解锁 CAS SciFinder-n 新功能

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美国化学文摘社（CAS）北京代表处

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  - 物质检索
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  - 设置、项目管理和历史记录

登录

CAS SciFinder^{n}: https://scifinder-n.cas.org

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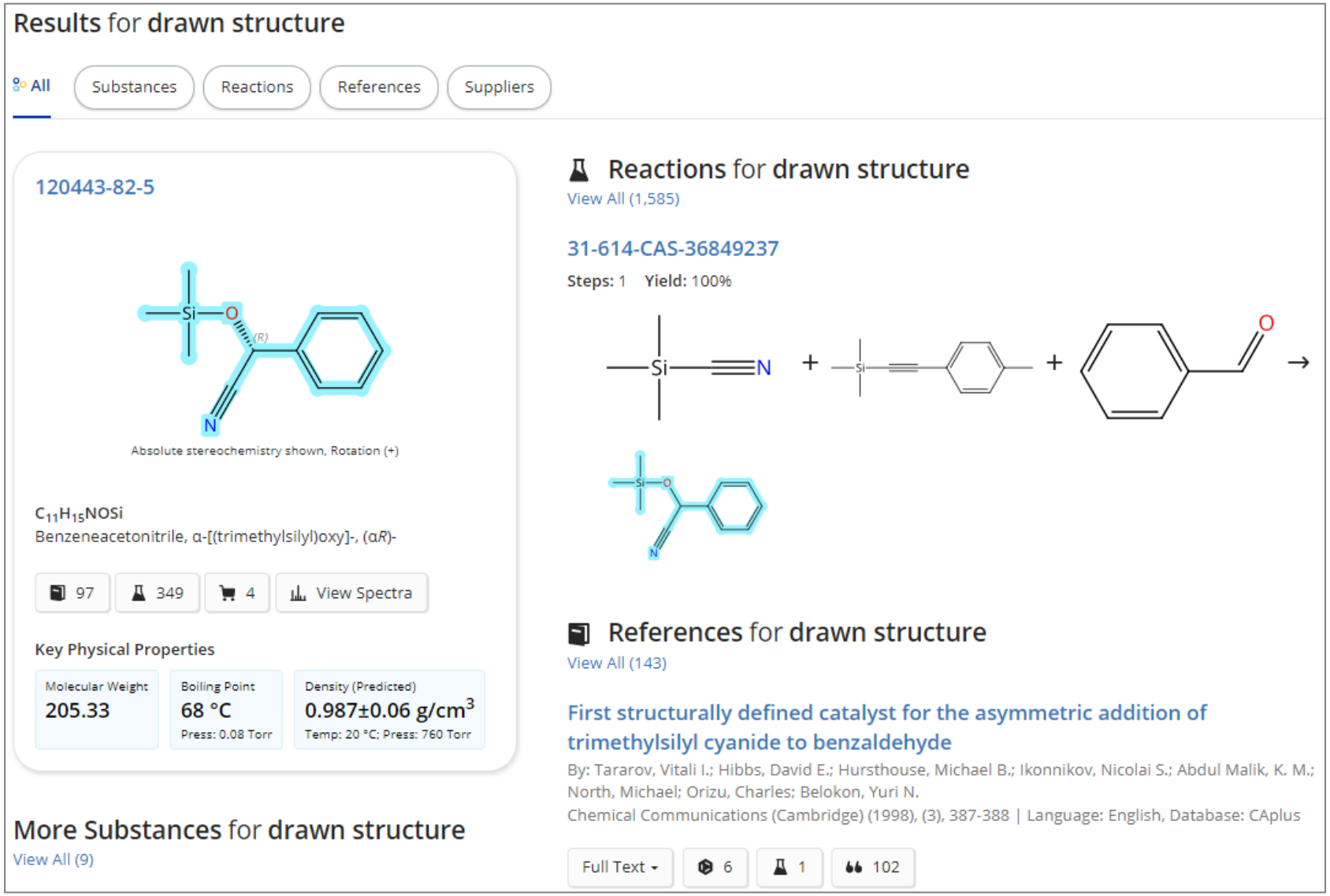
一站式检索功能增强



一站式检索“All”界面更新，最大限度地减少滚动页面的需要，提高界面整体可用性。

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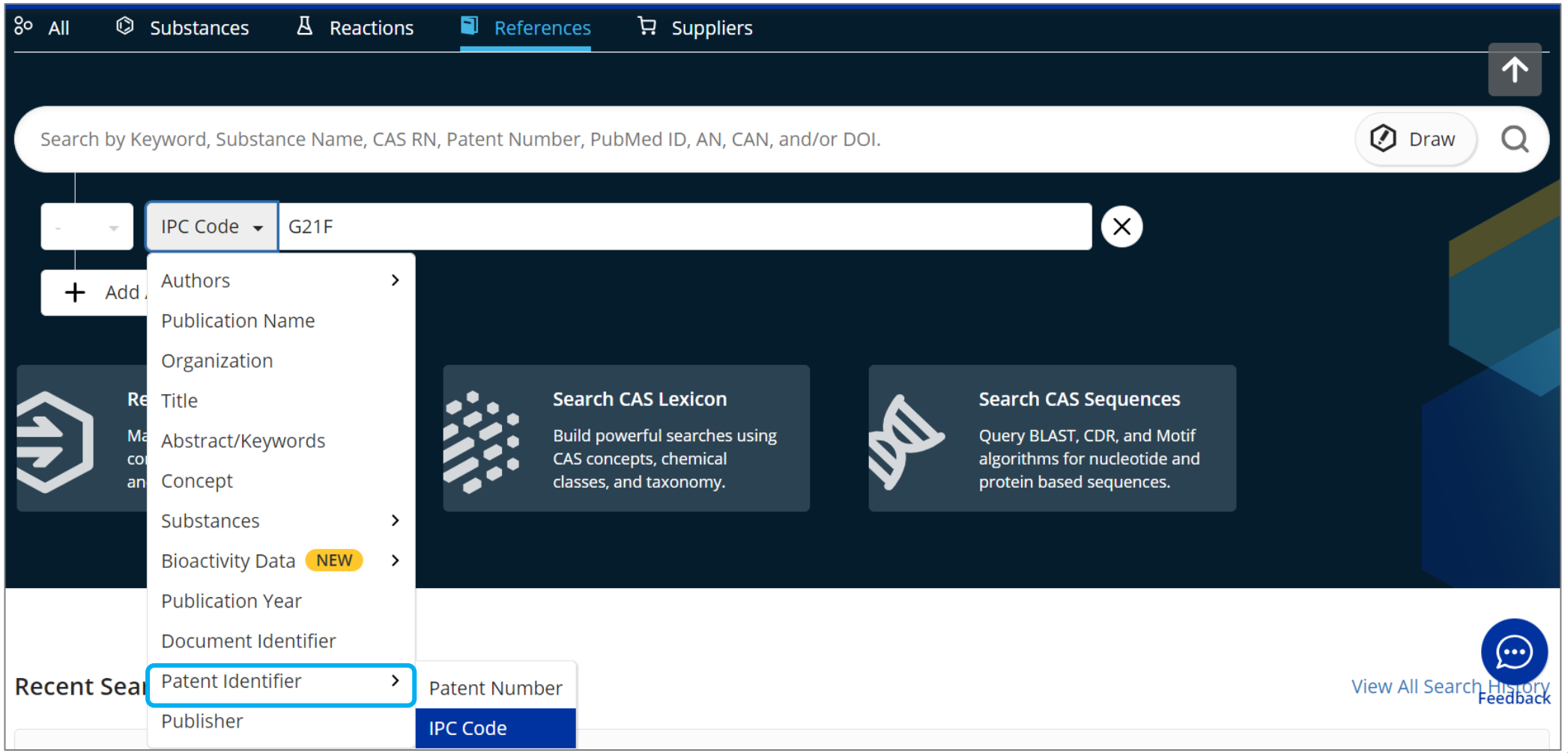
通过 IPC 分类号检索专利

高级检索项选择 Patent Identifier，点击 IPC Code 检索专利



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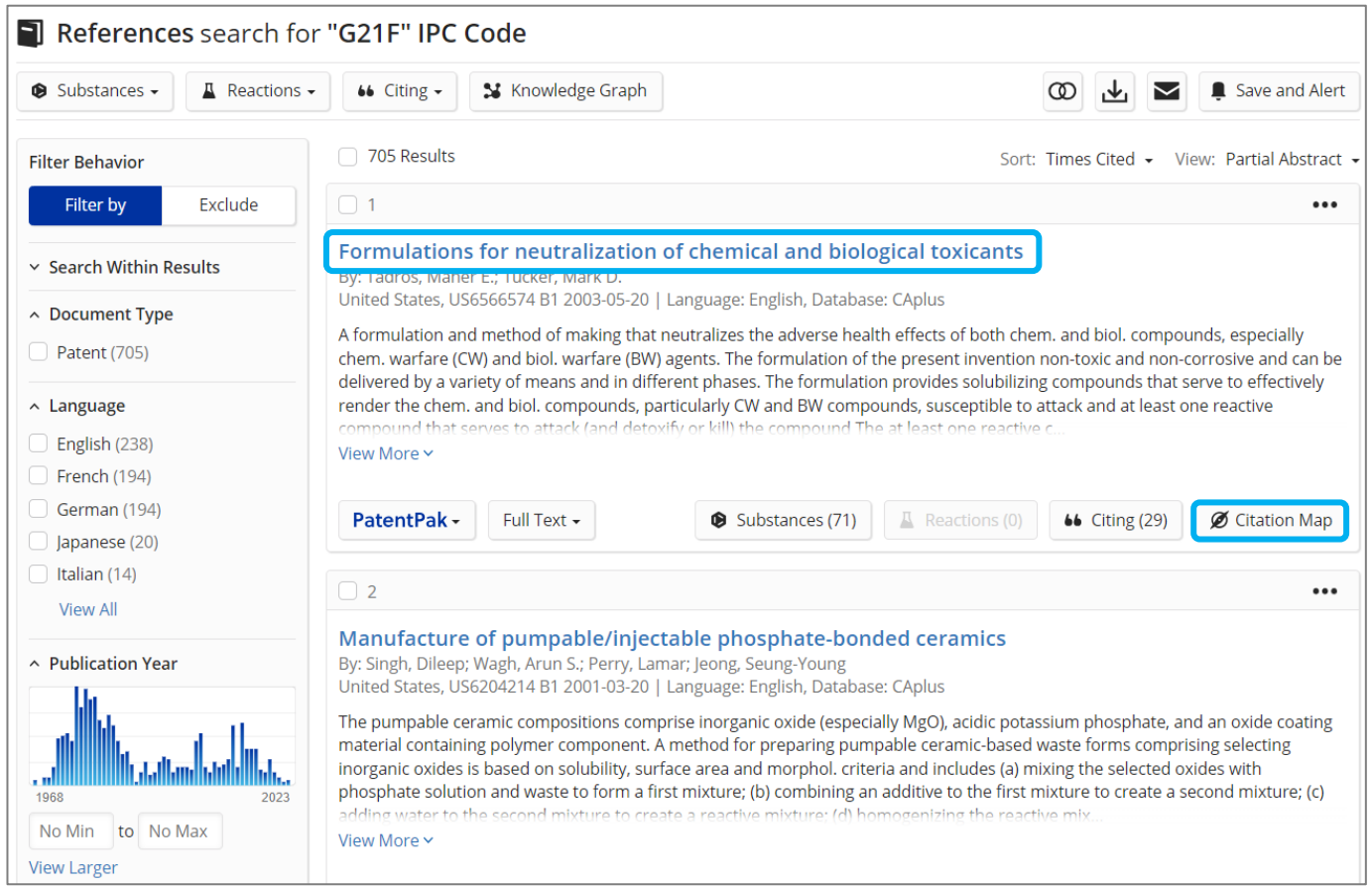
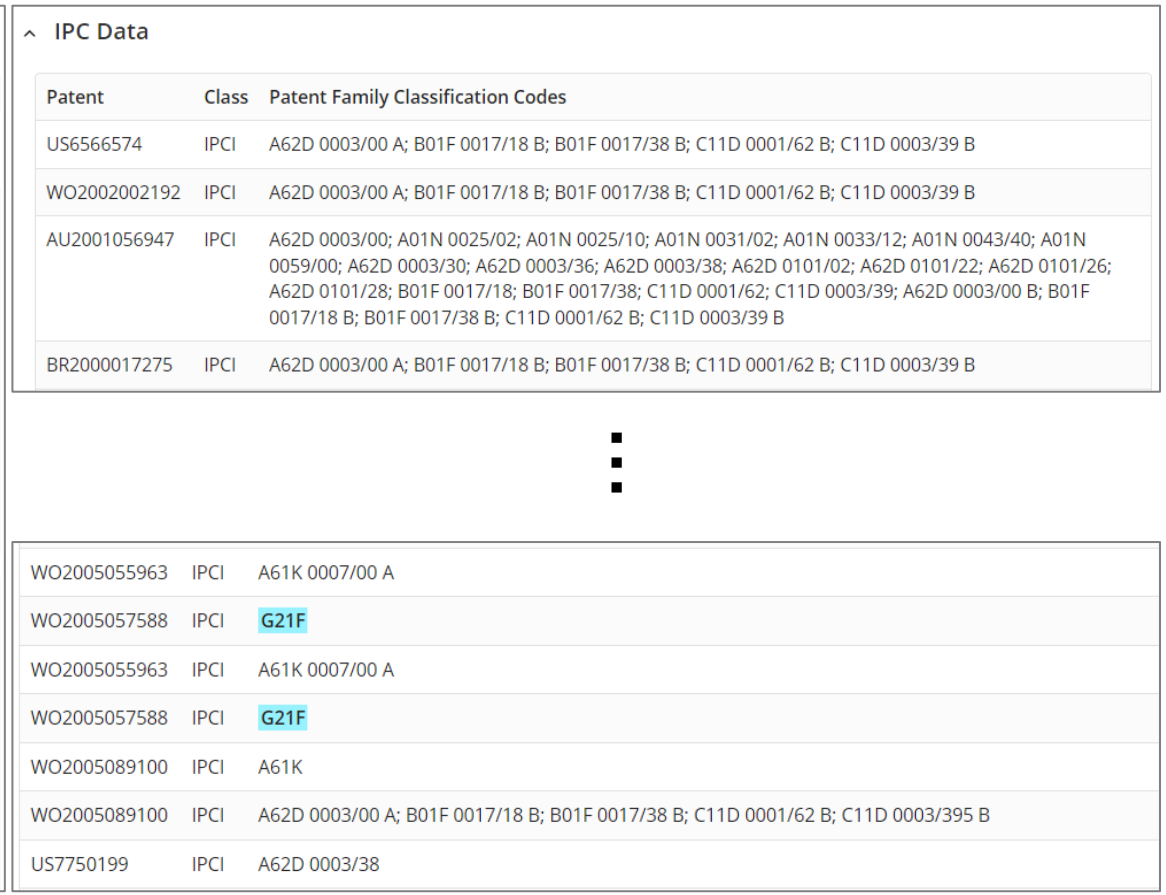
浏览 IPC Data 及其他专利信息

点击标题进入文献详情页面，查看 IPC Data 相关信息





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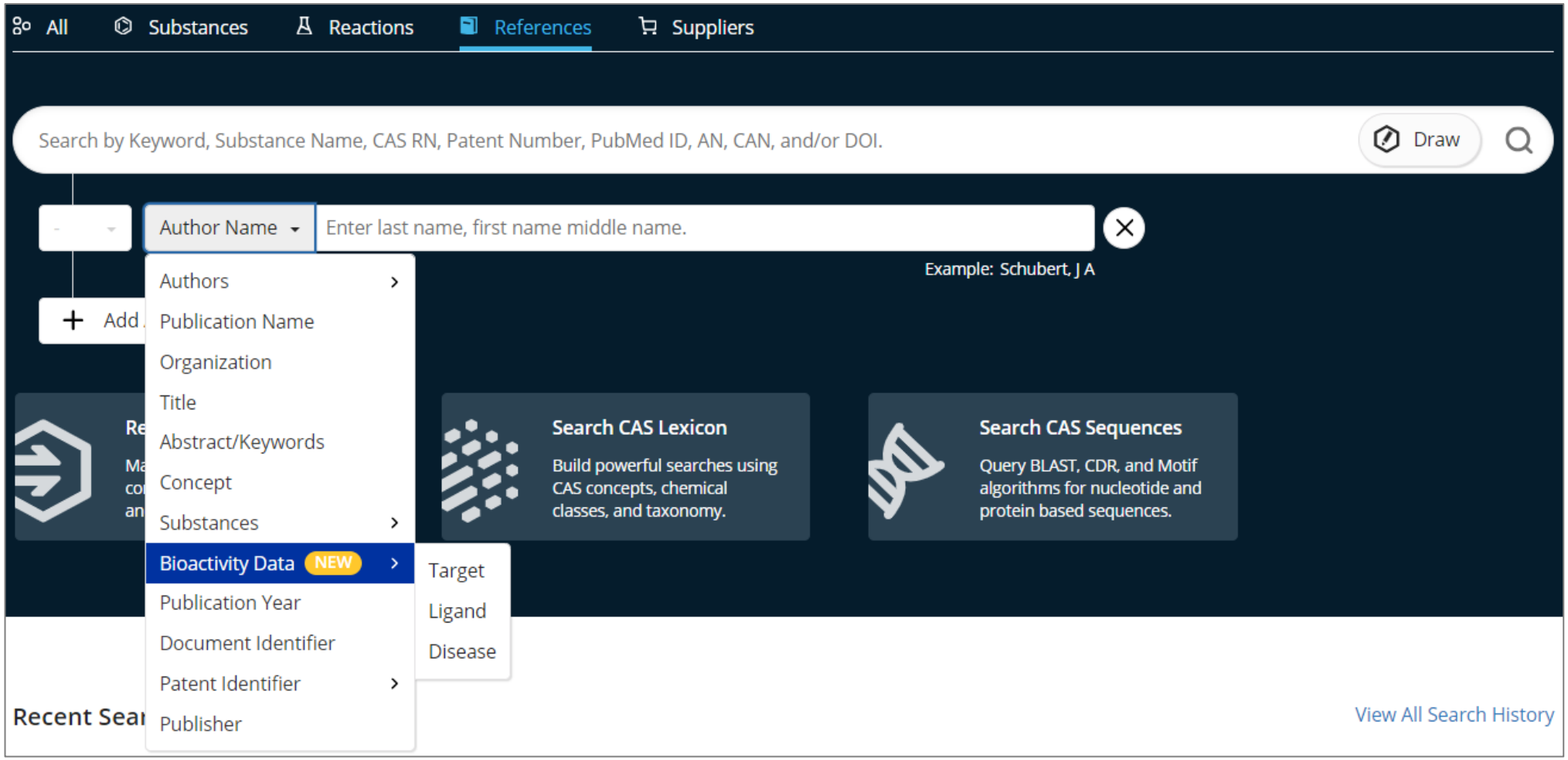
文献检索支持根据生物活性数据检索文献

根据生物活性数据（靶点、疾病、配体/药物）等检索



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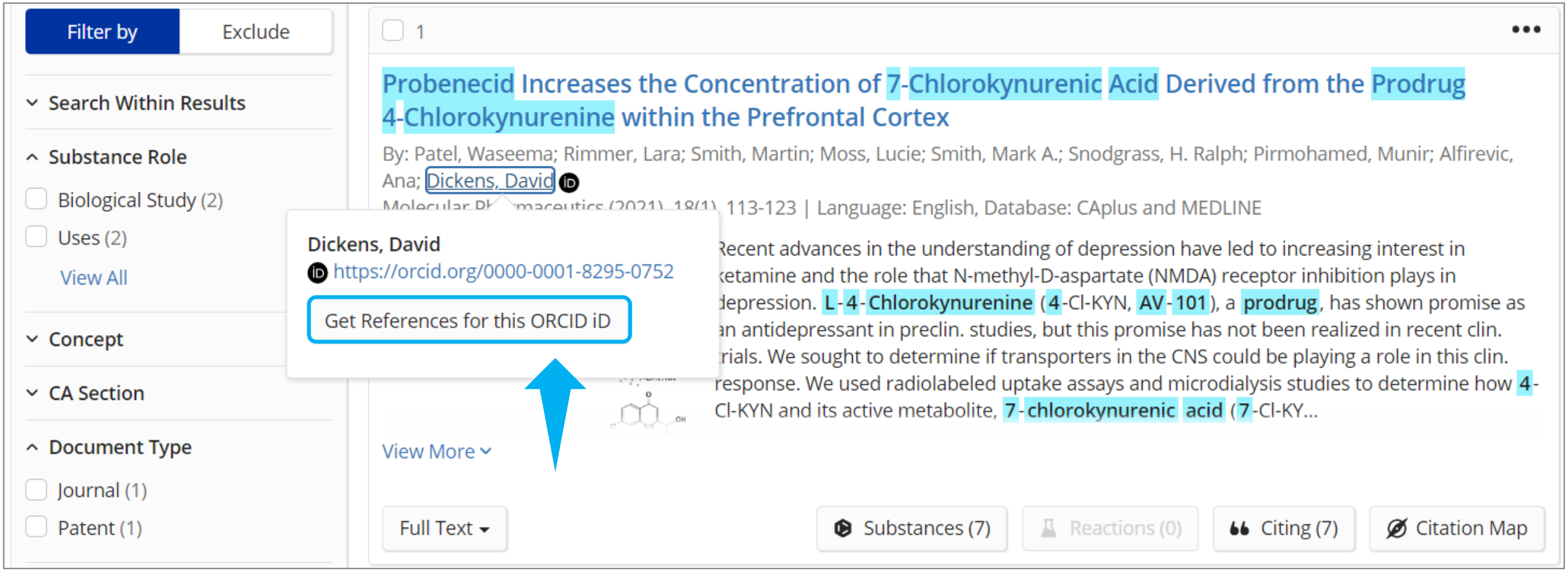
通过作者 ORCID iD 链接至其他出版物



支持检索与作者 ORCID iD 相关的参考文献

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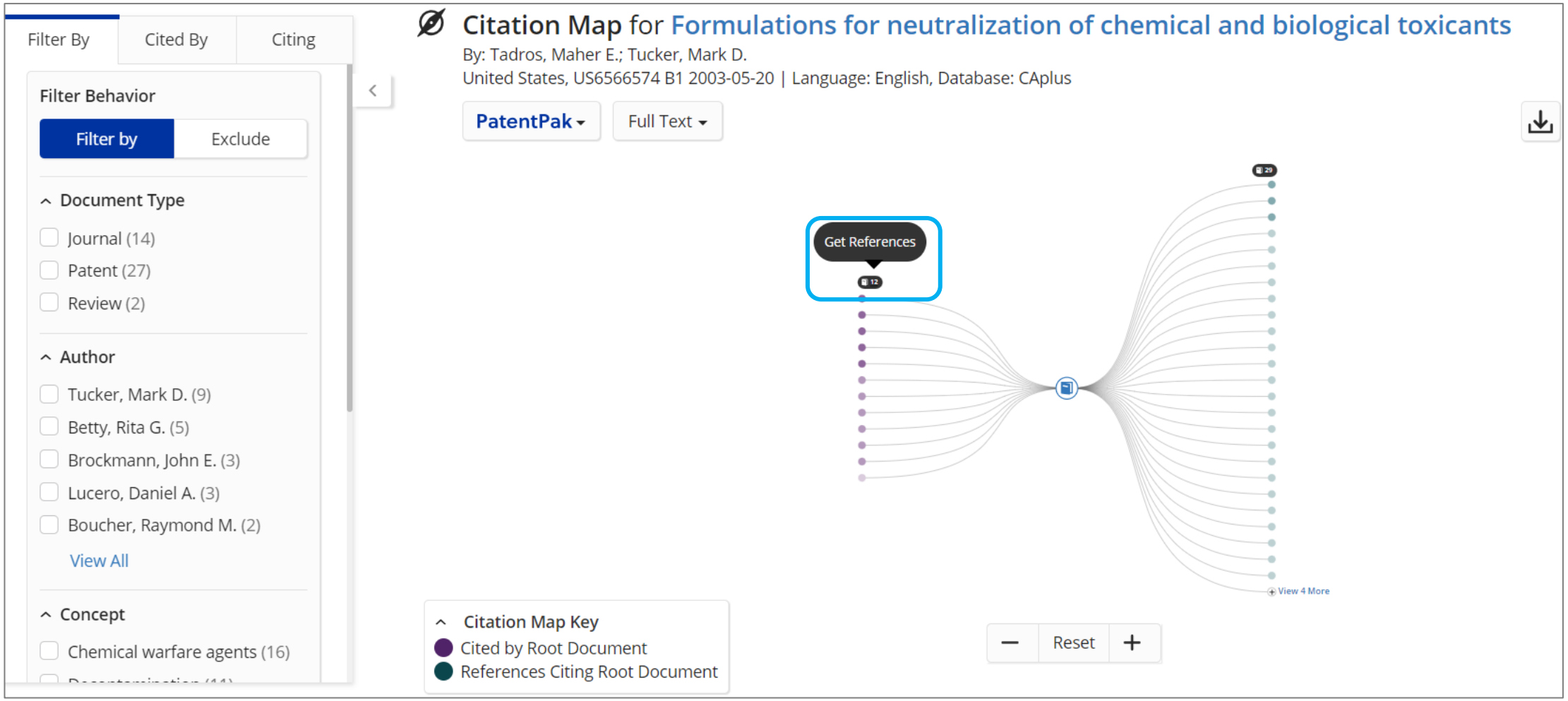
获取引文地图中的关联文献

点击被引/施引文献上方数字获取文献结果集



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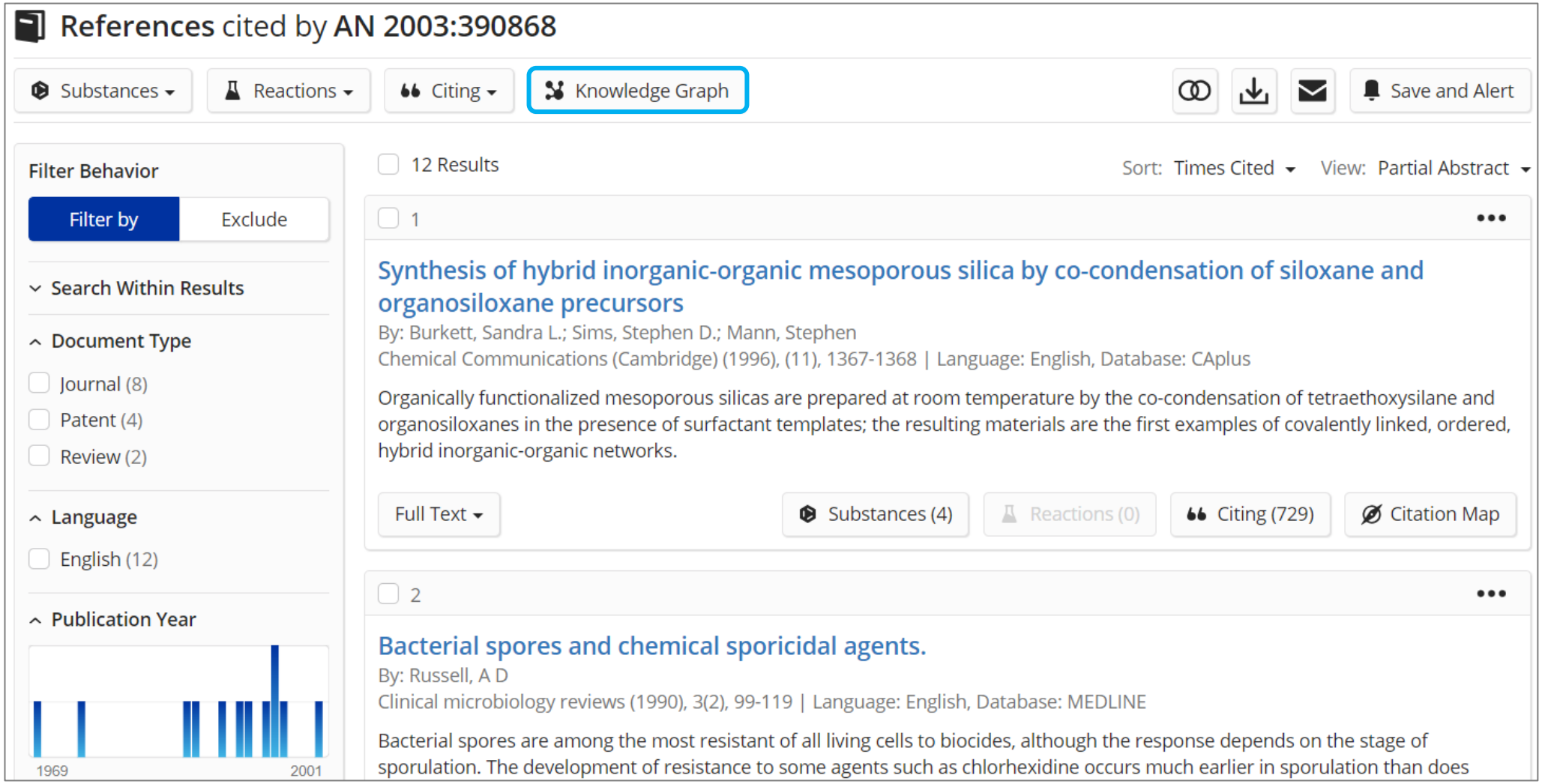
获取文献知识谱图

点击 Knowledge Graph 获取文献知识谱图



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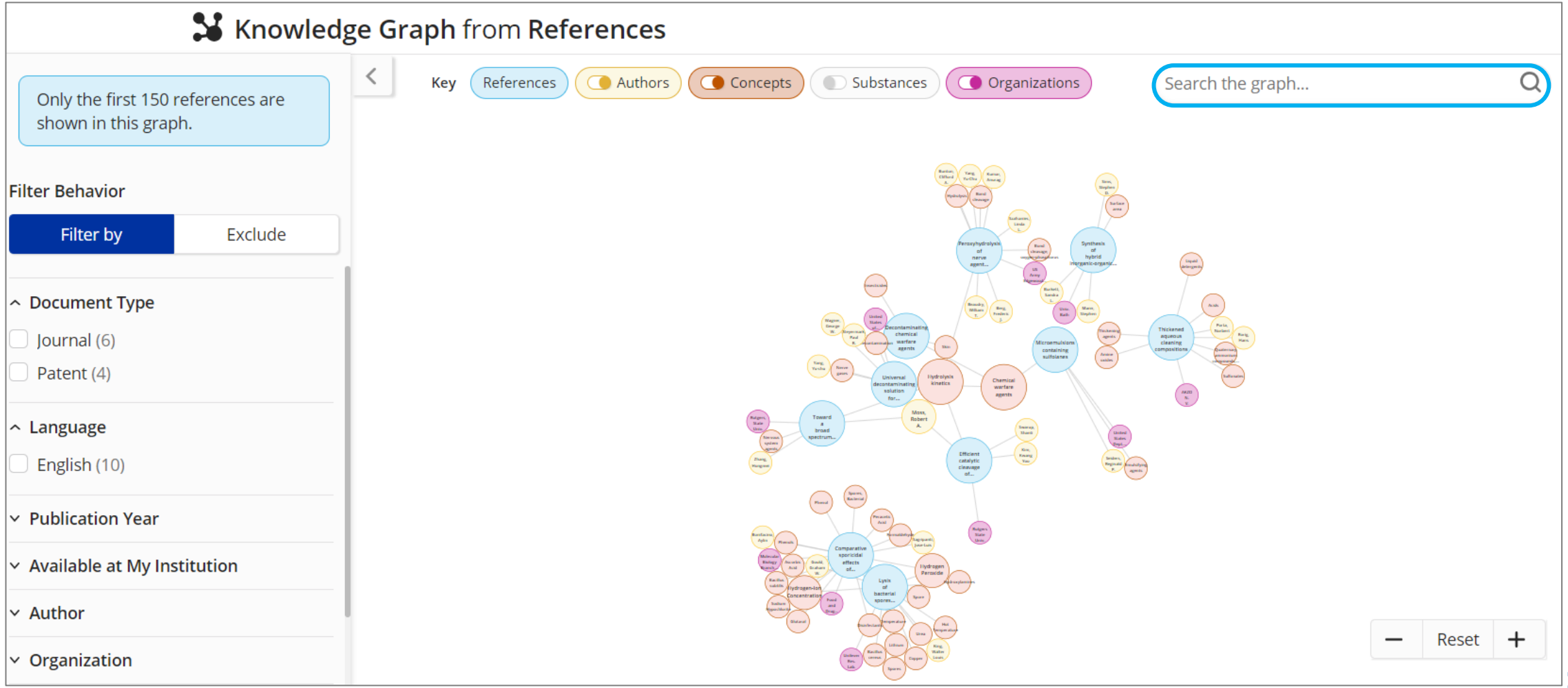
检索文献知识谱图

通过输入框对图谱信息进行关键词检索



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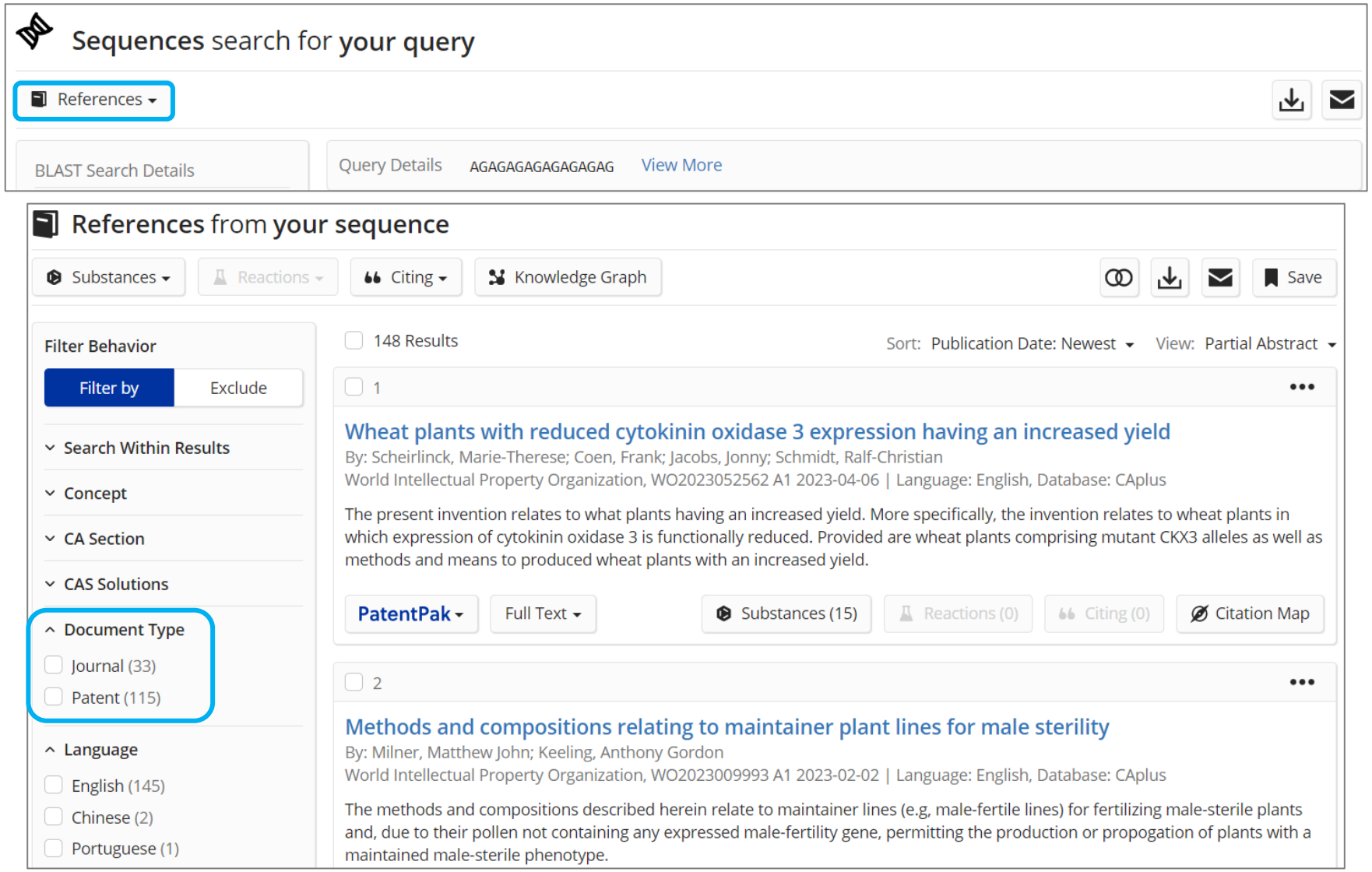
从序列结果获得的文献结果页面新增显示非专利文献



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文献详情页面推荐相似文献

点击“get similar references”
浏览最多500篇相似文献

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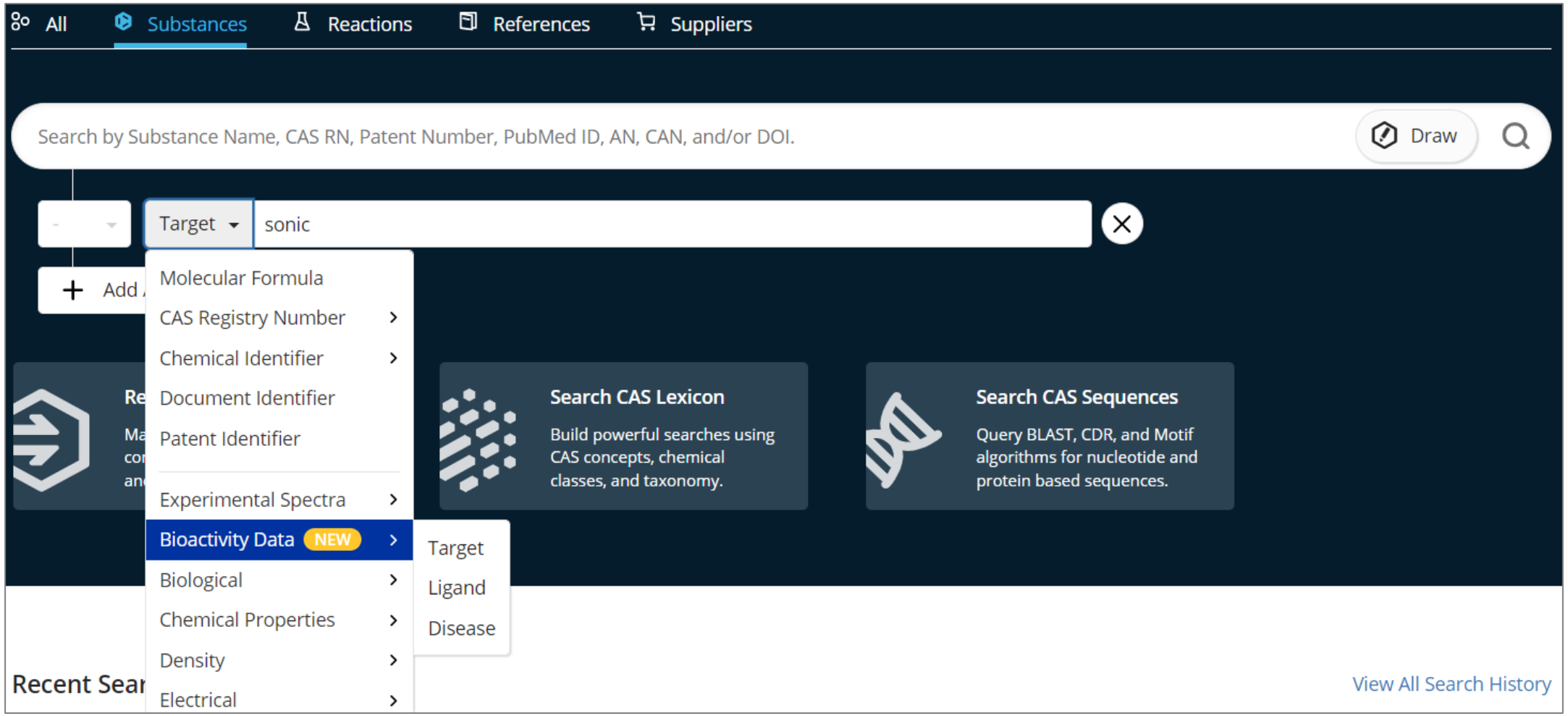
物质检索支持根据生物活性数据检索物质

根据生物活性数据（靶点、疾病、配体/药物）等检索



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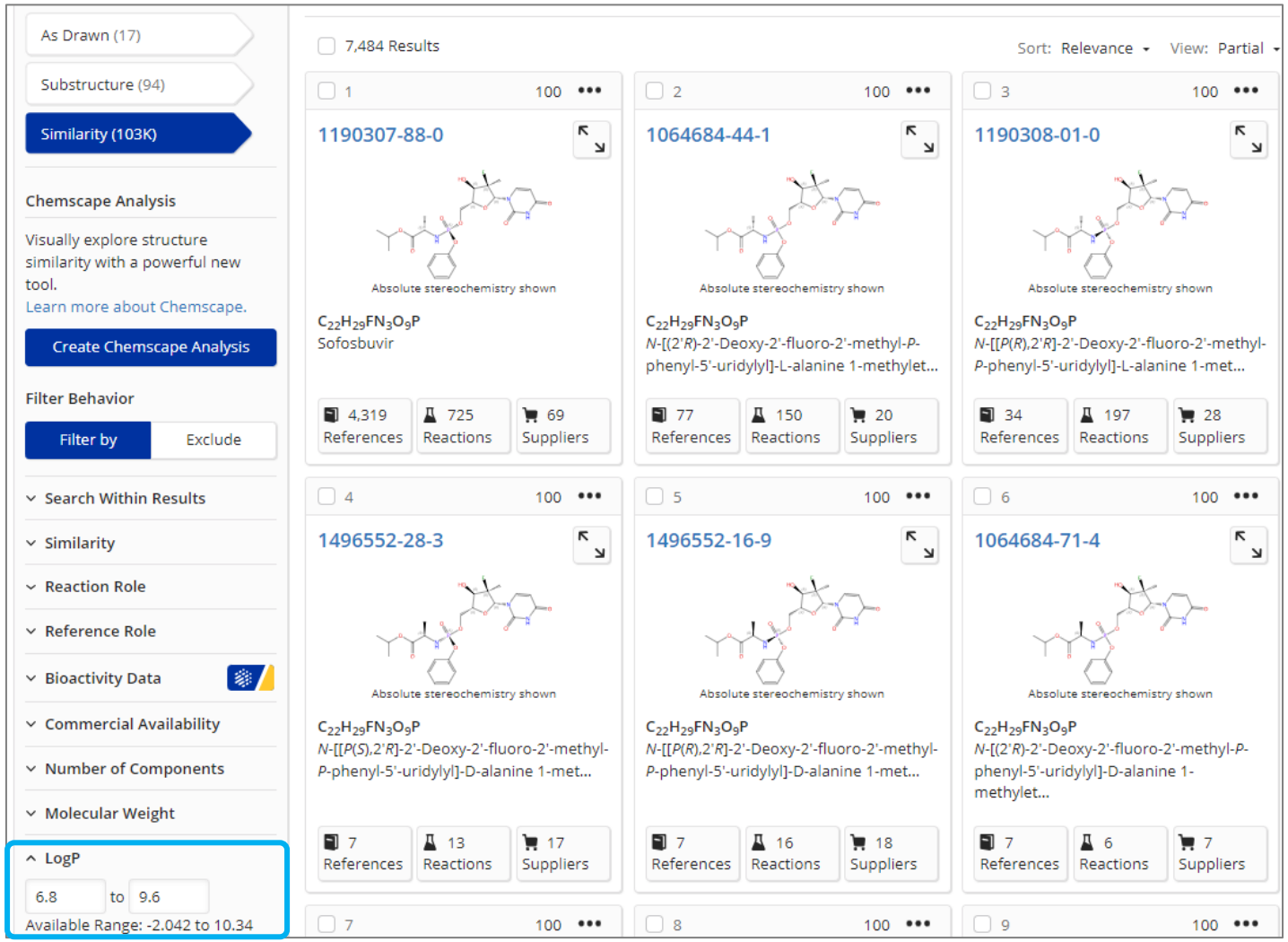
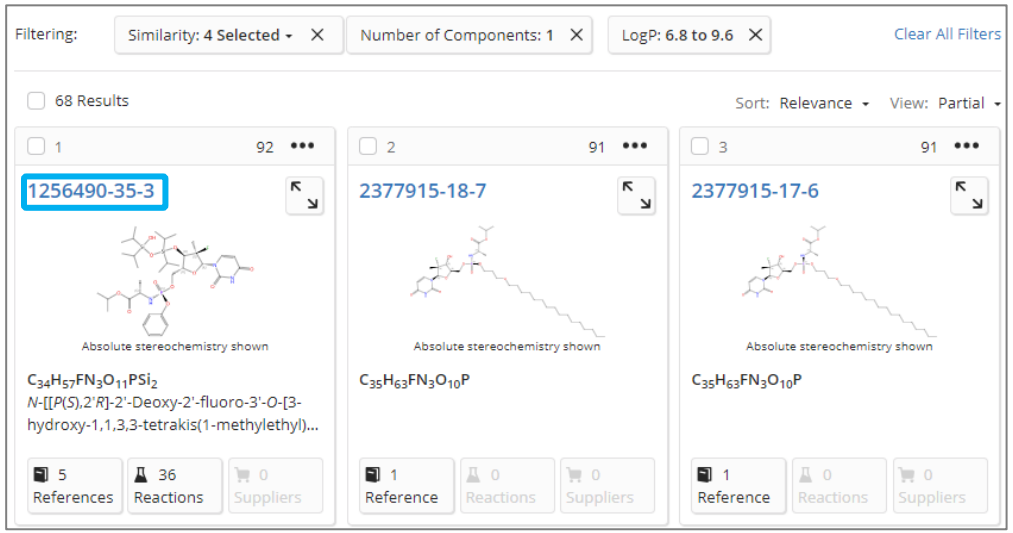
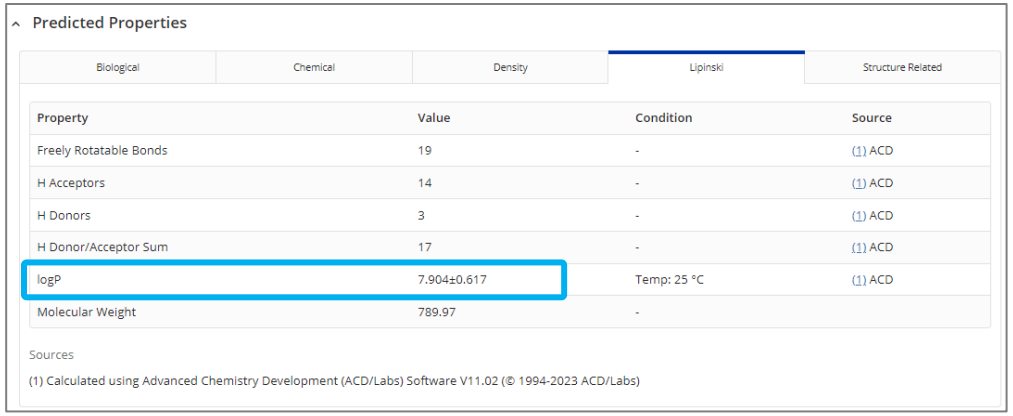
LogP 值筛选物质结果集

了解当前物质结果集 LogP 分布范围，输入范围或具体数值筛选物质







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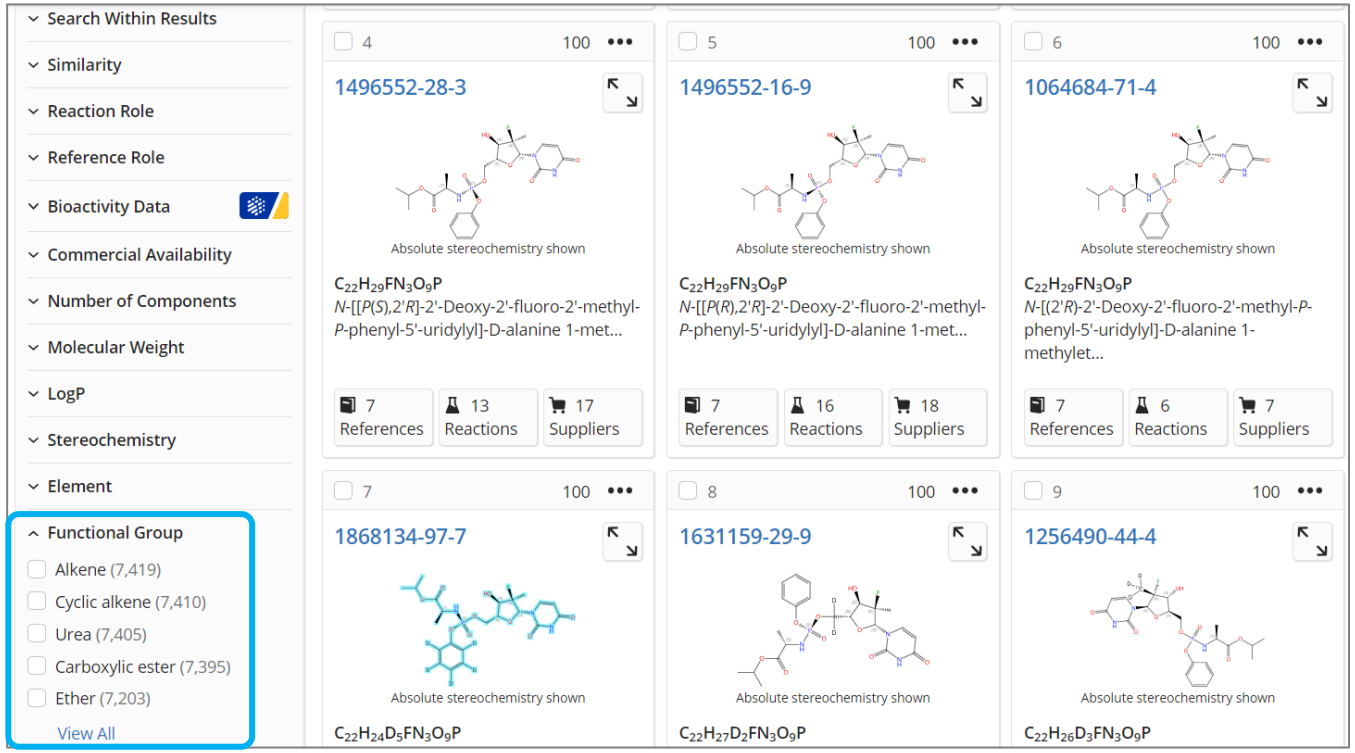
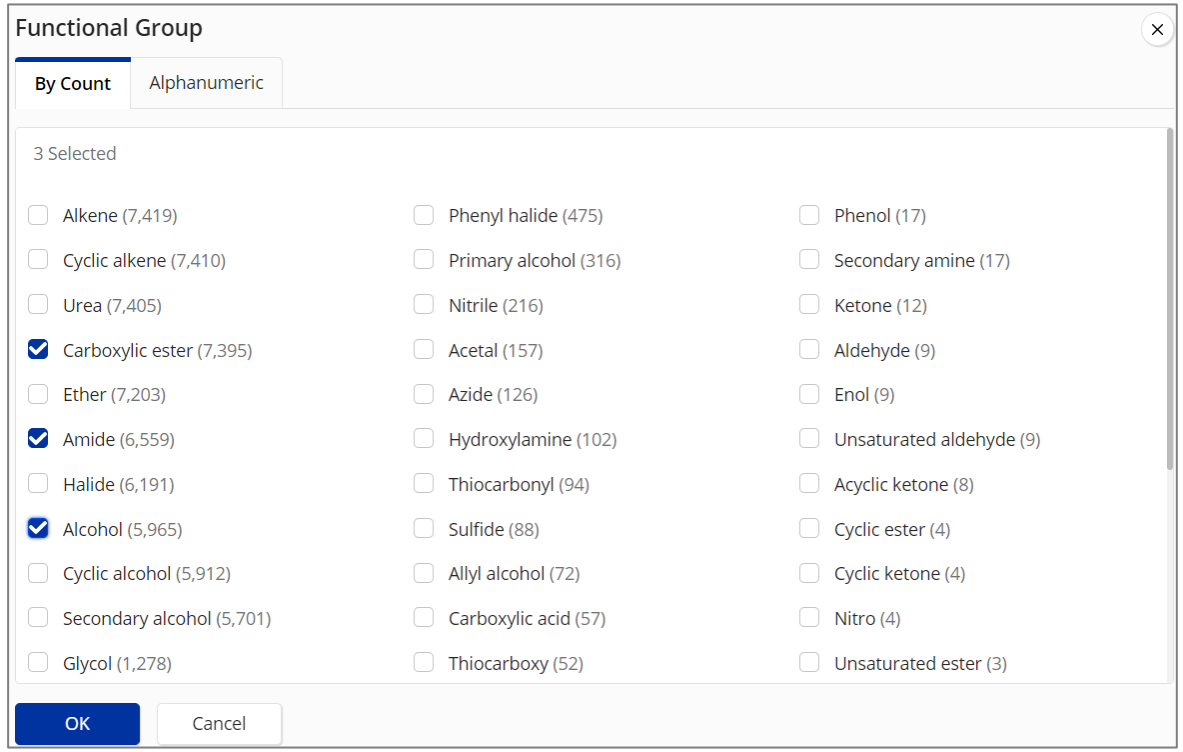
官能团筛选物质结果集

查看或筛选包含特定官能团的物质





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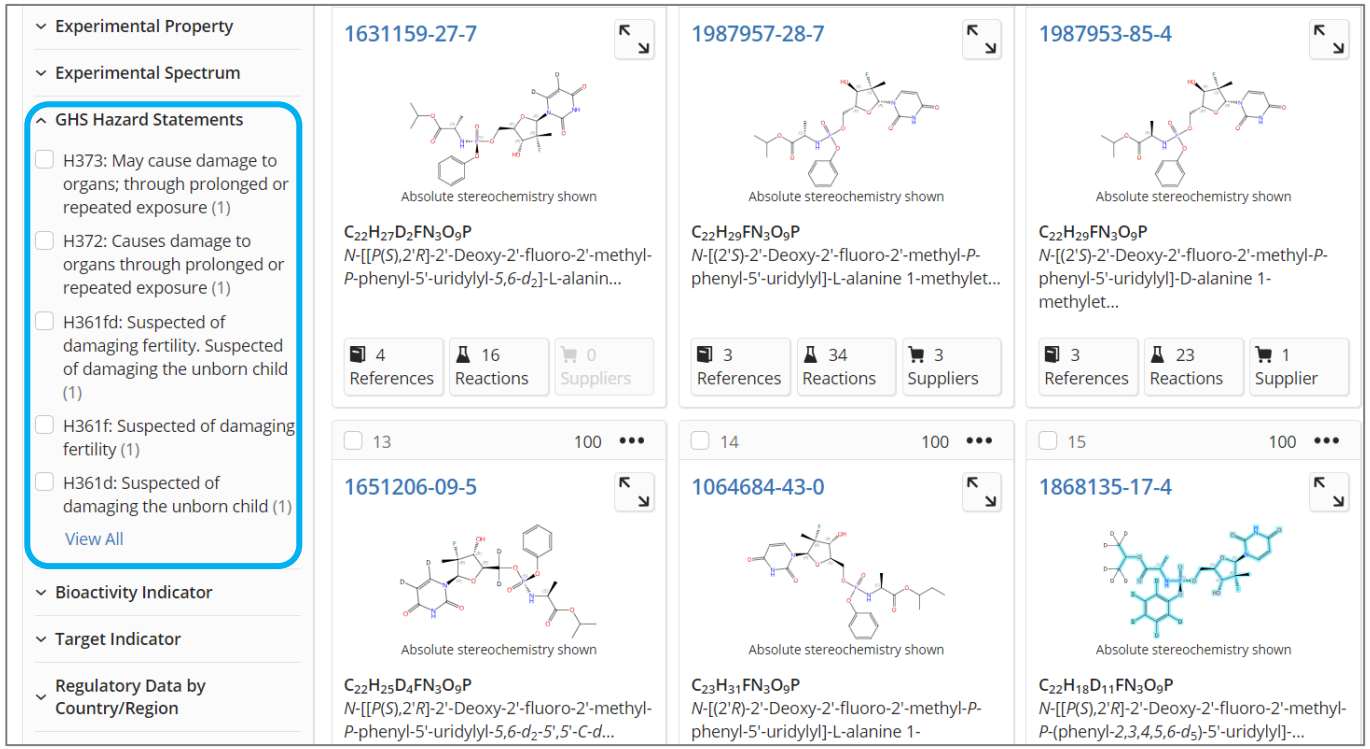
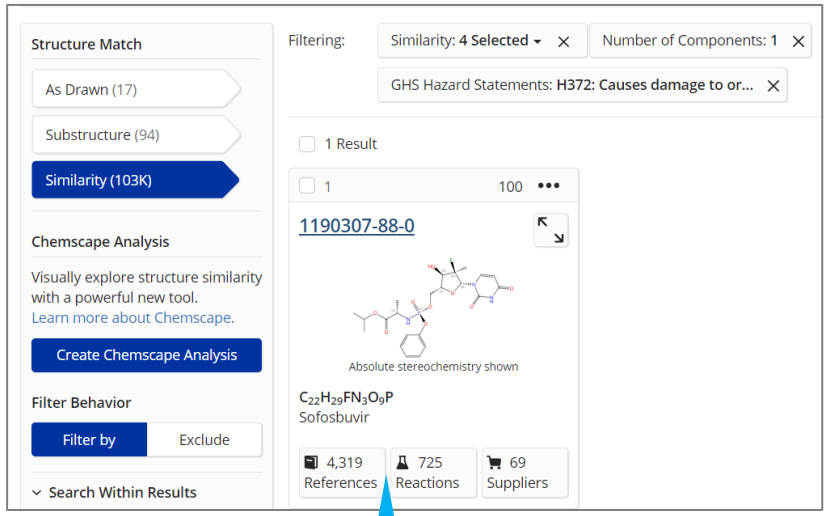
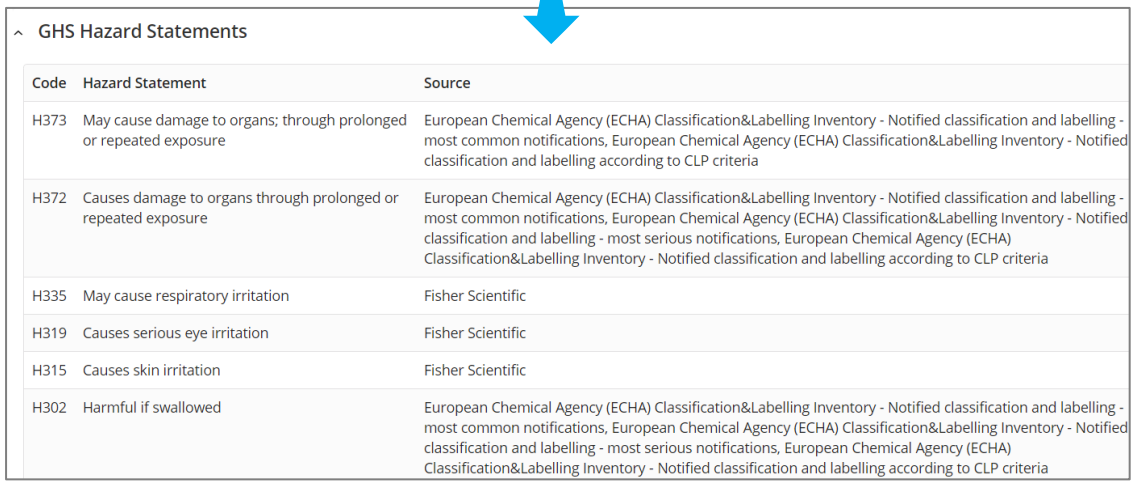
GHS 危害说明筛选物质结果集

支持根据 GHS 分类代码筛选结果







GHS Hazard Statements

Code	Hazard Statement	Source
H373	May cause damage to organs; through prolonged or repeated exposure	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most common notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria
H372	Causes damage to organs through prolonged or repeated exposure	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most common notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria
H335	May cause respiratory irritation	Fisher Scientific
H319	Causes serious eye irritation	Fisher Scientific
H315	Causes skin irritation	Fisher Scientific
H302	Harmful if swallowed	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most common notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria

物质详情界面展示 GHS 标识图标和详细的危害说明

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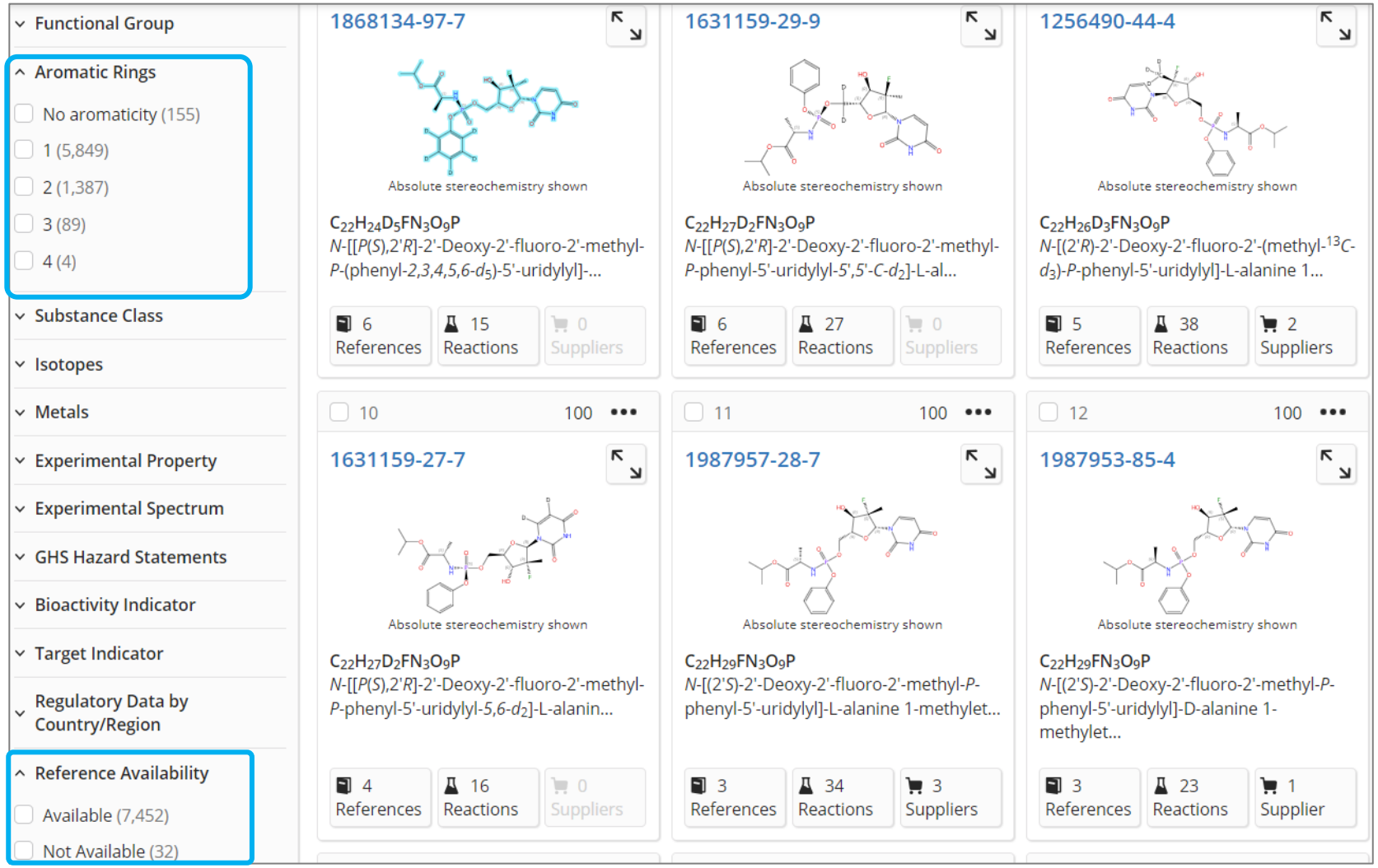
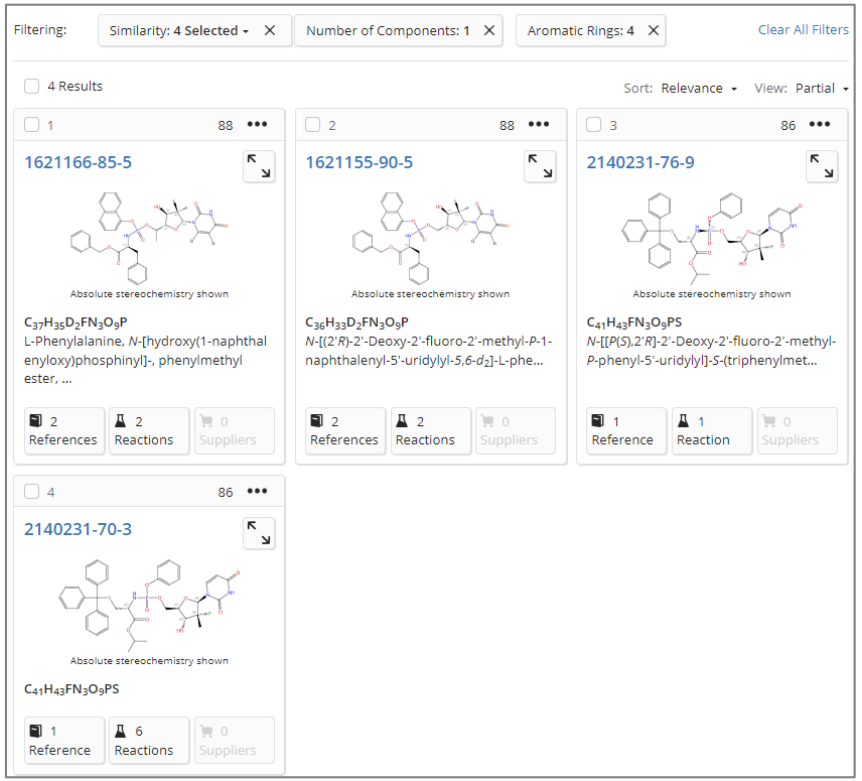
芳香环数量 & 是否有关联文献筛选物质结果集





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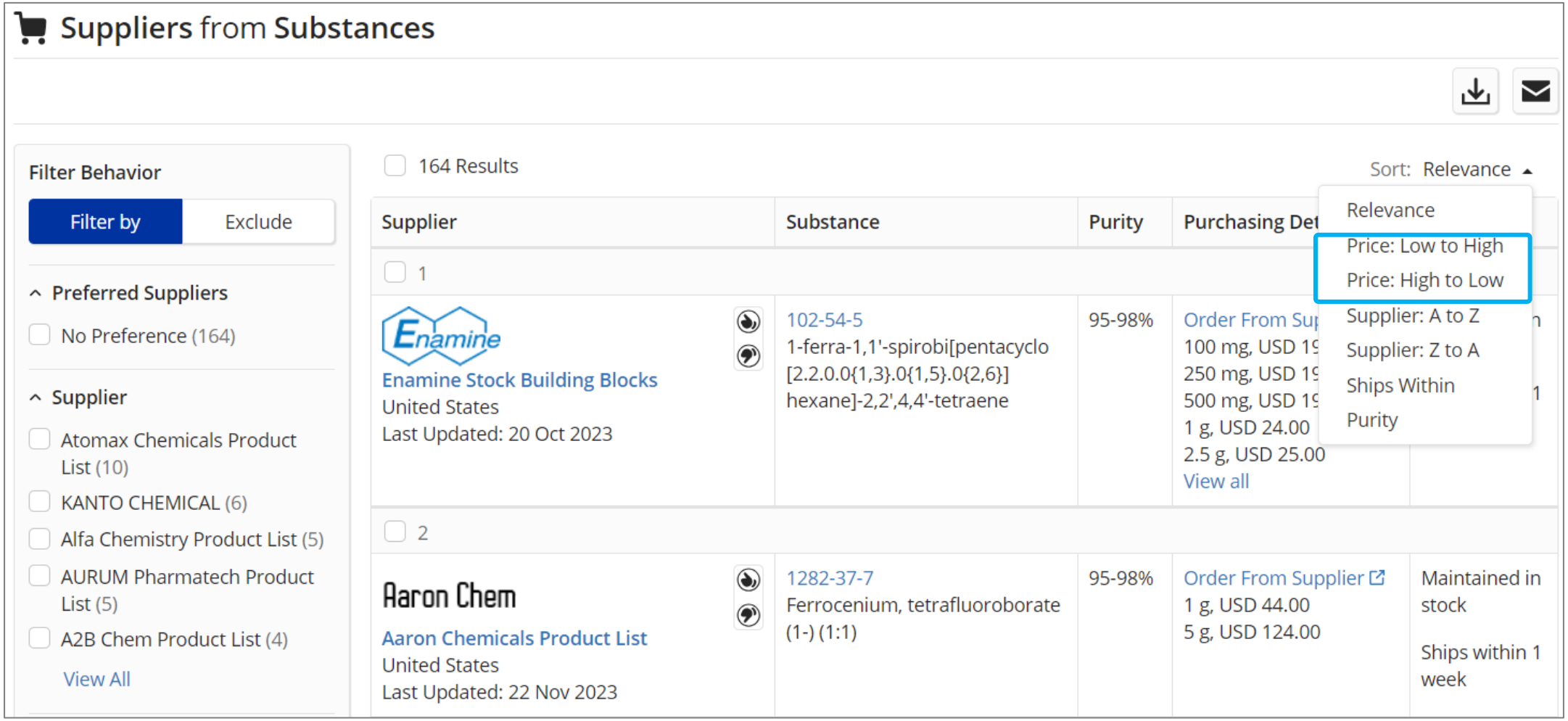
根据价格高低筛选供应商信息



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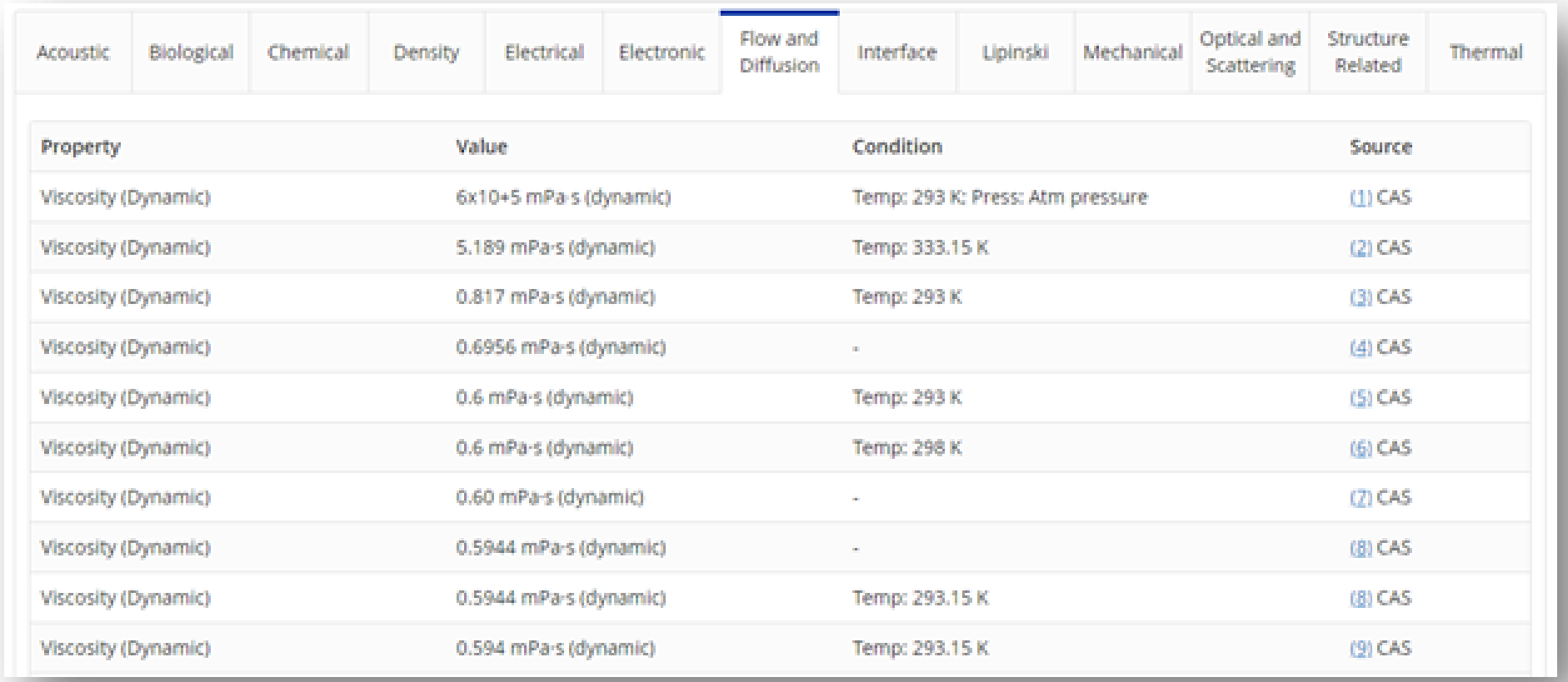
新增多种物质实验属性

新增转化温度、流体属性、解离常数、偶极距数据，以及热动力学参数等实验属性



Acoustic | Biological | Chemical | Density | Electrical | Electronic | Flow and Diffusion | Interface | Lipinski | Mechanical | Optical and Scattering | Structure Related | Thermal

Property	Value	Condition	Source
Viscosity (Dynamic)	6x10+5 mPa·s (dynamic)	Temp: 293 K; Press: Atm pressure	(1) CAS
Viscosity (Dynamic)	5.189 mPa·s (dynamic)	Temp: 333.15 K	(2) CAS
Viscosity (Dynamic)	0.817 mPa·s (dynamic)	Temp: 293 K	(3) CAS
Viscosity (Dynamic)	0.6956 mPa·s (dynamic)	-	(4) CAS
Viscosity (Dynamic)	0.6 mPa·s (dynamic)	Temp: 293 K	(5) CAS
Viscosity (Dynamic)	0.6 mPa·s (dynamic)	Temp: 298 K	(6) CAS
Viscosity (Dynamic)	0.60 mPa·s (dynamic)	-	(7) CAS
Viscosity (Dynamic)	0.5944 mPa·s (dynamic)	-	(8) CAS
Viscosity (Dynamic)	0.5944 mPa·s (dynamic)	Temp: 293.15 K	(8) CAS
Viscosity (Dynamic)	0.594 mPa·s (dynamic)	Temp: 293.15 K	(9) CAS

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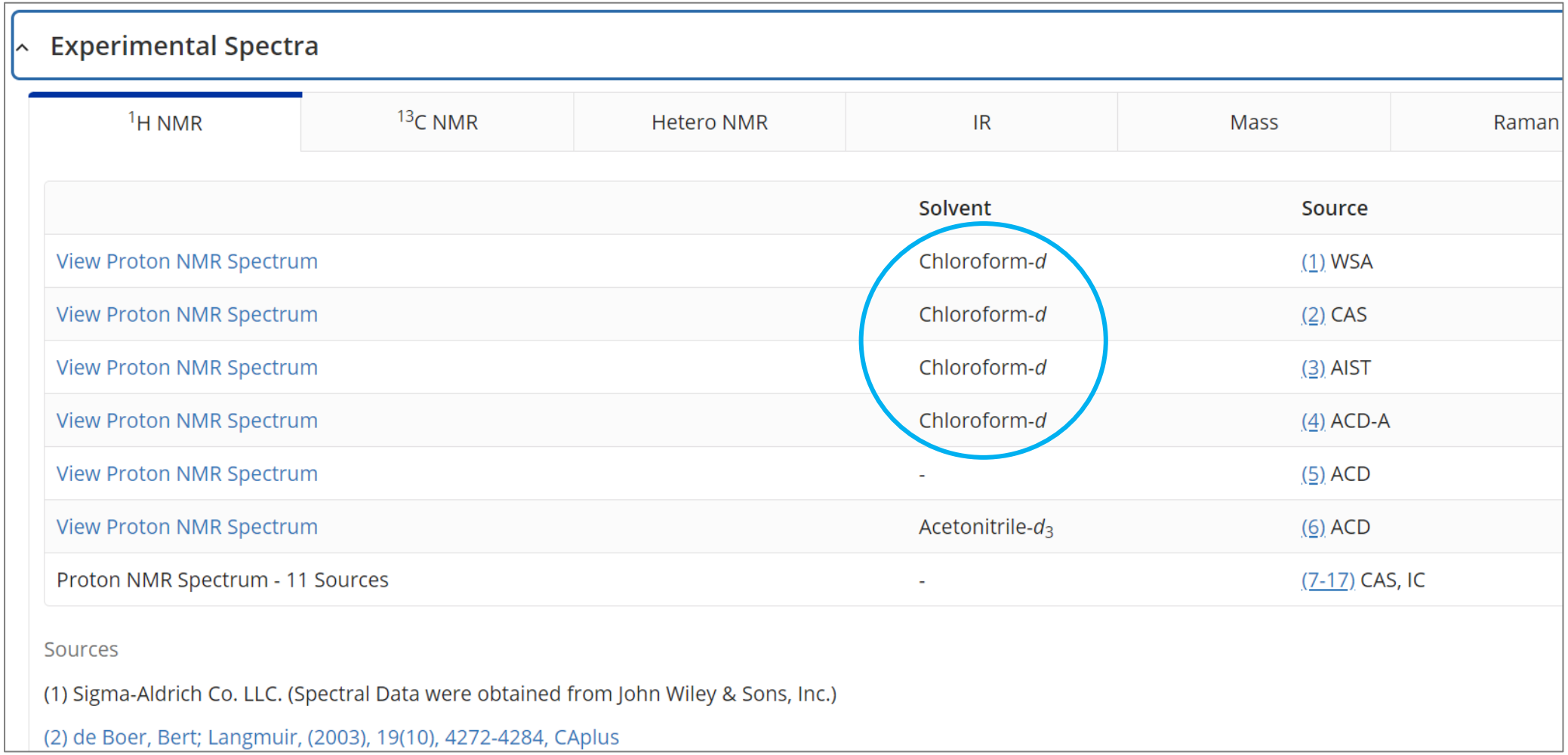
物质实验谱图中显示溶剂信息

在物质详情页中，实验谱图部分新增显示所用溶剂信息，比如氘代溶剂



Experimental Spectra

^{1}H NMR | ^{13}C NMR | Hetero NMR | IR | Mass | Raman

	Solvent	Source
View Proton NMR Spectrum	Chloroform-*d*	(1) WSA
View Proton NMR Spectrum	Chloroform-*d*	(2) CAS
View Proton NMR Spectrum	Chloroform-*d*	(3) AIST
View Proton NMR Spectrum	Chloroform-*d*	(4) ACD-A
View Proton NMR Spectrum	-	(5) ACD
View Proton NMR Spectrum	Acetonitrile-d_3	(6) ACD
Proton NMR Spectrum - 11 Sources	-	(7-17) CAS, IC

Sources

(1) Sigma-Aldrich Co. LLC. (Spectral Data were obtained from John Wiley & Sons, Inc.)

(2) de Boer, Bert; Langmuir, (2003), 19(10), 4272-4284, CAplus

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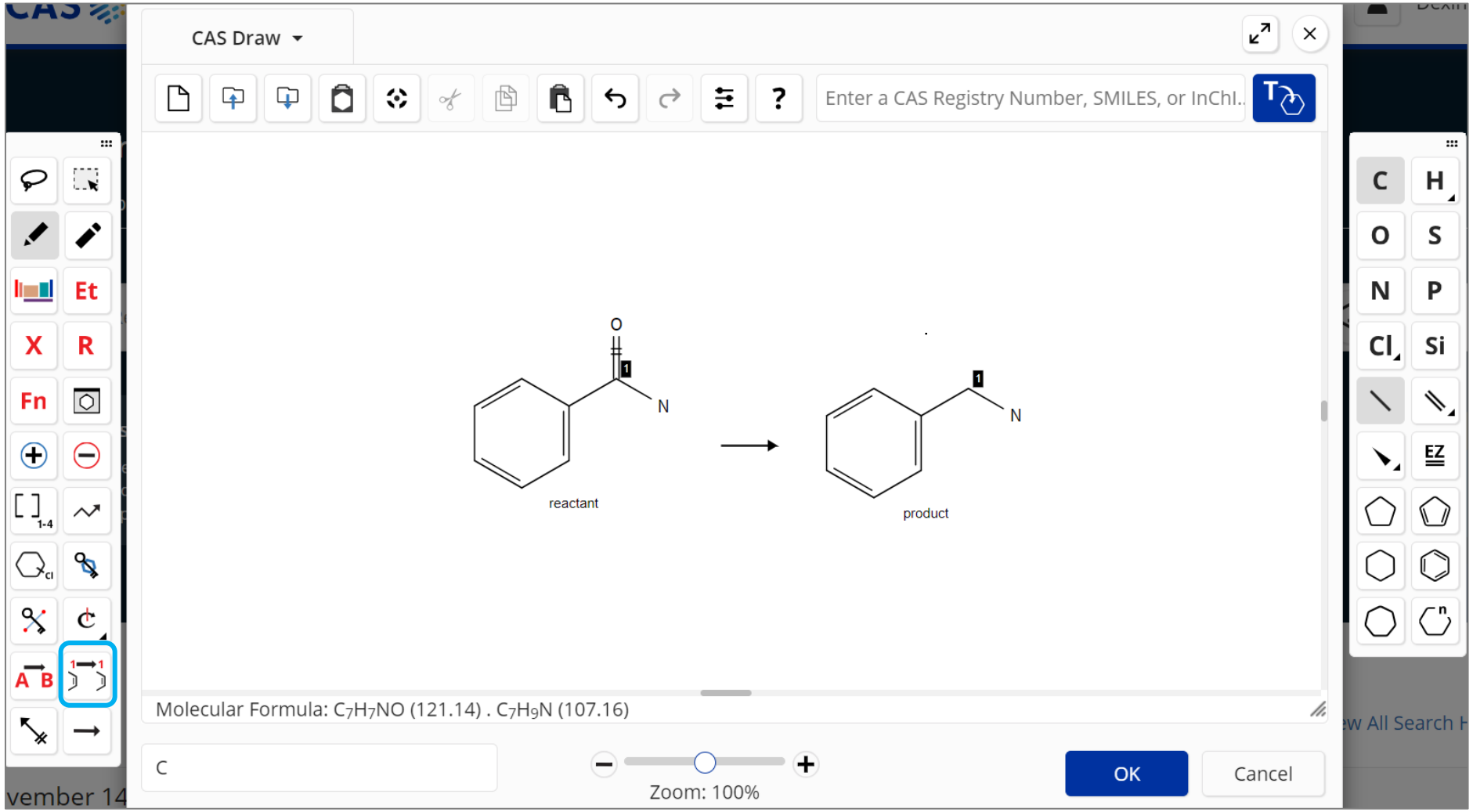
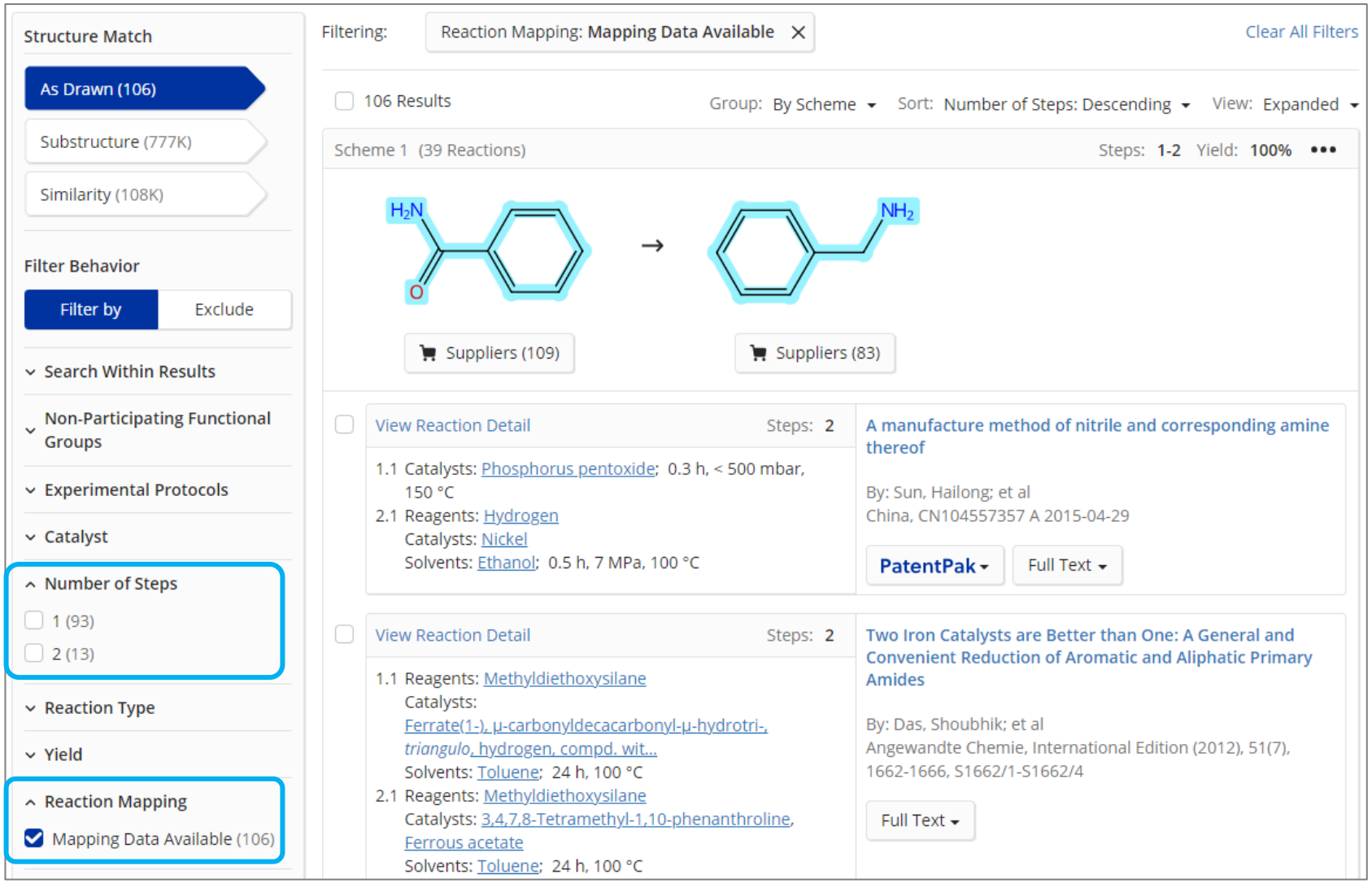
可对多步反应进行原子对标记筛选

在CAS SciFinderⁿ 结构绘制面板的左侧工具栏中，使用原子标记工具对原料和产物中同一原子进行对应标记



可对多步反应进行原子对标记筛选

对是否含有原子对标记的反应进行分类，适用于单步和多步反应



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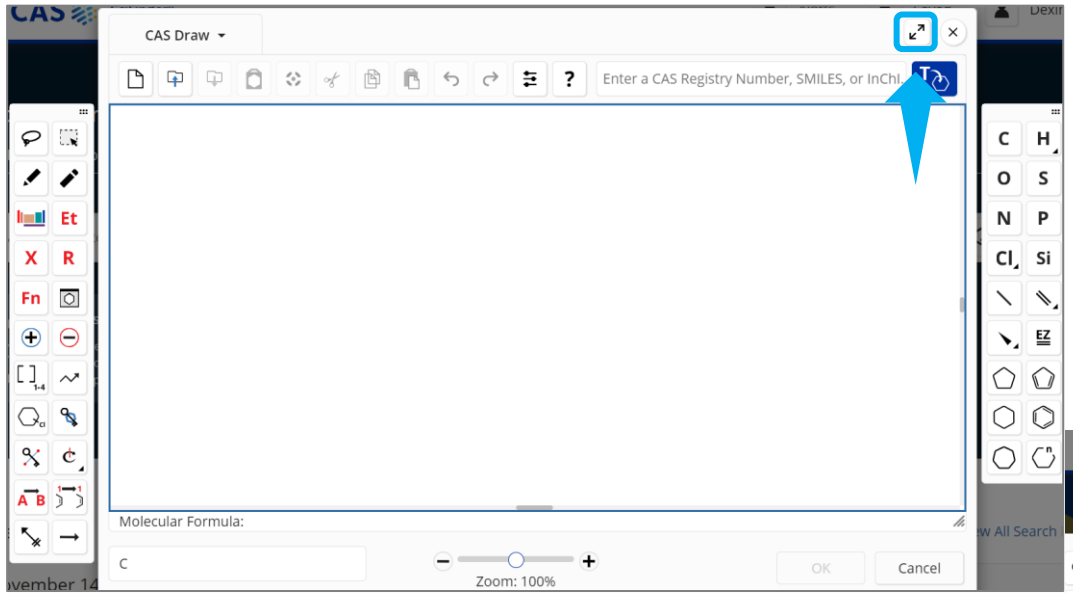
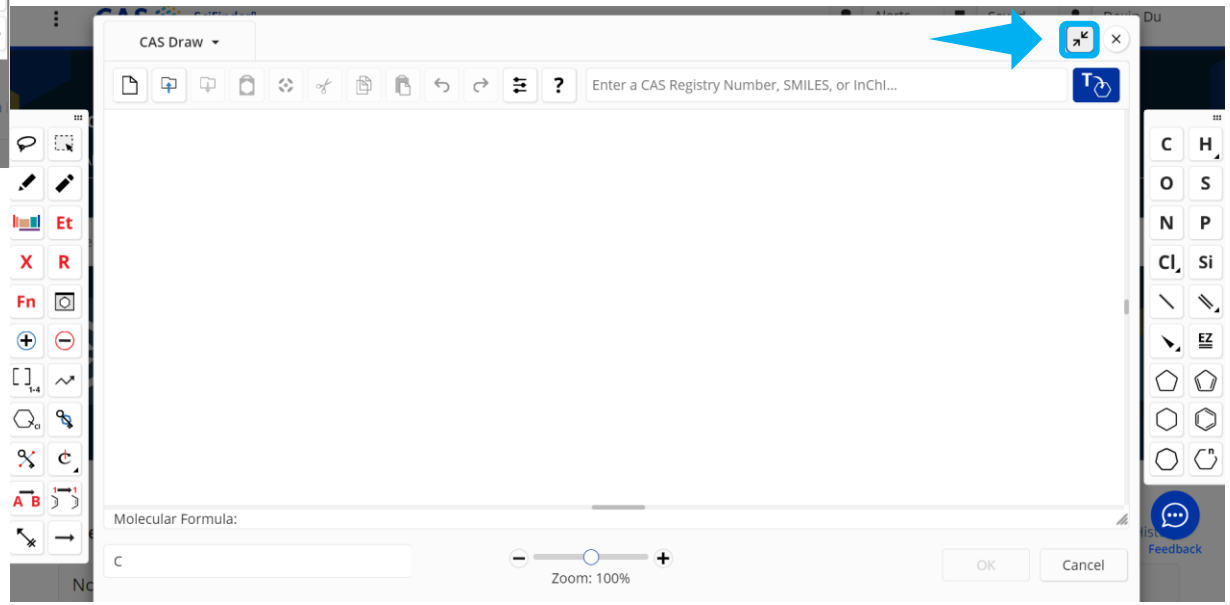
结构编辑器可自由缩放



- 点击右上角图标可将绘制面板最大化，再次点击可恢复初始大小
- 退出 CAS SciFinder^{n} 后，再次访问时会默认使用上次的设置



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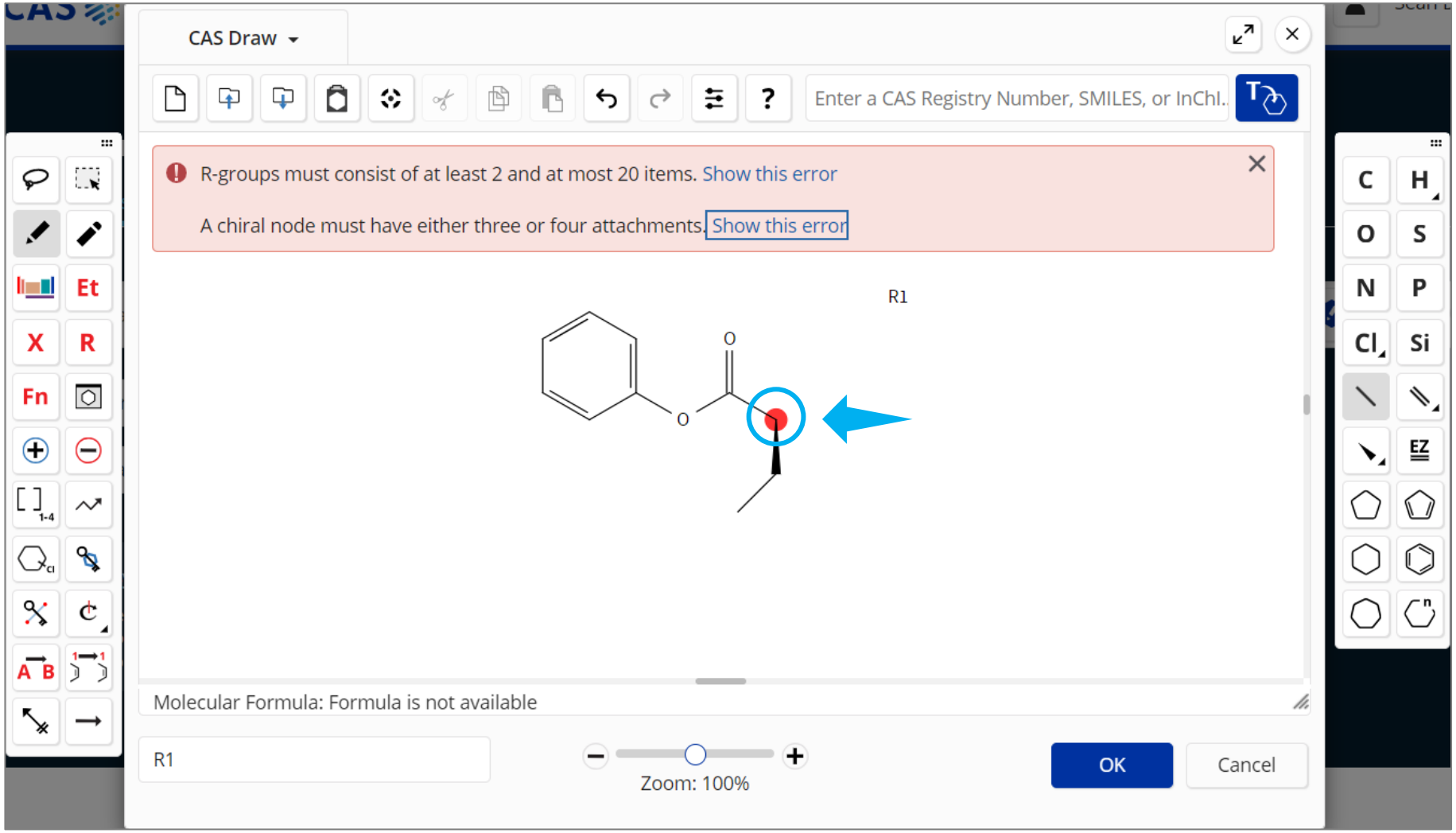
CAS Draw 对出错信息添加描述

增加出错信息描述，出错位置高亮显示



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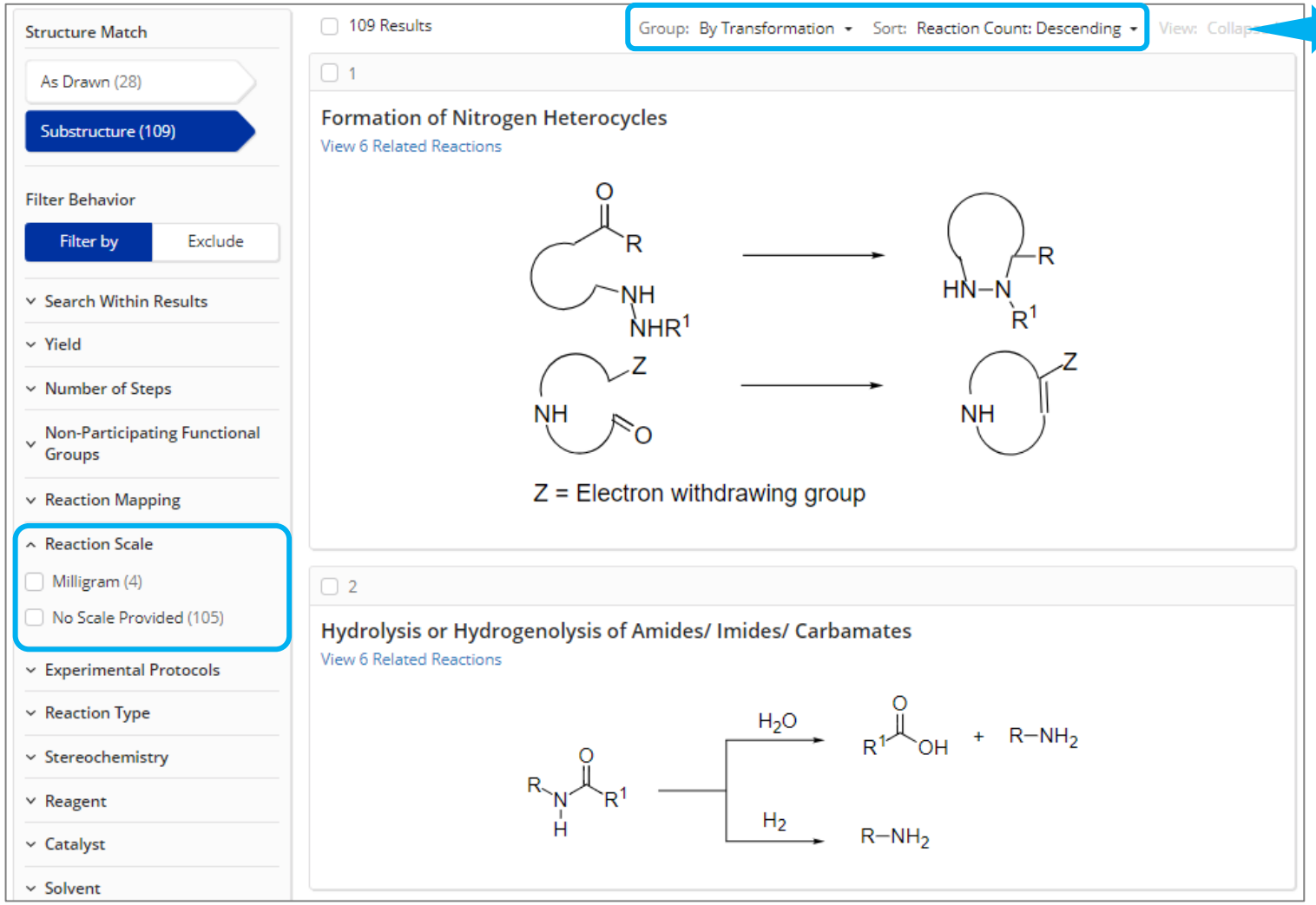
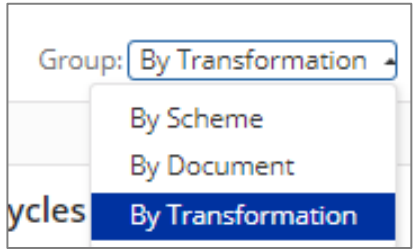
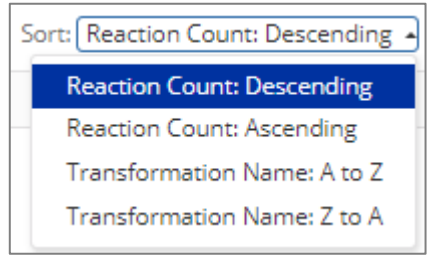
反应结果集排序和筛选新功能

按转化类型（Transformation）分组后，可根据转化类型名称或反应数量排序







反应规模（Reaction Role）筛选不同反应规模的反应结果

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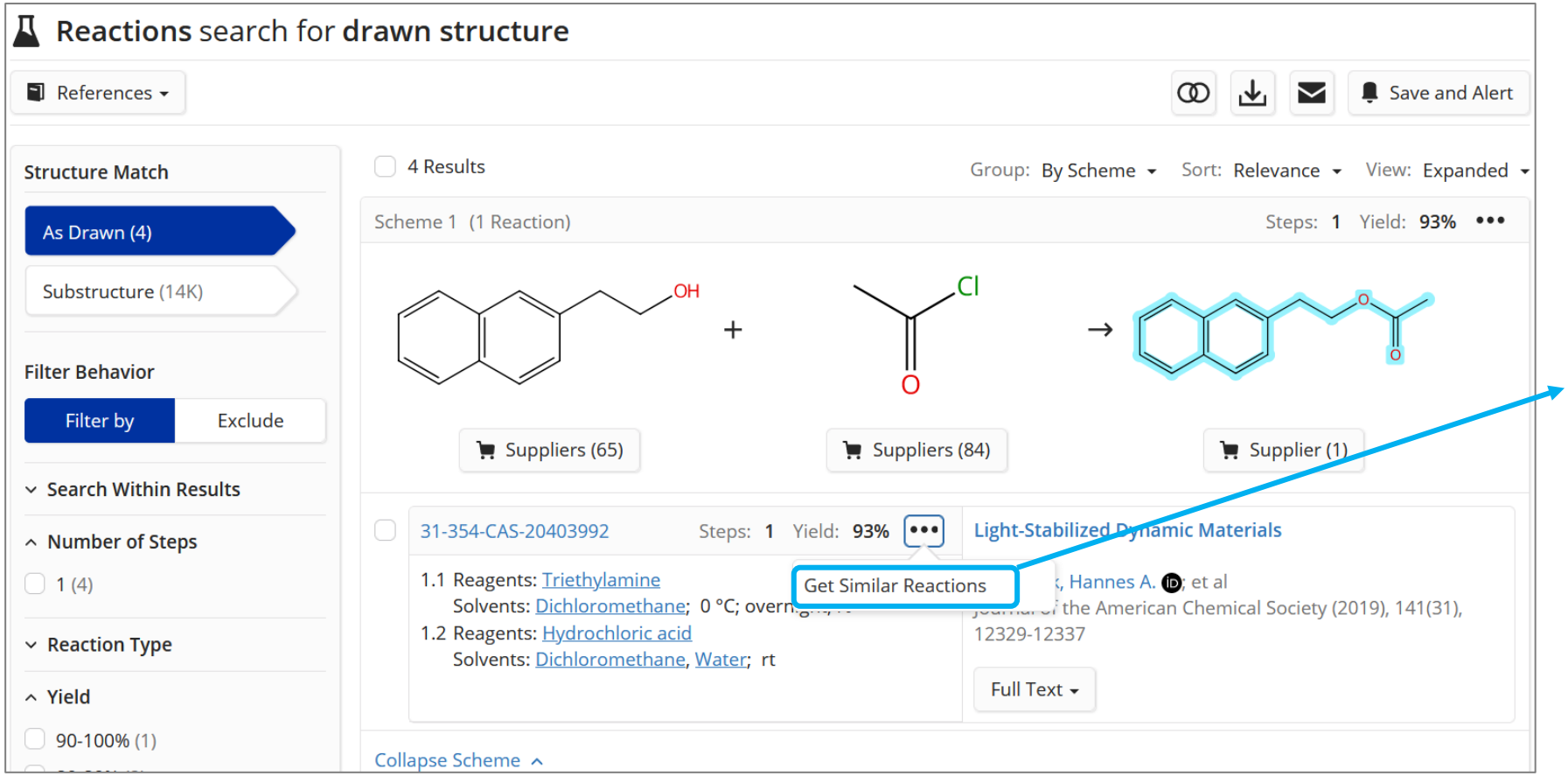
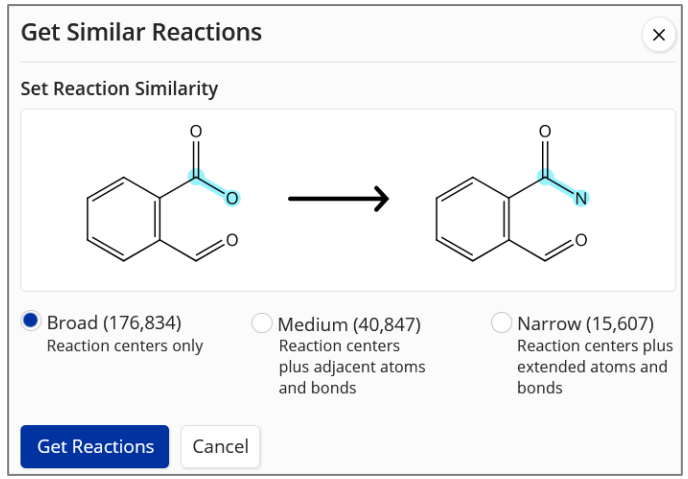
获取指定反应的相似反应结果

反应中心一致，周边原子和化学价特征较相似的反应





选择相似度范围

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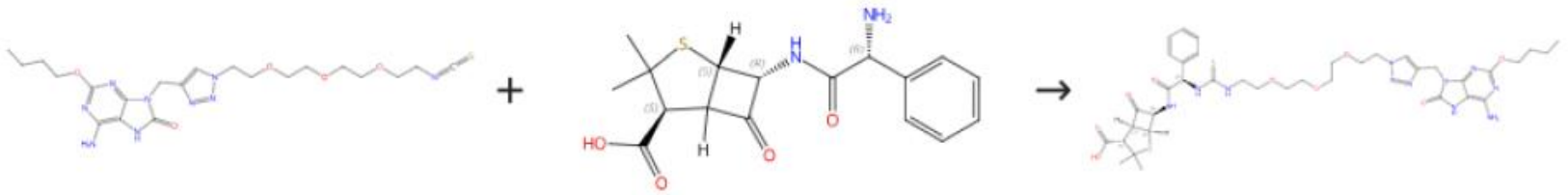
反应详情页获取相似反应

CAS Reaction Number: 31-316-CAS-23145310

Get Similar Reactions

Save



10%

Reaction Overview

Steps: **1** Yield: **10%**

PATENT

Preparation of purine derivatives as immune agonists

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Triethylamine	-	Dimethyl sulfoxide	overnight, rt

Alternative Steps (0)

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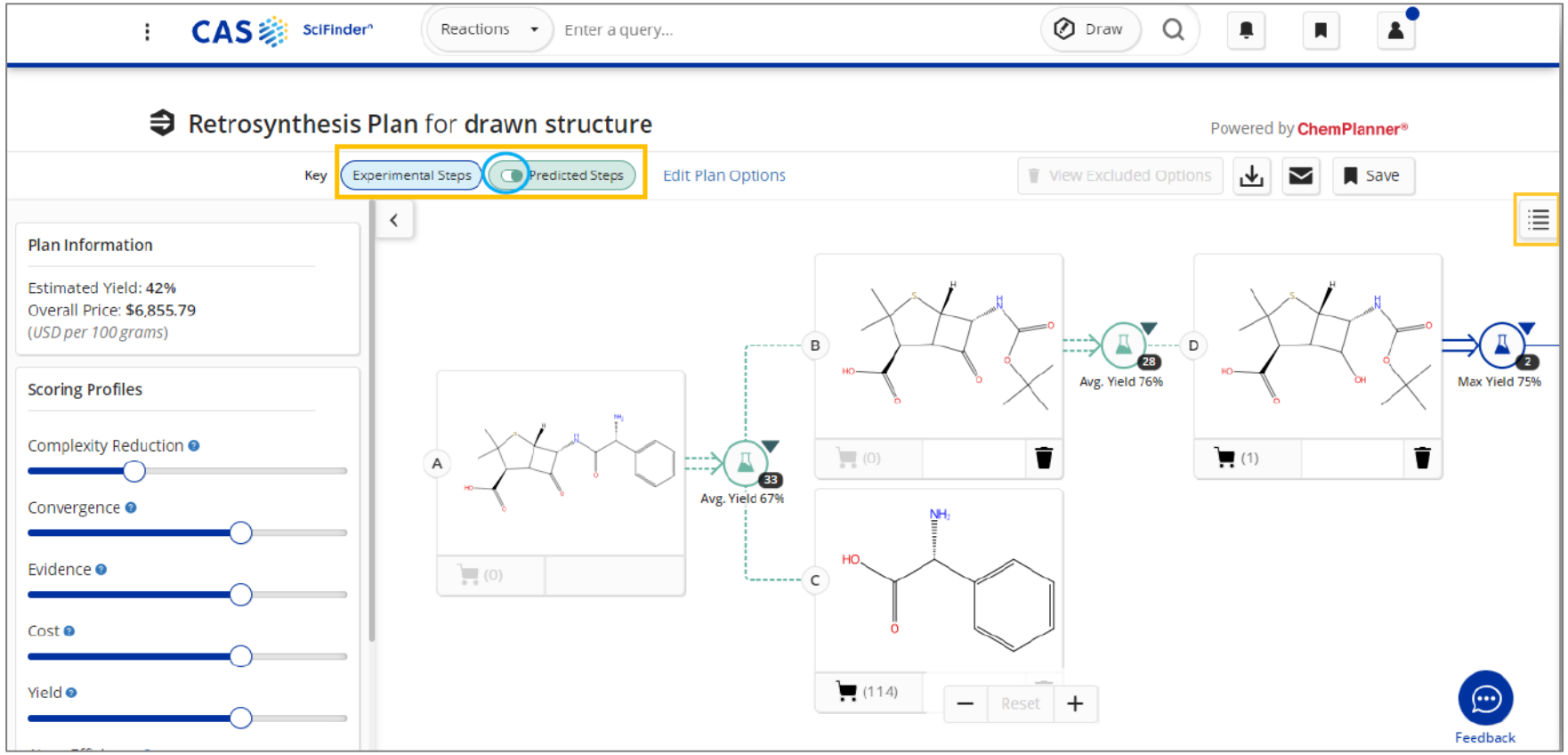
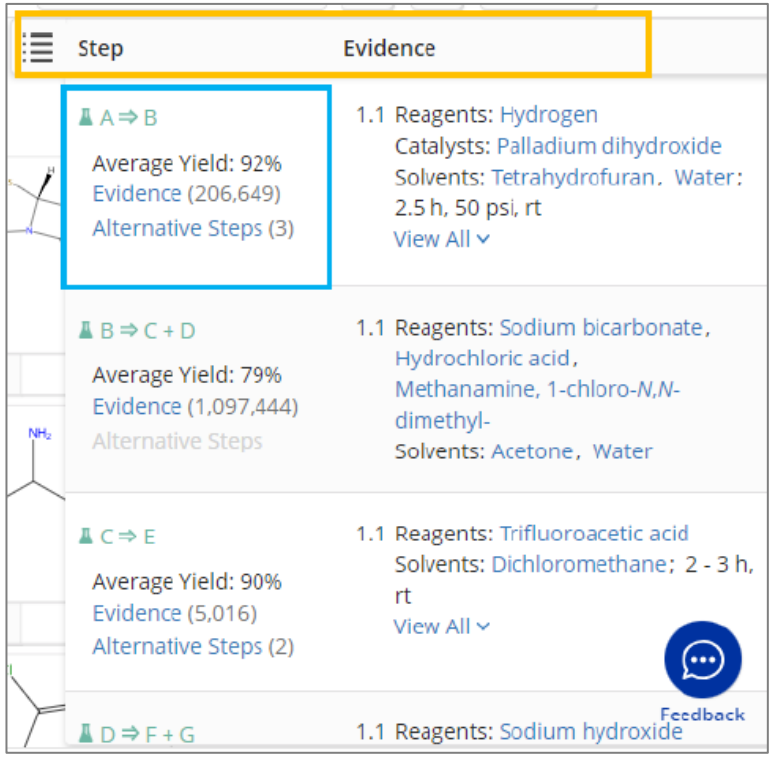
逆合成路线结果页面展示更新





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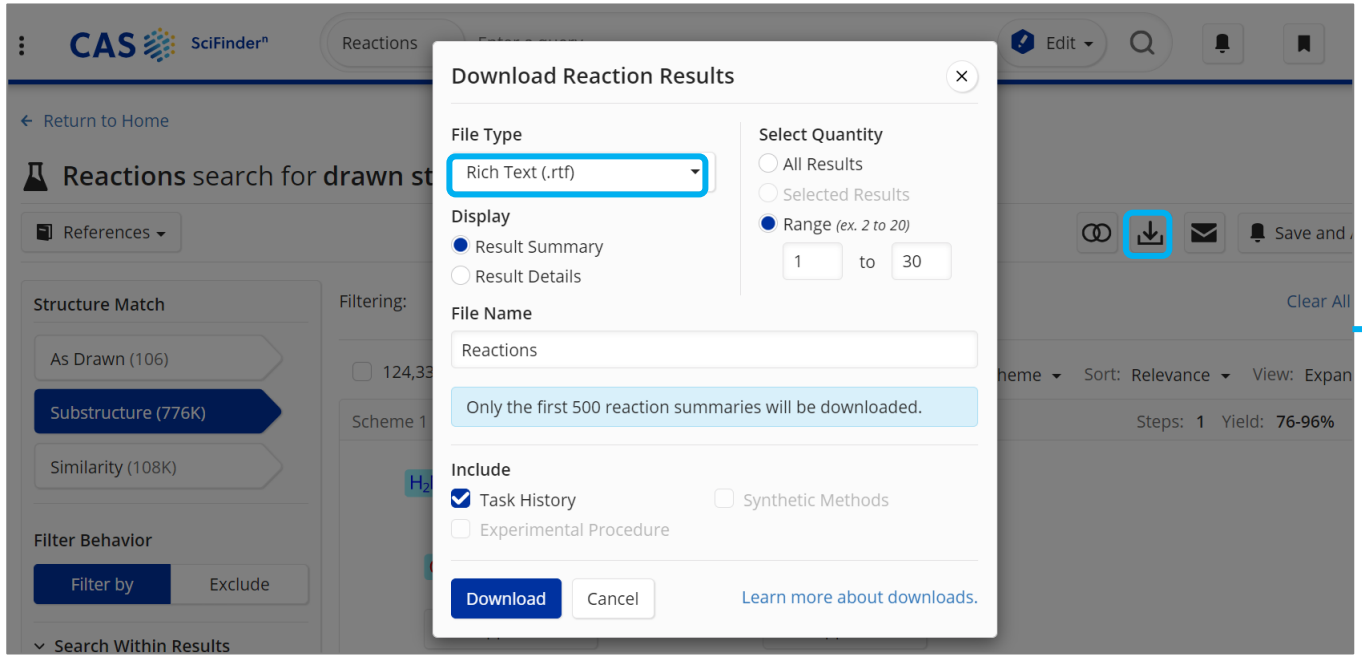
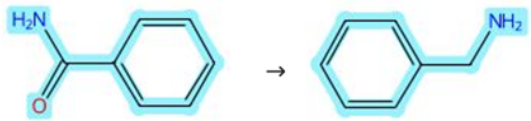
以可编辑的 RTF 格式下载反应检索结果



View in SciFinder^n

Reactions (30)

1. Scheme 1 (14 Reactions)



Ultrasound mediated functional group reduction and chemoselective studies by DMAB
By: Jayakumar, Venkatesan; et al
Chemical Science Transactions (2019), 8(3), 418-424.
10.7598/cst2019.1581
View All Sources in SciFinder^n

Steps: 1-2, Yield: 29-96%
CAS Reaction Number: 31-541-CAS-20665946
1.1 **Reagents:** (*T*-4)-(*N*,*N*-Dimethylbenzenamine)trihydroboron
Solvents: Tetrahydrofuran; 5 min; 21 min
1.2 **Reagents:** Potassium carbonate
Solvents: Water

A Convenient and General Reduction of Amides to Amines with Low-Valent Titanium
By: Zhang, Tongxin; et al
Advanced Synthesis & Catalysis (2013), 355(14-15), 2775-2780.

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目录

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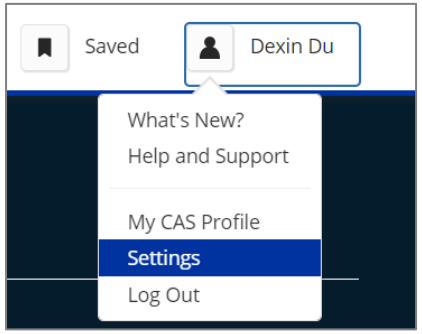
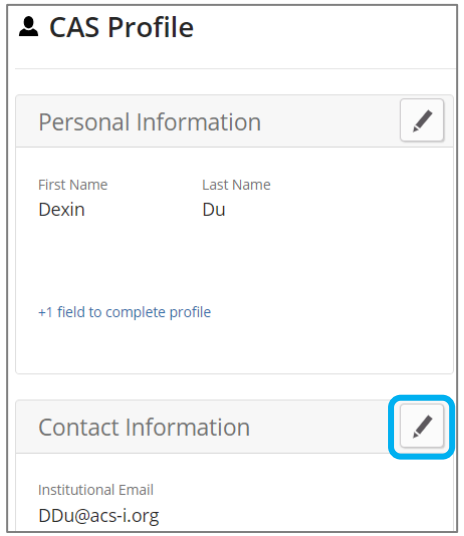
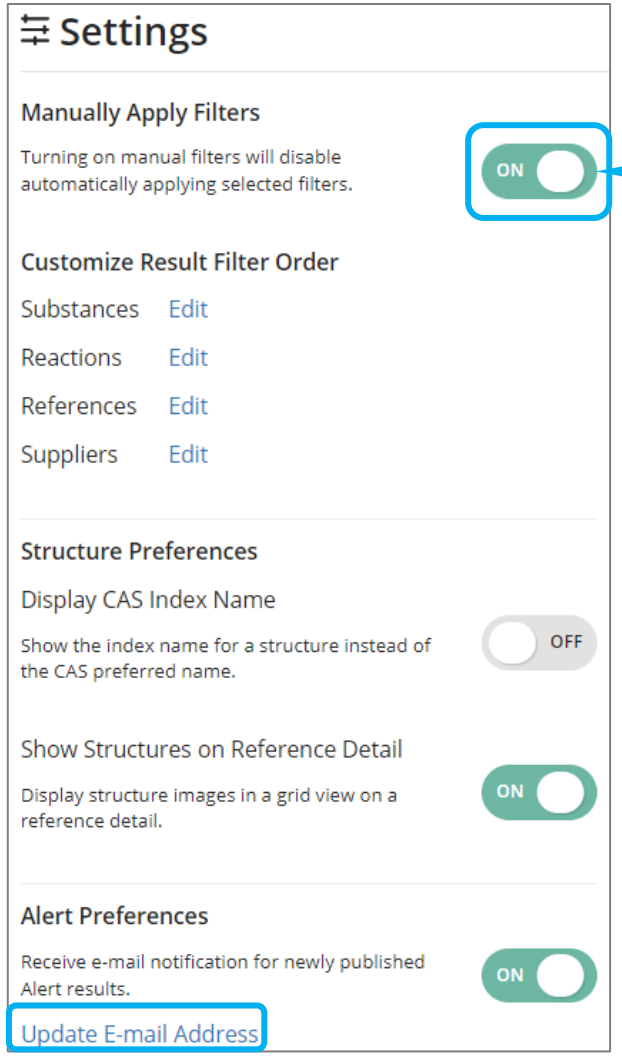
自定义设置功能

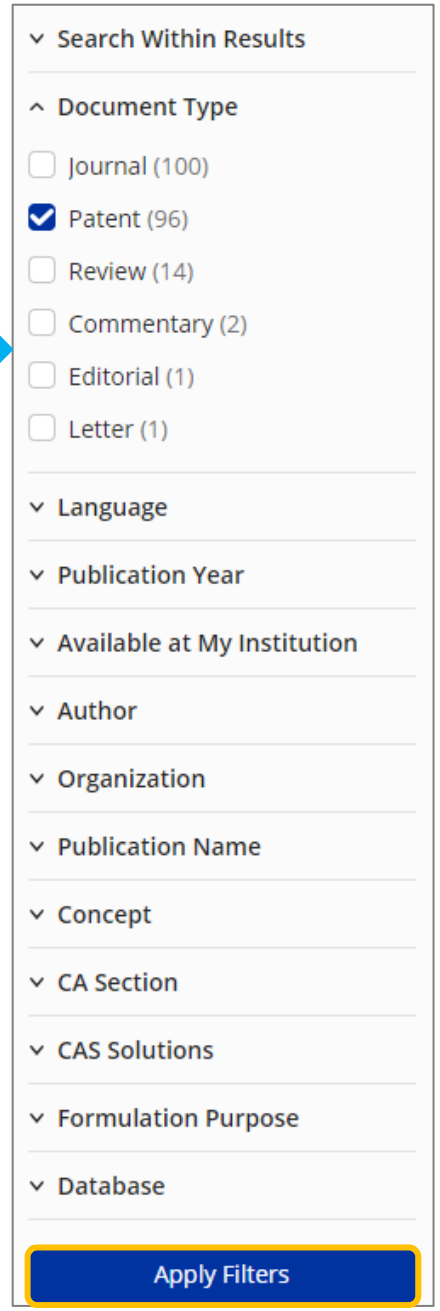
Manually Apply Filters: 手动筛选检索结果

Alert Preferences: 更改提醒邮箱









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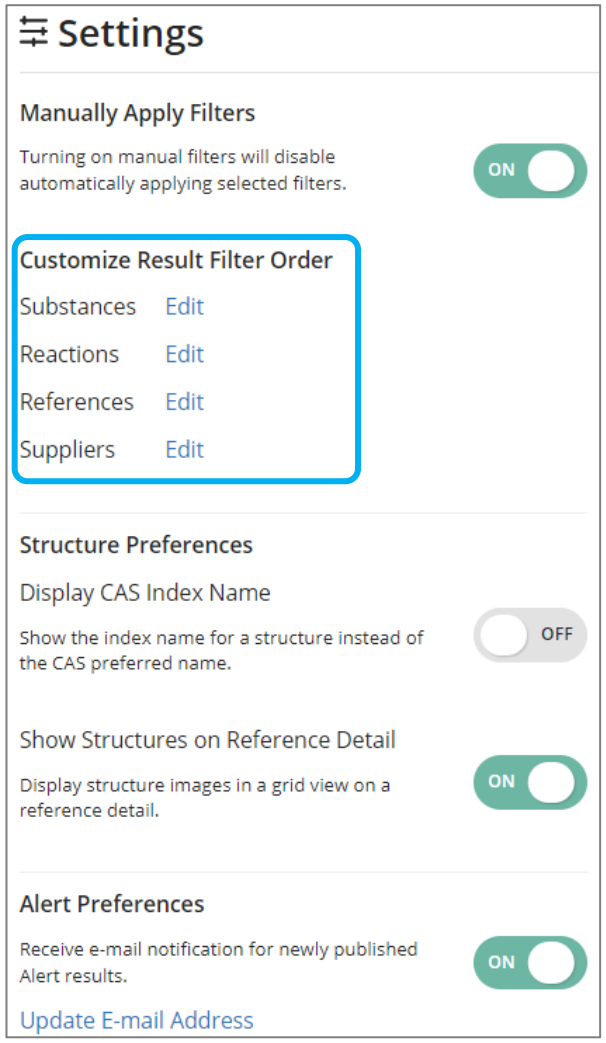
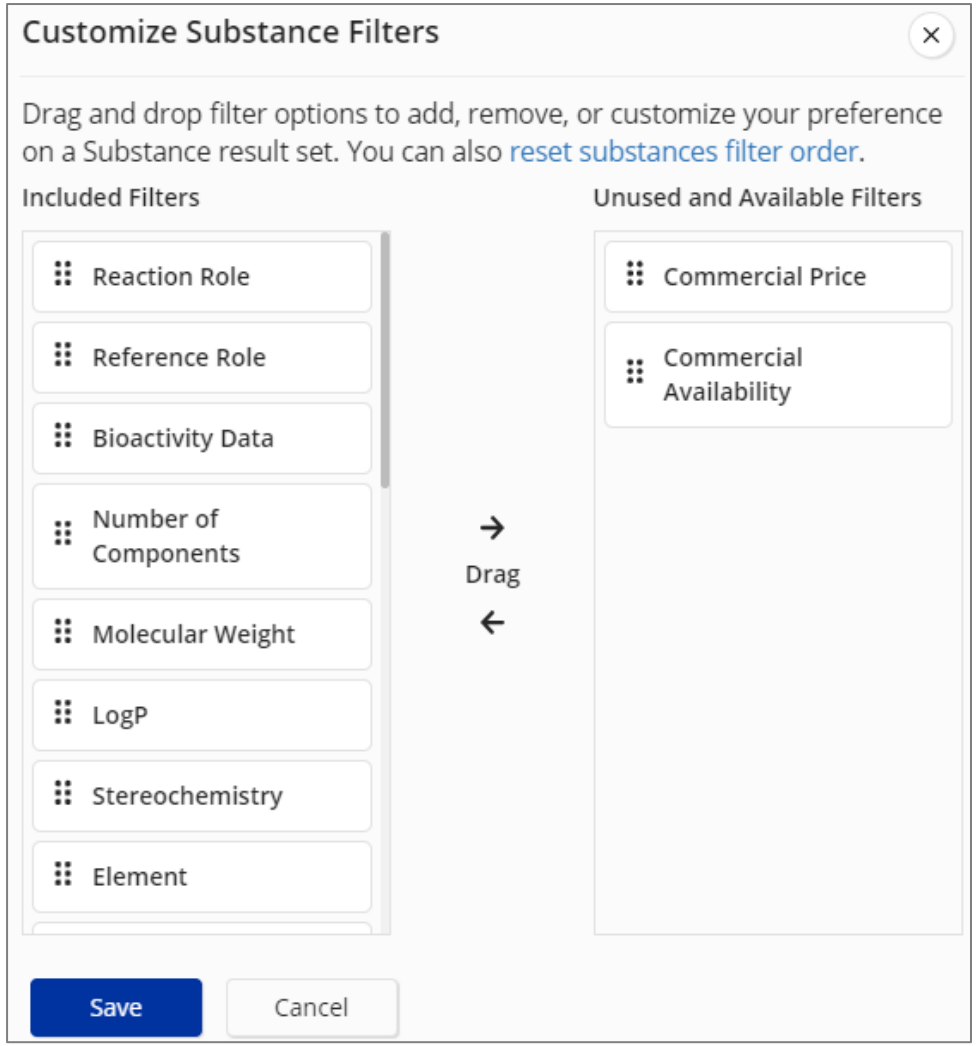
自定义设置检索结果筛选项及排序

拖拽筛选项进行选择或排序





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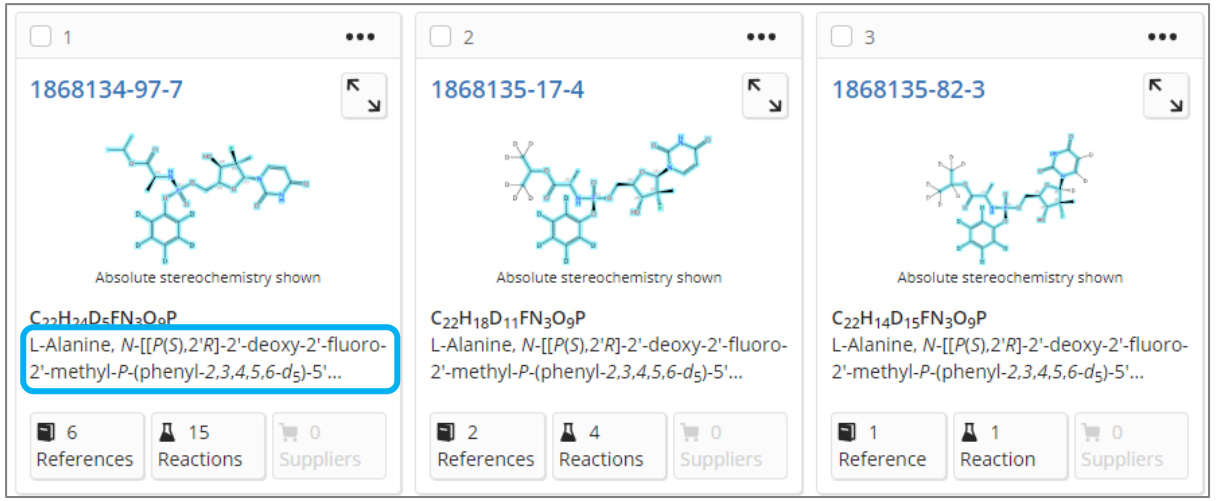
优先展示 CAS Index Name

Structure Preferences

Display CAS Index Name

Show the index name for a structure instead of the CAS preferred name.

ON

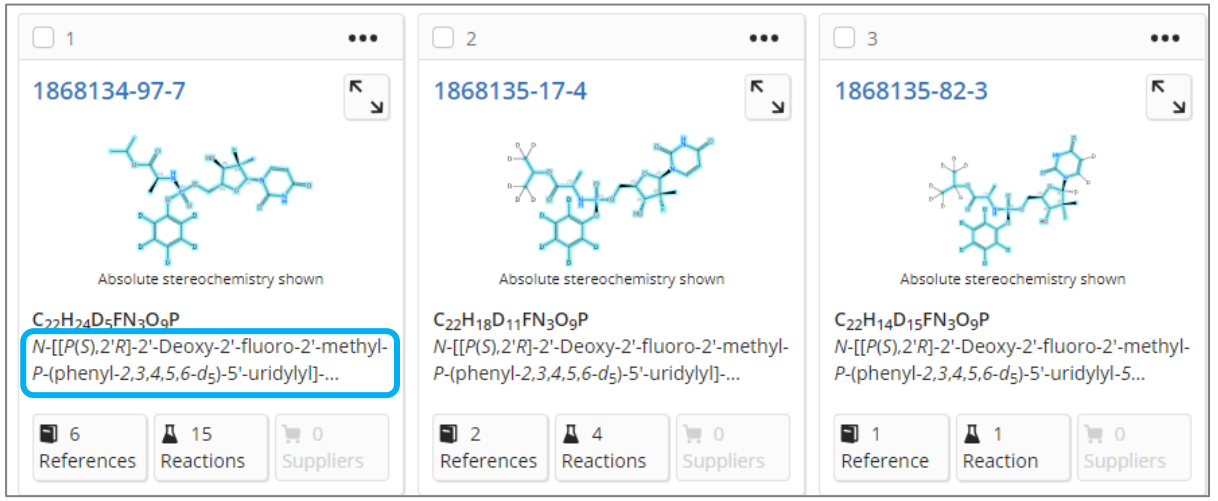


Structure Preferences

Display CAS Index Name

Show the index name for a structure instead of the CAS preferred name.

OFF



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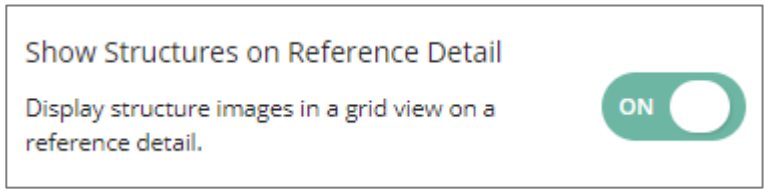
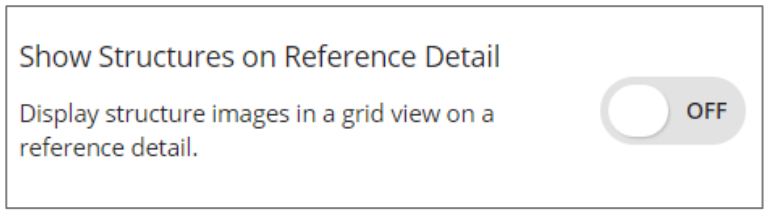
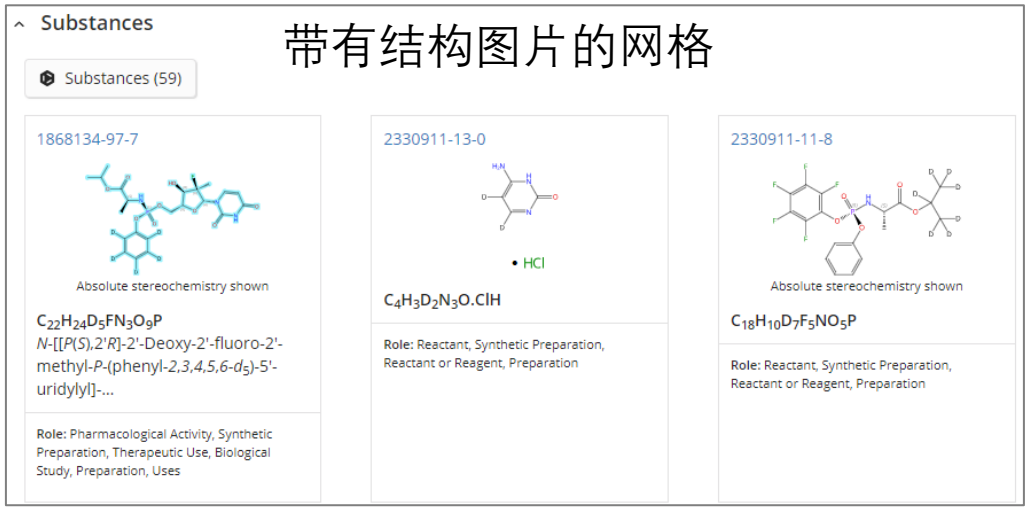
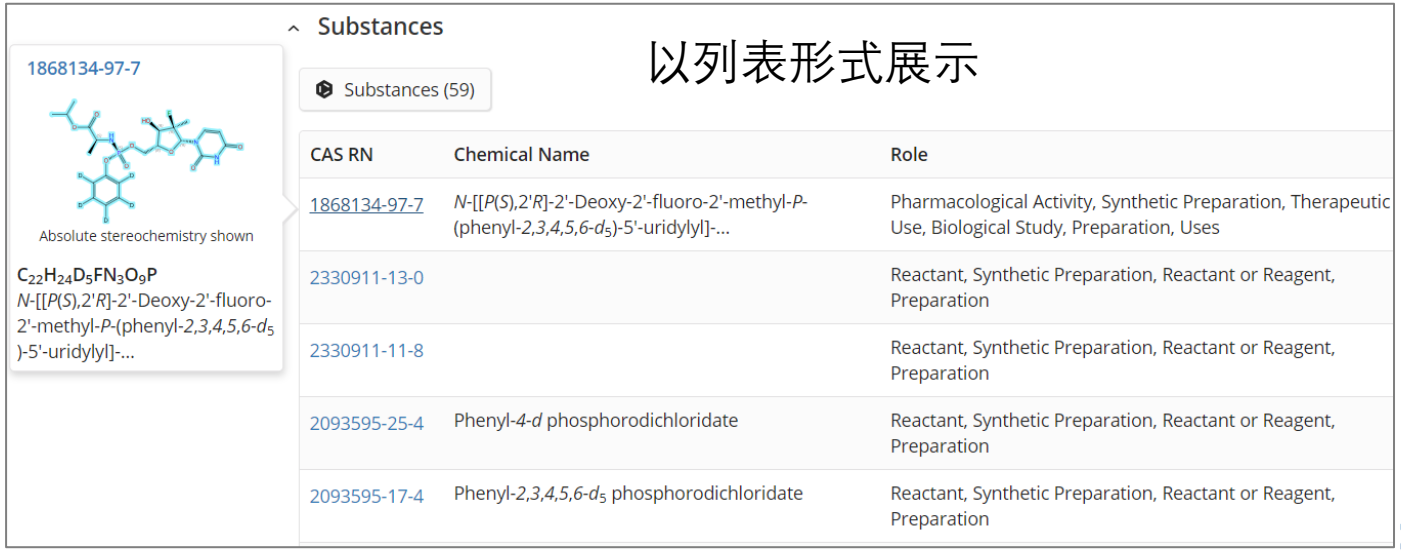
文献详情页面物质信息展现形式







带有结构图片的网格



以列表形式展示

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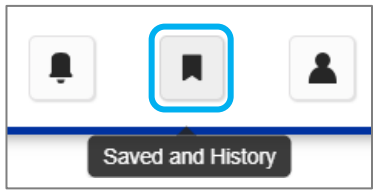
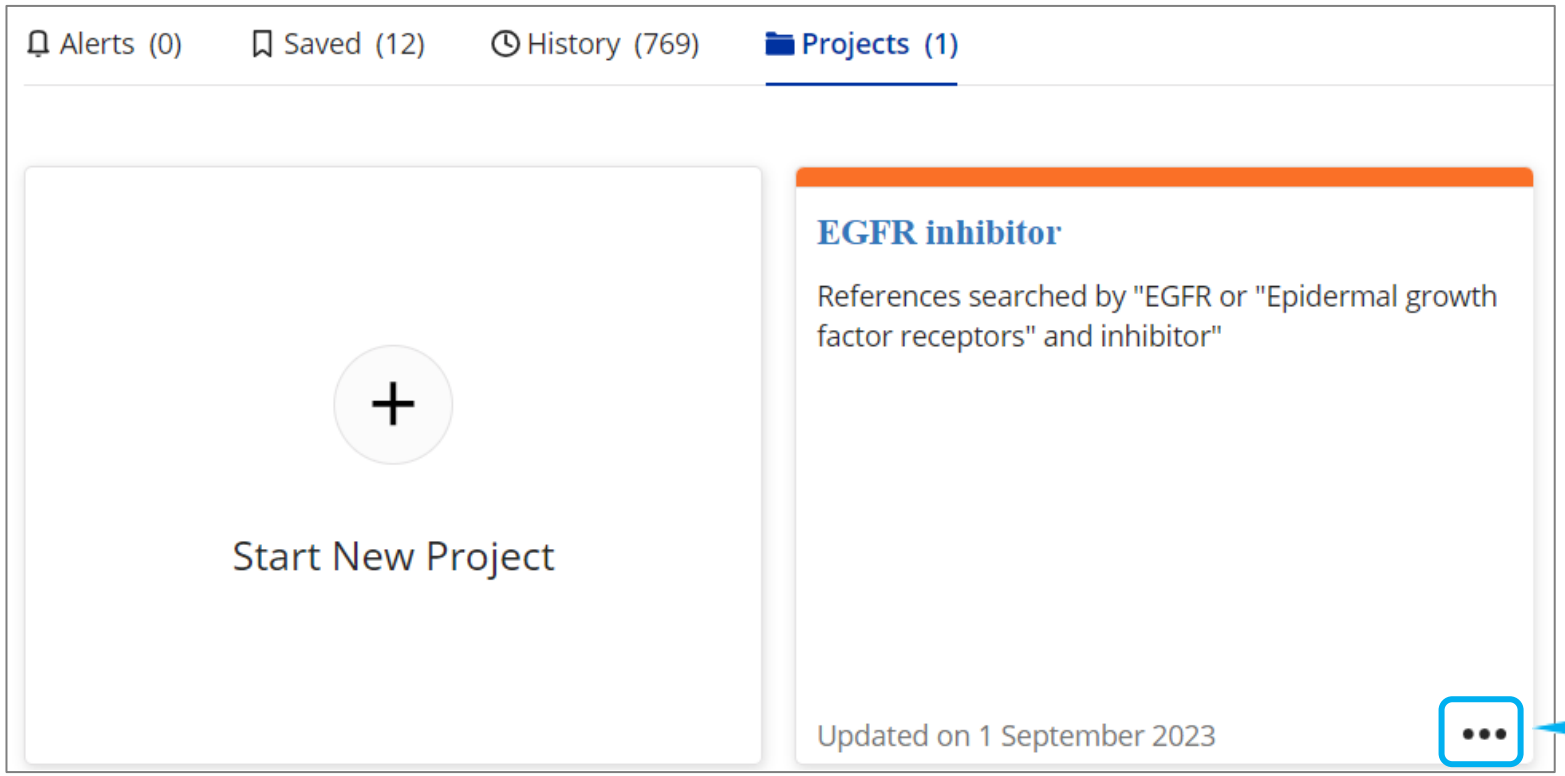
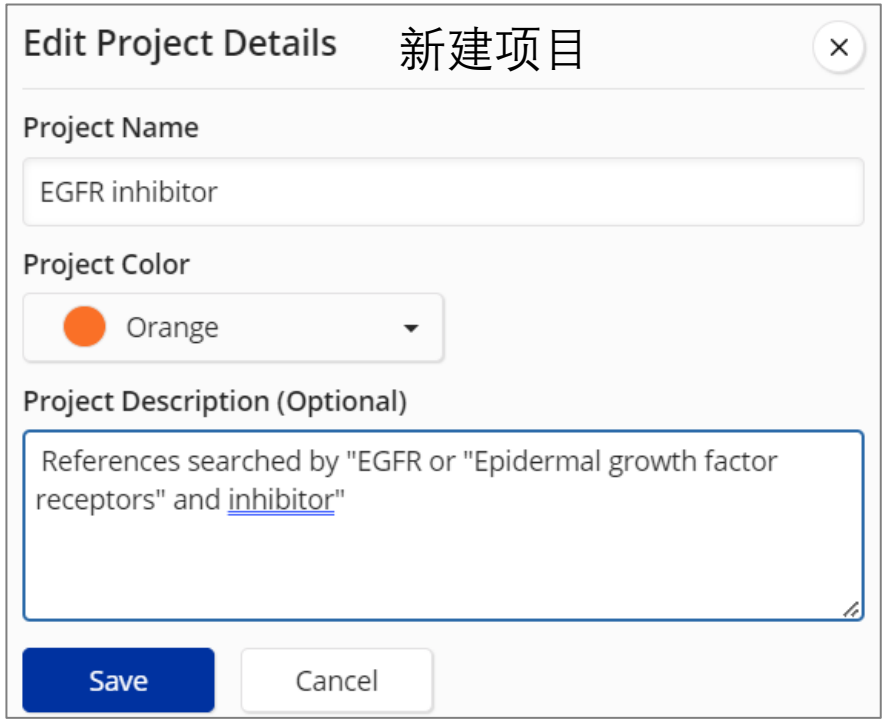
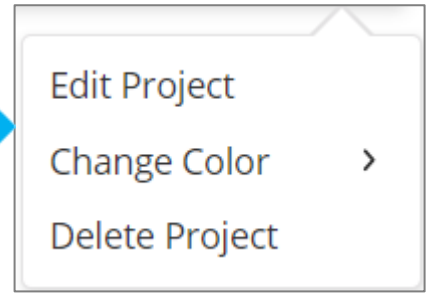
结果项目管理









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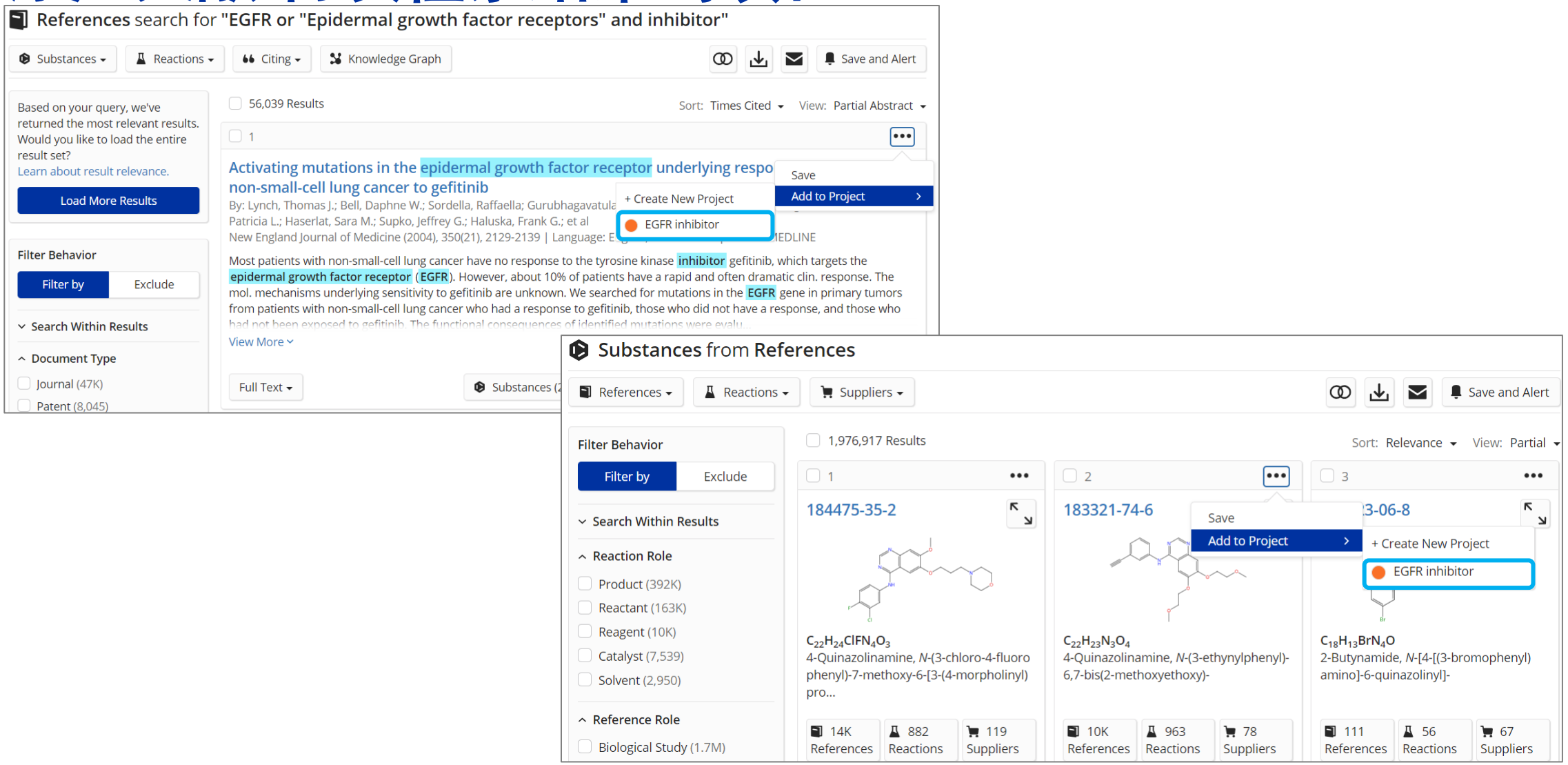
添加文献/物质检索结果到项目



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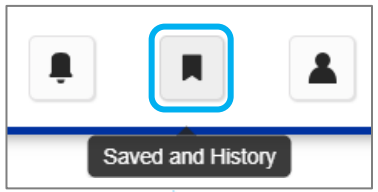
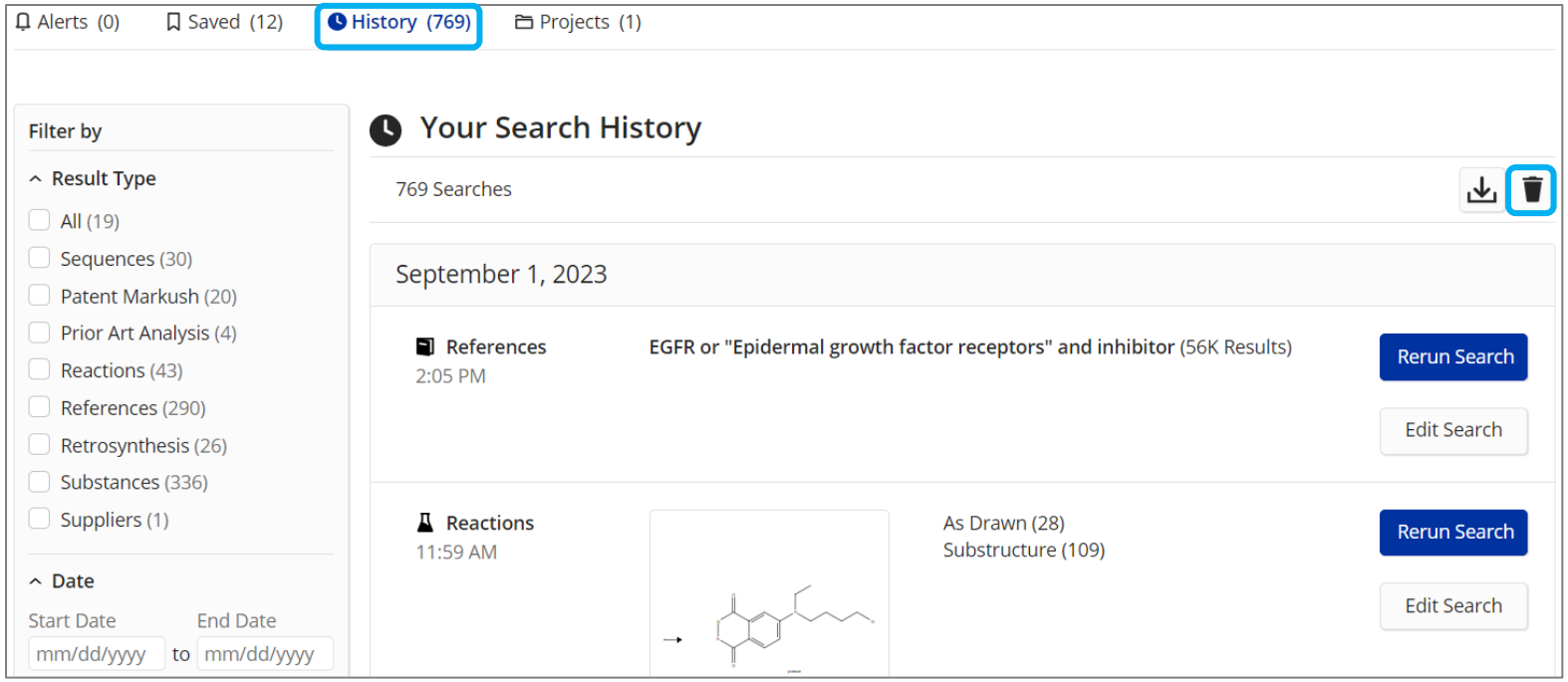
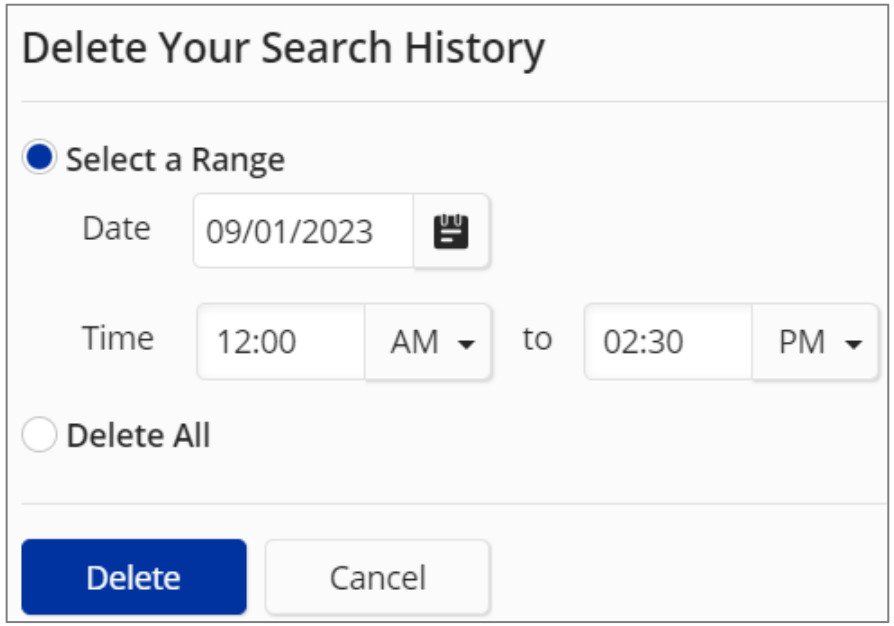
删除特定时间段历史记录







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CAS SciFinder^{n} 新功能总结

- 文献检索
  - 支持高级检索项 IPC Data 检索专利文献
  - 文献结果页面支持检索与作者 ORCID iD 相关的参考文献
  - 从序列结果获得的文献结果页面新增显示非专利文献
  - 文献检索支持根据生物活性数据检索文献
  - 文献详情页面推荐相似文献，引文地图可直接查看文献合集
  - 知识谱图可直接搜索关注内容
- 物质检索
  - 支持按 LogP 值、官能团、芳香环数量、GHS Code 和是否有文献关联等筛选结果
  - 新增多种物质实验属性，核磁谱图支持显示溶剂信息
  - 物质检索支持根据生物活性数据检索物质
  - CAS Draw 对出错信息添加描述
  - 支持根据价格高低筛选供应商信息

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CAS SciFinder^{n} 新功能总结

- 反应检索
  - 按转化类型（Transformation）分组后，支持根据转化类型名称或反应数量排序
  - 支持按反应规模筛选结果
  - 可直接查看相似反应
  - 支持对多步反应进行原子对标记和筛选
  - 支持下载可编辑RTF格式的反应检索结果
  - 逆合成路线结果页面展示更新
- 设置、项目管理和历史记录
  - 支持自定义设置功能和排序
  - 文献/物质结果集支持项目管理
  - 支持删除特定时间历史记录

Between problems and progress are connections that matter

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