CAS SciFinder Discovery Platform (Academic)

全面高效获取科技信息

杜德鑫

ddu@acs-i.org

美国化学文摘社 (CAS) 北京代表处

CAS
A division of the
American Chemical Society

大纲

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

CAS SciFinder Discovery Platform 查找路径

学校官网
（图书馆）

图书馆官网
（电子资源）
（外文数据库）

外文数据库
（SciFinder Academic 数据库）

CAS
A division of the American Chemical Society

CAS SciFinder Discovery Platform 简介与注册说明

注册和登录方式

开通时间：2023年01月01日至2025年12月31日。

1. 在校园网IP地址范围内用学校域名邮箱注册SciFInder帐号后在校园网IP地址范围内登陆网站：https://scifinder.cas.org/

2. SciFinder注册须知：

读者在使用SciFinder之前须使用学校的后缀名邮箱注册账号密码。注册后系统将自动发送一个链接到您所填写的email邮箱中，48小时内激活此链接即可完成注册。参考“SciFinder用户注册指南”。

SciFinder注册地址：

https://scifinder.cas.org/registration/index.html?corpKey=3A35186EX86F35055X1AA5171E17AE354E59

3. 特别提示：

1)如果进入系统后20分钟没有操作，系统将自动断开您与服务器的连接。2)SciFinder经常更新，请大家留意图书馆或美国化学文摘社主页(**www.cas.org**)的相关消息。

3)注意保护知识产权，合理使用数据库，只用于学术研究，实名使用，不与他人分享，禁止过量下载（以电子形式存储不超过5,000条记录），禁止在商业机构使用。

4)在使用过程中出现问题，请参考“SciFinder常见问题解答”，如无法解决，请填写“SciFinder问题报告”，并发送至**China@acs-i.org**或联系图书馆。

4. 附件：

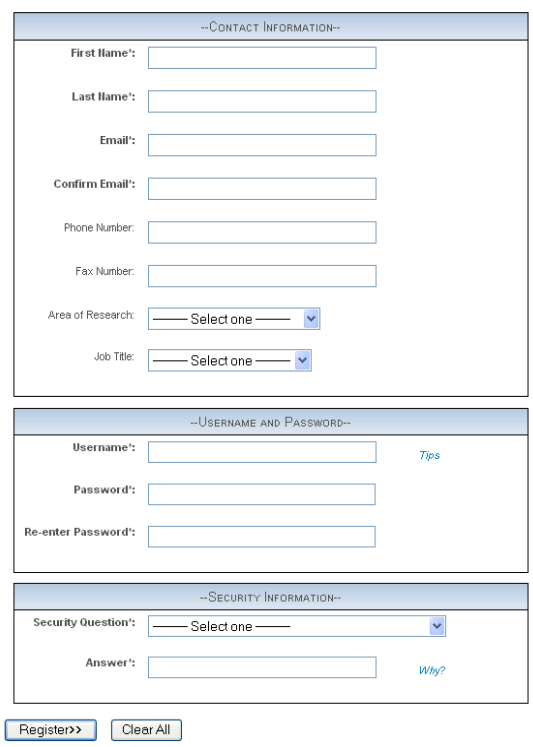
1) SciFinder用户注册指南.pdf：提供了详细的注册流程介绍，便于用户顺利完成账号注册。

2) SciFinder常见问题解答.docx：总结了用户在使用SciFinder数据库时常见的问题及解决办法，便于用户遇到问题时快速自查和应对。

3) SciFinder 问题报告.doc：用户在遇到账号问题时，

CAS
A division of the American Chemical Society

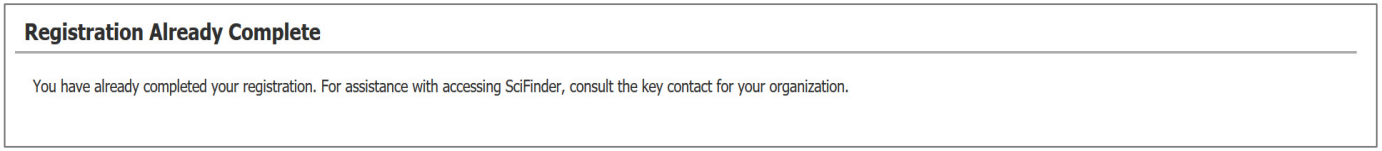
如何获取 CAS SciFinder^n 账号 （登录贵校图书馆网站，查看注册相关的链接和说明）



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 @、#、%、&、*）

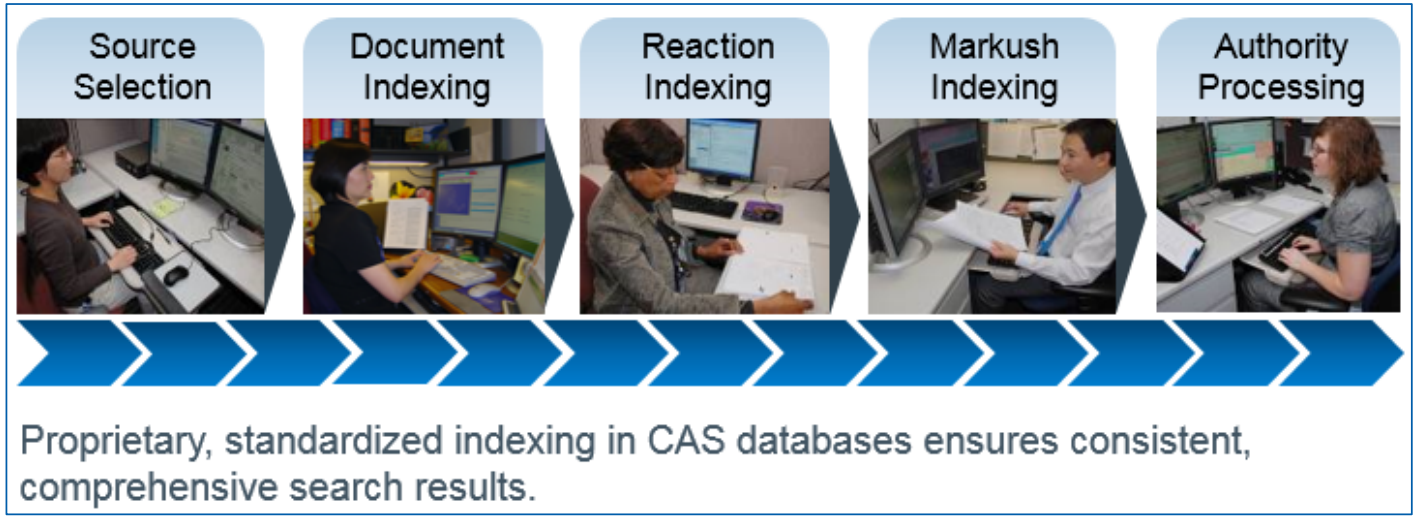
例：abc@123
4.从下拉列表中选择一个密码提示问题并给出答案
单击 Register（注册）



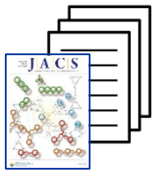
点击激活链接后注册成功；之后直接点击 https://scifinder-n.cas.org 访问

CAS
A division of the American Chemical Society

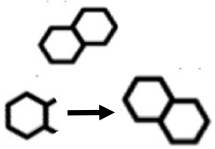
CAS 科学家智力标引

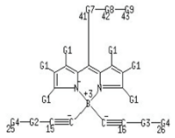


Data pre-repository



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

CAS
A division of the American Chemical Society

CAS 具有最全面的学科连接内容合集

Over
50K
scientific journals and documents

Over
279
million substances

Over
50
languages translated

109
patent offices worldwide

CAS
A division of the American Chemical Society

内容合集

CAS SciFinder Discovery Platform 涵盖的工作流程解决方案

CAS SciFinder^{n}

新一代的权威科学研究工具，是化学及相关学科智能研究平台，提供全球全面、可靠的化学及相关学科研究信息和分析工具

CAS Formulus

专业的配方数据库， 助力配方研究科学家快速评估配方、寻找可替代供应商和探索监管信息

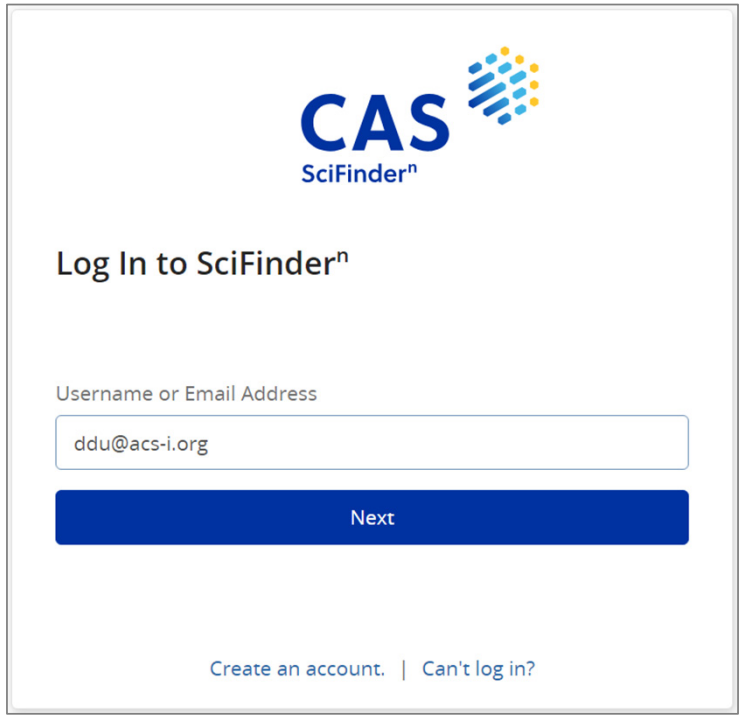
CAS Analytical Methods

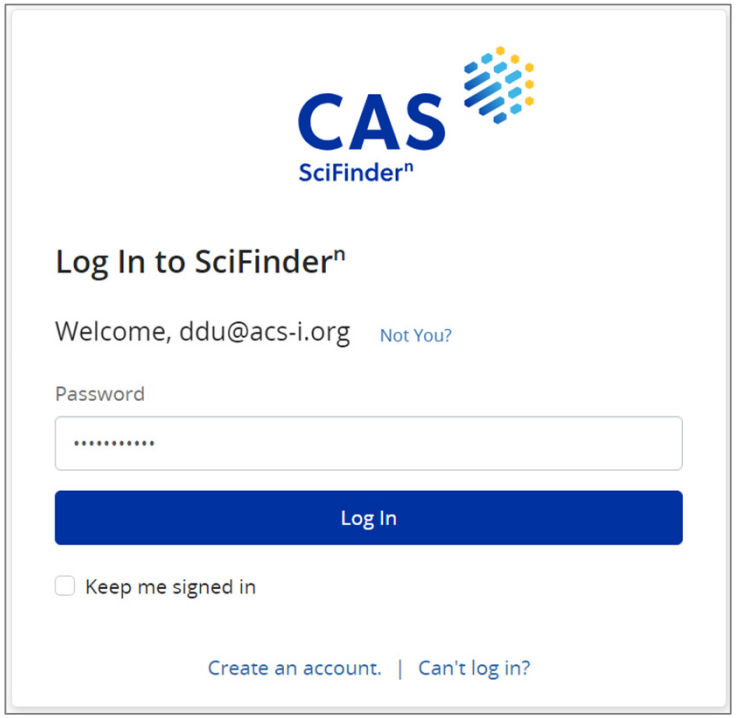
独特的分析方法详情数据库，有助于分析科学家快速获取详尽的分析方法信息、直接用于实验，并启发新方法的建立

CAS
A division of the American Chemical Society

CAS SciFinder^{n} 登录

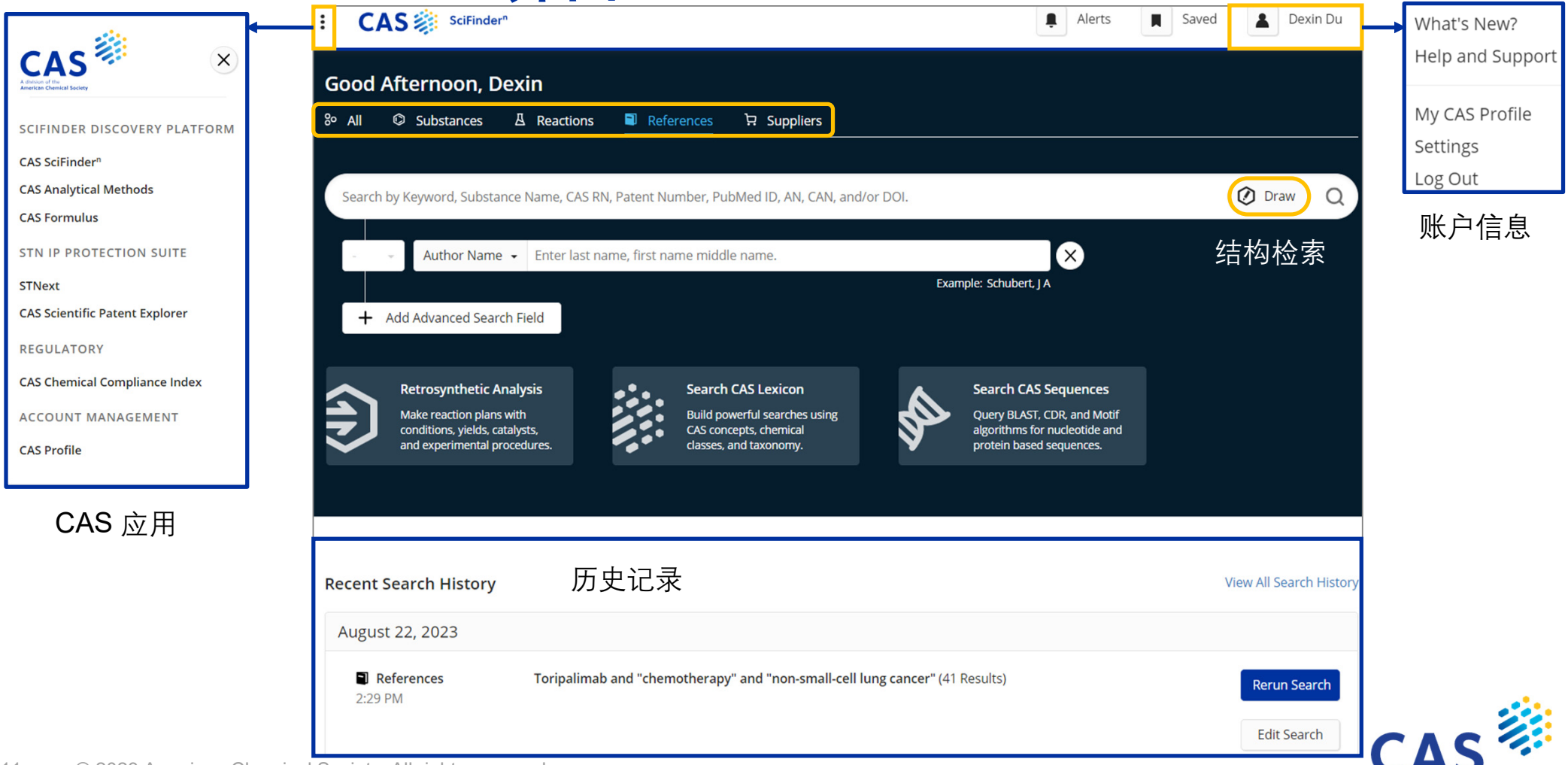
https://scifinder-n.cas.org





CAS
A division of the American Chemical Society

CAS SciFinder^n 主界面



大纲

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

CAS
A division of the American Chemical Society

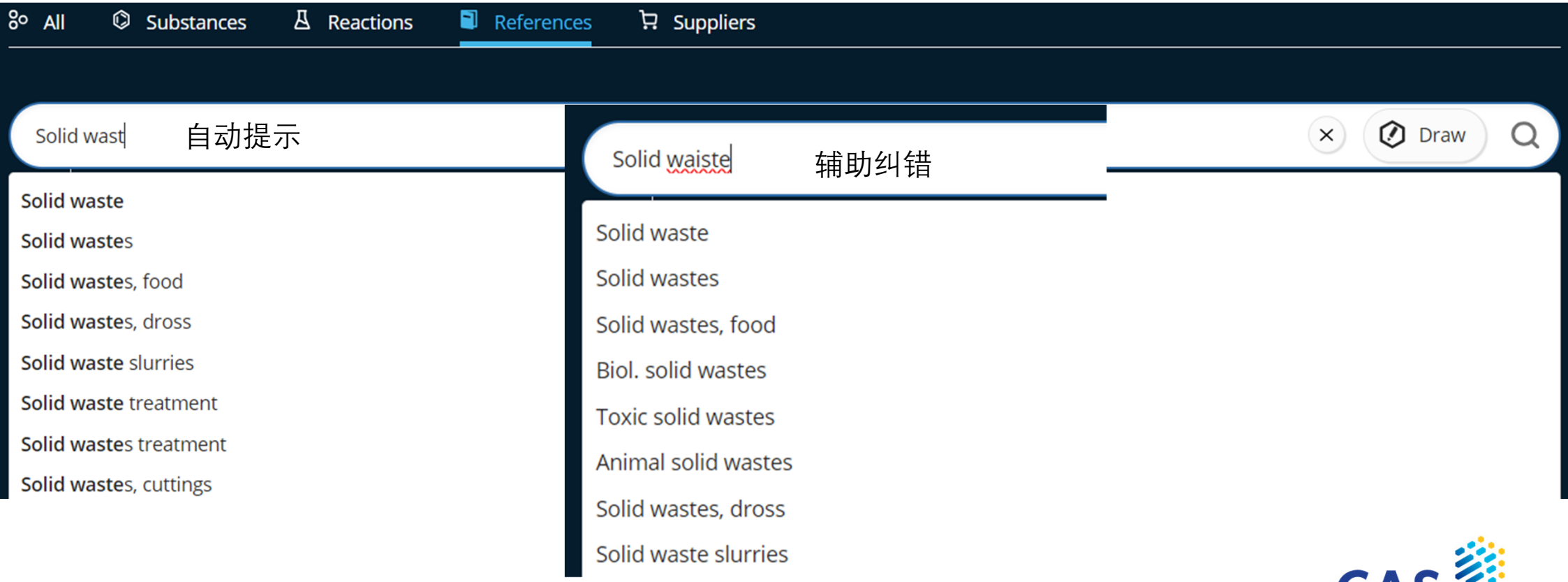
如何拓展文献检索?

- 主题词怎么选择？如何构建?
- 研究某结构相关的文献?
- 如何筛选文献？追踪最新进展?
- 关注某篇文献的被引文献和引文——引文地图

CAS
A division of the American Chemical Society

检索目标课题研究文献

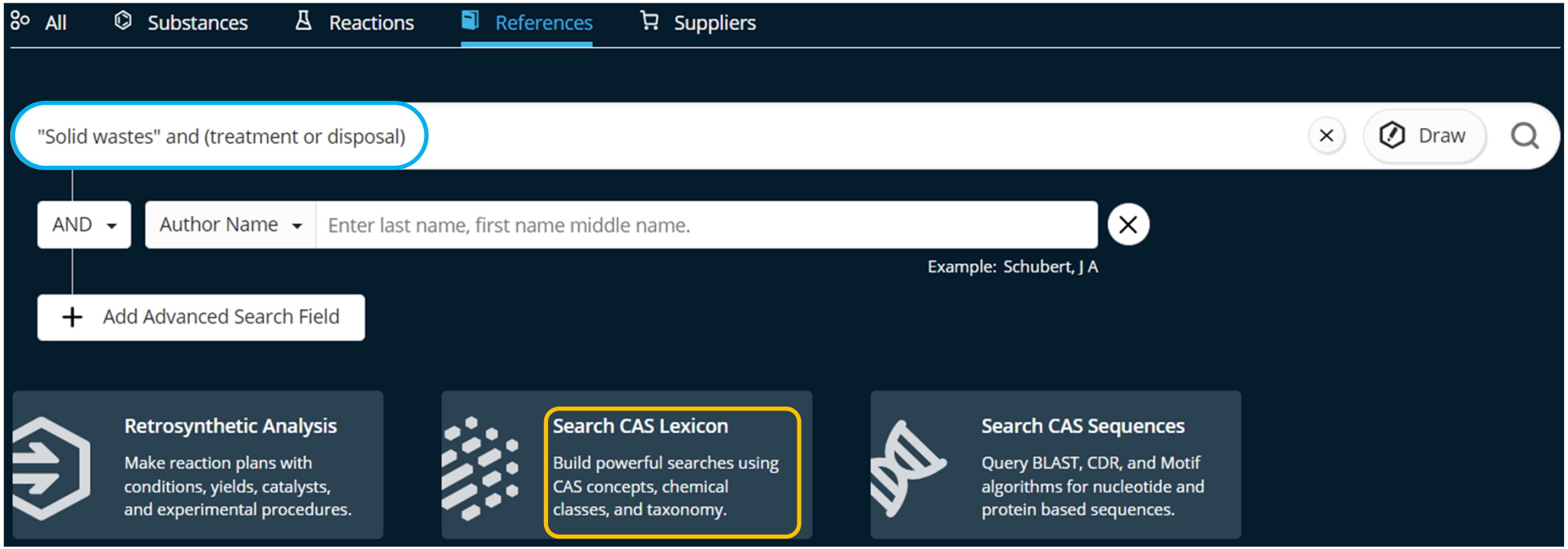
主题词、物质名称、CAS 登记号、专利号、PubMed ID、文献号、DOI 号



CAS
A division of the American Chemical Society

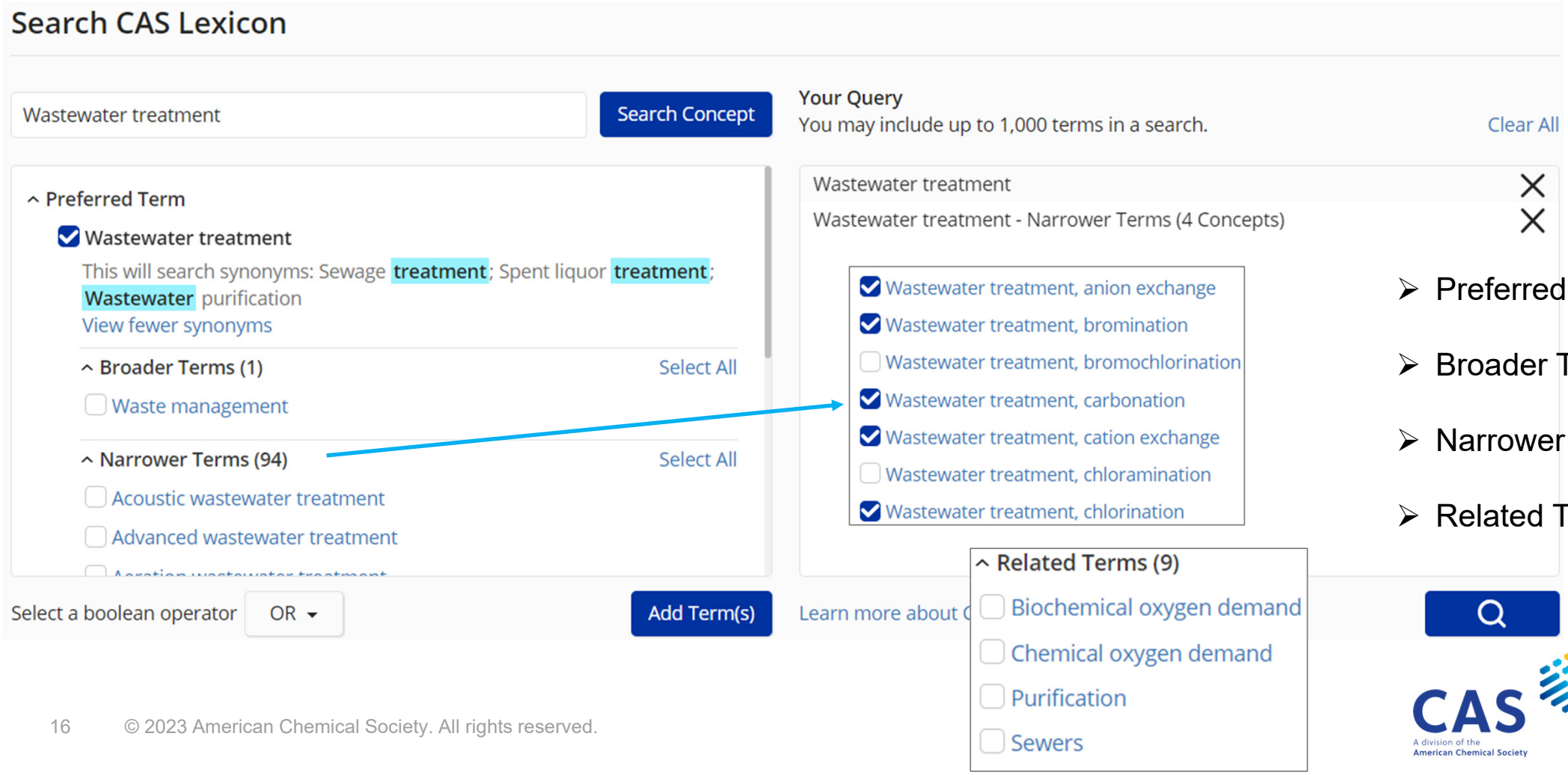
利用布尔逻辑运算符 & 通配符精准检索相关文献

- 支持布尔逻辑运算符 (or/and/not)，默认运算顺序 or > and > not
- “ ” 不允许词形变化，但可出现单数或复数； ( ) 优先运算，括号中表达式还可以和其他术语交互
- 支持通配符 * 或 ?, * 代表 0 或多个字符，？代表 0 或 1 个字符



CAS
A division of the American Chemical Society

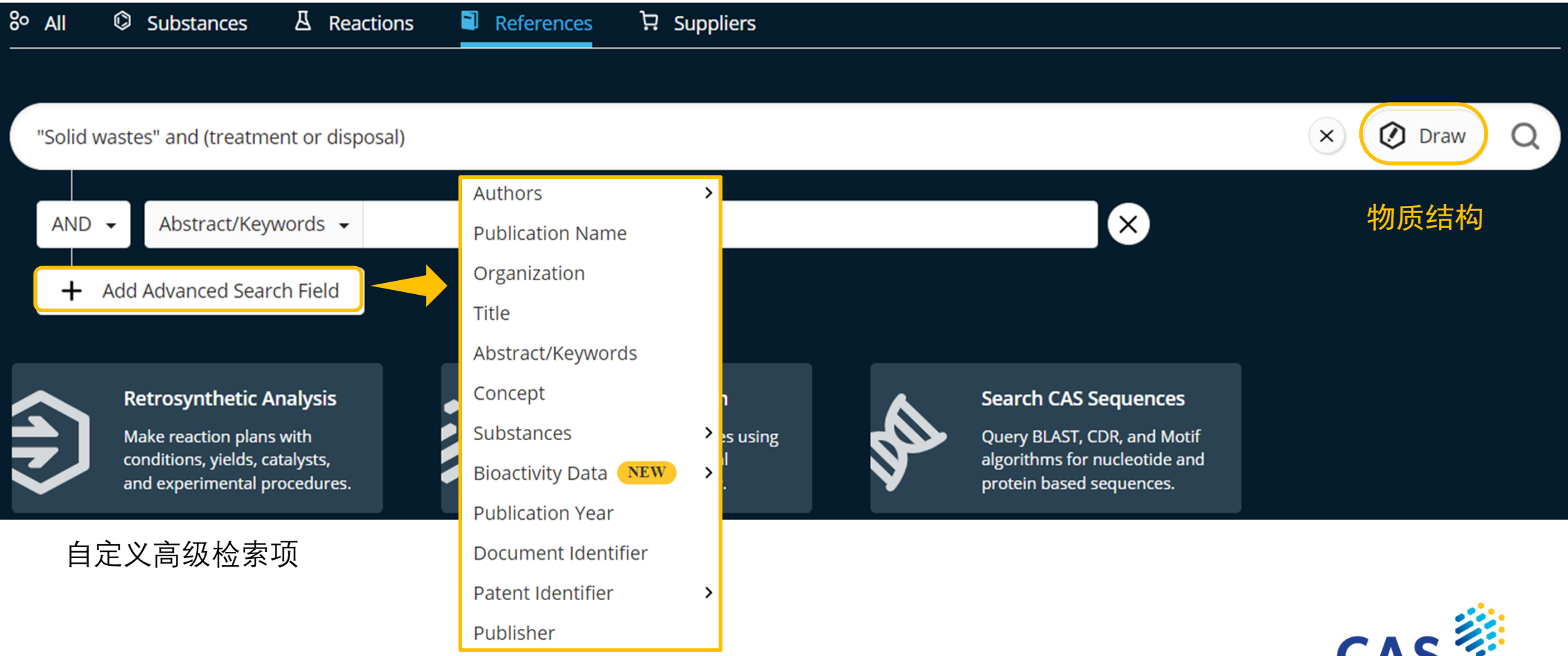
CAS Lexicon 词库检索近义词和相关技术术语



- Preferred Terms
- Broader Terms
- Narrower Terms
- Related Terms

CAS
A division of the American Chemical Society

根据作者/出版物/研究机构/物质结构检索相关文献



自定义高级检索项

CAS
A division of the American Chemical Society

物质结构与关键词联合检索文献

文本与物质结构检索是 “and” 关系

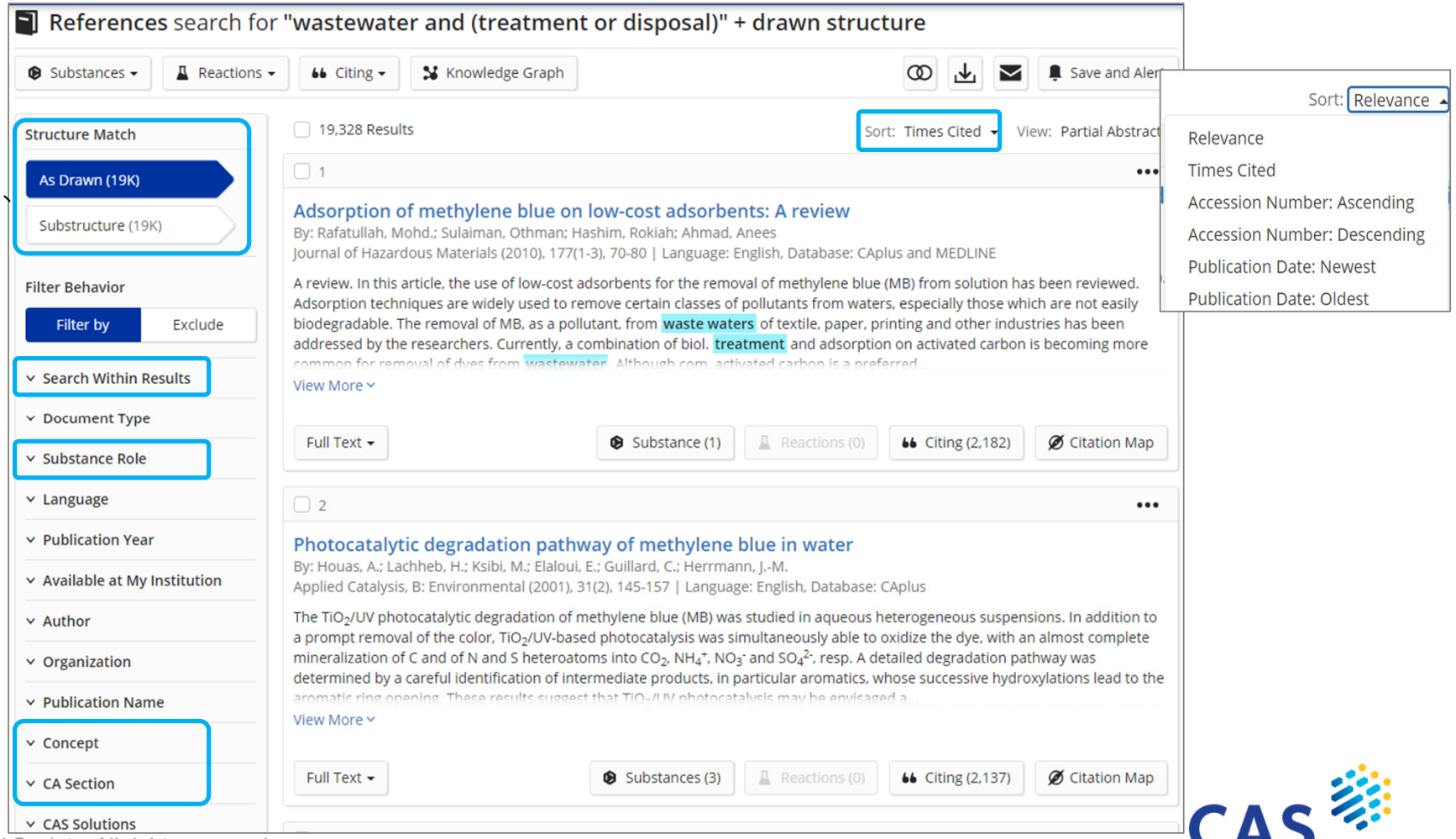
检索结果分析与筛选

- As Drawn 精确结构

  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

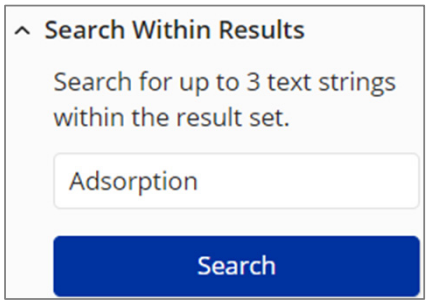
- Substructure 亚结构

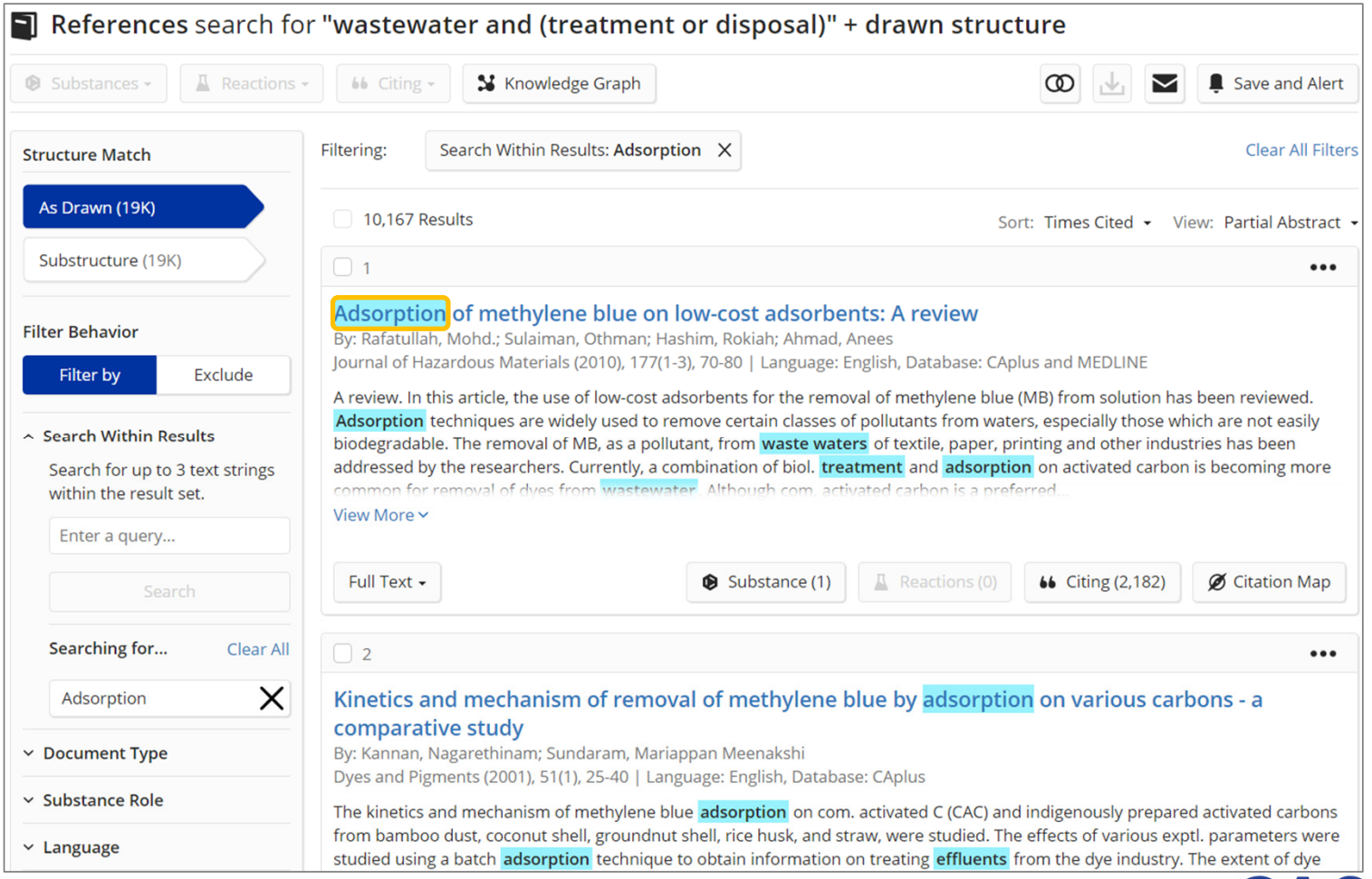
  包括 As Drawn 检索结果，价态未达饱和的原子可以连接氢以外的其他原子；如果有环系，可形成其他环



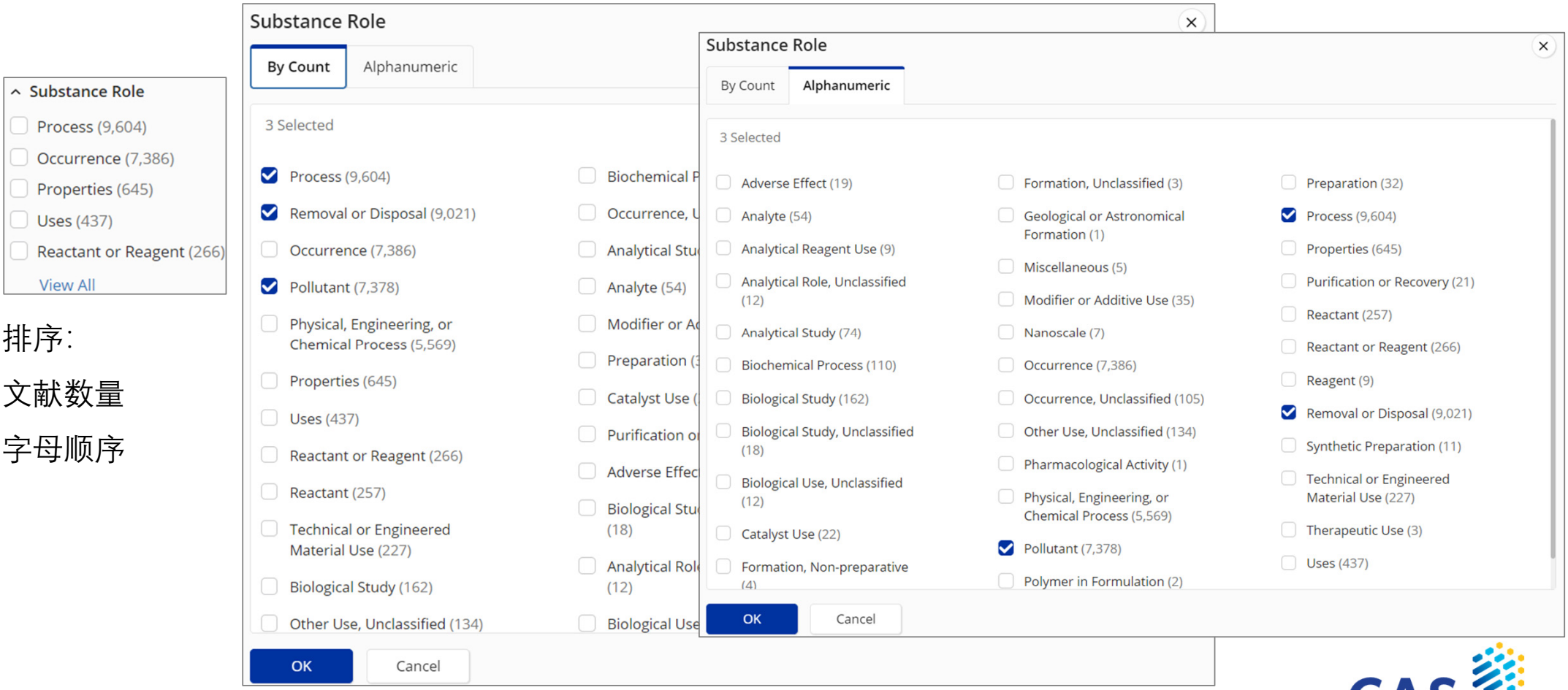
CAS
A division of the American Chemical Society

结果集二次检索研究内容：Search Within Results





物质角色筛选文献：Substance Role



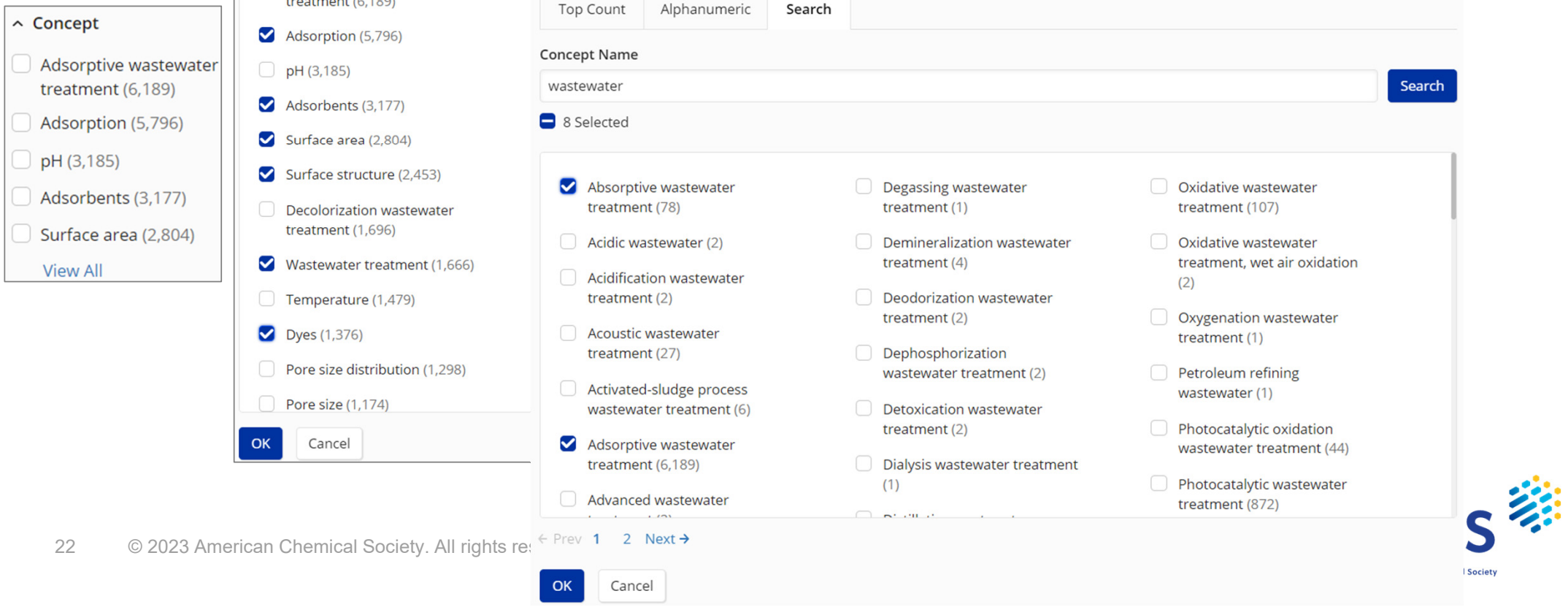
排序：

文献数量

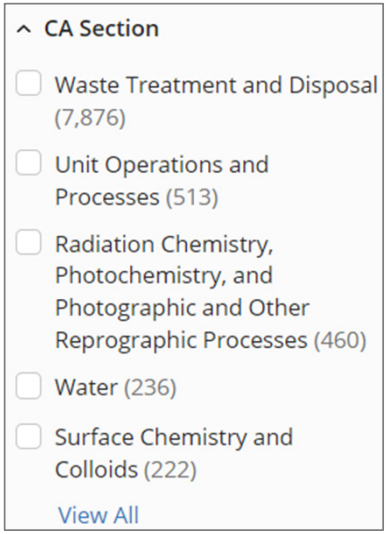
字母顺序

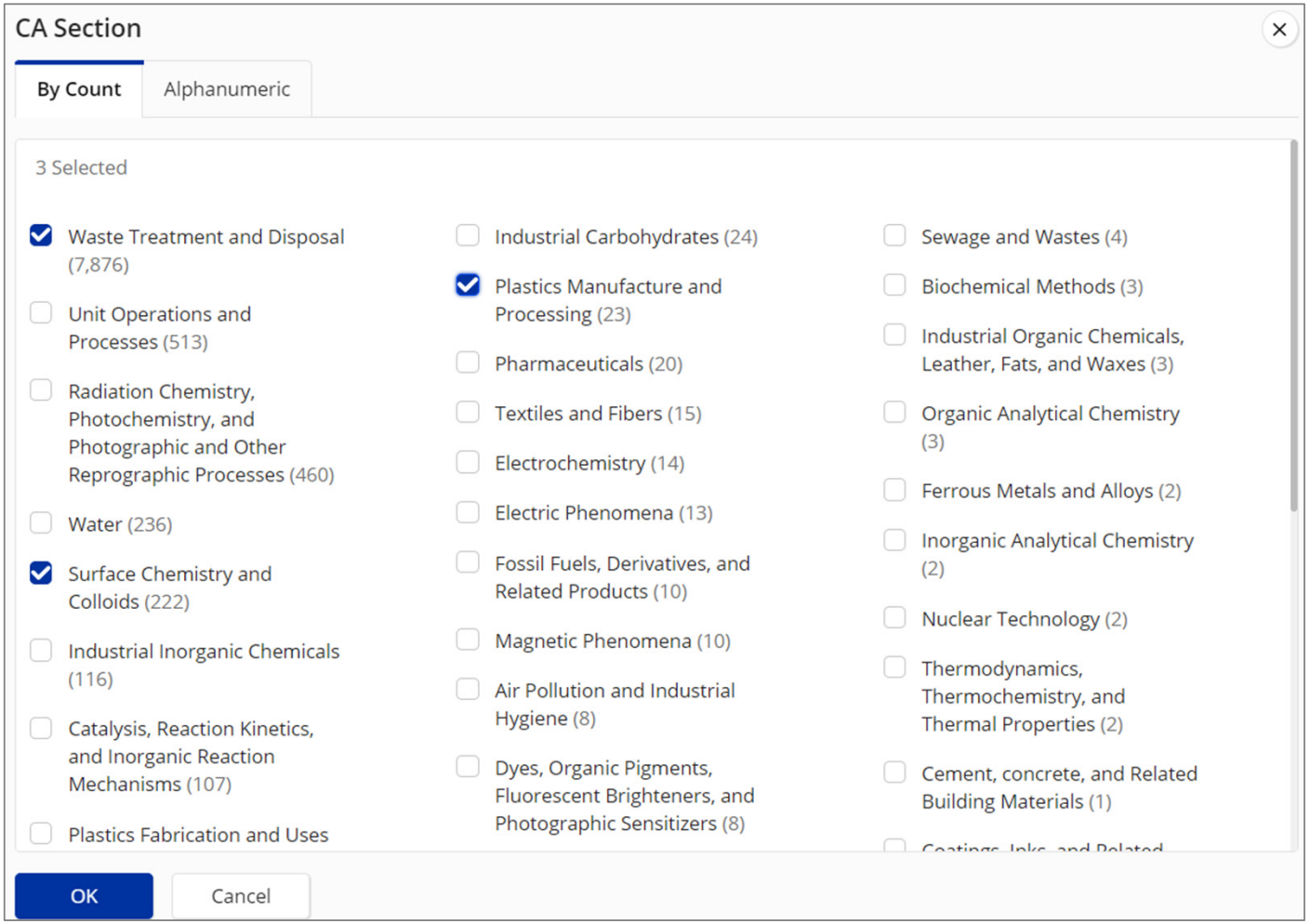
CAS
A division of the American Chemical Society

确定文献核心研究内容：Concept



筛选不同研究领域文献：CA Section

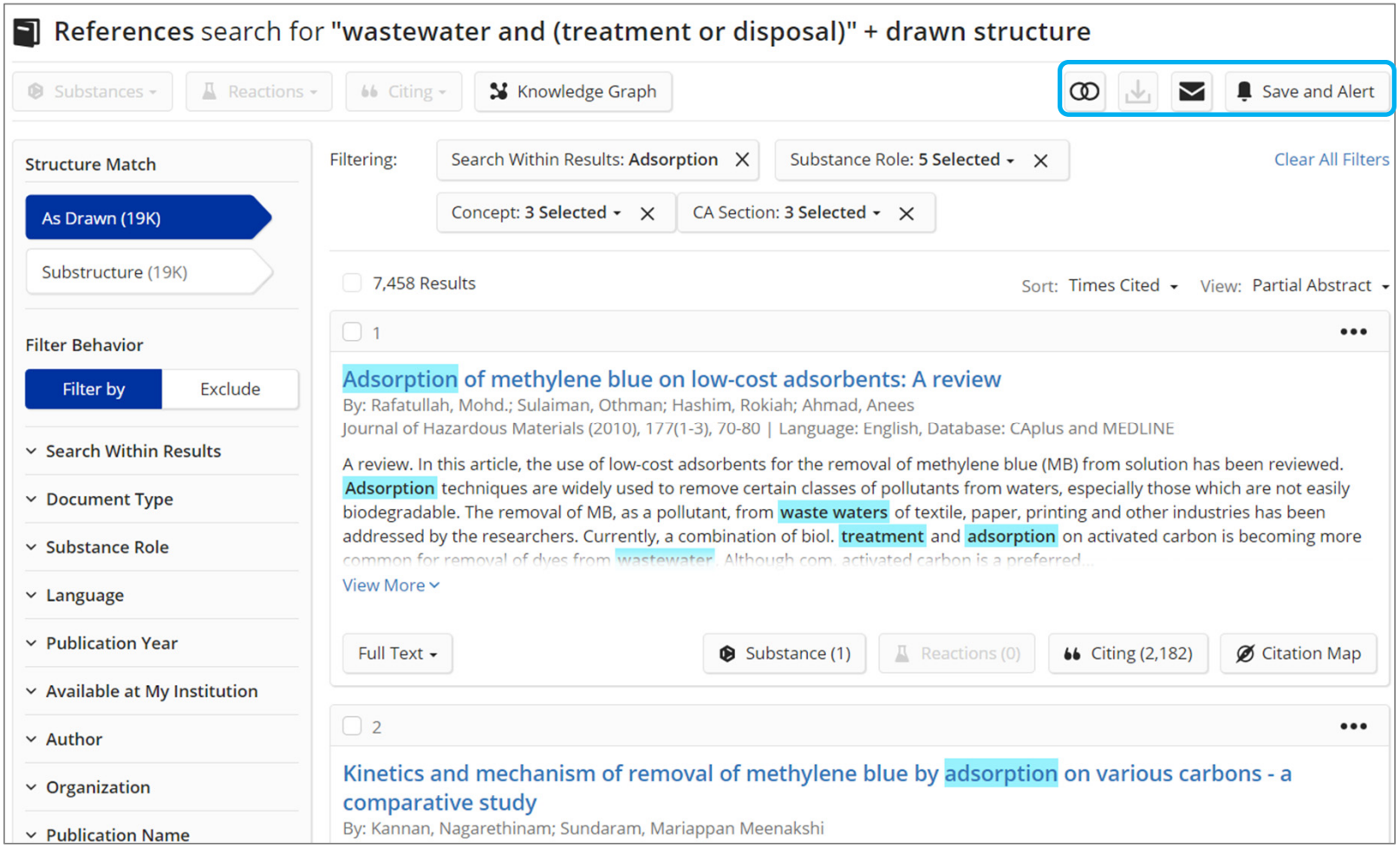




CAS
A division of the American Chemical Society

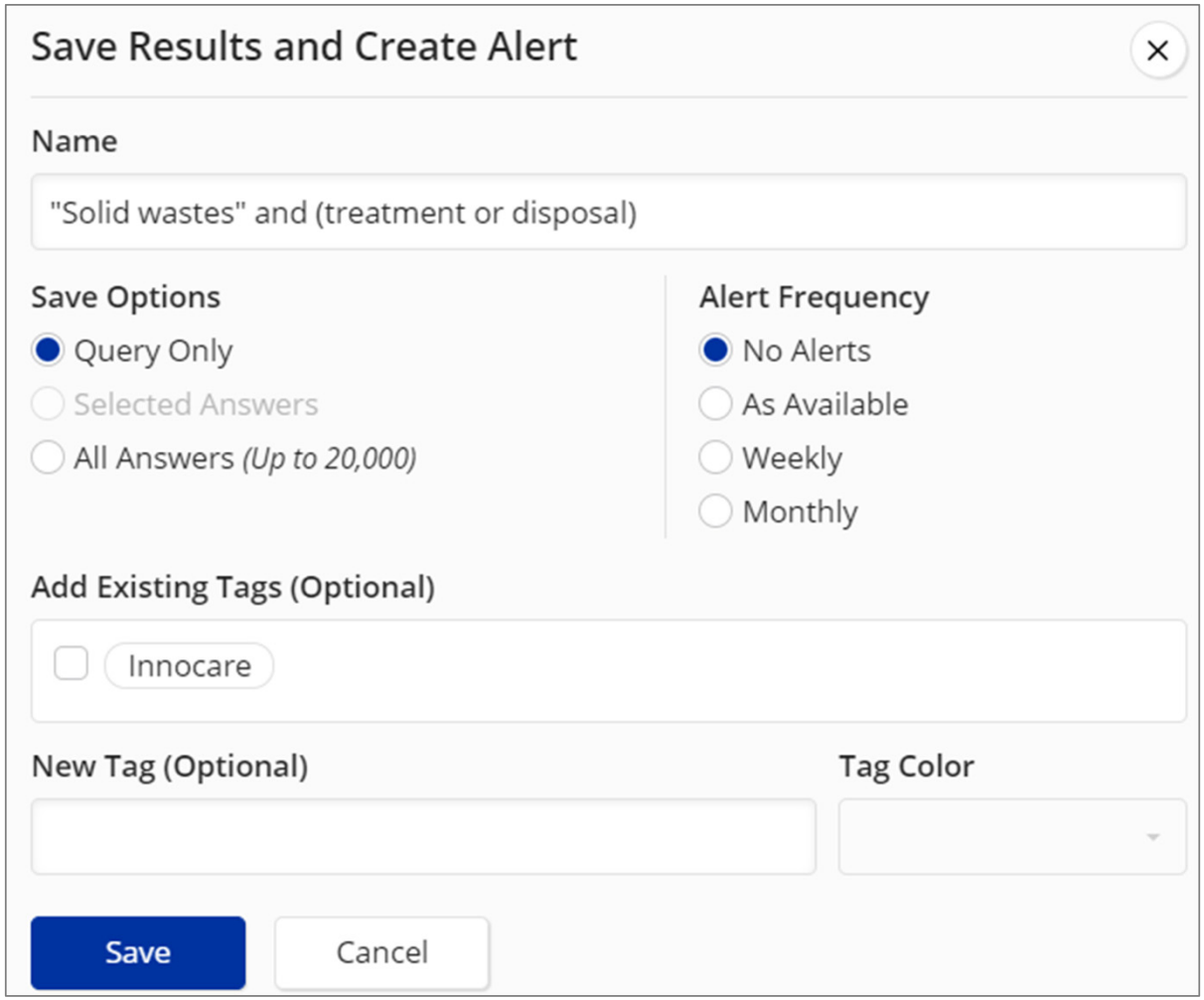
文献结果集管理

合并、下载、分享和保存



CAS
A division of the American Chemical Society

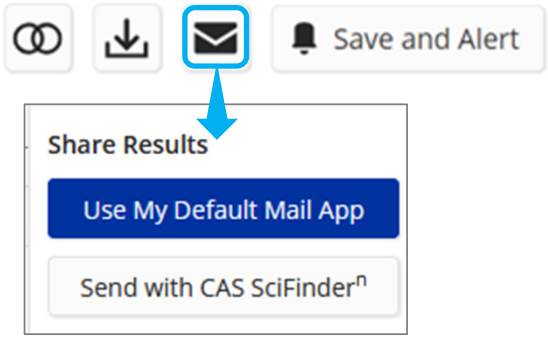
保存和提醒

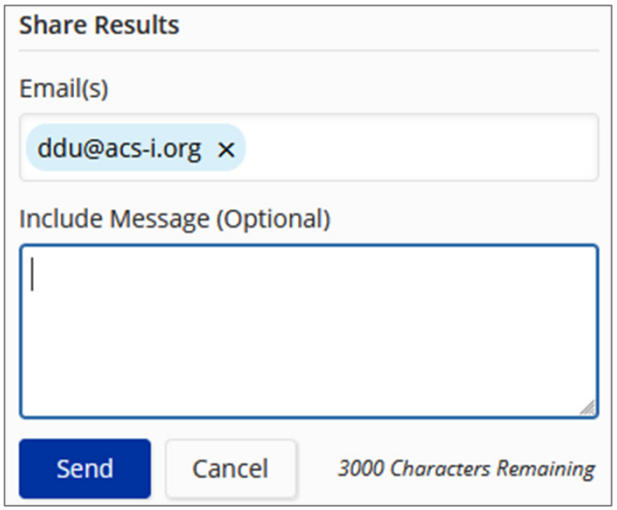


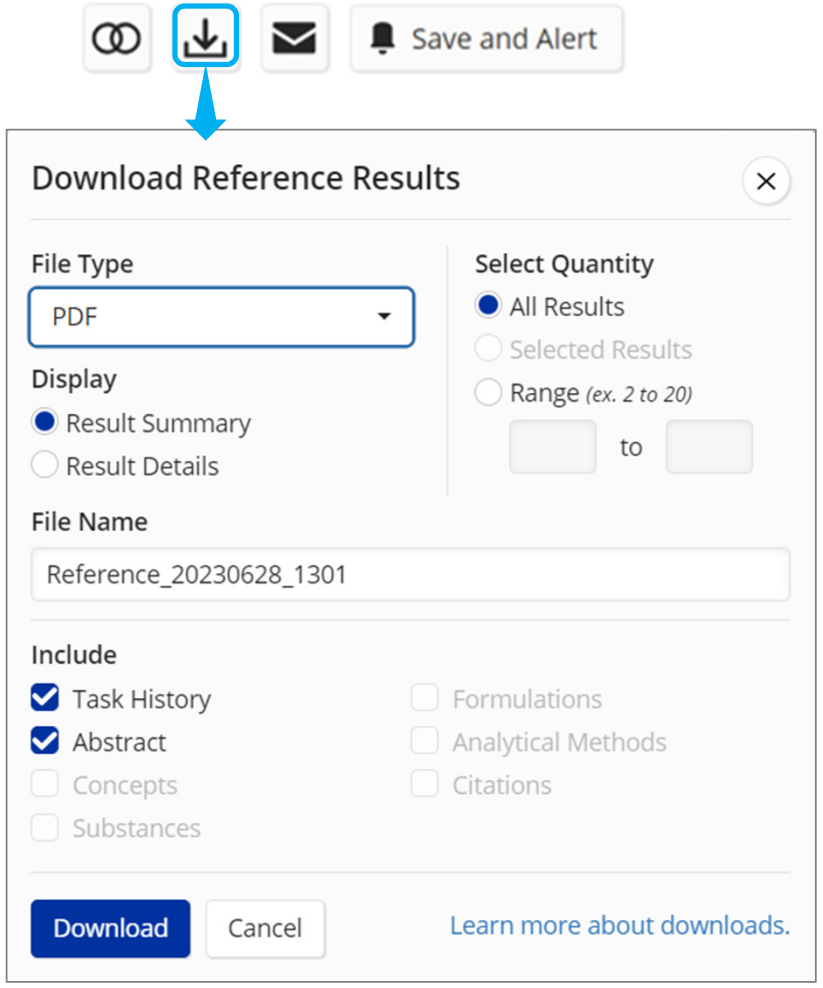
- 结果保存
- 自定义提醒频率
- 标签分类

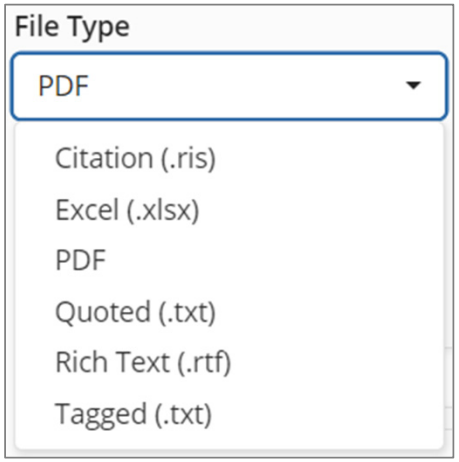
CAS
A division of the American Chemical Society

下载和分享



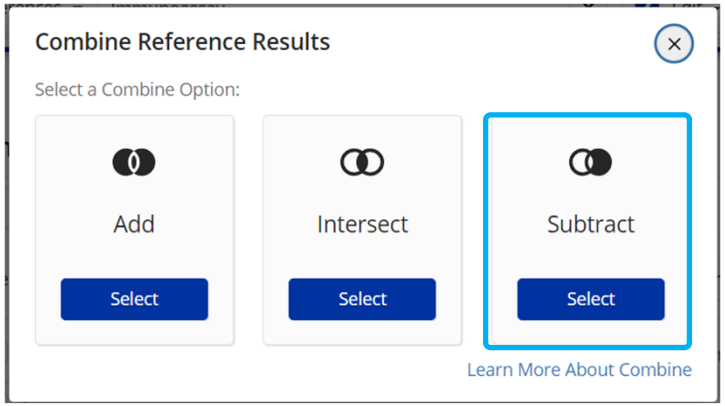




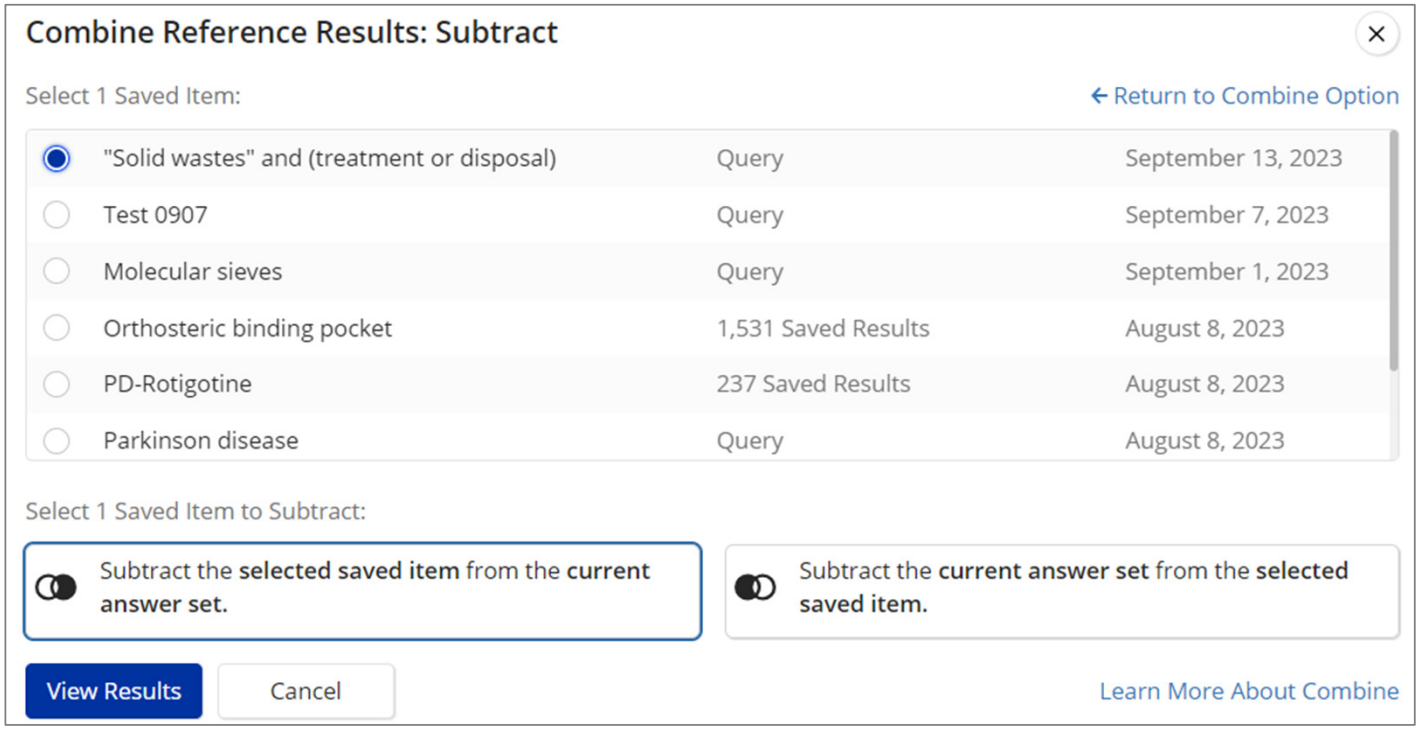


CAS
A division of the American Chemical Society

合并

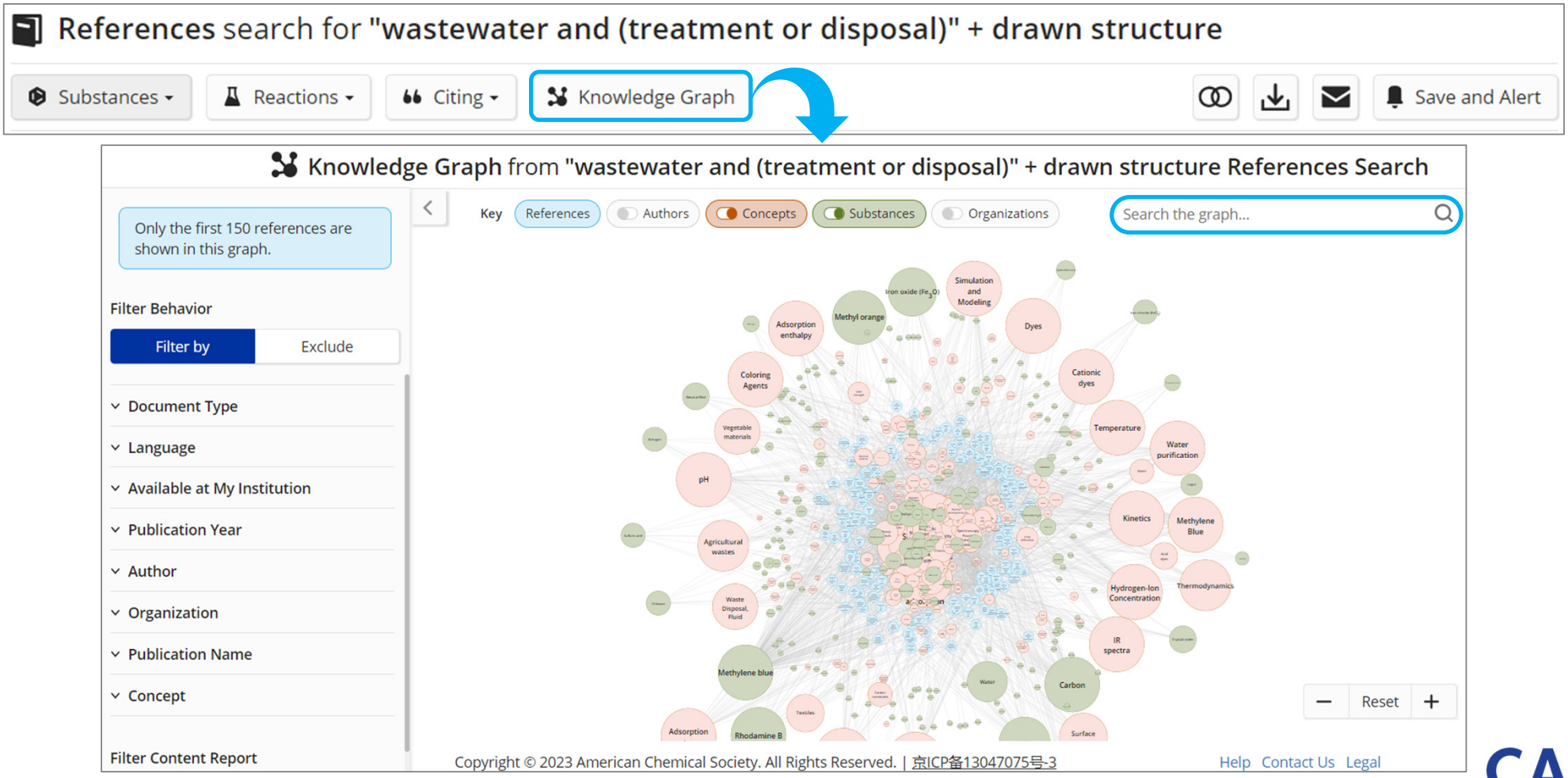


- 并集
- 交集
- 差集



CAS
A division of the American Chemical Society

绘制知识谱图：Knowledge Graph



CAS
A division of the American Chemical Society

查看目标文献详情

Use of cellulose-based wastes for adsorption of dyes from aqueous solutions

Substances (7) | Reactions (0) | Citing (1,175) | Citation Map | Save

JOURNAL

Source
Journal of Hazardous Materials
Volume: 92
Issue: 3
Pages: 263-274
Journal; Article; Research Support, Non-U.S. Gov't
2002
DOI: 10.1016/s0304-3894(02)00017-1

CODEN: JHMAD9
ISSN: 0304-3894
ISSN-L: 0304-3894

Database Information
AN: 2002:372829
CAN: 137:205692
PubMed ID: 12031611
CAplus and MEDLINE

Company/Organization
Department of Chemical Engineering
National Taiwan University
Taipei 106
Taiwan

By: Annadurai, Gurusamy; Juang, Ruey-Shin; Lee, Duu-Jong

Low-cost banana and orange peels were prepared as adsorbents for the adsorption of dyes from aqueous solutions Dye concentration and pH were varied. The adsorption capacities for both peels decreased in the order methyl orange > methylene blue > Rhodamine B > Congo Red > methyl violet > Amido Black 10B. The isotherm data could be well described by the Freundlich and Langmuir equations at concentrations 10-120 mg/L. An alk. pH was favorable for the adsorption of dyes. Based on the adsorption capacity, it was shown that banana peel was more effective than orange peel. Kinetic parameters of adsorption such as the Langergren rate constant and the intraparticle diffusion rate constant were determined For the present adsorption process intraparticle diffusion of dyes within the particle was identified to be rate limiting. Both peel wastes were promising materials for adsorption of dyes from aqueous solutions

Keywords: cellulose waste adsorption dye wastewater

View Source | Full Text

Similar References NEW | Get Similar References

- Adsorption of dyes from aqueous solution by chromium-containing leather waste
  Zhongguo Pige (2004), 33(13), 10-13 | Language: Chinese, Database: CAplus
- Adsorptive removal of Methylene blue dye from an aqueous solution using wter hyacinth root powder as a low cost adsorbent
  International Journal of Chemical Sciences and Applications (2012), 3(3), 338-345 | Language: English, Database: CAplus
- Equillibrium modelling of adsorptive removal of methylene blue using BGA
  Oriental Journal of Chemistry (2012), 28(1), 519-524 | Language: English, Database: CAplus

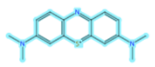
Expand All | Collapse All

Concepts — CAS 科学家提供的核心研究点

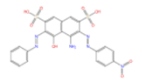
- Adsorption
- Adsorptive wastewater treatment
- Citrus sinensis
  Modifier: peel of
- Decolorization wastewater treatment
- Dyes
- Musa
  Modifier: peel of
- Orange
  Modifier: peel of

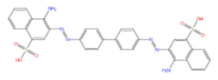
Substances — 重点研究物质

Substances (7)

61-73-4

• Cl⁻
$C_{16}H_{18}N_3S.Cl$
Phenothiazin-5-ium, 3,7-bis(dimethylamino)-, chloride (1:1)
Role: Removal or Disposal, Process

9004-34-6
Image Not Available
Unspecified
Cellulose
Role: Unspecified

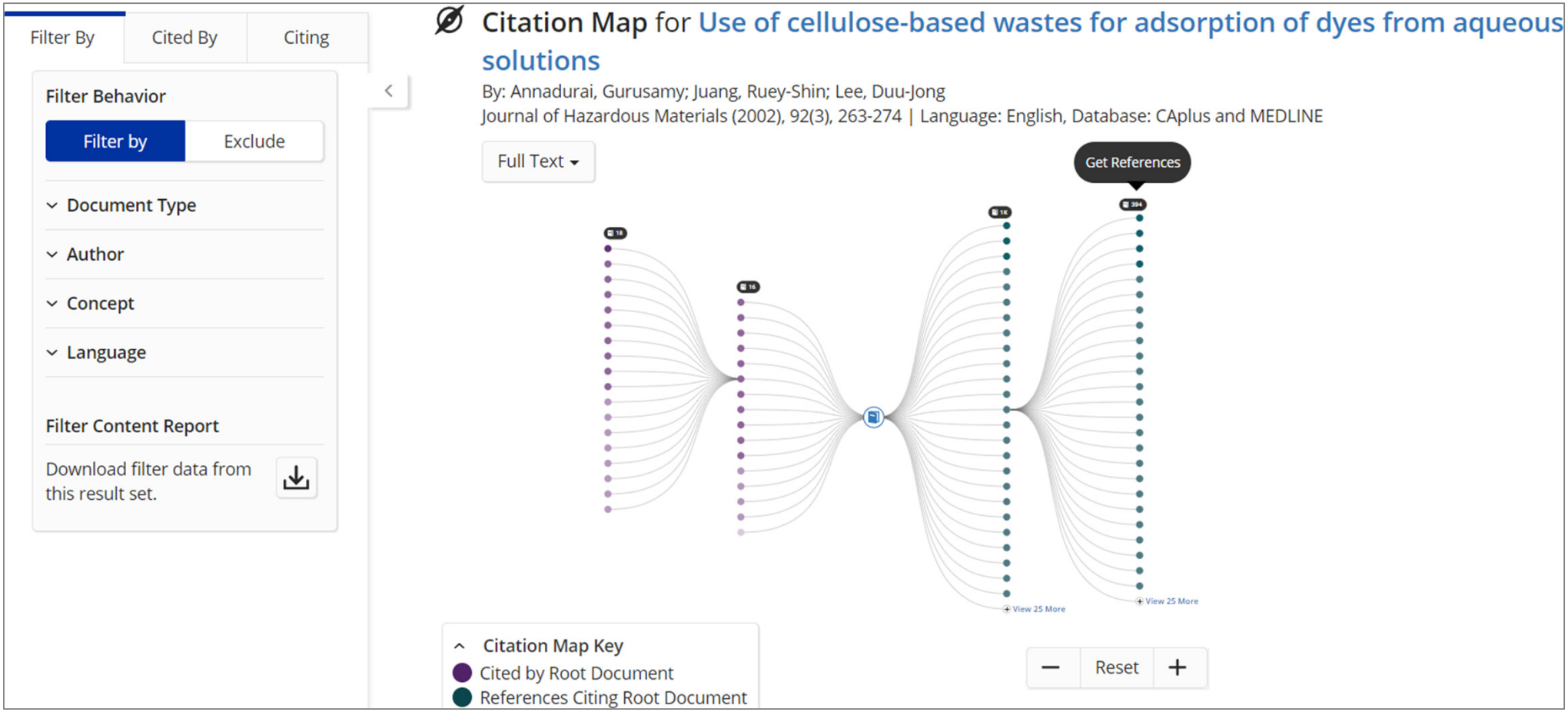
1064-48-8

• 2 Na
$C_{22}H_{16}N_6O_9S_2.2Na$
2,7-Naphthalenedisulfonic acid, 4-amino-5-hydroxy-3-[2-(4-nitrophenyl)diazenyl]-...
Role: Removal or Disposal, Process

573-58-0

• 2 Na
$C_{32}H_{24}N_6O_6S_2.2Na$
1-Naphthalenesulfonic acid, 3,3'-[[1,1'-biphenyl]-4,4'-diylbis(2,1-diazenediyl)]...
Role: Removal or Disposal, Process

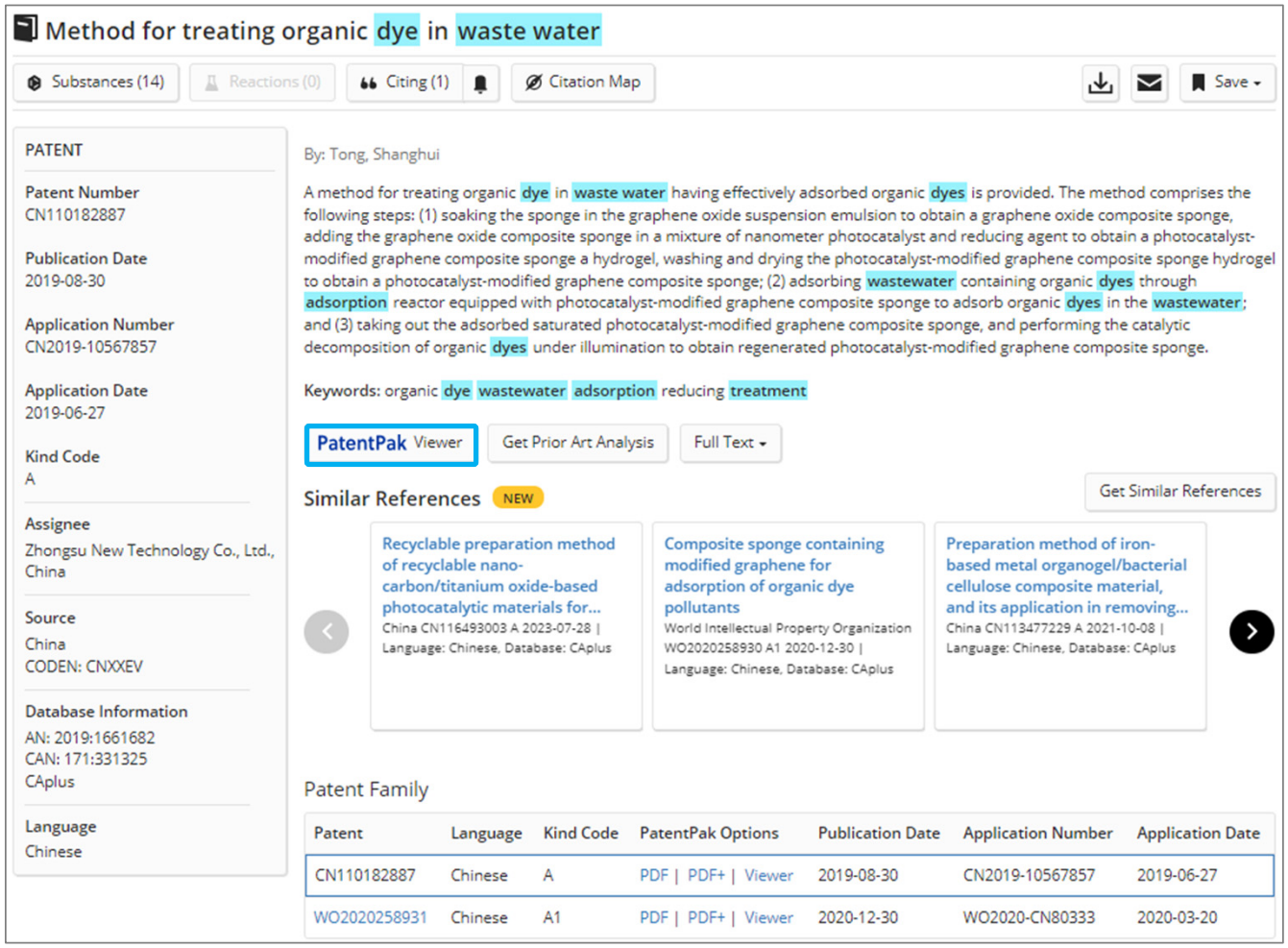
物质角色

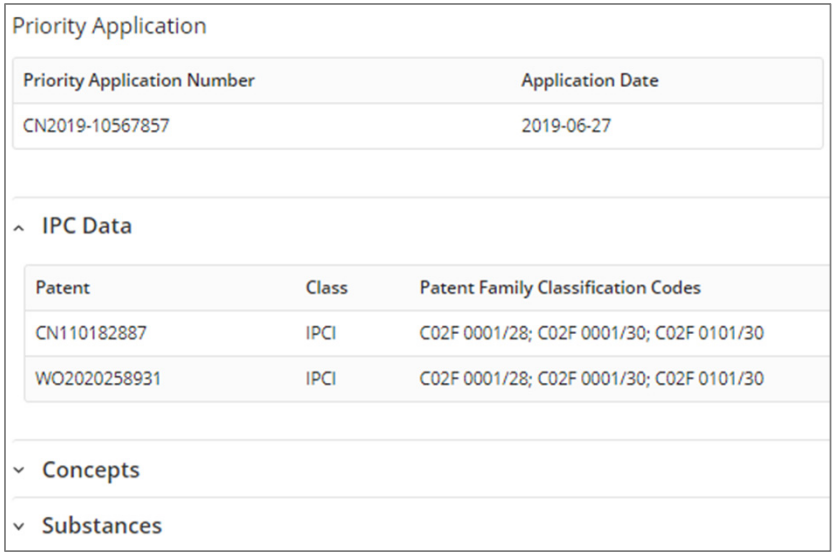
CAS
A division of the American Chemical Society

绘制引文地图：Citation Map



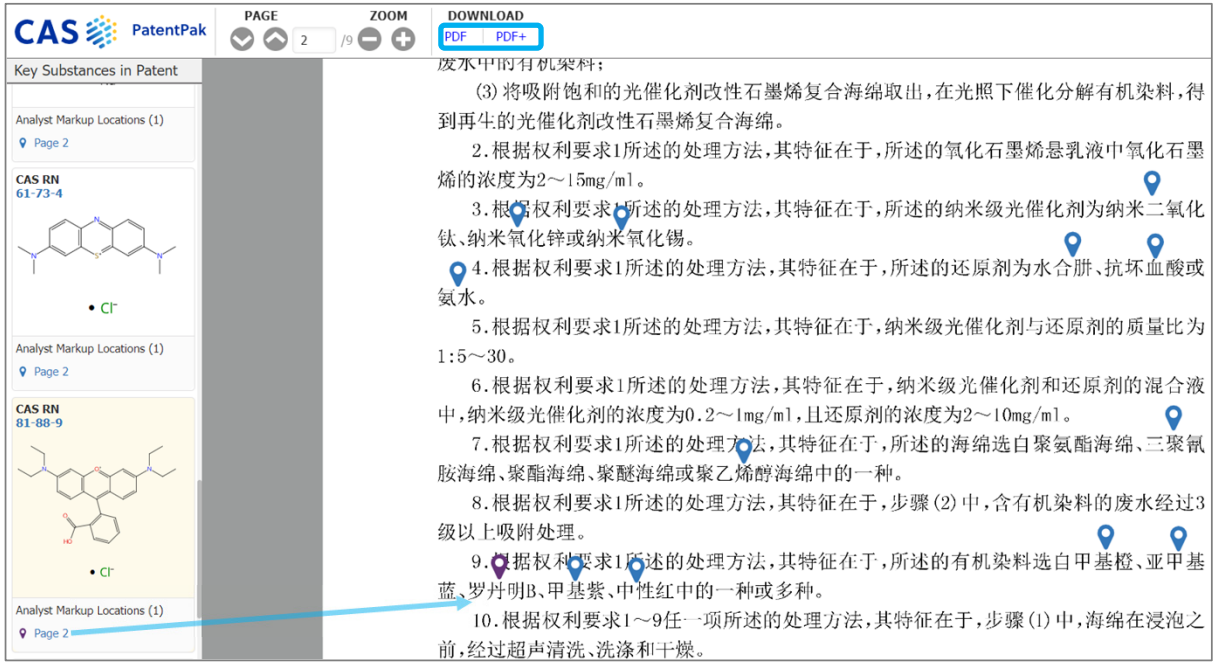
查看专利详情





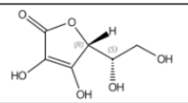
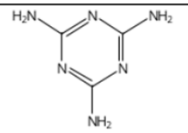
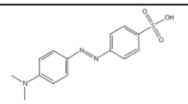
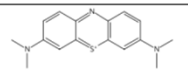
CAS
A division of the American Chemical Society

PatentPak Viewer 高效阅读专利



精准定位

Key Substances in Patent

Mark	Page #	CAS RN	Name	Structure
2	p.2	1034343-98-0D	Graphene oxide	
4	p.2	1034343-98-0	Graphene	
5	p.2	13463-67-7	Titanium oxide (TiO_2)	O═Ti═O
6	p.2	1314-13-2	Zinc oxide (ZnO)	Zn═O
7	p.2	1332-29-2	Tin oxide	
8	p.2	302-01-2	Hydrazine	$H_2N—NH_2$
9	p.2	50-81-7	L-Ascorbic acid	
10	p.2	1336-21-6	Ammonium hydroxide ($(NH_4)(OH)$)	$H_4N—OH$
12	p.2	108-78-1	1,3,5-Triazine-2,4,6-triamine	
15	p.2	9002-89-5	Ethenol, homopolymer	
16	p.2	547-58-0	Benzenesulfonic acid, 4-[2-[4-(dimethylamino)phenyl]diazenyl]-, sodium salt (1:1)	
17	p.2	61-73-4	Phenothiazin-5-ium, 3,7-bis(dimethylamino)-, chloride (1:1)	

CAS 科学家增值标引的信息

CAS
A division of the American Chemical Society

小结

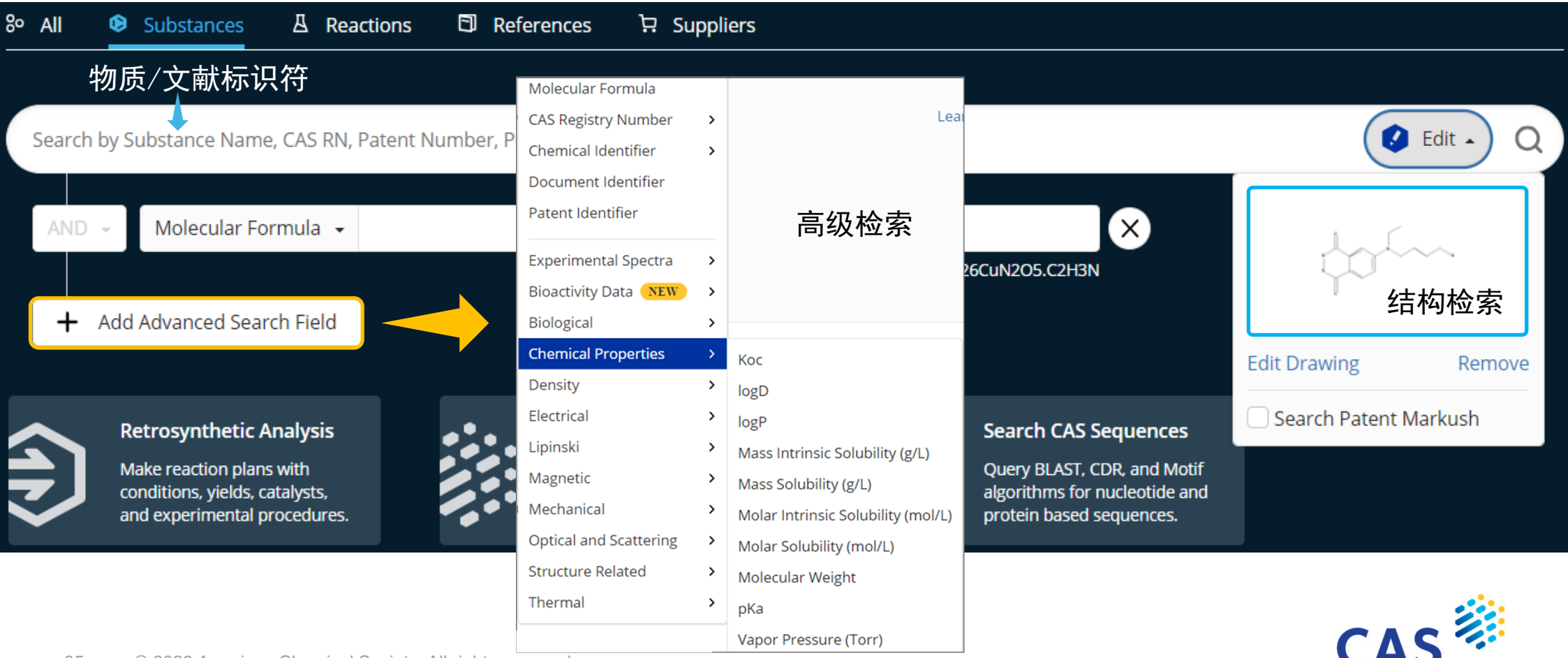
1. 检索词的构建：使用布尔逻辑算符及通配符连接主题词，CAS Lexicon 丰富选词
2. 利用高级检索选项以及文本与结构联合进行自定义组合检索
3. 通过聚类筛选工具快速获得目标文献
4. 利用引文地图拓展检索
5. 使用 PatentPak 高效阅读专利

如何调研某类物质?

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

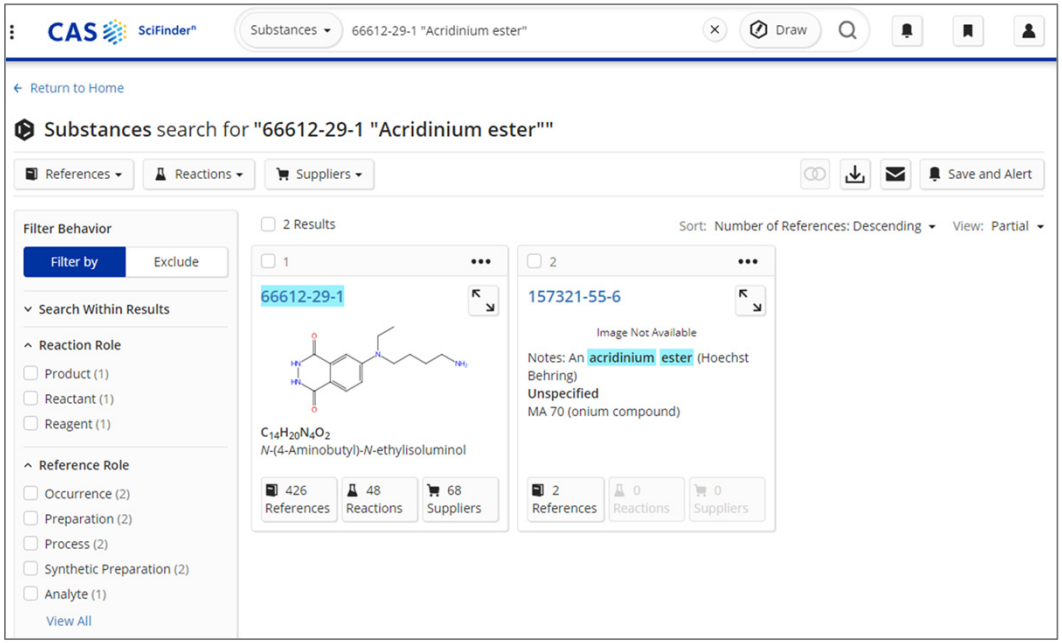
CAS
A division of the
American Chemical Society

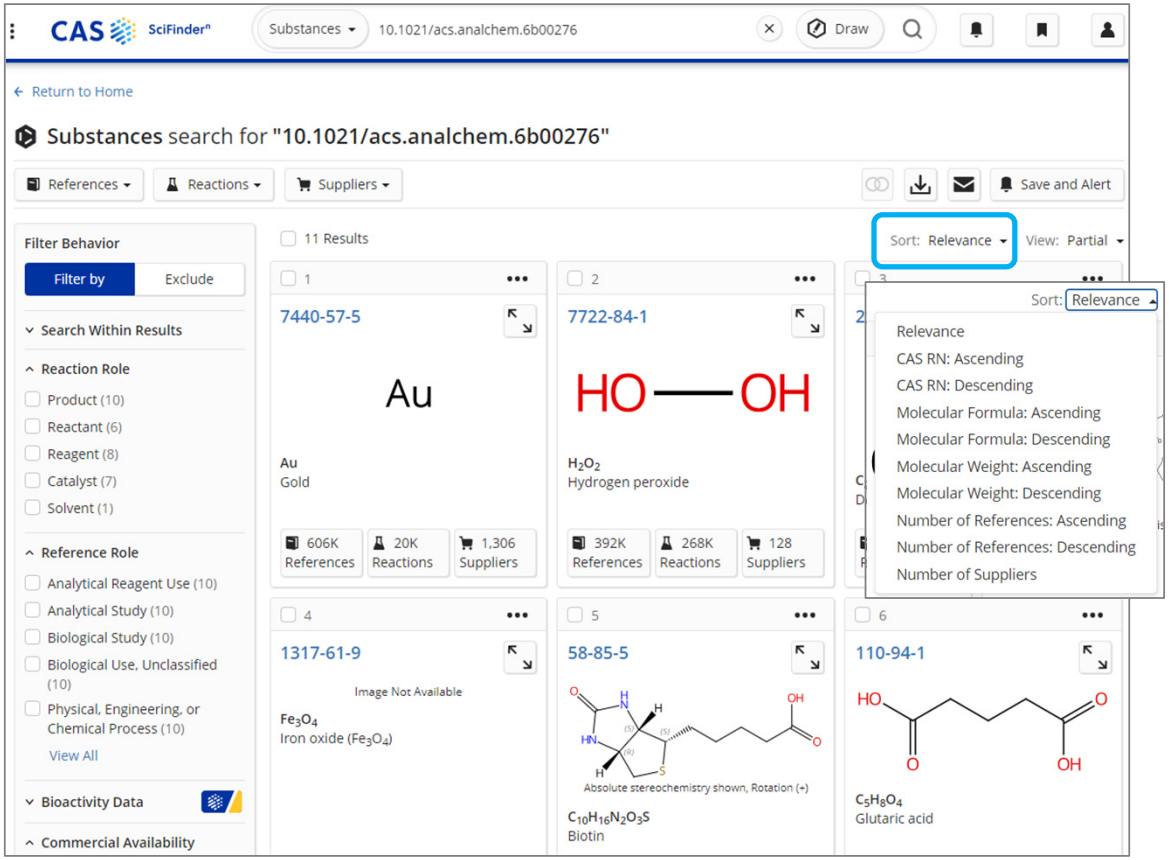
检索研究所需物质



CAS
A division of the American Chemical Society

物质/文献标识符检索与结果集排序





- 可同时检索多个物质识别符（物质名称或 CAS 登记号）
- 双引号“ ”可精确识别物质识别符
- 不同物质用空格隔开，支持 **2000** 个字符

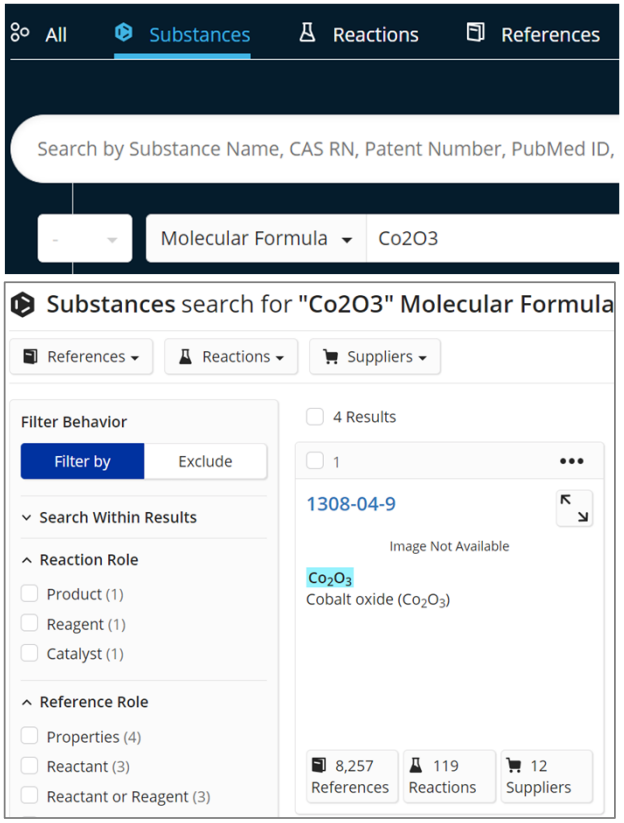
CAS
A division of the American Chemical Society

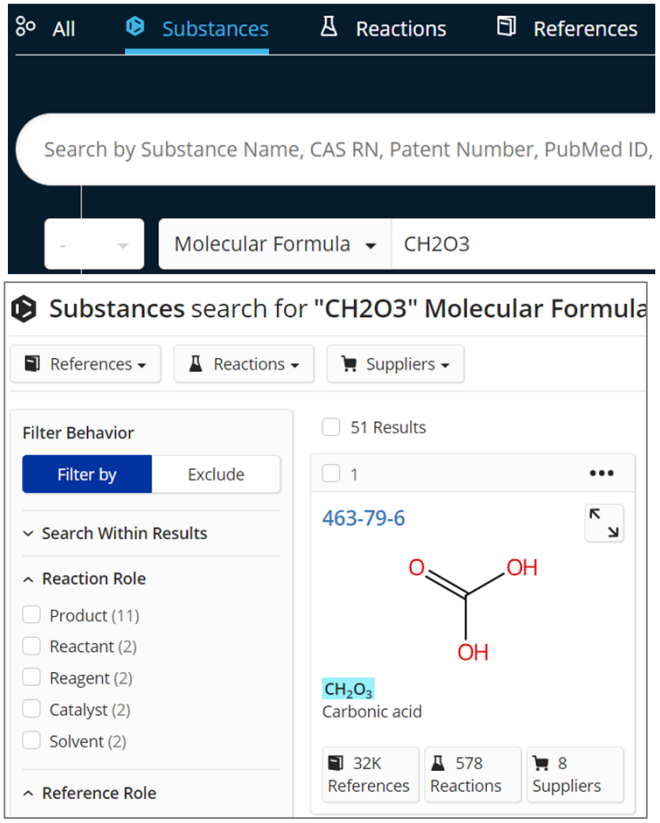
分子式检索物质

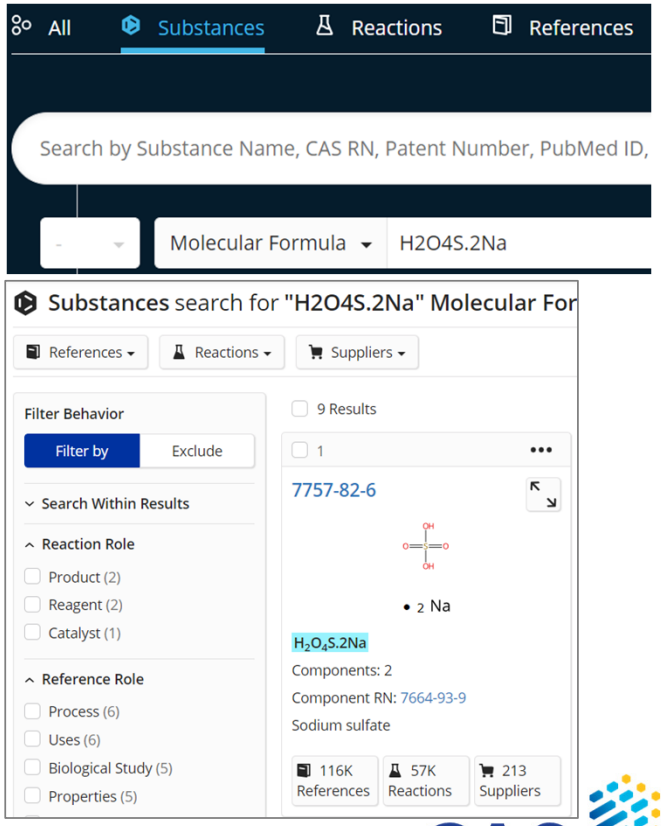
不含碳元素，按元素符号首字母顺序书写

含碳元素，碳排第一位，氢排第二位，其他元素符号按首字母顺序书写

金属离子和阴离子间用点·隔开，补充和阳离子等同个数的氢原子



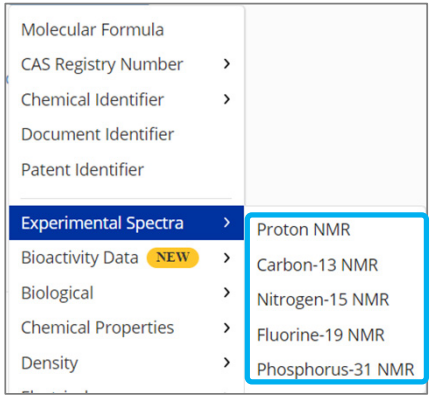


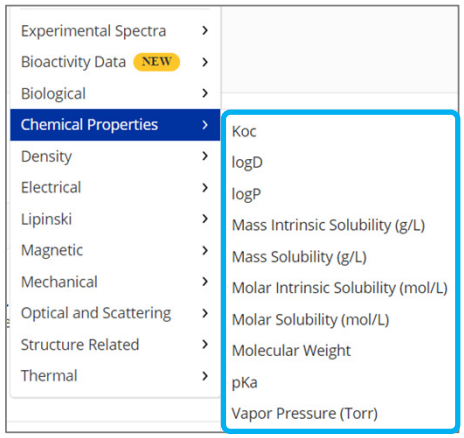


适合聚合物或无机化合物

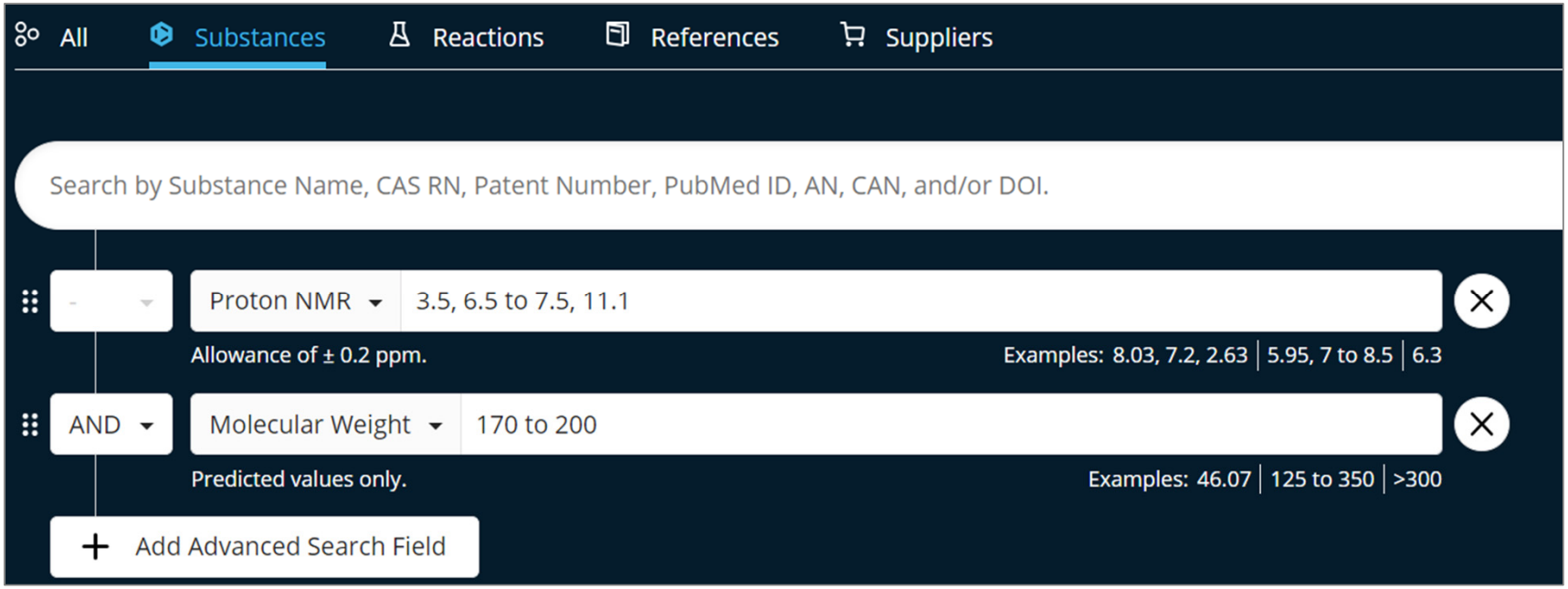
CAS
A division of the American Chemical Society

谱图和分子量联合检索物质



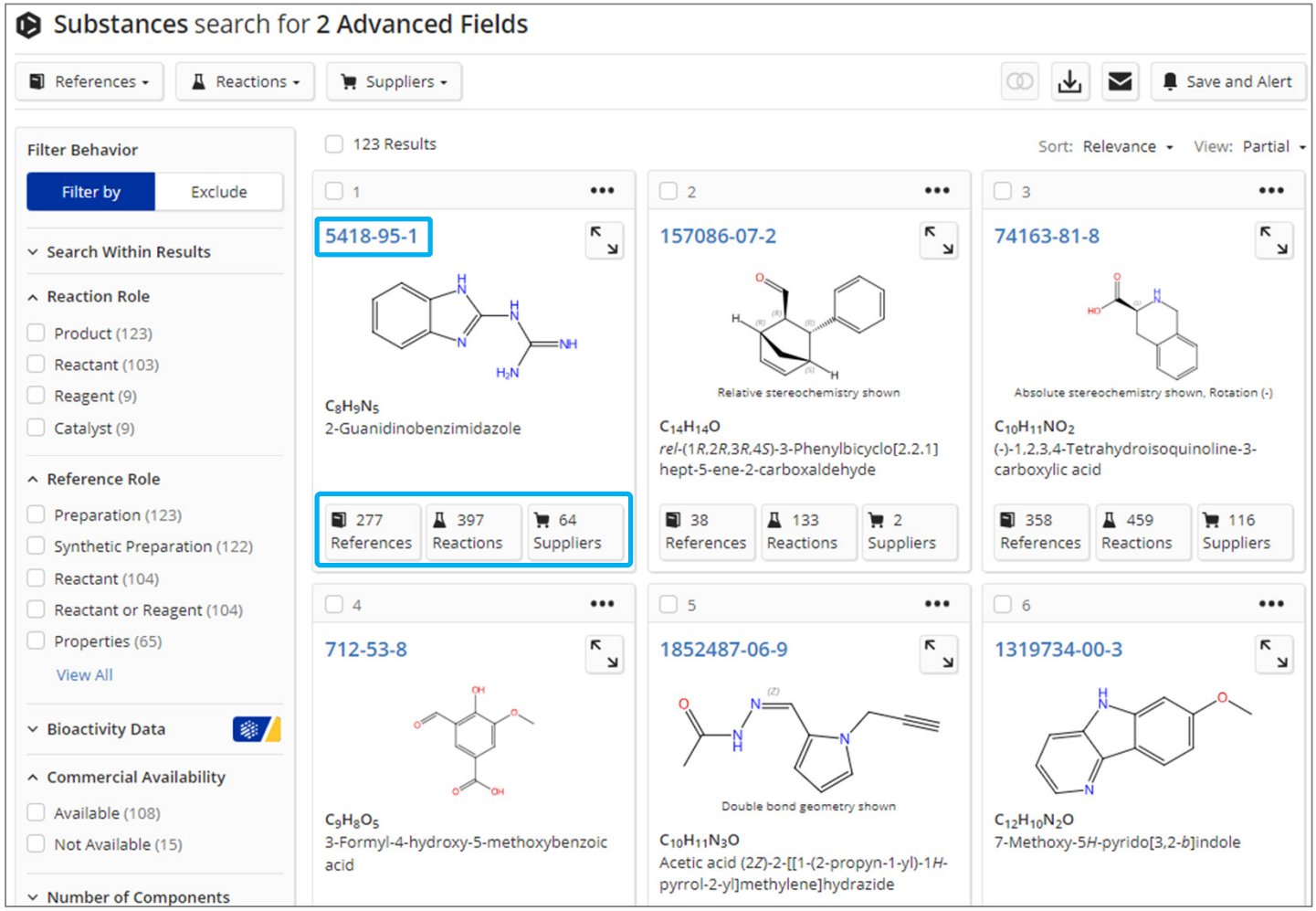


- H 谱化学位移：3.5, 6.5 至 7.5, 11.1
- 分子量：170 至 200



- 从小到大的顺序输入检索信息
- 英文模式下输入逗号和空格

谱图和分子量联合检索物质



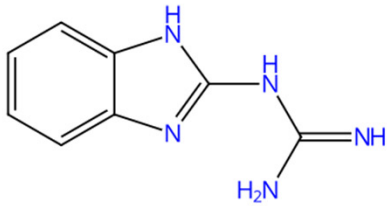
- 点击 CAS 登记号查看物质详情
- 查看物质相关的文献、反应和供应商信息

CAS
A division of the American Chemical Society

查看物质详情

CAS Registry Number: 5418-95-1

References (277) | Reactions (397) | Suppliers (64) | Save



$C_8H_9N_5$

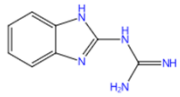
Guanidine, *N*-1*H*-benzimidazol-2-yl- (ACI)

Key Physical Properties	Value	Condition
Molecular Weight	175.19	-
Melting Point (Experimental)	245 °C (decomp)	-
Boiling Point (Predicted)	392.7±25.0 °C	Press: 760 Torr
Density (Predicted)	1.56±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.67±0.30	Most Basic Temp: 25 °C

Experimental Properties | Spectra

Proton NMR Spectrum for 5418-95-1

5418-95-1



$C_8H_9N_5$

CAS Name
2-Guanidinobenzimidazole

Conditions

Working Frequency
300 MHz

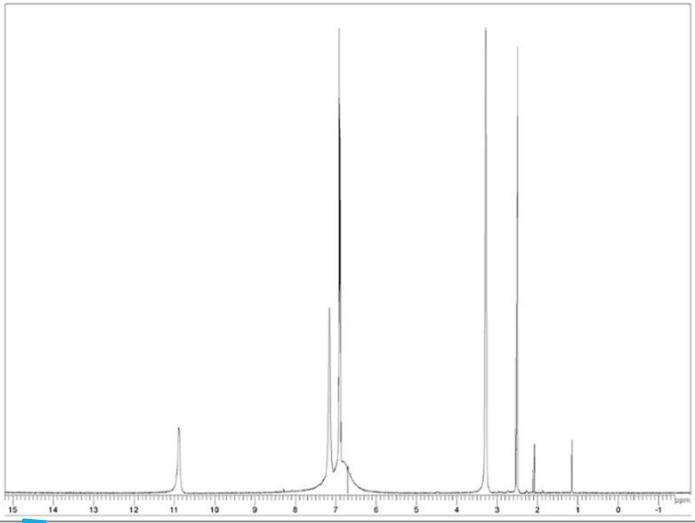
Solvent
DMSO-d_6 (2206-27-1)

Temperature
24 °C

Spectrum Summary

Spectrum ID
ASI_6014117

Source
Spectral data were obtained from John Wiley & Sons, Inc.



Experimental Spectra

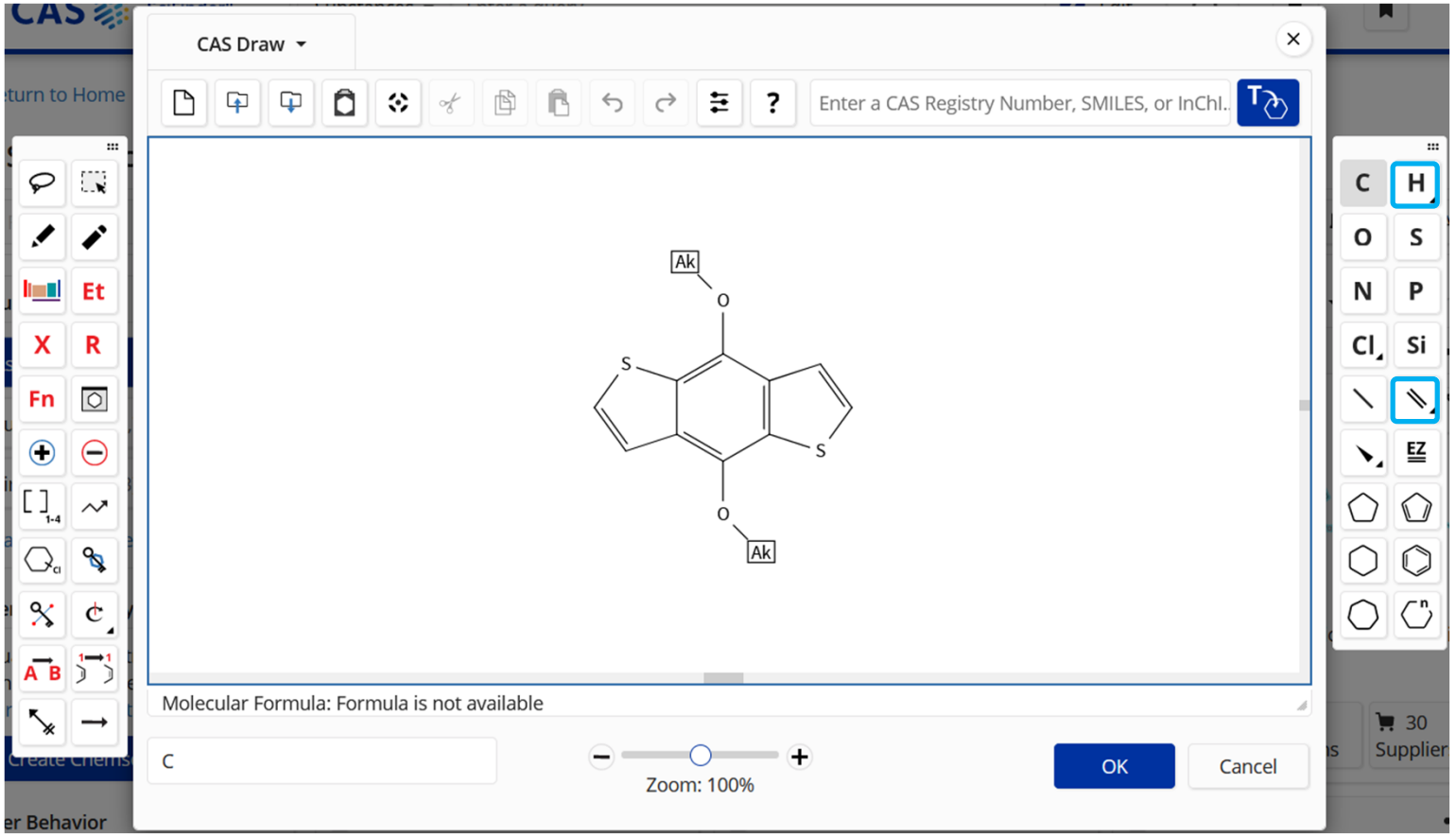
^{1}H NMR	^{13}C NMR	IR	Mass	Raman

	Source
View Proton NMR Spectrum	(1) WSS
View Proton NMR Spectrum	(1) WSS
View Proton NMR Spectrum	(2) ENAMINE

CAS
A division of the American Chemical Society

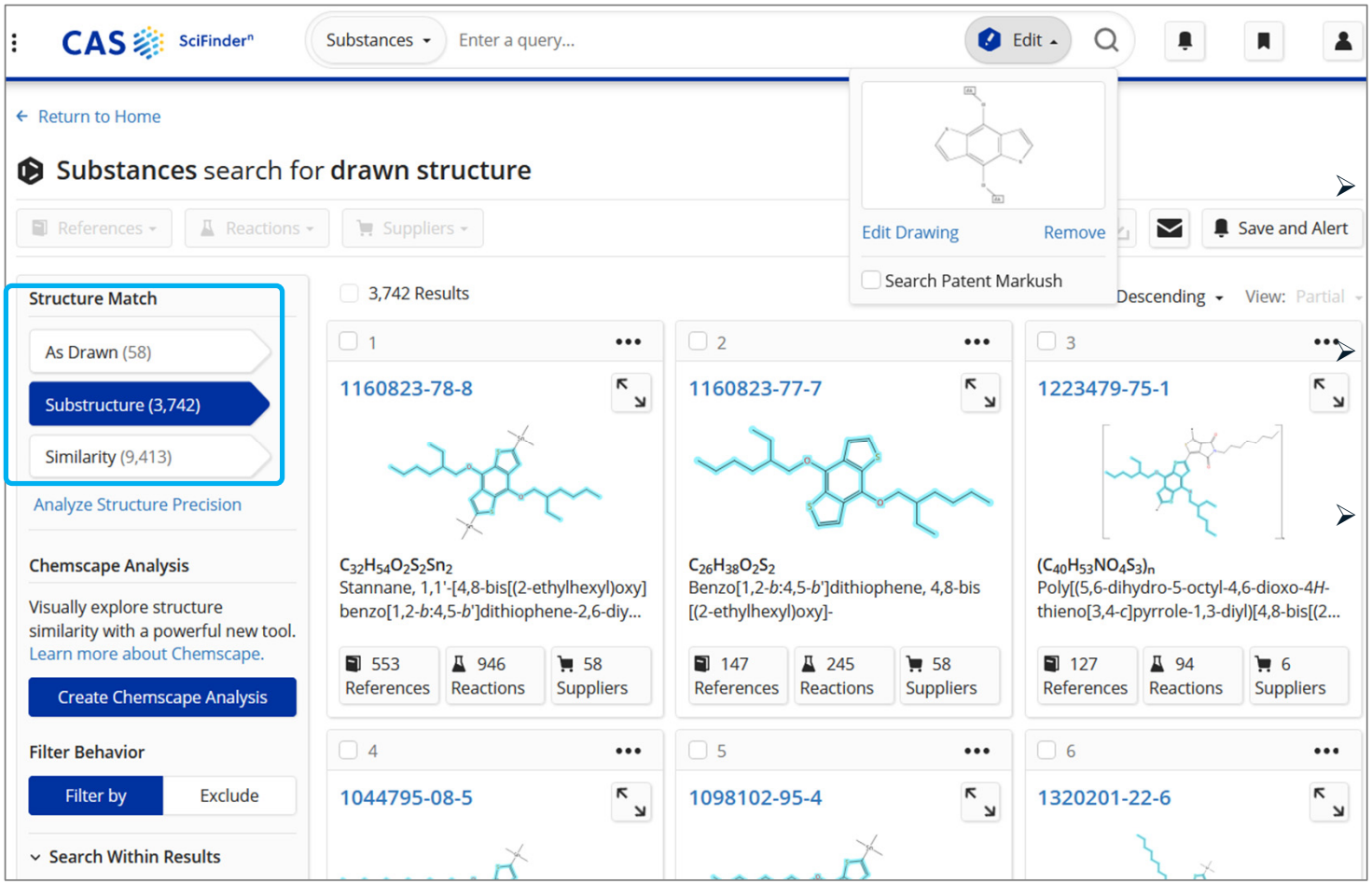
利用结构信息检索物质

- 可变基团
- 自定义基团
- 片段结构
- 重复工具
- 取代位点可变
- 反应角色标记
- 锁定工具



[CAS Draw 使用技巧]

检索结果集：Structure Match



As Drawn：绘制结构中可出现 R 基团和可变基团。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。

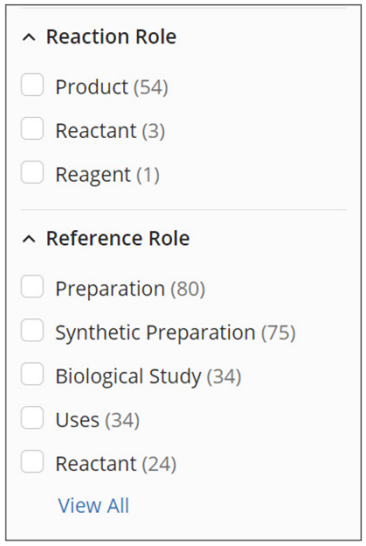
Substructure：包括 As Drawn 的检索结果，另外价态未达饱和的原子可以连接氢以外的其他原子，环系（如有）可以与其他环稠合或成桥环。

Similarity：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和改变。

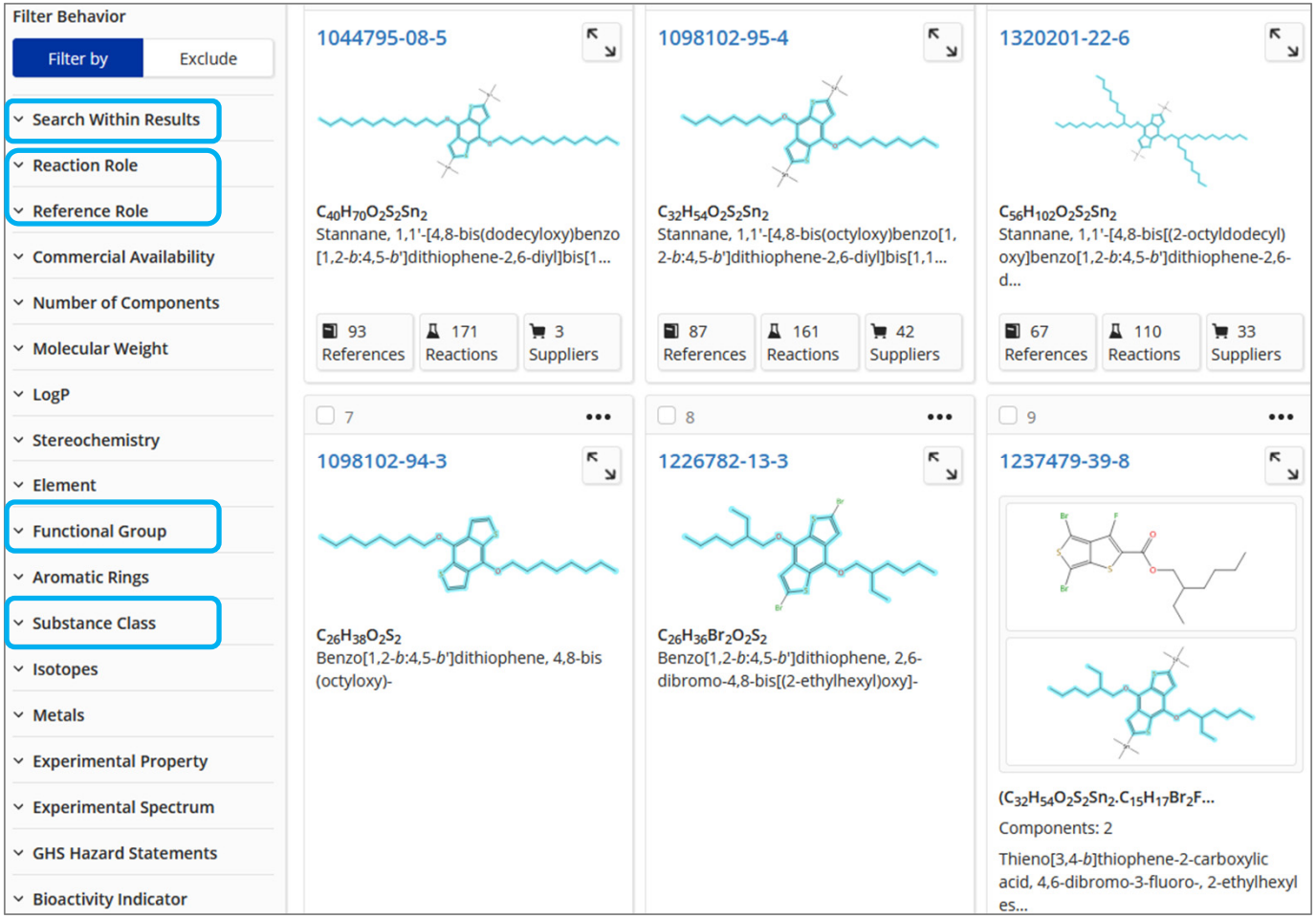
注意：Similarity 条件下不要绘制通式结构

检索结果集筛选目标物质：Filter Behavior

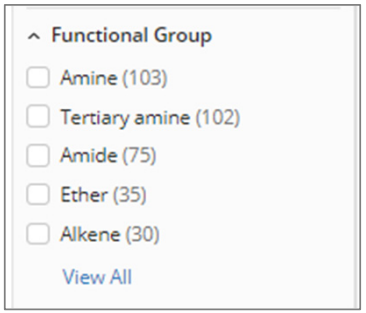
物质在反应中的角色

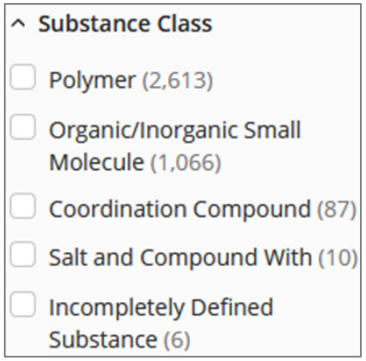


物质在文献中的研究角色



特定官能团





物质类别

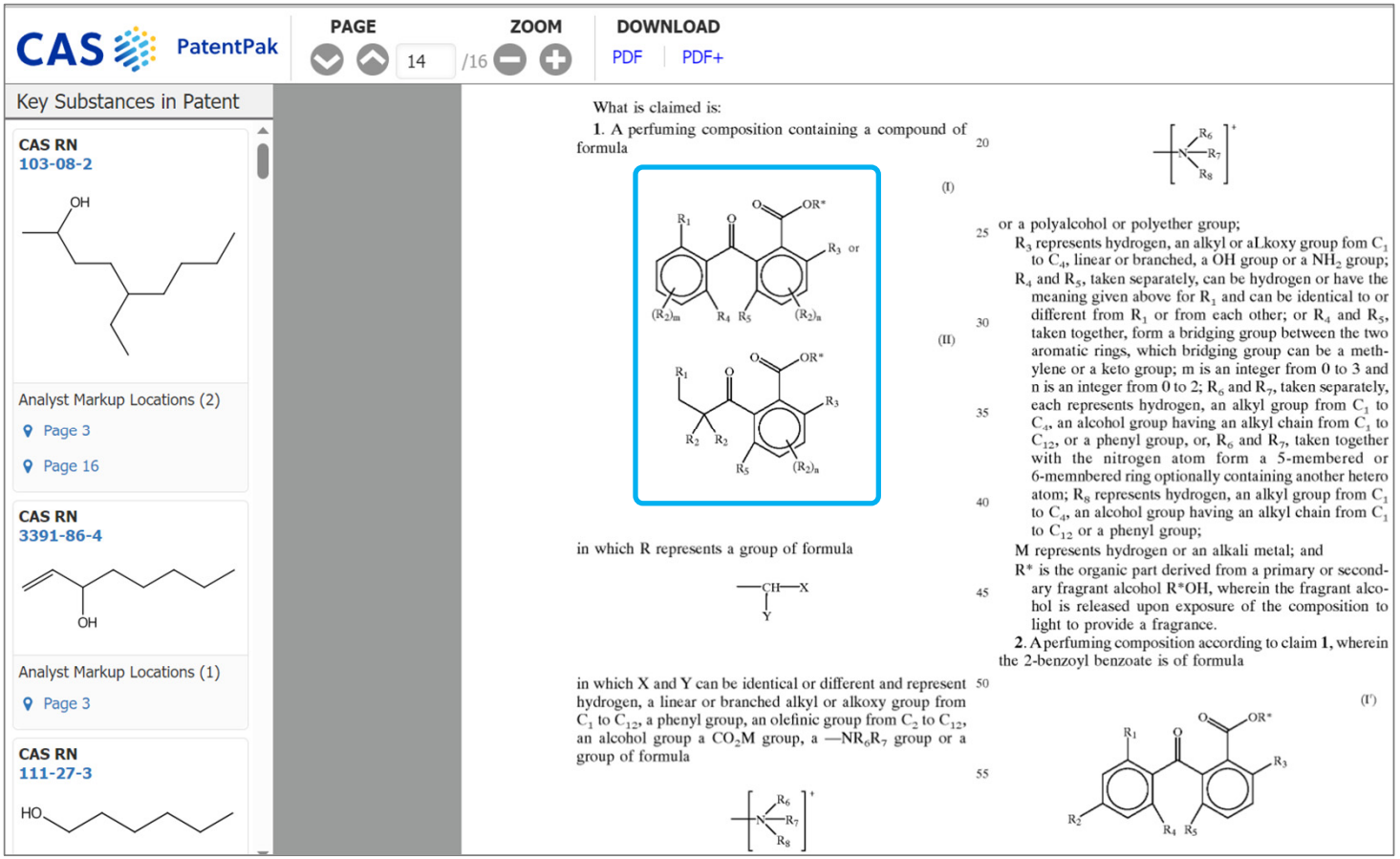
CAS Markush 检索，结构查新

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 登记号

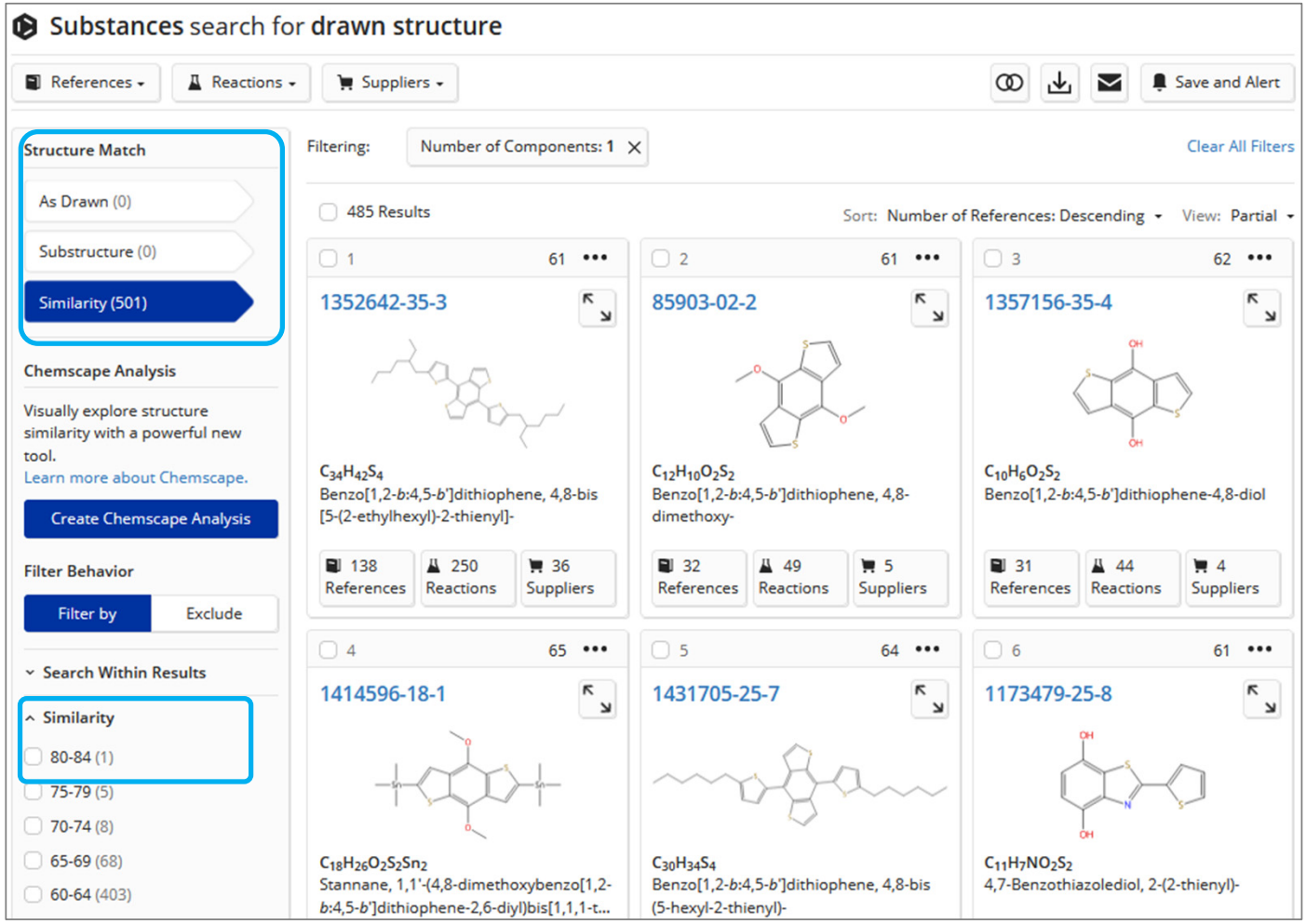
预测性物质 (Prophetic Substance)

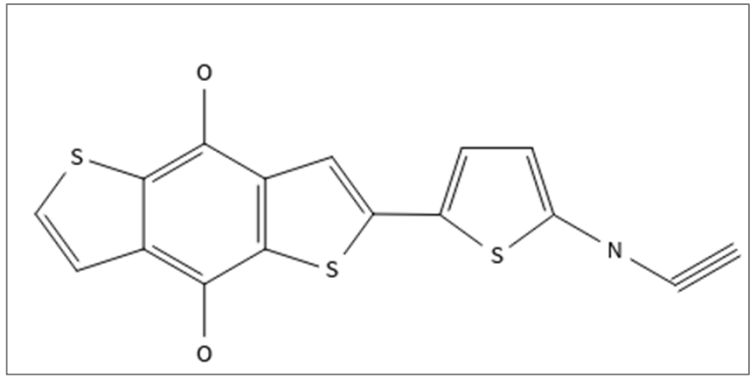
- 使用 Markush 结构陈述的预测物质，一个 Markush 可以陈述数千甚至更多的化学物质
- 被 Markush 结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，则不会被分配 CAS 登记号
- Markush 检索能够检索到仅通过 Substance 可能检索不到的结构



CAS
A division of the American Chemical Society

完整的结构检索流程



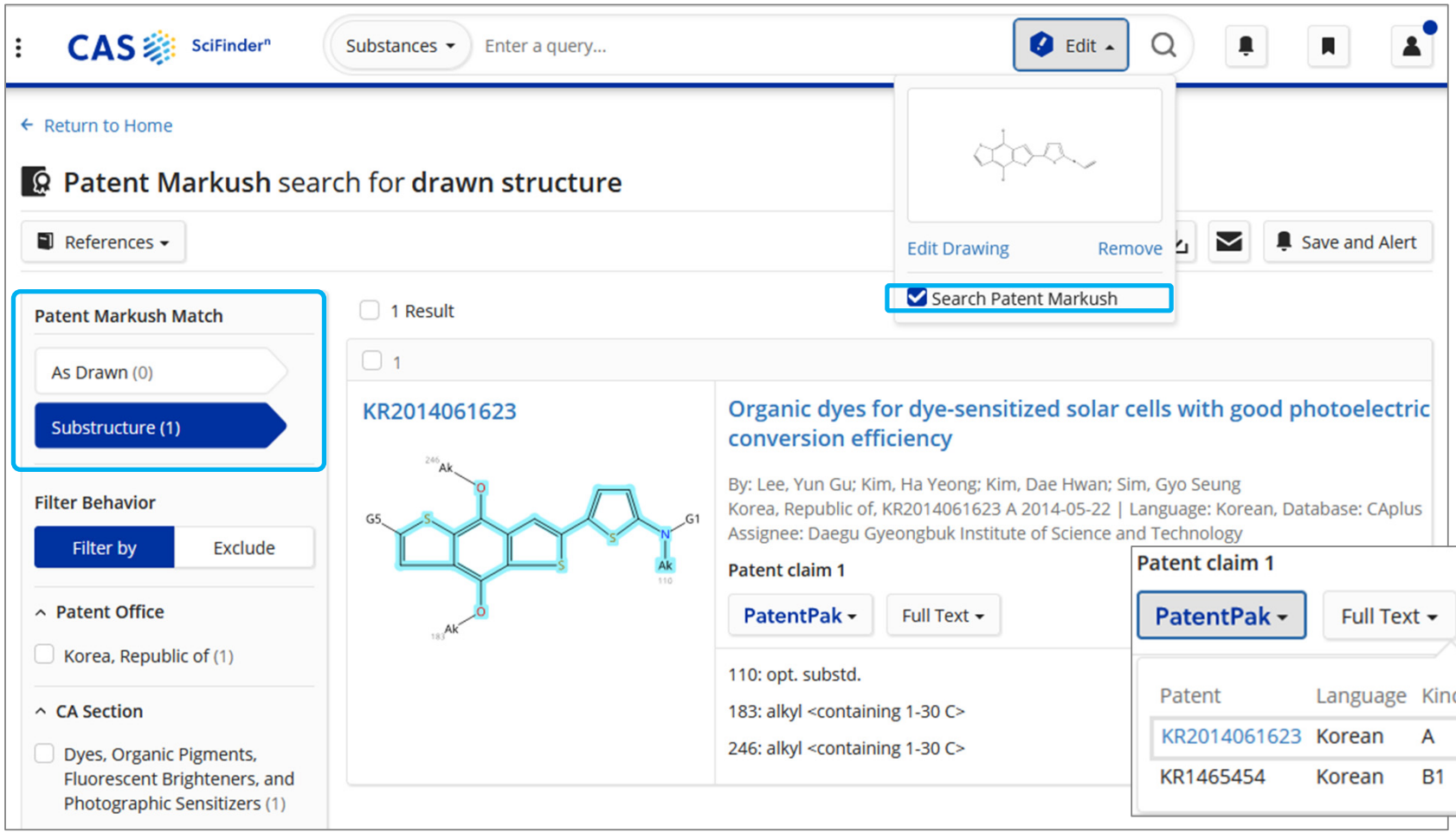


Step 1: 物质结构检索

- As Drawn, Substructure 结果为 0
- Similarity 结果中物质最大相似度

仅 80-84%

完整的结构检索流程



Step 2: Markush 结构检索

- 直观呈现检索的结构与专利原文中 Markush 匹配的部分
- 标引结构在专利中的位置
- 详细的结构取代信息描述

CAS
A division of the American Chemical Society

物质检索小结

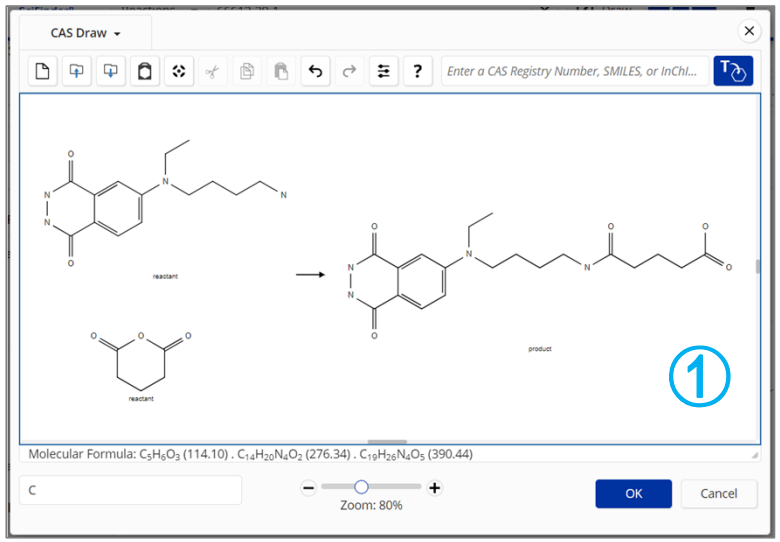
1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 正确理解 As Drawn、Substructure、Similarity检索结果集的意义和范围
3. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
4. 利用CAS Markush检索尽可能全面的获得结构的公开信息

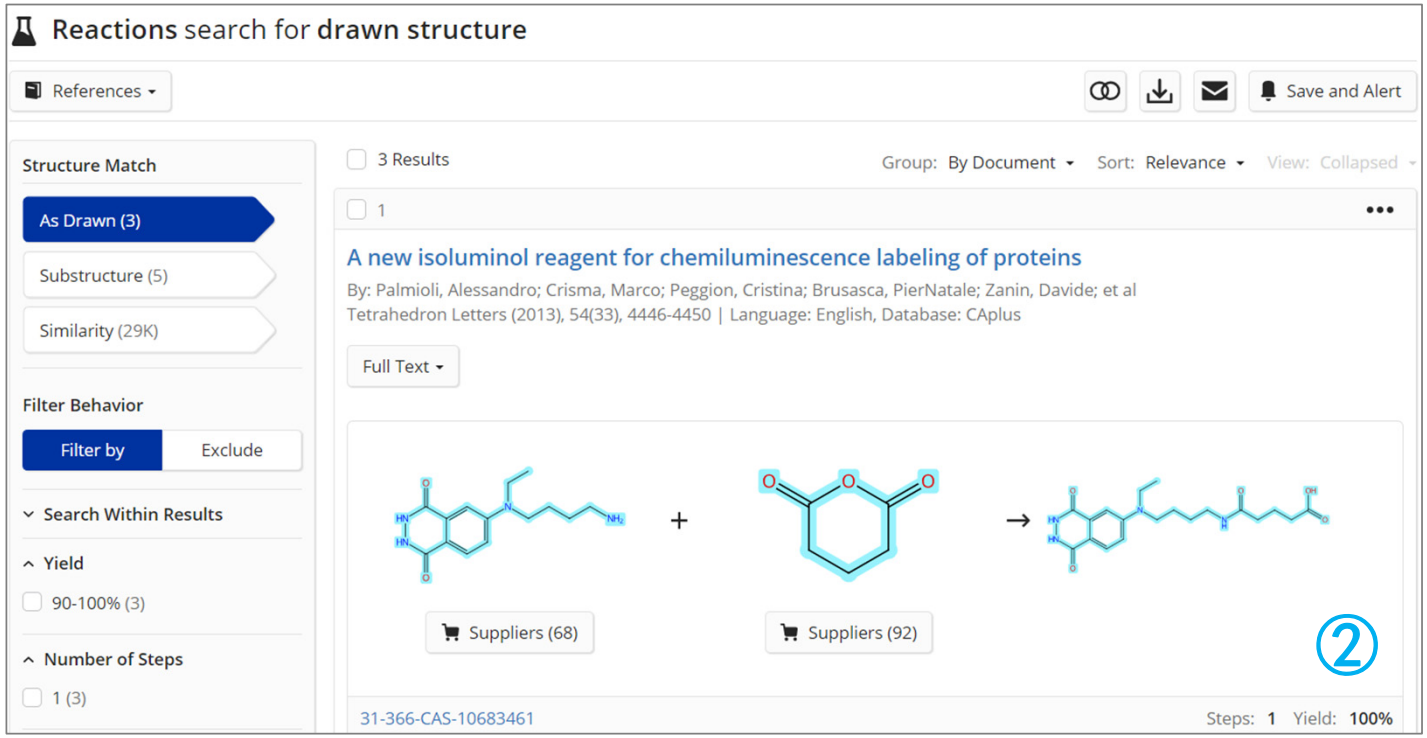
3. 如何进行反应调研?

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

反应检索

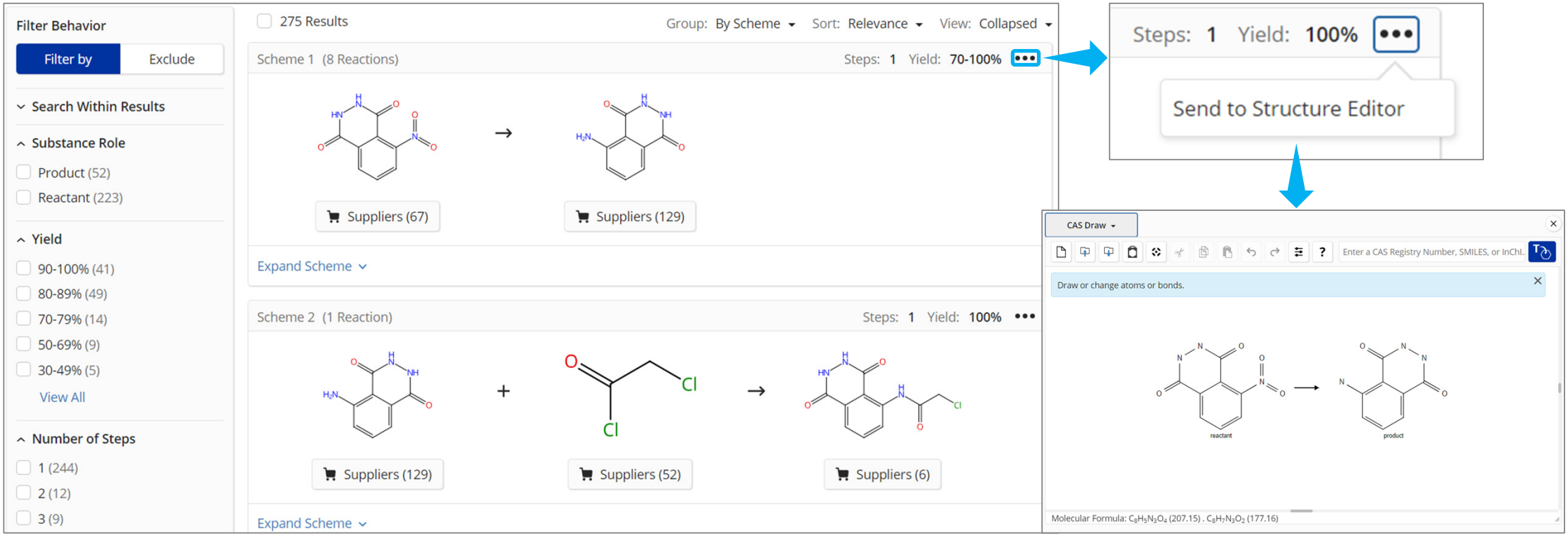
直接反应检索





CAS
A division of the American Chemical Society

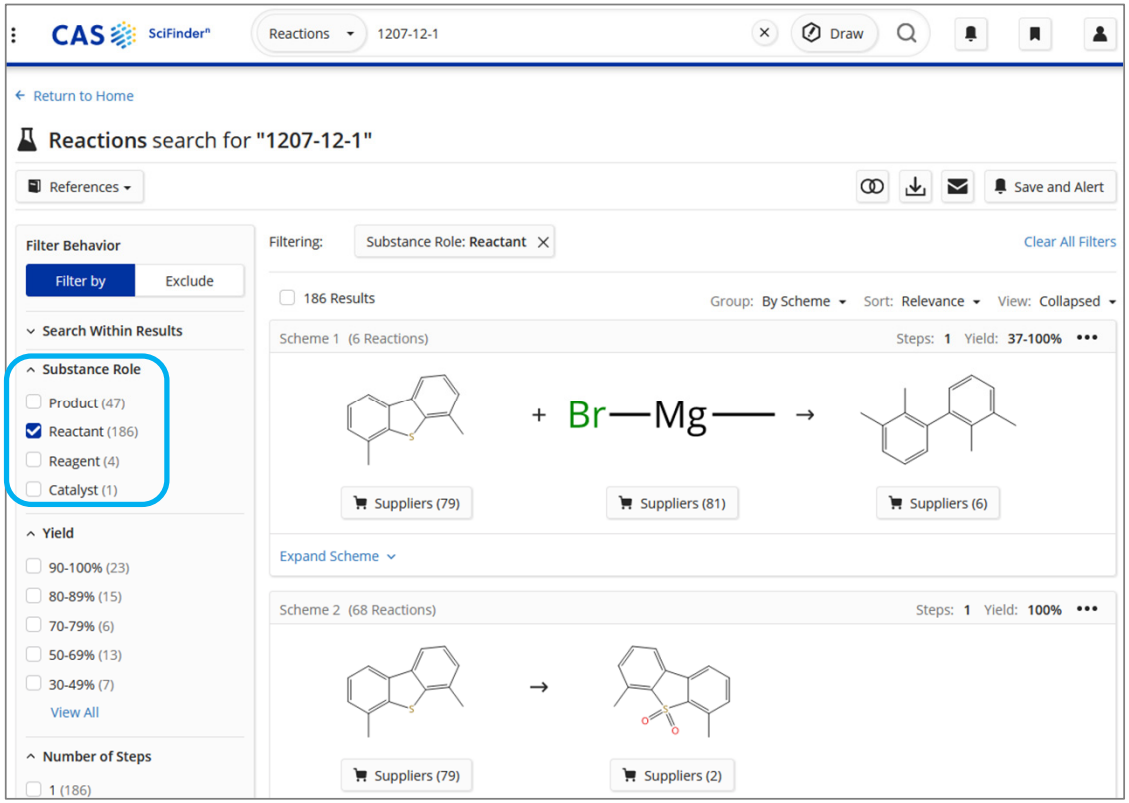
反应检索结果再编辑



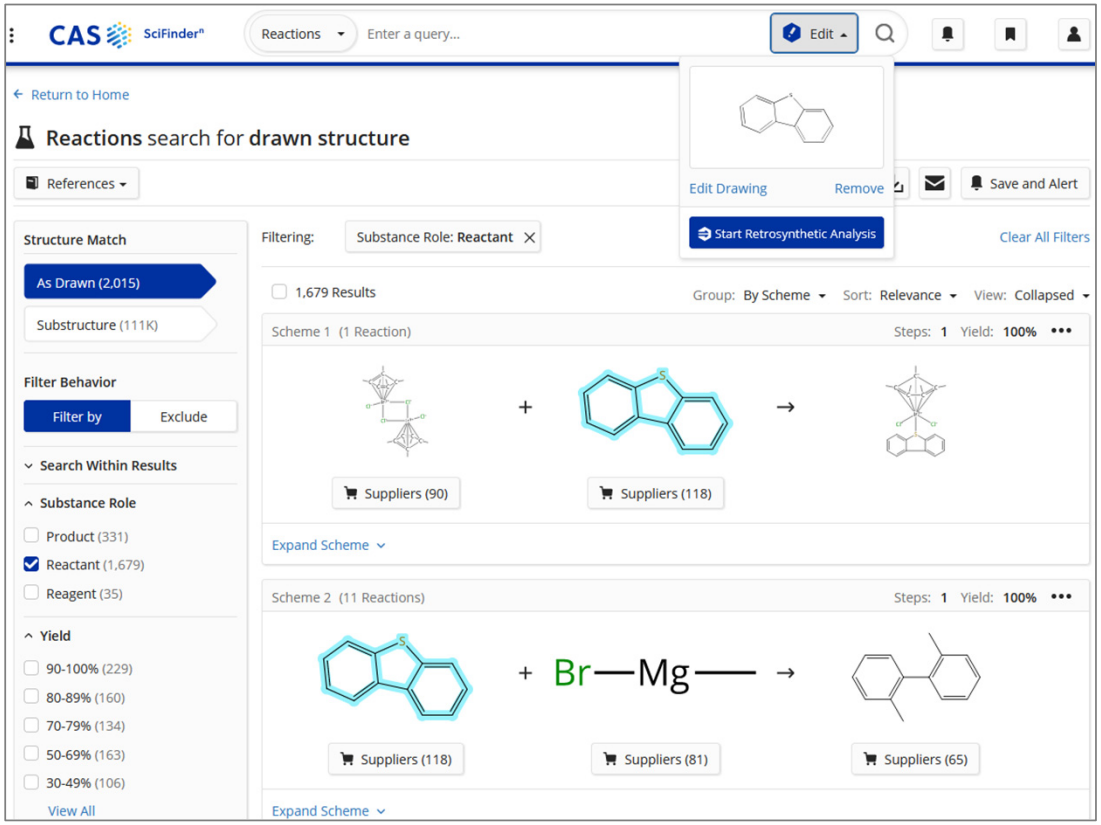
反应式再编辑

CAS
A division of the American Chemical Society

检索物质能够发生的反应



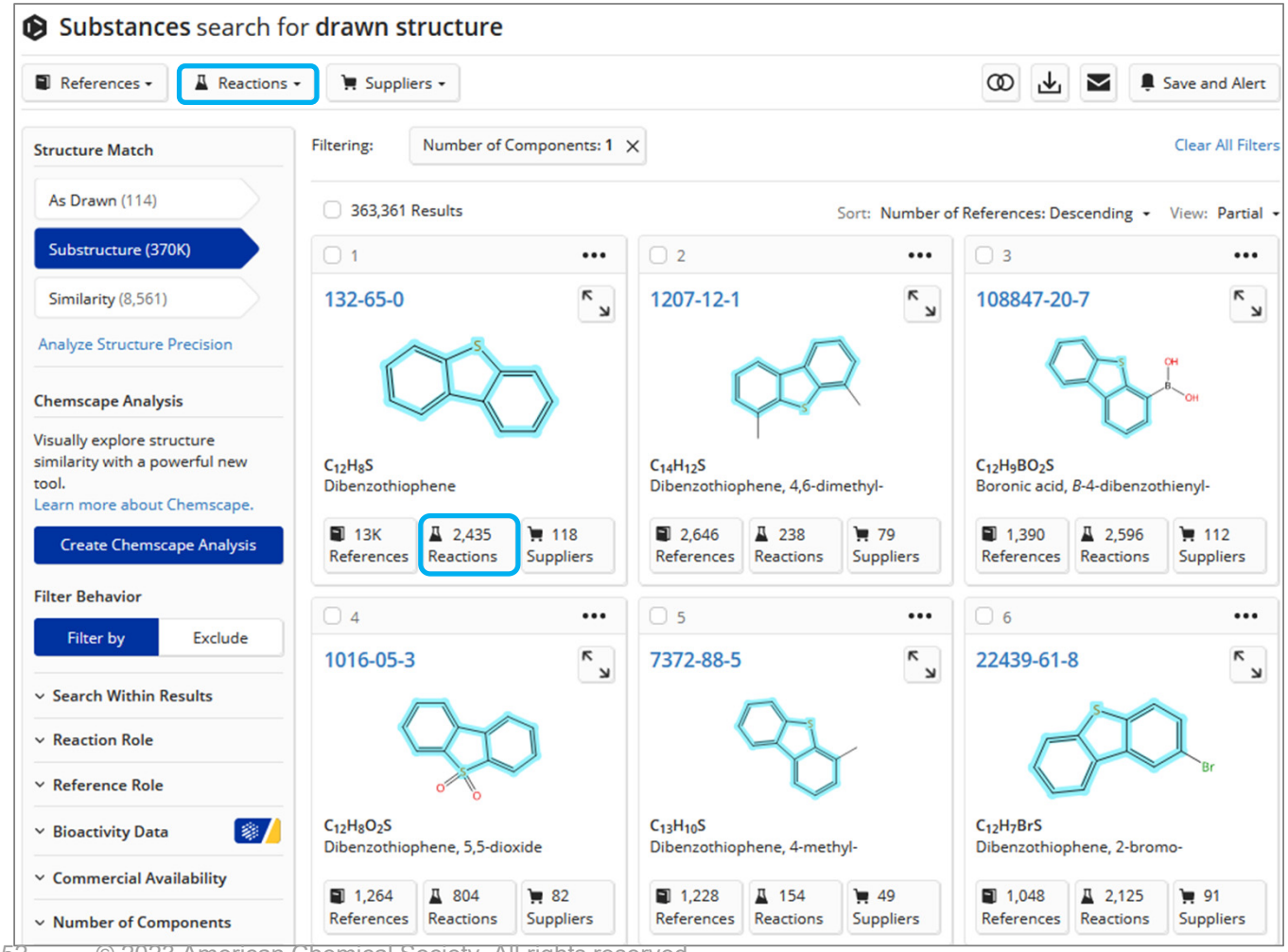
物质标识符



物质结构式

CAS
A division of the American Chemical Society

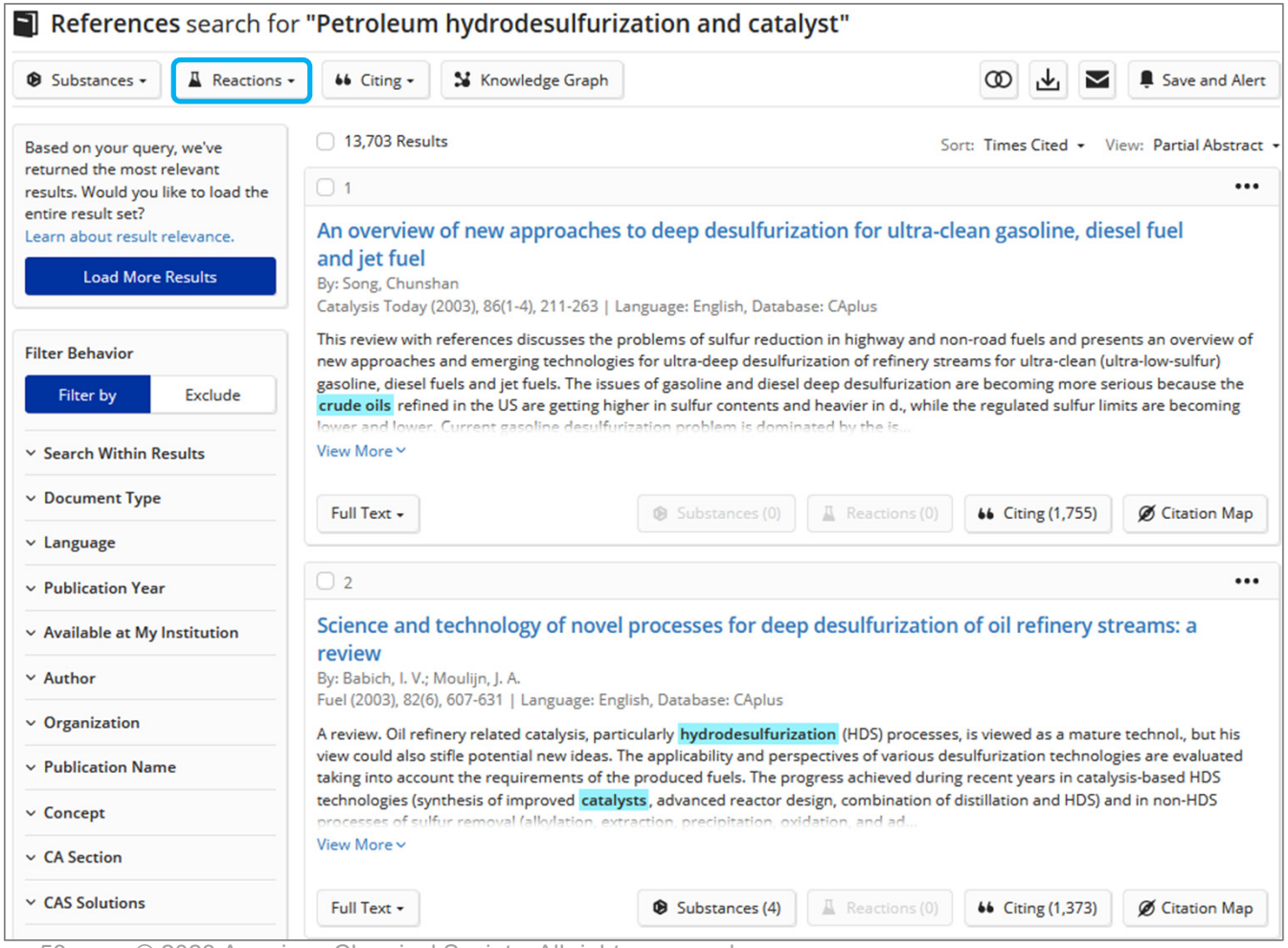
在物质结果集中查看能够发生的反应



- 查找系列衍生物
- 数据关联查阅相关反应

CAS
A division of the American Chemical Society

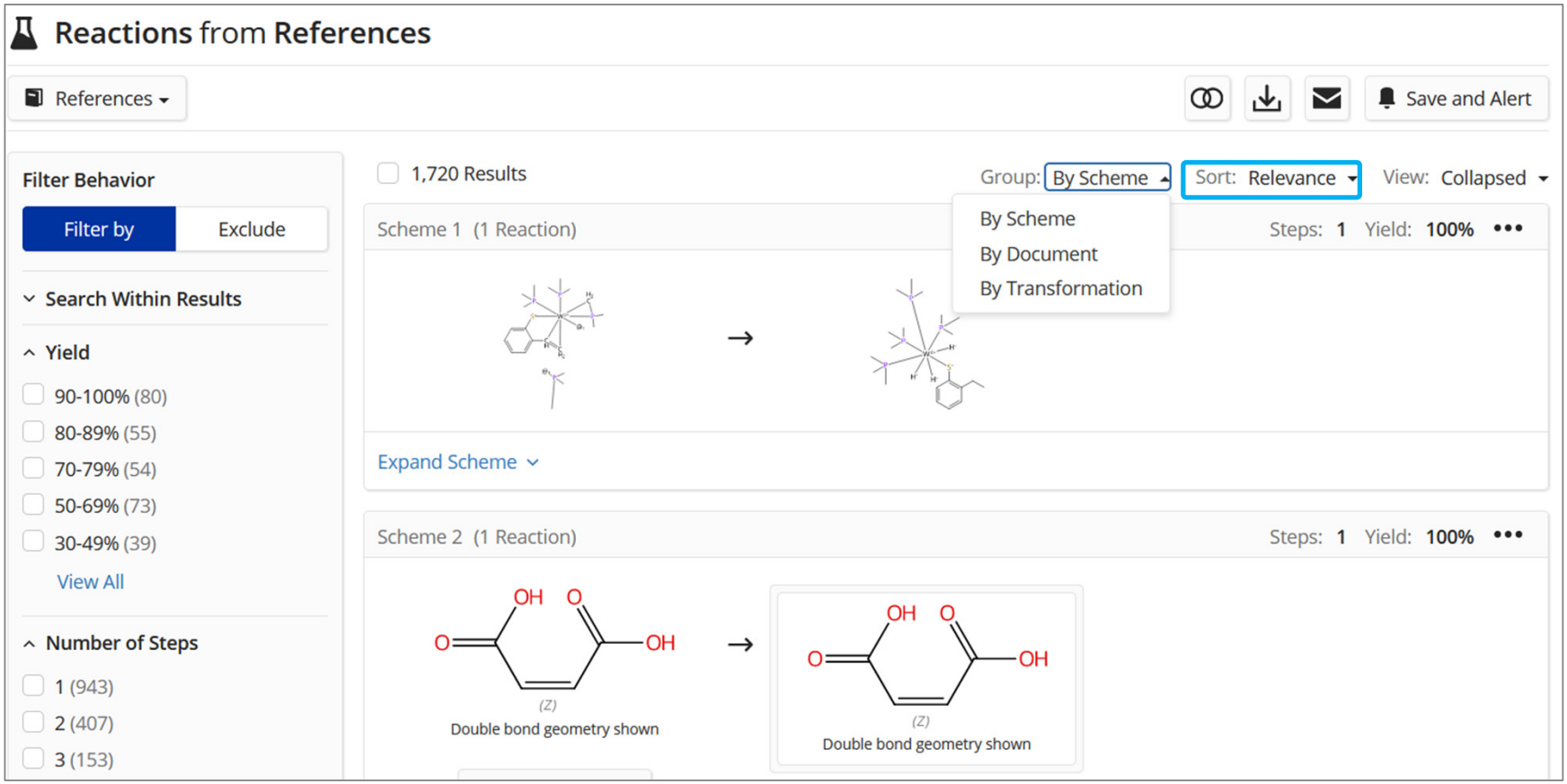
关注反应的催化剂/机理研究或人名反应?



- 查找特定研究领域中的文献
- 数据关联查阅文献中的反应

CAS
A division of the American Chemical Society

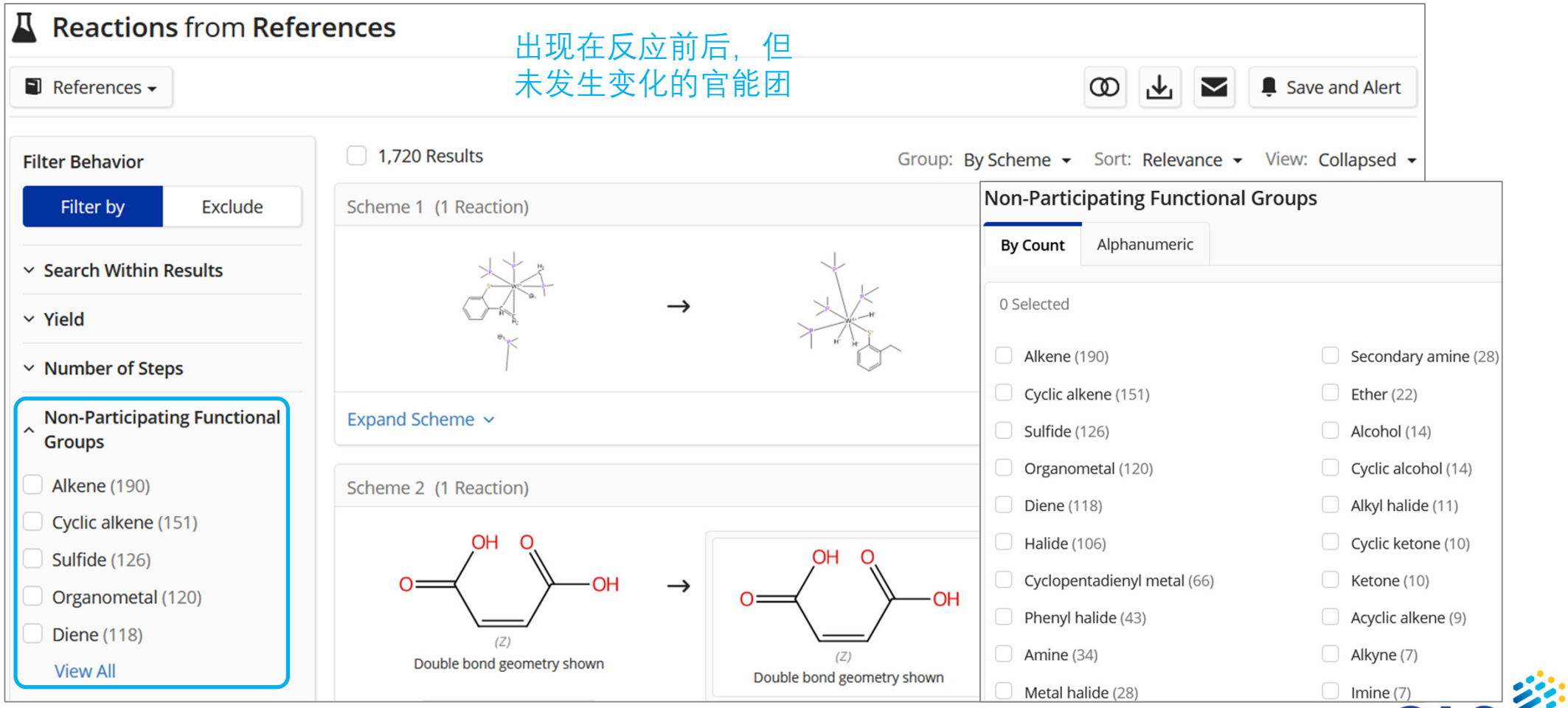
反应检索结果集分组与排序



Relevance
Publication Date: Newest
Publication Date: Oldest
Yield
Number of Steps: Ascending
Number of Steps: Descending

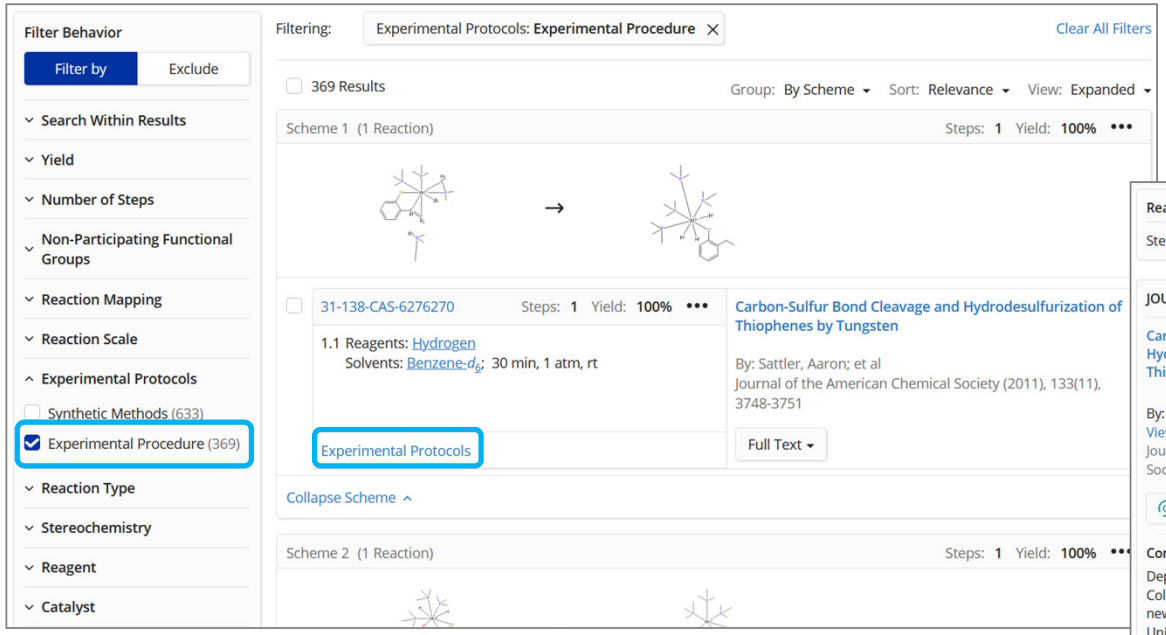
CAS
A division of the American Chemical Society

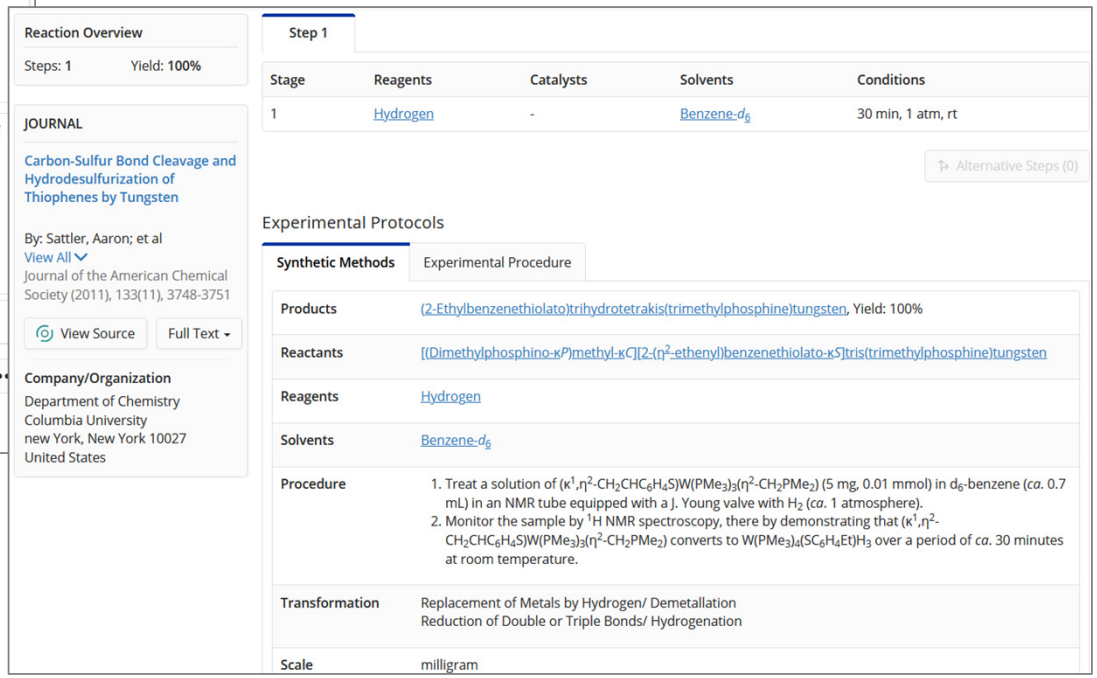
根据不参与反应的官能团筛选反应



CAS
A division of the American Chemical Society

便捷查看详细反应操作



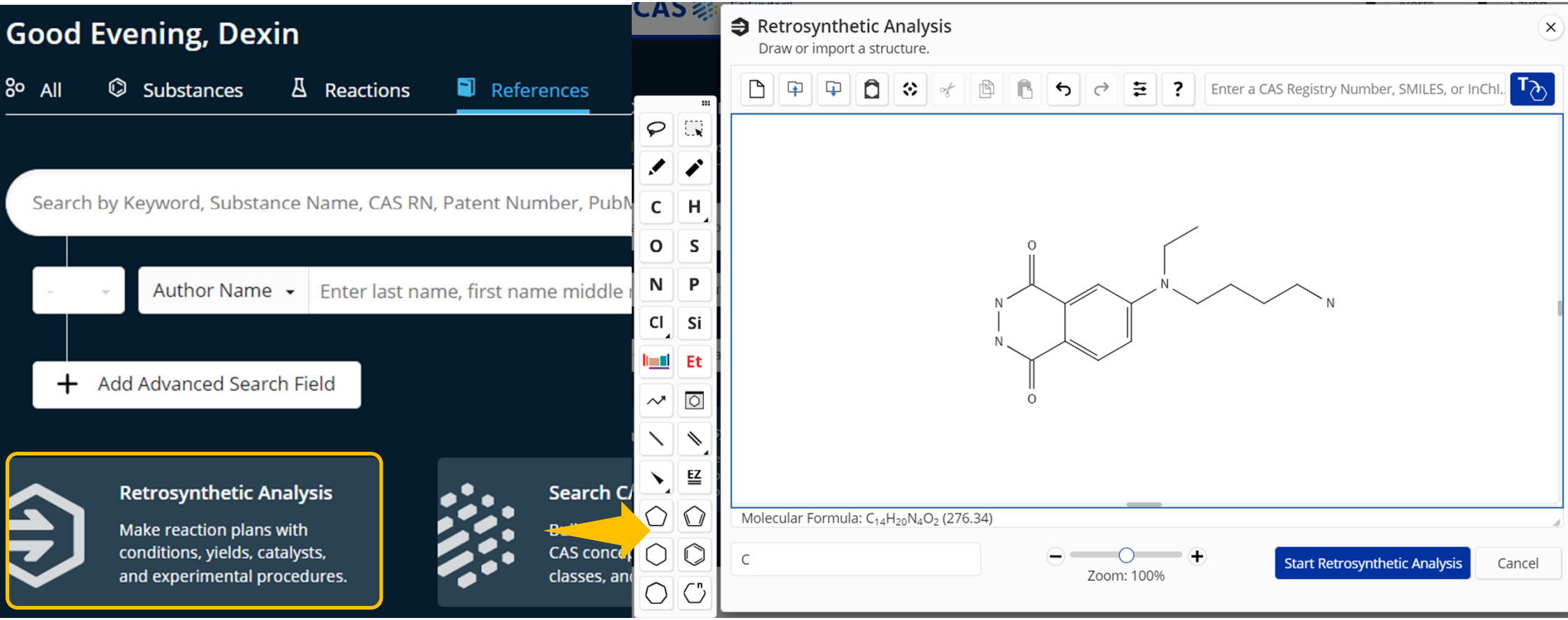


- Experimental Protocols
- 查看详细合成方法或实验过程

无需浏览原文即可获取详细的实验信息

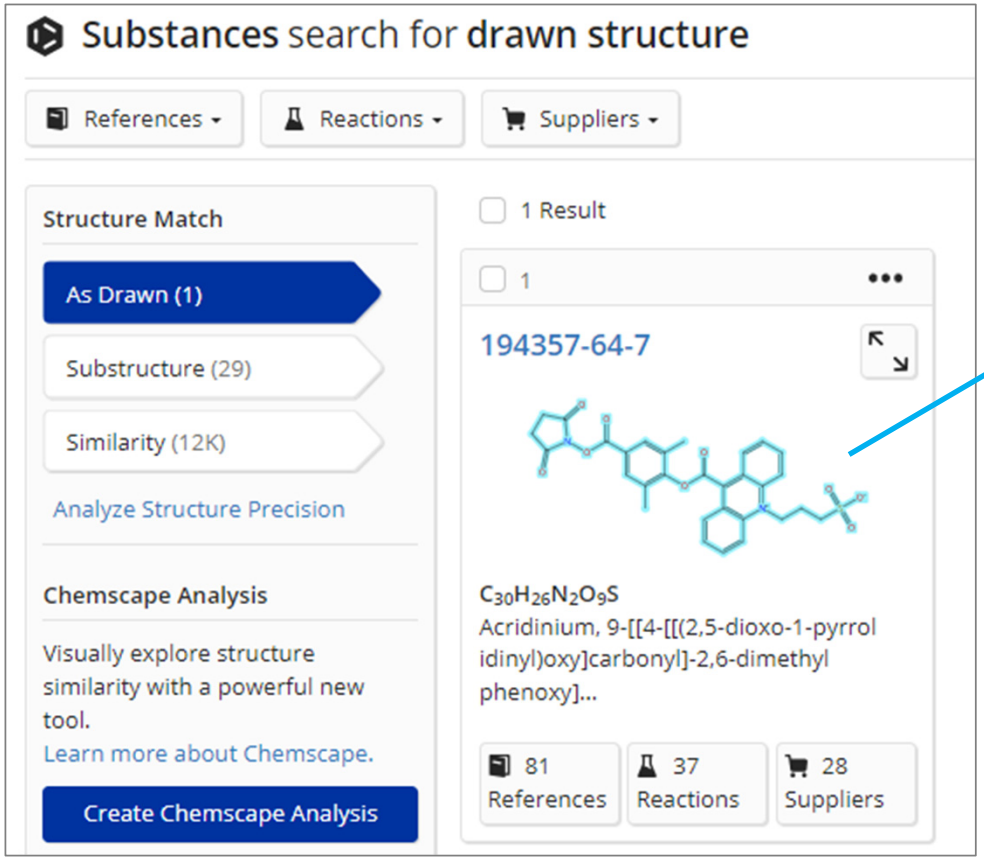
CAS
A division of the American Chemical Society

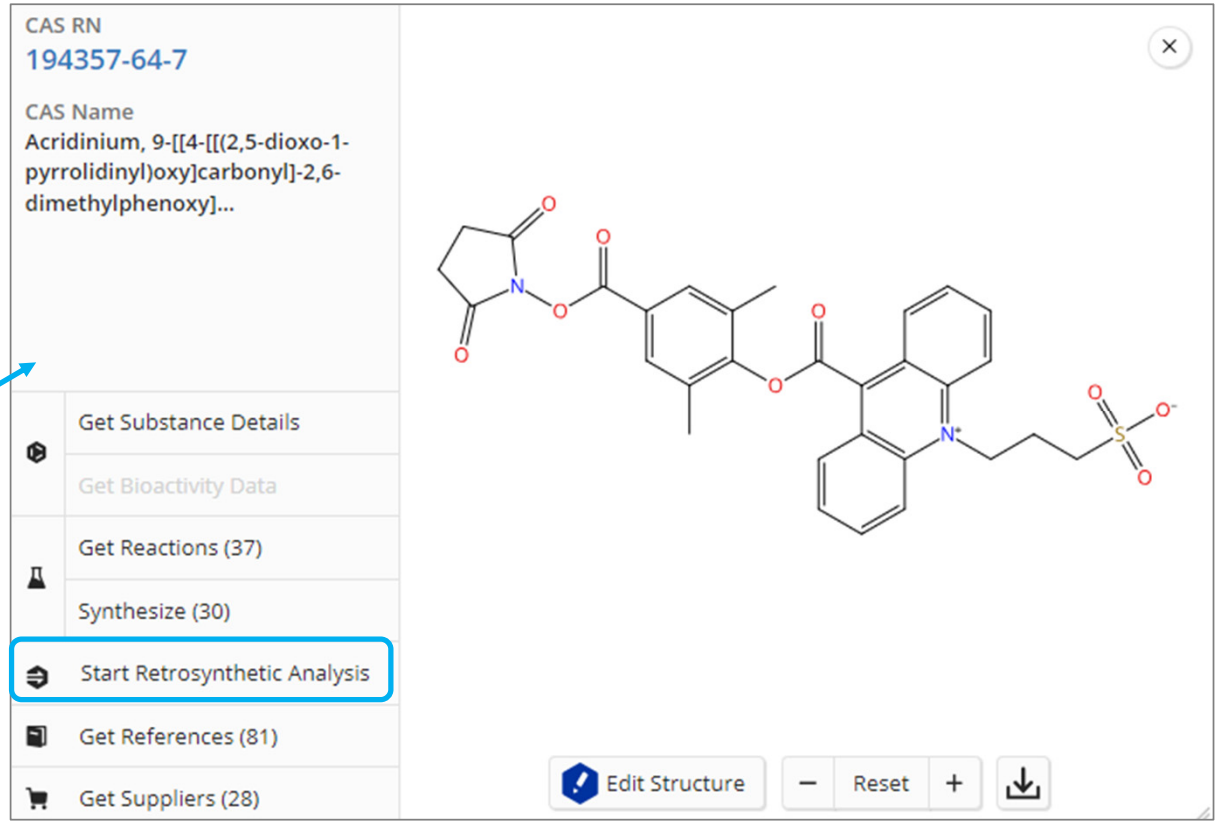
逆合成反应路线设计



CAS
A division of the American Chemical Society

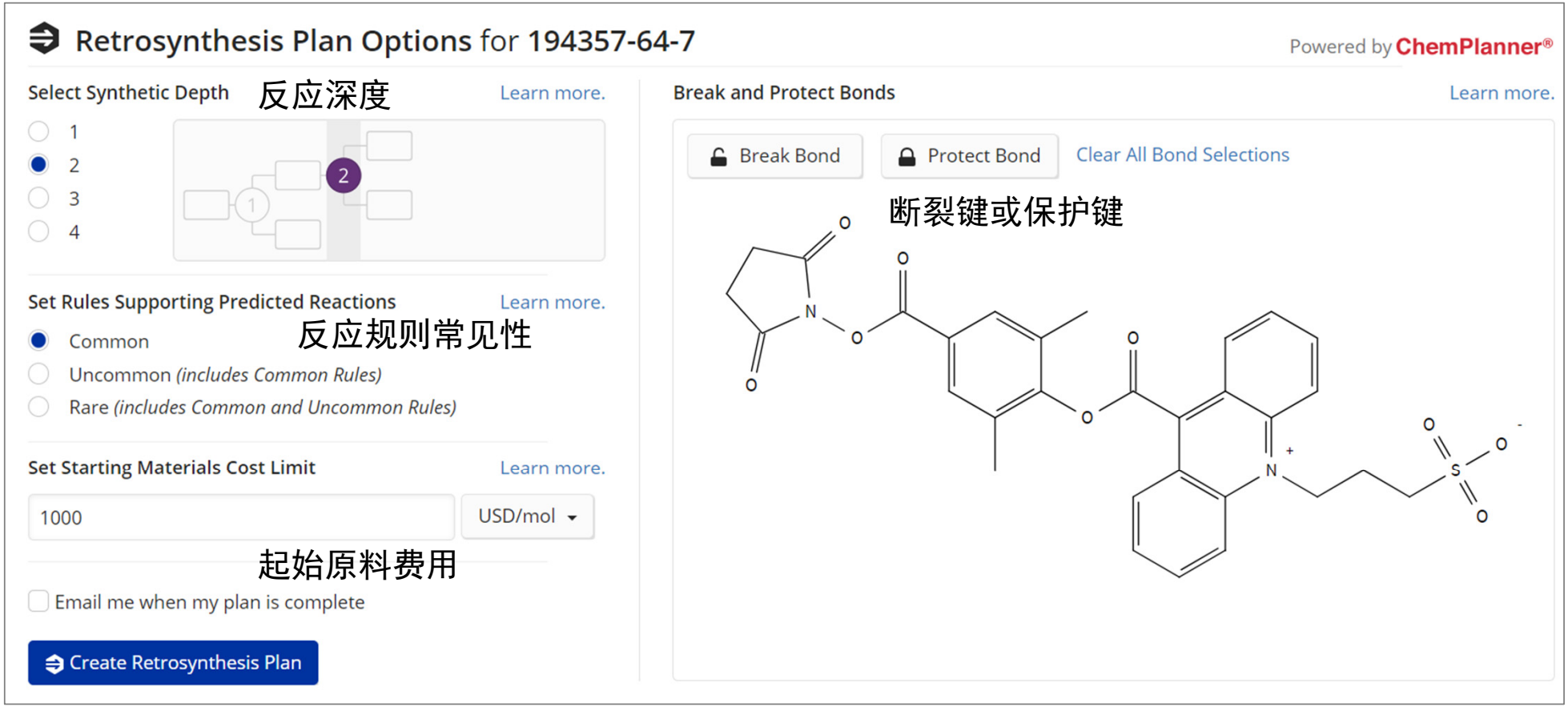
逆合成反应路线设计



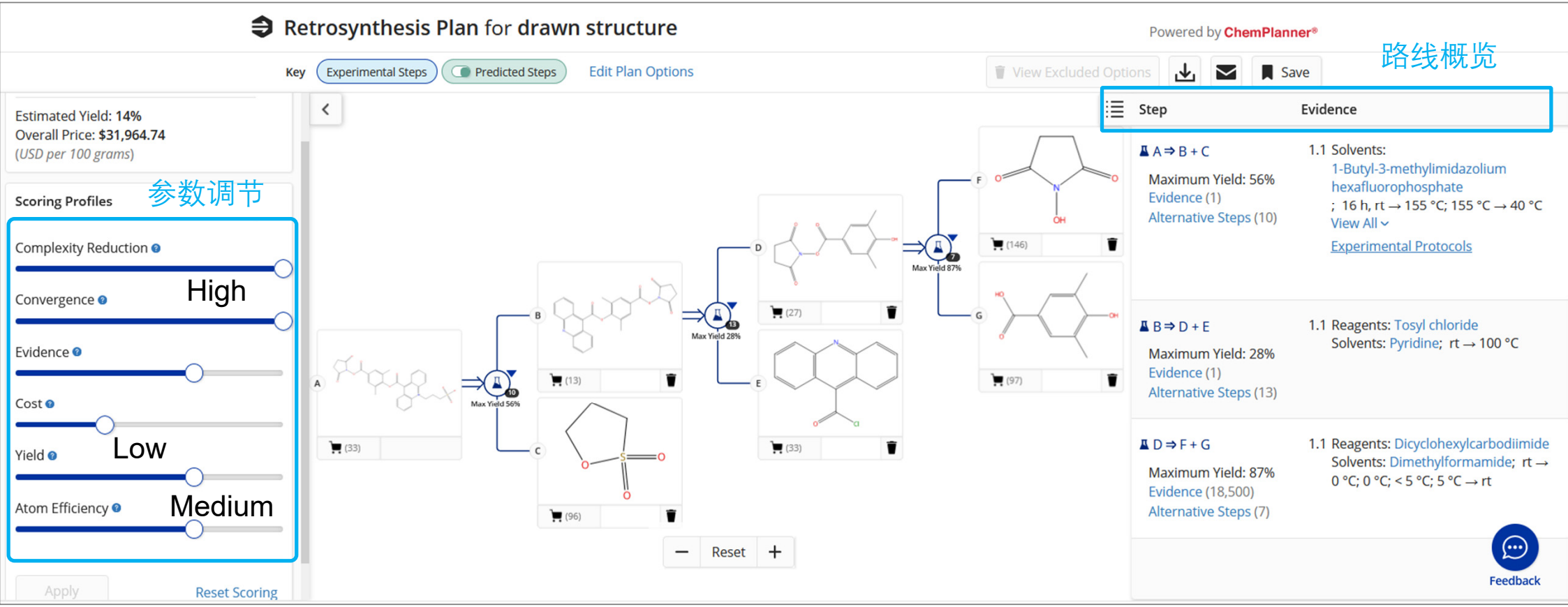


- 先进行物质检索
- 点击目标化合物，弹出物质菜单
- 点击 Start Retrosynthetic Analysis

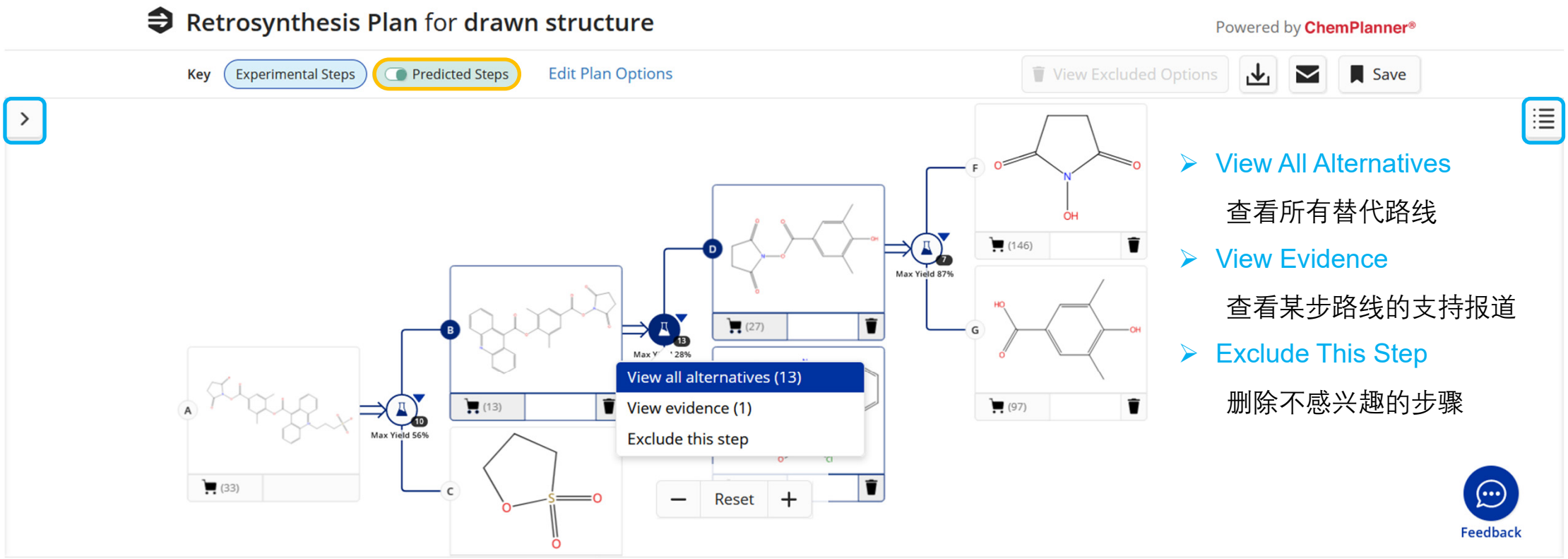
预设路线参数



路线概览和参数调节

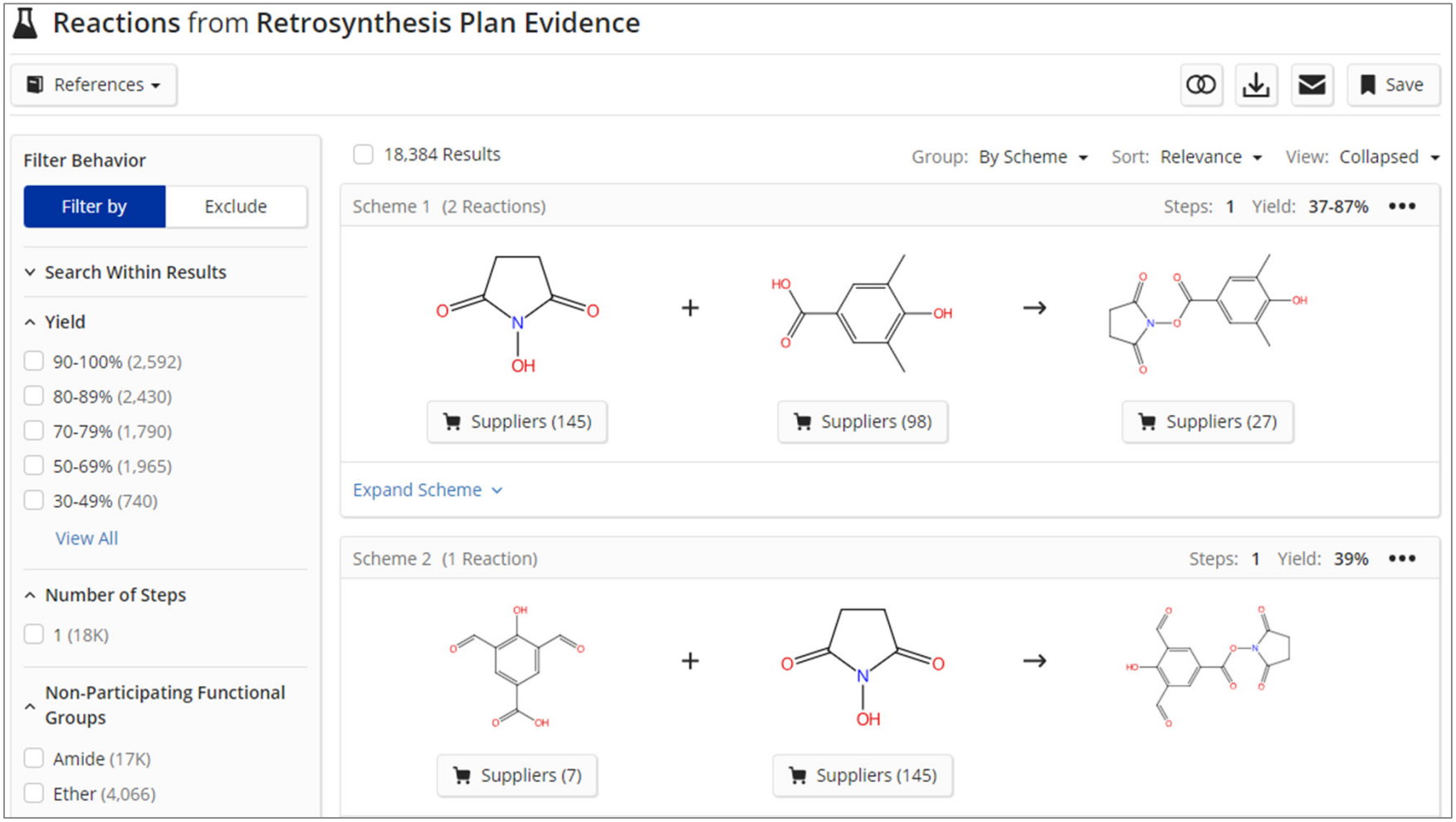


路线详情



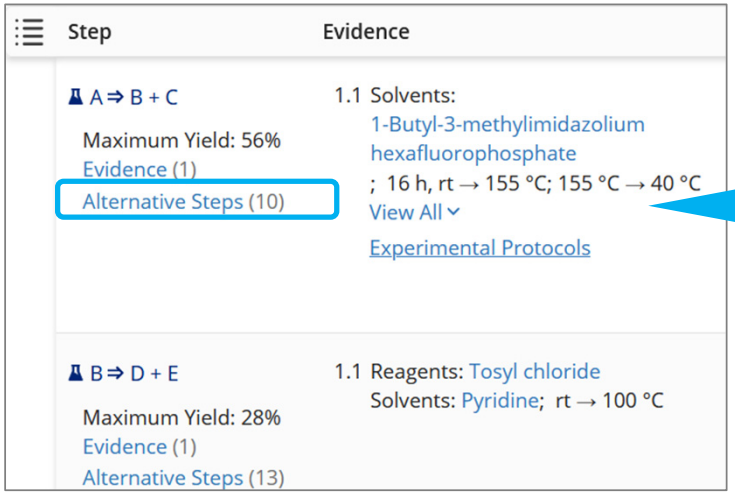
- View All Alternatives
  查看所有替代路线
- View Evidence
  查看某步路线的支持报道
- Exclude This Step
  删除不感兴趣的步骤

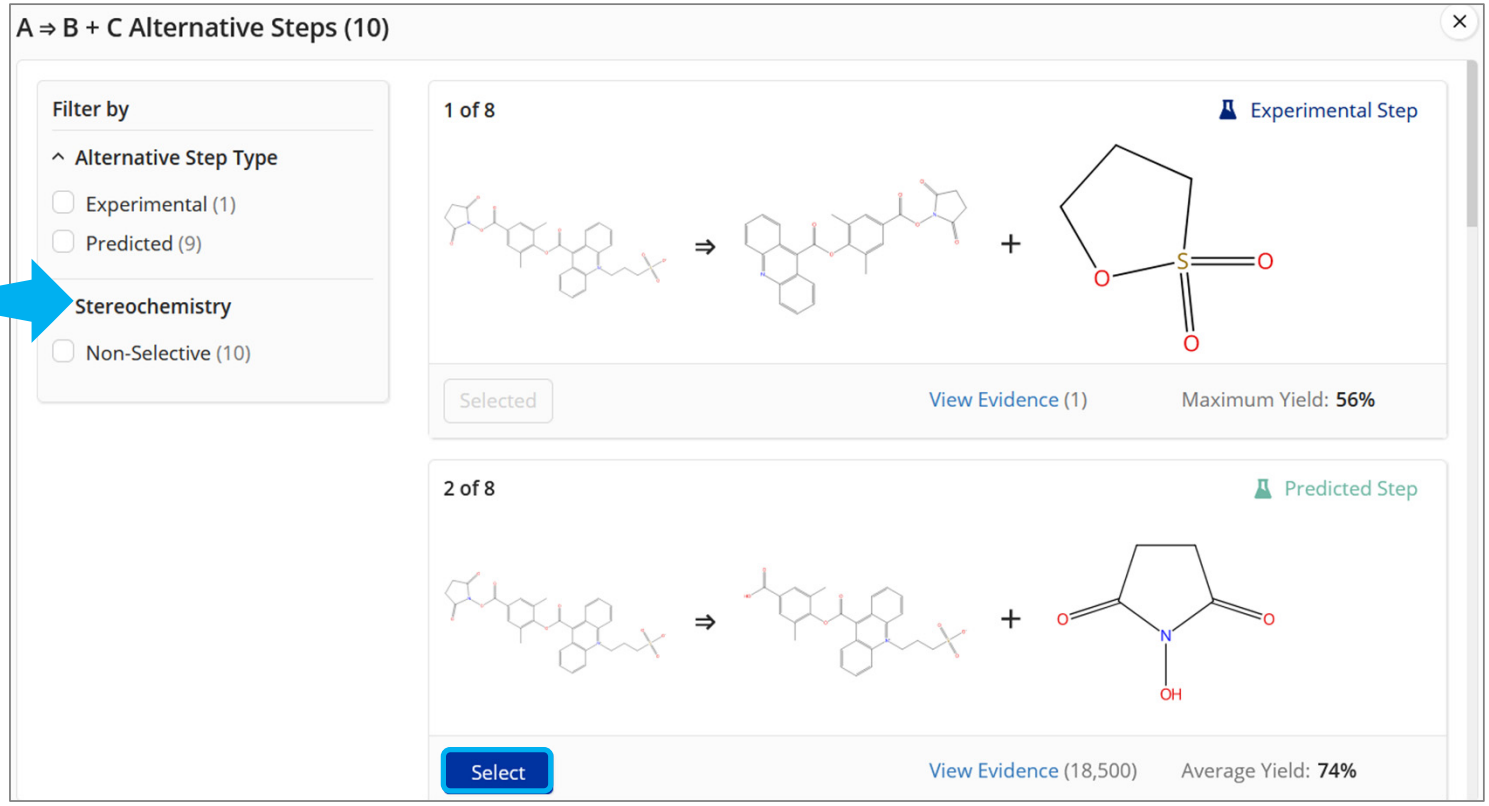
查看逆合成反应路线中的实验报道



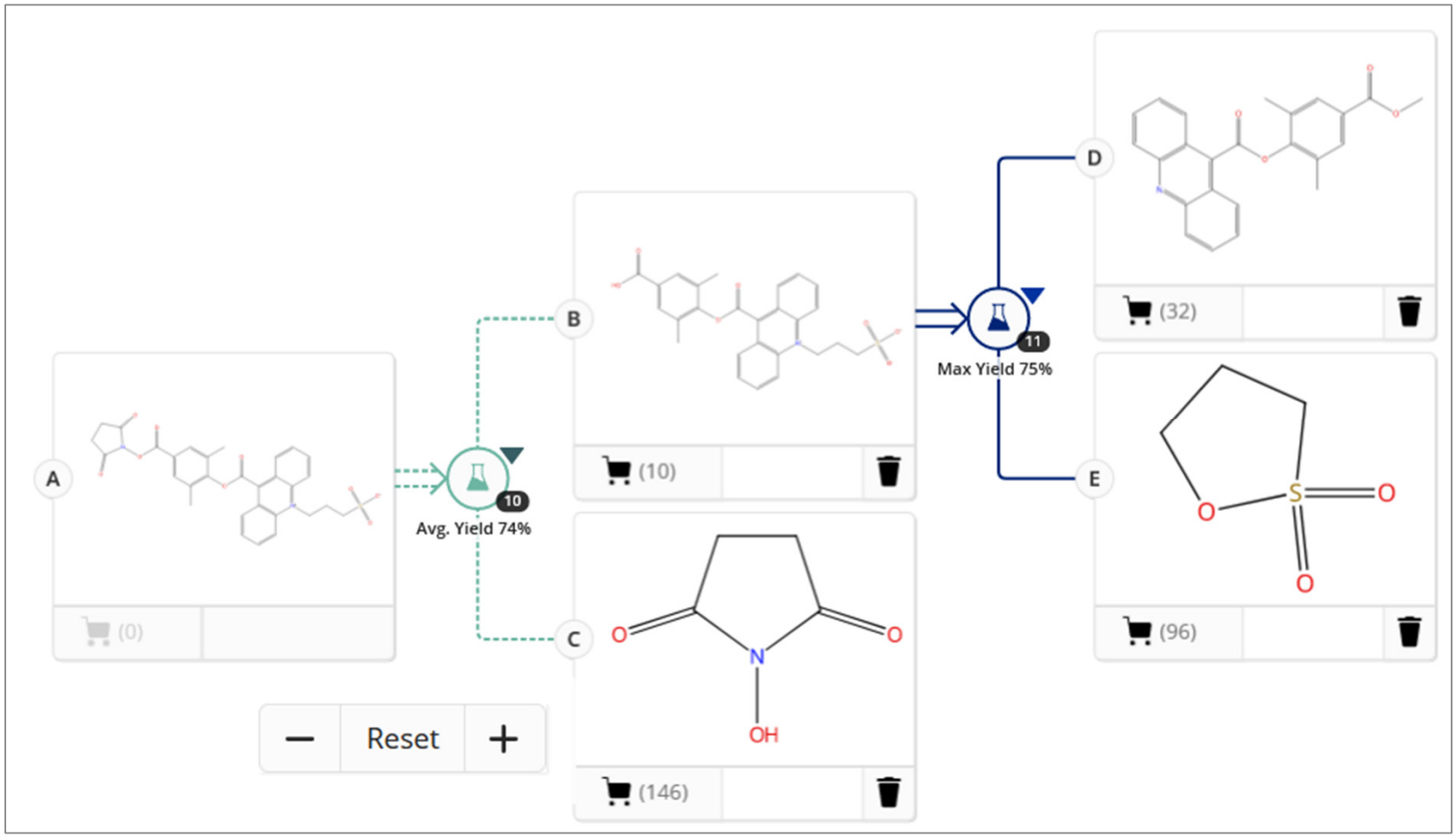
CAS
A division of the American Chemical Society

选择替代路线





新的逆合成反应路线



反应检索小结

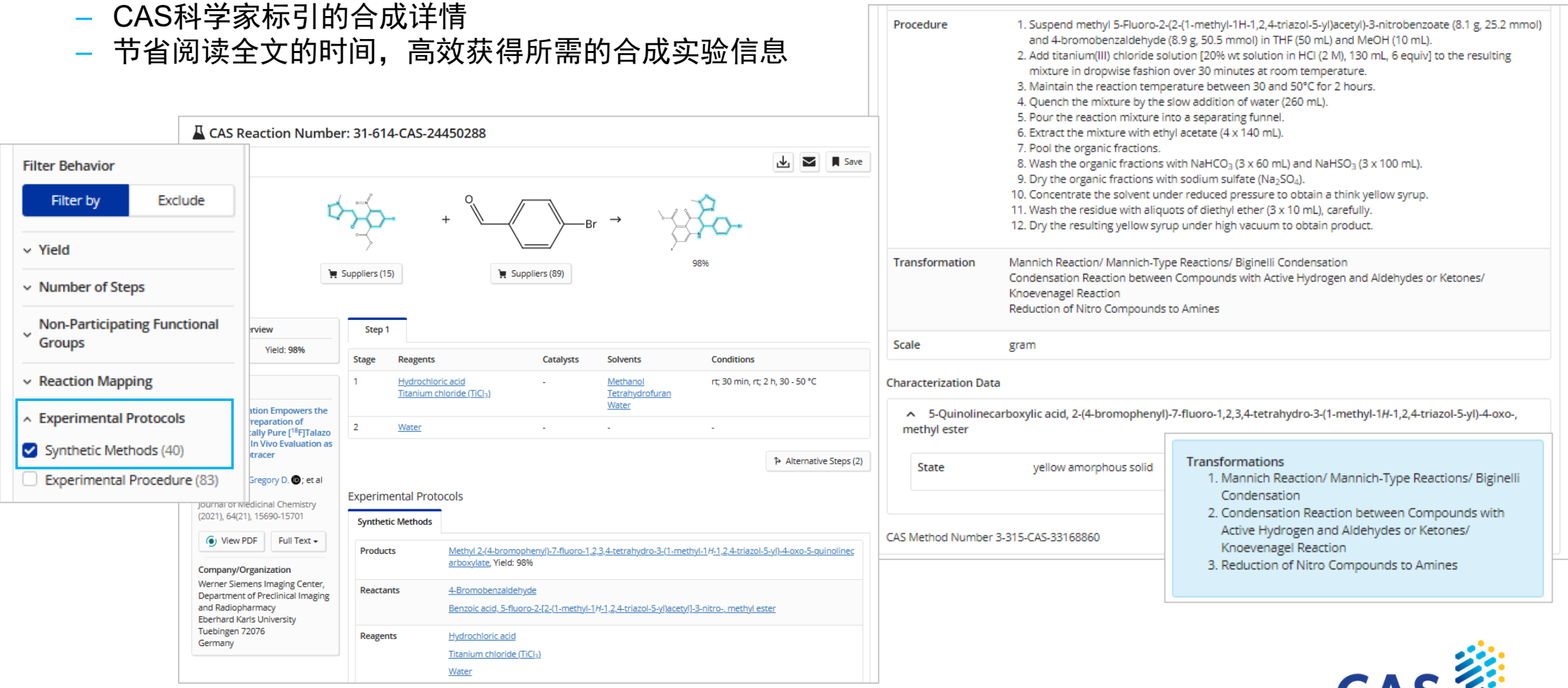
1. 反应检索方法：通过物质标识符、文献标识符、结构式以及文本信息等进行检索
2. 反应结果集筛选精炼：
   - Non-Participating Functional Groups 确定不参与反应的官能团
   - Search Within Results 可在结果集中进行二次筛选
3. 反应详情：Experimental Protocols 获取 CAS 科学家增值标引的反应详情
4. Retrosynthesis 支持化合物的反应路线预测（未知和已知化合物）
5. 支持查看反应路线详情和文献支持，也可以自定义选择替代路线或删除不感兴趣的路线

具体的实验方案怎么查、怎么选?

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

直观的合成实验详情 Synthetic Methods™

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



CAS
A division of the American Chemical Society

CAS 分析实验方法详情

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

Analysis of Vanadium in Stainless steel by Electrochemical extraction

CAS MN: 1-119-CAS-286328

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

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

实验原料

Source

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

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

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

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

Full Text | View in CAS SciFinder

Abstract

文献来源

Equipment Used

Cutting machine, Secotom-10, Struers
Ultrasonic cleaning unit, P 30 H, Elmasonic
Grinding machine, Labopol-6, Struers
Potentiostat, SP-150, BioLogic
Vacuum pump, BUSCHI
Graphite furnace atomic absorption spectrometer, AAnalyst 600, PerkinElmer
Autosampler, AS-800, PerkinElmer

分析仪器

Conditions

Instrument

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

分析条件

Instructions

Preparation of stainless steel process samples

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

Electrolytic extraction of stainless steel using 10% acetylacetone

1. Perform electrolytic extraction on a BioLogic SP-150 potentiostat.
2. Use 10% acetylacetone (10 v/v% acetylacetone, 1 w/v% tetramethylammonium chloride and methanol) as the electrolyte.
3. Use the sample as the working electrode and set the potential to 0.150 V vs. the standard calomel electrode (SCE).
4. Suspend the sample in the electrolyte in a platinum basket and use a platinum ring as a counter electrode.
5. Filter the electrolyte through a 0.05 µm pore size polycarbonate filter with the help of a BUSCHI vacuum pump.
6. Expose the sample to ultrasound in methanol and filter the methanol with the electrolyte.

Decomposition of inclusions

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

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

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

操作步骤

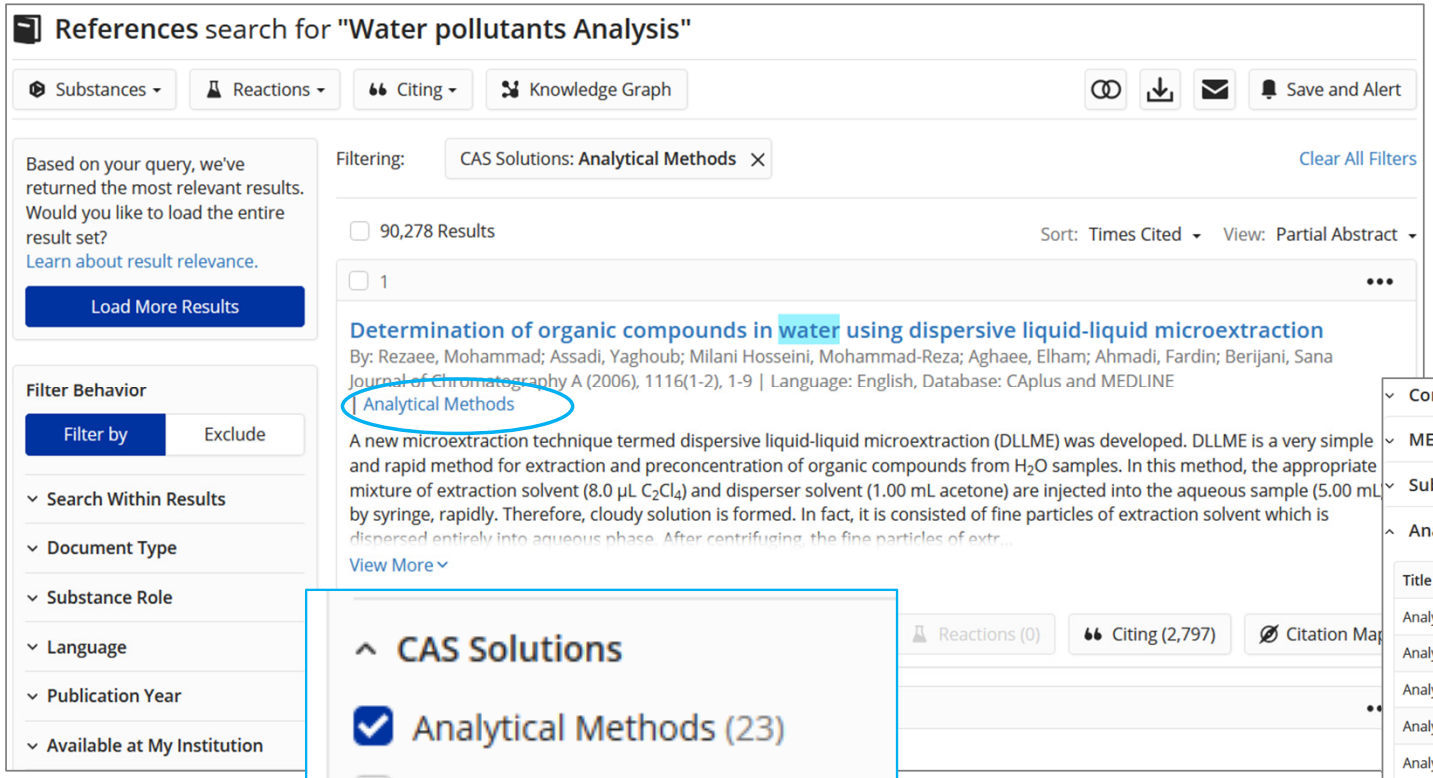
Validation

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

数据有效性

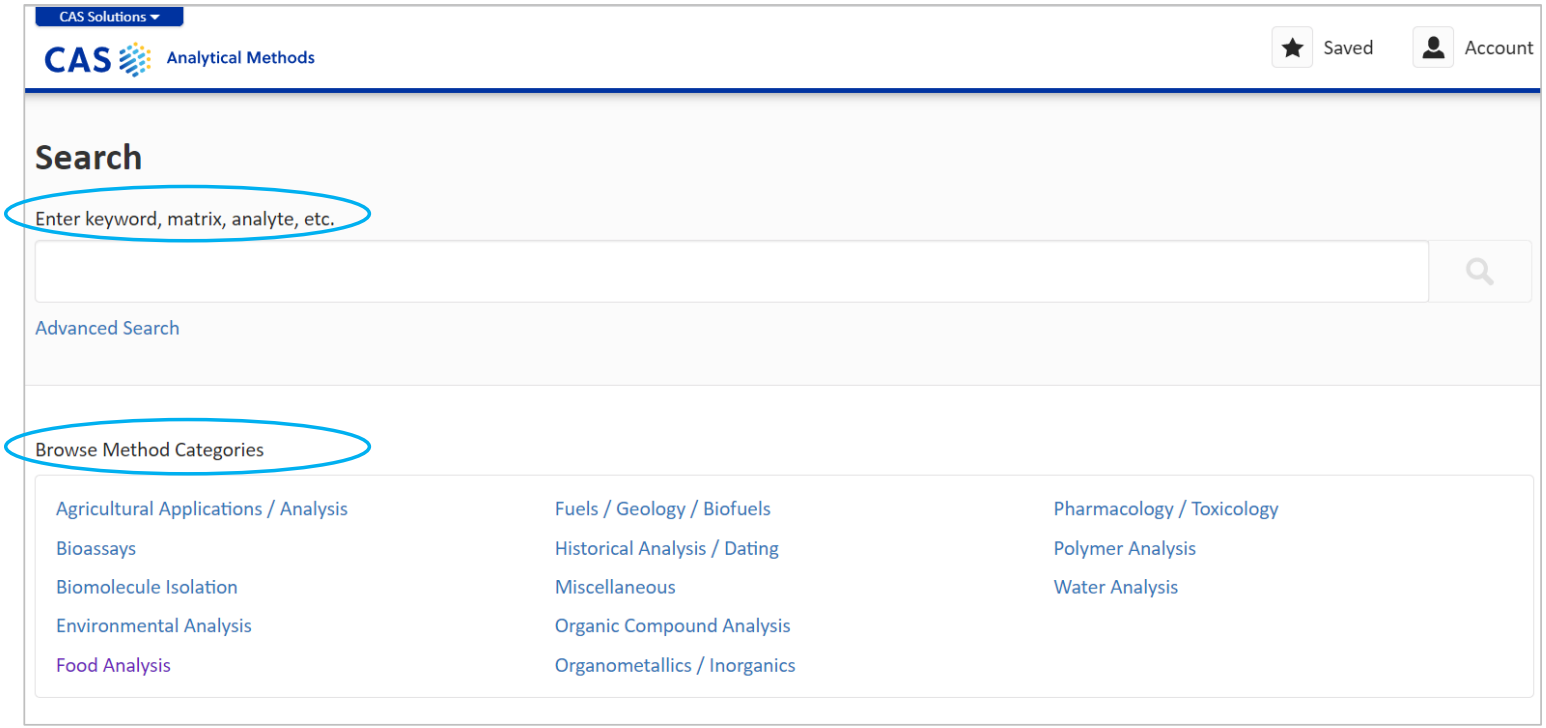
关注文献关联的分析实验方法?

方法一：文献结果集页面点击 CAS Solutions中的 Analytical Methods获得有具体分析实验方法的文献，从文献详情页中链接至分析实验方法



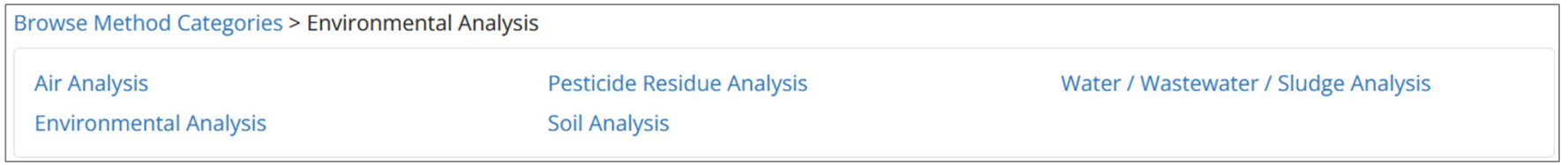
直接检索感兴趣的分析实验方法

方法二：登录 https://methods.cas.org 进行主题检索或分类浏览



方法分类: 13大类，45小类

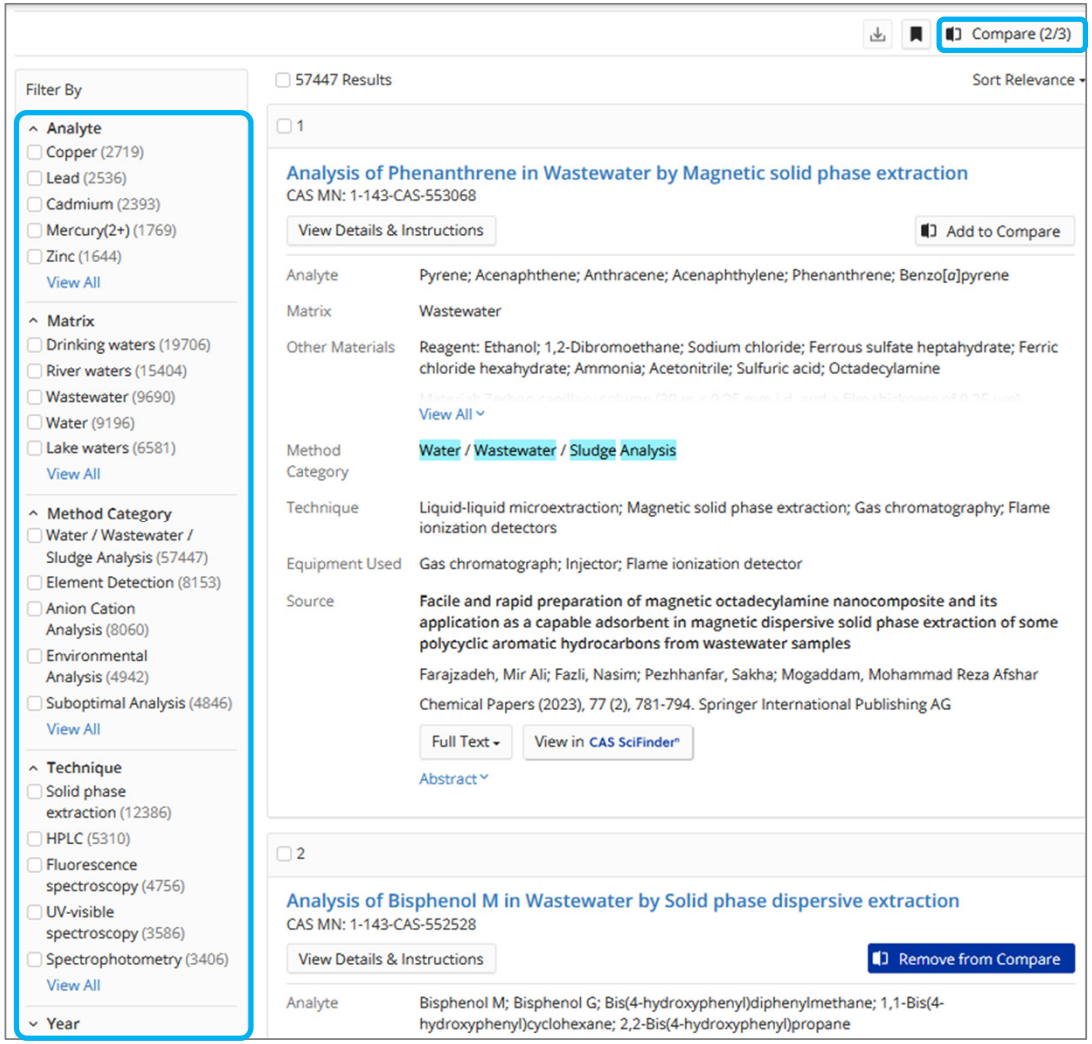
农业应用、生物鉴定、生物分子分离、环境、食品、考古、有机物、药学、毒理学等



气体/土壤/废水/杀虫剂残留分析

CAS
A division of the American Chemical Society

如何选择合适的分析方法?



- 根据待分析物、基质、方法类别、分析技术和发表年份筛选
- 查看分析原料、所用仪器和方法来源
- 支持多种分析实验方法对比

CAS
A division of the American Chemical Society

如何选择合适的分析实验方法?

	1	2	3
Title	Analysis of Phenanthrene in Wastewater by Magnetic solid phase extraction	Analysis of Bisphenol M in Wastewater by Solid phase dispersive extraction	Analysis of Anthracene in Drinking waters by Solid phase extraction
CAS Method Number	1-143-CAS-553068	1-143-CAS-552528	1-143-CAS-552414
Method Category	Water / Wastewater / Sludge Analysis	Water / Wastewater / Sludge Analysis	Water / Wastewater / Sludge Analysis
Technique	Liquid-liquid microextraction; Magnetic solid phase extraction; Gas chromatography; Flame ionization View All	Solid phase dispersive extraction	Gas chromatography; Solid phase extraction
Analyte	Pyrene; Acenaphthene; Anthracene; Acenaphthylene; Phenanthrene; Benzo[*a*]pyrene	Bisphenol M; Bisphenol G; Bis(4-hydroxyphenyl)diphenylmethane; 1,1-Bis(4-hydroxyphenyl)cyclohexane; 2,2- View All	Pyrene; Anthracene; Acenaphthylene; Benzanthracene; Acenaphthene; Naphthalene; Fluorene
Matrix	Wastewater	Wastewater; River waters; Bottled drinking water	Wastewater; River waters; Well waters; Drinking waters
Other Materials	Ethanol; 1,2-Dibromoethane; Sodium chloride; Ferrous sulfate heptahydrate; Ferric chloride View All	Sodium chloride; Sodium hydroxide; Thenoyltrifluoroacetone; Methanol; Iron chloride ($FeCl_3$); Ethanol; View All	Sodium chloride; 1*H*-Pyrrole; Methanol; Hydrofluoric acid; Sulfuric acid; Toluene; CBP-5 column (25 m × View All

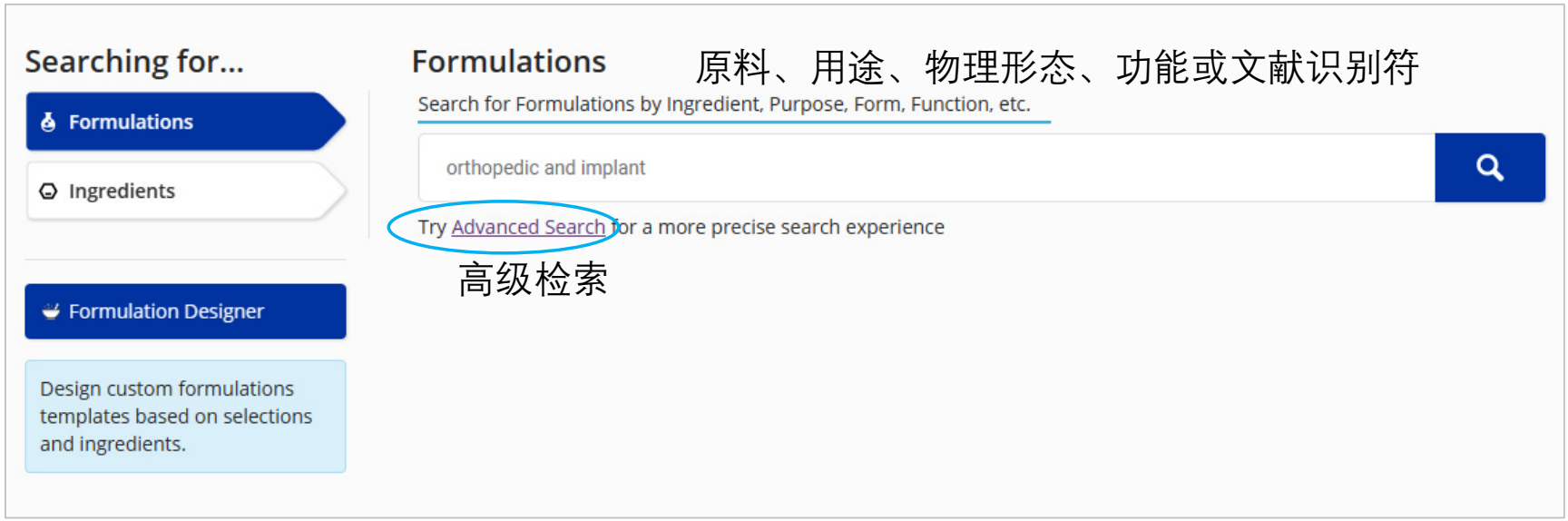
Preparation			
	Preparation of stock and working standard solutions of polycyclic aromatic hydrocarbons (PAHs) 1. Preapare a mixture stock solution of the selected PAHs at a concentration of 100 mg/L in acetonitrile (ACN). 2. Dilute this solution with deionized water to obtain working standard solutions. **Preparation of magnetic octadecylamine nanocomposite (octadecylamine@Fe_3O_4) by chemical co–precipitation method** 1. Add 100 mg of octadecylamine to 50 mL sulfuric acid solution (2 mol/L). 2. Adjust the temperature of the mixture to 80 °C, stir at a rate of 300 rpm for 20 min to dissolve octadecylamine and obtain a clear solution. 3. Add 0.53 g of ferric chloride hexahydrate ($FeCl_3.6H_2O$) and 0.36 g of ferrous sulfate heptahydrate ($FeSO_4.7H_2O$) to the solution. 4. Add 20 mL concentrated ammonia solution dropwise to obtain stable brownish color, indicating the generation of Fe_3O_4 nanoparticles. 5. Maintain the solution temperature at 80 °C and stir at 300 rpm. 6. Separate the produced magnetic	**Collection of water samples** 1. Collect waste water treatment plant (WWTP) effluent sample, a river water sample and a bottled water sample for analysis. 2. Allow the sample to stand overnight in the dark so that the sedimentation of particulate matter would occur. 3. Spike the decanted supernatants at three concentration levels (25, 75, 125 mg/L) in triplicate and then analyze. **Preparation of bisphenol standard solutions** 1. Prepare individual stock solutions of 500 ppm in methanol and store at 4 °C in the dark until use. 2. Prepare the working solutions of 1 ppb daily by appropriate dilution with 1:10 diluted NH_4Cl–NH_4OH buffer, pH 8.0. **Synthesis of solid phase Fe(TTA)$_3$ complex** 1. Weigh 4 mmol of HTTA into a 20 mL glass vial and dissolve in 10 mL ethanol. 2. Add 3 mL of 1 mol/L NaOH to dissociate thenoyltrifluoroacetone (HTTA) to its enolate, TTA. 3. Place a magnetic stirrer in the vial and stir the mixture for 5	**Preparation of standard solution of polycyclic aromatic hydrocarbons (PAHs)** 1. Prepare a stock solution of PAHs (10 mg/mL) in methanol and keep in the dark at 4 °C. **Preparation of polypyrrole (PPy) coated stainless steel mesh** 1. Dip bare stainless steel mesh in hydrofluoric acid for 30 min, rinse with deionized water to produce a rough surface. 2. Cut a circle with an inner diameter equal to the syringe's inner diameter from the etched stainless steel mesh. 3. Deposit PPy coating on the pretreated meshes by electrochemical deposition by a Metrohm electroanalyzer Model 797 VA computrace. 4. Perform deposition by cyclic voltammetry based on the three-electrode system including stainless steel mesh as the working electrode, an Ag/AgCl electrode as the reference electrode and a platinum wire electrode as the auxiliary electrode. 5. Perform electropolymerization of PPy film on the meshes in a nitrogen-saturated solution containing 0.1 mol/L pyrrole monomer and 0.5 mol/L sulfuric

详细的分析实验方法对比

CAS
A division of the American Chemical Society

研究课题在产品中的应用？配方/制剂的检索与设计

方法一：登https://formulus.cas.org 输入检索式



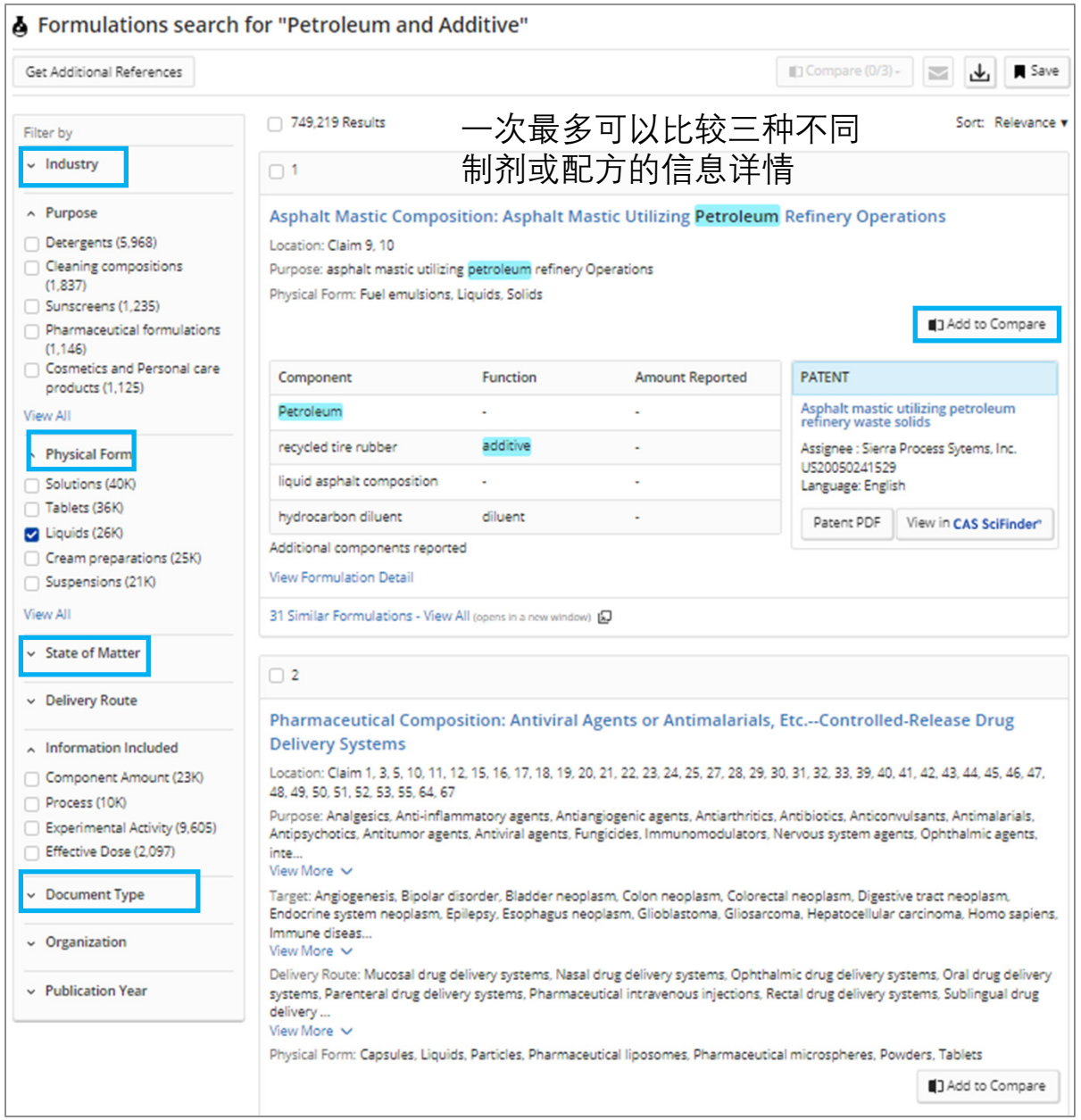
- 制药、化妆品、食品、农化、油墨、涂料等多领域中的配方
- 工艺、成分、目标成分的常见配伍成分、设计配方、探索合规要求等

配方/制剂结果集

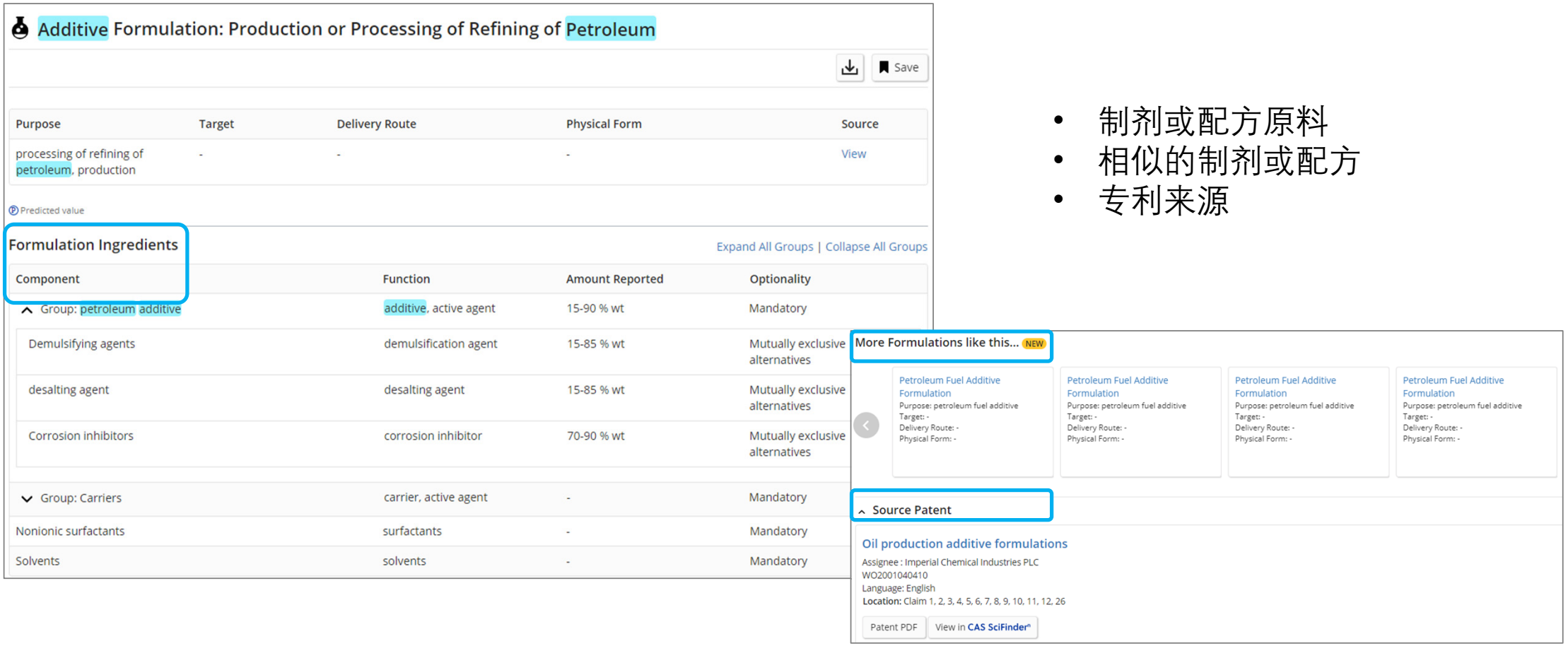
- 利用聚类项精简结果:

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

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



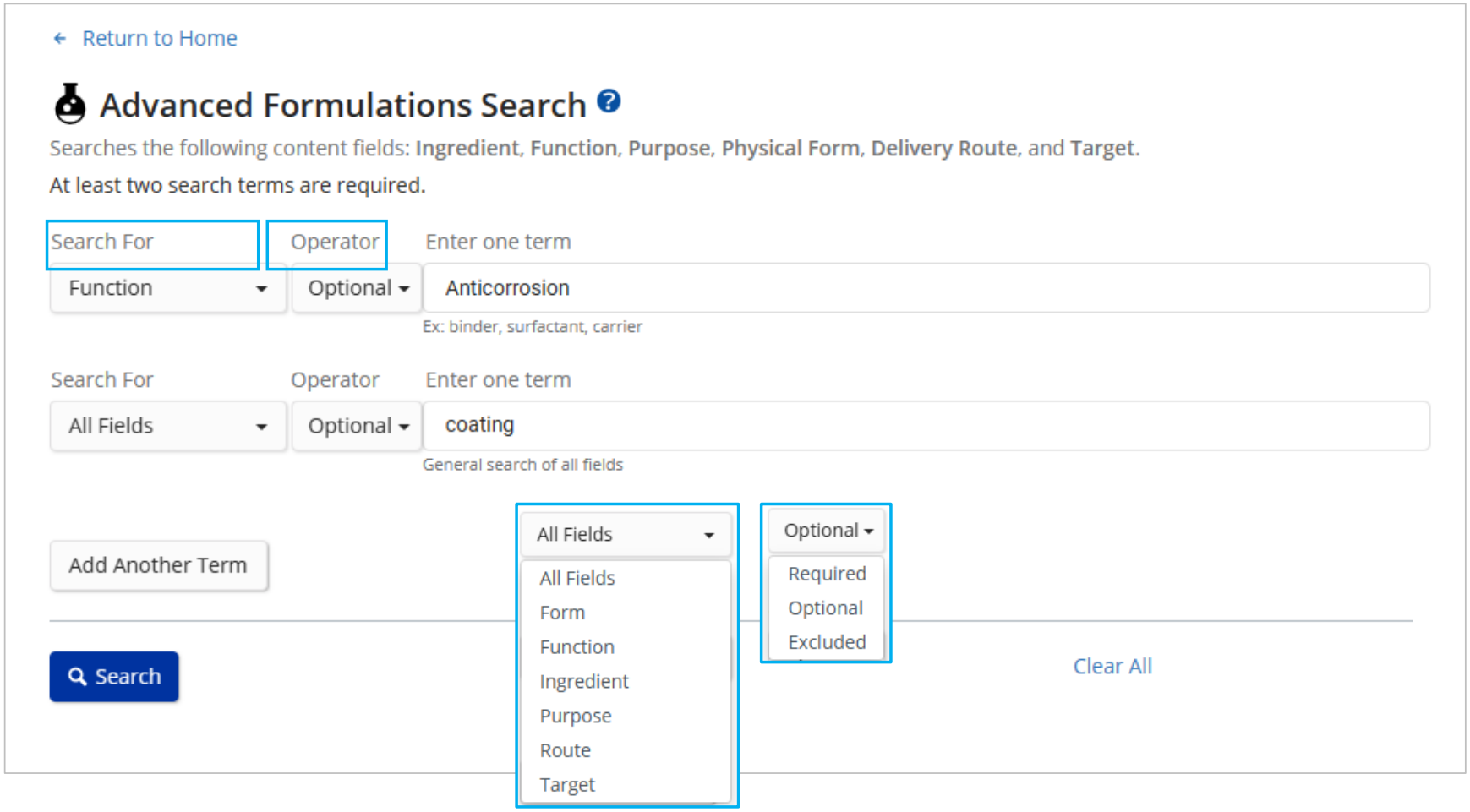
配方/制剂的制备？实验评估？



- 制剂或配方原料
- 相似的制剂或配方
- 专利来源

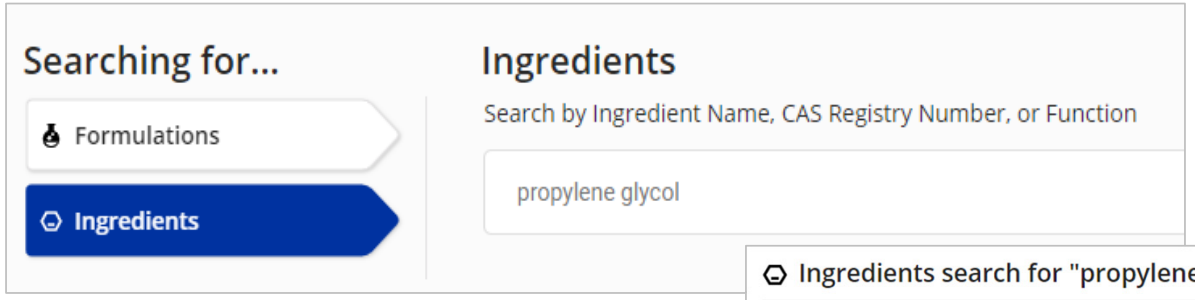
CAS
A division of the American Chemical Society

高级检索

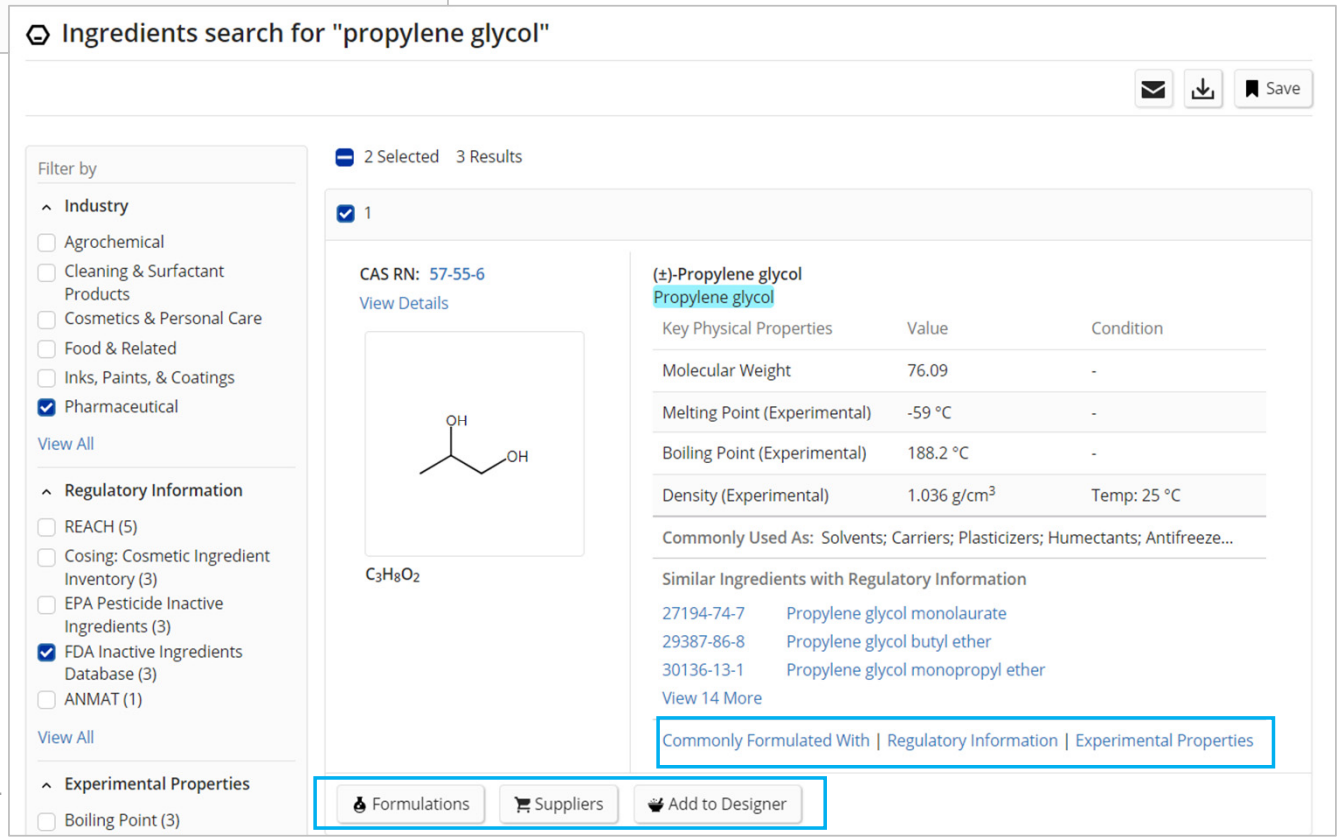


CAS
A division of the American Chemical Society

检索原料

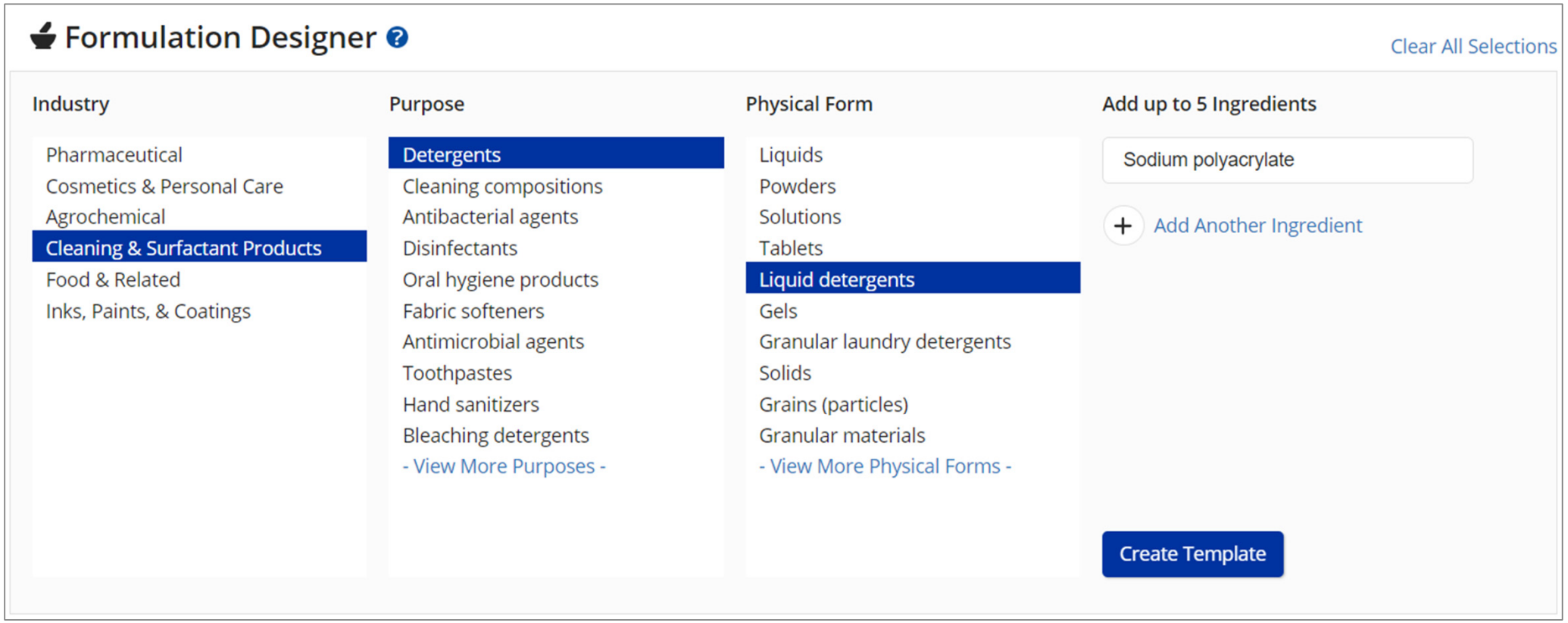


- 制剂或配方中，与该原料同时使用的其它配伍成分
- 管控信息及清单
- 实验属性



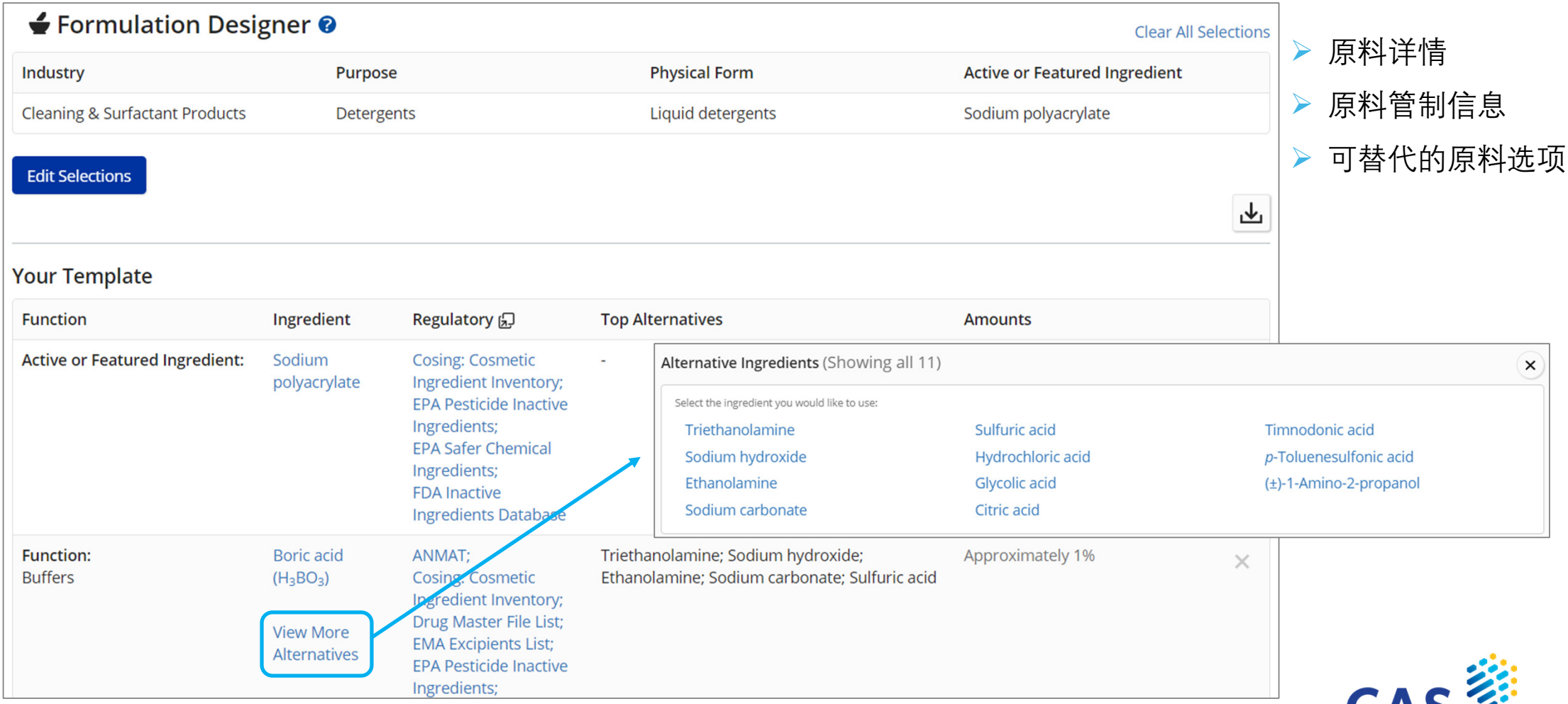
- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至设计工具 Formulation Designer

设计配方/制剂



CAS
A division of the American Chemical Society

设计配方/制剂

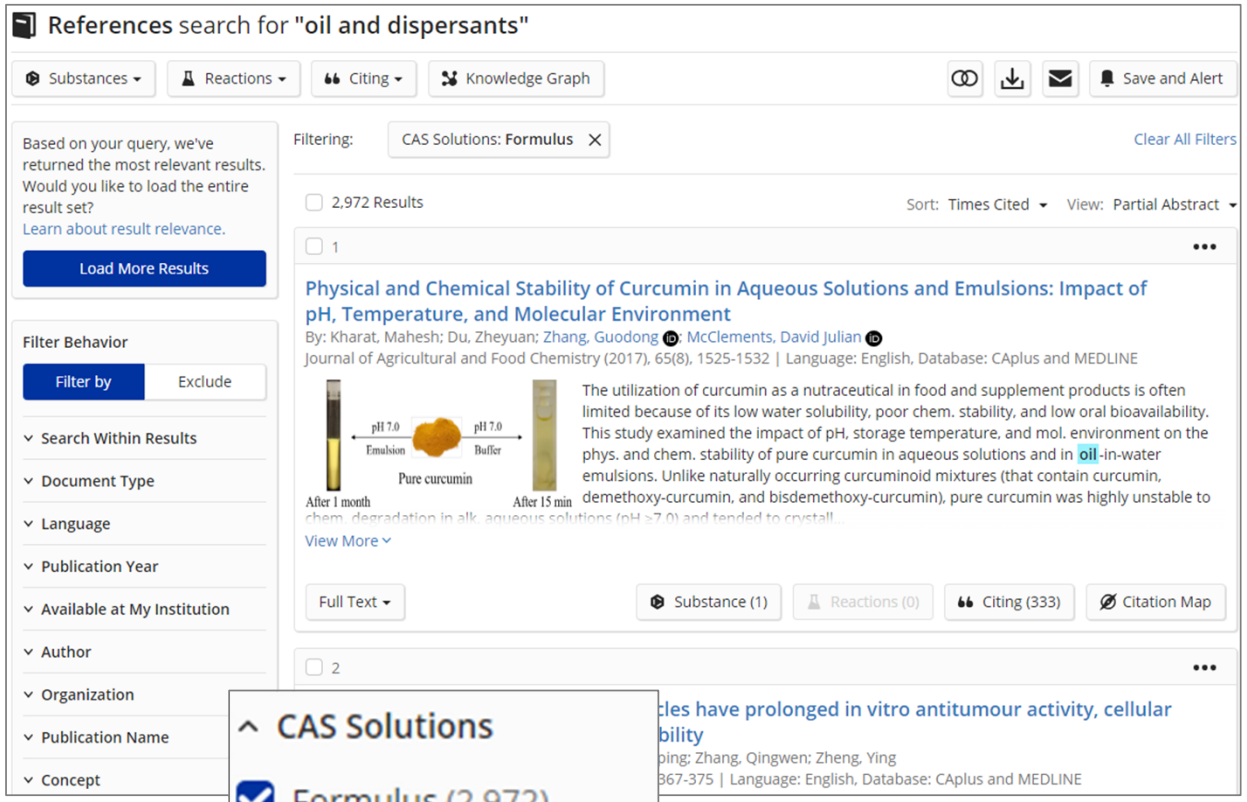


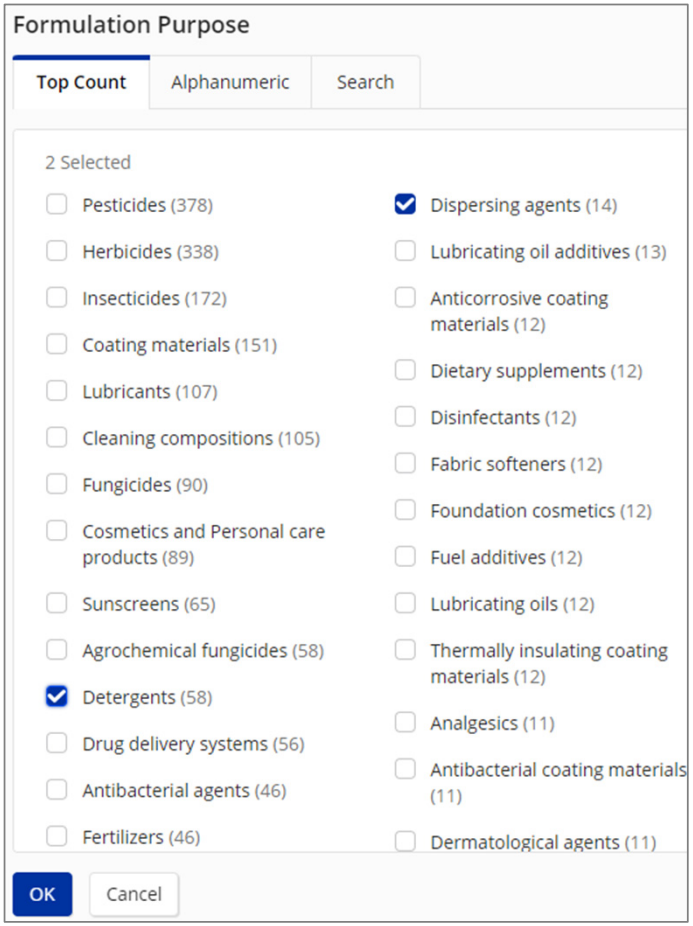
- 原料详情
- 原料管制信息
- 可替代的原料选项

CAS
A division of the American Chemical Society

文献关联的配方/制剂

方法二：在文献结果集页面，点击 CAS Solutions 中的 Formulus 获得有具体配方或制剂信息的文献，从文献详情页中链接获取





定位配方或制剂的功能目标

文献关联的配方/制剂

Formulations

Dispersant Composition: Dispersing Agents

View CAS Formulus® Detail

Location: Claim 1, 12, 14
Purpose: Dispersing agents

Component	Function	Amount Reported
Group: hydrocarbon fluid	active agent	-
polyamine-polyester reaction products	-	-

成分 功能 用量

Dispersant Composition: Dispersing Agents

View CAS Formulus® Detail

Location: Claim 1, 12, 14, 15
Purpose: Dispersing agents

Component	Function	Amount Reported
Group: hydrocarbon fluid	active agent	-
polyamine-polyester reaction products	-	-
metal dialkyldithiophosphate	-	<0.6 w %

Dispersant Composition: Dispersing Agents

View CAS Formulus® Detail

Location: Table 1
Purpose: Dispersing agents

Component	Function	Amount Reported
Maleic anhydride	-	-
pilot 900 oil	-	40 %
Polyaziridine	-	-

Dispersant Composition: Dispersing Agents

View CAS Formulus® Detail

Location: Table 1
Purpose: Dispersing agents

Component	Function	Amount Reported
Maleic anhydride	-	-
pilot 900 oil	-	40 %
Polyaziridine	-	-

CAS
A division of the American Chemical Society

实验方案检索小结

1. 利用 Synthetic Methods™ 查看文献中合成方法详情
2. 利用 CAS Analytical Methods 进行主题检索或分类浏览获得分析方法，或通过文献查看关联的分析实验及数据详情
3. 利用 CAS Formulus 检索原料、配方/制剂，或通过文献结果集获得关联的配方/制剂信息；利用配方设计工具启发产品配方的开发

学习资源

ACS Chemistry for Life®

运用化学的力量改善人们的生活

订阅号

服务号

CAS SciFinderⁿ 学习中心

2023 CAS SciFinder Discovery Platform 论坛录课

日期	主题
3月1日	解锁CAS SciFinder Discovery Platform新功能
3月8日	巧用CAS SciFinder Discovery Platform文献检索快速进阶
3月15日	万物互联 | CAS SciFinder Discovery Platform物质检索更高效
3月22日	CAS SciFinder Discovery Platform反应检索，不止A to B
4月4日	不止化学: CAS SciFinder Discovery Platform序列检索技巧
4月12日	新手入门开题和文献综述？ 巧用CAS SciFinder Discovery Platform事半功倍
4月19日	实验进展太慢？ 巧用CAS SciFinder Discovery Platform寻找启发
5月10日	毕业季|CAS SciFinder Discovery Platform助力论文写作及答辩准备
5月24日	毕业季|巧用CAS SciFinder Discovery Platform 做足升学与择业准备

CAS
A division of the American Chemical Society

CAS SciFinder Discovery Platform 专题论坛时间表

2023 年 9 月 — 12 月

CAS SCIFINDER DISCOVERY PLATFORM专题论坛涵盖多个科学研究领域，为您带来全面的检索思路和丰富的检索技巧。

直播时间为周五14:00 - 15:00。点击论坛主题即可注册、观看直播。

9月15日 | 专利专题论坛

9月22日 | 生物制药专题论坛

10月13日 | 高分子材料专题论坛

10月27日 | 金属有机与无机化学专题论坛

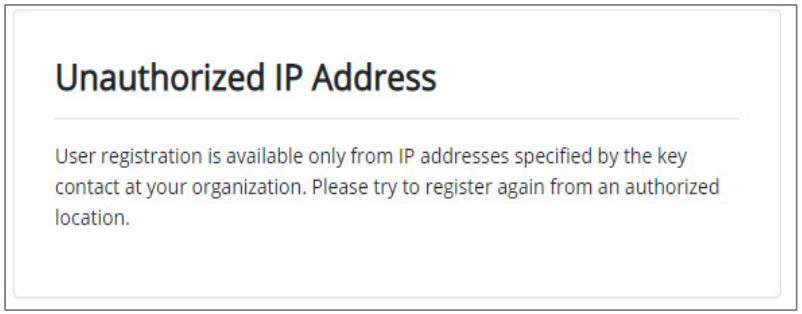
11月10日 | 食品与个人护理品专题论坛

11月24日 | 药物设计与合成专题论坛

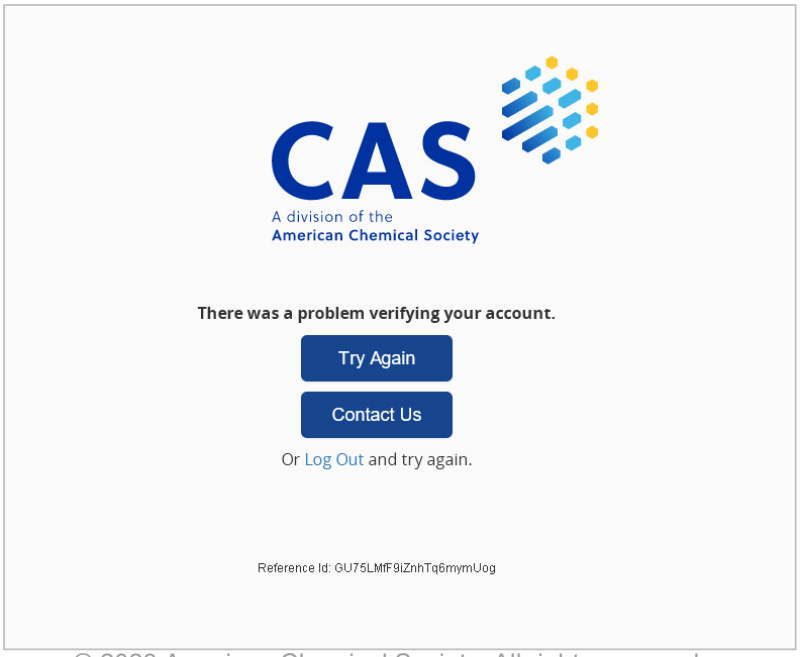
12月8日 | 电子信息与能源材料专题论坛

CAS
A division of the American Chemical Society

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



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

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

- 一人注册一个账号
- 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

THANK YOU!

CAS
A division of the American Chemical Society

美国化学文摘社北京代表处
ACS International, Ltd. – Representing CAS
Unit 1010, Tower B, Raycom InfoTech Park
2 Kexueyuan Nanlu, Haidian District, Beijing, China
+86-10-6250 8026/7
cas.org

CAS
A division of the American Chemical Society

扫描上方二维码答题

CAS
A division of the
American Chemical Society