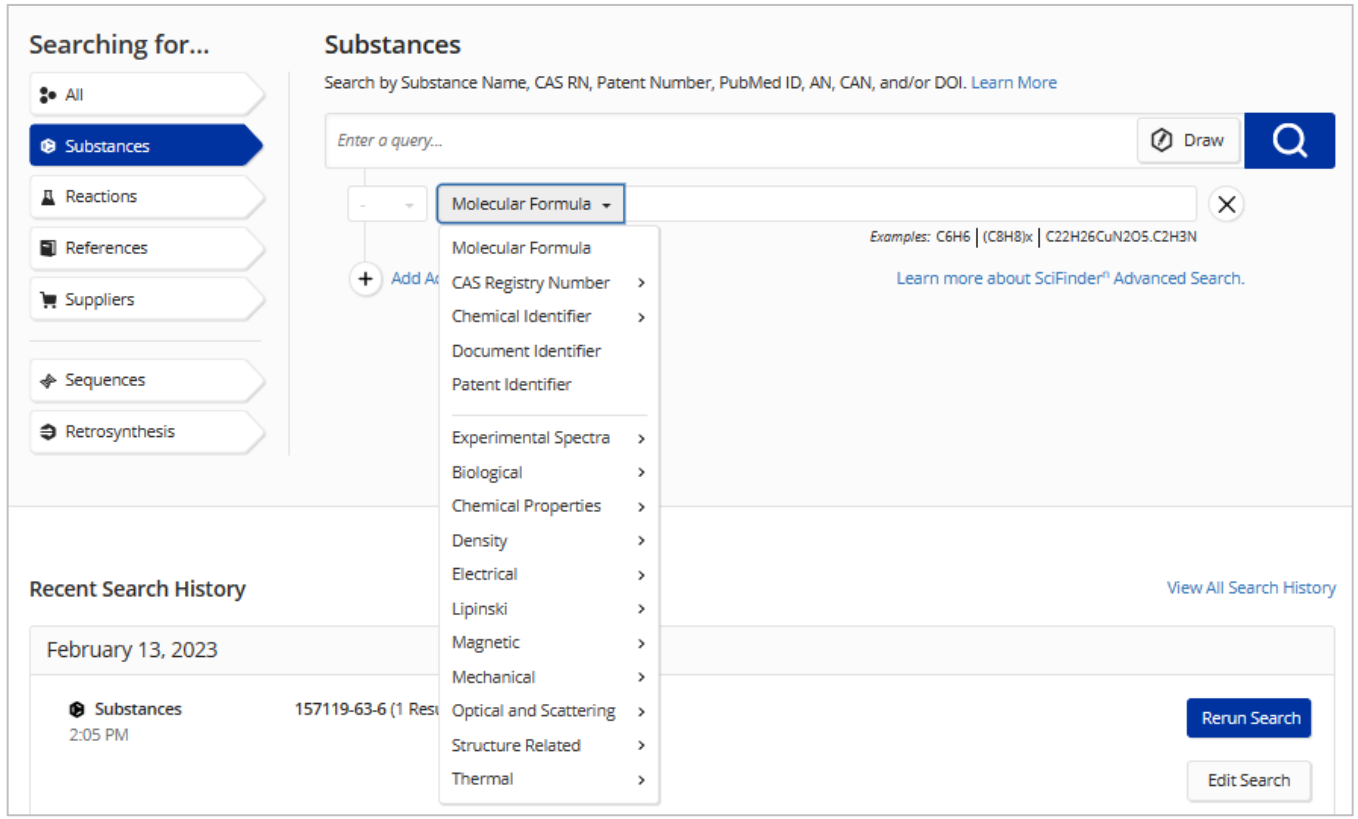
物质检索—Advanced Search



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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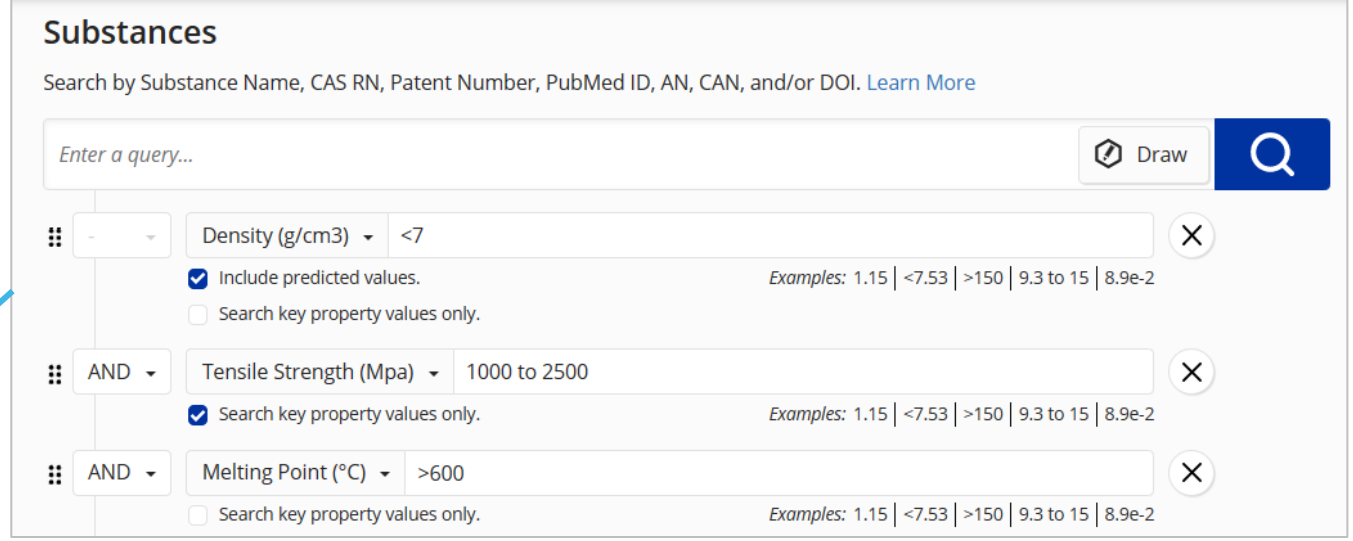
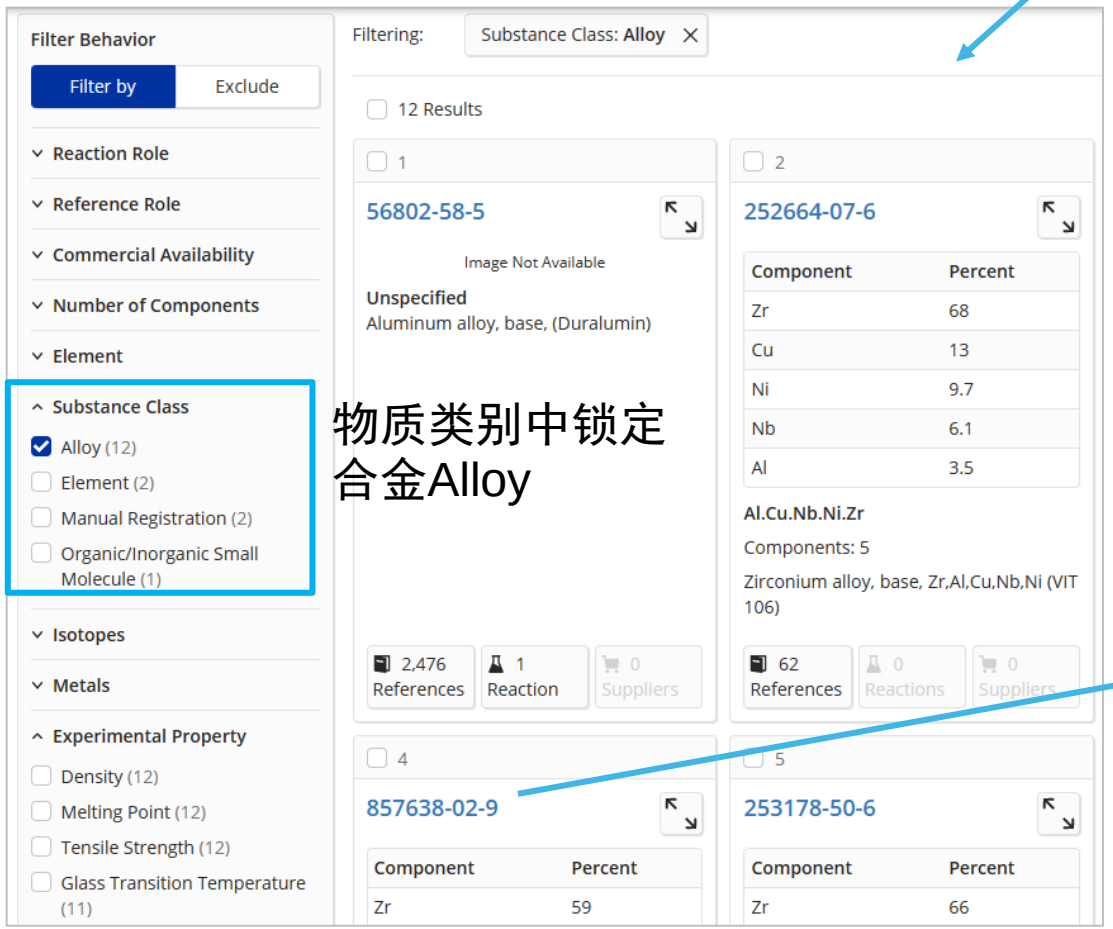
物质检索—联用检索(1)

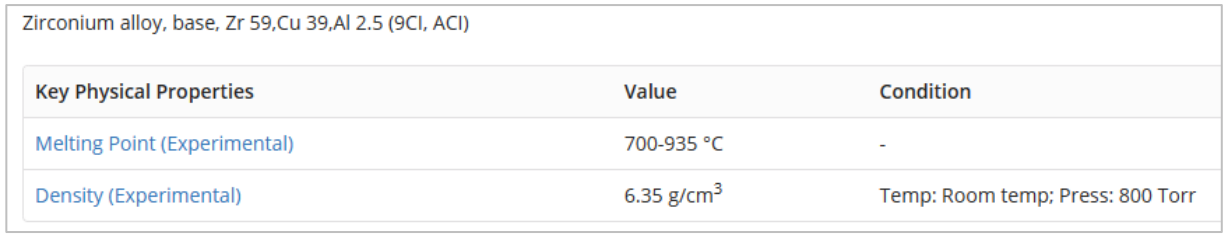
查找满足以下属性要求的合金：

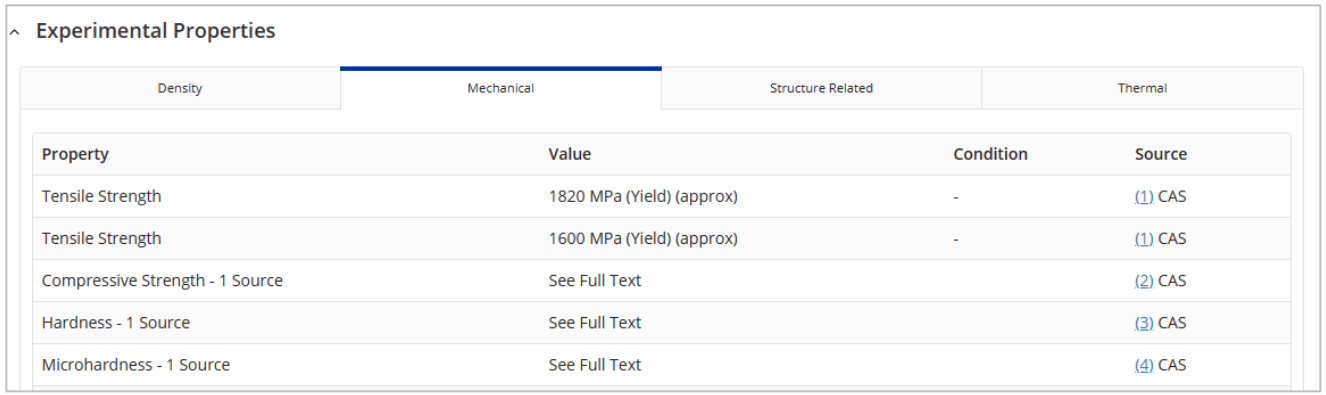
1. 密度<7g/cm^3
2. 拉伸强度>1000MPa
3. 熔点>600





物质类别中锁定合金Alloy





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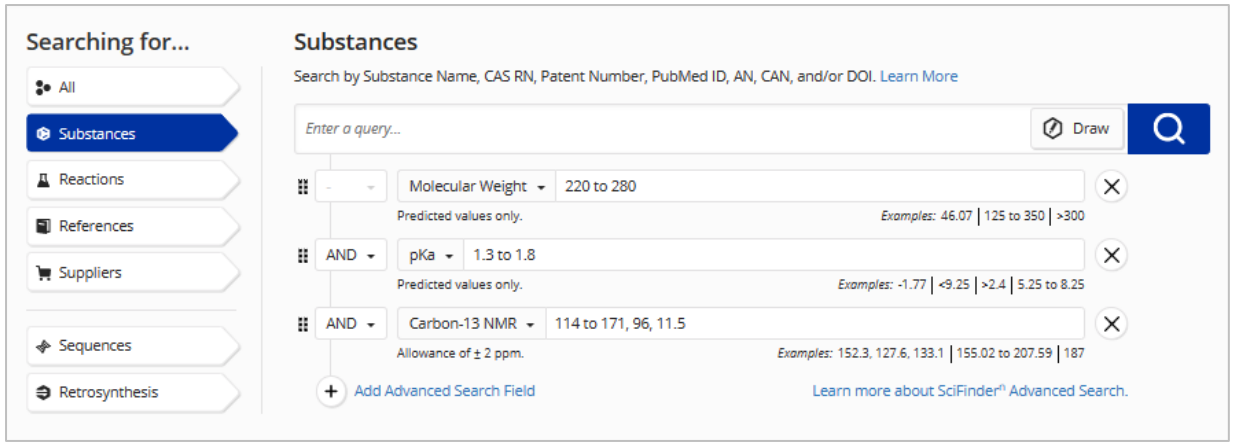
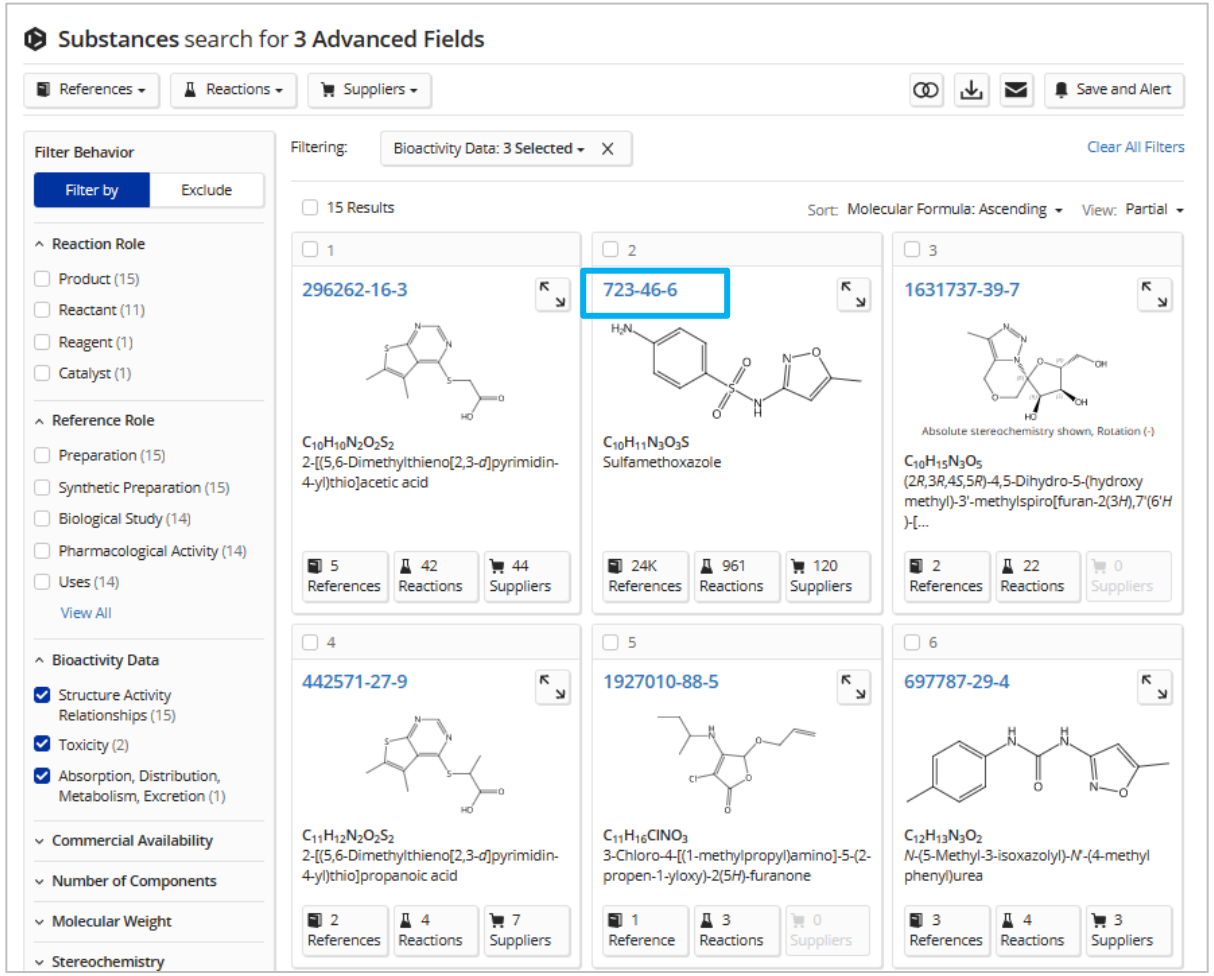
物质检索—联用检索(2)

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





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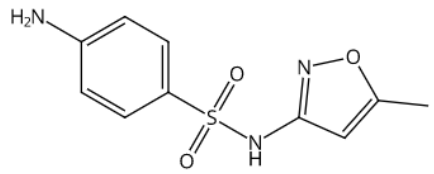
物质详情

CAS Registry Number: 723-46-6

References (24K) | Reactions (961) | Suppliers (120) | Save



$C_{10}H_{11}N_3O_3S$

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 Point (Predicted)	482.1±55.0 °C	Press: 760 Torr
Density (Experimental)	1.4895 g/cm^3	-
pKa (Predicted)	5.81±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- 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

折叠菜单显示物质各类信息

Experimental Spectra

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

	Source
View Proton NMR Spectrum	(1) LC
View Proton NMR Spectrum	(2) ENAMINE
View Proton NMR Spectrum	(2) ENAMINE
View Proton NMR Spectrum	(3) CAS
View Proton NMR Spectrum	(4) CAS
View Proton NMR Spectrum	(5) CAS
View Proton NMR Spectrum	(6) BIORAD
View Proton NMR Spectrum	(6) BIORAD
View Proton NMR Spectrum	(7) AIST
Proton NMR Spectrum - 4 Sources	(8-11) CAS

Sources

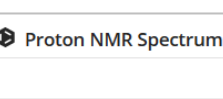
(1) Spectral data were obtained from Life Chemicals

(2) Spectral data were obtained from Enamine Ltd.

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

Proton NMR Spectrum for 723-46-6

723-46-6



$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

Working Frequency
400 MHz

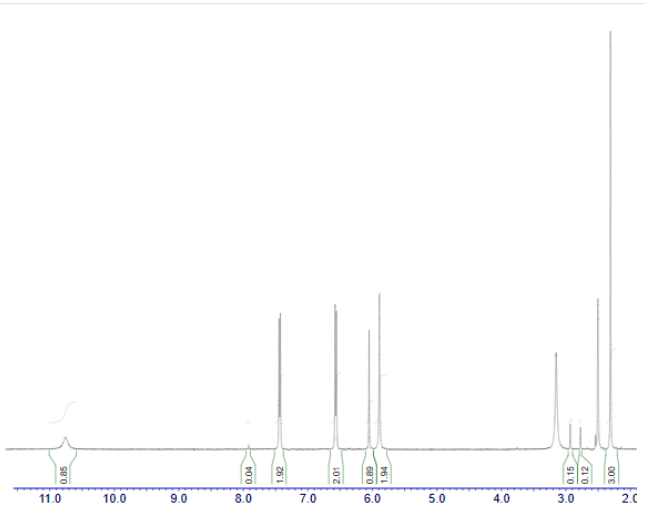
Solvent
Dimethyl sulfoxide (67-68-5)
Carbon tetrachloride (56-23-5)

Temperature
20 °C

Spectrum Summary

Spectrum ID
F0175-0013

Source
Spectral data were obtained from Life Chemicals



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物质详情

Structure Activity Relationships

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Target | Function | Parameter | Disease | Organism

Filter Disease
- Bacterial infection (273)
- Microbial infection (206)
- Oxidative stress (76)
- Toxoplasmosis (46)
- Bacterial infections

Apply | Clear All

Target	Function	Paramet		Disease	Organism	Assay	Source
1132187-M	Inhibitor	Drug ren		-	-	View Detail	(1) CAS
207419-N	Inhibitor	Drug ren		-	-	View Detail	(1) CAS
226605-F	Inhibitor	Drug ren		-	-	View Detail	(1) CAS
A. baumannii	Inhibitor	MIC		Microbial infections	-	View Detail	(2) CAS
Acanthamoeba	Inhibitor	IC50		Acanthamoeba keratitis	-	View Detail	(3) CAS
Acanthamoeba	Inhibitor	IC50	0.8 ug/mL	Acanthamoeba keratitis	-	View Detail	(3) CAS

Absorption, Distribution, Metabolism, and Excretion Data

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Target | Function | Parameter | Disease

Filter Parameter
- Drug concentration (7)
- Cell uptake (2)
- Serum concentration (2)
- fAUC(0-24 h) (2)
- fCmax (2)
- t1/2 (2)

Apply | Clear All

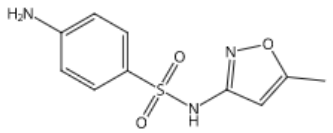
Target	Func	Value	Disease	Organism	Assay	Source
Methicillin-resistant Staphylococcus aureus	-	217.5 mg x h/L	Bacterial infections	-	View Detail	(1) CAS
Methicillin-resistant Staphylococcus aureus	-	13 mg/L	Bacterial infections	-	View Detail	(1) CAS
Methicillin-resistant Staphylococcus aureus	-	10 h	Bacterial infections	-	View Detail	(1) CAS
Methicillin-sensitive Staphylococcus aureus	-	217.5 mg x h/L	Bacterial infections	-	View Detail	(1) CAS

Assay Data

CAS LIFE SCIENCES

← Prev (2 of 1,031) Next →

Ligand
723-46-6



$C_{10}H_{11}N_3O_3S$
Sulfamethoxazole

Target	207419-N
Assay Name	-
Assay Type	Functional
Procedure	Laccase degradation assay
Function	Inhibitor
Parameter	Drug removal
Value	0.00 %
Ligand Dose	-
Disease	-
Biological System	in vitro
Source	Evaluation of bezafibrate, gemfibrozil, indomethacin, sulfamethoxazole, and diclofenac removal by ligninolytic enzymes By: Camarillo Ravelo, Dante; Loera Corral, Octavio; Gonzalez-Martinez, Ignacio; Chan Cupul, Wilberth; Rodriguez Nava, Celestino Odin Preparative Biochemistry & Biotechnology (2020), 50(6), 592-597 | Language: English, Database: CAplus and MEDLINE

Toxicity

CAS LIFE SCIENCES

Parameter

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	1.917 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS

(1) Plouffe, David M.; Cell Host & Microbe (2016), 19(1), 114-126, CAplus and MEDLINE

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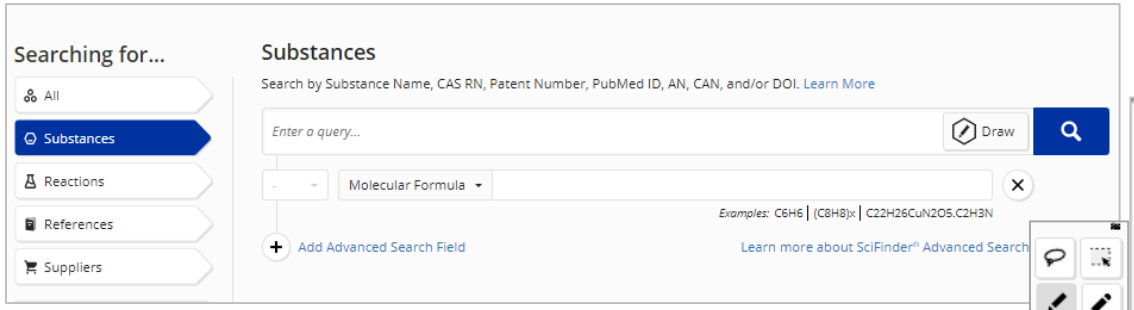
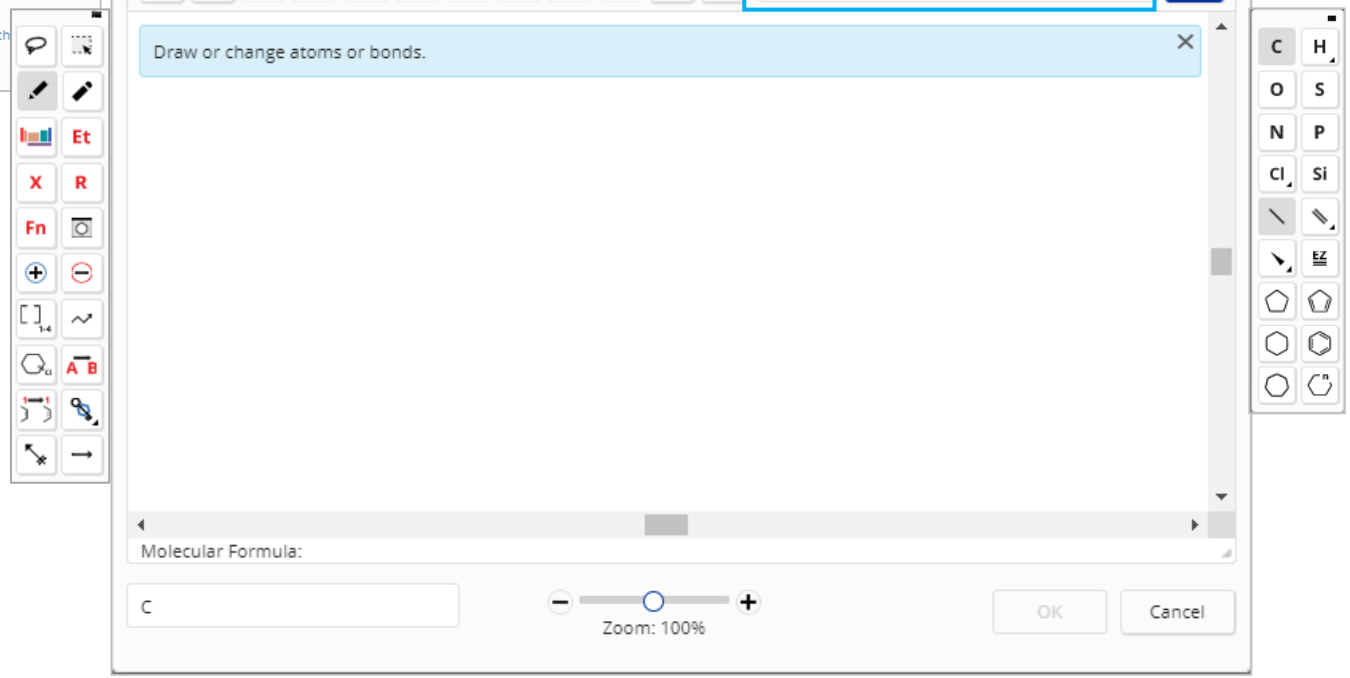
物质检索—结构检索



选择可变基团　取代位点可变

自定义R基团　锁工具

重复片段工具　片段结构



CAS Draw和ChemDoodle的使用指南
https://scifinder-n.cas.org/help/#t=Drawing_Search_Queries%2FDrawing_Structure_Queries.htm https://www.cas.org/support/training/scifinder-n/structure-search
https://www.cas.org/support/training/scifinder-n/chemdoodle-structure-search

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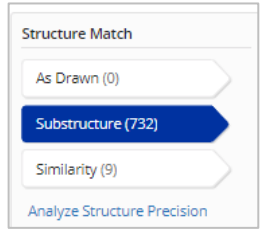
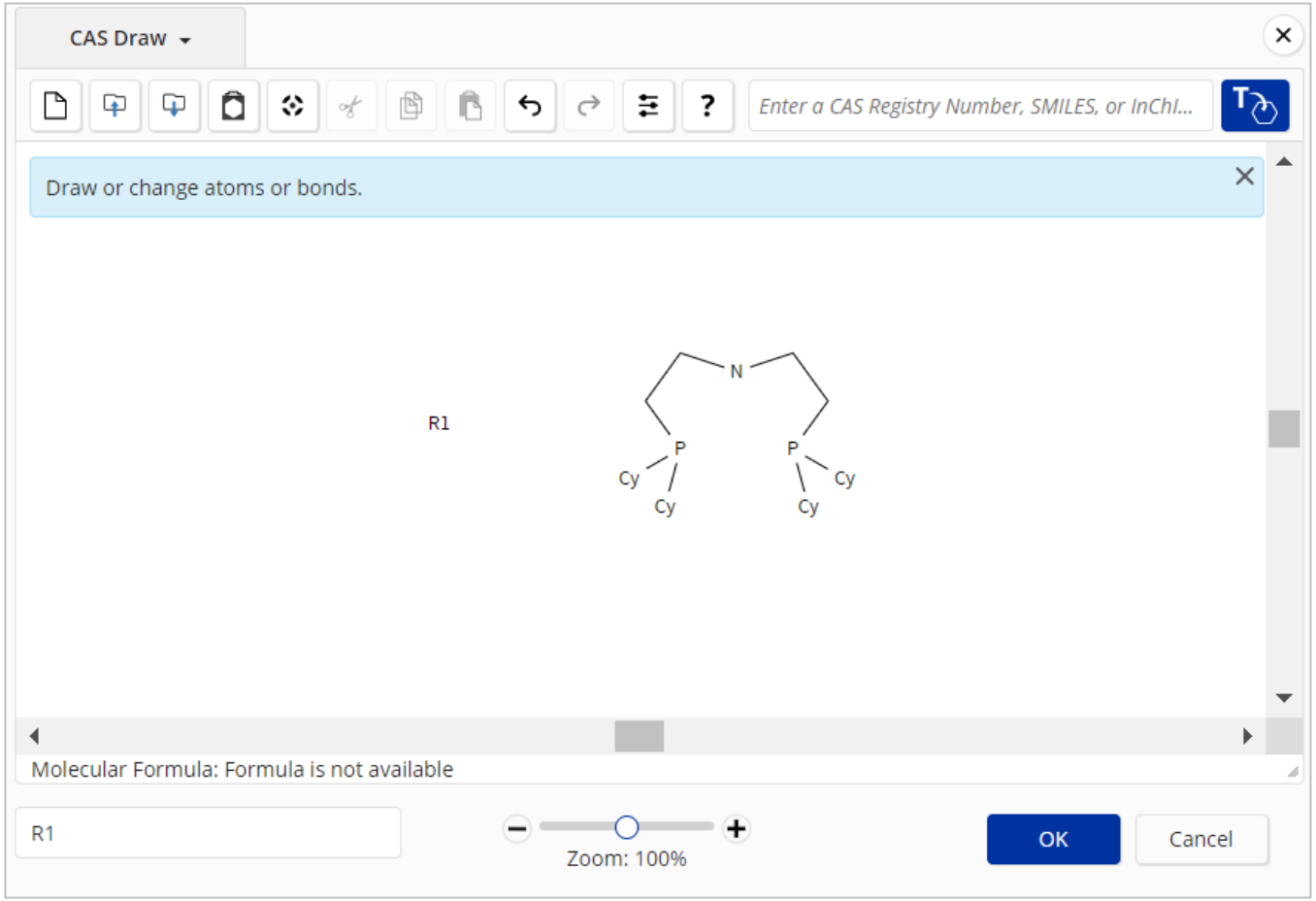
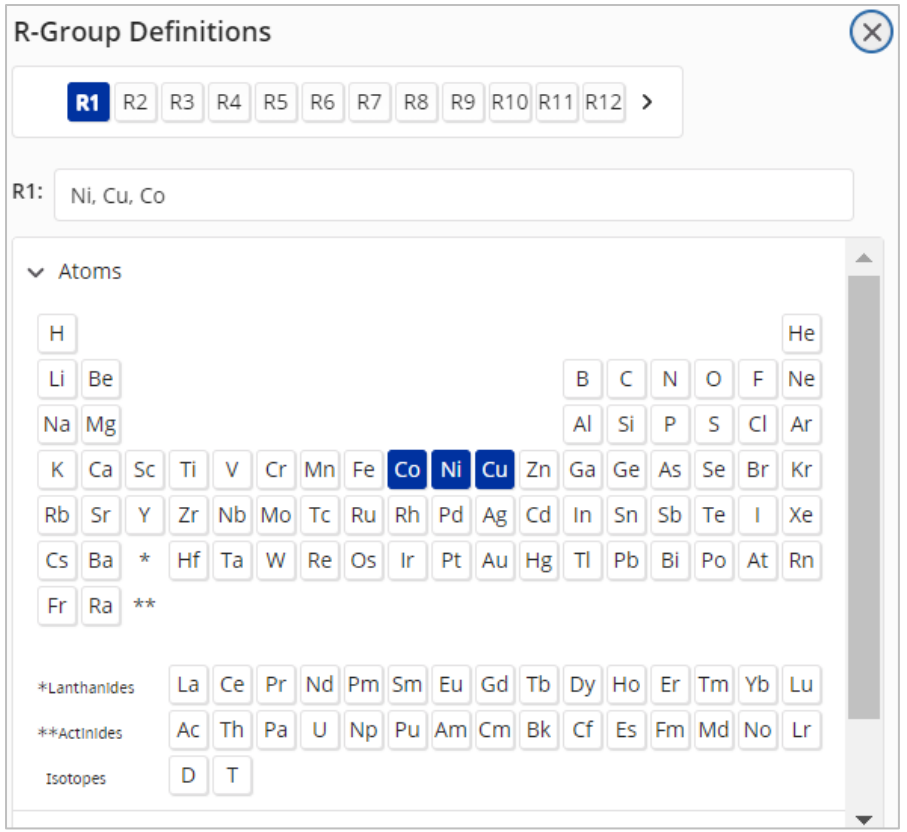
物质检索—结构检索



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





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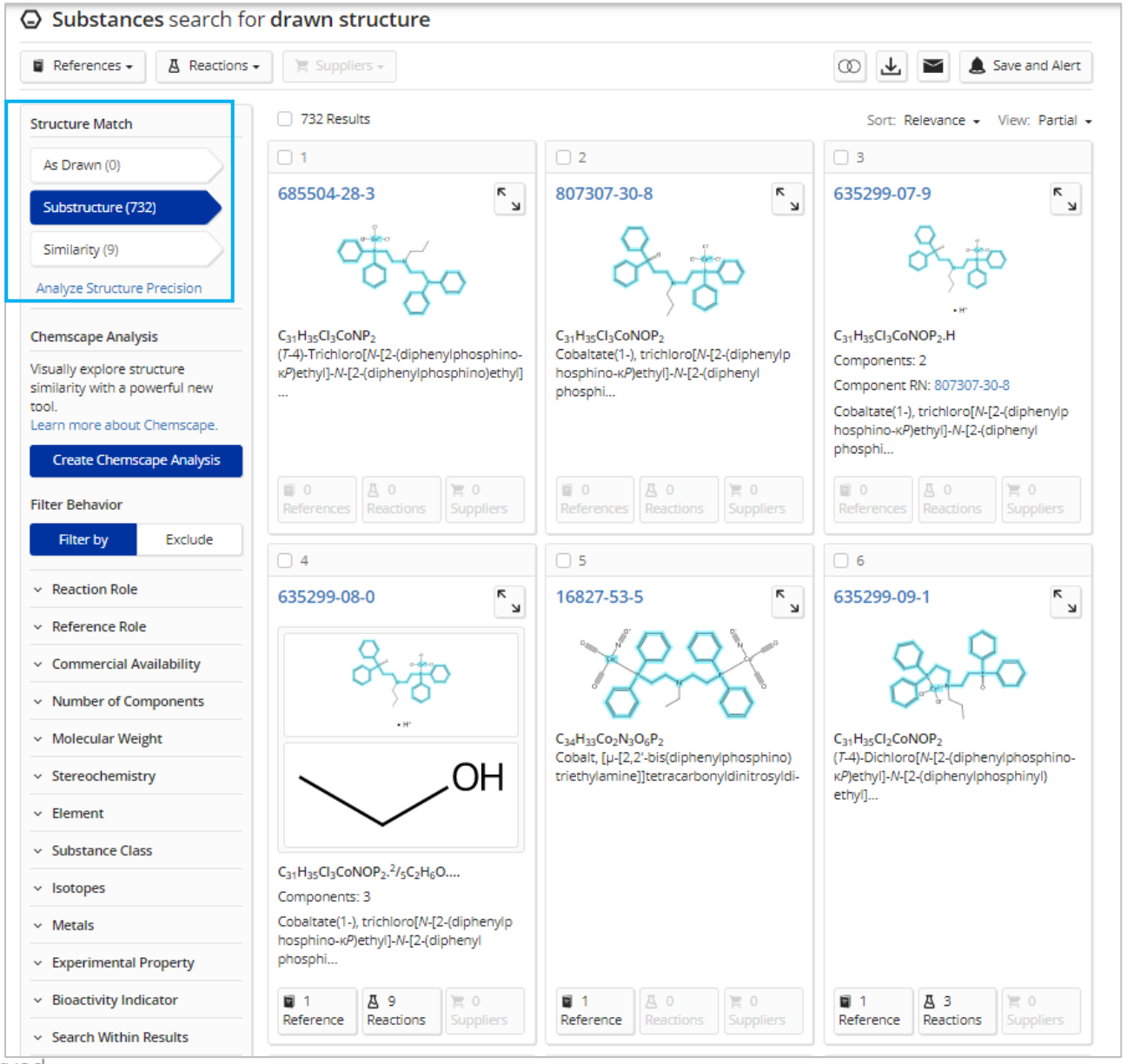
物质检索—检索结果集筛选

结构检索类别：
As Drawn
亚结构
相似结构

Chemscape分析

Filter by & Exclude

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……



物质检索—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

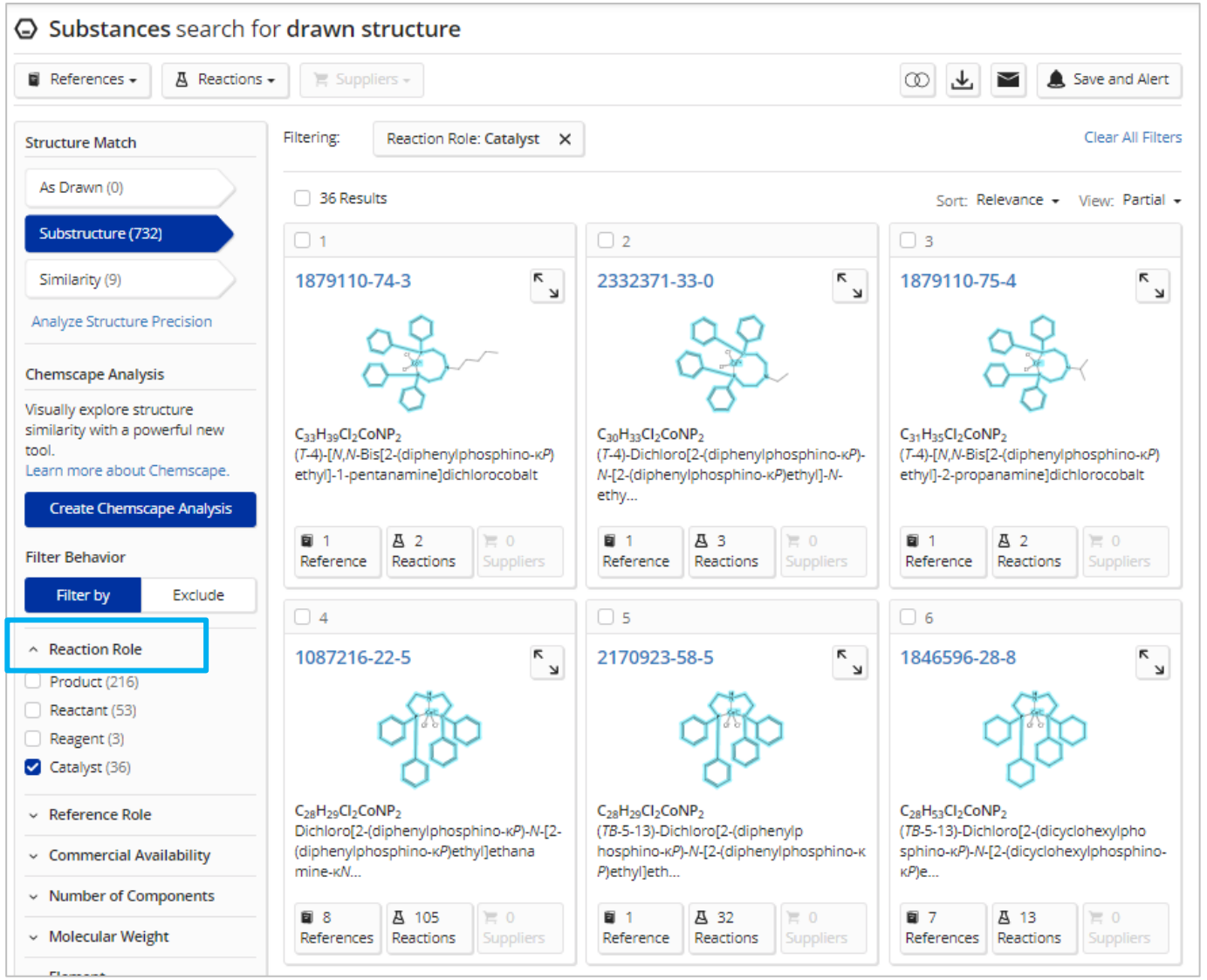
- Similarity 相似结构

  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--检索结果集筛选：Reaction Role

利用物质在反应中的角色精准定位相应的物质



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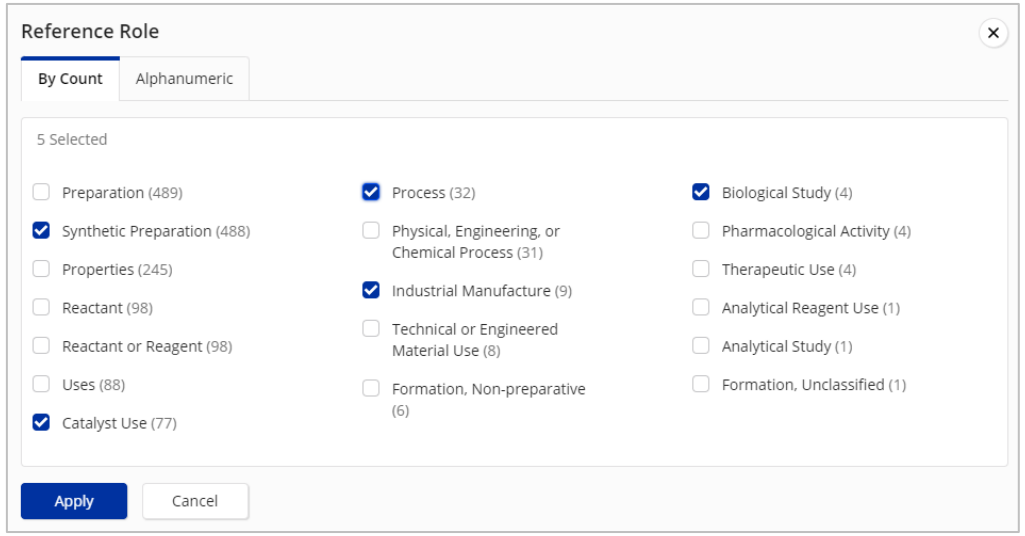
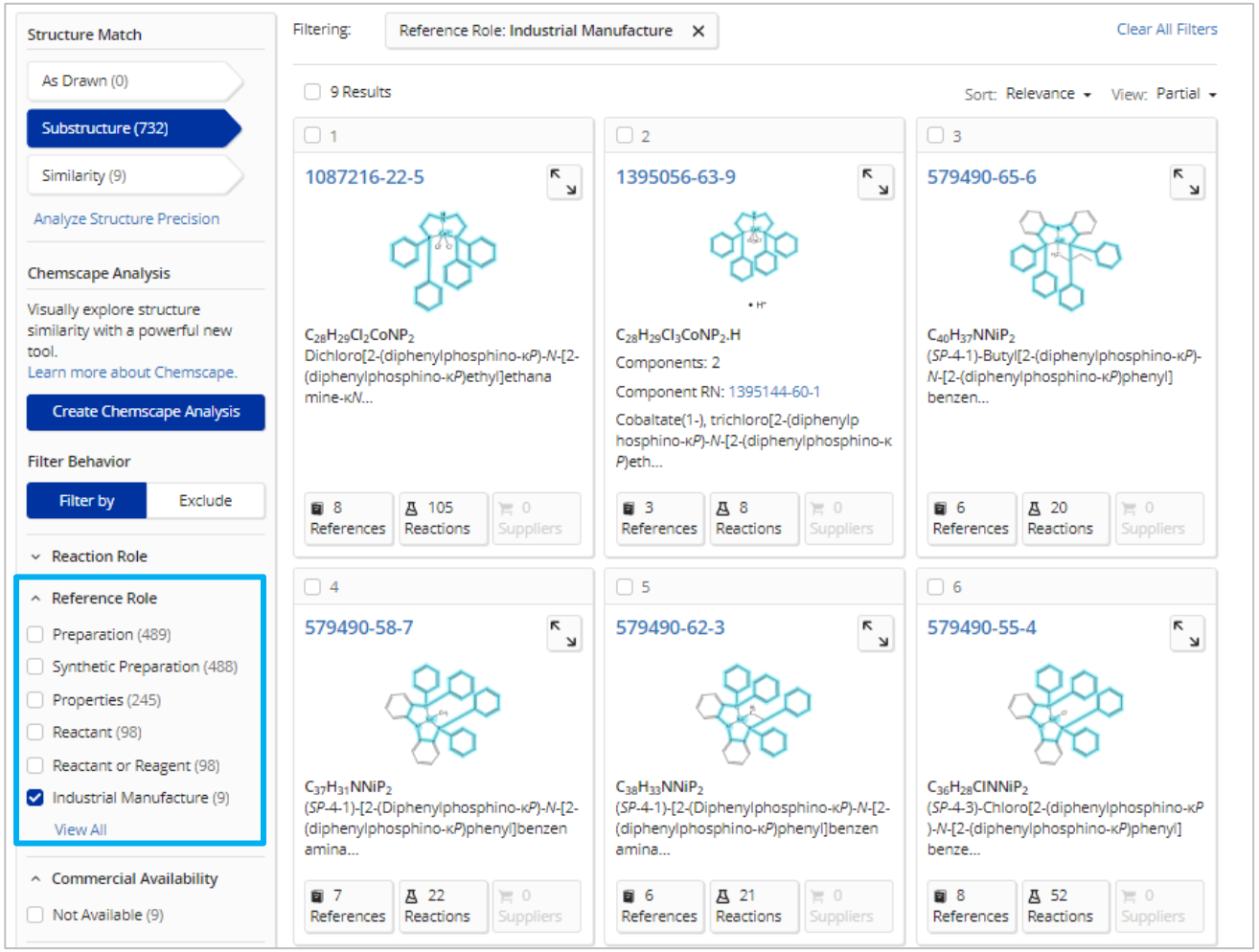
物质检索—检索结果集筛选：Reference Role

利用物质的研究角色精准定位相应的物质





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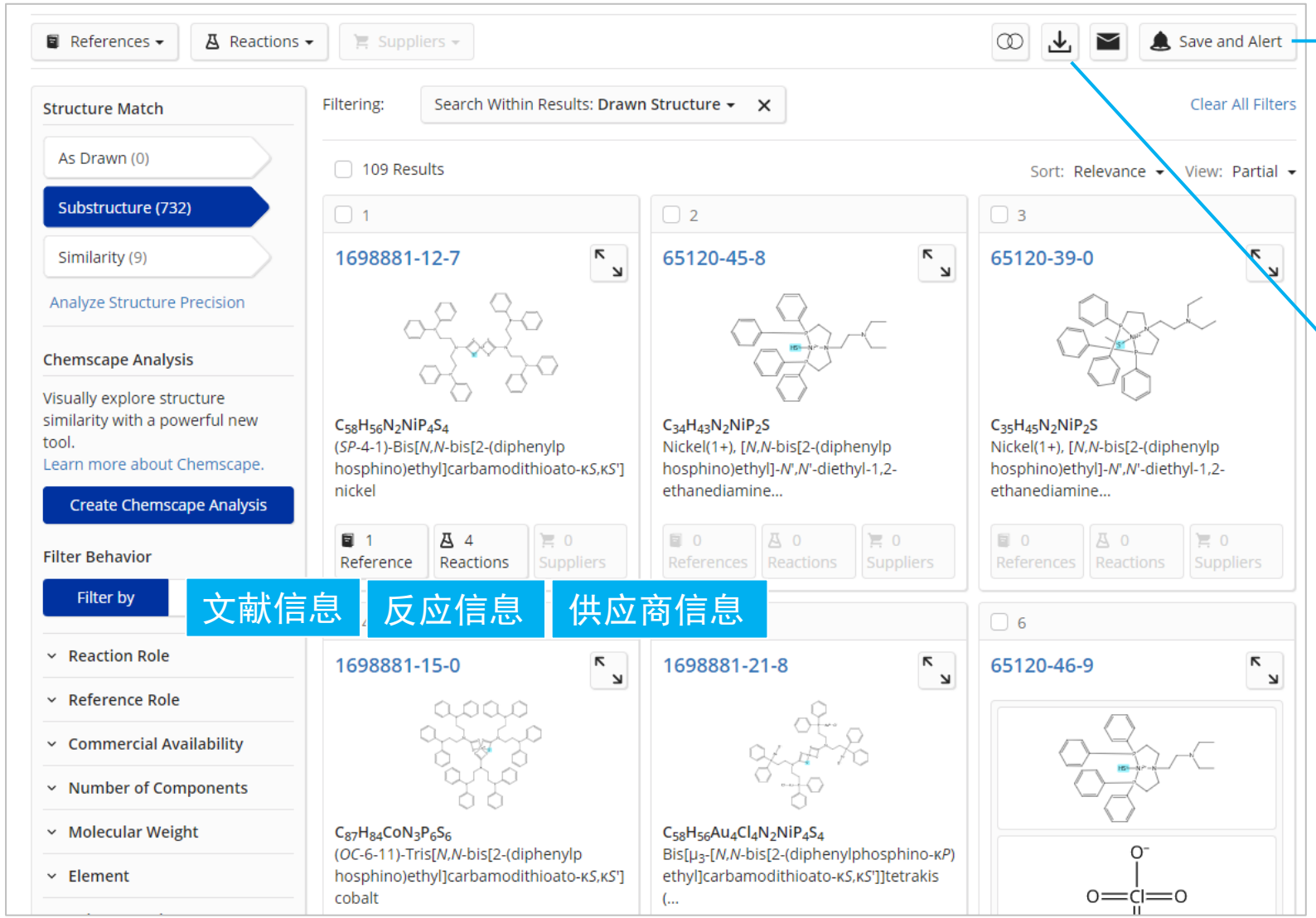
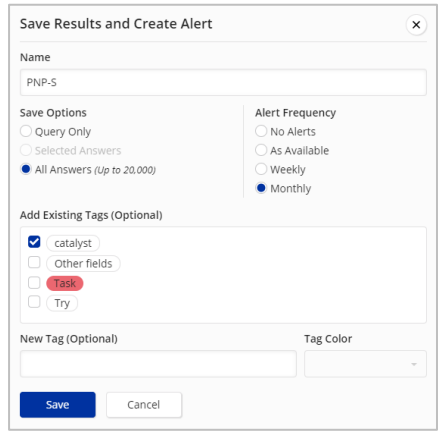
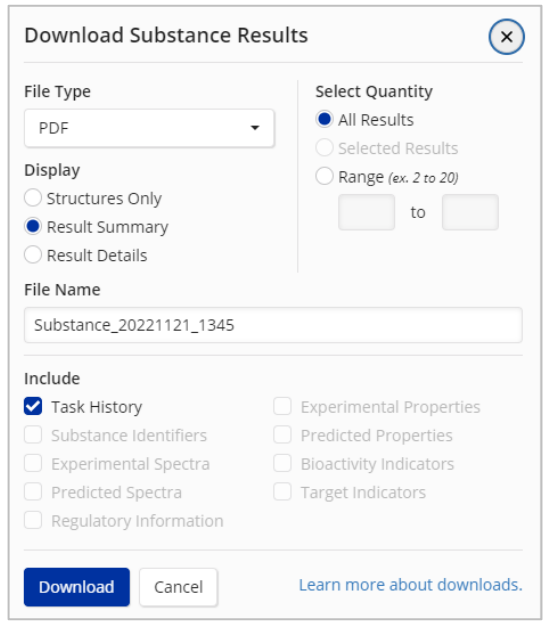
物质检索—检索结果集的保存







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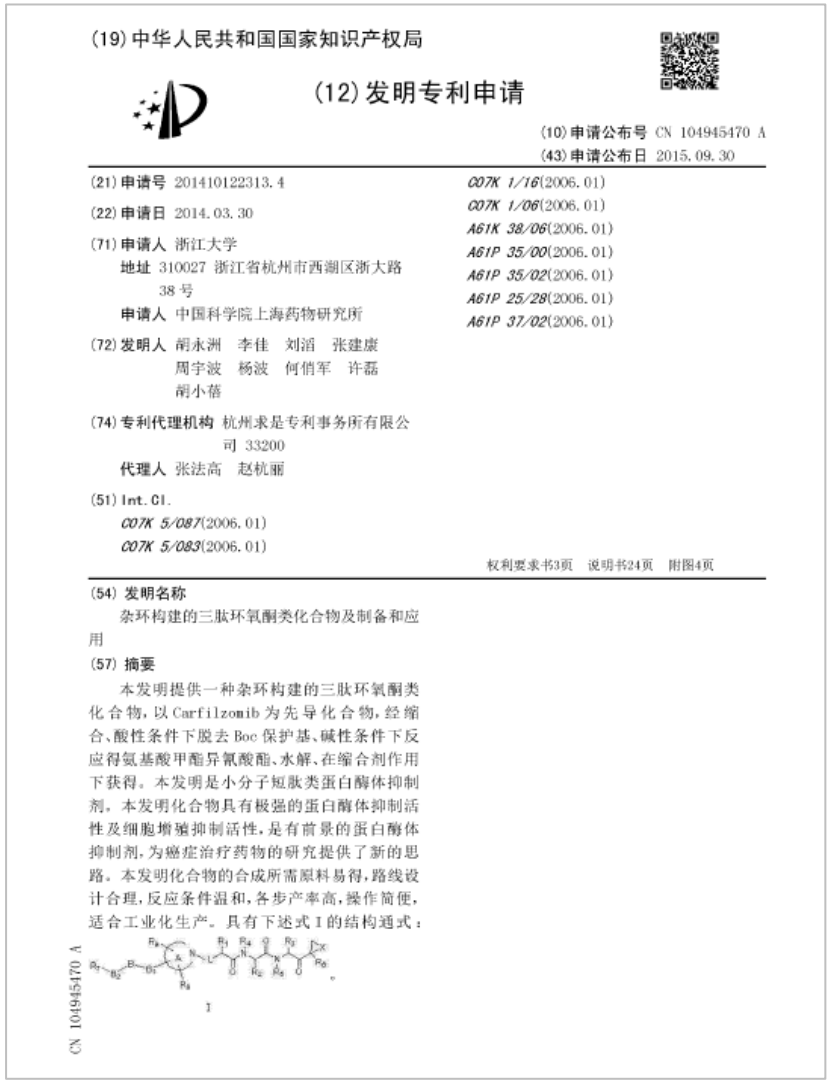
CAS Markush检索



(19)中华人民共和国国家知识产权局

(12)发明专利申请

(10)申请公布号 CN 104945470 A
(43)申请公布日 2015.09.30

(21)申请号 201410122313.4
(22)申请日 2014.03.30
(71)申请人 浙江大学
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(54)发明名称

杂环构建的三肽环氧酮类化合物及制备和应用

(57)摘要

本发明提供一种杂环构建的三肽环氧酮类化合物，以Carfilzomib为先导化合物，经缩合、酸性条件下脱去Boc保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶体抑制剂。本发明化合物具有极强的蛋白酶体抑制活性及细胞增殖抑制活性，是有前景的蛋白酶体抑制剂，为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得，路线设计合理，反应条件温和，各步产率高，操作简便，适合工业化生产。具有下述式I的结构通式：

I

CN 104945470 A

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

具体实施方式

[0026] 本发明结合附图和实施例作进一步的说明，以下实施例仅是说明本发明，而不是以任何方式限制本发明。

[0027] 制备实施例1、4-(吡嗪-2-基氨甲酰基)哌啶-1-甲酸叔丁酯(1a,1b)

将1-(叔丁氧羰基)哌啶-4-甲酸(2.75g,12mmol)置于50mL三颈瓶中，N_2保护下加入25mL无水CH_2Cl_2，然后缓缓滴入吡啶(2.5mL,30mmol)和二氯亚砜(1.1mL,14mmol)，该反应液置于室温反应半小时。随后，2-氨基吡嗪(0.95g,10mmol)和三乙胺(5.7mL,40mmol)溶于15mL CH_2Cl_2后缓缓滴入上述反应液，室温反应6小时。反应液加30mL饱和食盐水稀释，分出有机层，水层CH_2Cl_2提取(15mL×3)，合并有机层，无水硫酸钠干燥后减压除去溶剂，柱层析分离得白色固体2.3g，收率74%。m.p.：134-136℃；^1H NMR (500MHz, $CDCl_3$)：δ = 9.55 (s, 1H, pyrazine-H), 8.35 (d, 1H, J=2.0Hz, pyrazine-H), 8.23 (s, 1H, pyrazine-H), 7.97 (s, 1H, NH), 4.20 (m, 2H, CH_2), 2.81 (m, 2H, CH_2), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH_2), 1.76 (m, 2H, CH_2), 1.47 (s, 9H, CH_3) ppm; ESI-MS: m/z = 307$[M+H]^+$。

[0028] 制备实施例2、4-(吡嗪-2-酰基)哌嗪-1-甲酸叔丁酯(1c,1d)

吡嗪-2-羧酸(1.5g,12mmol)置于50ml反应瓶中，加入35mL无水CH_2Cl_2溶解，随即加入1-羟基苯并三氮唑(1.6g,12mmol)和N-(3-二甲氨基丙基)-N'-乙基碳二亚胺盐酸盐(3.5g,18mmol)，室温反应半小时。随后，哌嗪-1-甲酸叔丁酯(1.9g,10mmol)加入反应液中，室温反应3小时。反应液加入30mL饱和碳酸氢钠水溶液稀释，分出有机层，饱和食盐

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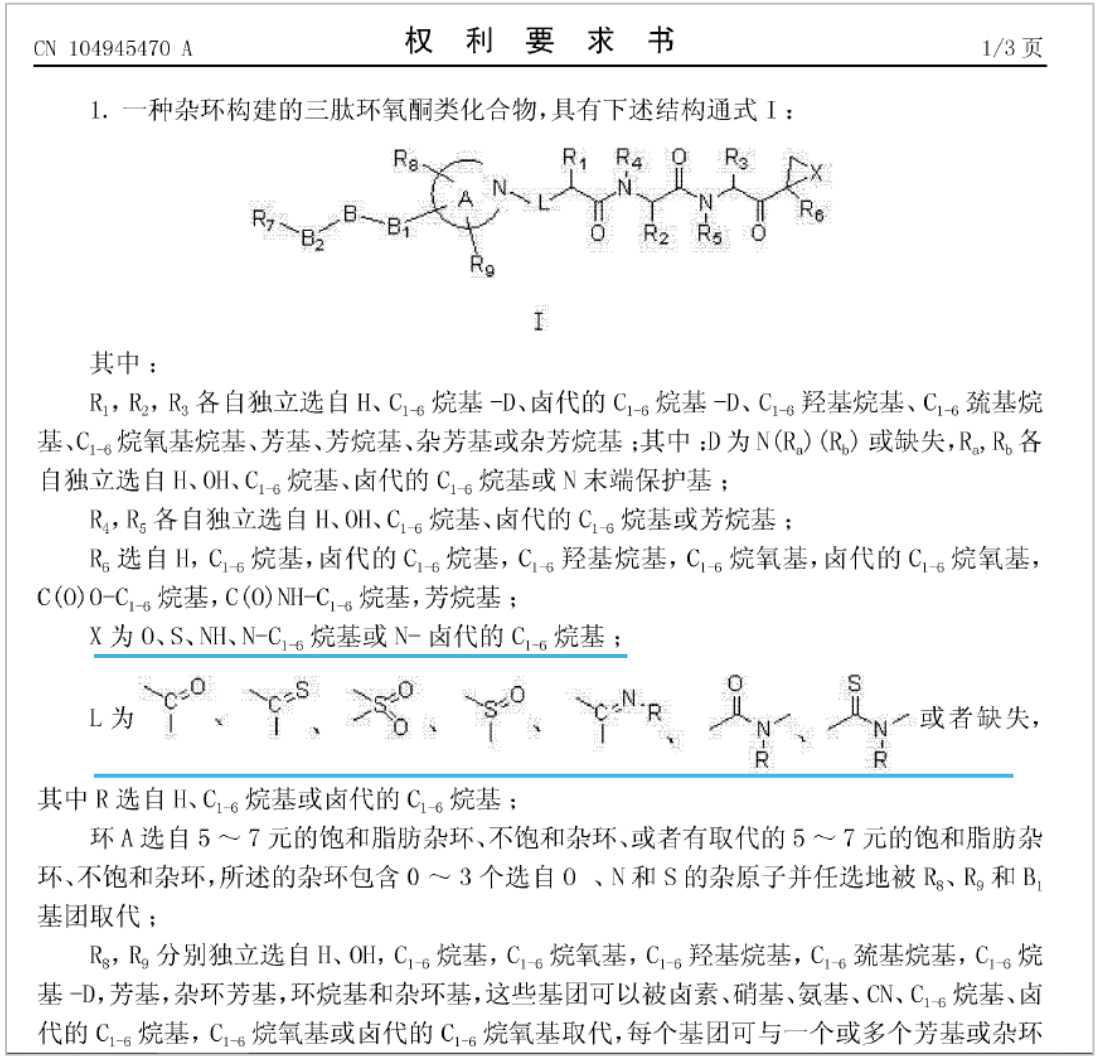
CAS Markush检索

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



CN 104945470 A　　权 利 要 求 书　　1/3 页

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} 烷基 -D，芳基，杂环芳基，环烷基和杂环基，这些基团可以被卤素、硝基、氨基、CN、C_{1-6} 烷基、卤代的 C_{1-6} 烷基，C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代，每个基团可与一个或多个芳基或杂环

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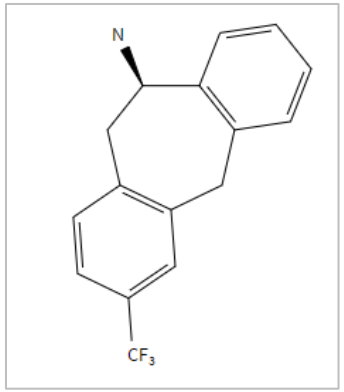
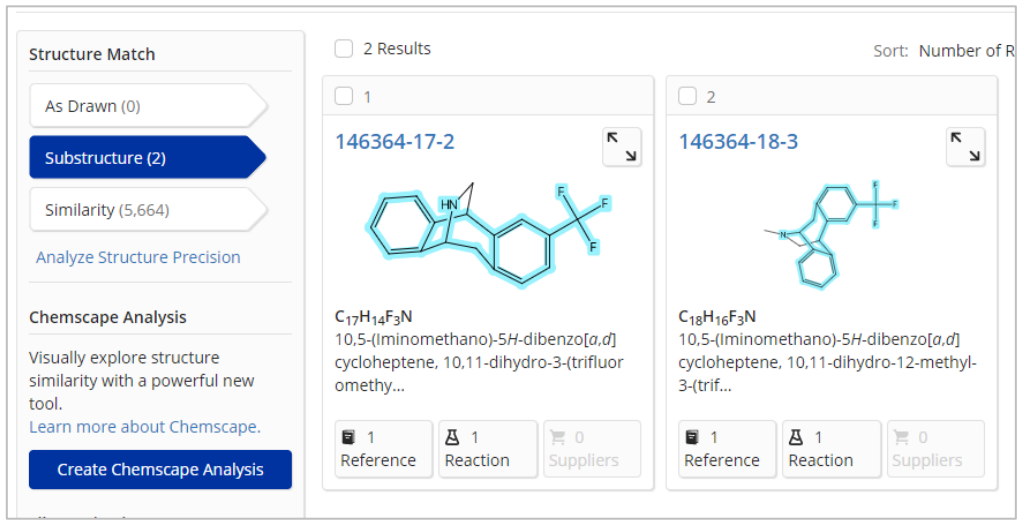
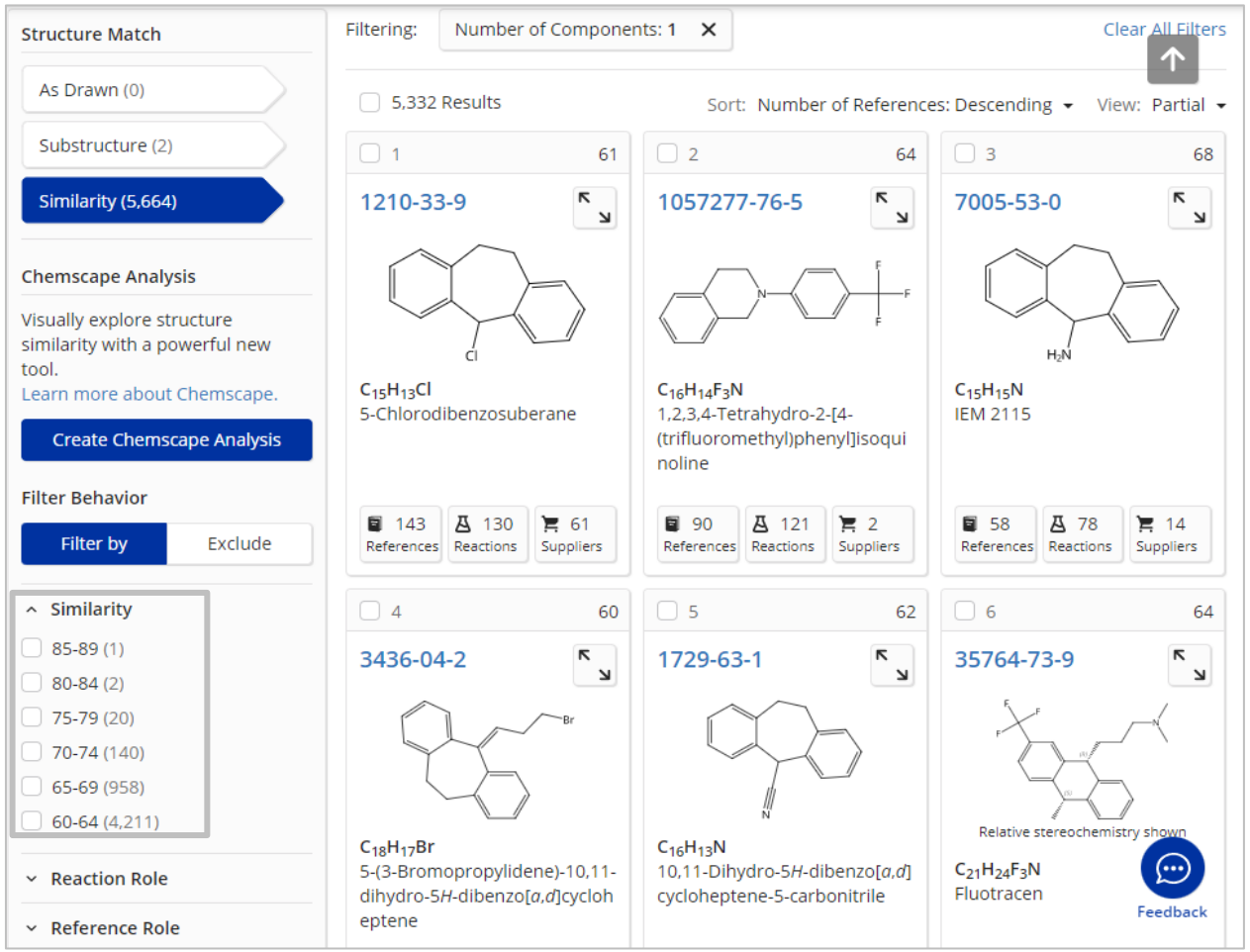
CAS Markush检索

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%







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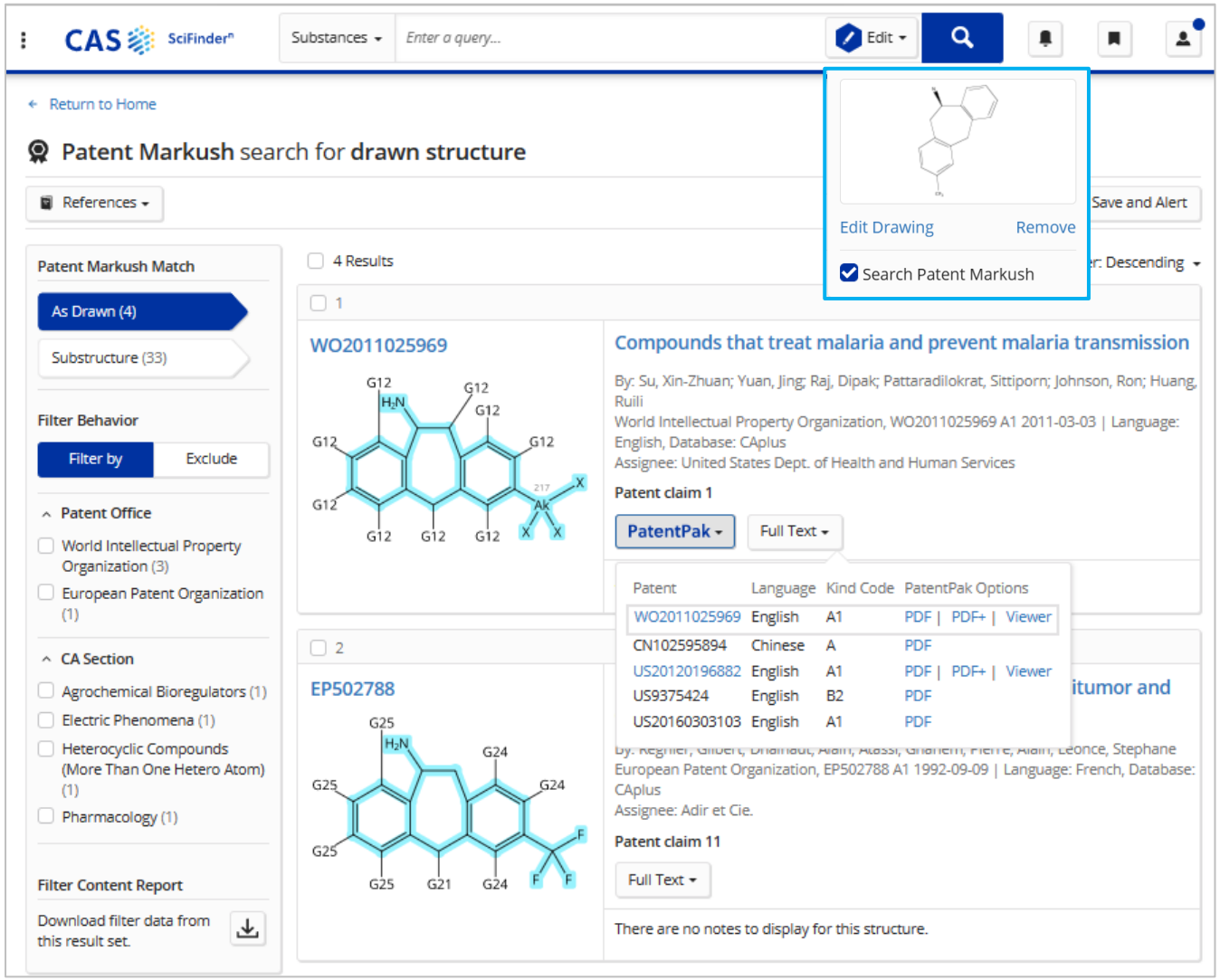
CAS Markush检索

第二步：Markush结构检索
获得四件专利文献

- 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



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

物质检索小结

1. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
2. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
3. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
4. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
5. 利用CAS Markush检索尽可能全面的获得结构的公开信息

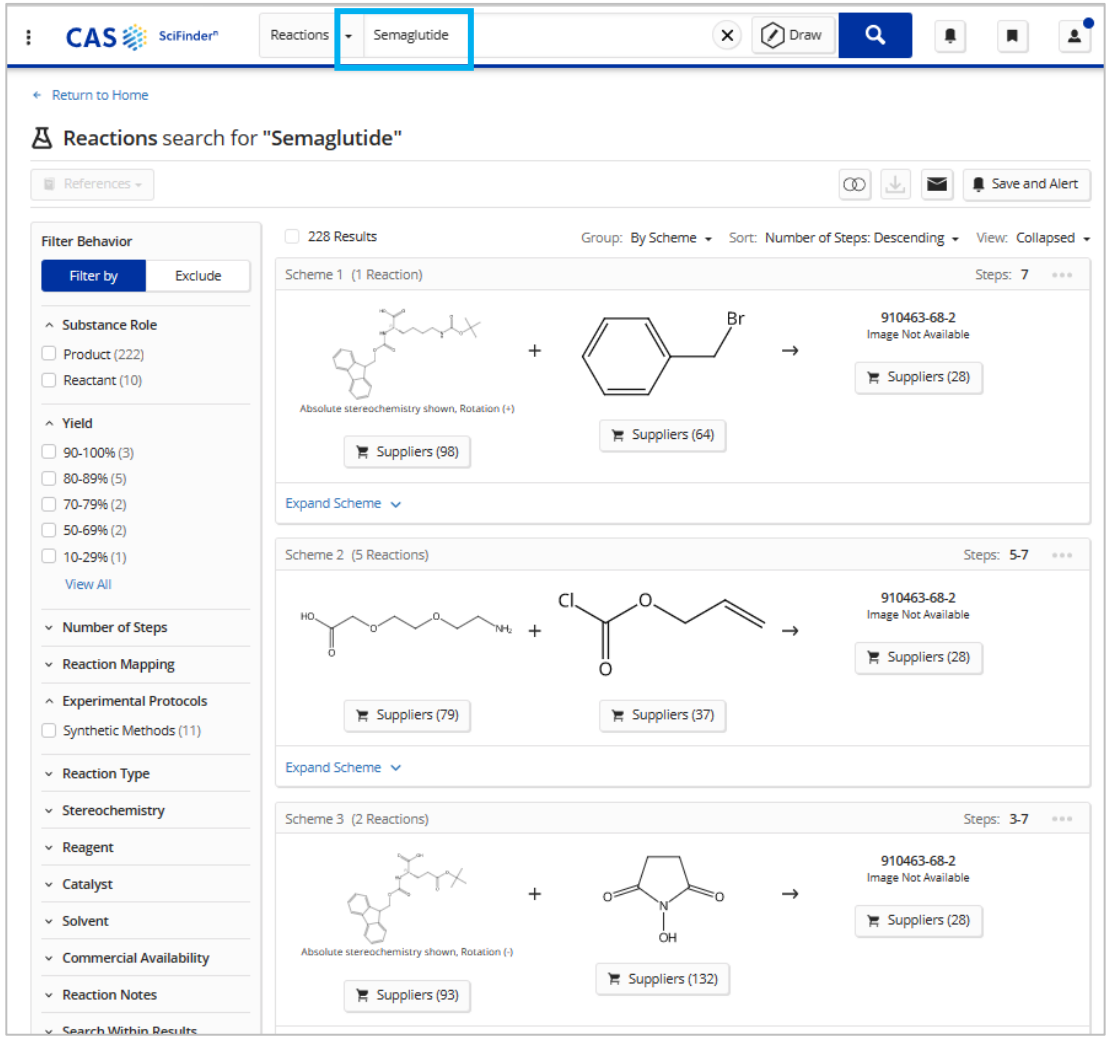
反应检索

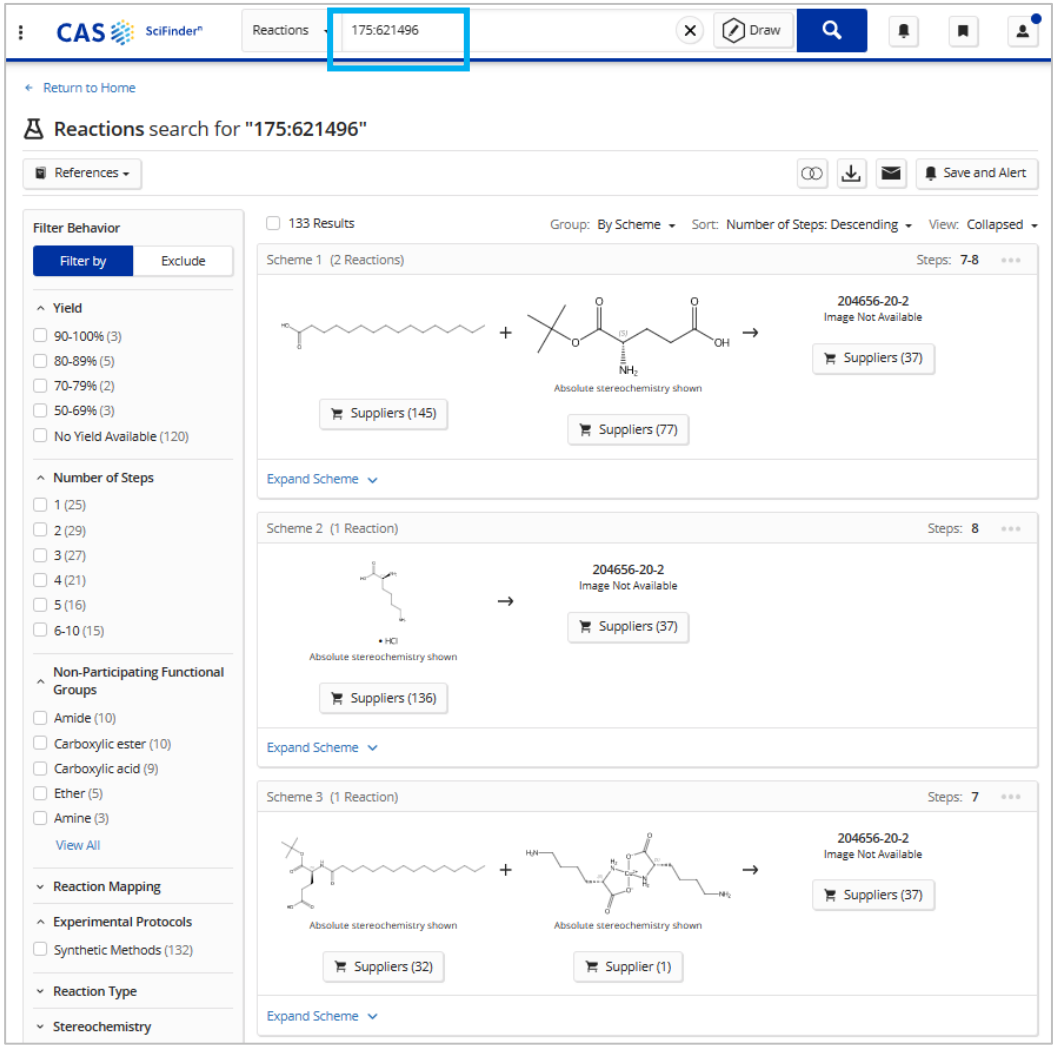
- 反应检索方法
  - 物质或文献标识符
  - 结构式
  - 关键词与结构联用

- 常用获取方法推荐
  - 已知物质：由物质获取反应
  - 已知文献：从文献中获取反应
  - 精确结构反应检索
  - 亚结构反应检索

反应检索

通过物质或文献标识符进行检索





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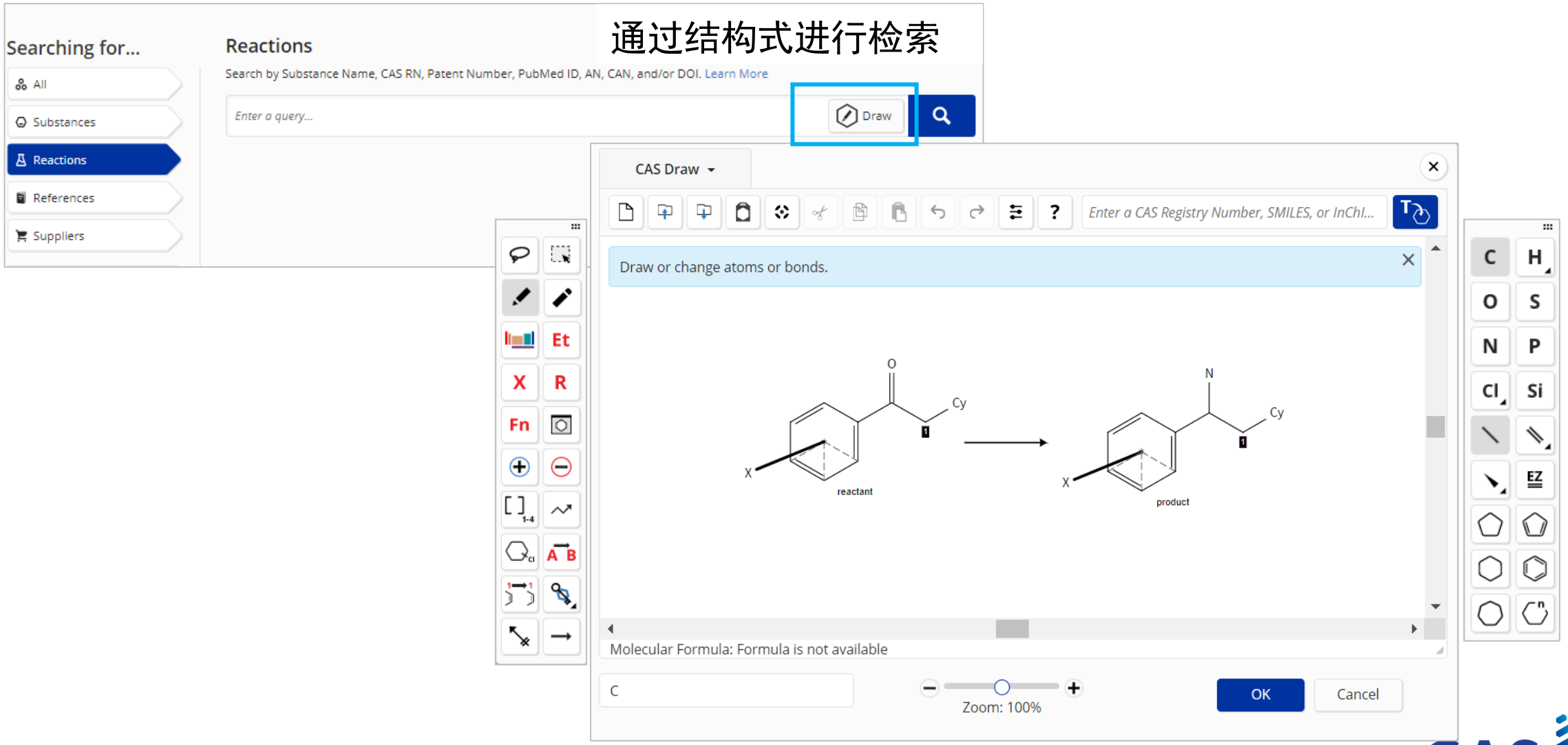
反应检索



X = Cl, Br

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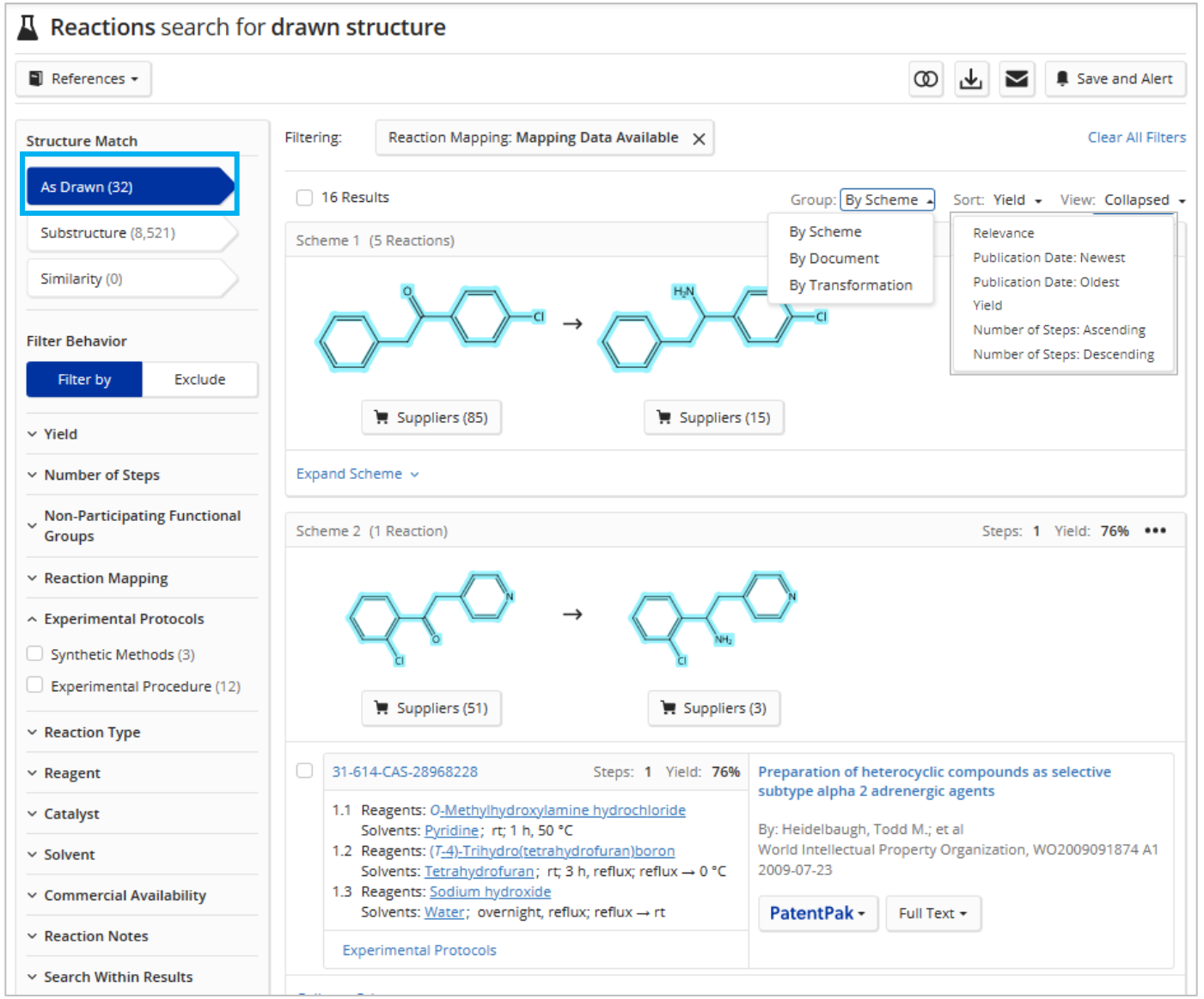
反应检索—结果集的分组与排序

As drawn结果为32



反应分组：
按类型分组
按文献分组

反应排序：
相关度
公布时间
产率
步数

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反应检索—结果集筛选

Substructure结果8521

As Drawn反应检索

亚结构反应检索

相似反应检索

反应筛选类别：

产率、反应步数

不参与反应的官能团

实验步骤

反应类型

立体化学

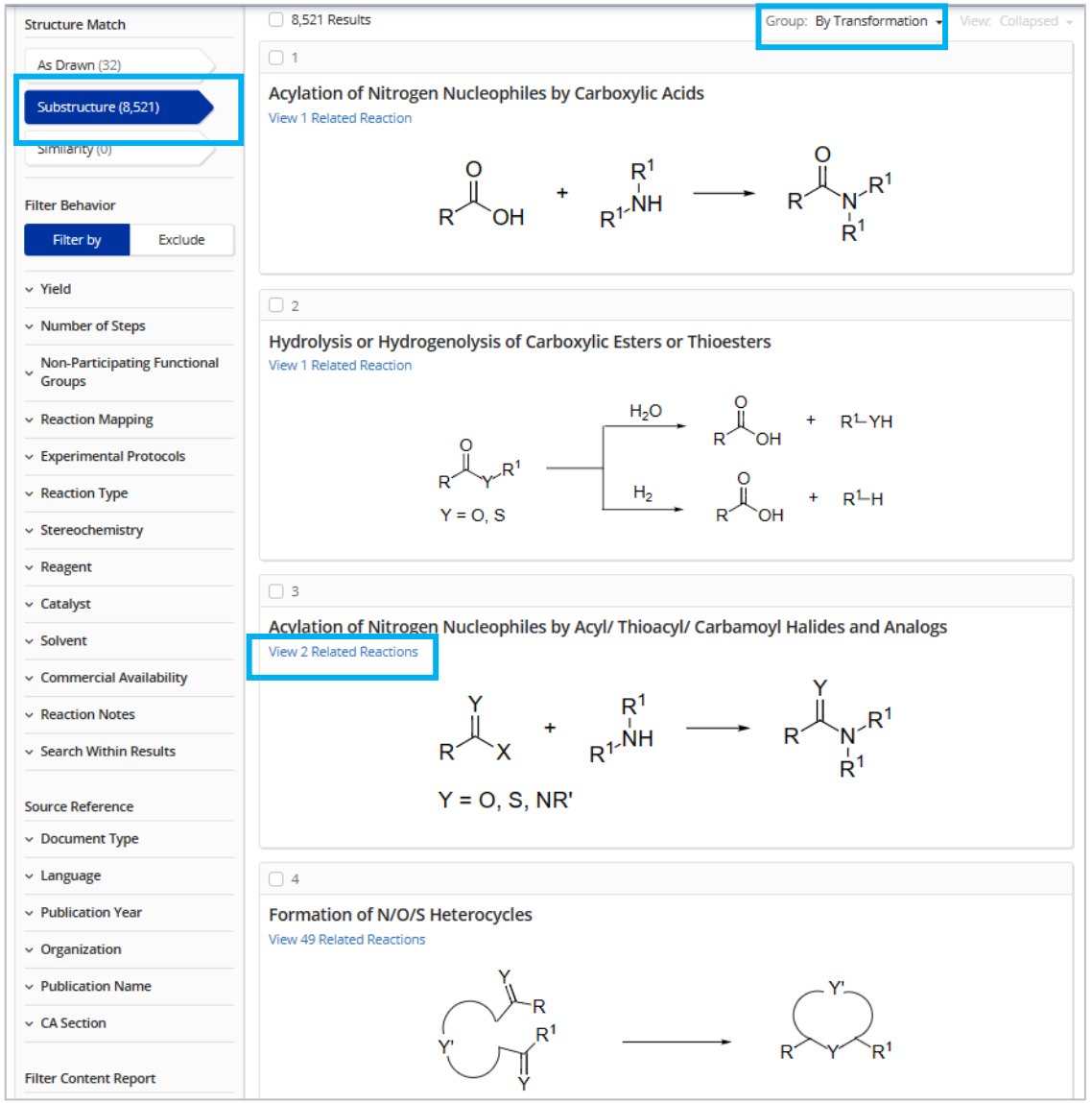
试剂、催化剂、溶剂

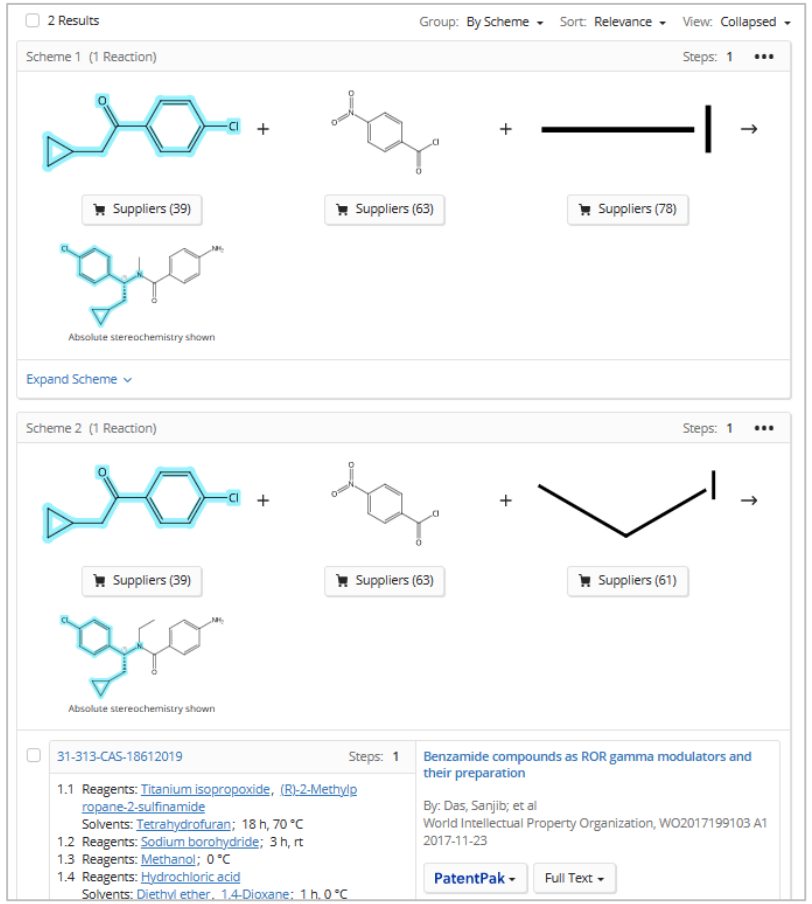
商品信息……

文献筛选类别：

文献类型、语言

出版年份、刊物名





折叠菜单显示：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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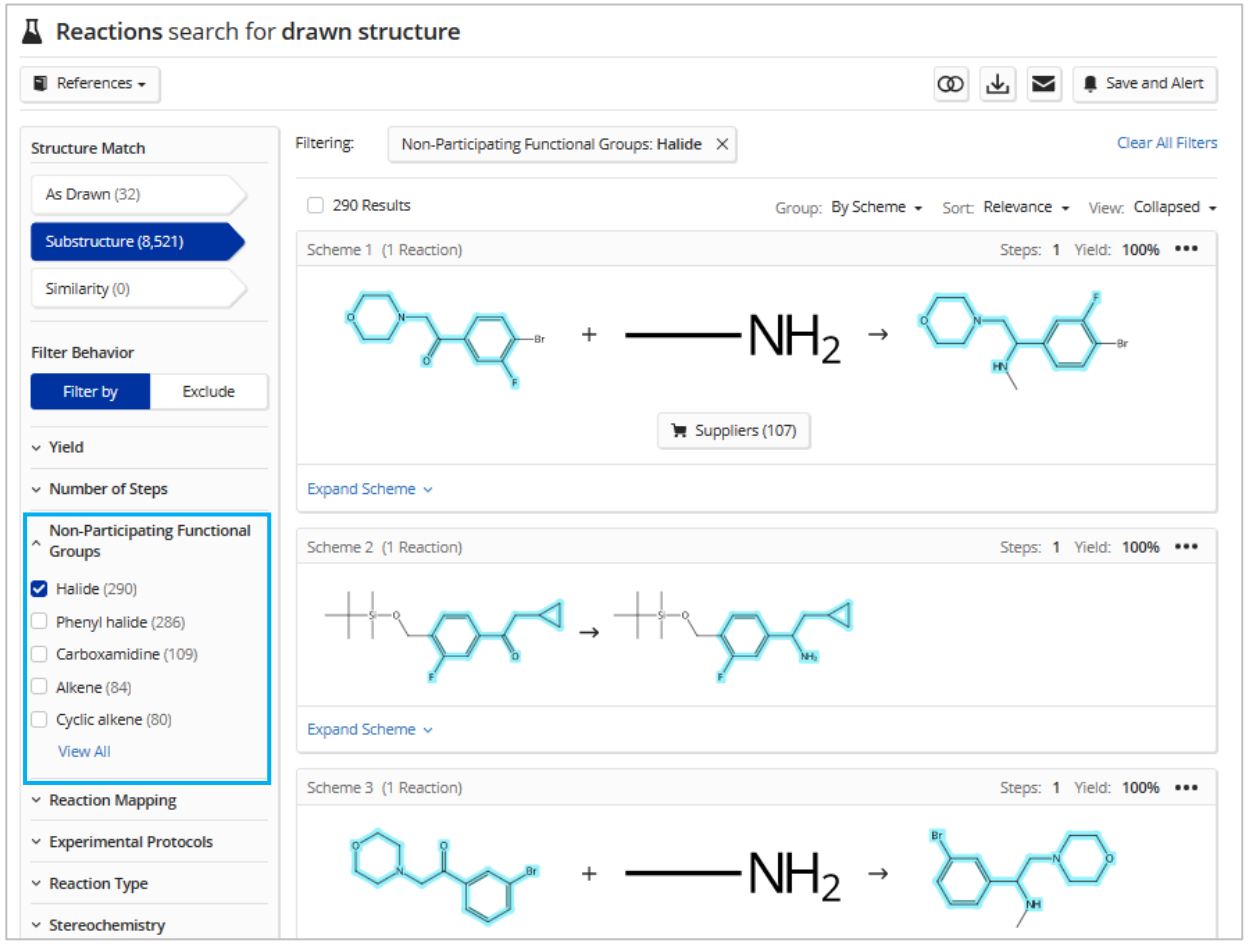
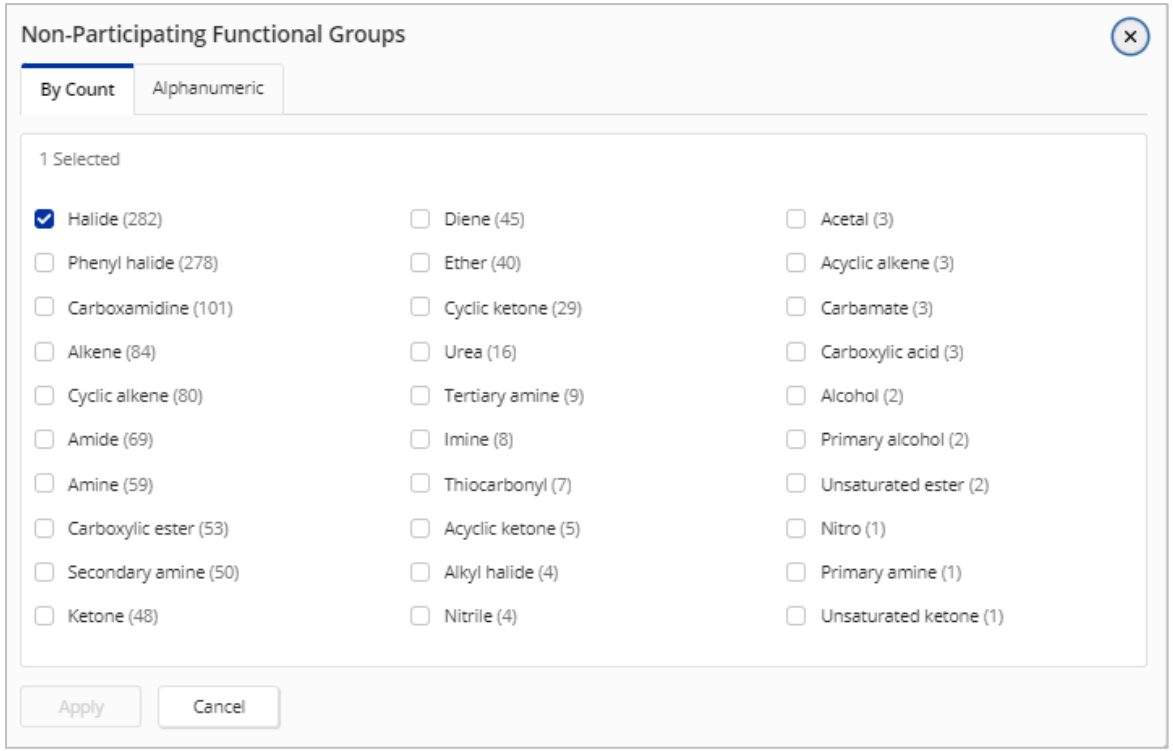
反应检索—结果集筛选：不参与反应官能团



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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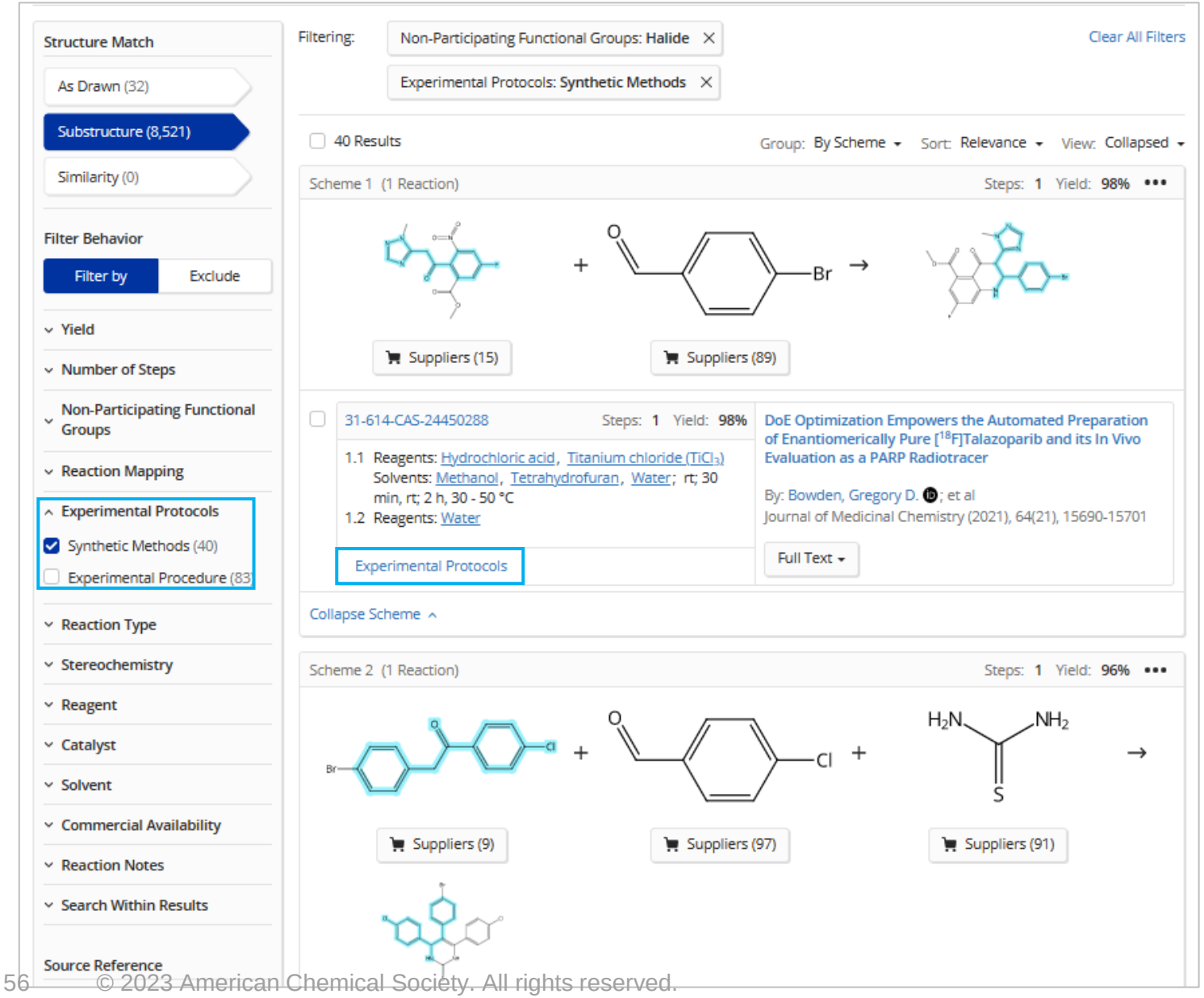
反应检索—结果集筛选：Synthetic Methods™



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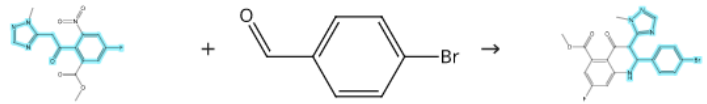
反应检索—结果集筛选：Synthetic Methods™

Synthetic Methods™：查看文献详情，分类显示详尽信息，方便操作

CAS Reaction Number: 31-614-CAS-24450288

Save



Suppliers (15) Suppliers (89) 98%

Reaction Overview

Steps: 1 Yield: 98%

JOURNAL

DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [^{18}F]Talazoparib and its In Vivo Evaluation as a PARP Radiotracer

By: Bowden, Gregory D.; et al

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Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

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Company/Organization

Werner Siemens Imaging Center, Department of Preclinical Imaging and Radiopharmacy
Eberhard Karls University
Tuebingen 72076
Germany

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrochloric acid Titanium chloride ($TiCl_3$)	-	Methanol Tetrahydrofuran Water	rt; 30 min, rt; 2 h, 30 - 50 °C
2	Water	-	-	-

Alternative Steps (2)

Experimental Protocols

Synthetic Methods

Products	Methyl 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1*H*-1,2,4-triazol-5-yl)-4-oxo-5-quinolinecarboxylate, Yield: 98%
Reactants	4-Bromobenzaldehyde Benzoic acid, 5-fluoro-2-[2-(1-methyl-1*H*-1,2,4-triazol-5-yl)acetyl]-3-nitro-, methyl ester
Reagents	Hydrochloric acid Titanium chloride ($TiCl_3$) Water

Procedure	1. Suspend methyl 5-Fluoro-2-(2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl)-3-nitrobenzoate (8.1 g, 25.2 mmol) and 4-bromobenzaldehyde (8.9 g, 50.5 mmol) in THF (50 mL) and MeOH (10 mL). 2. Add titanium(III) chloride solution [20% wt solution in HCl (2 M), 130 mL, 6 equiv] to the resulting mixture in dropwise fashion over 30 minutes at room temperature. 3. Maintain the reaction temperature between 30 and 50°C for 2 hours. 4. Quench the mixture by the slow addition of water (260 mL). 5. Pour the reaction mixture into a separating funnel. 6. Extract the mixture with ethyl acetate (4 x 140 mL). 7. Pool the organic fractions. 8. Wash the organic fractions with $NaHCO_3$ (3 x 60 mL) and $NaHSO_3$ (3 x 100 mL). 9. Dry the organic fractions with sodium sulfate (Na_2SO_4). 10. Concentrate the solvent under reduced pressure to obtain a think yellow syrup. 11. Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully. 12. Dry the resulting yellow syrup under high vacuum to obtain product.
Transformation	Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/ Knoevenagel Reaction Reduction of Nitro Compounds to Amines
Scale	gram

Characterization Data

5-Quinolinecarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1*H*-1,2,4-triazol-5-yl)-4-oxo-, methyl ester

State	yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

Transformations
1. Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
2. Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/ Knoevenagel Reaction
3. Reduction of Nitro Compounds to Amines

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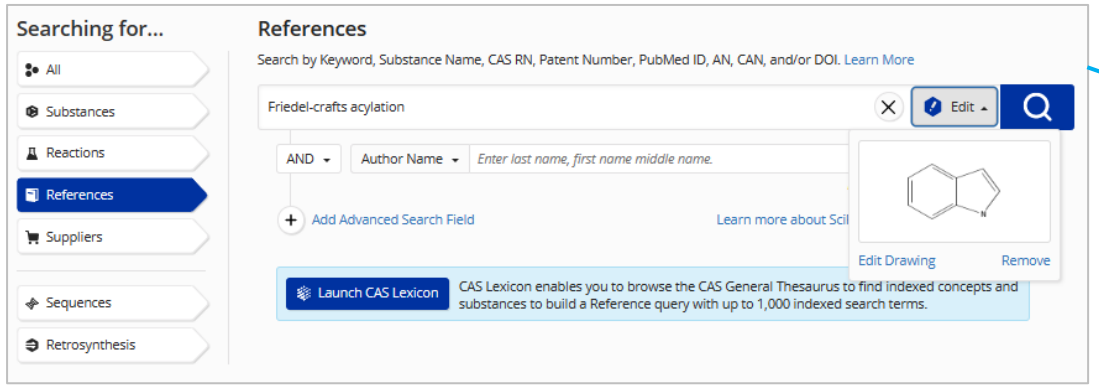
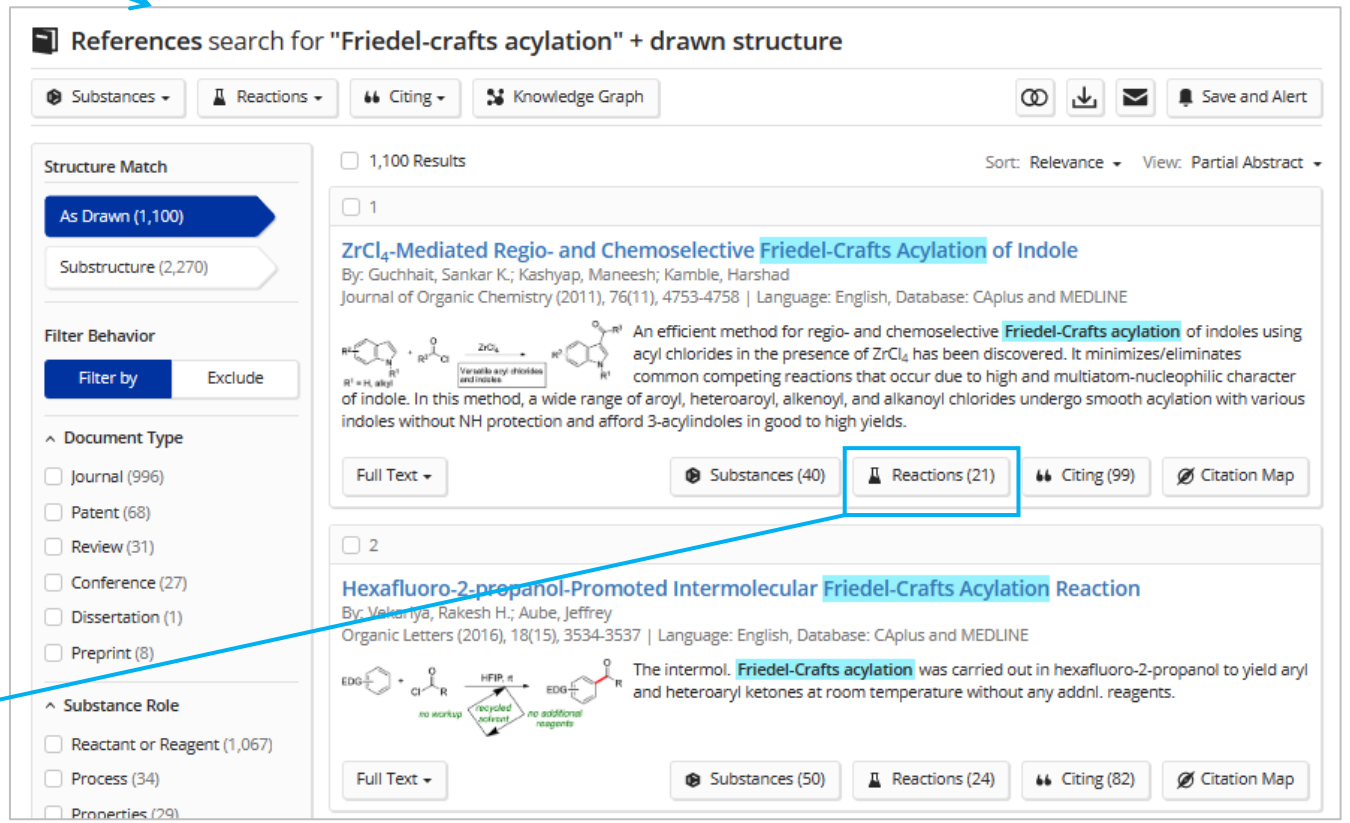
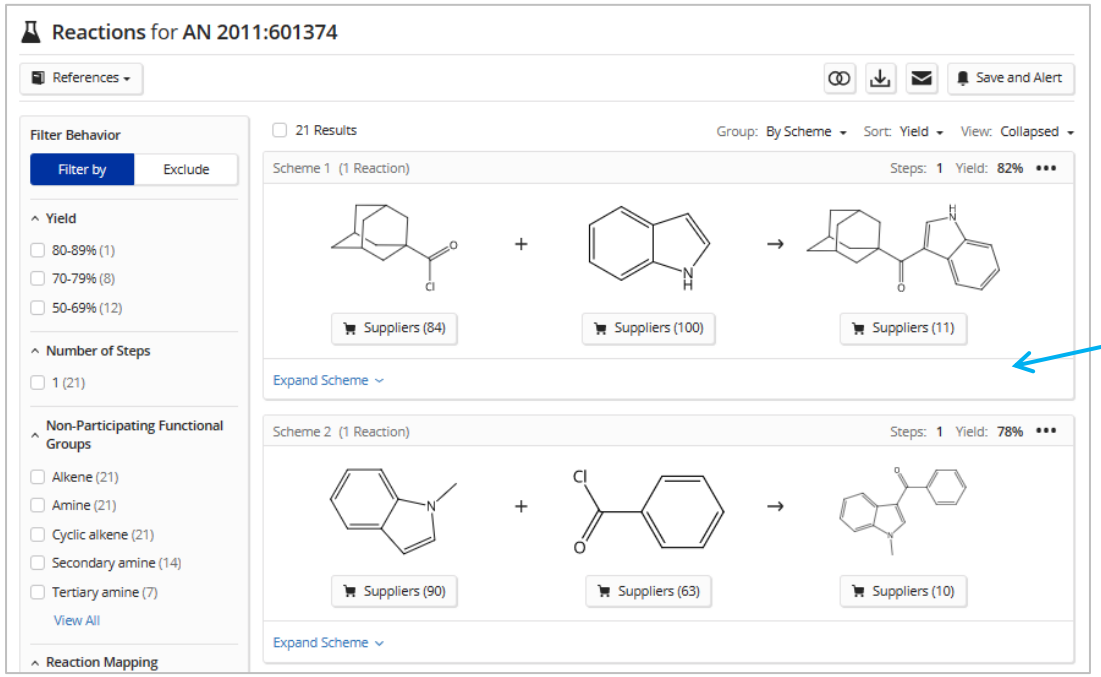
联合检索—结构与关键词

联用检索提高检索效率







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反应检索小结

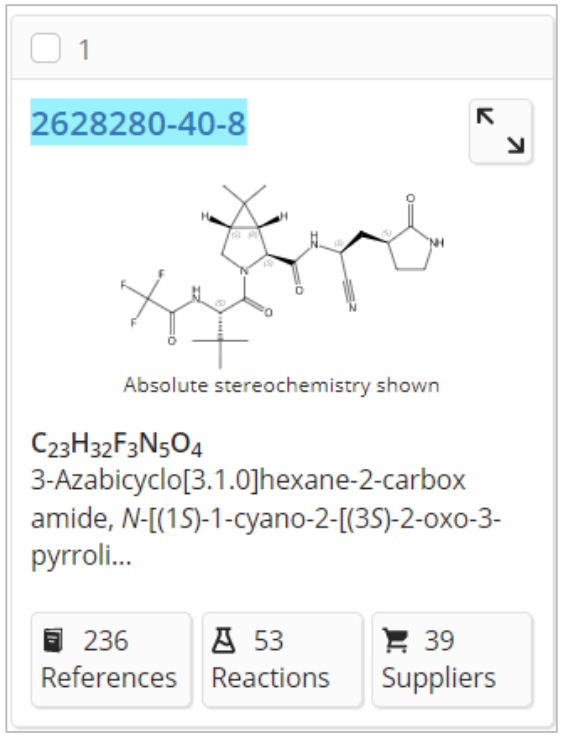
1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 利用Synthetic Methods™查看文献中合成方法详情
4. 关键词与反应式的联合检索

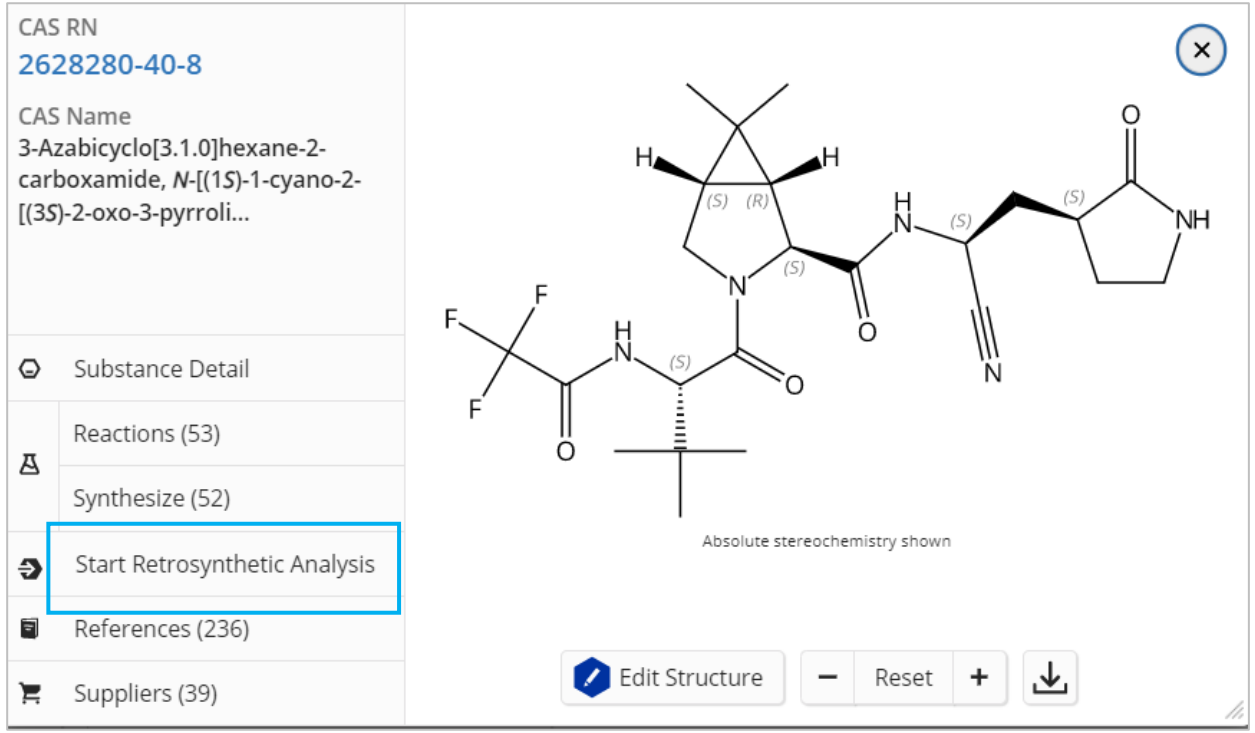
大纲

- CAS Retrosynthesis Tool的使用
  - 获得已知化合物的逆合成反应路线
  - 获得未知化合物的逆合成反应路线

CAS Retrosynthesis Tool—由物质获得

获得已知化合物的逆合成路线（1）：
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

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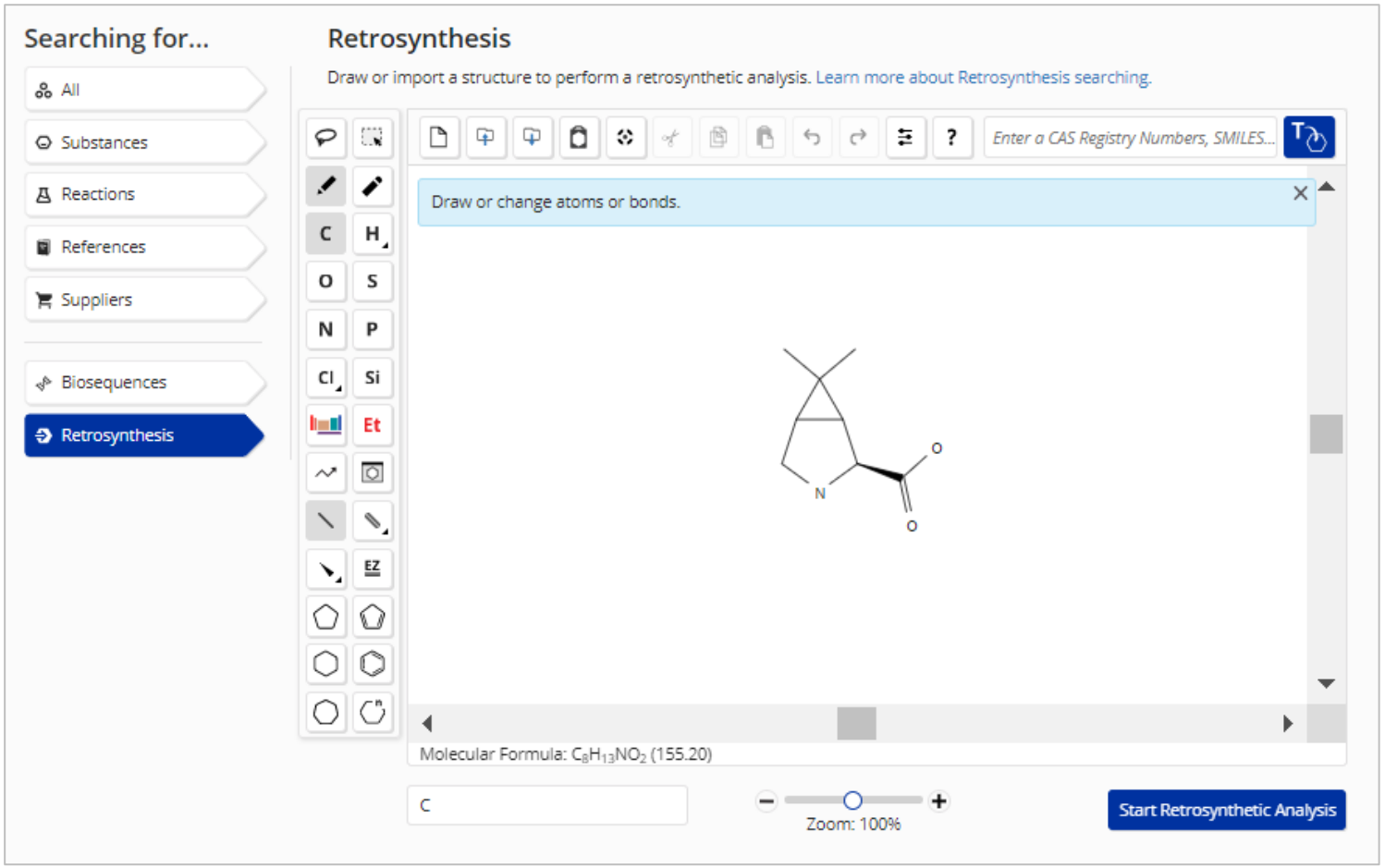
CAS Retrosynthesis Tool—直接绘制

获得已知化合物的逆合成路线（2）：
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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CAS Retrosynthesis Tool—预设参数

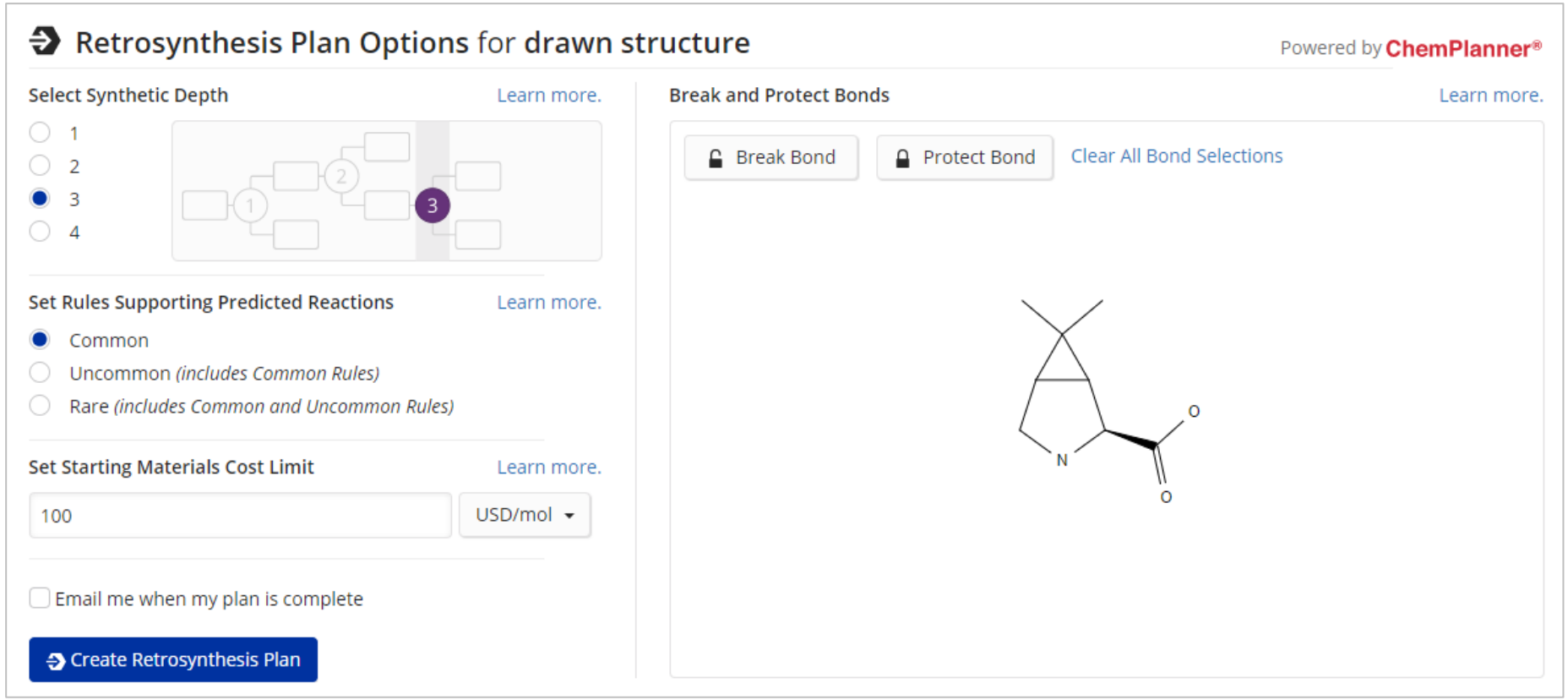
预设反应路线参数：

反应深度

反应规则常见性

起始原料费用

设置断裂键或保护键



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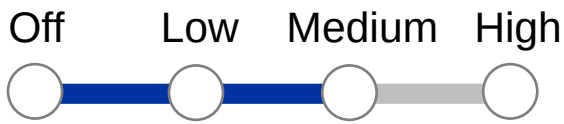
CAS Retrosynthesis Tool—路线概览



Scoring Profiles：

降低每步原料结构的复杂性

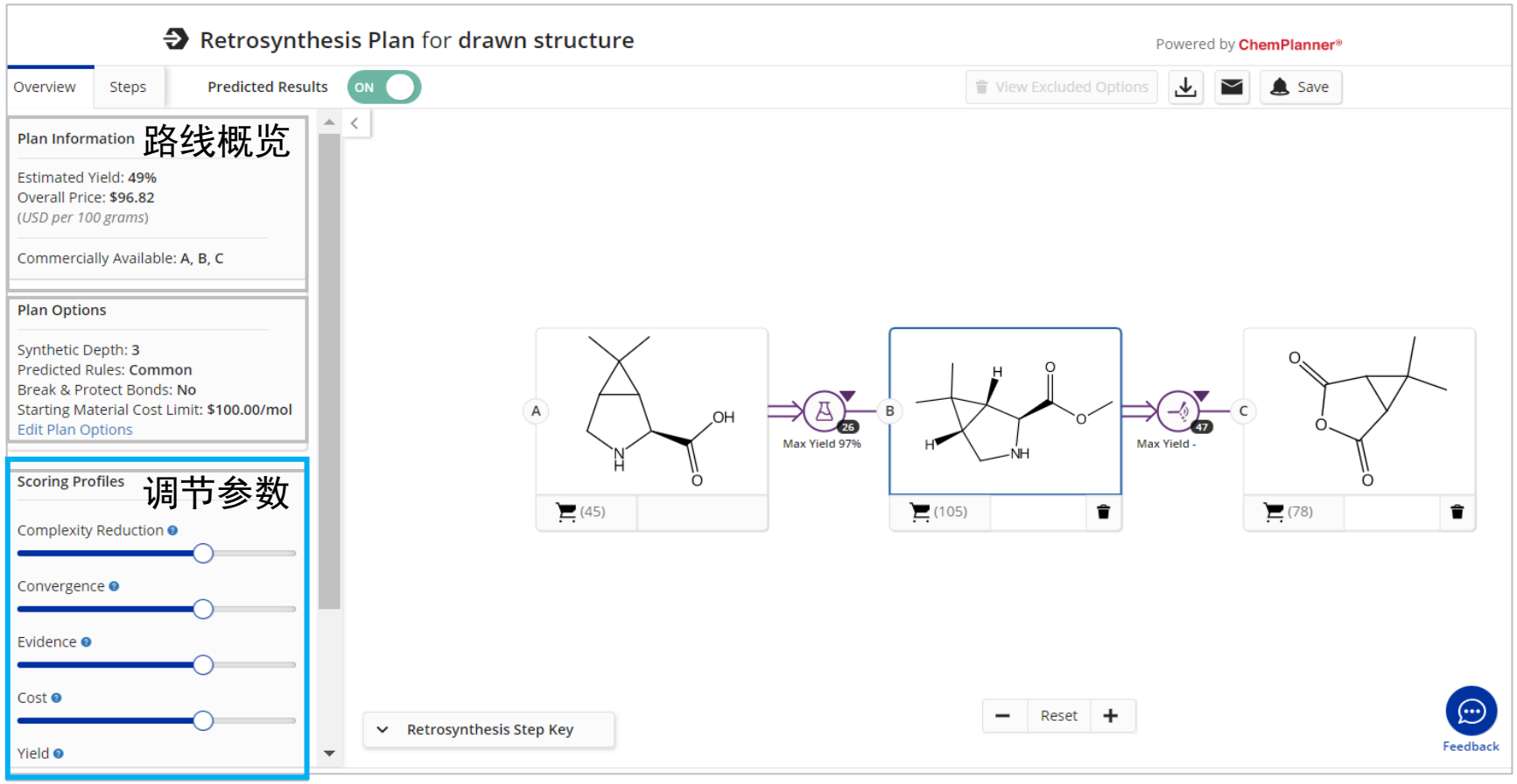
逆合成路线中前体的数量

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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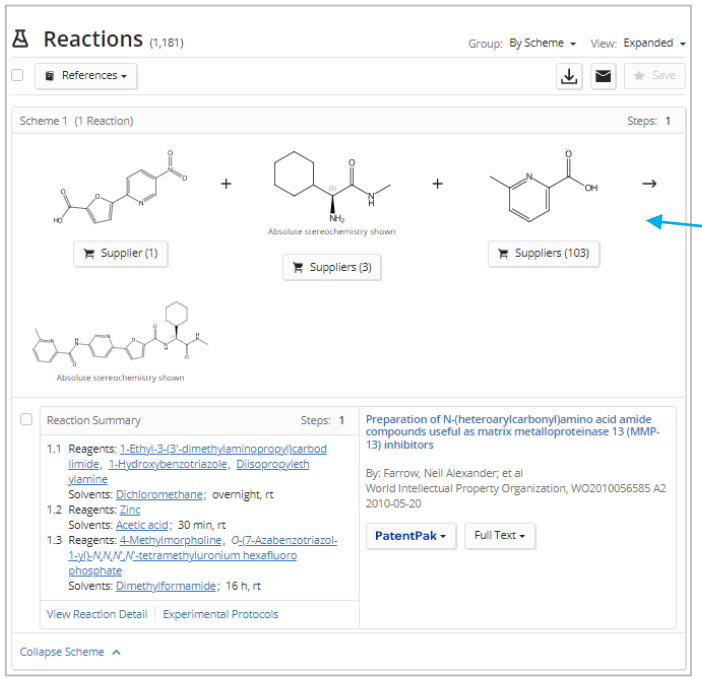
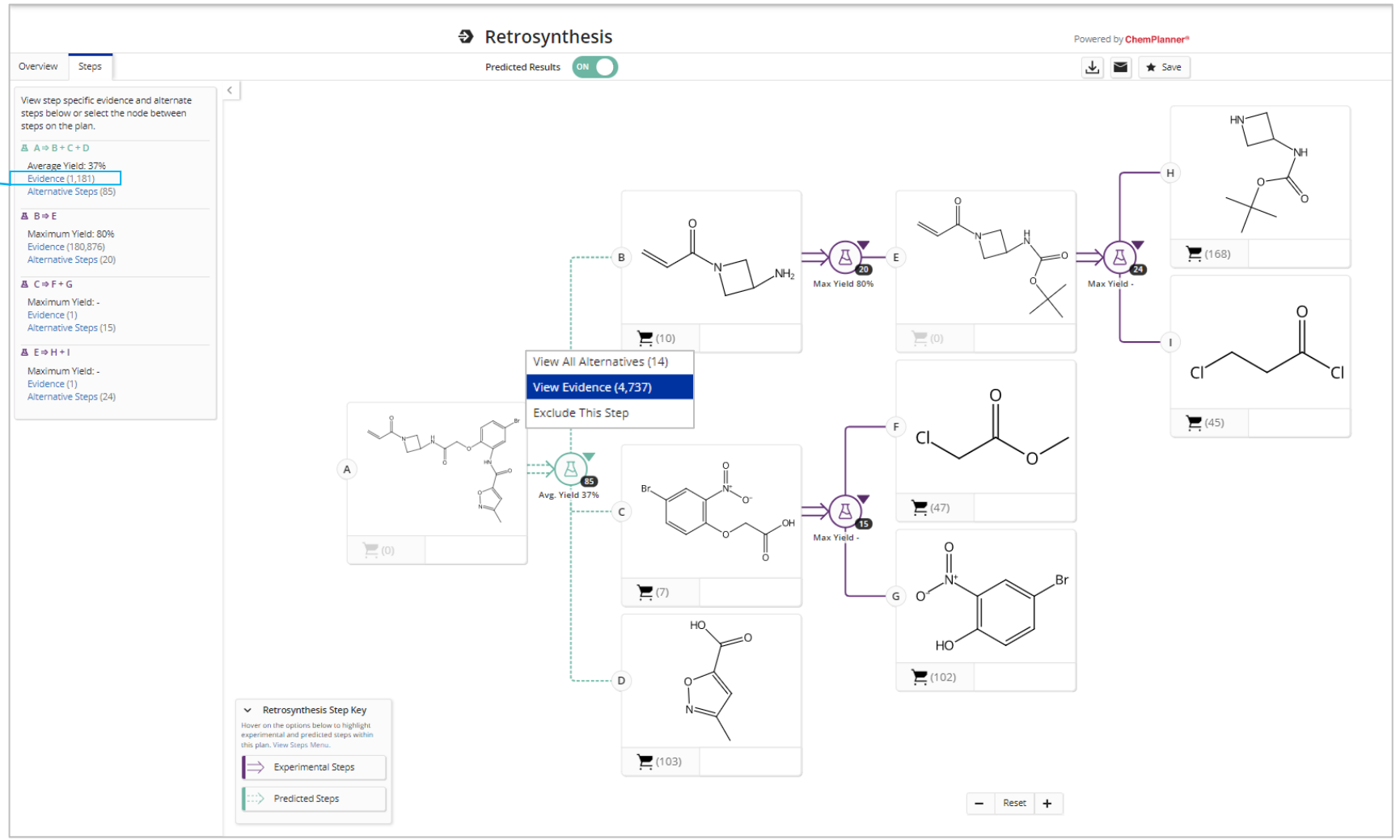
CAS Retrosynthesis Tool—路线详情





- 快速获取最优的逆合成路线
- 可获取预测逆合成路线
- 可查看每步路线的详细条件
- 可自定义选择替代路线

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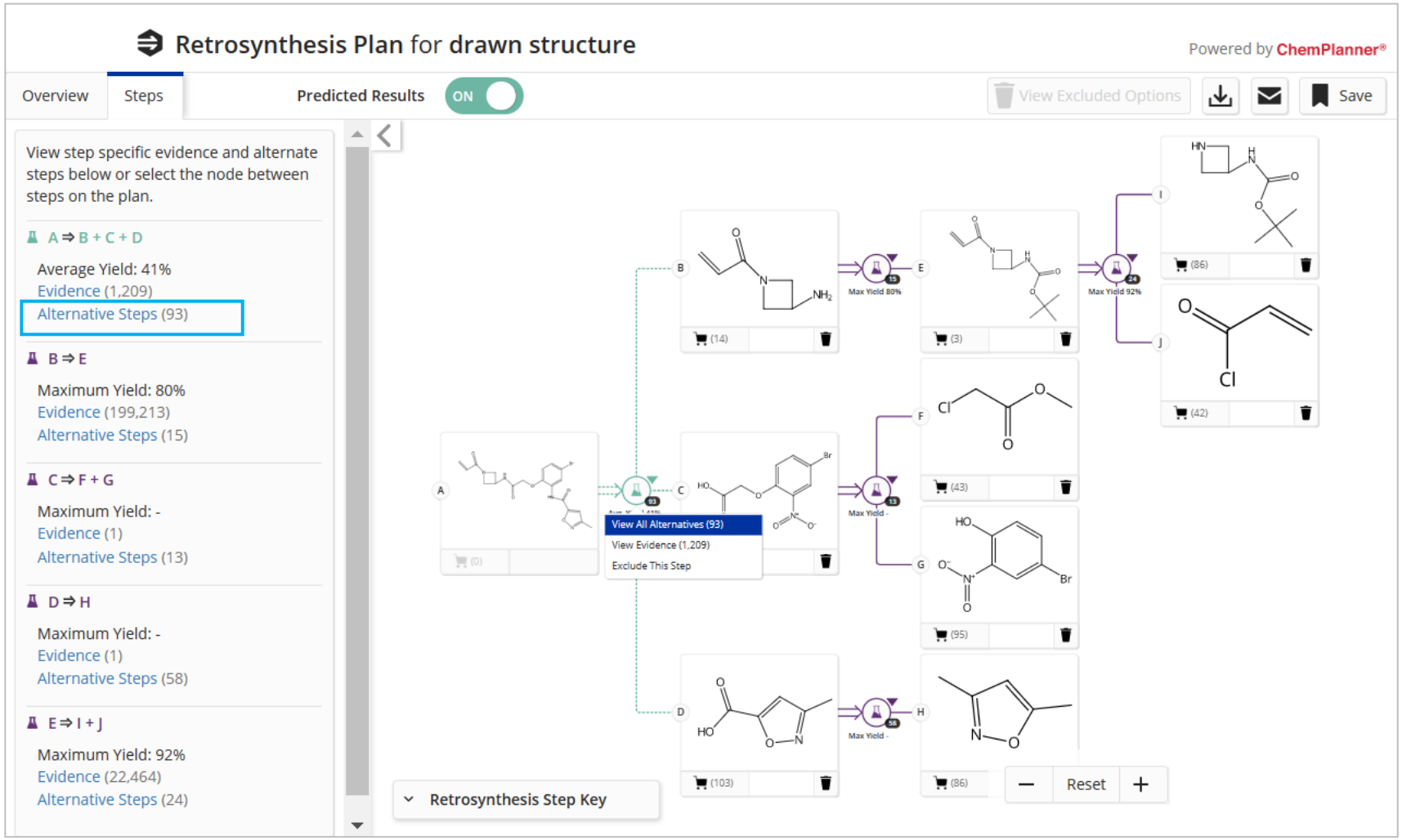
CAS Retrosynthesis Tool—路线详情

点击Alternative Steps查看并选择替换路线，得到自定义的合成路线



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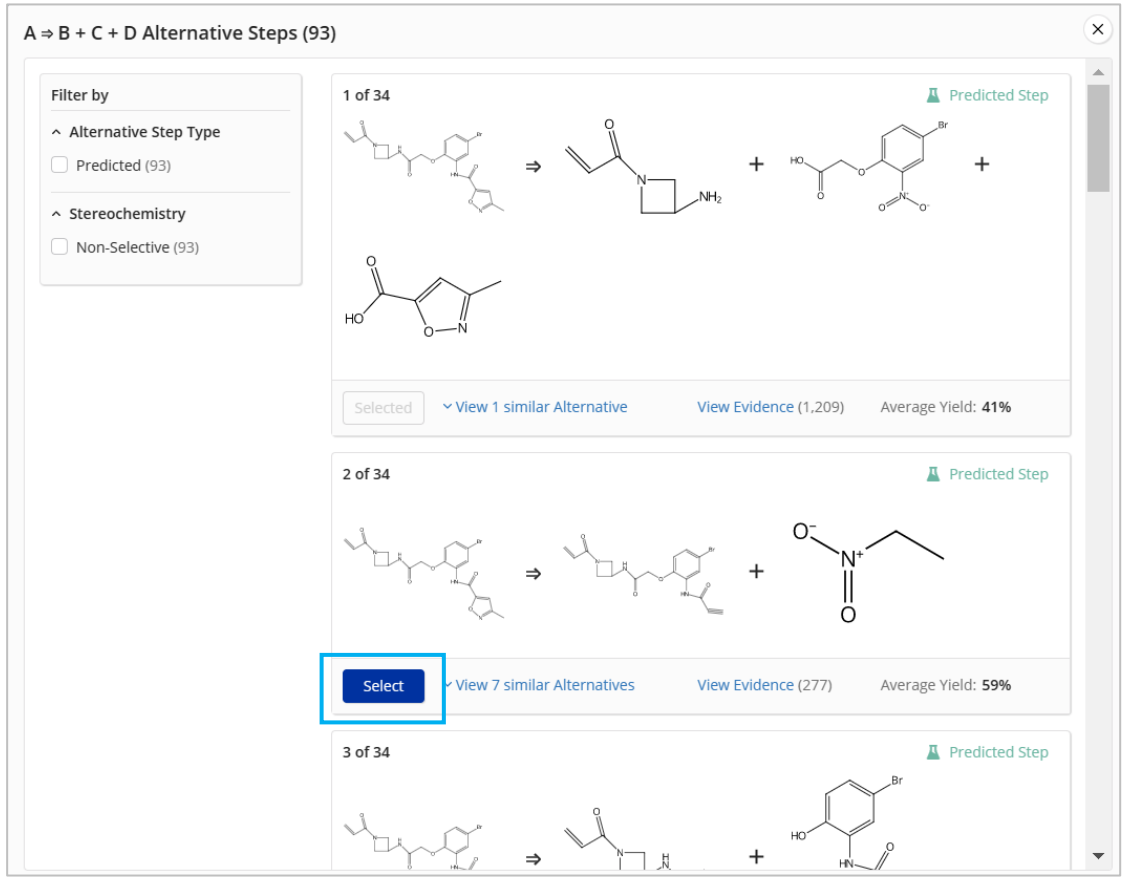
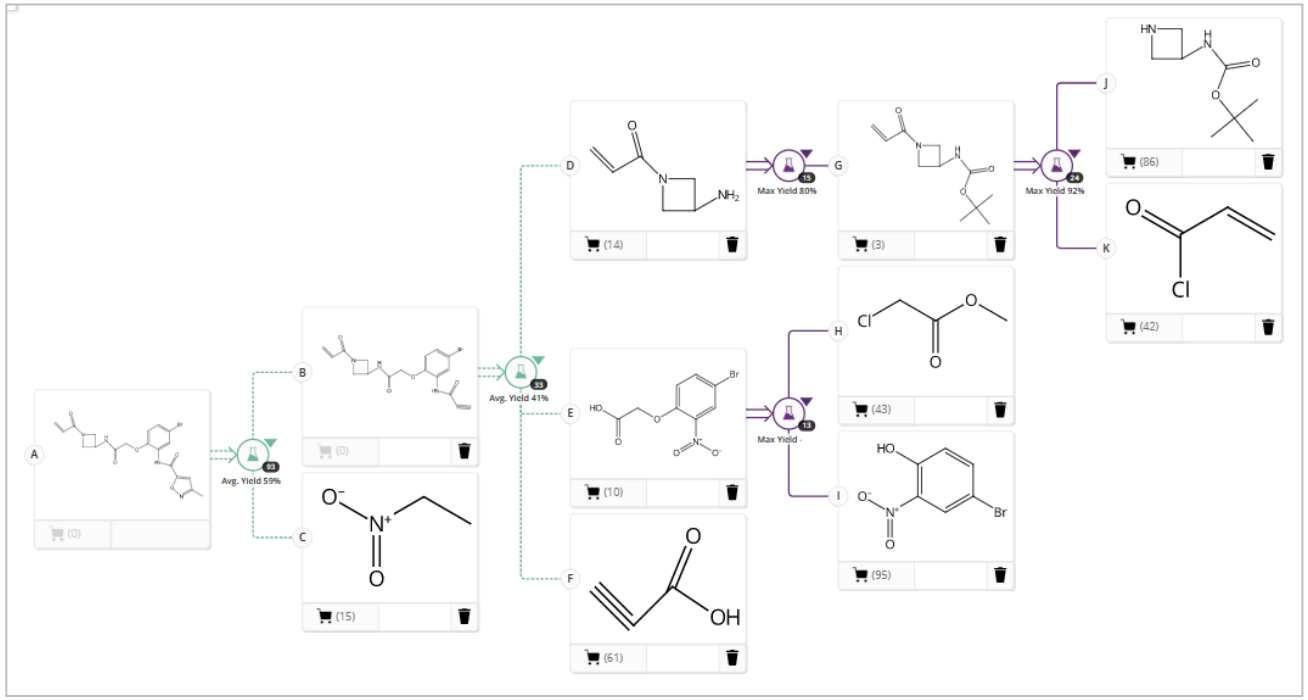
获取替代路线





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逆合成路线小结

1. 通过物质结构获取已知化合物的逆合成路线
2. 获取预测的逆合成路线
3. 反应路线参数的预先设定与调节
4. 查看反应路线详情和文献支持，自定义选择替代路线

大纲

- CAS SciFinder^{n}中的序列检索
  - BLAST
  - CDR
  - Motif

视频链接：
https://american-chemical-society.zoom.us/rec/share/JPoebb74K7-dbzGw2Aj8vRqqeddGB5zzBnQTV8MYcW2E2QQqq2rkYWoBtkHy_tt2.ag1fUmL880MKBne3?startTime=1647943207000

下一节：反应检索

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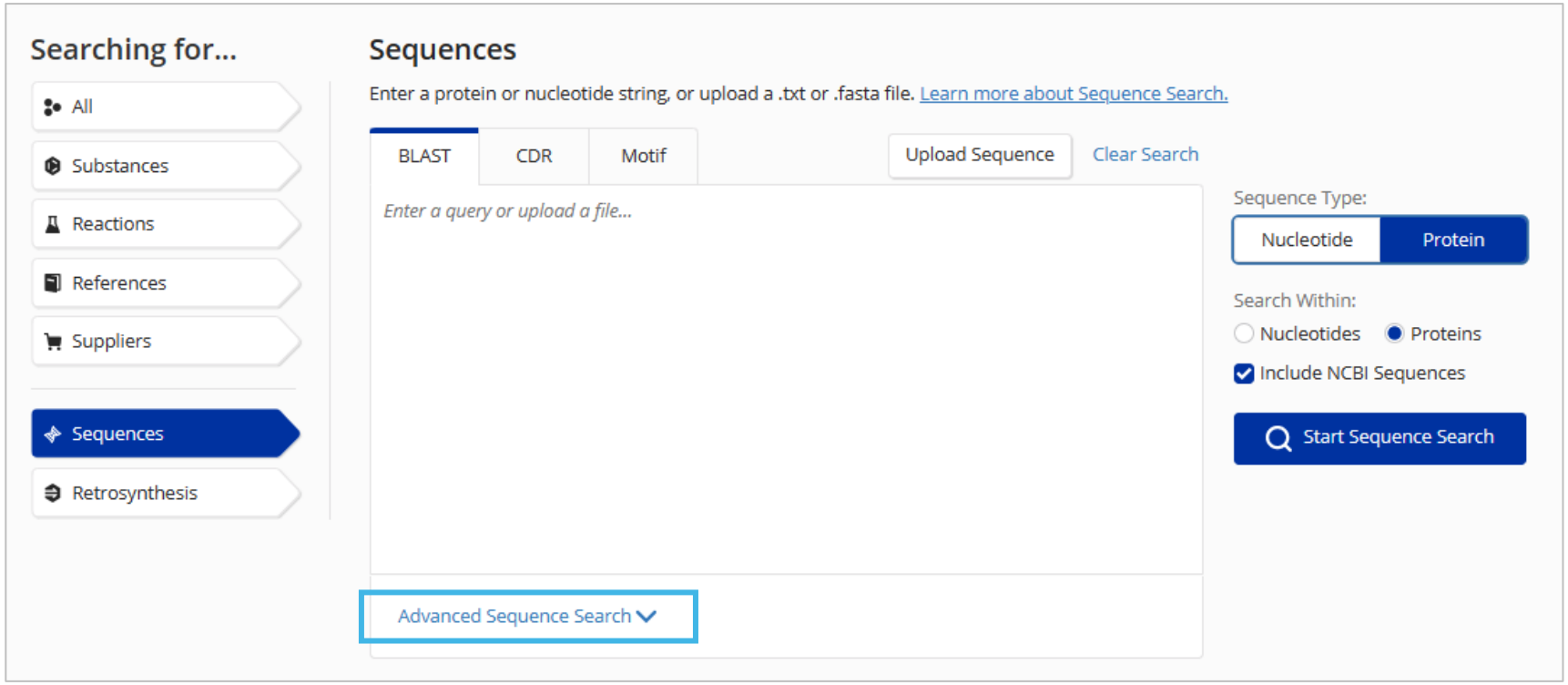
Sequences Search™ — Blast检索



可选择是否包含NCBI中的序列

支持四种检索选择：
Protein-Protein
Protein-Nucleotides
Nucleotide-Nucleotides
Nucleotide-Proteins

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高级检索—设置相关参数

Sequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. Learn more about Sequence Search.

BLAST | CDR | Motif

Upload Sequence | Clear Search

AACAACAACATATCAAATCCTACTGGTGGCACAACTTGA

Sequence Type: Nucleotide | Protein

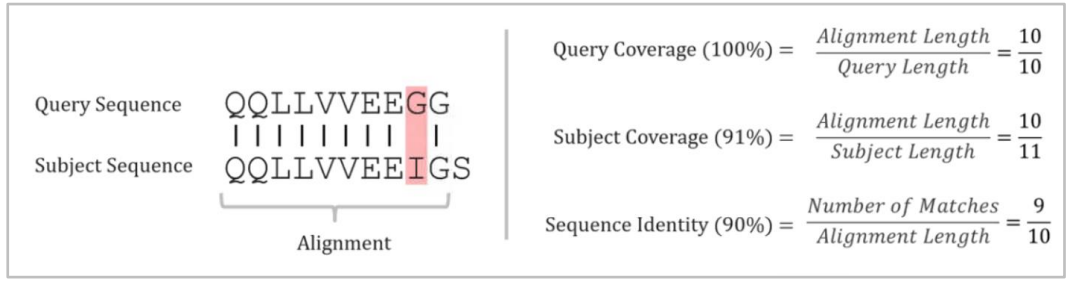
Search Within: Nucleotides | Proteins

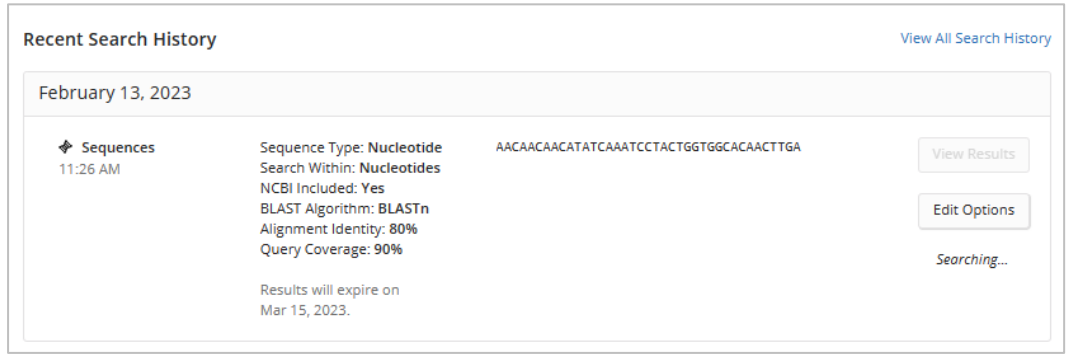
Include NCBI Sequences

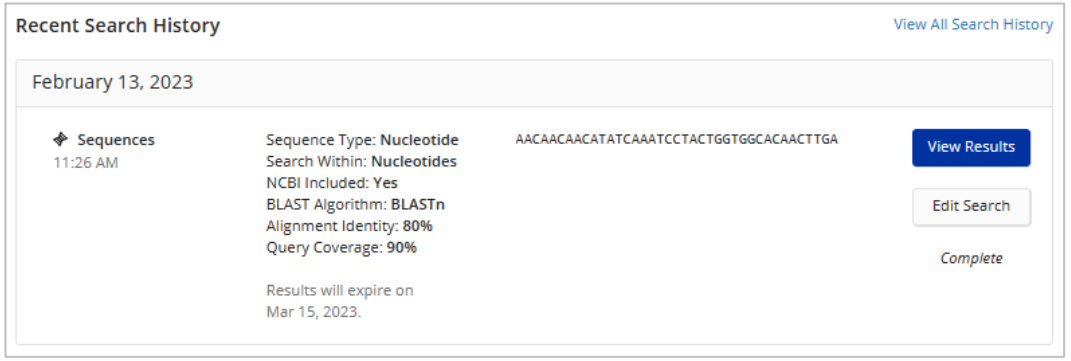
Start Sequence Search

Advanced Sequence Search | Adjust Parameters for Short Sequences | Reset All

Alignment Identity %: 80	Match with Gaps?: Yes / No	Gap Costs: Existence 5 Extension 2
Query Coverage %: 90	Word Size: 11	Reward for Match / Penalty for Mismatch: 2, -3
BLAST Algorithm: BLASTn	E-Value: 10	Exclude Low Complexity Regions: Yes / No







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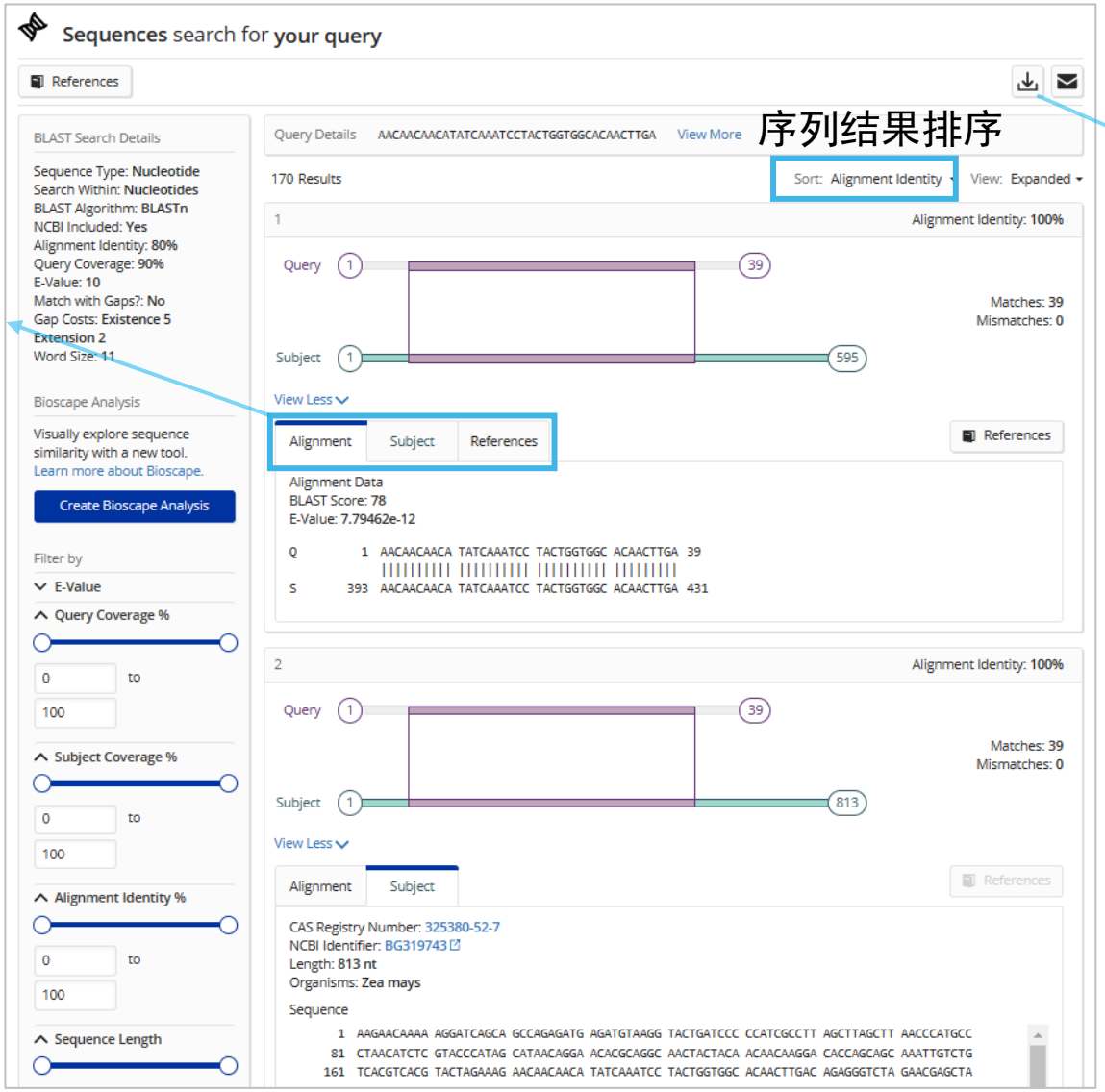
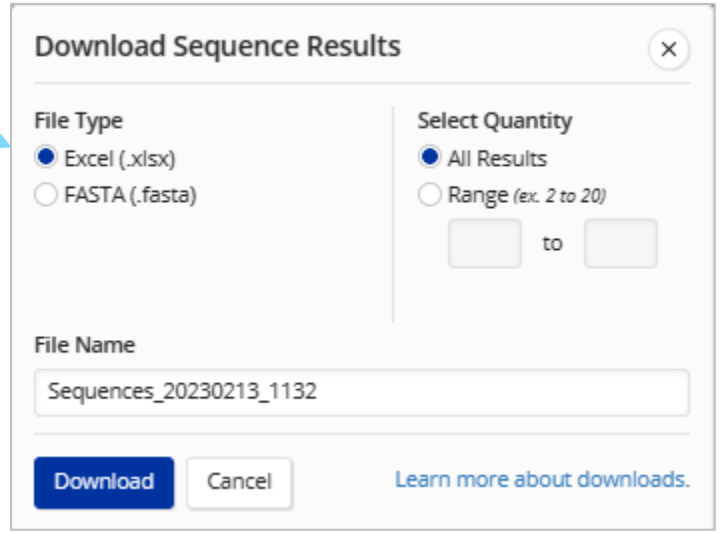
BLAST检索结果

- 序列一致性详情
- 目标序列
- 披露序列的专利文献

- 可视化地图

- 结果筛选





下载结果:

- 比对详情
- 序列长度参数
- 相关专利号
- 专利中的序列编号等

（Excel或FASTA格式）

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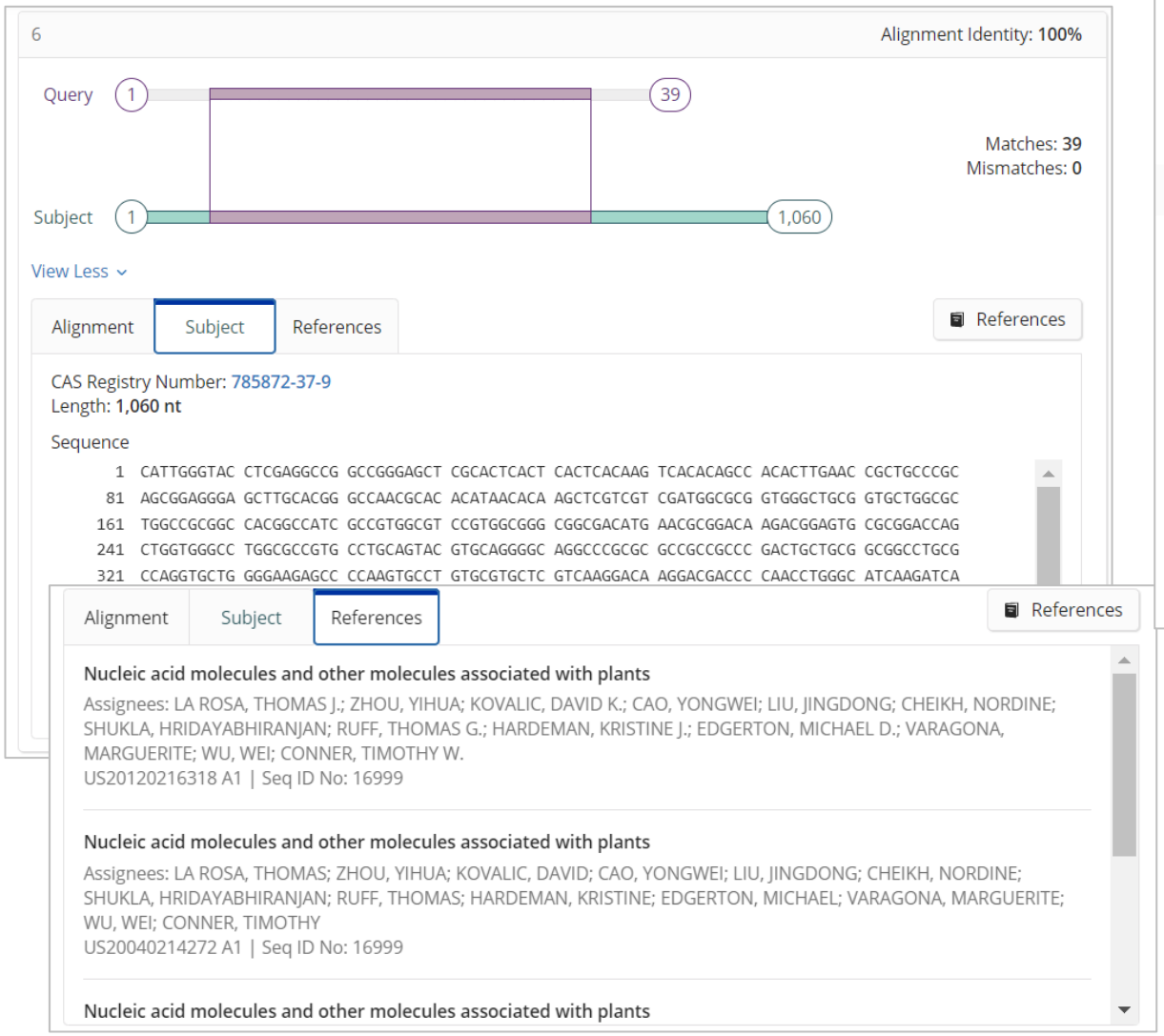
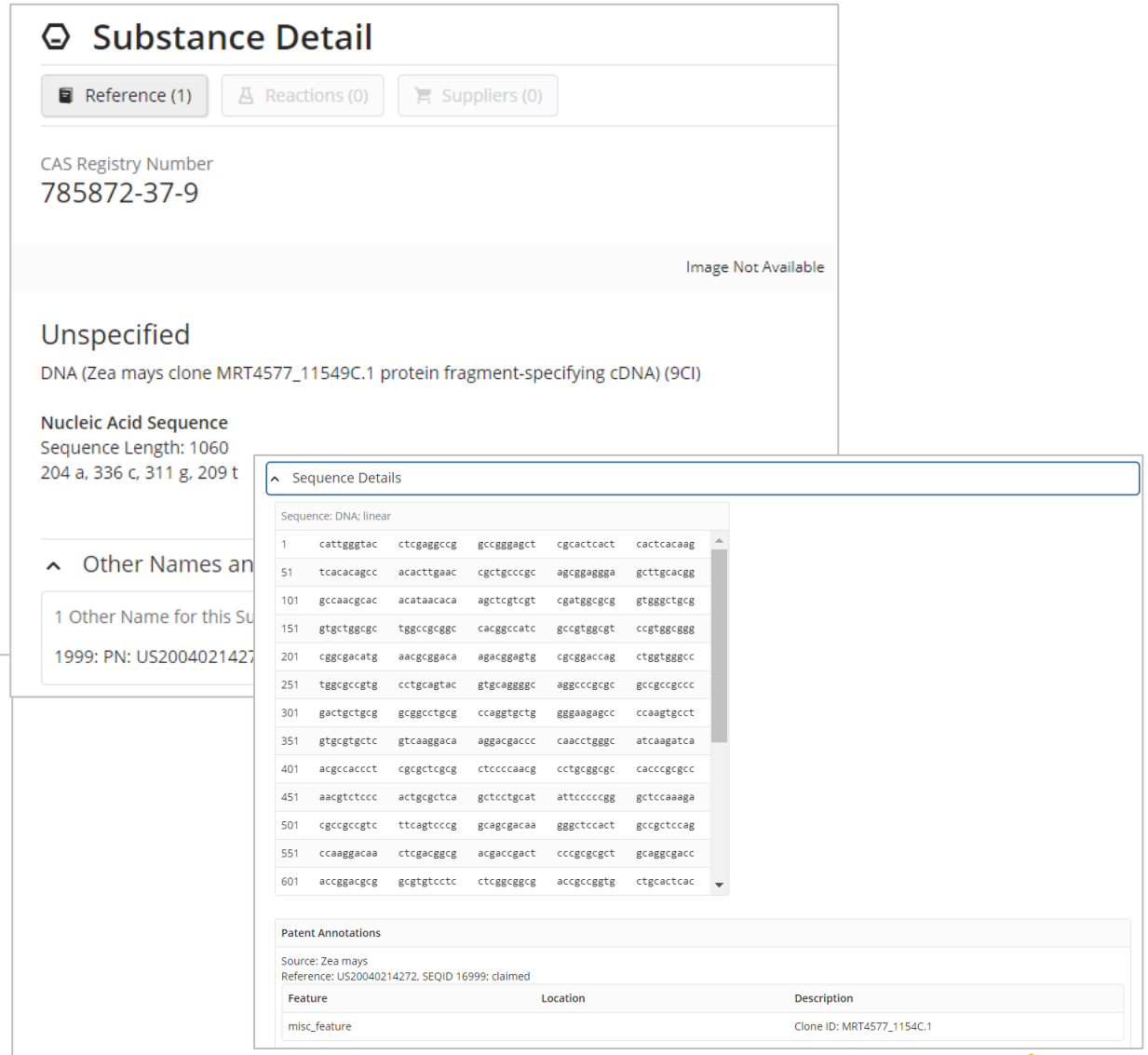
BLAST检索结果





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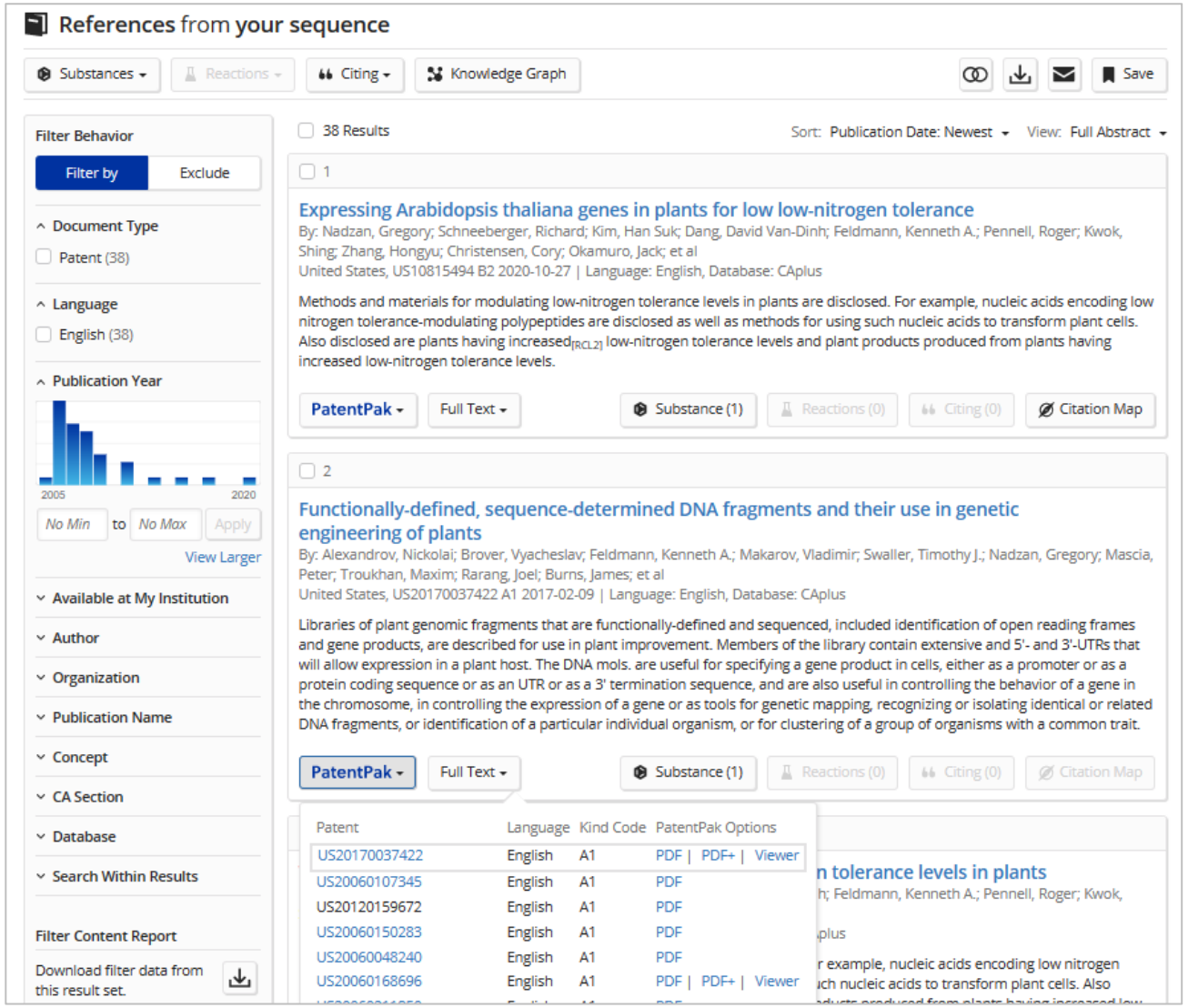
序列详情及相关的专利文献结果



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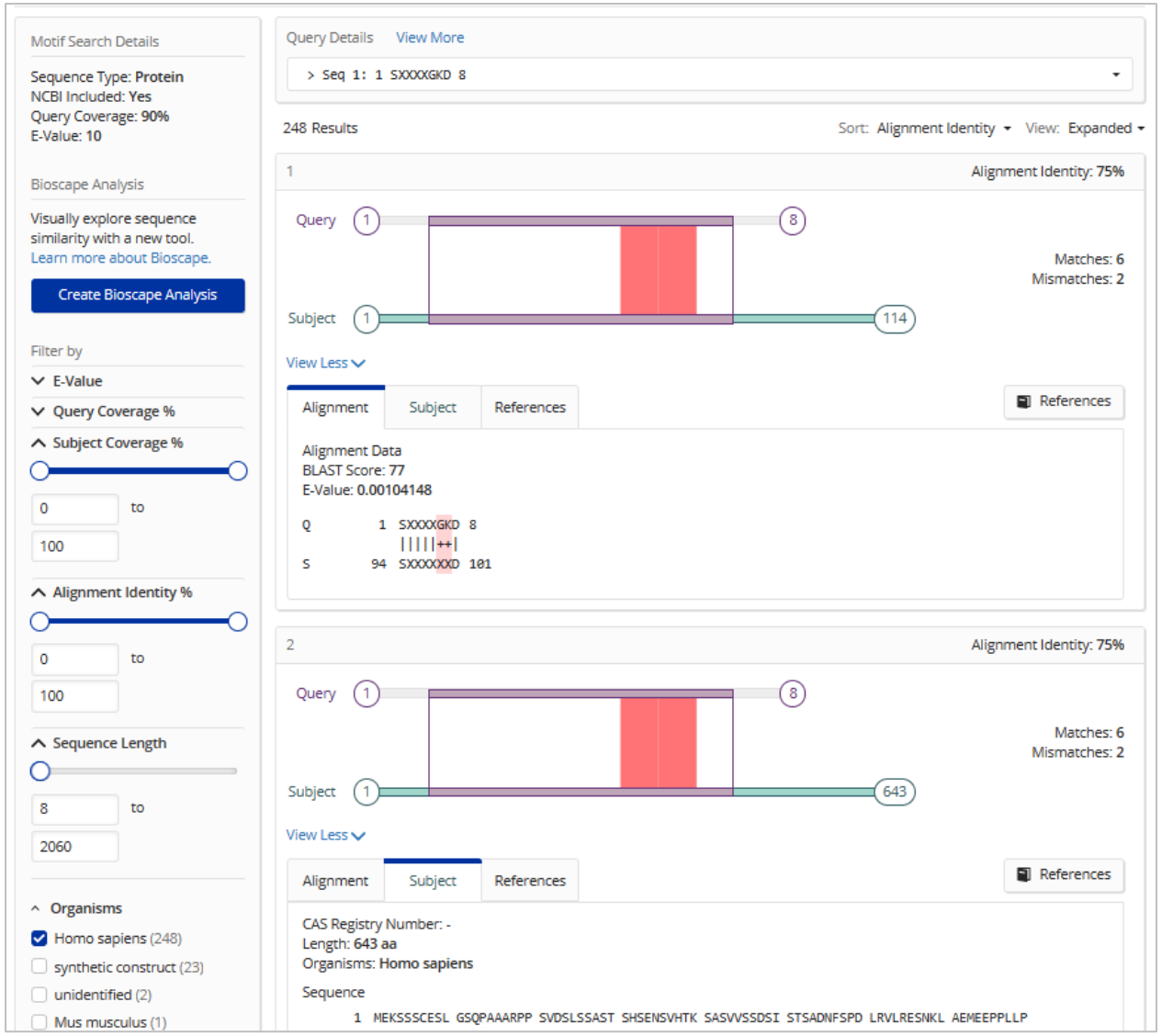
Sequences Search™—Motif检索

Motif中有可变部分，可借助符号来表示：
“[ ]”中括号：代表或者，表示出现在该位置的氨基酸或核苷酸是括号中的任意一个
“{ }”大括号：代表氨基酸或核苷酸的重复次数。其中字段可用逗号开，{2,6}表示在大括号左边紧密相连的氨基酸可重复2-6次

Motif检索结果



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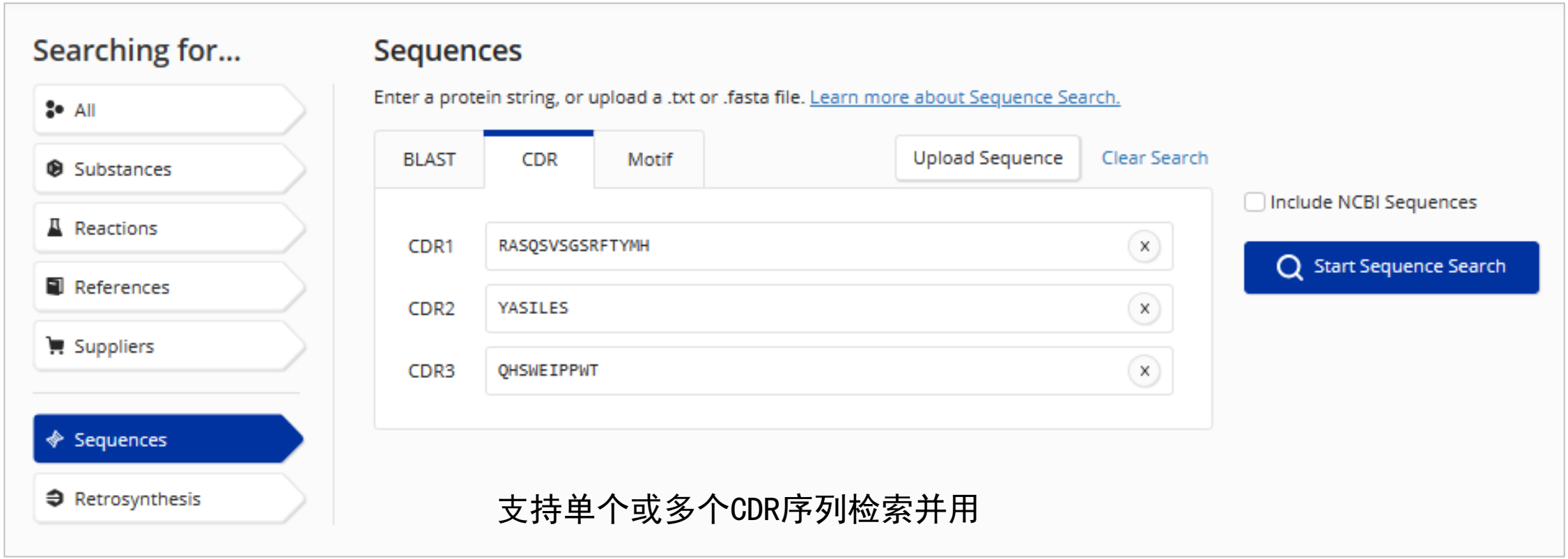
Sequences Search™—CDR检索

CDR（complementarity－determining regions）：抗体或细胞中的互补决定区



支持单个或多个CDR序列检索并用

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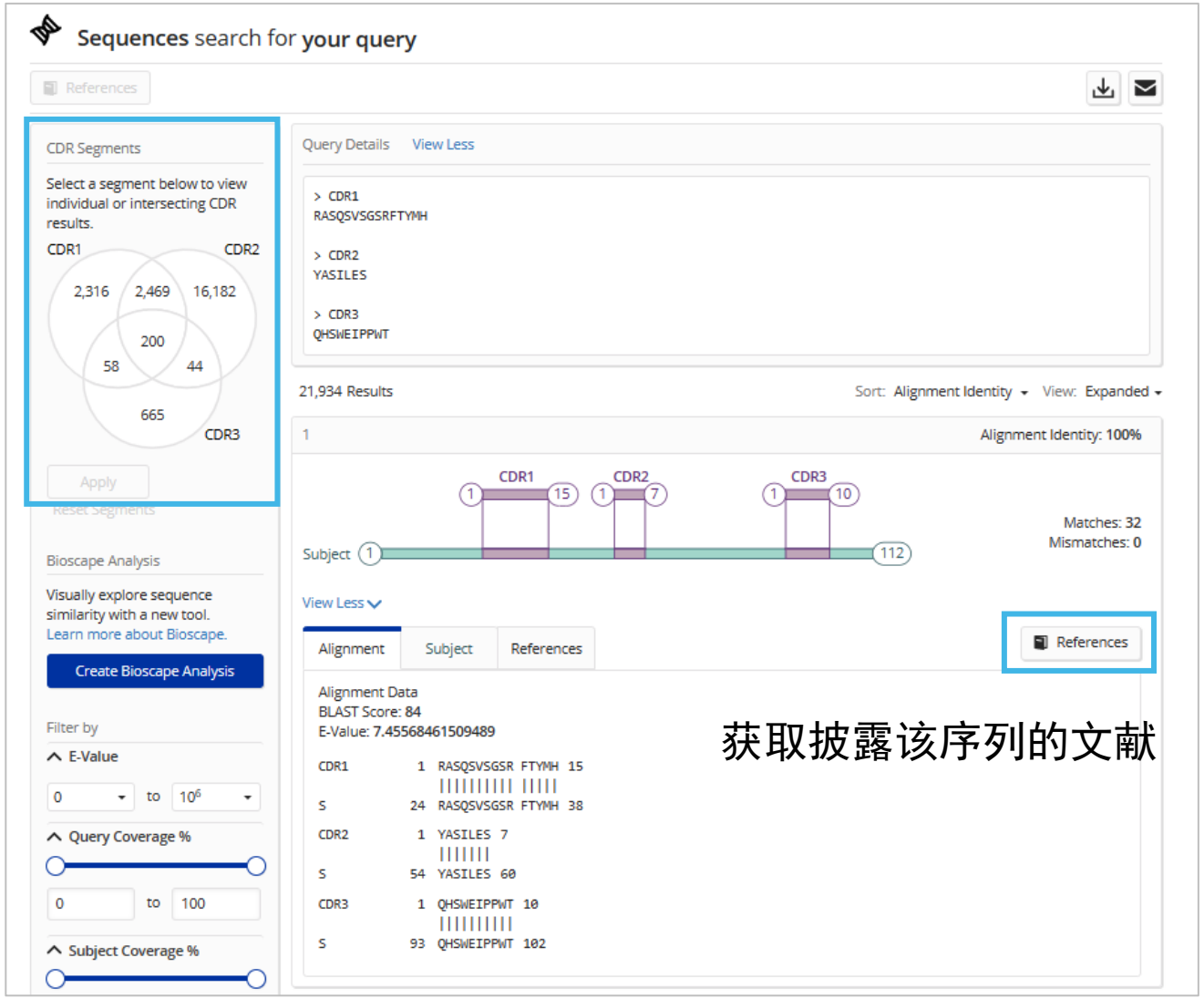
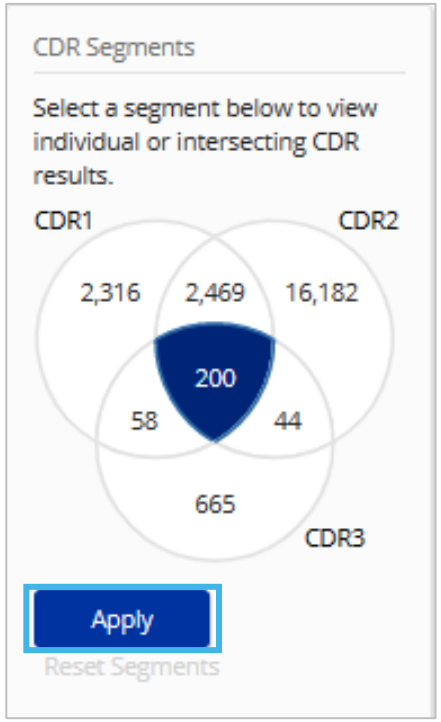
CDR检索结果



获取披露该序列的文献



CDR Segments：

- 匹配到一个或者多个CDR的subject序列的序列数量
- 可根据已知信息和需求查看1-3个CDR被包含的序列结果

Reset segments：

- 重新选择查看匹配的序列结果

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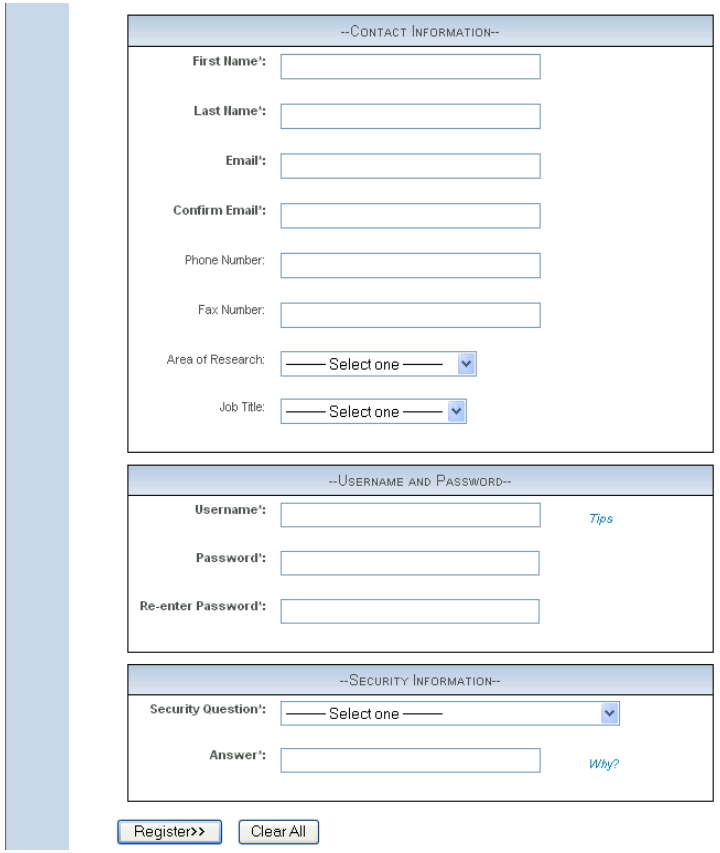
序列检索小结

- Sequences涵盖期刊、专利、NCBI当中的序列信息
- Sequences可以针对DNA/RNA的核苷酸序列、肽/蛋白的氨基酸序列进行检索
- 生物序列的获取方法：Sequences检索、物质名称/代码/结构式、关键词及文献-物质的数据关联
- Motif适合检索短序列，并支持可变部分输入
  - ✓ X代表未指定氨基酸，N代表未指定核苷酸
  - ✓ [ ]表示出现在该位置的序列是括号里氨基酸/核苷酸中的任意一个
  - ✓ { } 代表氨基酸/核苷酸的重复次数，如重复次数是范围，用逗号将数字隔开，如{2,6}

大纲

- CAS及CAS SciFinder^{n}简介
- 常见检索方式
  - 文献检索
  - 物质检索 (CAS Markush*)
  - 反应检索
  - 逆合成反应路线设计 (CAS Retrosynthesis*)
  - 生物序列检索*
- 常见问题及解答

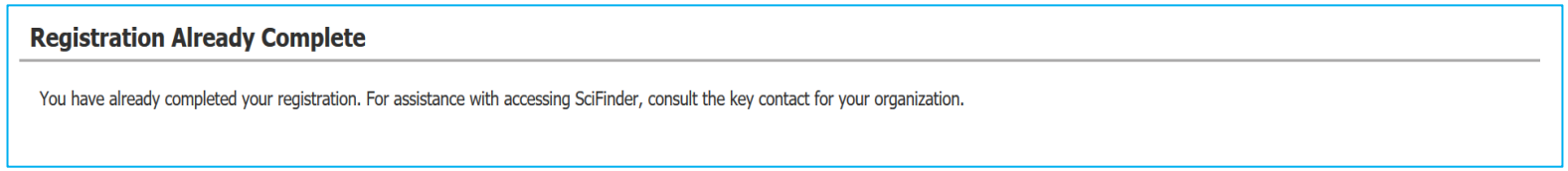
如何获取CAS SciFinder^{n}账号 （登录贵校图书馆网站，查看注册相关的链接和说明）



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）。



点击激活链接后注册成功；之后直接点击https://SciFinder-n.cas.org访问。

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CAS SciFinder^{n}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**

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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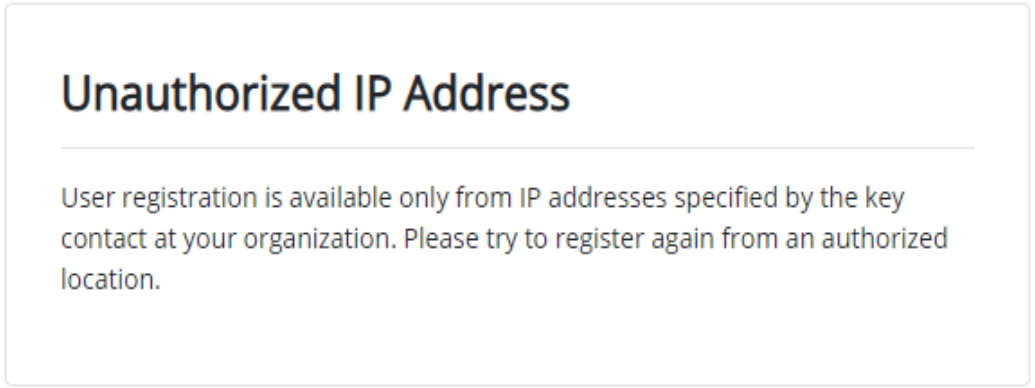
常见问题



- 检查注册链接是否正确
- 确认连入校园网，且不是通过VPN连接
- 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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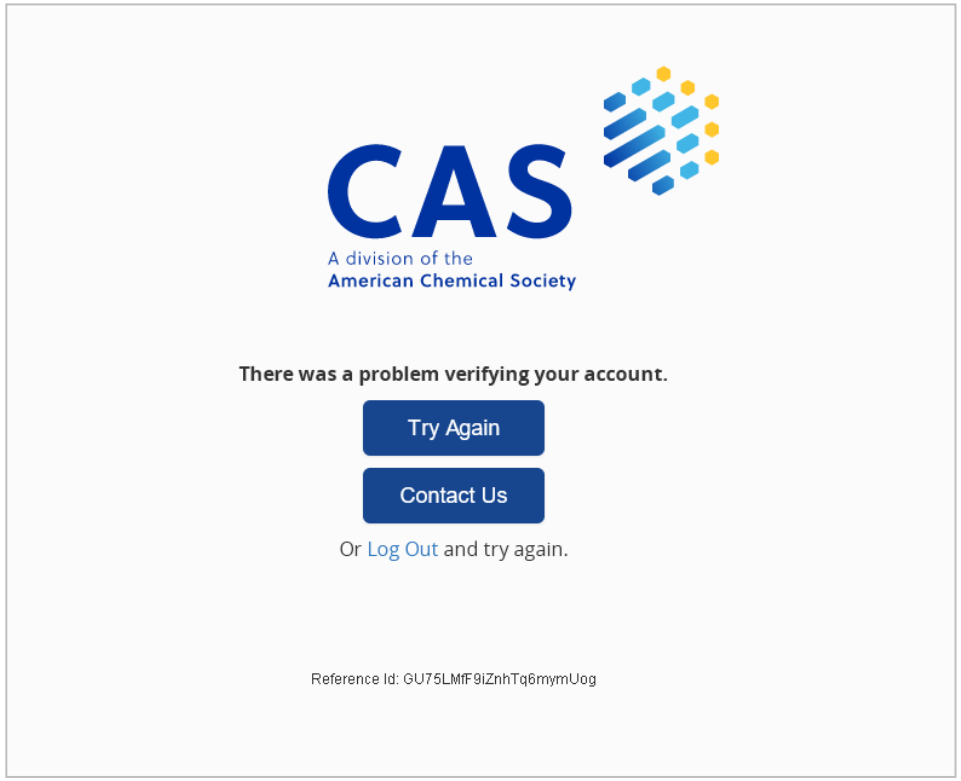
常见问题



- 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

学习资源

CAS SciFinderⁿ学习中心

预告：2023 CAS SciFinder Discovery Platform 论坛

https://mp.weixin.qq.com/s/TGX0QrkeYySH76nBx1QSaw

回顾：2022 CAS SciFinderⁿ论坛合集

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THANK YOU!

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