CAS SciFinder Discovery Platform™

全面高效获取科技信息

潘娜 博士
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美国化学文摘社(CAS)北京代表处

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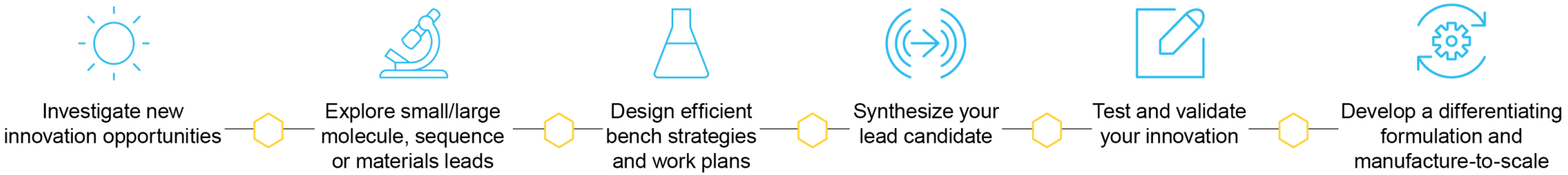
大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查找分析实验方法和制剂/配方详情?
- 常见问题Q&A

CAS 独特的解决方案和能力

助您加速创新之旅

Informing and accelerating the innovation process end-to-end



CAS SciFinder Discovery Platform™

为研究人员提供他们所需要的信息，加速科学发现市场化并优化利润率

STN IP Protection Suite™

确保知识产权得到保护，并找到机会拓展新市场

CAS Custom Services℠

定制数据、分析和见解，最大化信息资产的价值，推动数字化成功

独特的内容 |最大科学数据合集

专业技术 |为整个创新之旅提供信息

专业知识 | 多学科背景的科学家和技术专家

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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 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 Formulus

专业的制剂/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

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CAS 独特的内容合集

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

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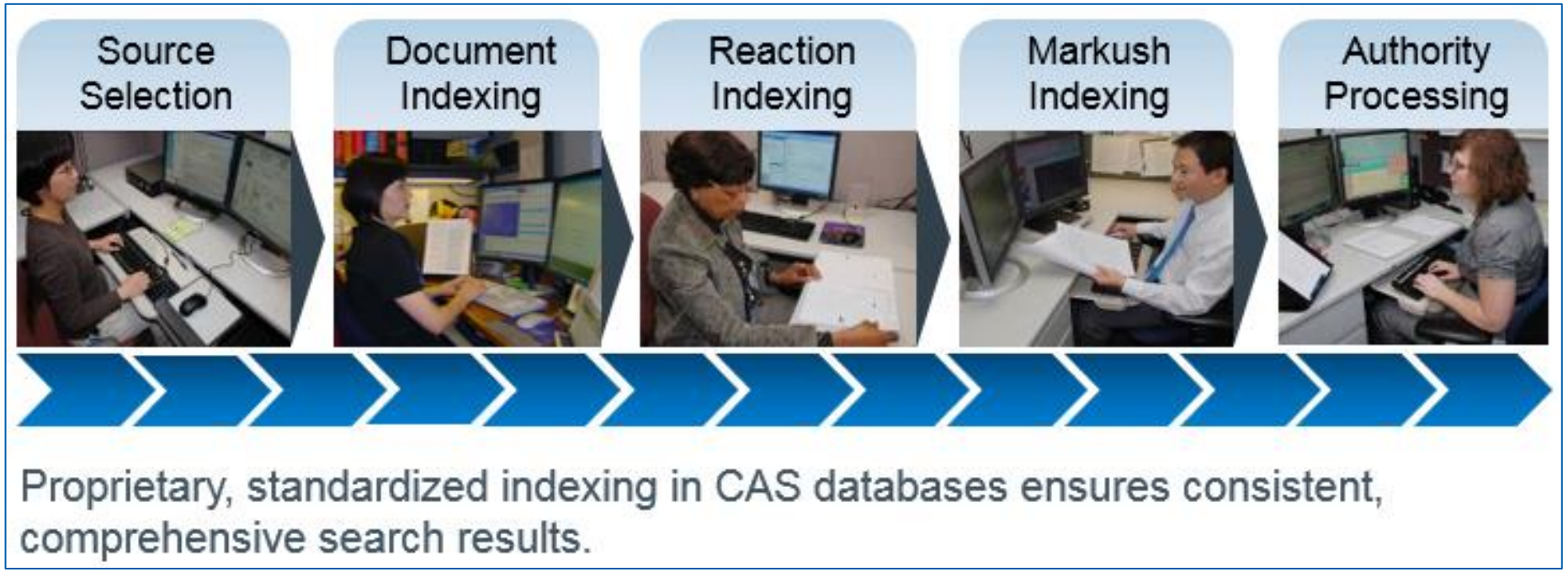
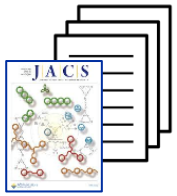
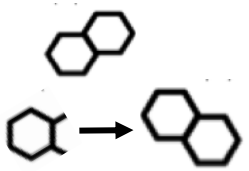
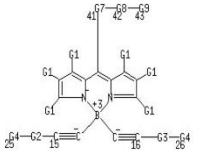
CAS 科学家的智力标引





1990
Smith, M.
anthracene





Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

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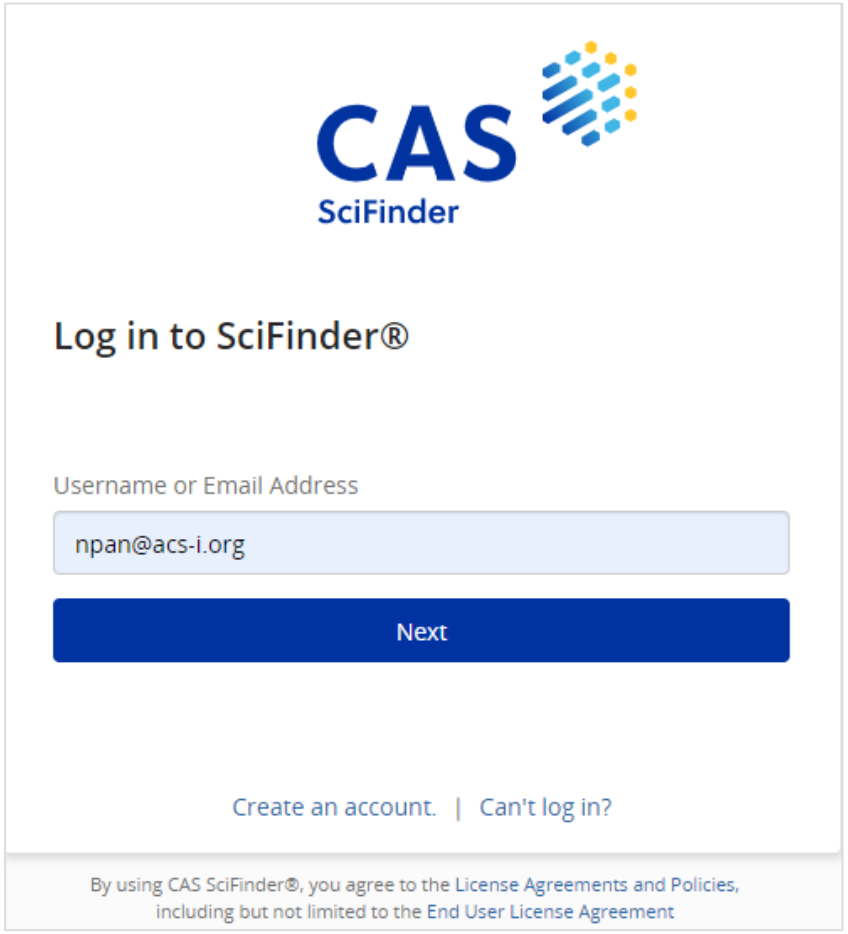
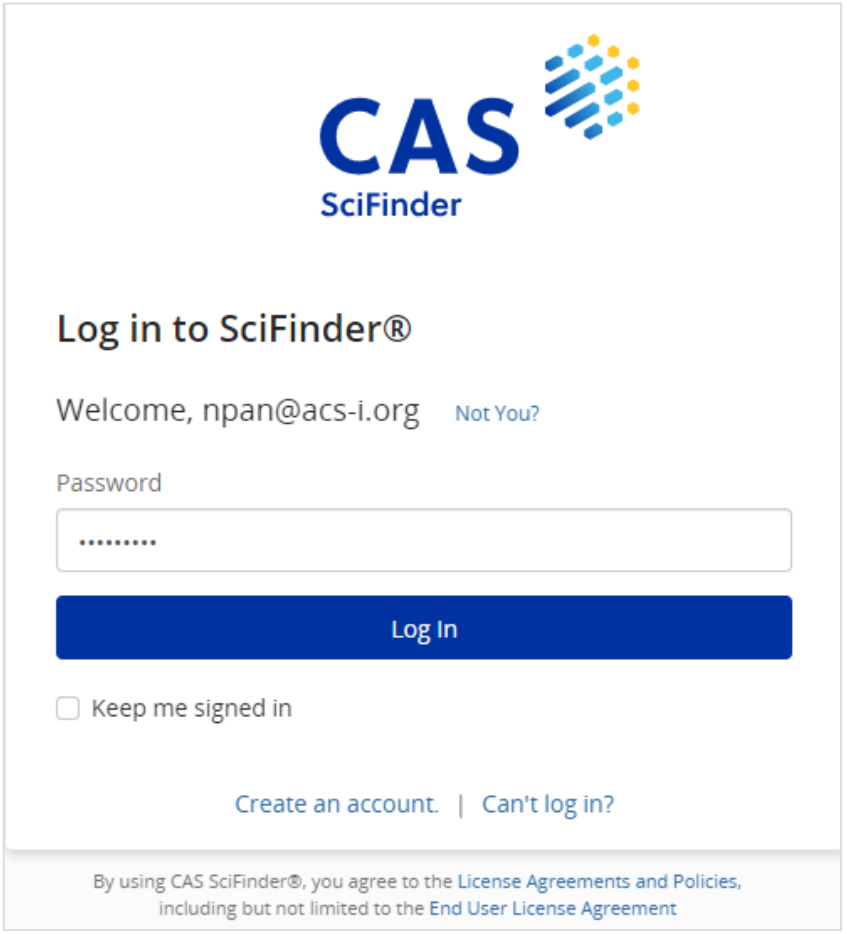
CAS SciFinder 登录网址：https://scifinder-n.cas.org/





使用CAS SciFinder账号登录

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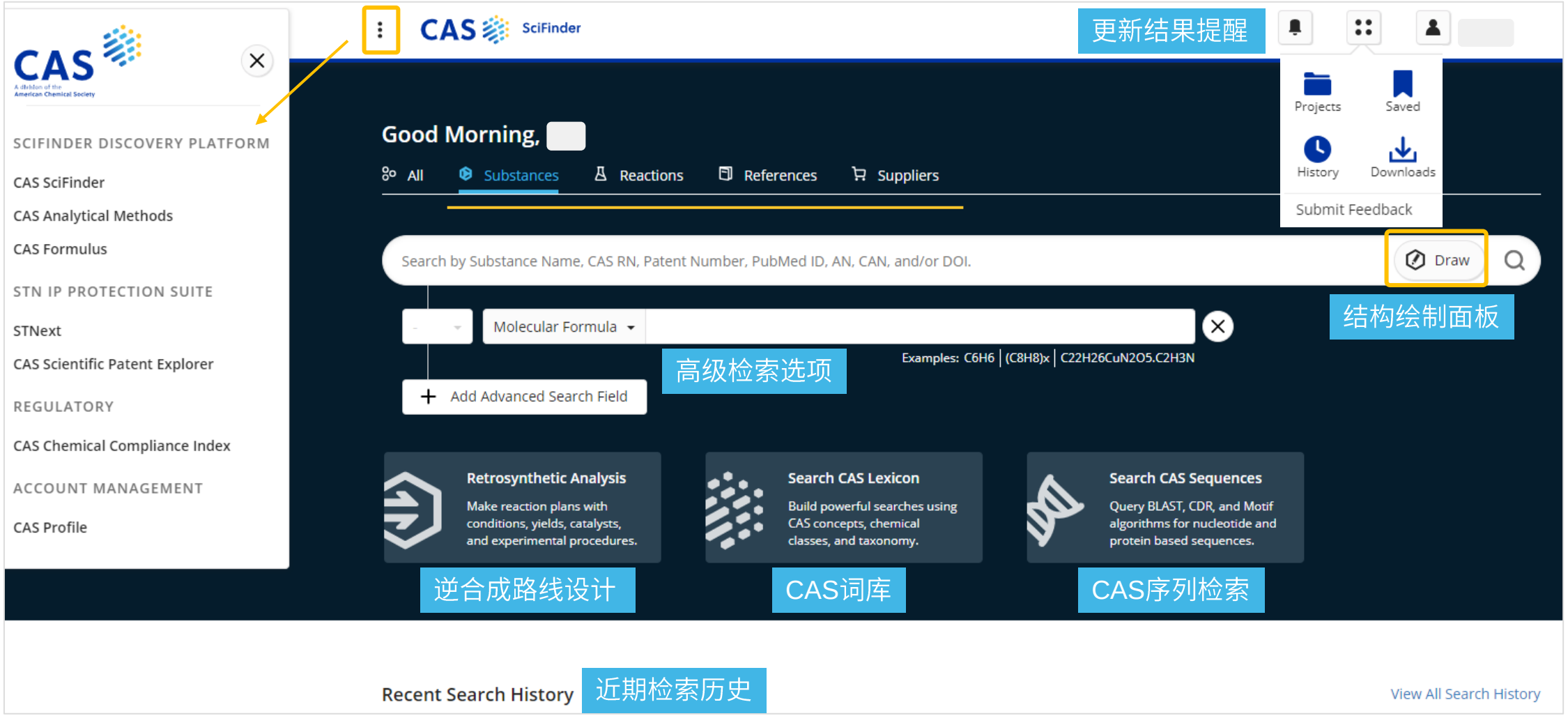
CAS SciFinder 主界面



大纲

- CAS SciFinder Discovery Platform 简介
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  - 如何开展文献调研?
  - 如何聚焦某类物质?
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  - 怎么查、怎么选具体的实验方案?
- 常见问题Q&A

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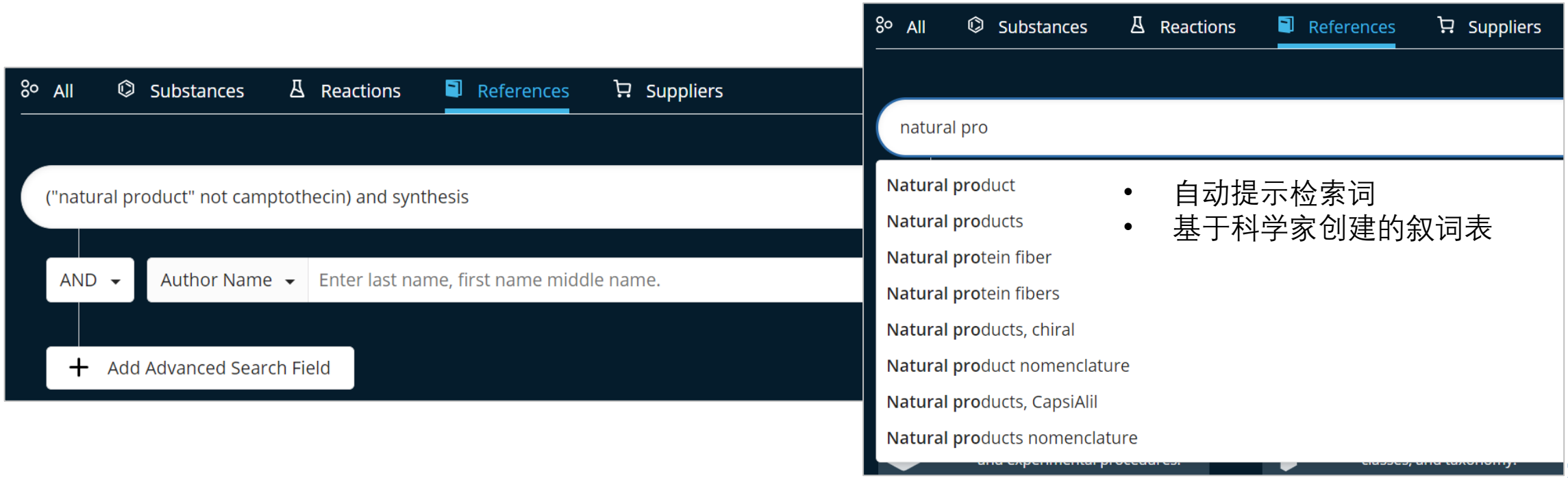
1. 如何开展文献检索?

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

1.1 如何精准构建检索主题?

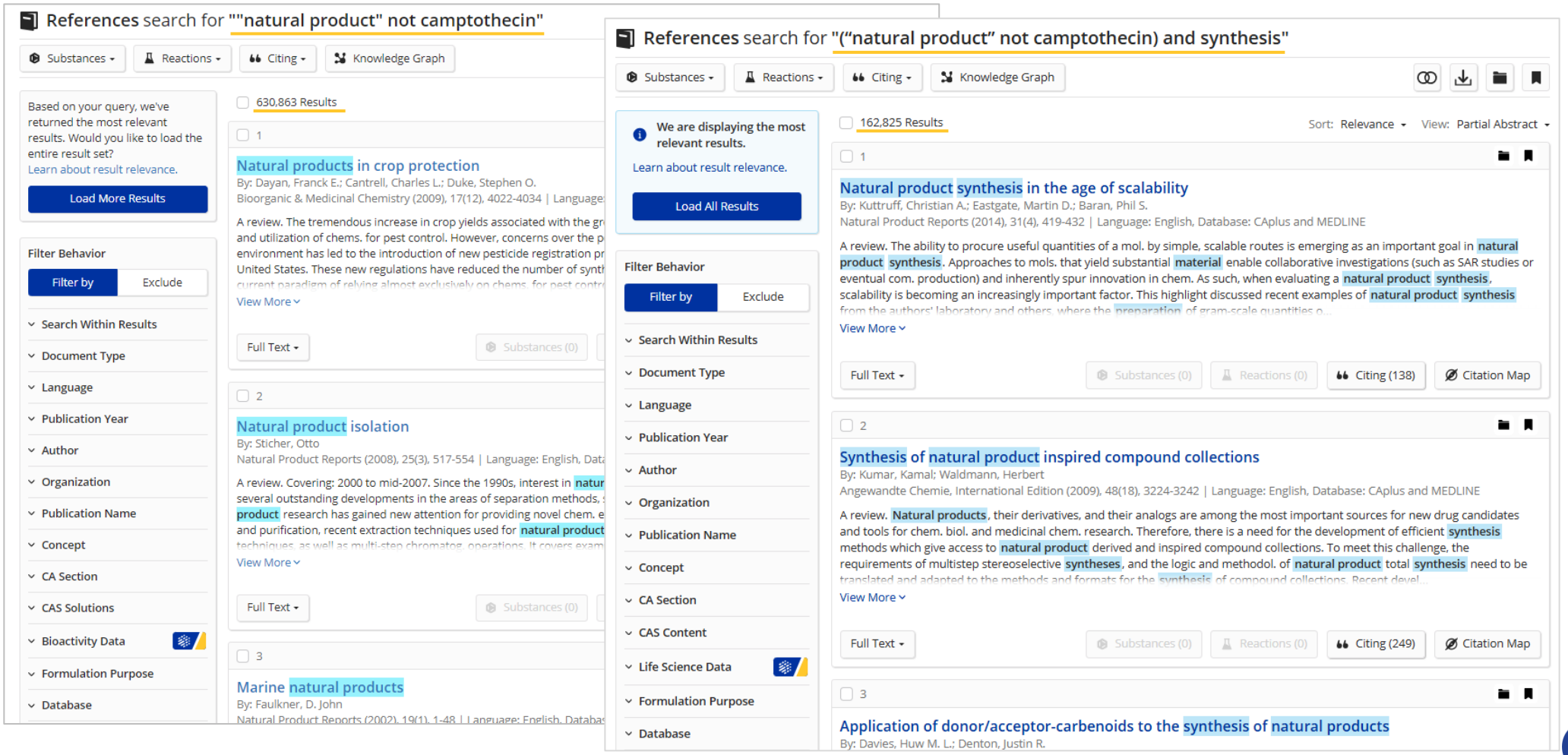
- 支持使用：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
- 布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not
- “ ”不允许词形变化，但可出现单数或复数；( ) 优先运算，括号中表达式还可以和其他术语交互
- 支持通配符*或？，*代表0或多个字符；？代表0或1个字符



1.1 如何精准构建检索主题?

主题词示例:

("natural product" not camptothecin) and synthesis（天然产物排除喜树碱，合成）



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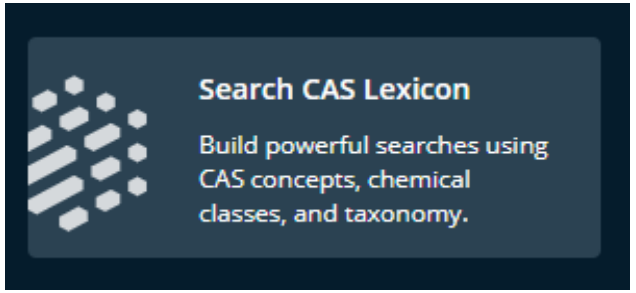
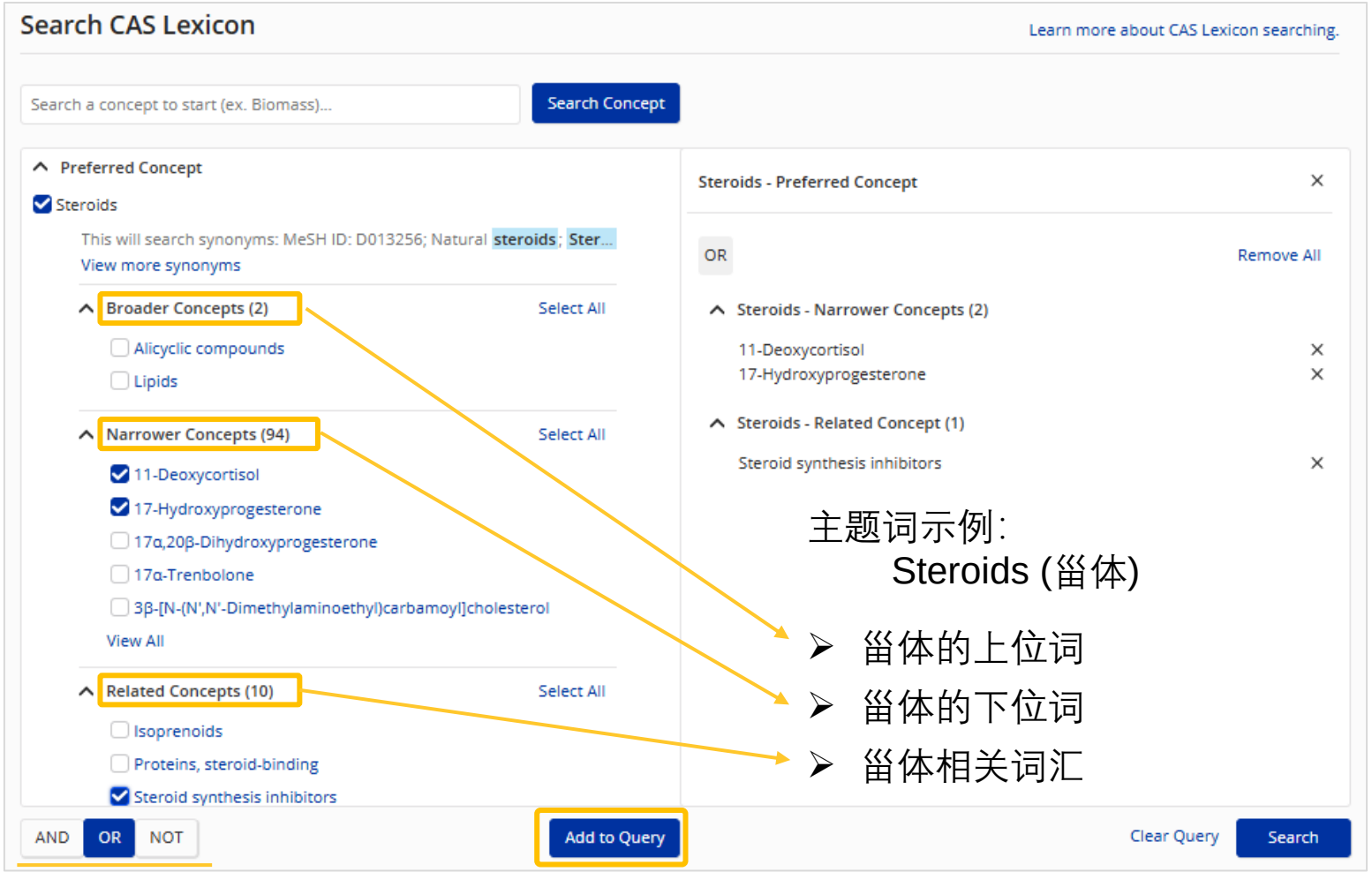
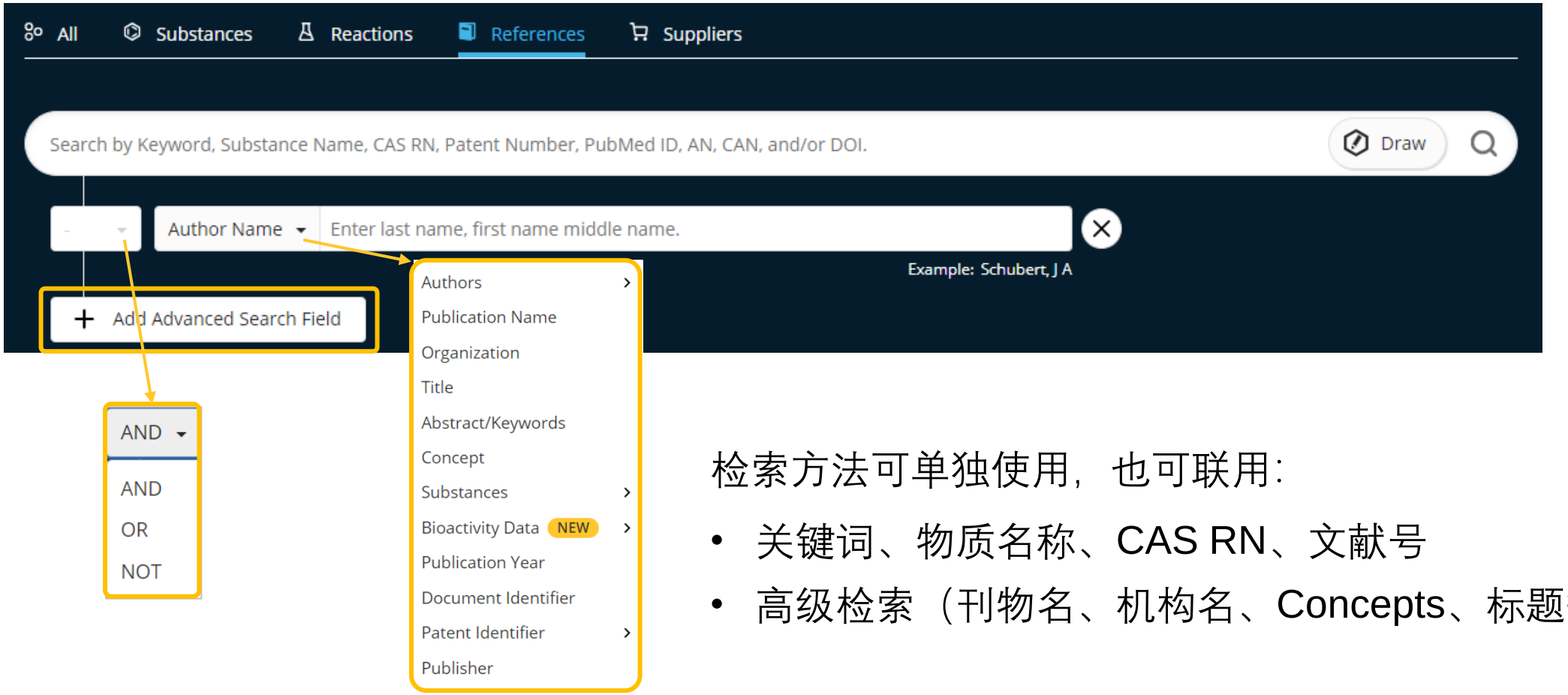
如何选择概念词？借助CAS Lexicon词库



- CAS科学家标引的概念词（Concepts）和重要物质
- 选择感兴趣的技术词来建立检索式（最多可用1000个词）



自定义组合检索



检索方法可单独使用，也可联用：

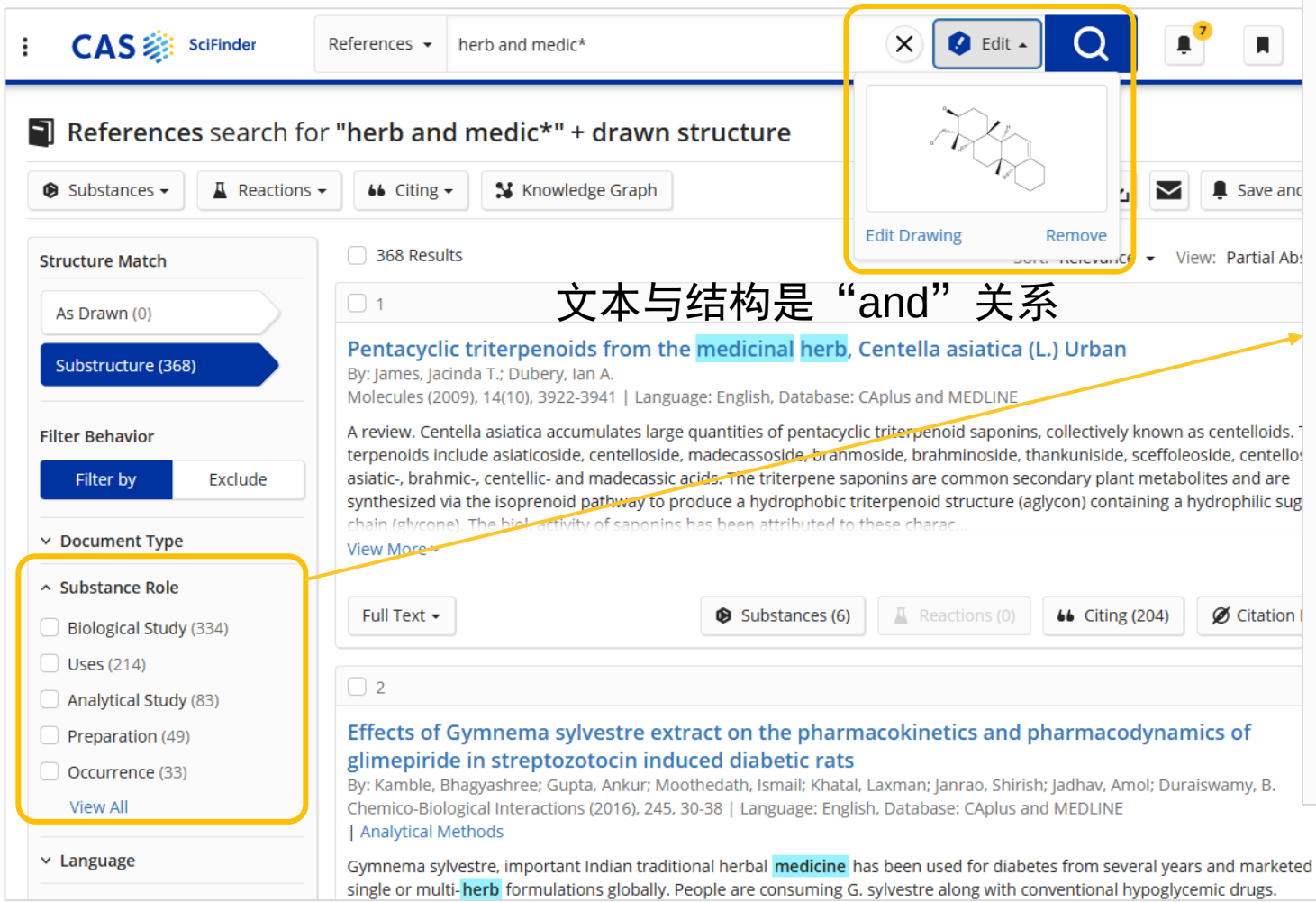
- 关键词、物质名称、CAS RN、文献号
- 高级检索（刊物名、机构名、Concepts、标题等）

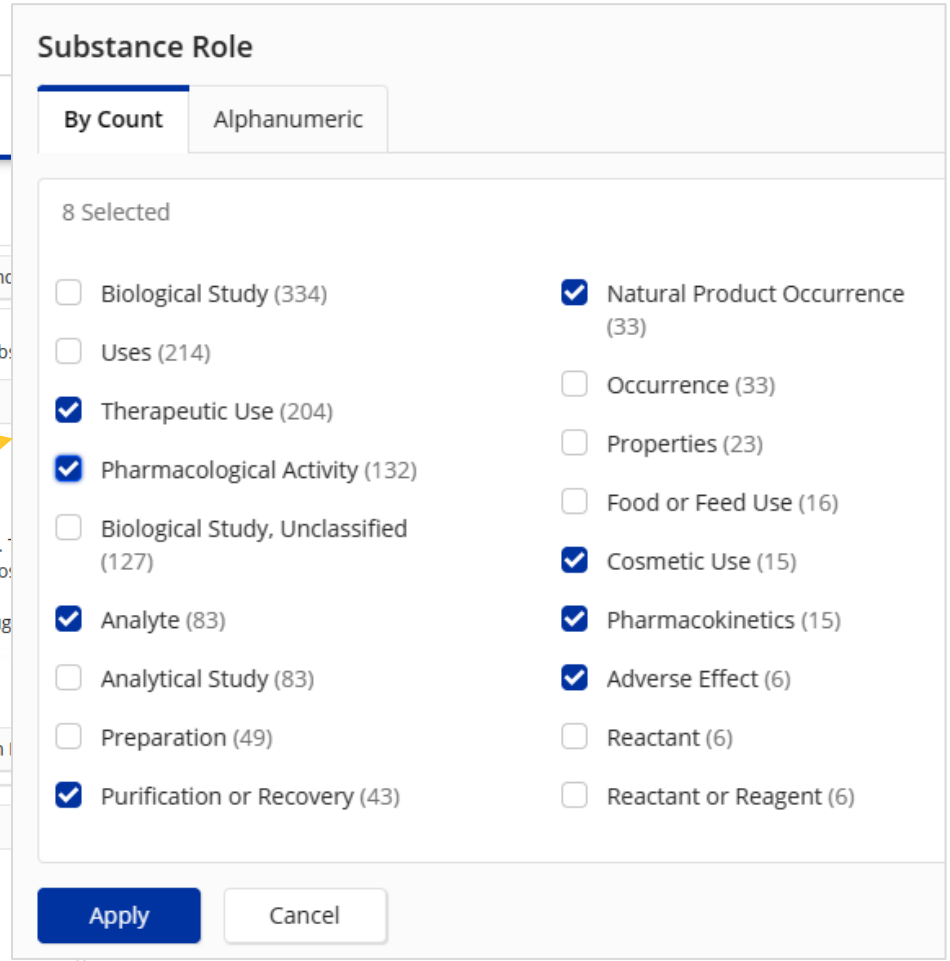
1.2 如何获得结构相关的文献?

示例：关注植物或药物中特定的结构骨架化合物

策略：从References出发，主题词+结构联用检索

定位物质在文献中的研究角色





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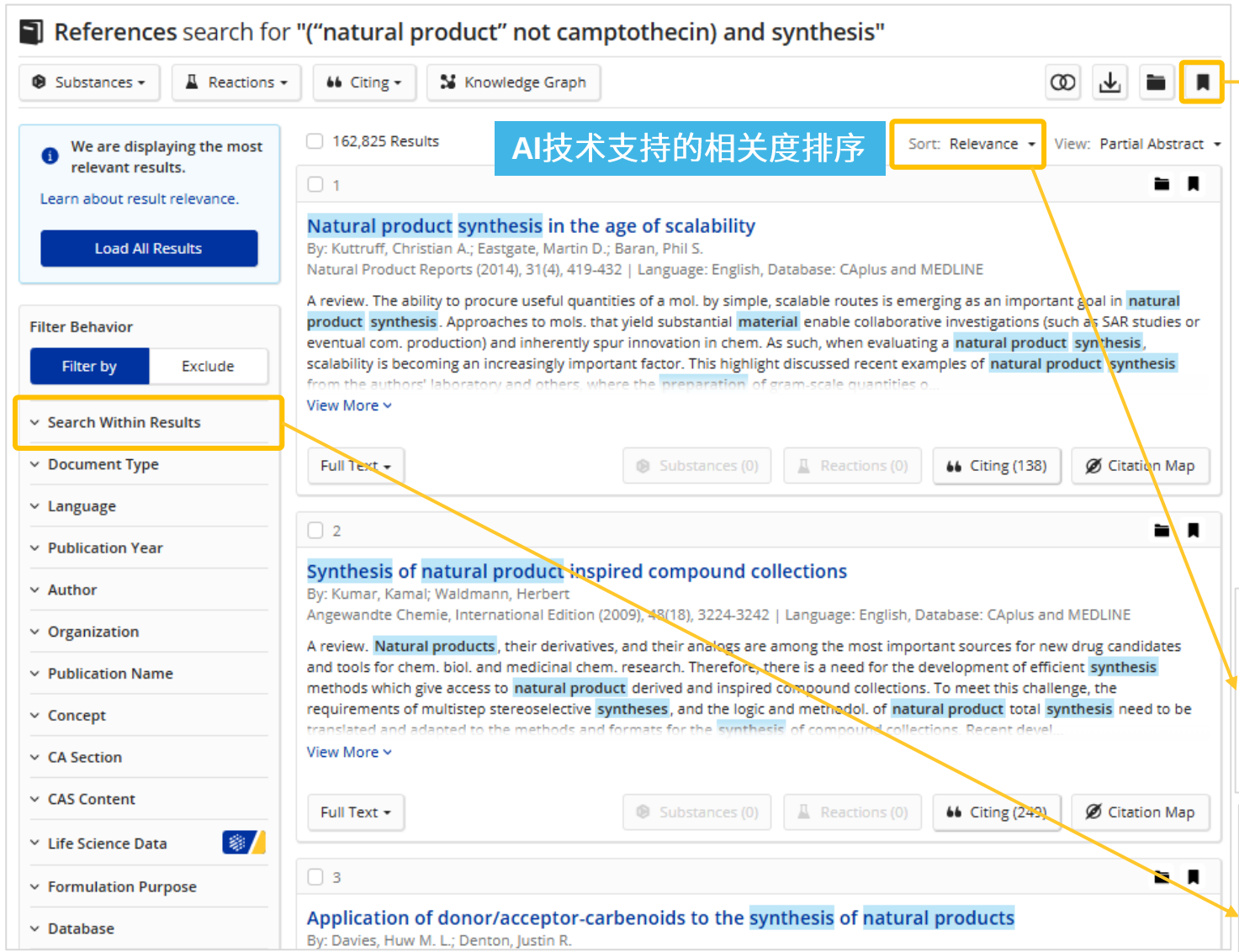
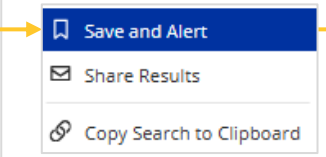
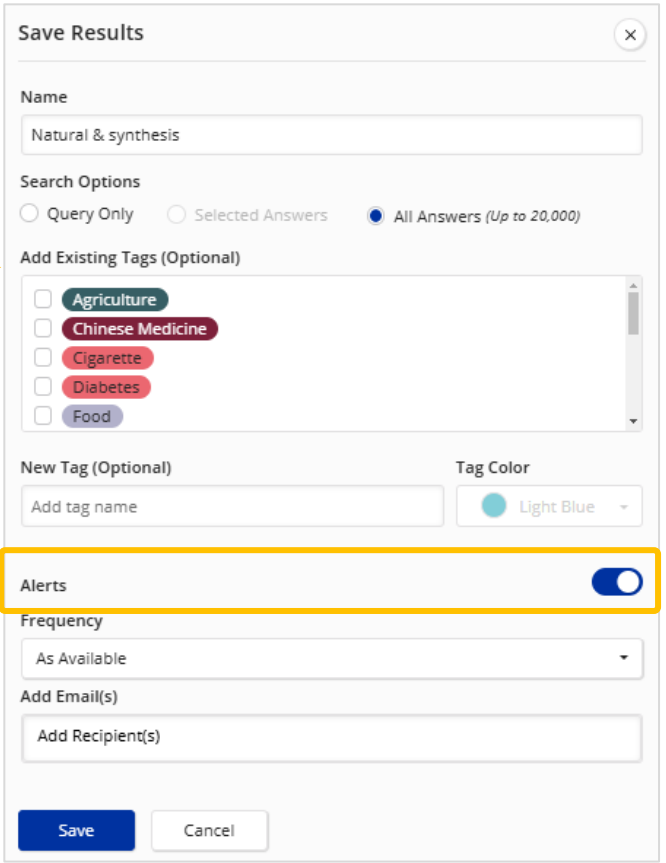
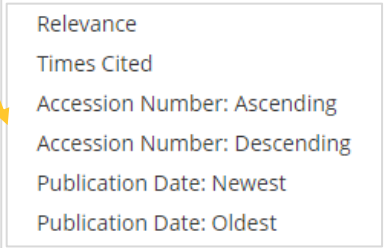
1.3 文献结果分析与筛选



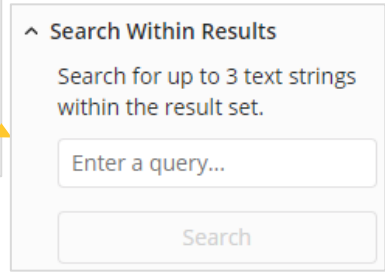




定题追踪



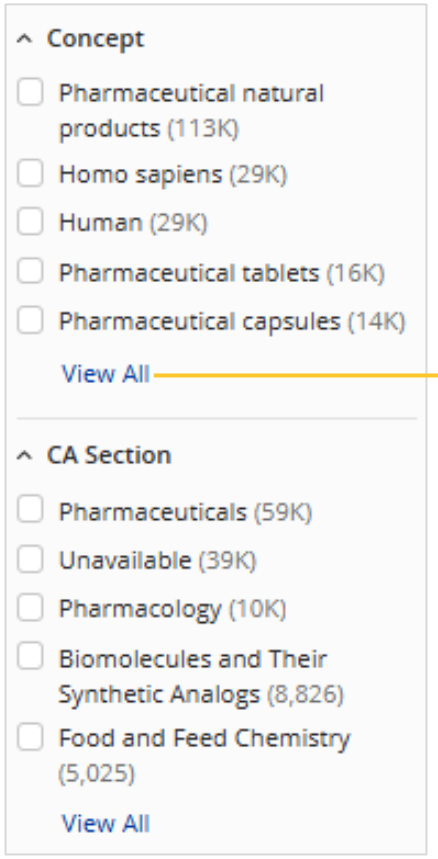
排序方式



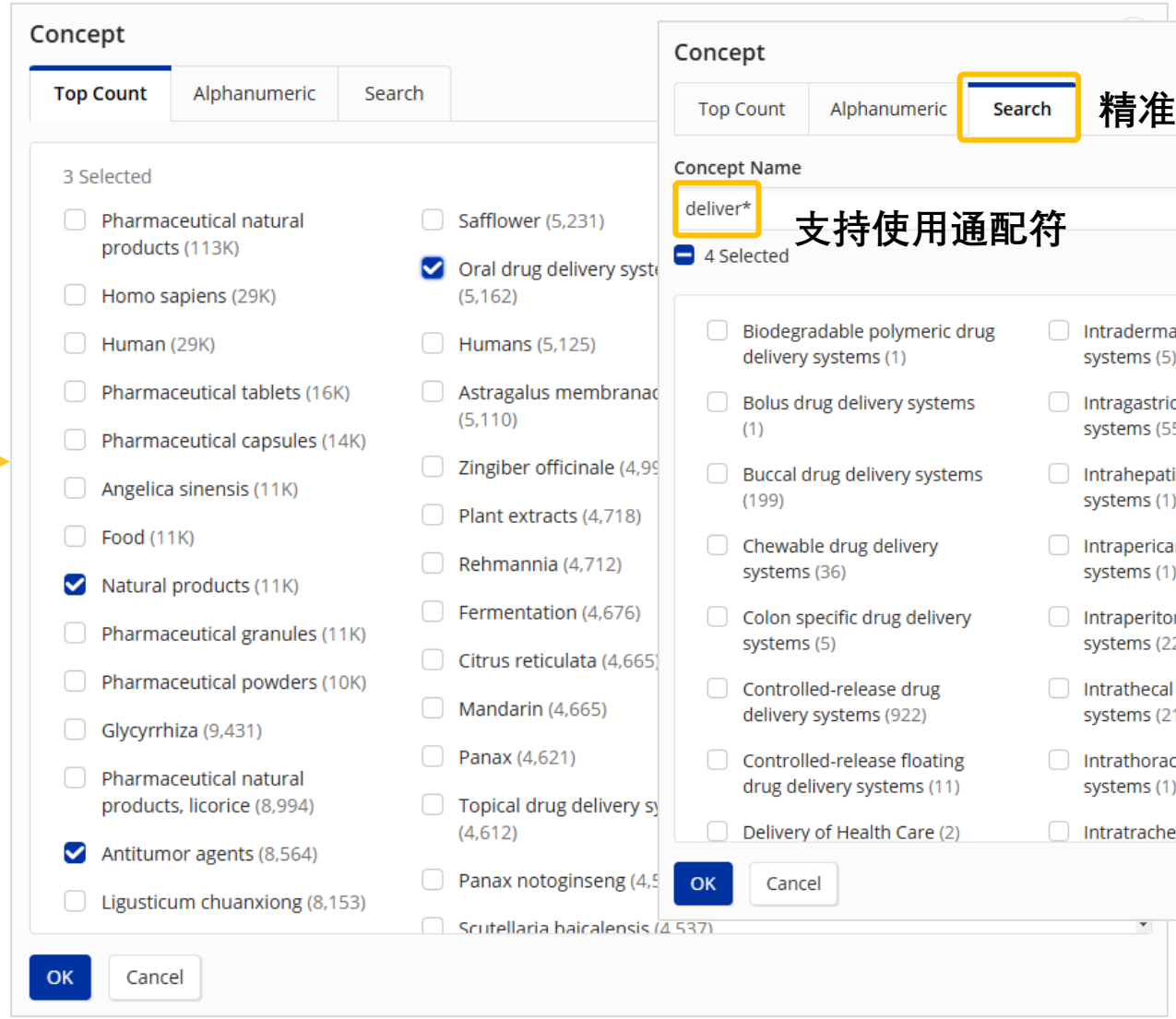
结果集的二次检索

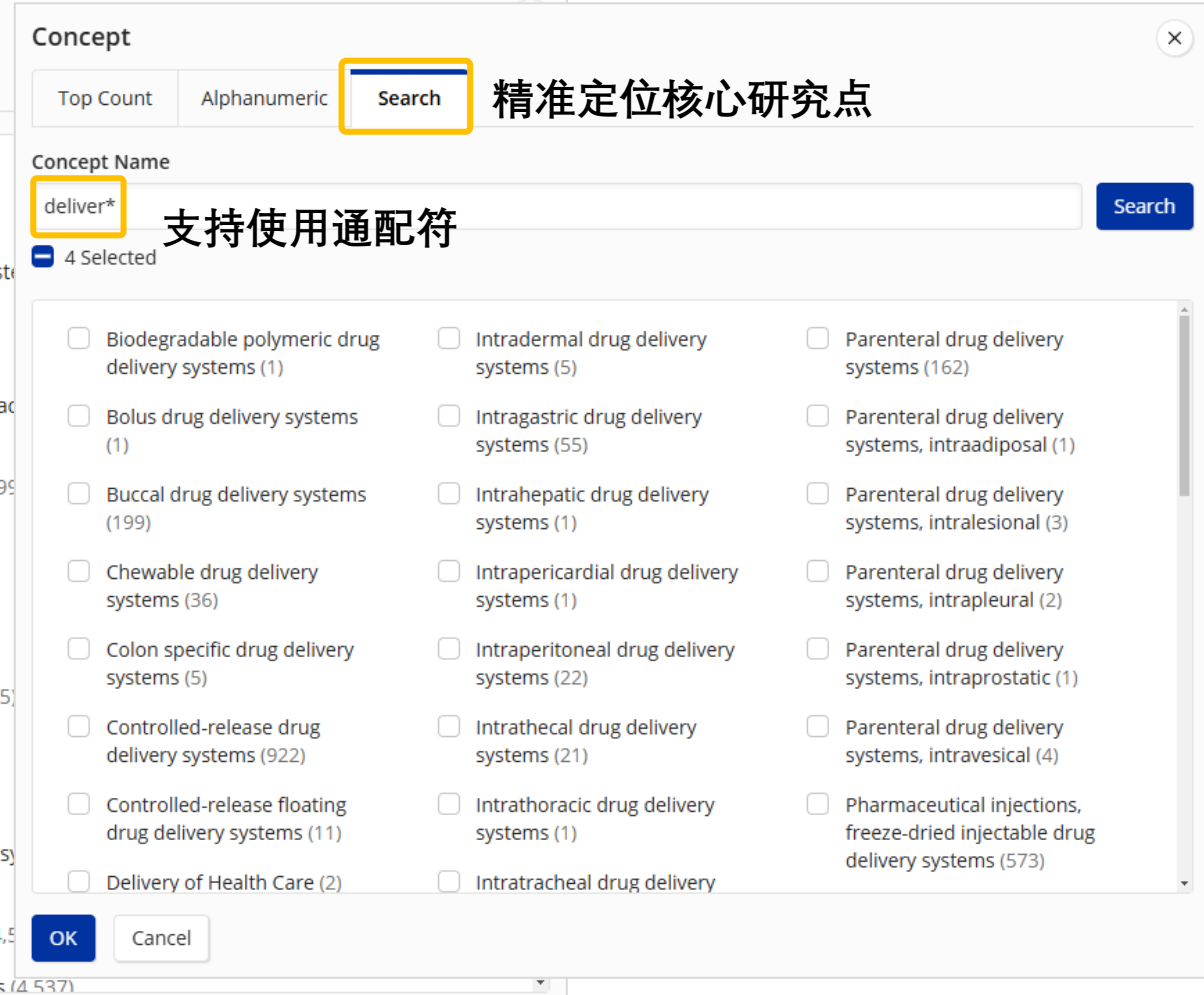
筛选工具 CA Section, Concept

聚焦核心研究点



纵览学科研究方向





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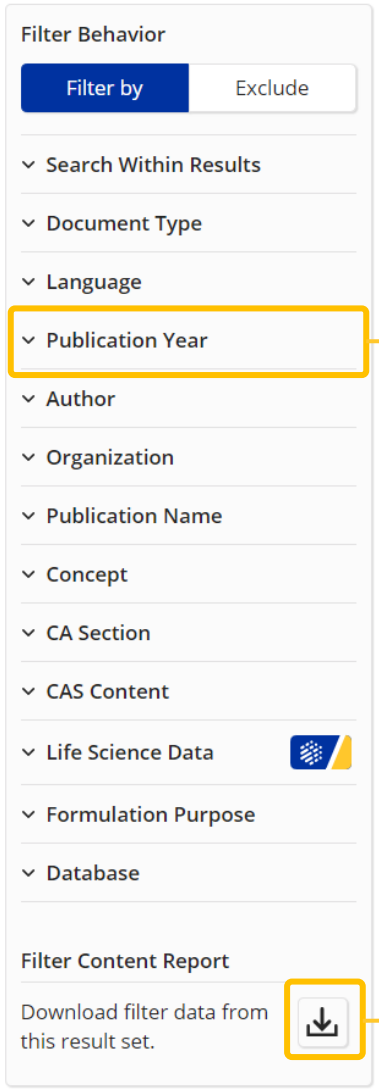
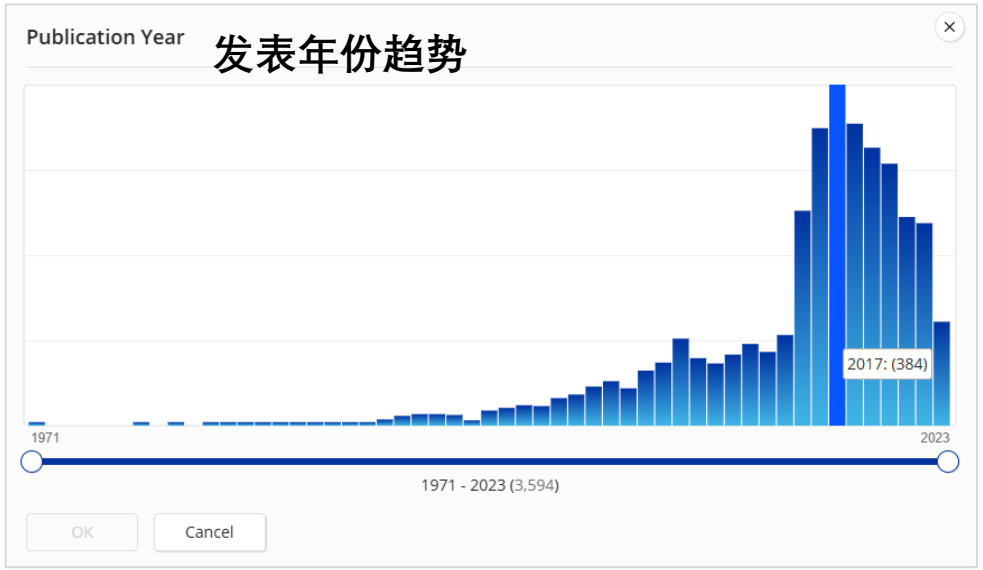
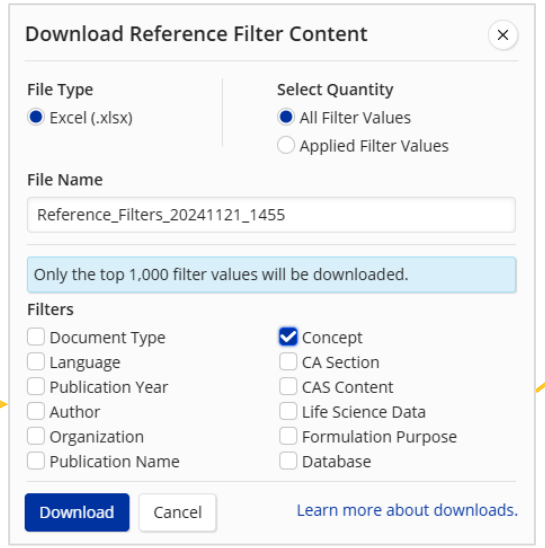
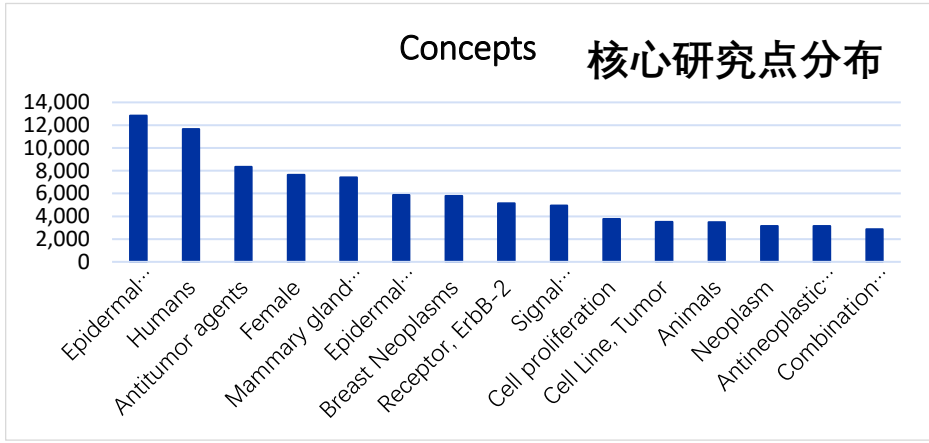
1.4 可视化分析——检索结果趋势分析





自主选择下载分析栏目





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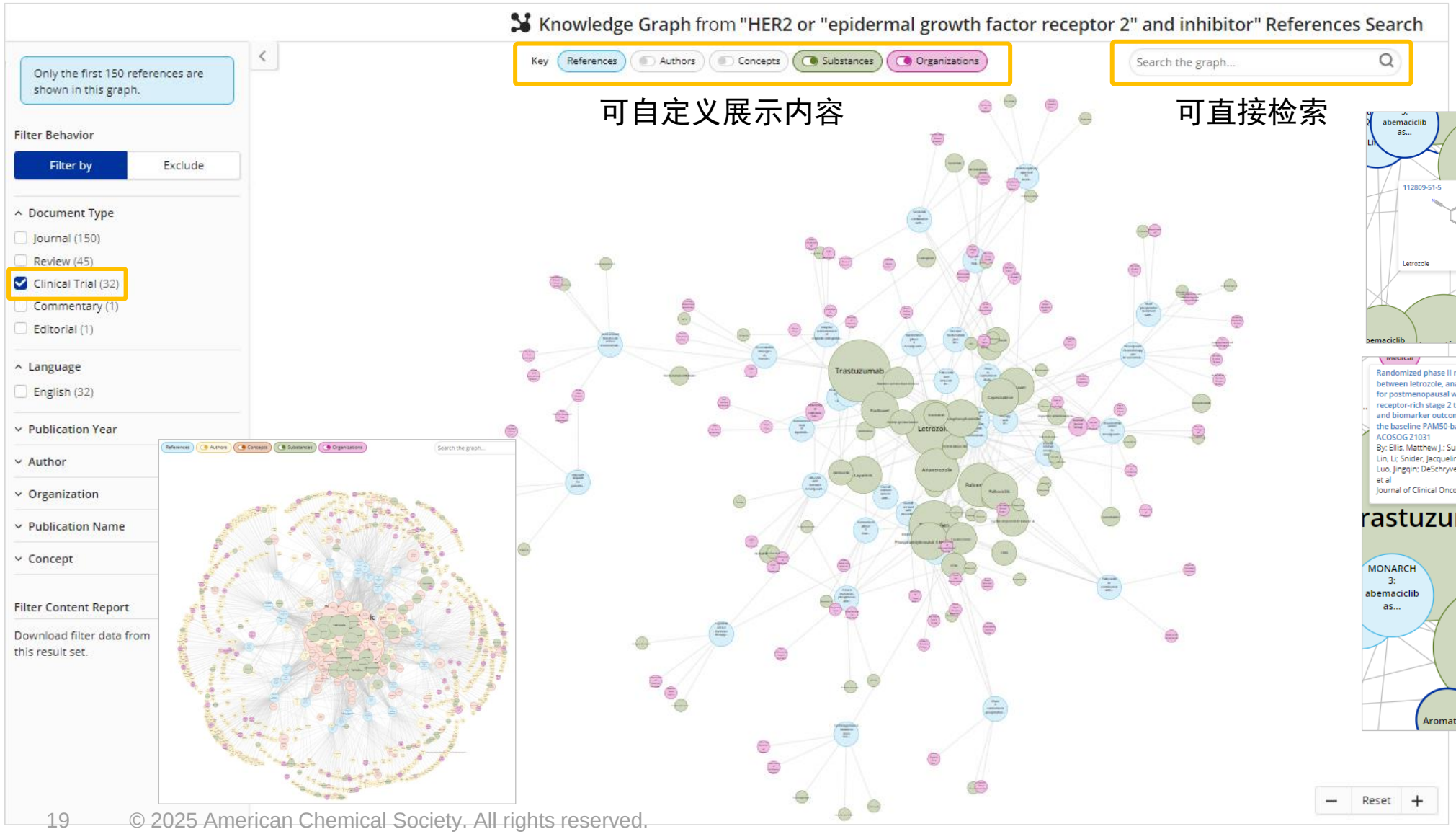
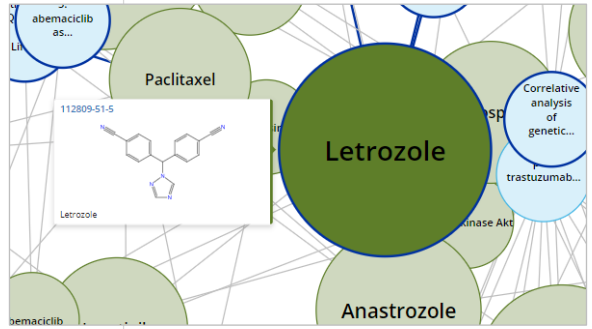
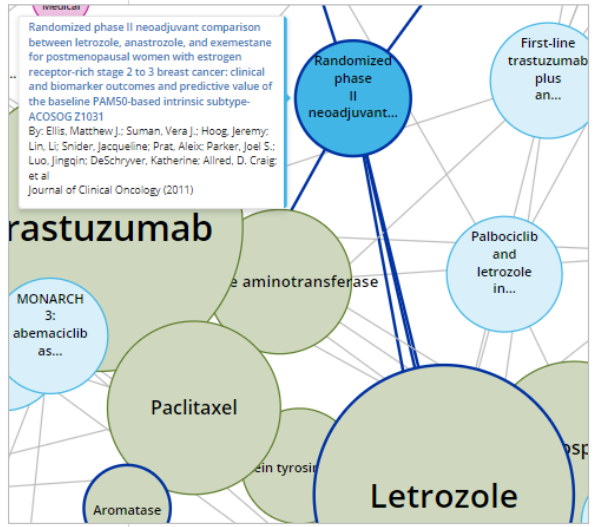
1.4 可视化分析——知识图谱

Knowledge Graph







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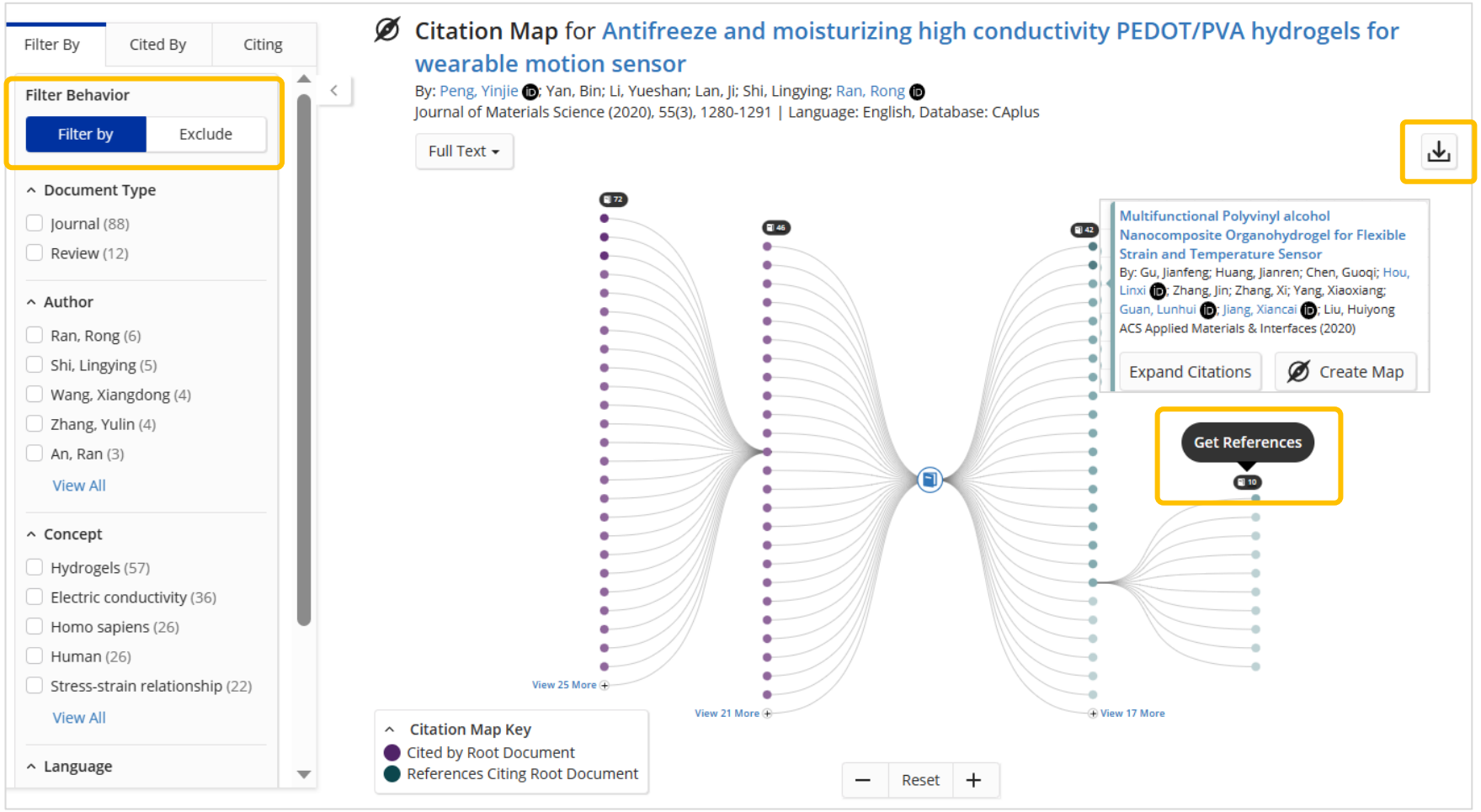
1.4 可视化分析——引文地图

便捷获得相关文献



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

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1.5 深入文献详情

Celecoxib, a selective cyclooxygenase 2 inhibitor, protects against human epidermal growth receptor 2 (HER-2)/neu-induced breast cancer

3 | 0 | 180 | Citation Map

In this Reference
- Concepts
- Substances
- Biomarkers
- Cited Documents

内容导航速览

By: Howe, Louise R.; Subbaramaiah, Kotha; Patel, Jay; Masferrer, Jaime L.; Deora, Aparna; Hudis, Clifford; Thaler, H… J.; Du, Baoheng; Brown, Anthony M. C.; et al
View All

Cyclooxygenase 2 (HER-2) (Cox-2), an inducible form of Cox, is over-expressed in HER-2/neu-pos. human breast … study was to determine whether celecoxib, a selective Cox-2 inhibitor, protected against HER-2/neu-induced exp… protein was detected in breast carcinomas from mouse mammary tumor virus (MMTV)/neu mice. Treatment with … significantly reduced the incidence of mammary tumors in MMTV/neu mice (P = 0.003) and caused about a 50% re… prostaglandin E_2 (PGE_2) levels. Because mammary glands from MMTV/neu mice expressed all four PGE_2 receptor … that signaling through PGE_2 receptors is important for mammary tumorigenesis. These results strengthen the rat… clin. trials to determine whether selective Cox-2 inhibitors possess anticancer properties in humans at risk for br…

Keywords: COX2 inhibitor celecoxib HER2 neu breast cancer

Full Text

Publication Information • Journal

Source	Database Information	Company/Organization	Email	Publisher
Cancer Research Volume: 62 Issue: 19 Pages: 5405-5407 Journal; Article; Research Support, Non-U.S. Gov't; Research Support, U.S. Gov't, P.H.S. 2002	AN: 2002:779608 CAN: 138:280829 PubMed ID: 12359744 CAplus and MEDLINE	Departments of Cell and Developmental Biology Weill Medical College of Cornell University New York, New York 10021 United States	lrhowe@med.cornell.edu	American Ass… for Cancer Re…

Concepts

CAS科学家提供的标准技术术语

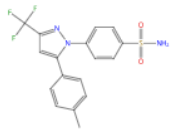
- Antitumor agents
- Epidermal growth factor receptor HER2 — Role: Biological Study, Unclassified
- Homo sapiens
- Human
- Mammary gland neoplasm
- Prostaglandin EP2 receptors — Role: Biological Study, Unclassified
- Prostanoid receptor PTGER4 — Role: Biological Study, Unclassified
- Prostanoid receptors, type EP_1 — Role: Biological Study, Unclassified
- Prostanoid receptors, type EP_3 — Role: Biological Study, Unclassified

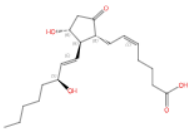
Substances

文献中的核心研究物质

Substances (3)

329900-75-6
Image Not Available
Unspecified
Cyclooxygenase 2
Role: Biological Study, Unclassified, Biological Study

169590-42-5

$C_{17}H_{14}F_3N_3O_2S$
Celecoxib
Role: Pharmacological Activity, Therapeutic Use, Biological Study, Uses

363-24-6

Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown
$C_{20}H_{32}O_5$
Prostaglandin E_2
Role: Biological Study, Unclassified, Biological Study

物质的研究角色

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1.5 深入文献详情

CAS PatentPak 快速定位专利中的物质

1

Intermediates for the preparation of halichondrin B

By: Austad, Brian; Chase, Charles E.; Fang, Francis G.

World Intellectual Property Organization, WO2005118565 A1 2005-12-15 | Language: English, Data

The present invention provides macrocyclic compounds I [PG^1, PG^2, PG^3 = H, protecting group (esp silylene, cyclic acetal, cyclic ketal, cyclic carbonate, cyclic boronate; R^1 = R, OR; R = H, C$_{1-4}$-haloalkyl, Me, CH$_2$Ph); LG^1 = leaving group (e.g., sulfonyloxy, (un)substituted alkylsulfonyloxy, alkenylsulfonyl mesyloxy or tosyloxy)], especially diastereomer II, synthesis of the same and intermediates theret = SiMe$_2$CMe$_3$, PG^3 = COCMe$_3$, LG^1 = OMs, Ms = SO$_2$Me, R^1 = OMe] was ...

View More

PatentPak | Full Text | Substances (152) | Reactions (1,160)

Patent	Language	Kind Code	PatentPak Options
WO2005118565	English	A1	PDF | PDF+ Viewer
AU2005250487	English	A1	PDF
CA2935786	English	A1	PDF
CA3028453	English	A1	PDF
CN1993342	Chinese	A	PDF
AU2005250487	English	B2	PDF
EP2522663	English	A1	PDF
JP5226304	Japanese	B2	PDF
KR1434673	Korean	B1	PDF
EP2522663	English	B1	PDF

View All on Reference Detail

thereof

ha N.

of making and using and com

hetic techniques. For example

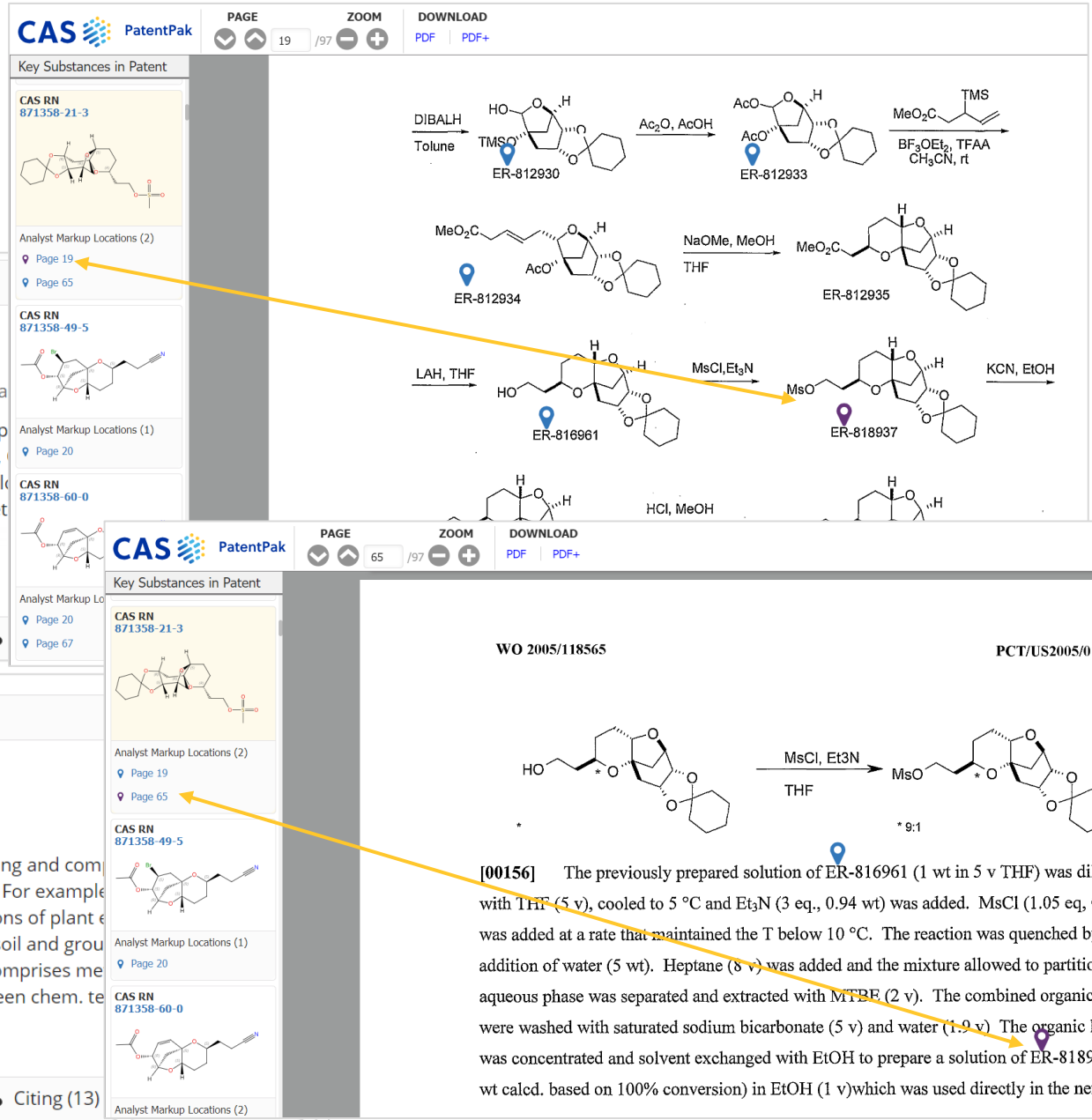
rmed with solutions of plant e

taminants from soil and grou

, the invention comprises me

formed using green chem. te

actions (0) | Citing (13)



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文献检索小结

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

大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查、怎么选具体的实验方案?
- 常见问题Q&A

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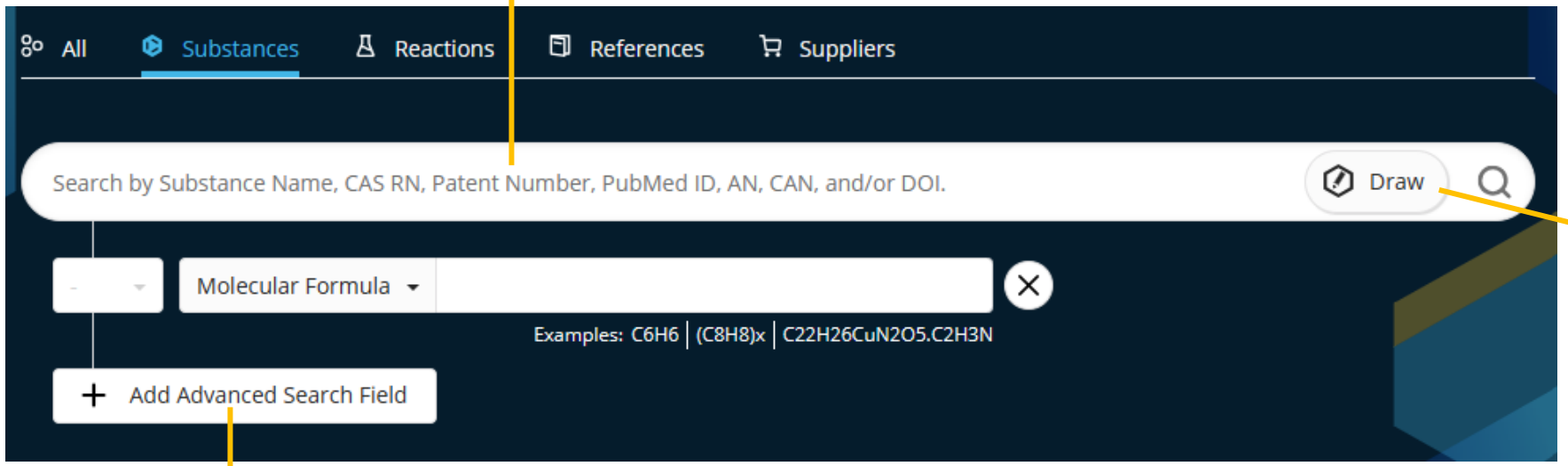
2. 如何聚焦某类物质?

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

研究某种/某类物质?

- 通过物质标识符、文献标识符检索物质

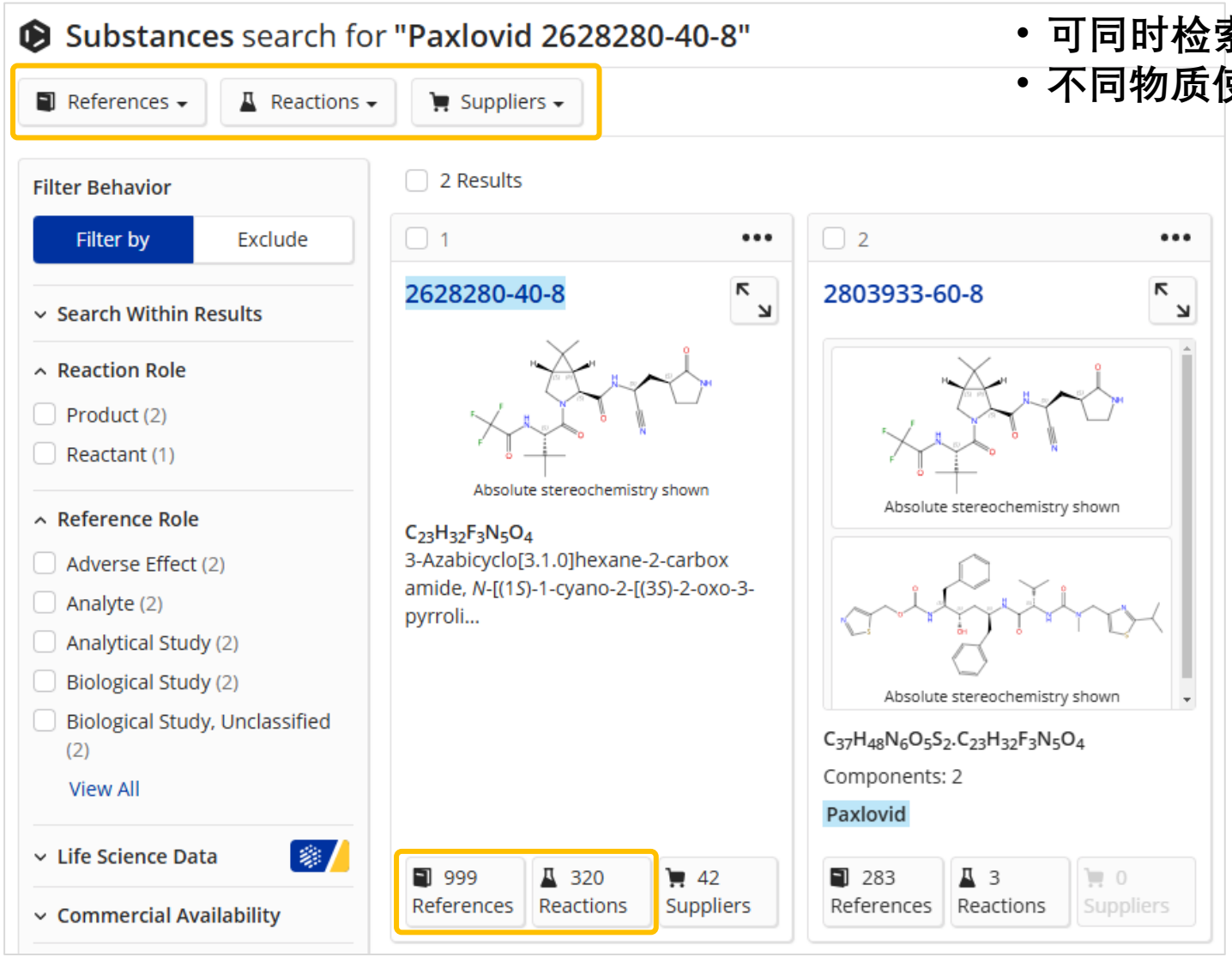


- 使用结构绘制面板进行结构检索

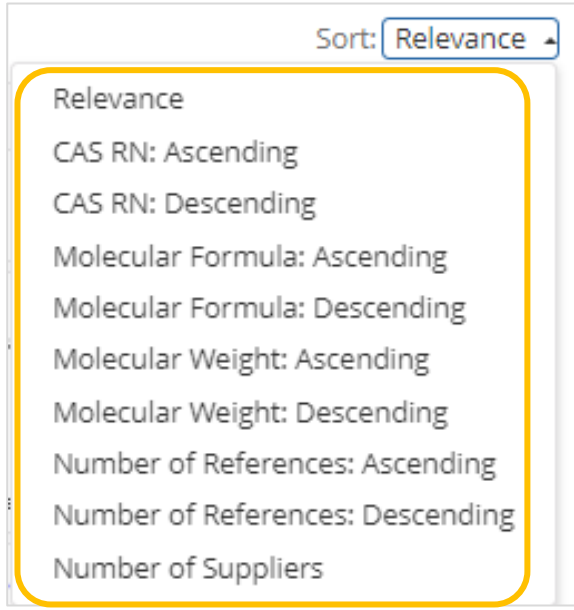
- 高级检索

➢ 检索策略推荐
  - 有机化合物，金属配合物，天然产物：结构检索
  - 无机物，合金：分子式检索
  - 高分子化合物：分子式检索和结构检索

物质检索——物质标识符



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



物质排序：相关度、CAS RN、分子式、分子量、文献量、供应商数量

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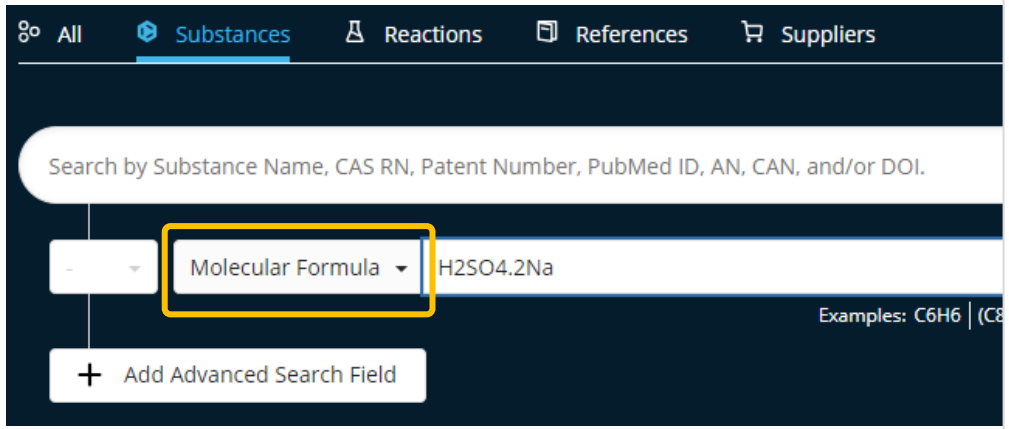
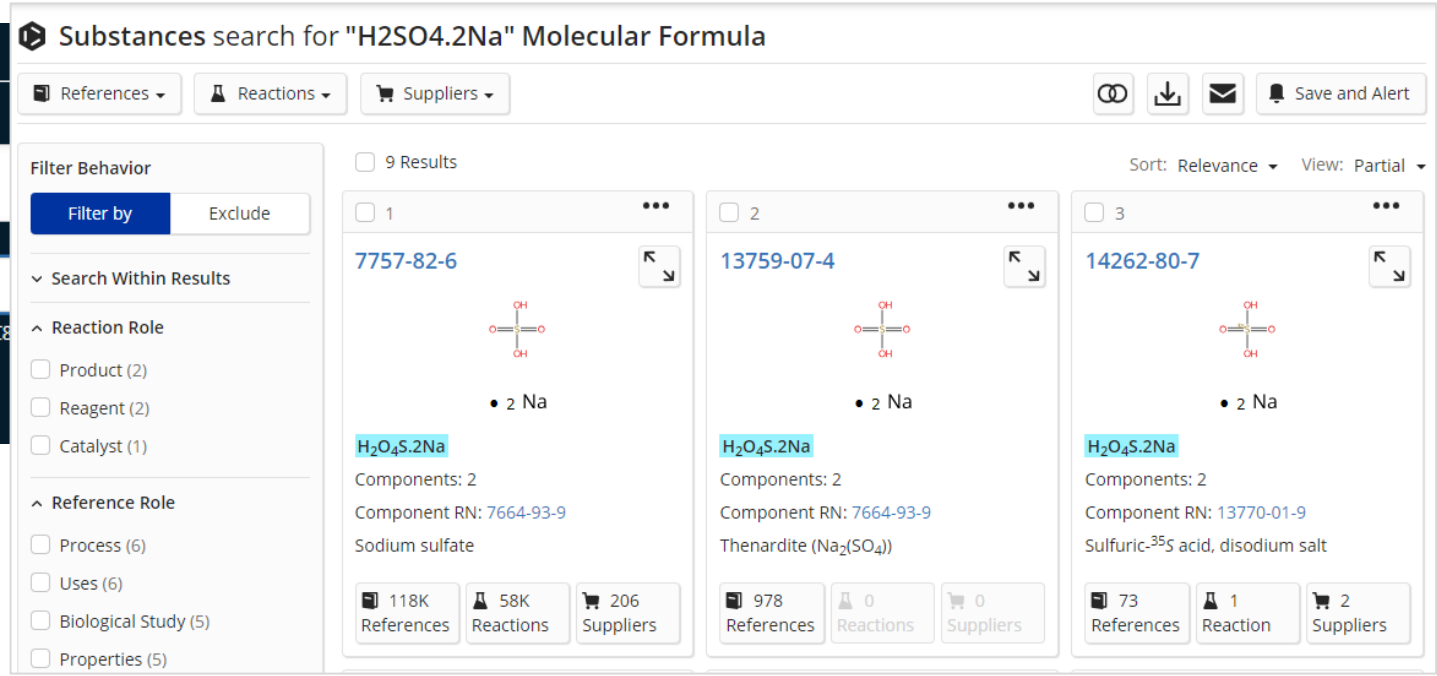
2.1 分子式检索：高效检索聚合物或无机化合物

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：铁钴镍合金 Fe.Co.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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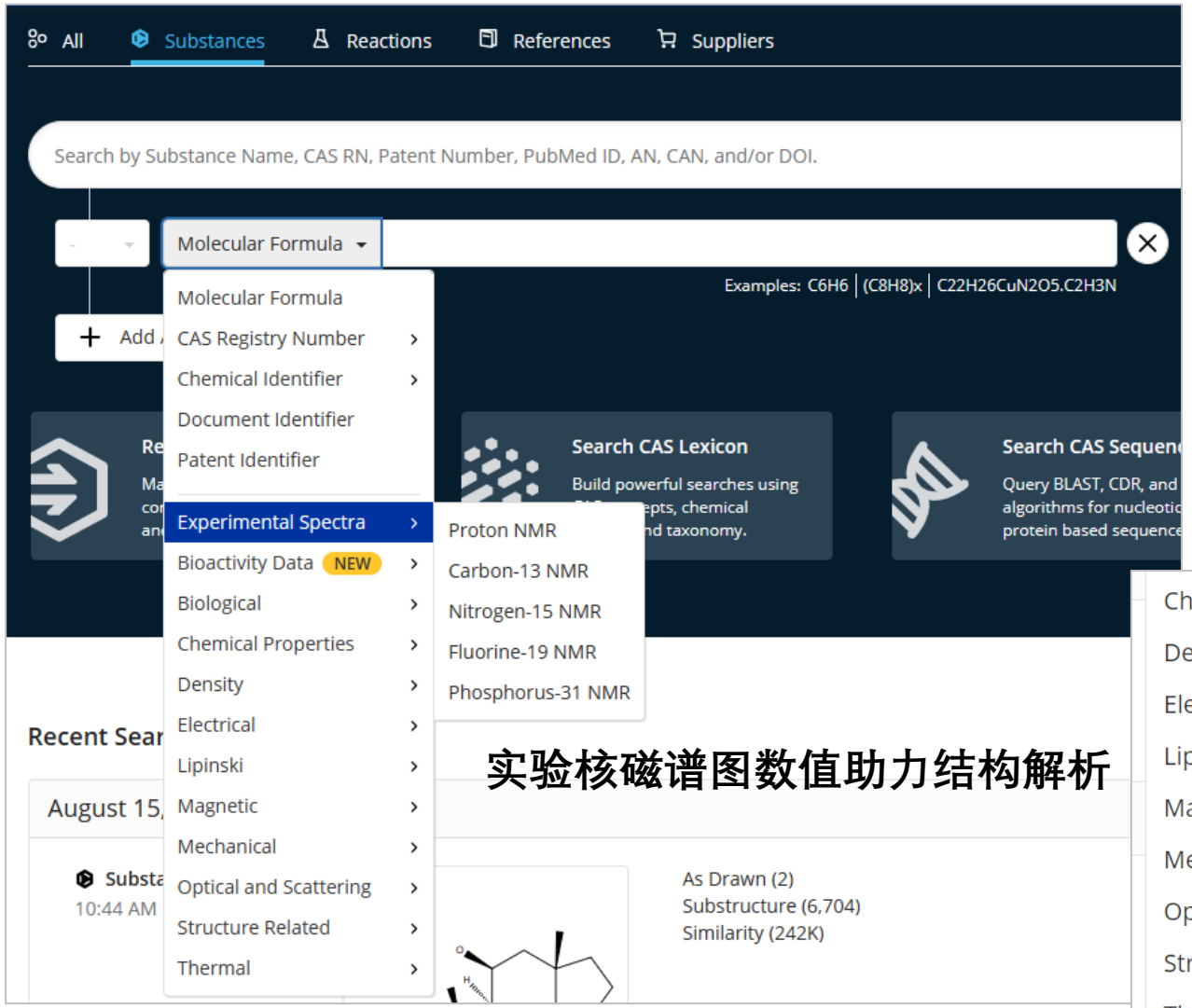
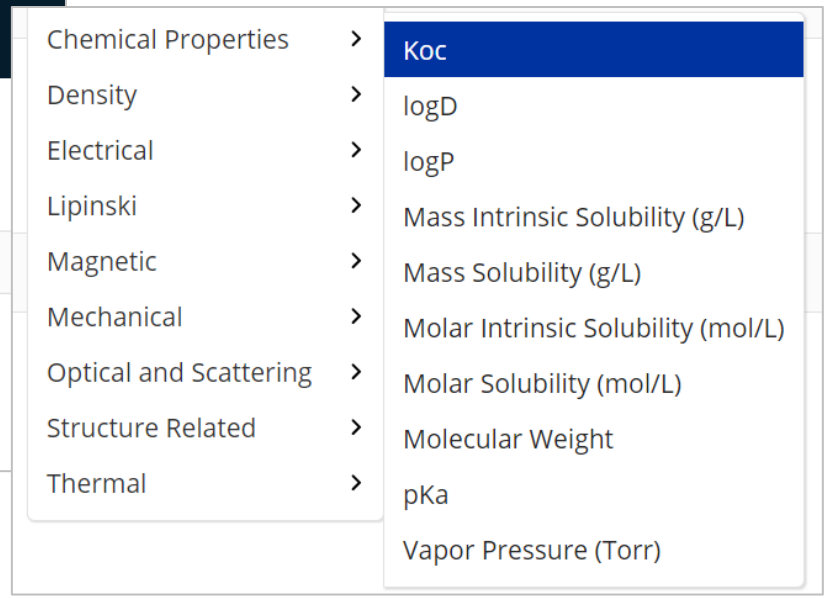
2.2 属性值联用检索物质



实验核磁谱图数值助力结构解析

高级检索字段：

- CAS RN（物质、组份）、物质标识符、分子式、文献号、专利号
- 实验谱图：^{1}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P NMR
- 化学标识符：化学名称、InChI key
- 生物：生物富集因子、LD50
- 化学：Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压
- 密度属性：密度、摩尔体积
- 电学：电导/电导率、电阻/电阻率
- Lipinski：自由旋转键、H受体/供体
- 磁：磁力矩
- 机械属性：拉伸强度
- 光散射：旋光性、折射率
- 结构：极性表面积
- 热学：熔点、沸点、闪电、玻璃转化温度、蒸发焓



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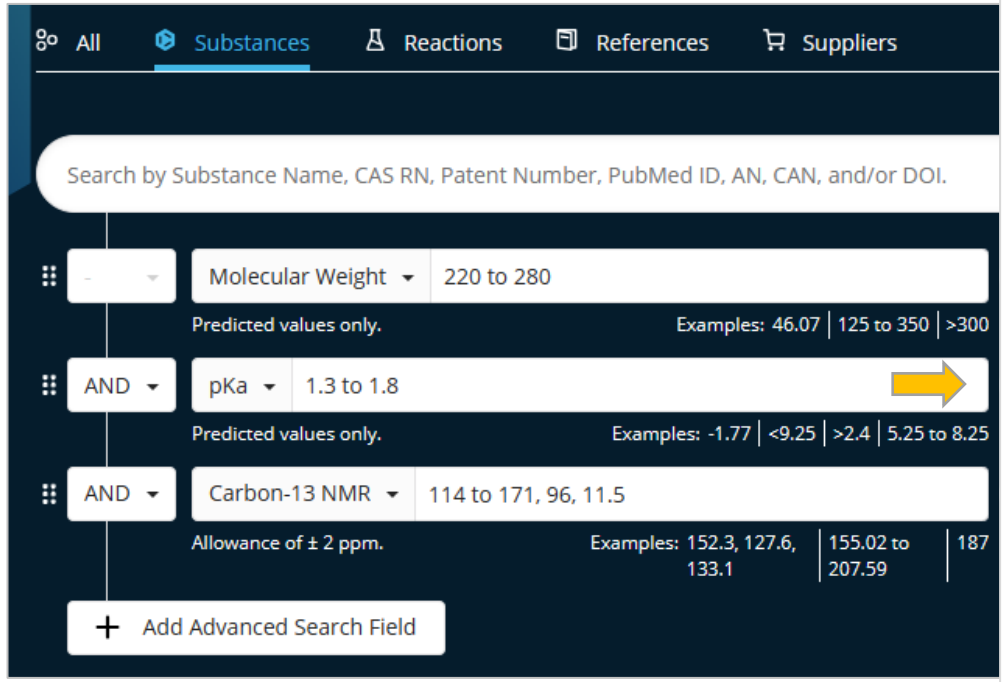
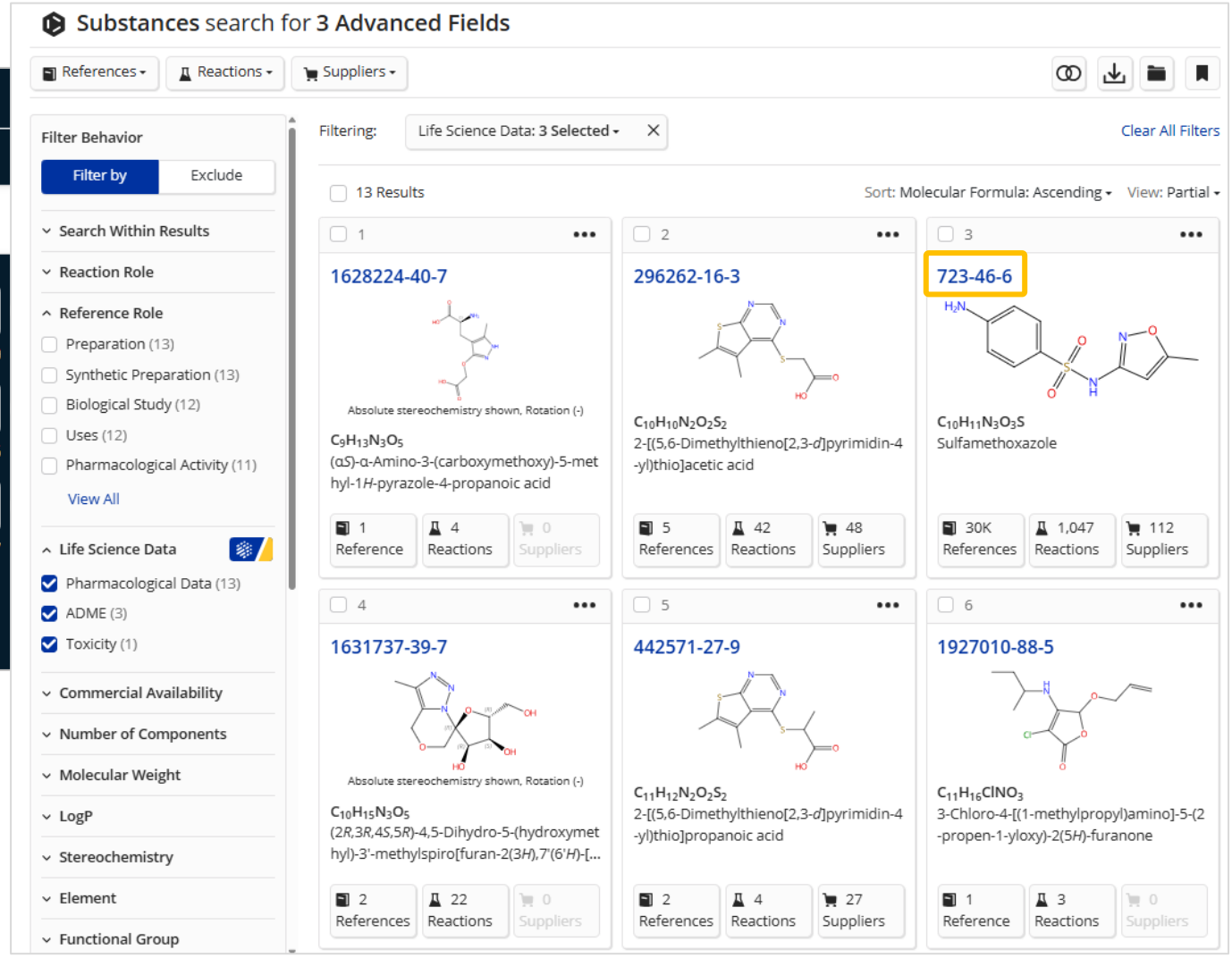
属性值、谱图数值联用检索物质





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

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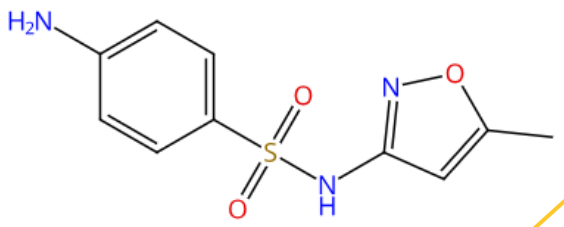
物质详情

CAS Registry Number: 723-46-6

30K | 1,047 | 112 | View in CAS BioFinder



$C_{10}H_{11}N_3O_3S$

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)	482.145±55.00 °C	Press: 760.00 Torr
Density (Experimental)	1.08 g/cm³	-
pKa (Predicted)	5.811±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra

Experimental Properties 实验属性

Biological | Chemical | Density | Electrical | Lipinski | Structure Related | Thermal

Property	Value	Condition	Source
Crystal Structure - 1 Source	See Full Text		(1) CAS
Molecular Structure - 2 Sources	See Full Text		(2-3) CAS
Particle Size - 1 Source	See Full Text		(4) CAS
Specific Surface Area - 1 Source	See Full Text		(5) IC
X-Ray Diffraction Pattern - 2 Sources	See Full Text		(6-7) CAS

Sources

(1) Perlovich, German L.; Crystal Growth & Design, (2013), 13(9), 4002-4016, CAplus

Experimental Spectra 实验谱图

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

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

Sources

(1) Kartashov, V. S.; Khimiko-Farmatsevticheskii Zhu

(2) Fruttero, Roberta; Journal of the Chemical Socie

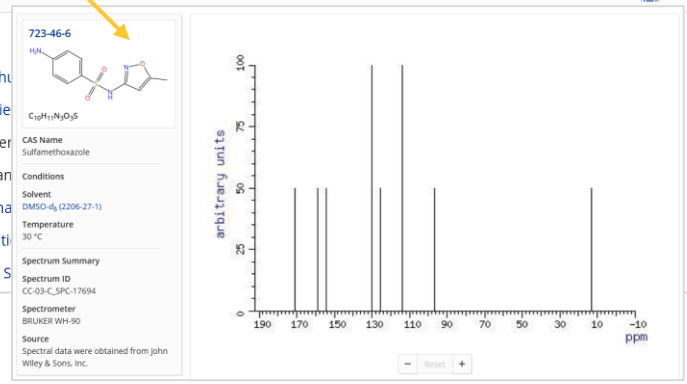
(3) Copyright Bio-Rad Laboratories. All Rights Reser

(4) "Integrated Spectral Data Base System of Organ

(5) Sunduru, Naresh; European Journal of Medicina

(6) Ham, Won Seok; Angewandte Chemie, Internati

(7) Blasioli, Sonia; Journal of Colloid and Interface S



Technology (Japan)

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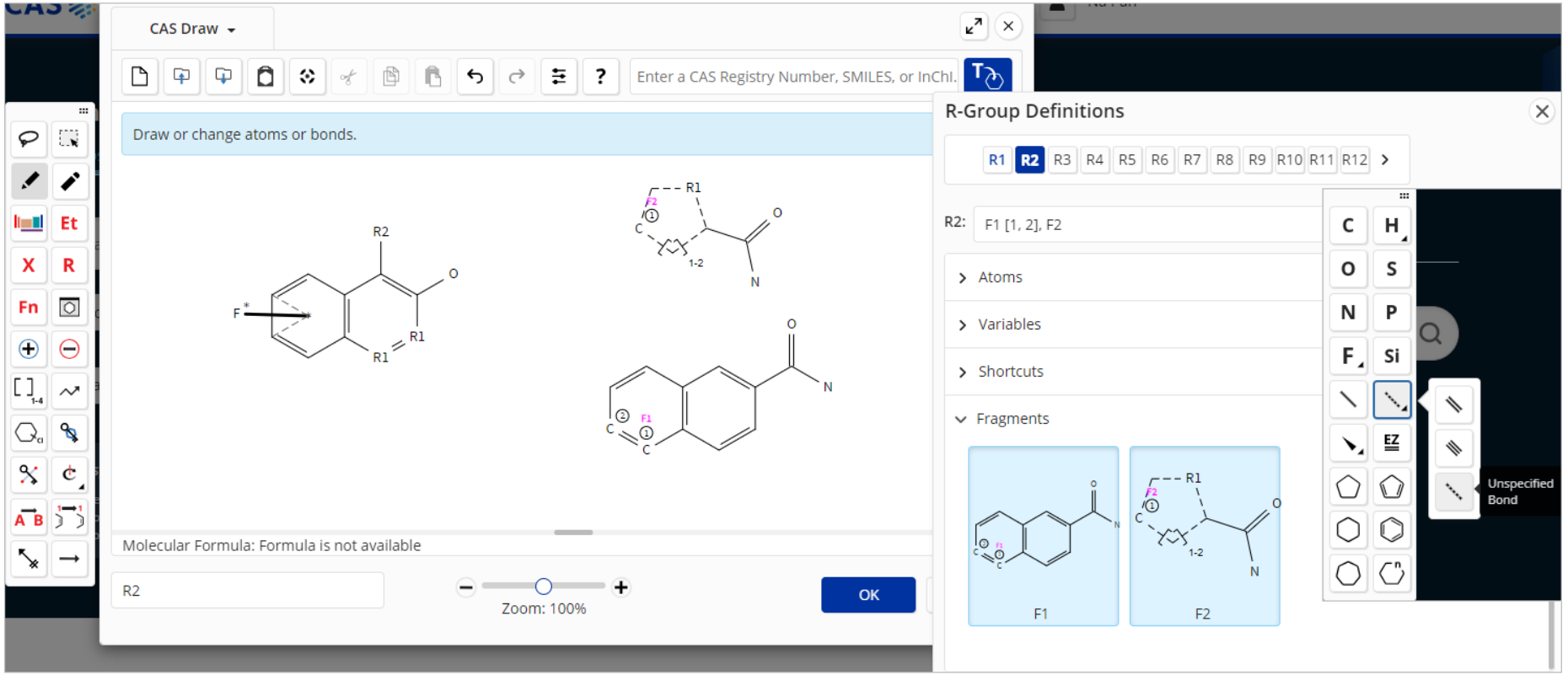
2.3 结构检索

灵活构建通式结构，提高物质/反应信息的检索效率

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



利用绘图工具自定义相似结构：

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

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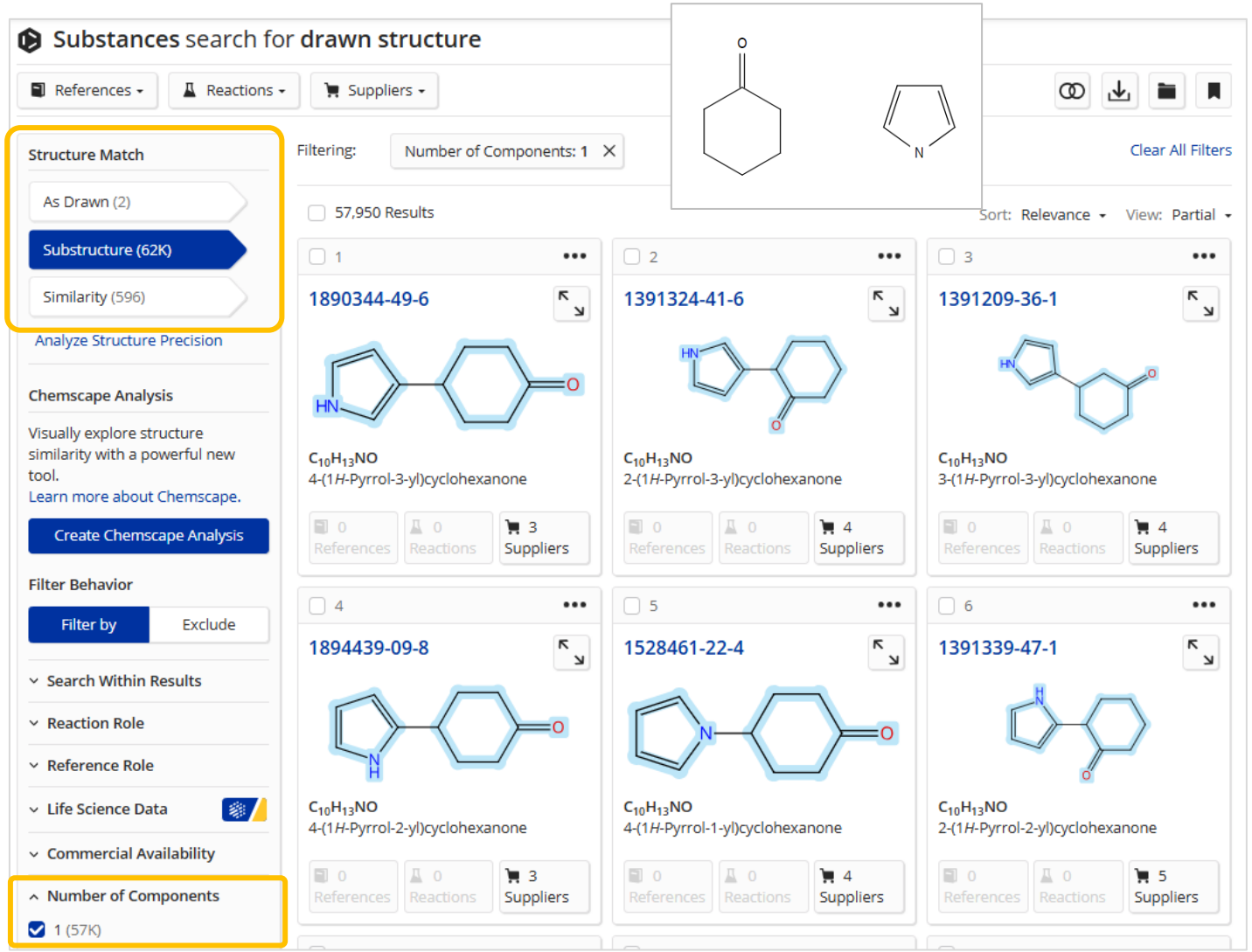
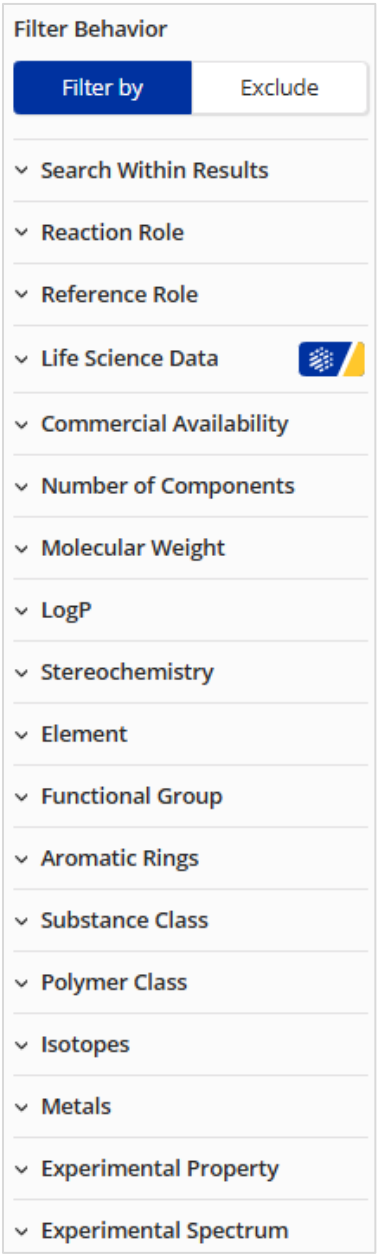
片段结构的检索



物质筛选类别：

二次检索
反应角色
文献角色
生命科学数据
是否商业可得
组分数量
分子量
油水分配系数
立体化学
所含元素
所含官能团
芳环数量
物质类别
聚合物类别
同位素
是否含金属
实验属性
实验谱图
……



https://cas-product-help.zendesk.com/hc/en-us/articles/9945764238477-Filter-Substances-by-Structure-Match

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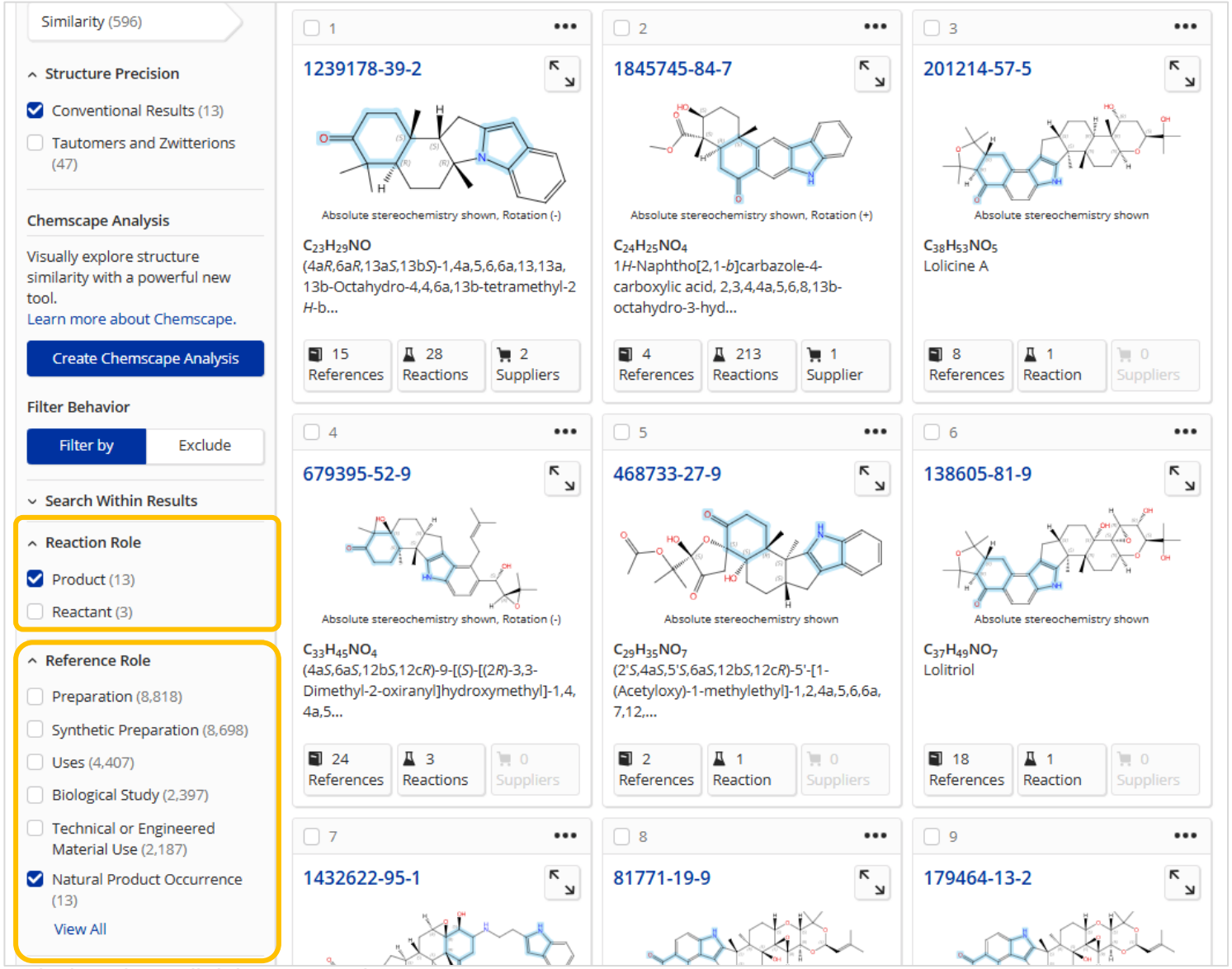
物质检索结果的筛选

思考：如何锁定尚未合成的天然产物结果？

Reaction Role：
物质在反应中的角色

Reference Role：
物质在文献中的研究角色



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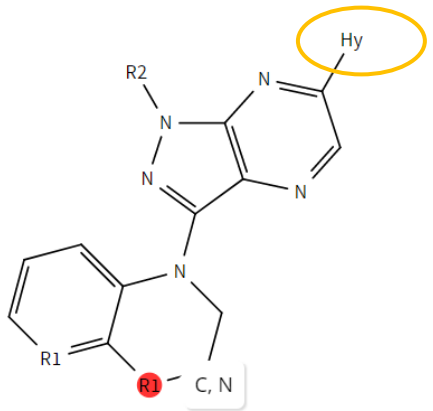
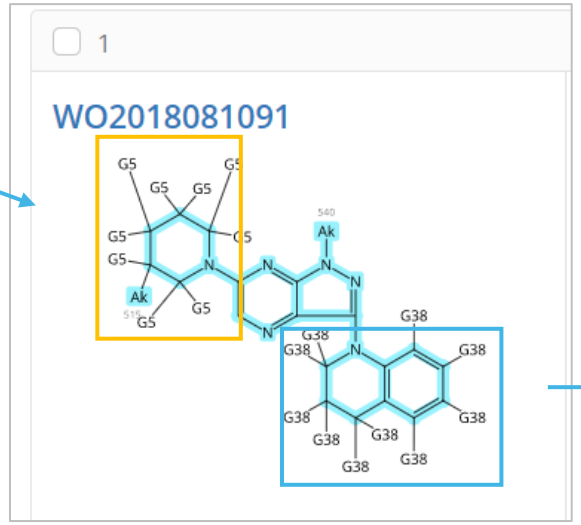
2.4 CAS Markush 检索，助力结构查新

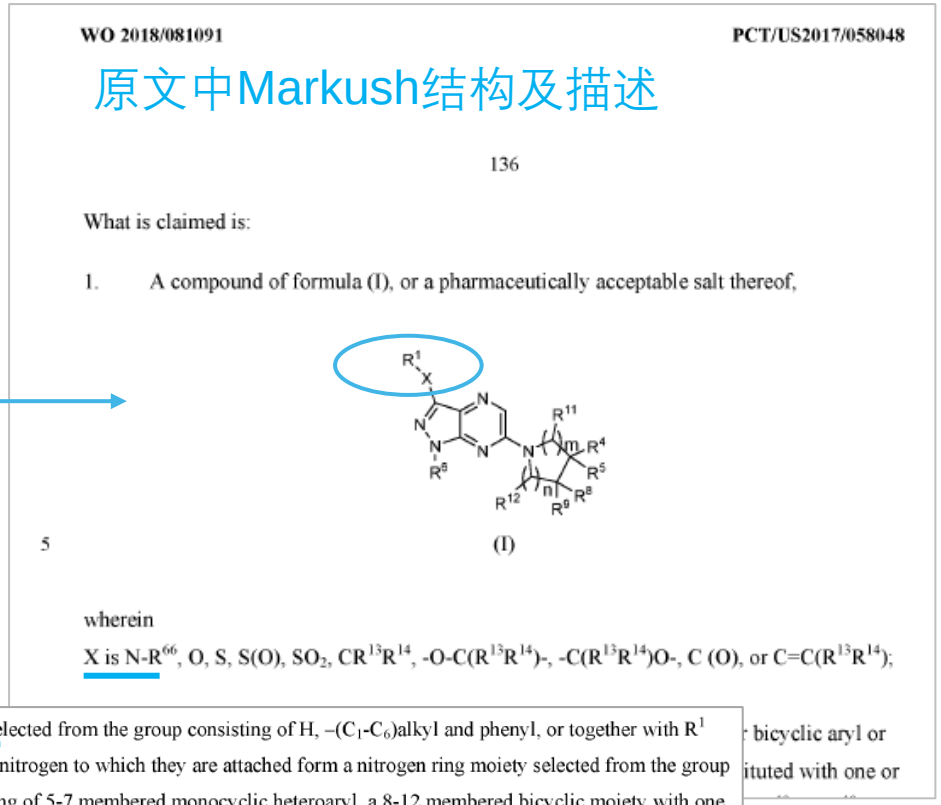
CAS科学家对文献的标引和解读





命中的Markush结构及解读

专利中的定位，专利权人、命中结构的特点等等



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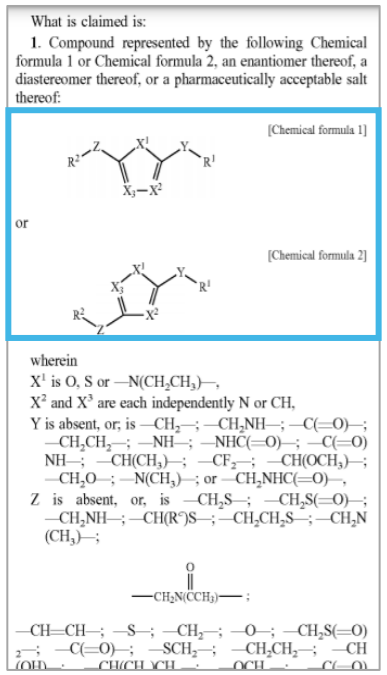
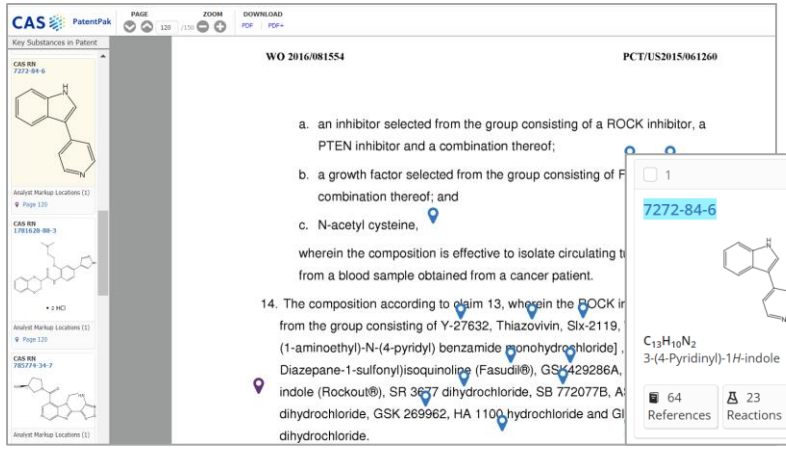
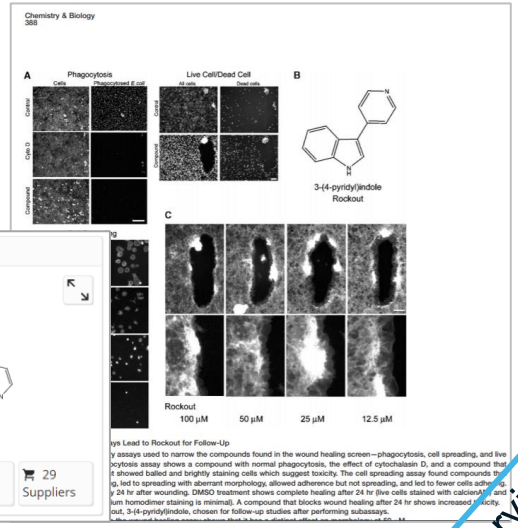
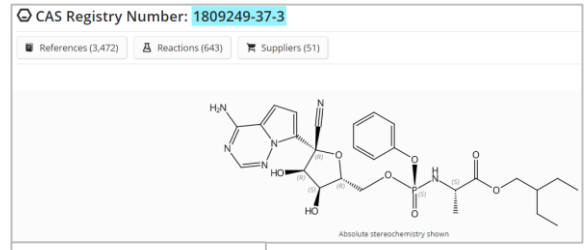
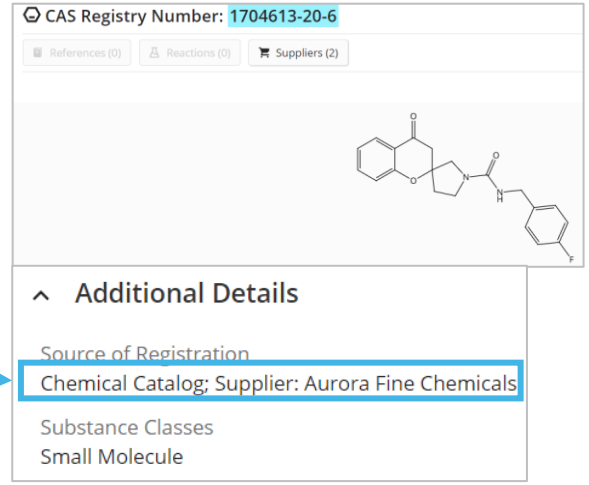
CAS结构层面的数据集

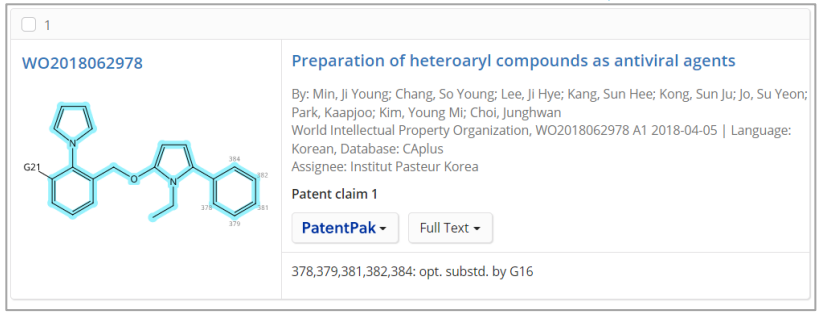












CAS Markush

Patent

Patent

Journal

CAS Client Service

CAS REGISTRY

Chemical catalog/library

Other web sources

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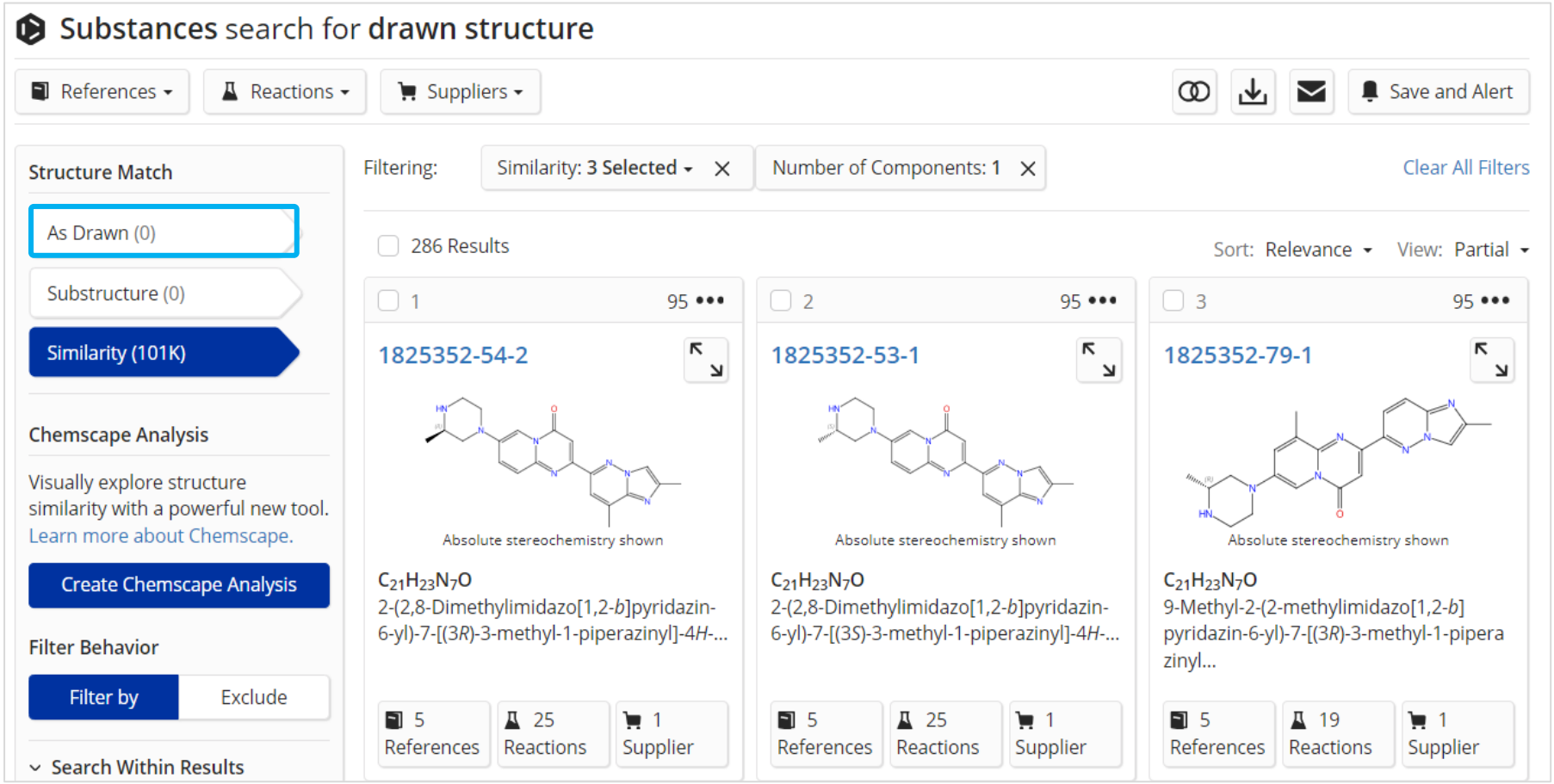
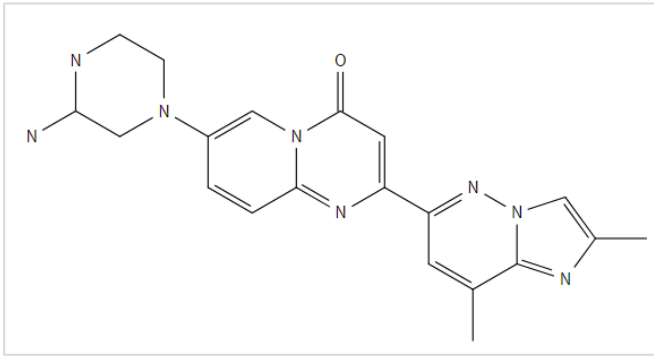
如何进行完整的分子结构检索?





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

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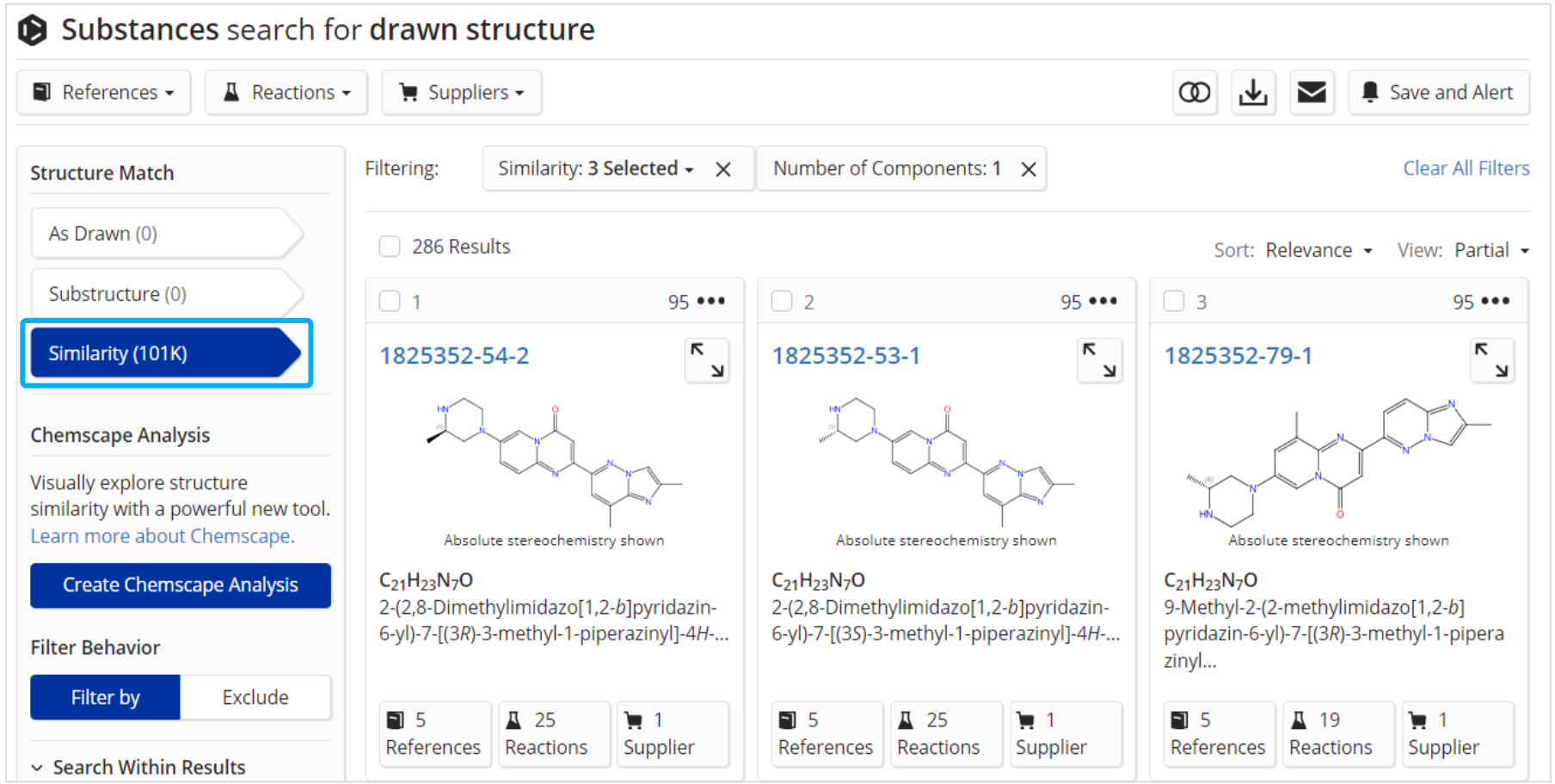
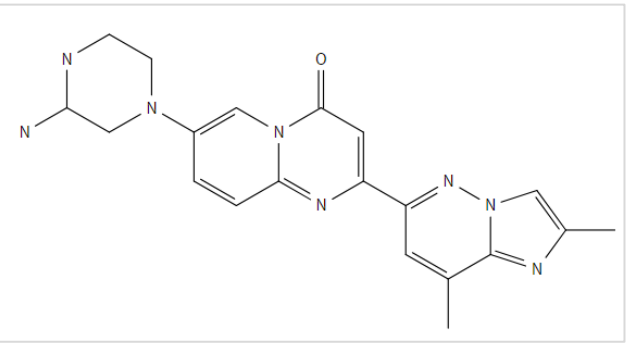
如何进行完整的分子结构检索?





查看相似结构，可参考Similarity score

https://cas-product-help.zendesk.com/hc/en-us/articles/11112258474125-What-are-similarity-scores

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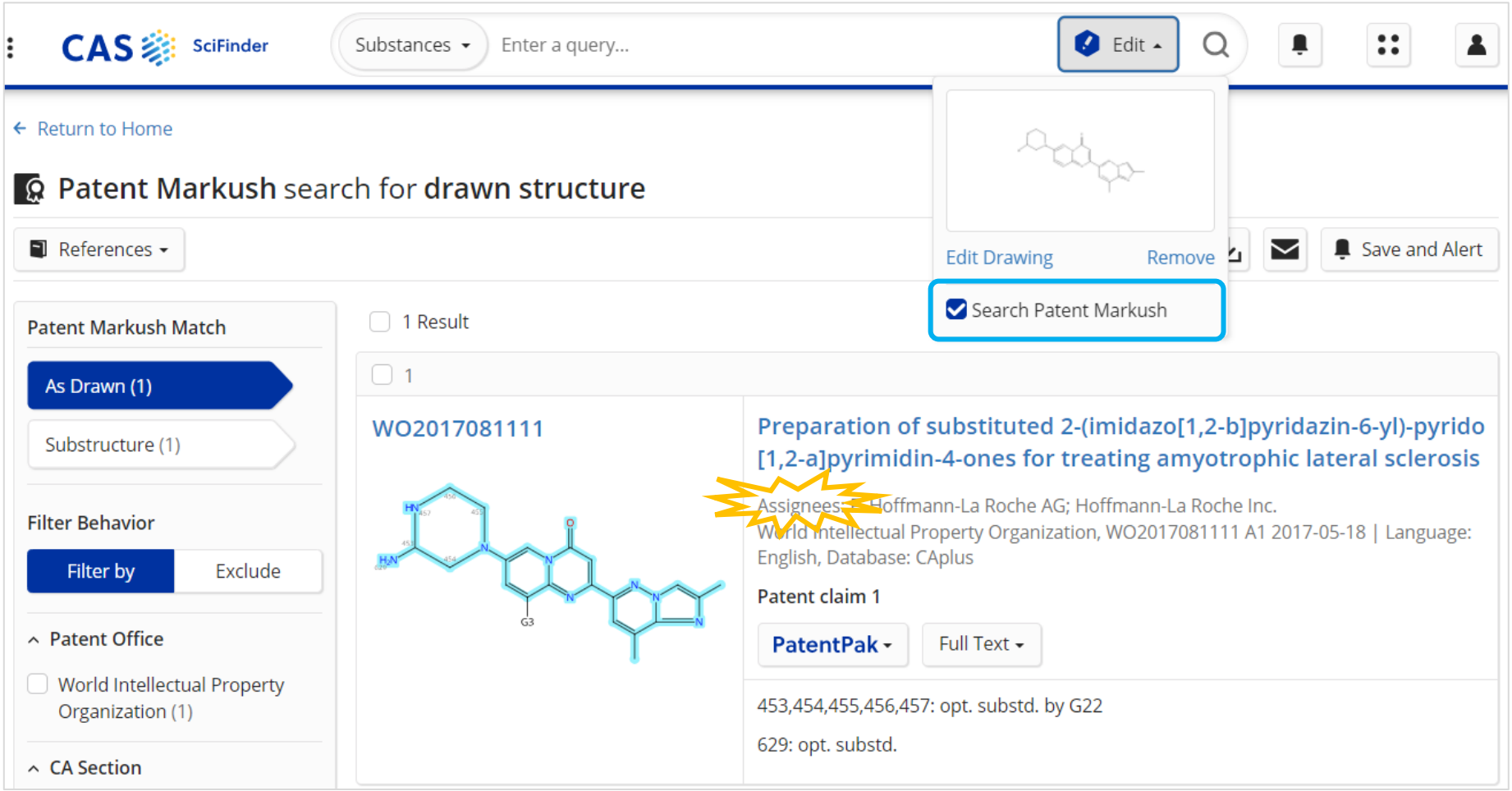
如何进行完整的分子结构检索?



- CAS 专利马库什数据集是专利审查员进行可专利性检索的重要参考依据
- 马库什检索可以使用具体结构、骨架结构和通式结构来进行迭代检索，确保获得完整的公开结构信息

用户可以根据必要性使用 CAS 文献数据集 CAplus 进行文本检索补充

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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

大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查、怎么选具体的实验方案?
- 常见问题Q&A

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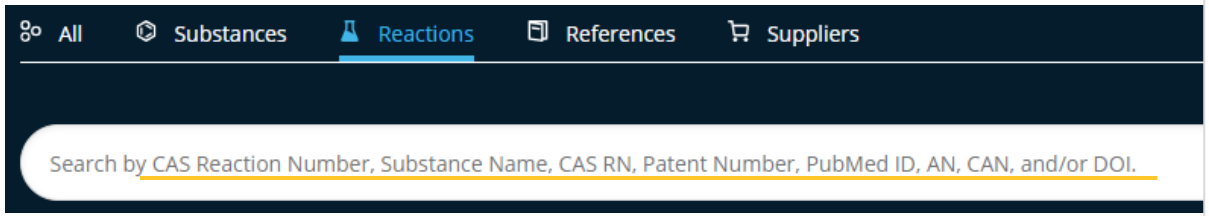
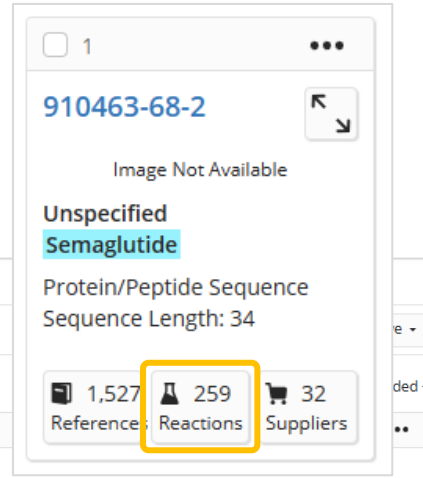
3. 如何进行反应调研?

- 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?

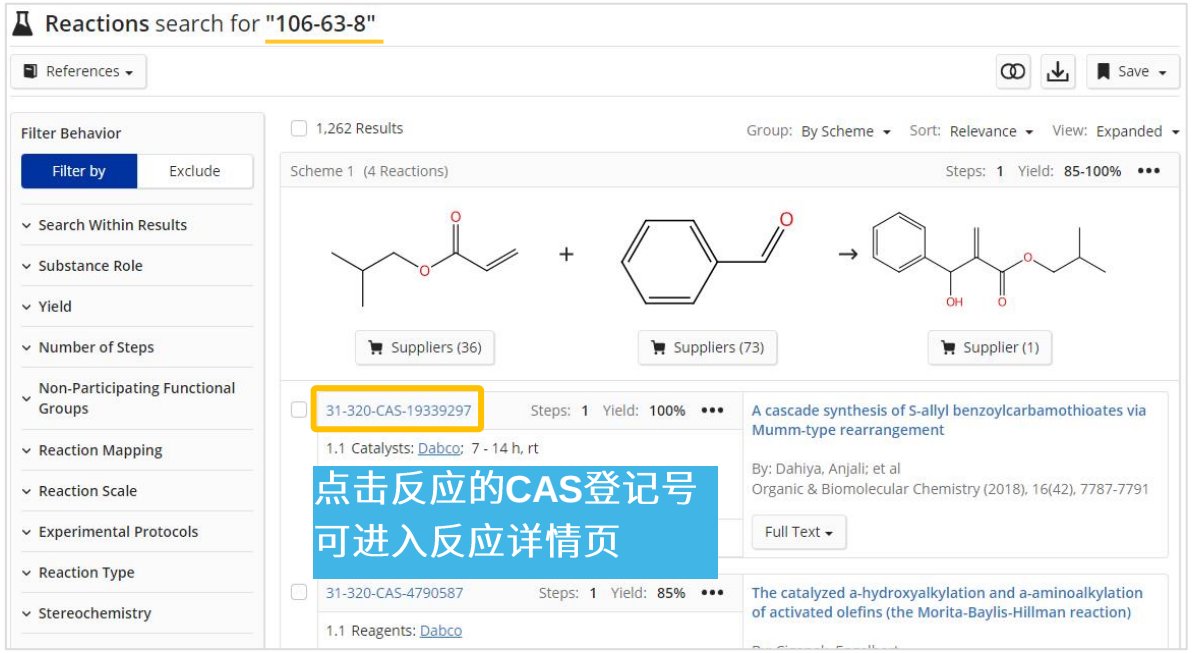
使用标识符直接检索

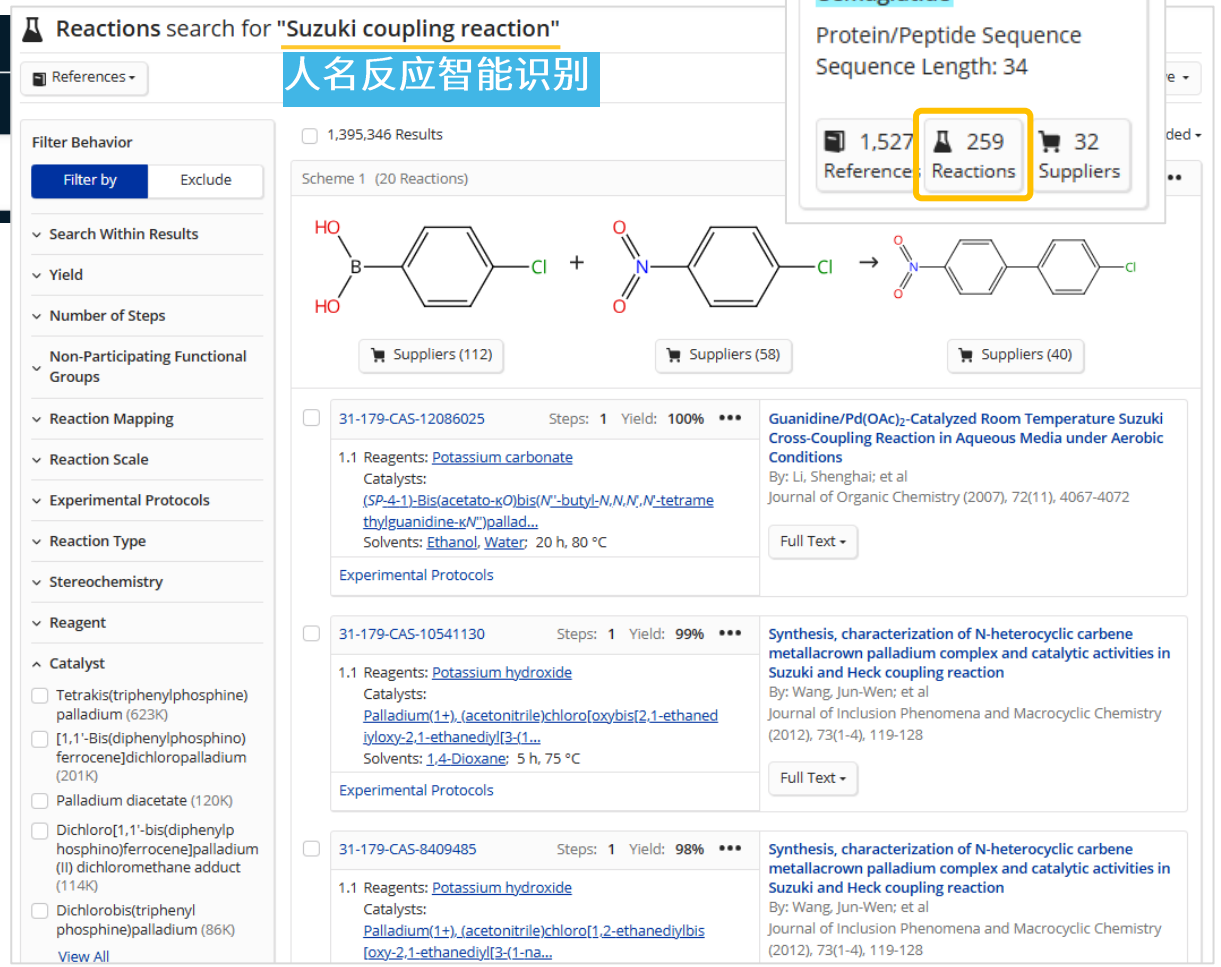
支持使用：CAS反应登记号、物质名称、CAS登记号、文献号等





示例：丙烯酸异丁酯的相关反应





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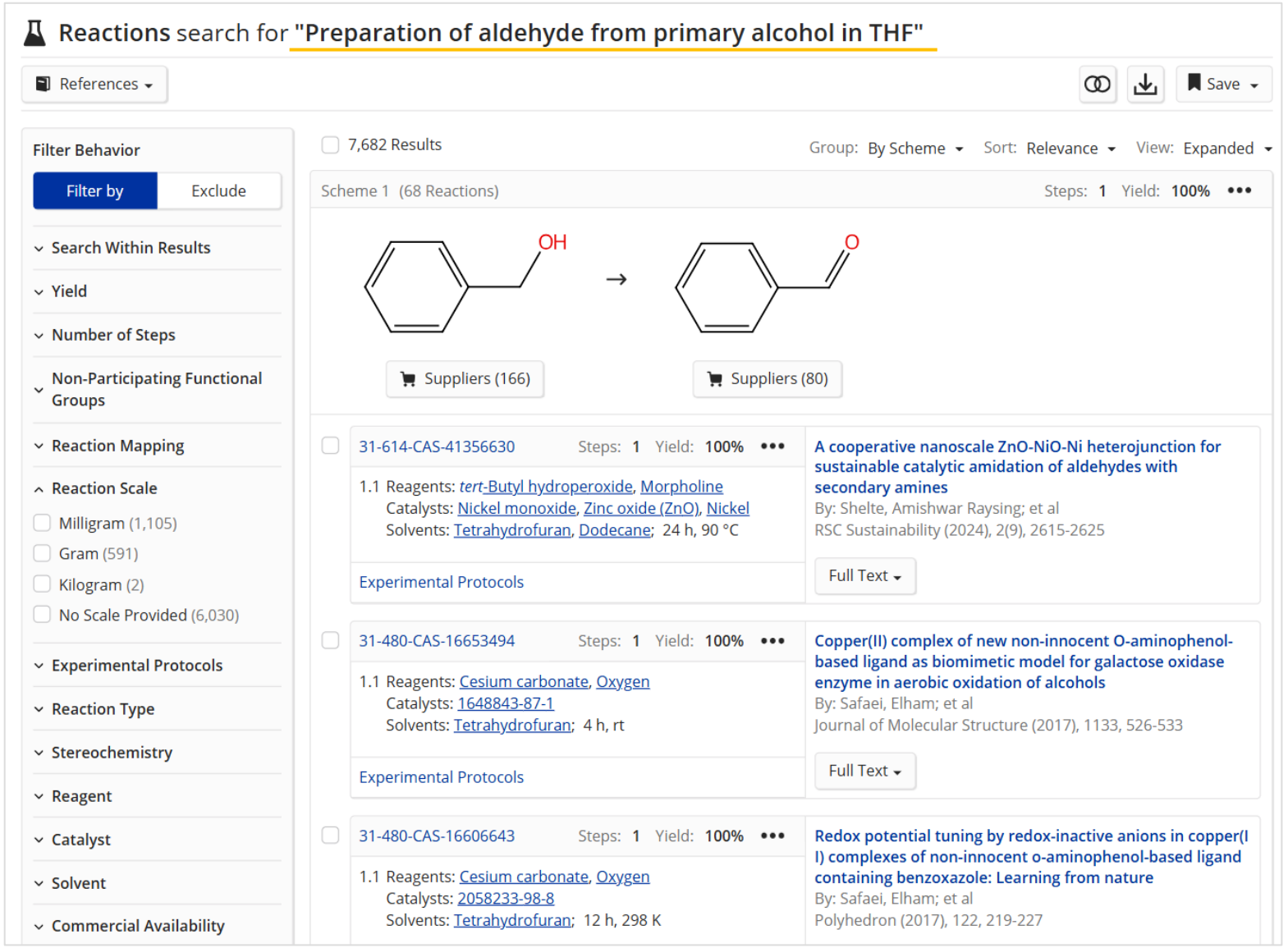
3.1 使用自然语言，检索某类反应



- 产物：synthesis / preparation / manufacture of
- 底物：from
- 溶剂：in
- 催化剂：catalyzed by
- 试剂：mediated by

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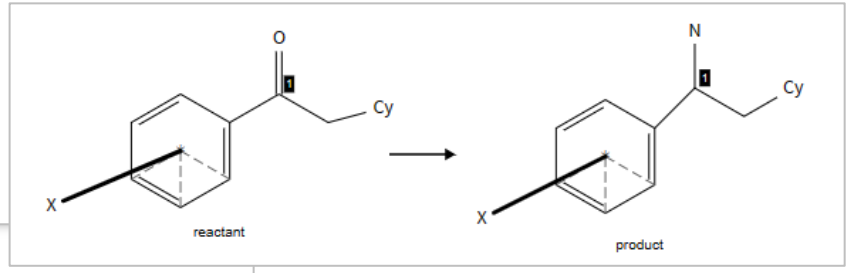
3.2 查找亚结构反应



As Drawn
亚结构反应
相似反应

Reactions search for drawn structure

References | Save and Alert

Structure Match
As Drawn (34)
Substructure (8,044)
Similarity (0)

Filtering: Reaction Mapping: Mapping Data Available | Clear All Filters

16 Results | Group: By Scheme | Sort: Relevance | View: Collapsed

By Scheme
By Document
By Transformation

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

Scheme 1 (5 Reactions)

Suppliers (93) | Suppliers (15)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 76%

Suppliers (53) | Suppliers (3)

Filter Behavior
Filter by | Exclude

Search Within Results

Yield
80-89% (4)
70-79% (2)
50-69% (1)
No Yield Available (9)

Reaction Scale
Milligram (2)
Gram (1)
No Scale Provided (13)

Non-Participating Functional Groups

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

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

Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

By: Heidelbaugh, Todd M.; et al

反应分组：
- 按反应式
- 按文献
- 按转化类型

反应排序：
- 相关度
- 公布时间
- 产率
- 步数

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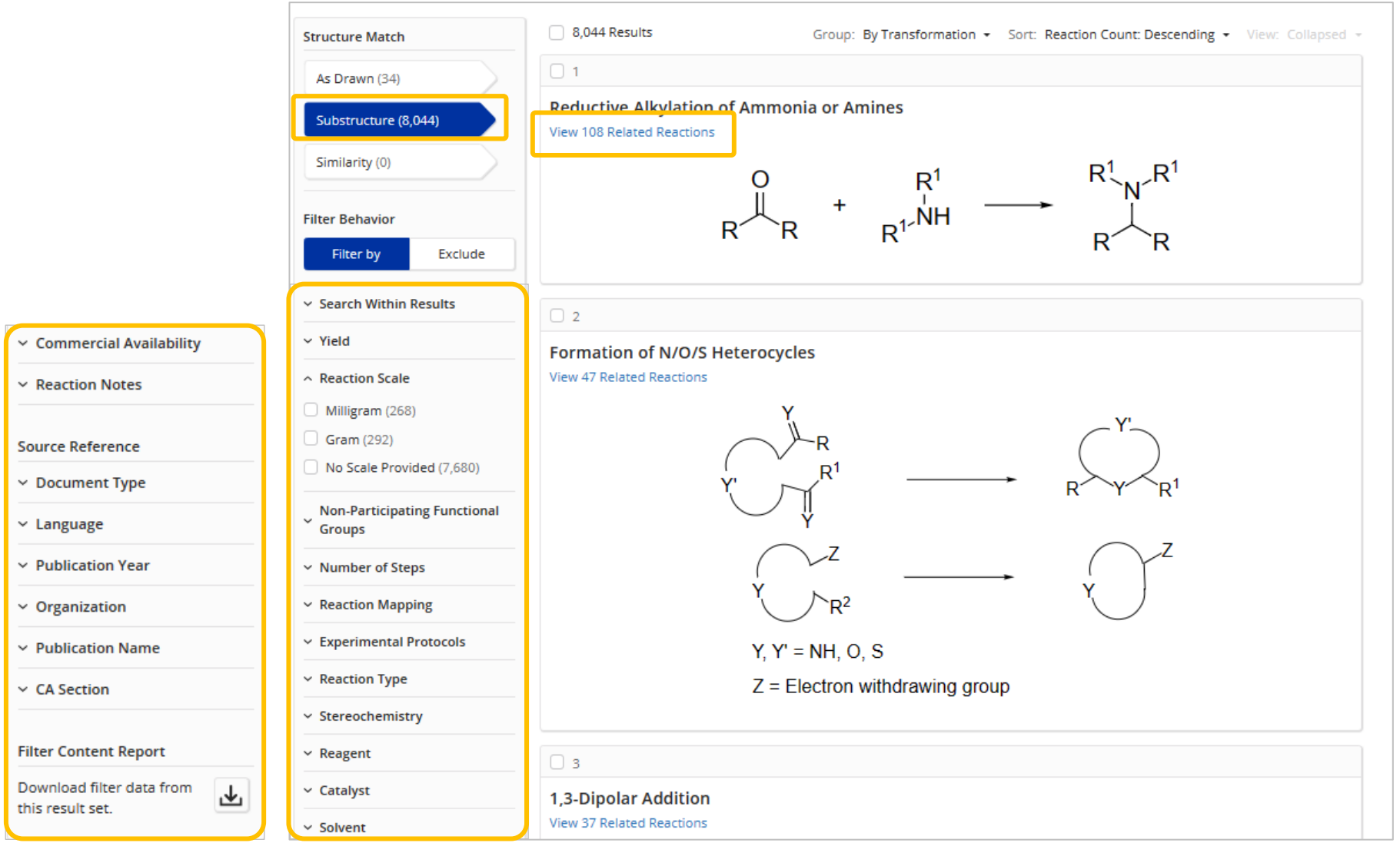
3.3 高效筛选目标反应

折叠菜单：相同反应类型的反应在同一菜单里，方便阅读和筛选

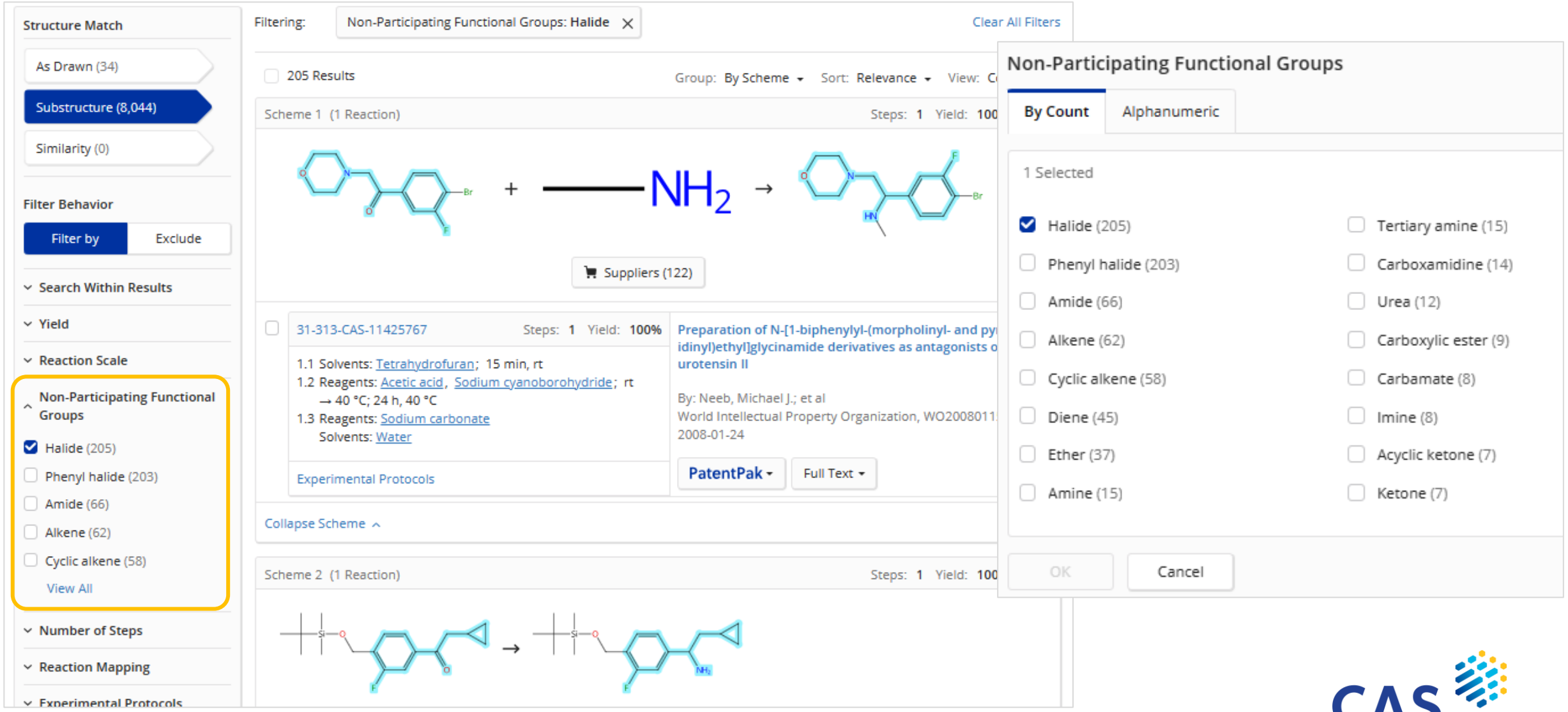
反应筛选类别：
产率、规模、步数
不参与反应的官能团
实验步骤
反应类型、立体化学
试剂、催化剂、溶剂
商品信息……

文献筛选类别：
文献类型、语言
出版年份、刊物名



筛选工具：不参与反应官能团

不参与反应官能团：出现在反应前后，但未发生变化的官能团



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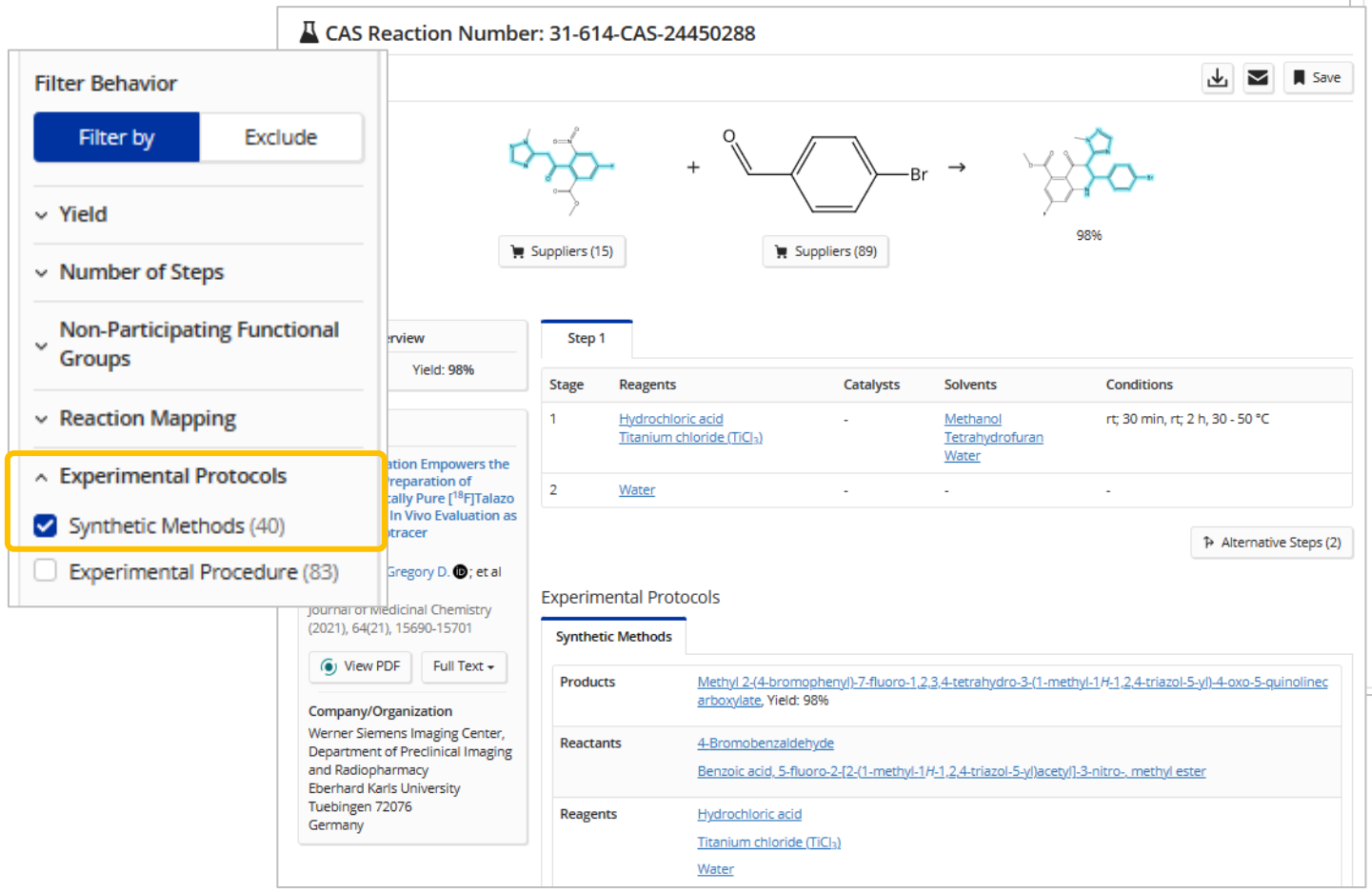
4.1 直观的合成实验详情 Synthetic Methods™

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



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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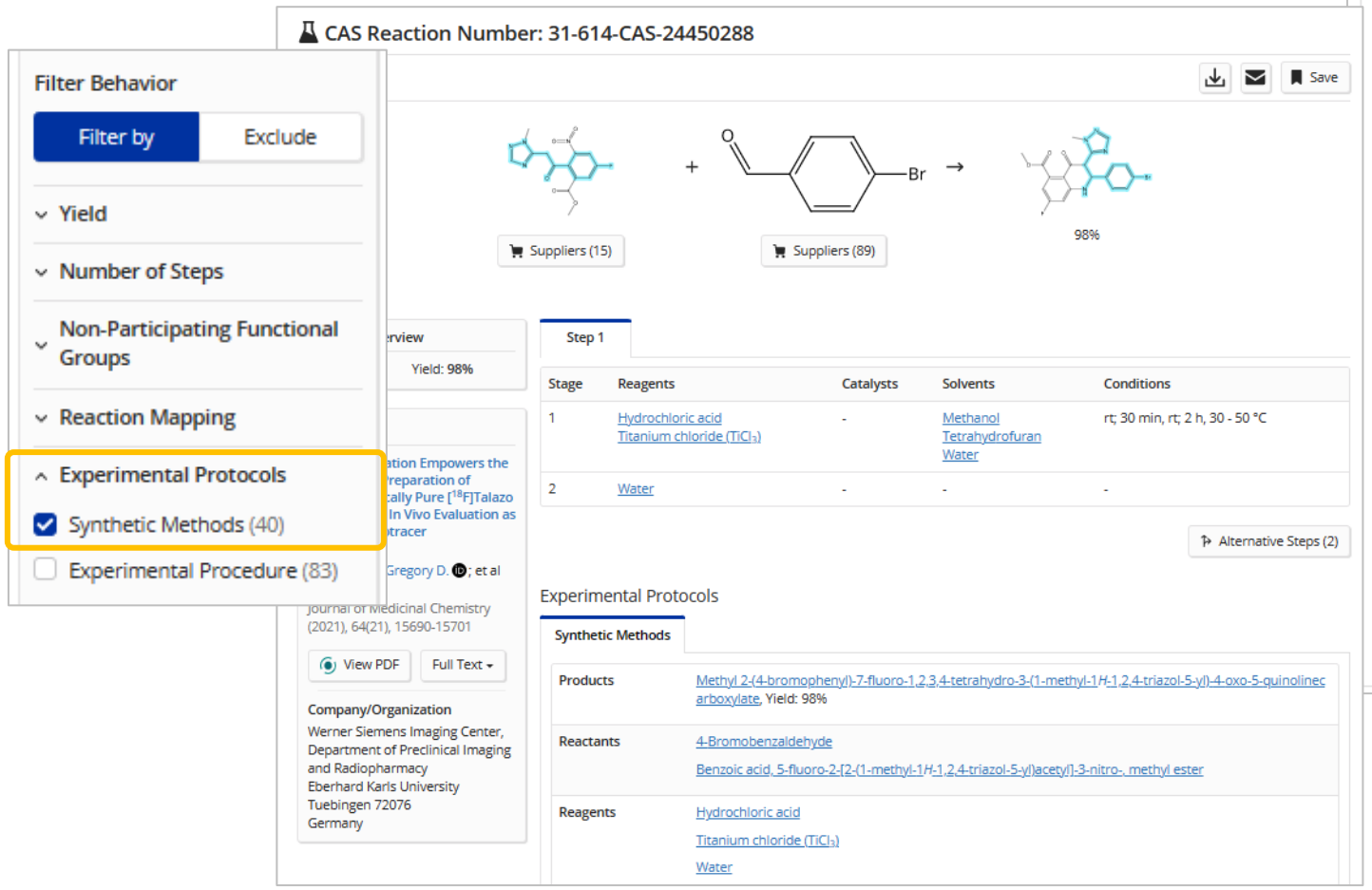
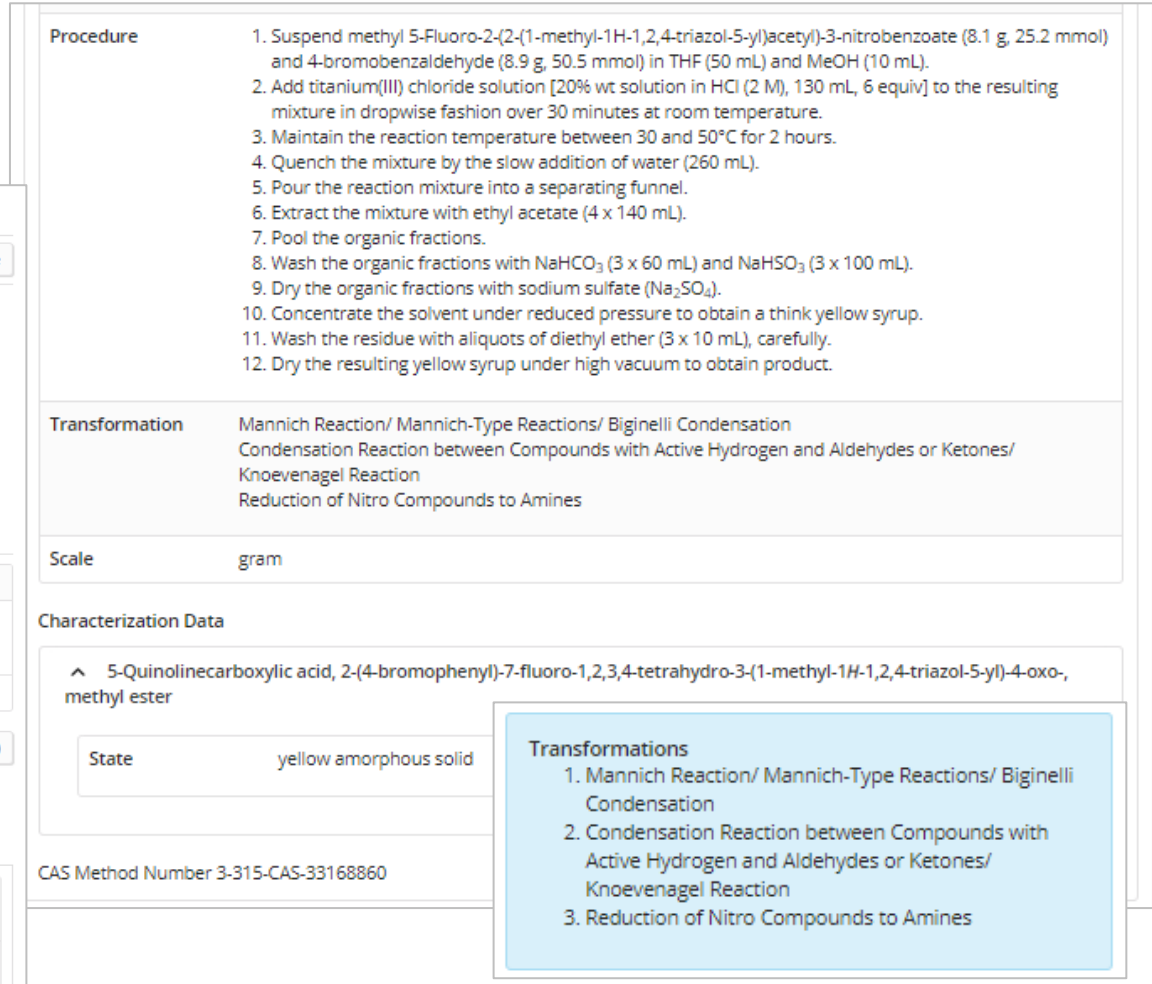
直观的合成实验详情 Synthetic Methods™

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





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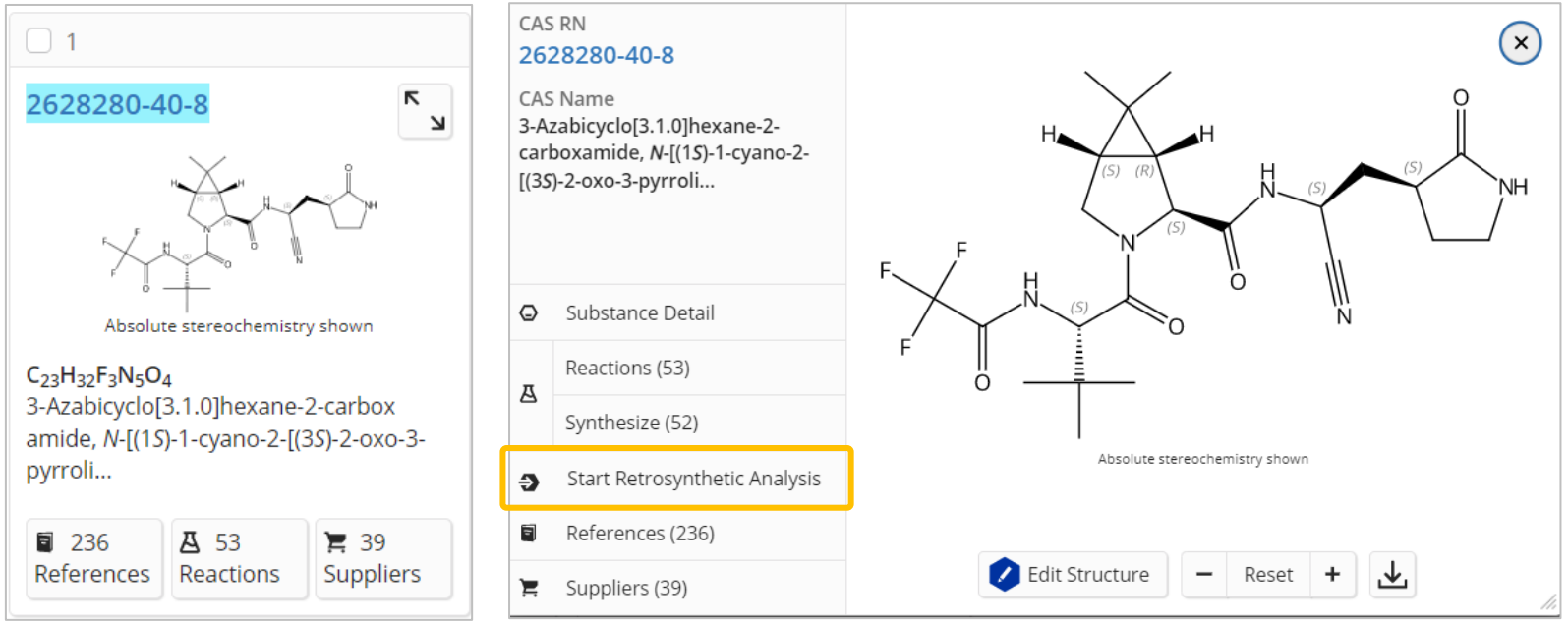
3.4 如何获得逆合成路线?

先进AI技术与CAS科学家标引的丰富反应信息相结合

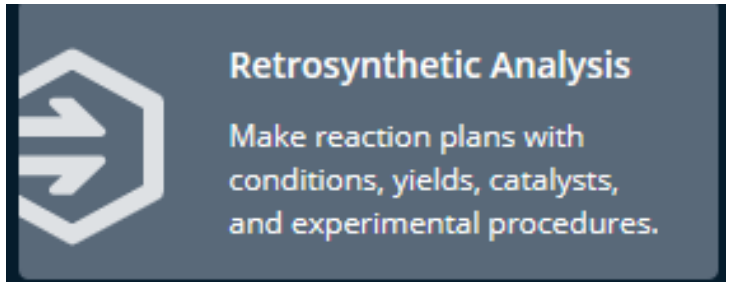
（1）已知化合物：点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis



CAS Retrosynthesis Tool：

- 逆合成反应路线设计功能
- 启发合成实验设计思路
- 高效获取逆合成反应路线

（2）已知/未知化合物：点击Retrosynthesis检索项，打开绘图板，绘制目标化合物，获得实验路线



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逆合成分析的预设参数

Retrosynthesis Plan Options for drawn structure

Set Rules Supporting Predicted Reactions Learn more

反应规则常见性

- (●) Common
- ( ) Uncommon (includes common rules)
- ( ) Rare (includes common and uncommon rules)

Set Starting Materials Cost Limit Learn more

起始原料费用

Set Starting Materials Cost Limit

1000 USD/mol

[ ] Email me when my plan is complete

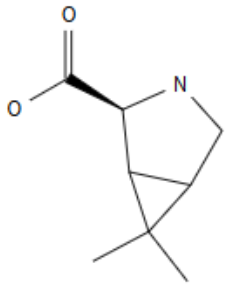
Continue to Retrosynthesis Plan

Break and Protect Bonds (Optional)

Select a bond within the box to break or protect. You may break a single bond or protect multiple bonds in the target molecule. Learn more

Break Bond | Protect Bond | Clear All Bond Selections

断裂键或保护键



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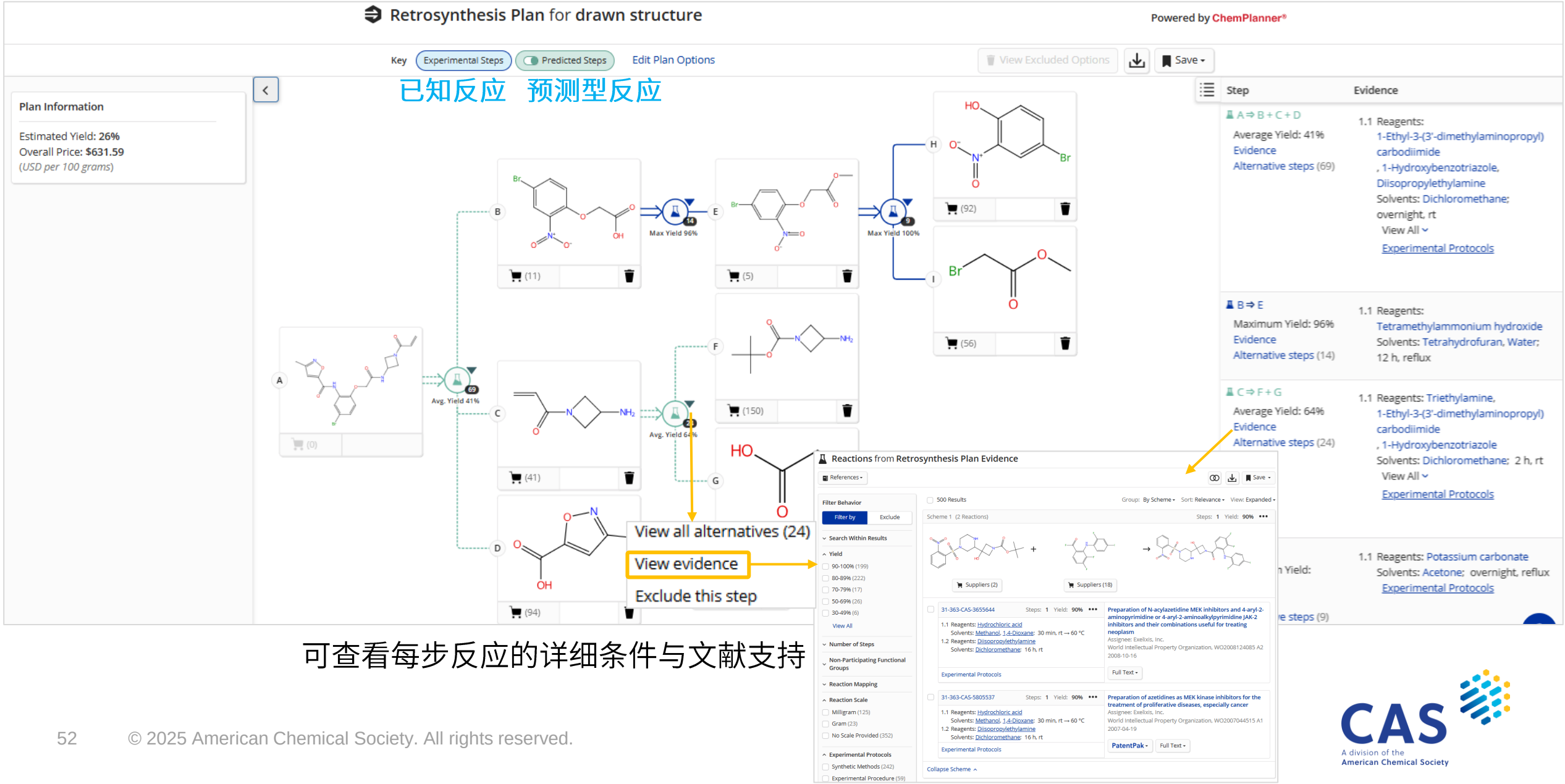
逆合成路线详情



可查看每步反应的详细条件与文献支持

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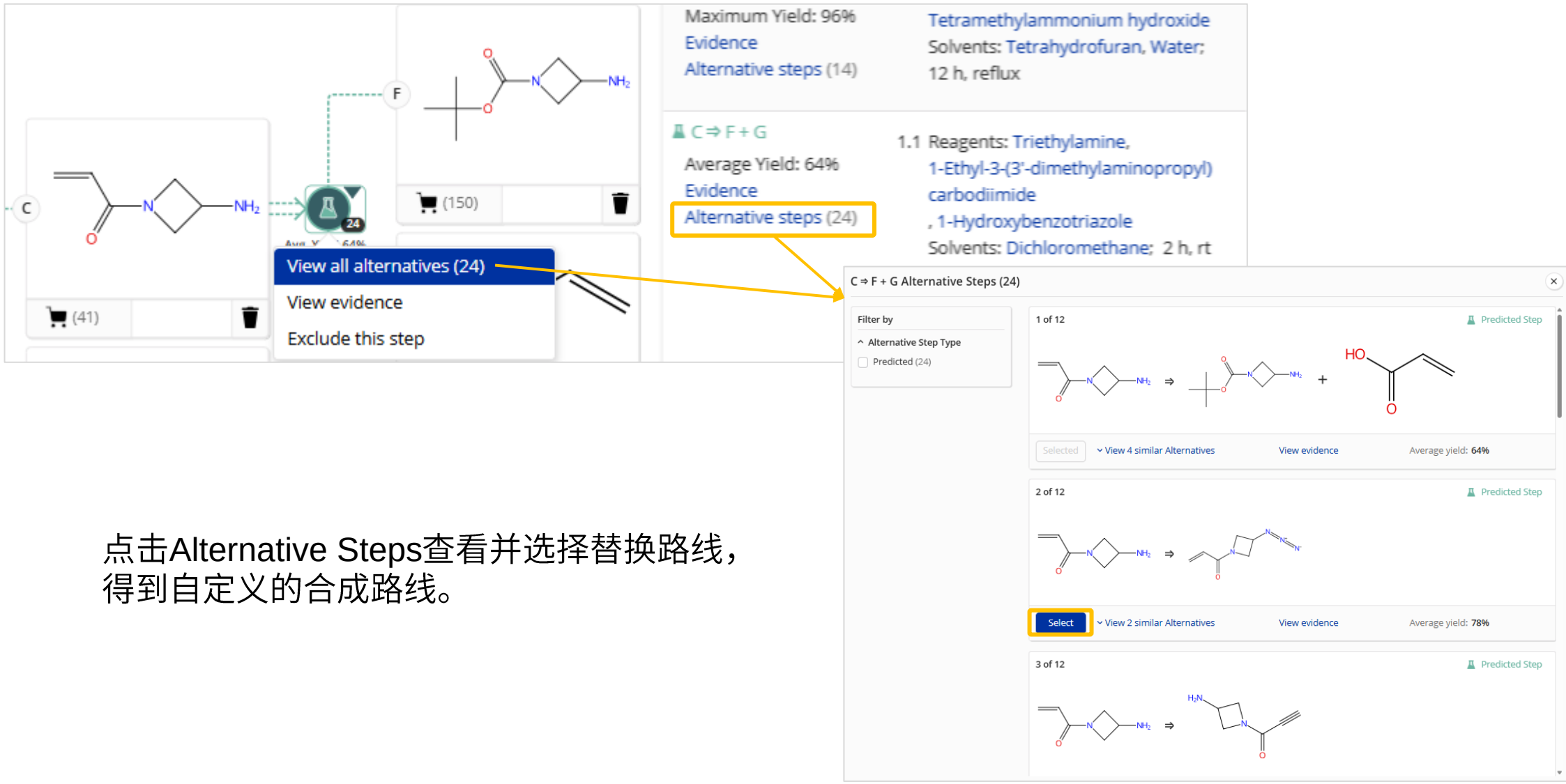
路线优化，考虑替换路线?



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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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. 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
5. 获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查找分析实验方法和制剂/配方详情?
- 常见问题Q&A

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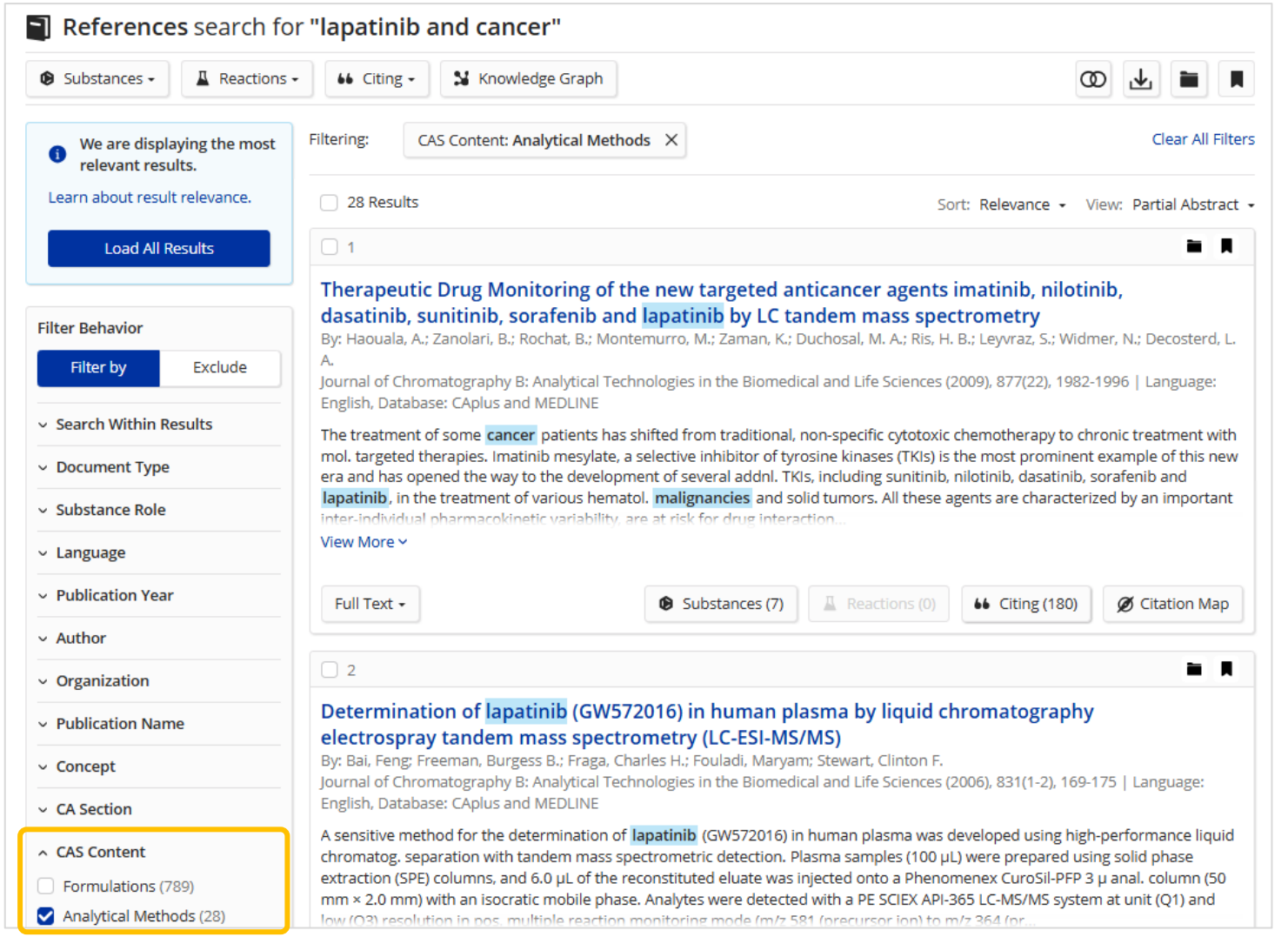
4. 怎么查找分析实验方法和制剂/配方详情?

- 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?

关注文献关联的分析方法?

方法 (1)：在CAS SciFinder的文献结果集页面，点击CAS Content中的 Analytical Methods筛选含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



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含有分析方法的文献详情页

Therapeutic Drug Monitoring of the new targeted anticancer agents imatinib, nilotinib, dasatinib, sunitinib, sorafenib and lapatinib by LC tandem mass spectrometry

7 | 0 | 180 | Citation Map

In this Reference

- Concepts
- Substances
- Analytical Methods
- Cited Documents

By: Haouala, A.; Zanolari, B.; Rochat, B.; Montemurro, M.; Zaman, K.; Duchosal, M. A.; Ris, H. B.; Levyraz, S.; Widmer, N.; Decosterd, L. A.

DOI: 10.1016/j.jchromb.2009.04.045

The treatment of some cancer patients has shifted from traditional, non-specific cytotoxic che
targeted therapies. Imatinib mesylate, a selective inhibitor of tyrosine kinases (TKIs) is the mos
has opened the way to the development of several addnl. TKIs, including sunitinib, nilotinib, da
treatment of various hematol. malignancies and solid tumors. All these agents are characteri
pharmacokinetic variability, are at risk for drug interactions, and are not devoid of toxicity. Ad
periods, anticipating the careful monitoring of their plasma exposure via Therapeutic Drug Mo
component of patients' follow-up. We have developed a liquid chromatog.-tandem mass spect
μL of plasma for the simultaneous determination of the six major TKIs currently in use. Plasma
supernatant is diluted in ammonium formate 20 mM (pH 4.0) 1:2. Reverse-phase chromatog. s
gradient elution of 20 mM ammonium formate pH 2.2 and acetonitrile containing 1% formic a
to the initial solvent composition up to 20 min. Analyte quantification, using matrix-matched c
spray ionization-triple quadrupole mass spectrometry by selected reaction monitoring detecti
validated according to FDA recommendations, including assessment of extraction yield, matrix
efficiency (87.1-104.2%), as well as TKIs short- and long-term stability in plasma. The method is
(-9.2 to +9.9%) and sensitive (lower limits of quantification comprised between 1 and 10 ng/mL
assay covering the major currently in-use TKIs. It is an improvement over previous methods in terms of convenience (a single extraction
procedure for six major TKIs, reducing significantly the anal. time), sensitivity, selectivity and throughput. It may contribute to filling the
current knowledge gaps in the pharmacokinetics/pharma
define their therapeutic ranges in different patient popul
these anticancer drugs could contribute to minimize the
lasting, therapeutic response.

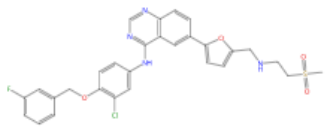
Keywords: imatinib nilotinib dasatinib sunitinib sorafenib
drug monitoring

View Source | Full Text | View in CAS Analytical Methods

Substances

Substances (7)

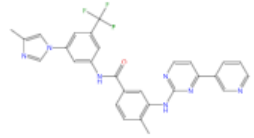
231277-92-2



$C_{29}H_{26}ClFN_4O_4S$
Lapatinib

Role: Analyte, Therapeutic Use, Analytical Study, Biological Study, Uses

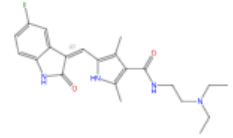
641571-10-0



$C_{28}H_{22}F_3N_7O$
Nilotinib

Role: Analyte, Therapeutic Use, Analytical Study, Biological Study, Uses

557795-19-4



Double bond geometry shown

$C_{22}H_{27}FN_4O_2$
Sunitinib

Role: Analyte, Therapeutic Use, Analytical Study, Biological Study, Uses

Analytical Methods

View All Methods

Method Title

Analysis of Imatinib mesylate in Blood plasma by HPLC-tandem mass spectrometry

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CAS Analytical Methods 分析方法详情

Analysis of Imatinib mesylate in Blood plasma by HPLC-tandem mass spectrometry

CAS Method Number
1-101-CAS-181855

Method Category
Active Pharmaceutical Ingredient and Metabolite Analysis

Technique
HPLC-tandem mass spectrometry; Extraction

Analyte
Dasatinib
Imatinib mesylate
Lapatinib
Nilotinib
Sorafenib
View All

Matrix
Blood plasma

Material
2.1 mm x 50 mm XTerra dC18 5 µm analytical column

Reagent
-

Biological Reagent
-

Equipment Used

LC system, Flux Instruments, AG, Thermo Fischer Scientific Inc, Waltham, MA

triple quadrupole (TSQ) Quantum Discovery mass spectrometer (MS), Thermo Fisher Scientific, Inc, Waltham, MA

thermostated column heater, Croco-Cil, Cluzeau Info Laboratory, Courbevoie, France

Centrifuge, J6B, Beckmann

benchtop Centrifuge, 16R, Hettich, Bach, Switzerland

Conditions

Chromatographic

mobile phase:20 mM ammonium formate in ultrapure water adjusted to pH 2.2 with formic acid (FA) 98-100% (solution A), and acetonitrile with 1% FA (solution B);flow rate:0.3-0.5 mL/min;

Instrument

ESI:positive mode;capillary temperature:350 °C;in source induced dissociation:10 V;tube lens voltages range:86-129 V;spray voltage:4 kV;sheath and auxiliary gas:nitrogen;flow-rate:60 psi and 5;Q2 collision gas (argon) pressure:1 mTorr (0.13 Pa)

Validation

Linearity Range	1-10000 ng/mL, Imatinib 1-200 ng/mL, Dasatinib 1-500 ng/mL, Nilotinib 100-15000 ng/mL, Sunitinib 1-5000 ng/mL, Sorafenib 5-5000 ng/mL, Lapatinib
Limit of Detection	0.3 ng/mL, Imatinib 0.3 ng/mL, Dasatinib 0.4 ng/mL, Nilotinib 0.1 ng/mL, Sunitinib 1 ng/mL, Sorafenib 0.4 ng/mL, Lapatinib
Limit of Quantitation	1 ng/mL, Imatinib 1 ng/mL, Dasatinib 1 ng/mL, Nilotinib 1 ng/mL, Sunitinib 10 ng/mL, Sorafenib 5 ng/mL, Lapatinib
Accuracy	7.2%, -7.6% and -1.9% (Intra-assay bias, in 3, 2000 and 8000 ng/mL concentrations respectively);6.5%, -9.2% and -2.9% (Inter-assay bias, in 3, 2000 and 8000 ng/mL concentrations respectively), Imatinib -2.1%, -8.7% and -0.5% (Intra-assay bias, in 3, 60 and 150 ng/mL concentrations respectively);2.4%, -5.3% and -1.2% (Inter-assay bias, in 3, 60 and 150 ng/mL concentrations respectively), Dasatinib 5.2%, 2.1% and 1.8% (Intra-assay bias, in 3, 800 and 3000 ng/mL concentrations respectively);4.2%, 4.0% and 9.9% (Inter-assay bias, in 3, 800 and 3000 ng/mL concentrations respectively), Nilotinib -8.7%, -1.4% and 0.1% (Intra-assay bias, in 3, 80 and 400 ng/mL concentrations respectively);-5.4%, -1.2% and -0.3% (Inter-assay bias, in 3, 80 and 400 ng/mL concentrations respectively), Sunitinib -0.2%, -7.3% and -1.2% (Intra-assay bias, in 15, 800 and 4000 ng/mL concentrations respectively);4.5%, -7.0% and 2.2% (Inter-assay bias, in 15, 800 and 4000 ng/mL concentrations respectively), Lapatinib -7.8%, 5.8% and -7.7% (Intra-assay bias, in 300, 1500 and 6000 ng/mL concentrations respectively);-6.6%, 5.6% and -8.1% (Inter-assay bias, in 300, 1500 and 6000 ng/mL concentrations respectively), Sorafenib
Precision	6.8%, 4.4% and 4.1% (Intra-assay CV, in 3, 2000 and 8000 ng/mL concentrations respectively);6.1%, 3.7% and 4.8% (Inter-assay CV, in 3, 2000 and 8000 ng/mL concentrations respectively), Imatinib

Source

JOURNAL

Therapeutic Drug Monitoring of the new targeted anticancer agents imatinib, nilotinib, dasatinib, sunitinib, sorafenib and lapatinib by LC tandem mass spectrometry

Haouala, A.; Zanolari, B.; Rochat, B.; Montemurro, M.; Zaman, K.; Duchosal, M. A.; Ris, H. B.; Leyvraz, S.; Widmer, N.; Decosterd, L. A.

Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2009), 877 (22), 1982 - 1996. Elsevier B.V.

CODEN : JCBAAI | ISSN : 15700232 | DOI : 10.1016/j.jchromb.2009.04.045

View Abstract | Full Text

Instructions

Preparation of plasma samples

1. Collect blood samples (5 mL) at random time after last drug intake in Monovettes (Sarstedt, Numbrecht, Germany, with K-EDTA as anticoagulant) from patients treated with one of the six analytes.
2. Centrifuge (1850 x g 3000rpm, + 4 °C, 10 min) (Beckmann Centrifuge, Model J6B) blood samples without delay and separate and transfer the plasma into polypropylene test tubes before storage at -20 °C.

Preparation of stock and standard solutions

1. Prepare stock solutions of imatinib and nilotinib at 1 mg/mL and dasatinib at 0.05 mg/mL by dissolution of 59.7 mg imatinib mesylate, 50 mg nilotinib base and 10 mg dasatinib base in 50.0 mL, 50.0 mL and 200.0 mL MeOH respectively.
2. Prepare sunitinib stock solution (1 mg/mL) in MeOH by extraction of Sutent capsules with MeOH.
3. Prepare sorafenib and lapatinib stock solutions after careful grounding in a mortar and extraction with MeOH of one Nexavar 200 mg tablet and one Tyverb 250 mg.Filter the resulting MeOH suspension and complete to the volume of 200 and 250 mL of MeOH respectively.
4. Store the stock solutions at 4 °C in glass flasks, with caps tightly wrapped with Parafilm.
5. Dilute the stock solutions with MeOH to obtain working solutions.

Plasma sample extraction

1. Mix a plasma sample aliquot (100 µL) with a 100 µL of internal standard solution.
2. Subject the resulting sample to protein precipitation with acetonitrile (600 µL) and carefully vortex-mix.
3. Centrifuge the mixture at 4 °C for 10 min at 20,000 x g (14000 rpm) on a benchtop Hettich Centrifuge (Benchtop Universal 16R centrifuge, Bach, Switzerland).
4. Add a 200 µL aliquot of the supernatant and 400 µL of buffer ammonium formate 20 mM pH adjusted to 4.0 with formic acid into 1.5 mL glass HPLC microvials and vortex-mix after secure closing with aluminium crimp seals.
5. Maintain processed samples at +10 °C in the thermostated autosampler rack.

LC-MS/MS analysis of the extracted plasma samples

1. Carry out chromatography on a LC system consisting of a Rheos 2200 quaternary pumps, equipped with an online degasser and a HTS PAL autosampler (CTC Analytics AG, Zwingen, Switzerland) controlled by Janeiro-CNS software (Flux Instruments, AG, Thermo Fischer Scientific Inc, Waltham, MA).
2. Separate the analytes on a 2.1 mm x 50 mm XTerra dC18 5 µm analytical column (Waters, Milford, MA, USA) placed in a thermostated column heater at 25 °C (Croco-Cil, Cluzeau Info Laboratory, Courbevoie, France).
3. Use 20 mM ammonium formate in ultrapure water adjusted to pH 2.2 with formic acid (FA) 98-100% (solution A), and acetonitrile with 1% FA (solution B) as the mobile phase.
4. Set up a gradient elution program as follows:5% of B at 0 min, 50% of B at 11 min, 100% of B at 14 min with a flow rate of 0.3 mL/min.
5. In the second part of the run carry out 3 min of intensive rinsing (100% B with 0.5 mL/min) and re-equilibration step to the initial solvent up to 20 min (at 17.01 with 0.3 mL/min).
6. Set the thermostated column heater at 25 °C and maintain the autosampler at 10 °C.
7. Carry out detection using a triple quadrupole (TSQ) Quantum Discovery mass spectrometer (MS) from Thermo Fisher Scientific, Inc. equipped with an Ion Max electrospray ionization (ESI) interface and operated with Xcalibur 2.0 software (Thermo Fischer Scientific Inc, Waltham, MA).
8. Set the MS conditions as follows: ESI in positive mode, capillary temperature: 350 °C, in source induced dissociation: 10 V, tube lens voltages range: 86-129 V, spray voltage: 4 kV and sheath and auxiliary gas (nitrogen) flow-rate: 60 psi and 5 respectively.Set the Q2 collision gas (argon) pressure at 1 mTorr (0.13 Pa).
9. Acquire the MS in selected reaction monitoring (SRM).
10. Perform chromatographic data acquisition, peak integration and quantification using the Xcalibur LC-Quan software package (version 2.0) (ThermoQuest, San Jose. CA, USA).

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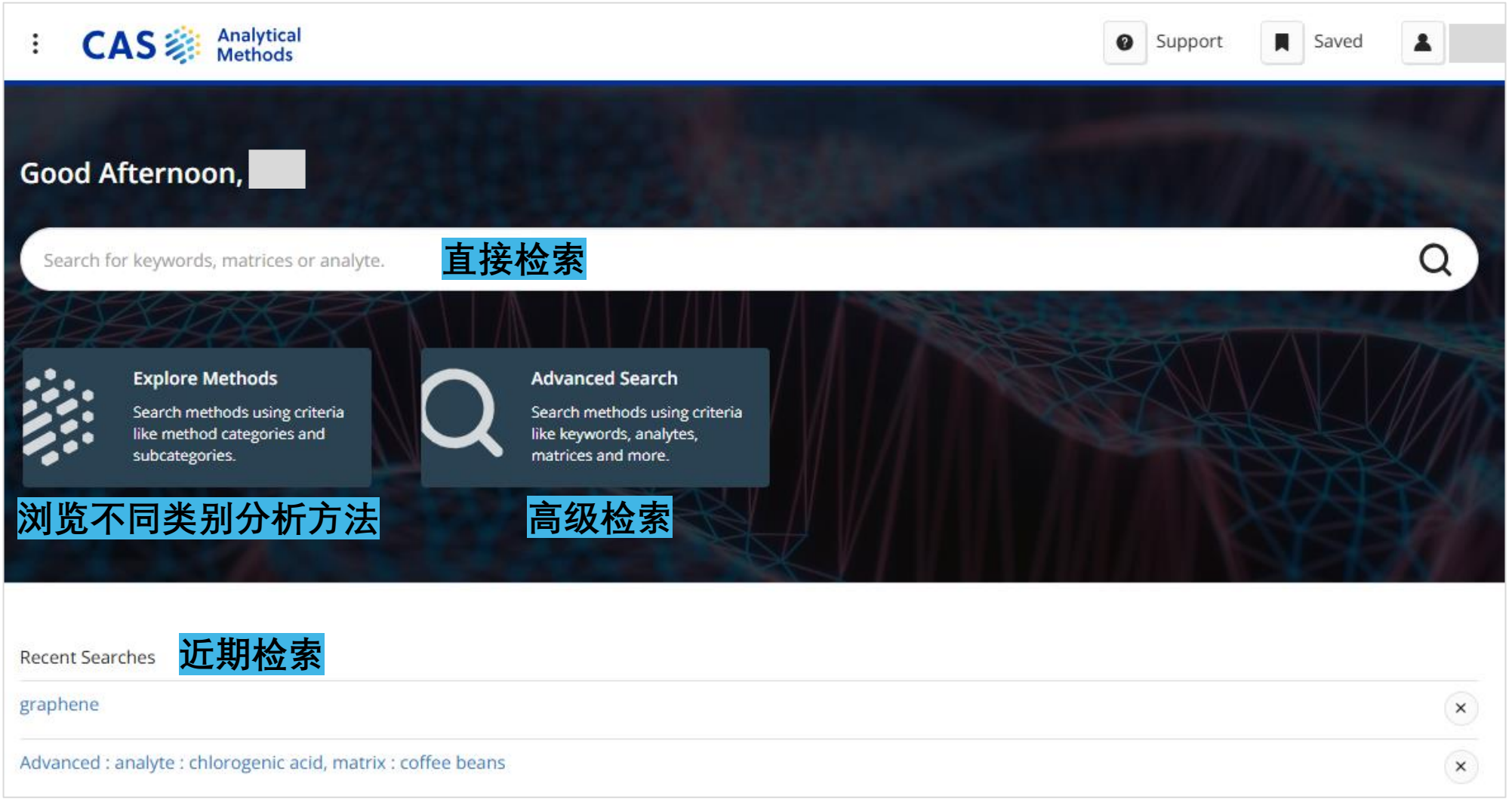
直接检索感兴趣的分析实验方法

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



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CAS Analytical Methods 分析方法类别

目前涵盖13个大类，45个小类；某些子分类属于多种方法分类。

Agricultural Applications / Analysis: 除草剂分析…

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

Biomolecule Isolation:天然产物分离分析，蛋白质分析…

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

Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析…

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

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

Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析…

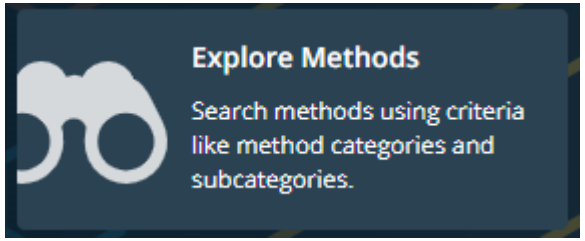
Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…

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

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

Polymer: 塑料加工

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



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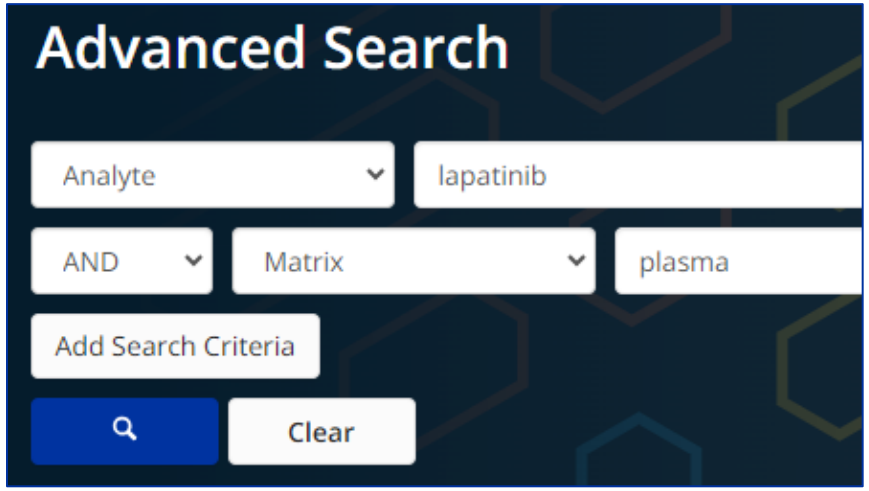
关键词检索分析方法

- **直接检索示例：**
  lapatinib 拉帕替尼

- **高级检索示例：**
  分析拉帕替尼血药浓度的方法



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检索结果分析与精炼

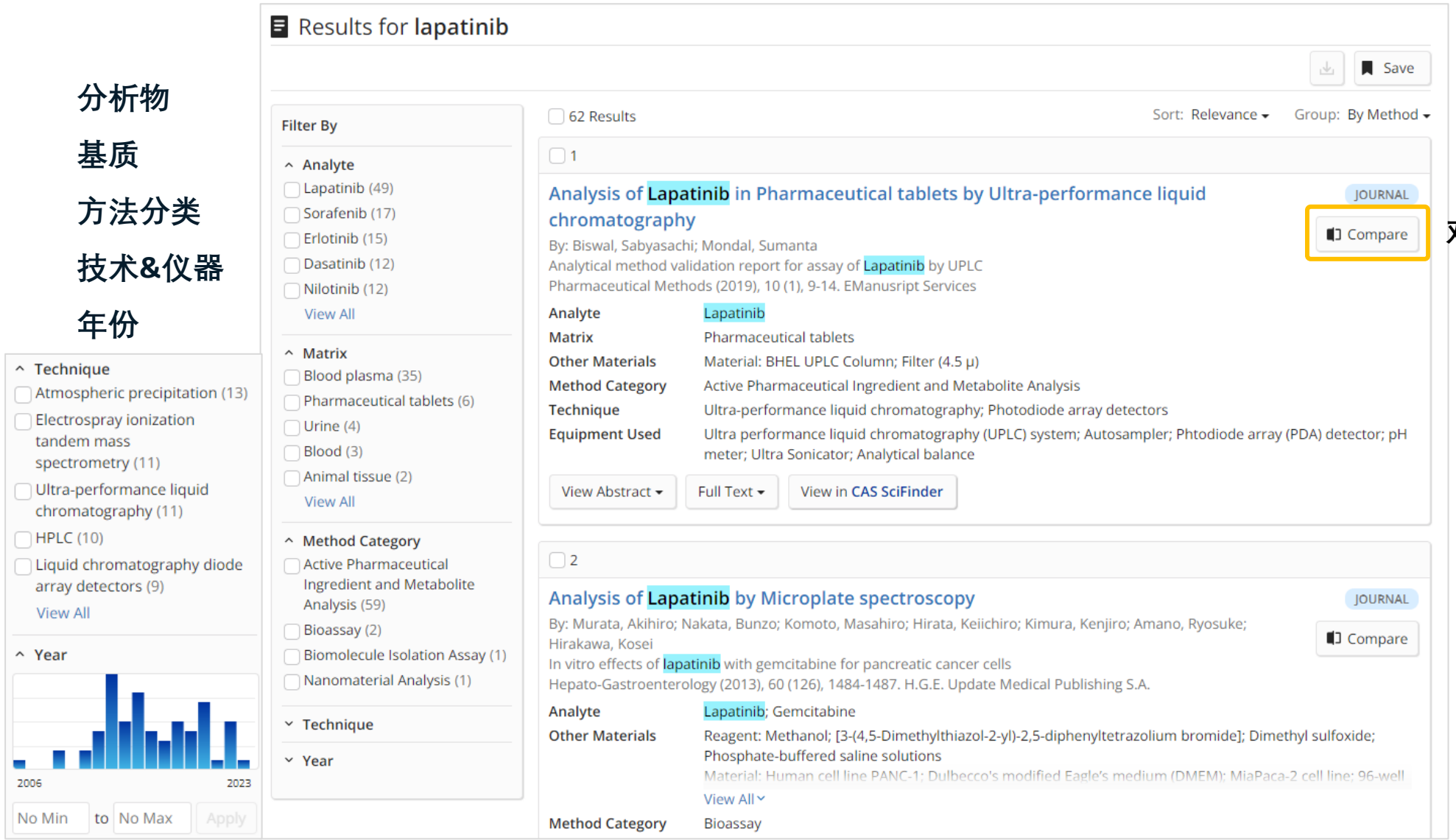
分析物

基质

方法分类

技术&仪器

年份



对比不同分析方法

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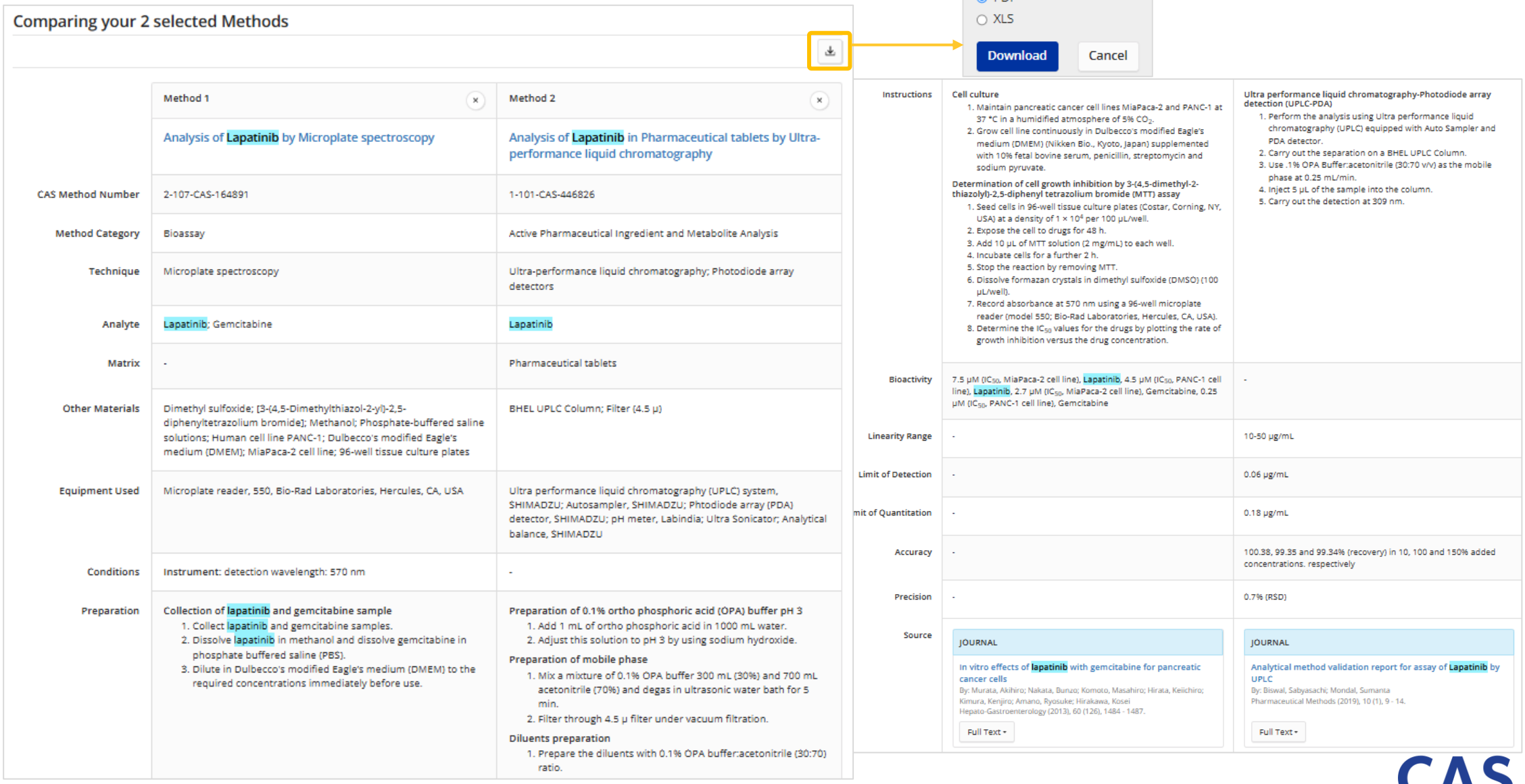
对照多个感兴趣的分析方法详情



	Method 1	Method 2
	Analysis of Lapatinib by Microplate spectroscopy	Analysis of Lapatinib in Pharmaceutical tablets by Ultra-performance liquid chromatography
CAS Method Number	2-107-CAS-164891	1-101-CAS-446826
Method Category	Bioassay	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Microplate spectroscopy	Ultra-performance liquid chromatography; Photodiode array detectors
Analyte	Lapatinib; Gemcitabine	Lapatinib
Matrix	-	Pharmaceutical tablets
Other Materials	Dimethyl sulfoxide; [3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide]; Methanol; Phosphate-buffered saline solutions; Human cell line PANC-1; Dulbecco's modified Eagle's medium (DMEM); MiaPaca-2 cell line; 96-well tissue culture plates	BHEL UPLC Column; Filter (4.5 µ)
Equipment Used	Microplate reader, 550, Bio-Rad Laboratories, Hercules, CA, USA	Ultra performance liquid chromatography (UPLC) system, SHIMADZU; Autosampler, SHIMADZU; Phtodiode array (PDA) detector, SHIMADZU; pH meter, Labindia; Ultra Sonicator; Analytical balance, SHIMADZU
Conditions	**Instrument:** detection wavelength: 570 nm	-
Preparation	**Collection of lapatinib and gemcitabine sample** 1. Collect lapatinib and gemcitabine samples. 2. Dissolve lapatinib in methanol and dissolve gemcitabine in phosphate buffered saline (PBS). 3. Dilute in Dulbecco's modified Eagle's medium (DMEM) to the required concentrations immediately before use.	**Preparation of 0.1% ortho phosphoric acid (OPA) buffer pH 3** 1. Add 1 mL of ortho phosphoric acid in 1000 mL water. 2. Adjust this solution to pH 3 by using sodium hydroxide. **Preparation of mobile phase** 1. Mix a mixture of 0.1% OPA buffer 300 mL (30%) and 700 mL acetonitrile (70%) and degas in ultrasonic water bath for 5 min. 2. Filter through 4.5 µ filter under vacuum filtration. **Diluents preparation** 1. Prepare the diluents with 0.1% OPA buffer:acetonitrile (30:70) ratio.
Instructions	**Cell culture** 1. Maintain pancreatic cancer cell lines MiaPaca-2 and PANC-1 at 37 °C in a humidified atmosphere of 5% CO_2. 2. Grow cell line continuously in Dulbecco's modified Eagle's medium (DMEM) (Nikken Bio., Kyoto, Japan) supplemented with 10% fetal bovine serum, penicillin, streptomycin and sodium pyruvate. **Determination of cell growth inhibition by 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl tetrazolium bromide (MTT) assay** 1. Seed cells in 96-well tissue culture plates (Costar, Corning, NY, USA) at a density of 1×10^4 per 100 µL/well. 2. Expose the cell to drugs for 48 h. 3. Add 10 µL of MTT solution (2 mg/mL) to each well. 4. Incubate cells for a further 2 h. 5. Stop the reaction by removing MTT. 6. Dissolve formazan crystals in dimethyl sulfoxide (DMSO) (100 µL/well). 7. Record absorbance at 570 nm using a 96-well microplate reader (model 550; Bio-Rad Laboratories, Hercules, CA, USA). 8. Determine the IC_{50} values for the drugs by plotting the rate of growth inhibition versus the drug concentration.	**Ultra performance liquid chromatography-Photodiode array detection (UPLC-PDA)** 1. Perform the analysis using Ultra performance liquid chromatography (UPLC) equipped with Auto Sampler and PDA detector. 2. Carry out the separation on a BHEL UPLC Column. 3. Use .1% OPA Buffer:acetonitrile (30:70 v/v) as the mobile phase at 0.25 mL/min. 4. Inject 5 µL of the sample into the column. 5. Carry out the detection at 309 nm.
Bioactivity	7.5 µM (IC_{50}, MiaPaca-2 cell line), Lapatinib, 4.5 µM (IC_{50}, PANC-1 cell line), Lapatinib, 2.7 µM (IC_{50}, MiaPaca-2 cell line), Gemcitabine, 0.25 µM (IC_{50}, PANC-1 cell line), Gemcitabine	-
Linearity Range	-	10-50 µg/mL
Limit of Detection	-	0.06 µg/mL
mit of Quantitation	-	0.18 µg/mL
Accuracy	-	100.38, 99.35 and 99.34% (recovery) in 10, 100 and 150% added concentrations. respectively
Precision	-	0.7% (RSD)
Source	JOURNAL In vitro effects of lapatinib with gemcitabine for pancreatic cancer cells By: Murata, Akihiro; Nakata, Bunzo; Komoto, Masahiro; Hirata, Keiichiro; Kimura, Kenjiro; Amano, Ryosuke; Hirakawa, Kosei Hepato-Gastroenterology (2013), 60 (126), 1484 - 1487. Full Text	JOURNAL Analytical method validation report for assay of Lapatinib by UPLC By: Biswal, Sabyasachi; Mondal, Sumanta Pharmaceutical Methods (2019), 10 (1), 9 - 14. Full Text

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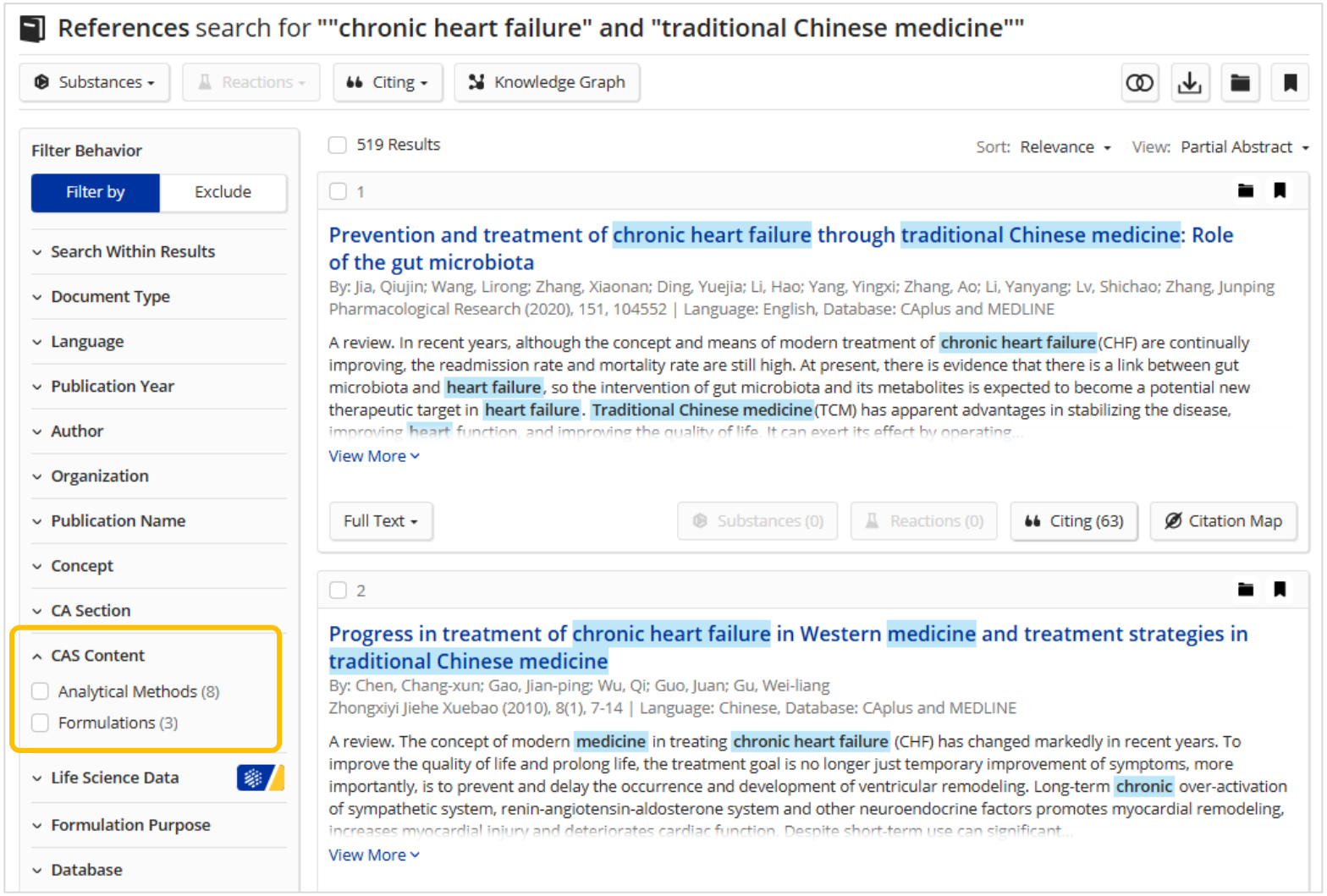
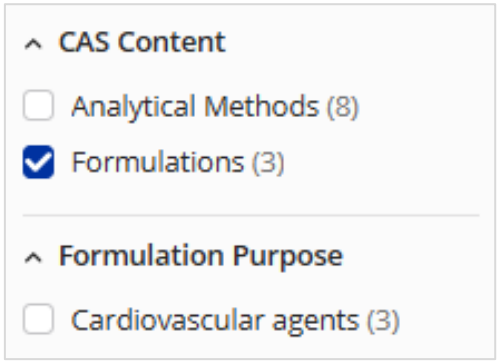
文献关联的制剂/配方

方法（1）：在CAS SciFinder的文献结果集页面，点击CAS Content中的 Formululations获得有具体制剂/配方信息的文献，从文献详情页中链接获取





定位制剂/配方的功能目标

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文献关联的制剂/配方

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

0 0 0 Citation Map

In this Reference

- IPC Data
- CAS Concepts
- Formulations

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

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

Keywords: myocardial hypertrophy prevention traditional Chinese medicine composition

PatentPak PDF | Get Prior Art Analysis | Full Text | View in CAS Formulus

Publication Information • **Patent** View Less

Patent Number
CN112190652

Publication Date
2021-01-08

Assignee
Capital Medical University, China

Source
China
CODEN: CNXXEV

Formulations

View All Formulations

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

Patent Family

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

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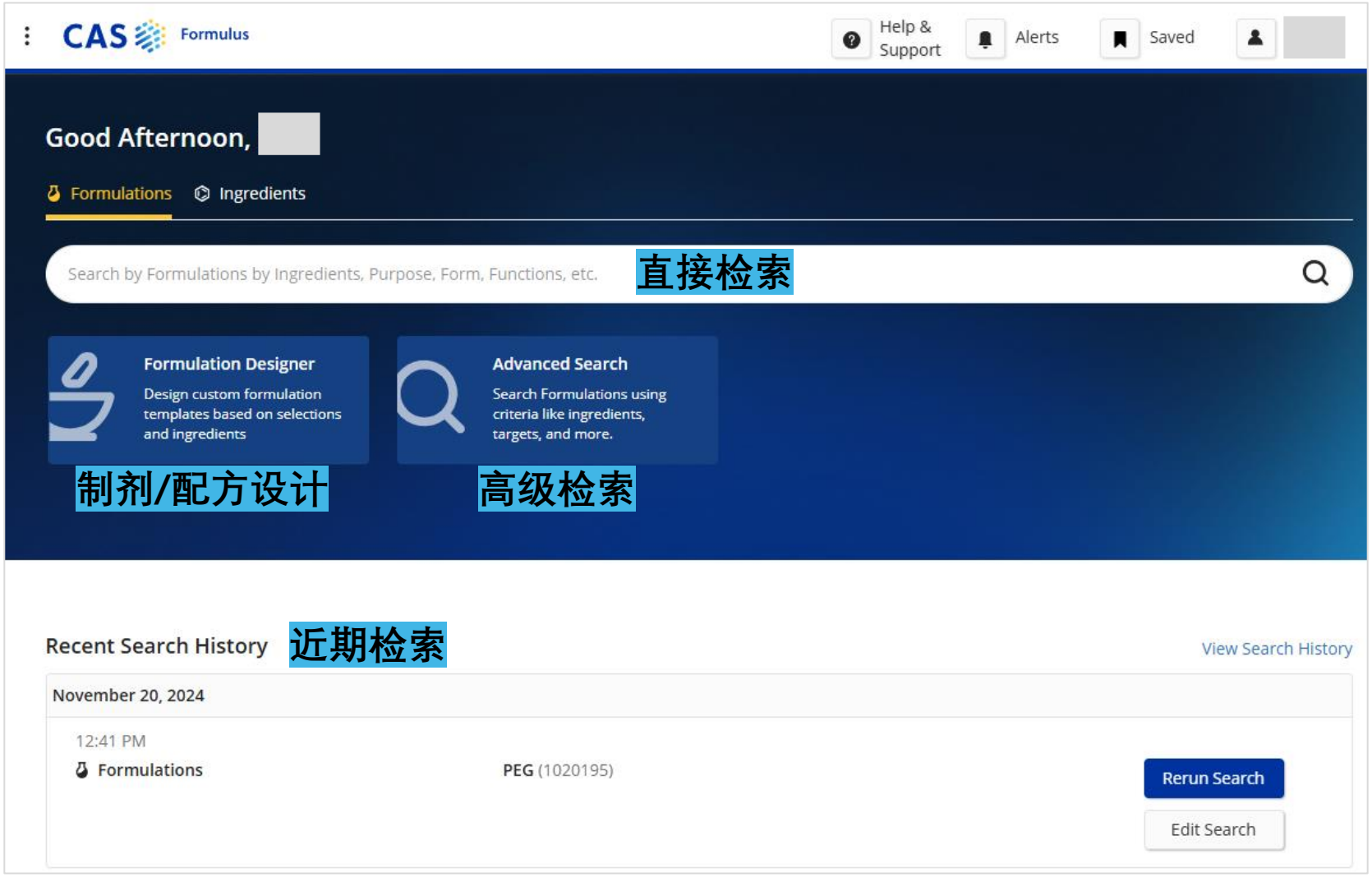
直接检索制剂/配方或配方成分

方法（2）：登录CAS Formulus主页（https://formulus.cas.org）进行直接检索或高级检索



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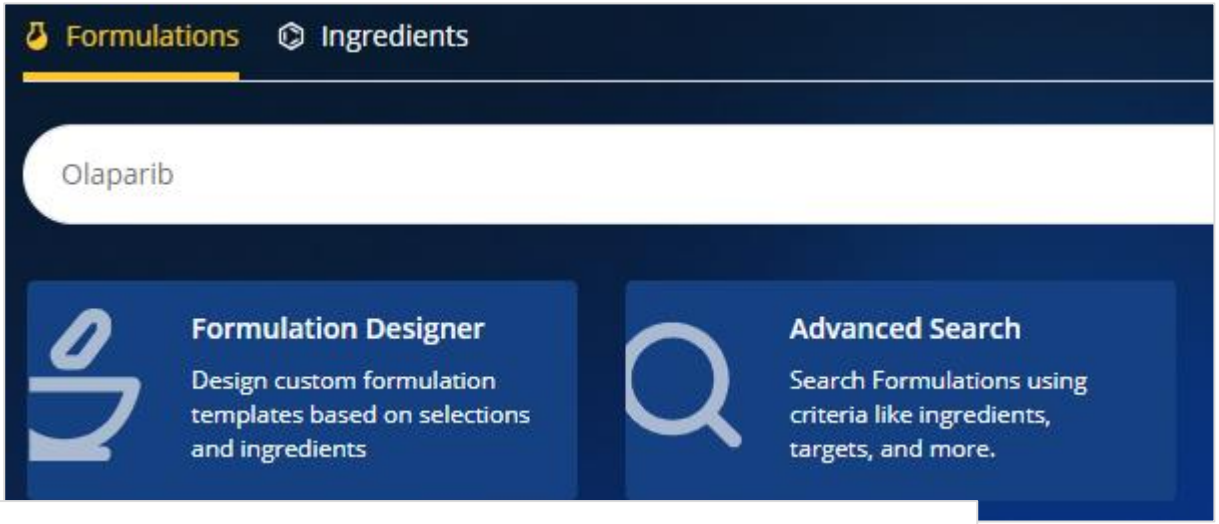
关键词检索制剂/配方

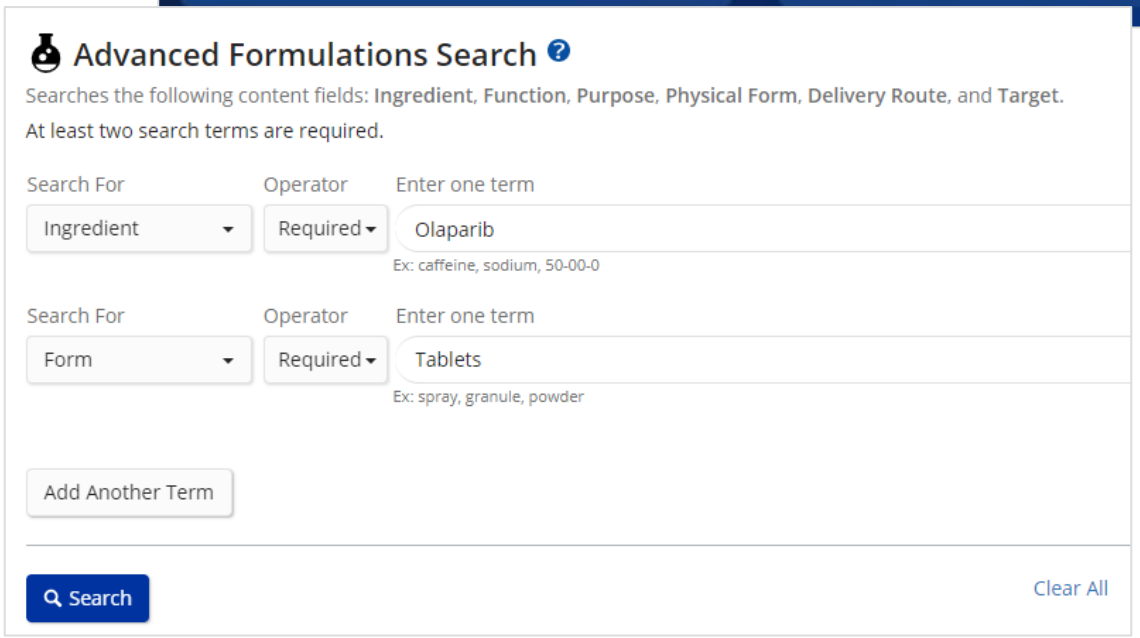
- 直接检索示例：

  Olaparib 奥拉帕尼



- 高级检索示例：

  奥拉帕尼片剂



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检索结果分析与精炼

应用领域

目的/用途

物理形态

物质状态

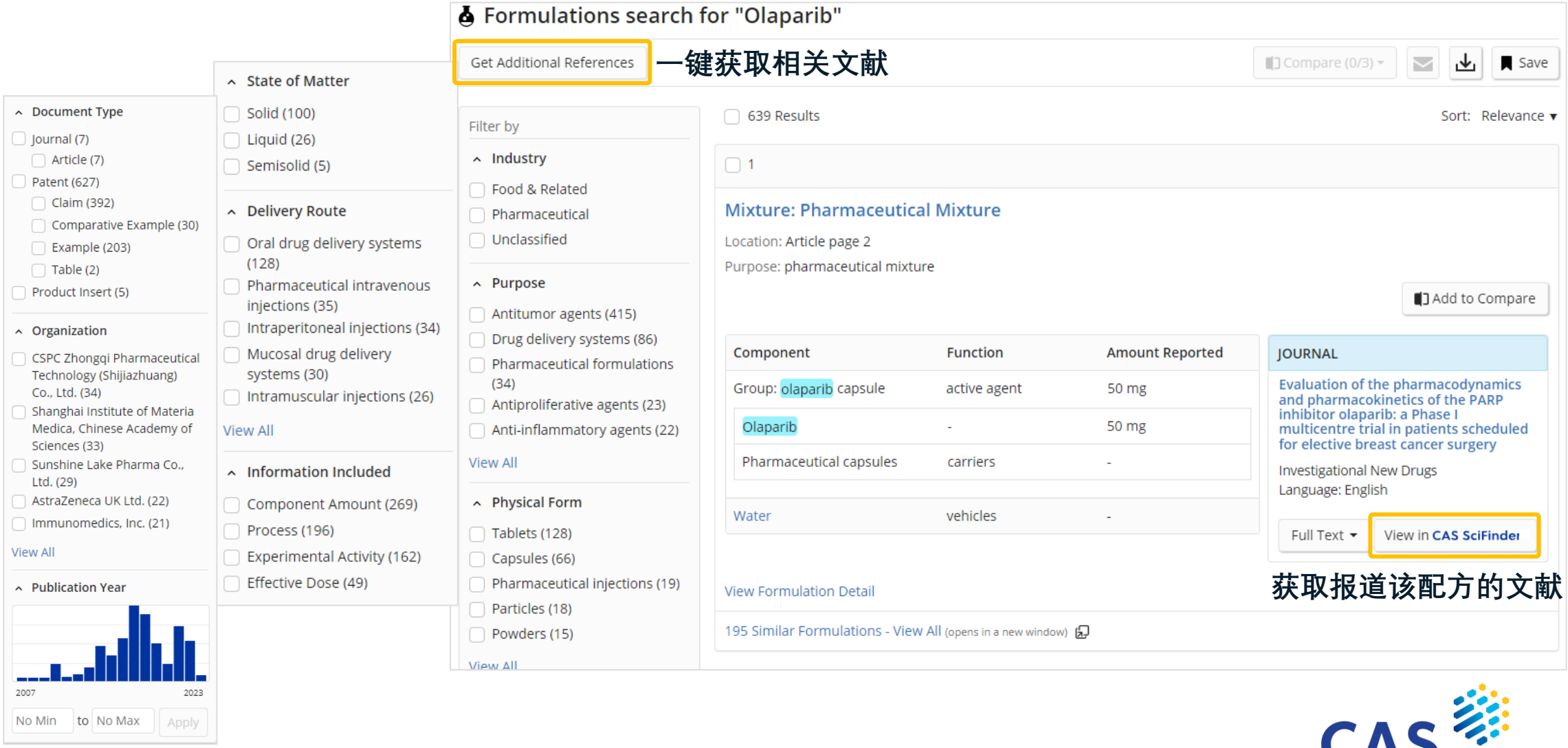
作用方式

制剂信息

文献类型

机构名

发表年份



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制剂、配方详情

Olaparib Solid Dispersion: Antitumor Agents

Save

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

Predicted value

Formulation Ingredients

制剂成分、功能、用量

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

More Formulations like this...

- **Lincomycin Solid Dispersion: Veterinary Drug**
  Purpose: Veterinary drugs
  Target: Homo sapiens, Livestock, Poultry
  Delivery Route: -
  Physical Form: Pharmaceutical solid di...
- **Olaparib Dispersible Tablets: Antitumor Agents**
  Purpose: Antitumor agents
  Target: Homo sapiens, Mammary glan...
  Delivery Route: Oral drug delivery syst...
  Physical Form: Pharmaceutical orally d...
- **Olaparib Dispersible Tablets: Antitumor Agents**
  Purpose: Antitumor agents
  Target: Homo sapiens, Mammary glan...
  Delivery Route: Oral drug delivery syst...
  Physical Form: Pharmaceutical orally d...
- **Lincomycin Solid Dispersion: Veterinary Drug**
  Purpose: Veterinary drugs
  Target: Homo sapiens, Livestock, Poultry
  Delivery Route: -
  Physical Form: Pharmaceutical solid di...

Process

工艺信息

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

Source Patent

Olaparib solid dispersion and preparation method ther

Assignee : Farmasino Pharmaceuticals (Jiangsu) Co., Ltd.
CN106692066
Language: Chinese
Location: Example 4

Patent PDF | View in CAS SciFinder

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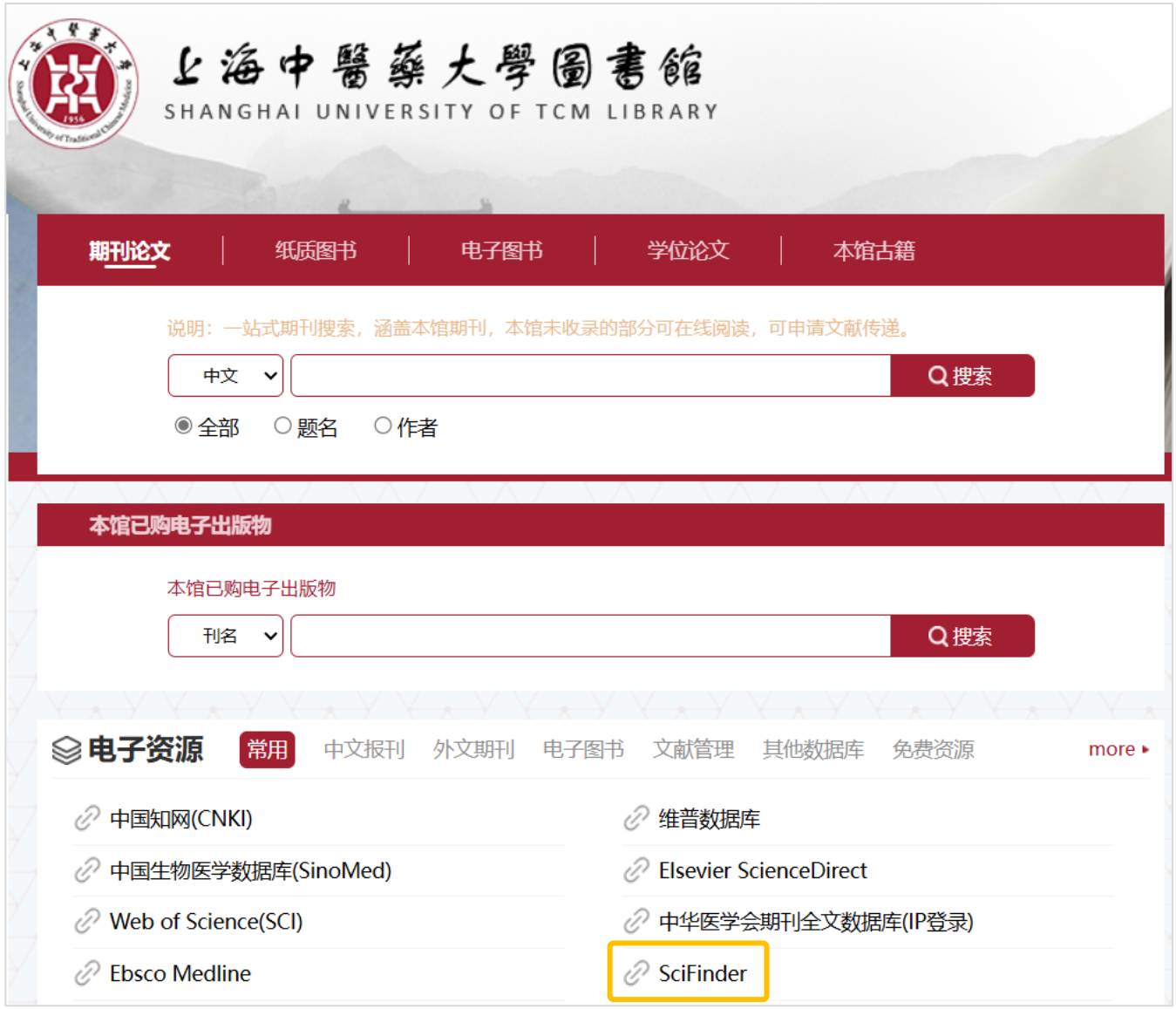
分析方法及制剂/配方检索小结

1. 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
2. 利用CAS Formulus检索制剂/配方、原料，或通过文献结果集获得关联的制剂/配方信息；利用配方设计工具启发产品配方的开发

大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查找分析实验方法和制剂/配方详情?
- 常见问题Q&A

如何获取CAS SciFinder账号



1、登录学校图书馆官网，在“电子资源”中点击“SciFinder”。

首页 > 电子资源 > 常用 > SciFinder >

一、数据库链接

访问链接：https://scifinder-n.cas.org/

账号注册地址：https://scifinder.cas.org/registration/index.html?corpKey=4A9382C4X86F350ABX229D311A5663BB09AC

二、数据库介绍

CAS SciFinder-n是美国化学会（American Chemical Society, 简称 ACS）旗下分支机构美国化学文摘社（CAS）出品的权威科学研究工具，是化学及相关学科智能研究平台，提供全球最全面、最可靠的化学及相关学科研究信息和分析工具。 CAS SciFinder-n由国际科学家团队追踪全球科技进展，每日收录汇总、标引、管理着世界上的专利、科技期刊等内容，并通过CAS SciFinder-n平台提供的先进检索技术高效揭示、发现重要的技术信息，确保研究人员及时同步全球最重要的研究进展。

CAS SciFinder-n涵盖了化学及相关领域，如化学、生物、医药、材料、食品、工程、农学、物理等多学科、跨学科的科技信息。CAS SciFinder-n收录的文献类型包括期刊、专利、会议论文、 学位论文、图书、技术报告、评论和网络资源等。

三、检索指南

CAS SciFinder-n使用指南，请登陆https://www.cas.org/support/training/scifinder-n，就可以看到相关功能的介绍及使用演示。

四、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. 注意保护知识产权，合理使用数据库，禁止过量下载，禁止在商业机构使用。
3. SciFinder经常更新，请大家留意图书馆或美国化学文摘社主页的相关消息。

2、进入详情介绍页面，点击账号注册地址进行注册。

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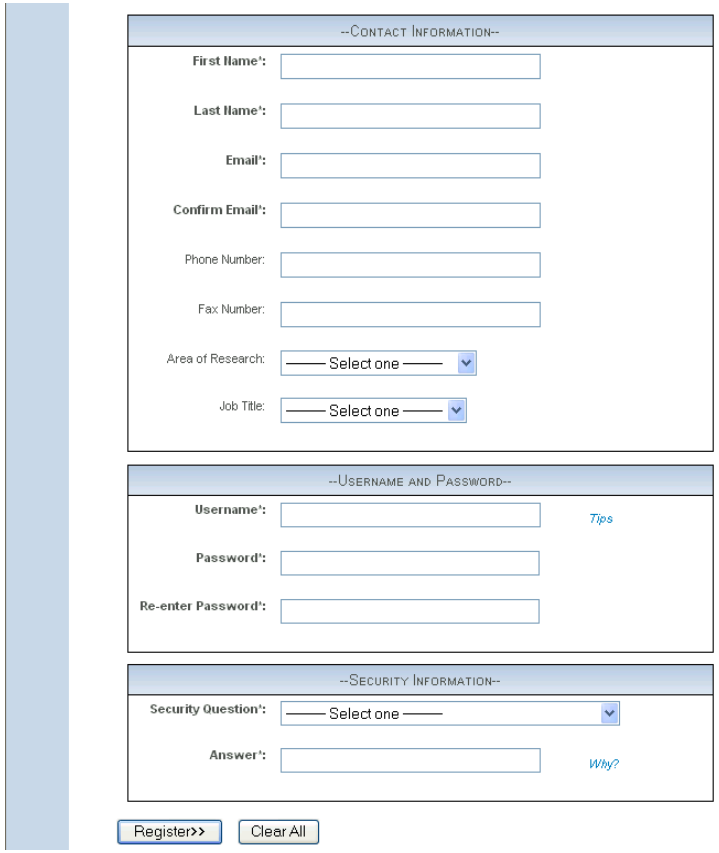


请注意：

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）

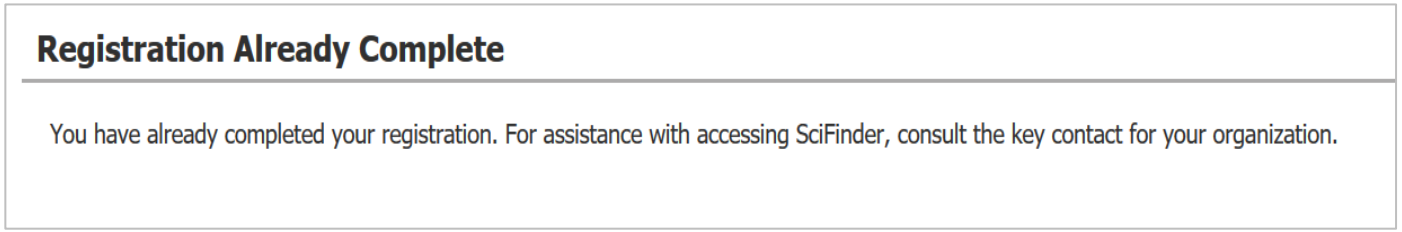
3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：

- 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

通过https://scifinder-n.cas.org/访问

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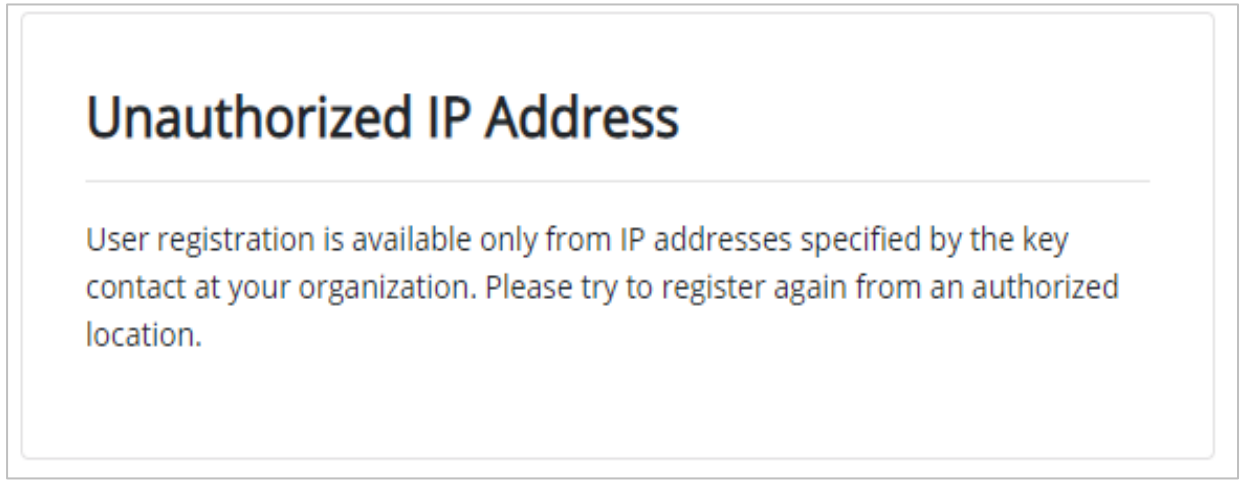

- 检查注册链接是否正确
- 确认连入校园网，且不是通过VPN连接
- 如果链接正确，且在校园内，请联系图书馆或China@acs-i.org

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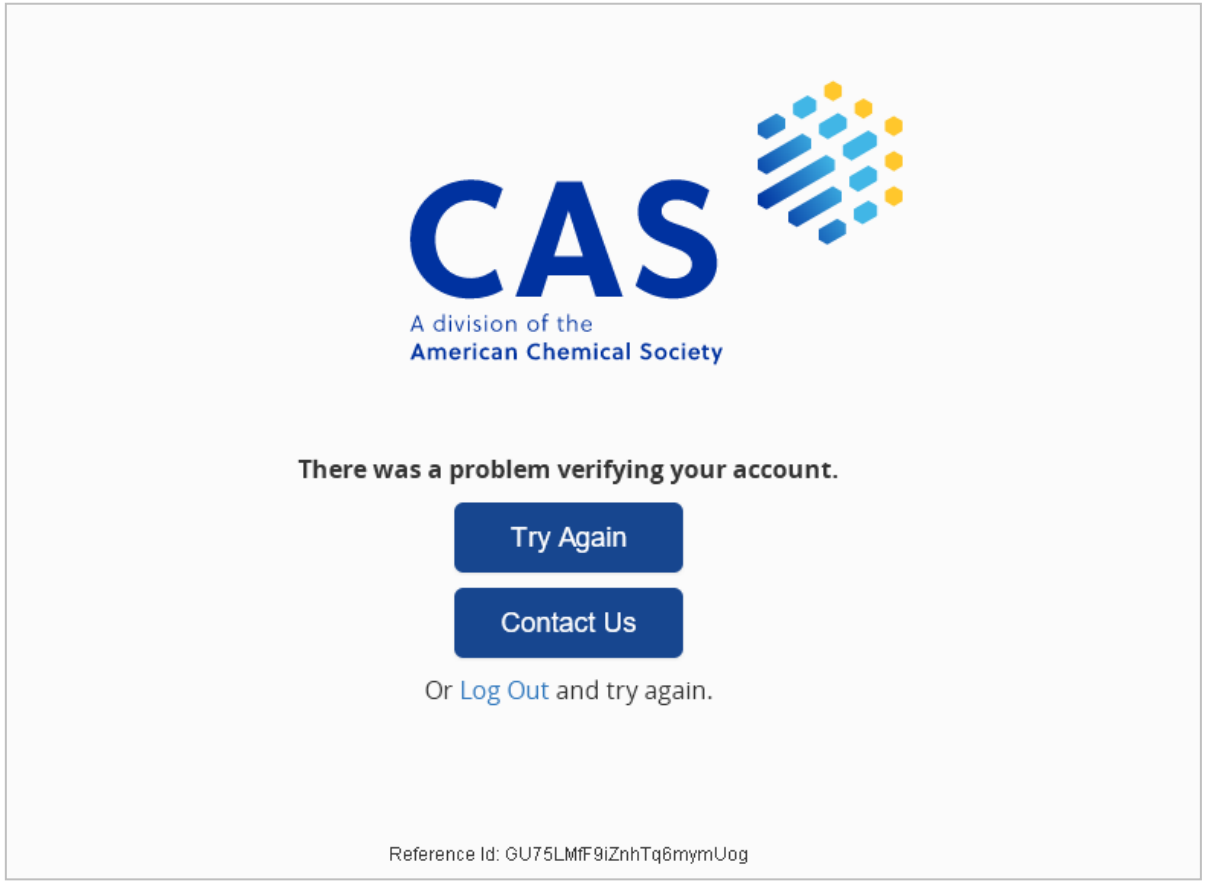
常见登录问题



- 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

CAS SciFinder 检索浏览器推荐

浏览器推荐：

- Windows (7, 8.1, 10)：Chrome 60及更高版本，Firefox 55及更高版本，Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13)：Safari 9.3及更高版本，Chrome 60及更高版本，Firefox 55及更高版本，Firefox 52 (ESR)
- **不建议使用360浏览器，相关功能或插件会被自动拦截**

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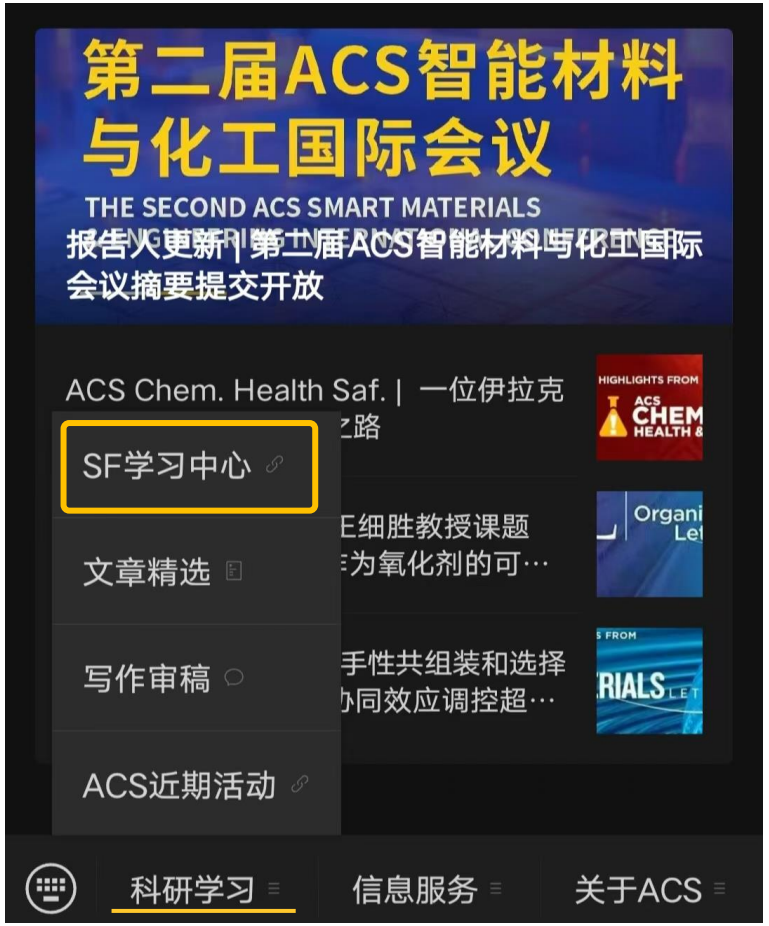

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演讲人：刘子露 博士

3 月 28 日 | 解锁新功能

演讲人：杜德鑫 博士

4 月 18 日 | 助攻论文写作

演讲人：潘娜 博士

4 月 25 日 | 探索科研成果转化

演讲人：钱欣 博士

5 月 9 日 | 结构绘制面板及案例详解

演讲人：刘子露 博士

5 月 23 日 | 反应检索策略及典型案例

演讲人：陈开乾 博士

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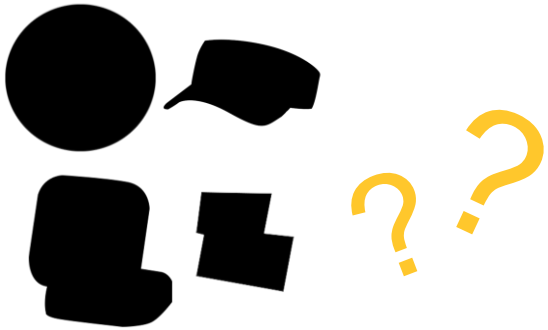

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