利用 CAS SciFinder Discovery Platform™

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

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- CAS 与 CAS SciFinder Discovery Platform 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

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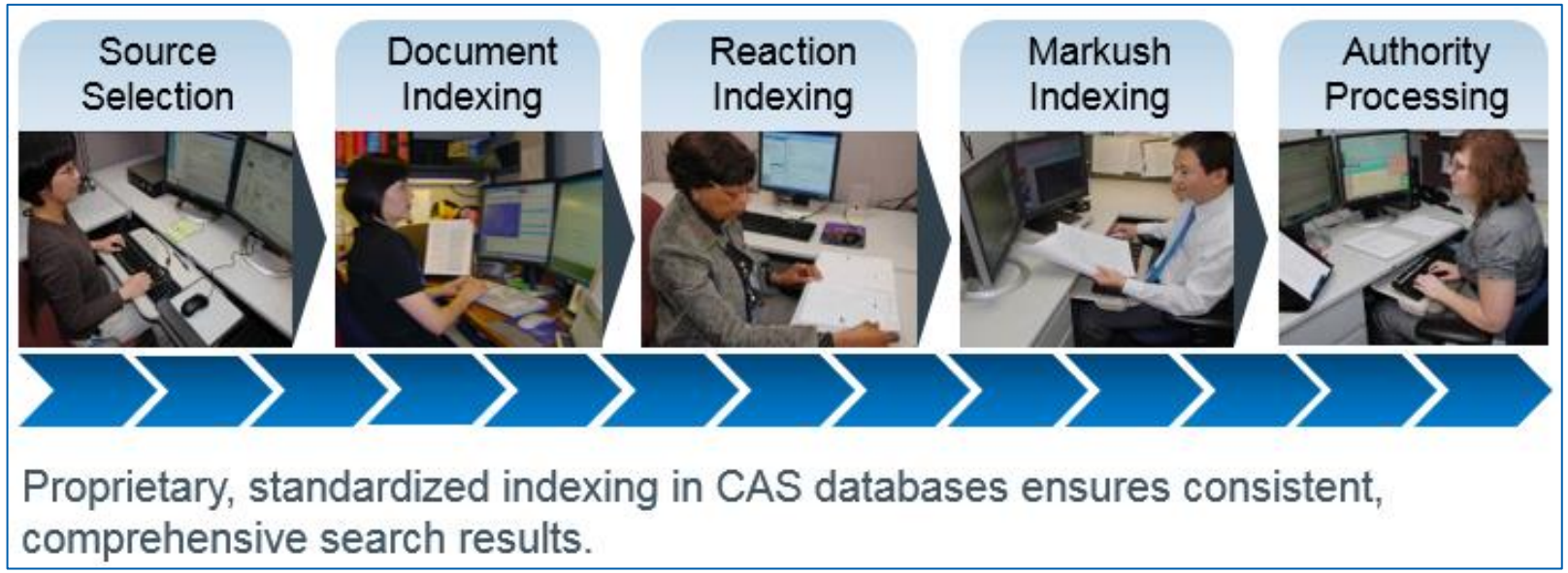
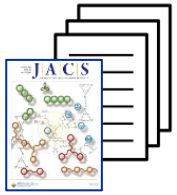
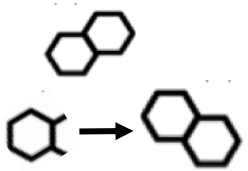
CAS 科学家智力标引

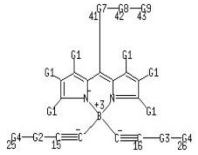


Data pre-repository



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

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

CAS SciFinder

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

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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

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https://lib.cmc.edu.cn/info/1006/2275.htm

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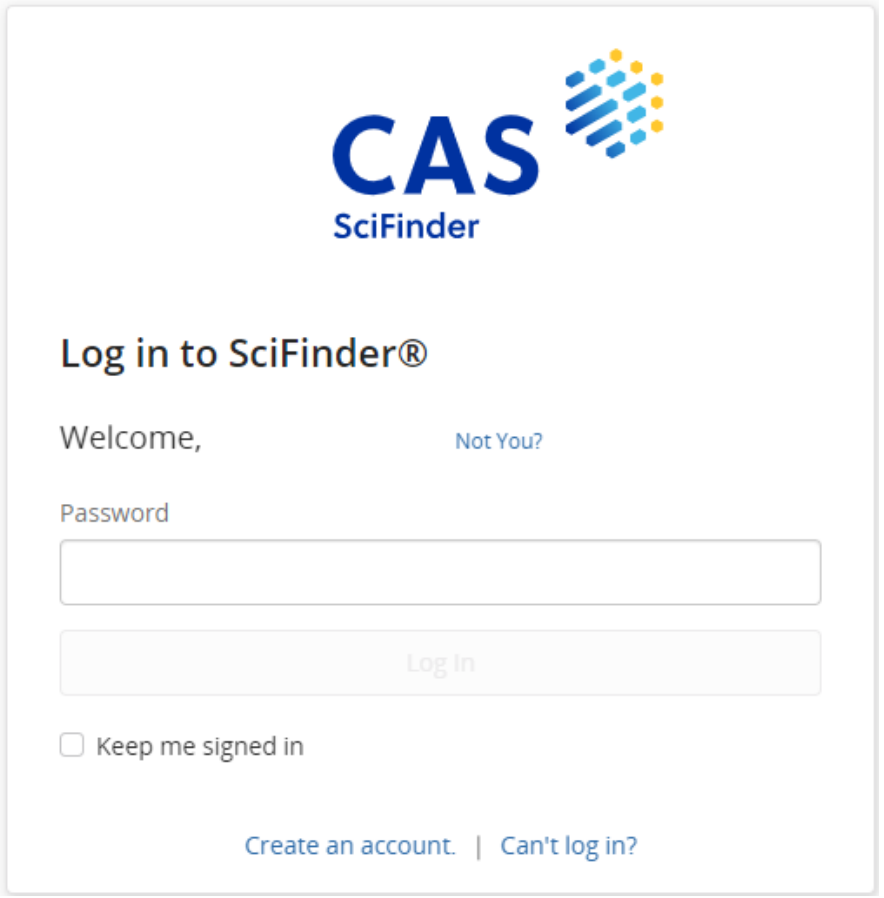
CAS SciFinder 登录

https://scifinder-n.cas.org



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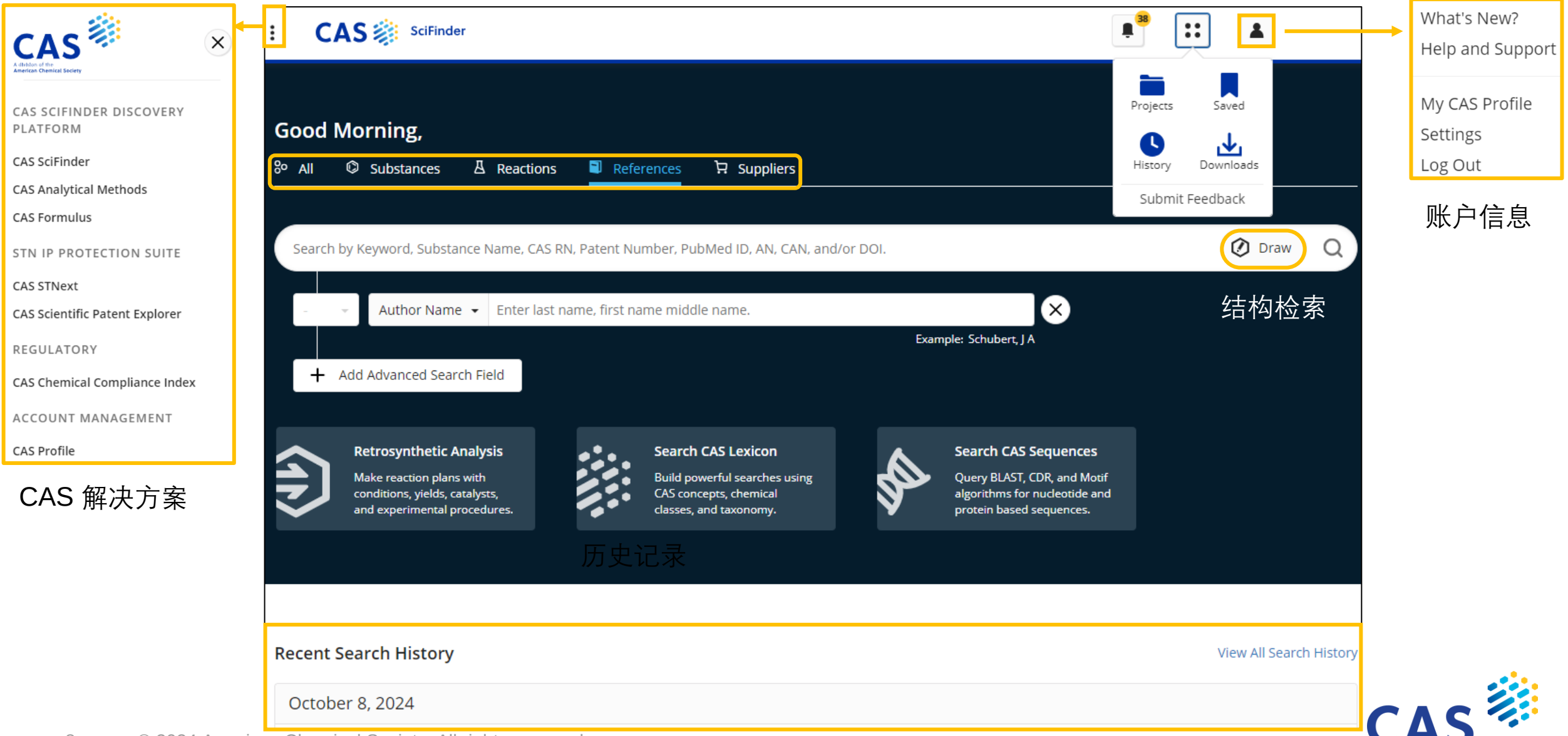
CAS SciFinder 主界面



CAS 解决方案

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- CAS 与 CAS SciFinder 简介
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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

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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
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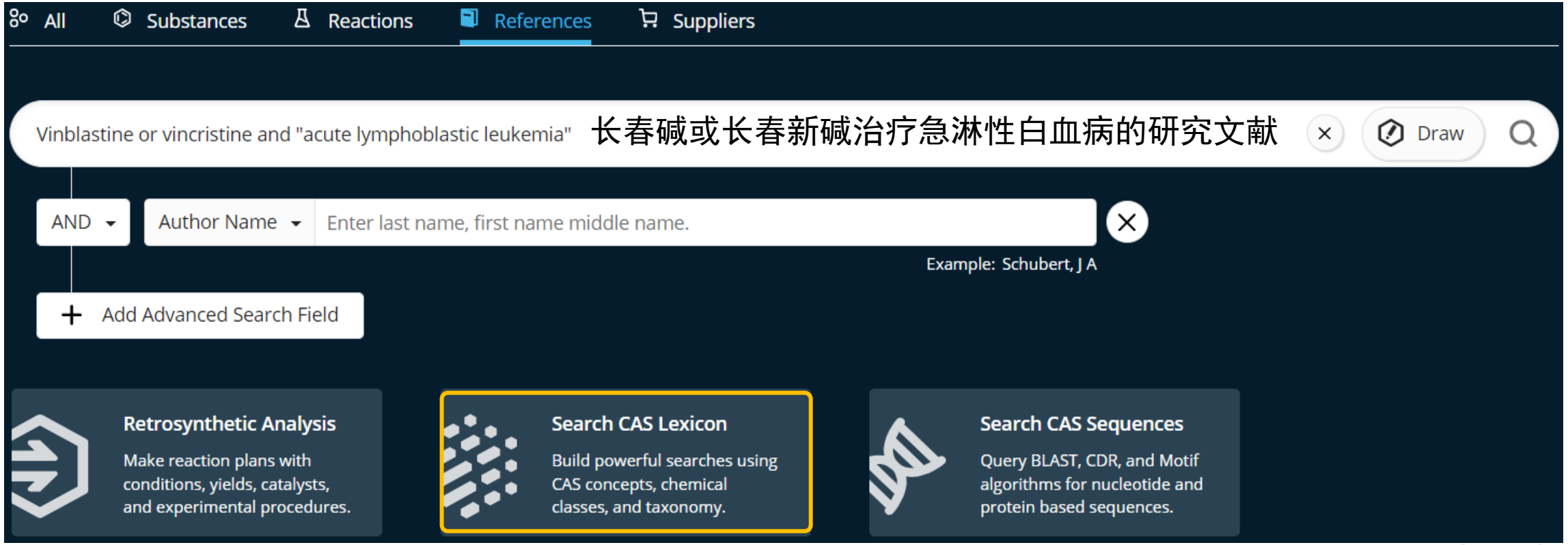

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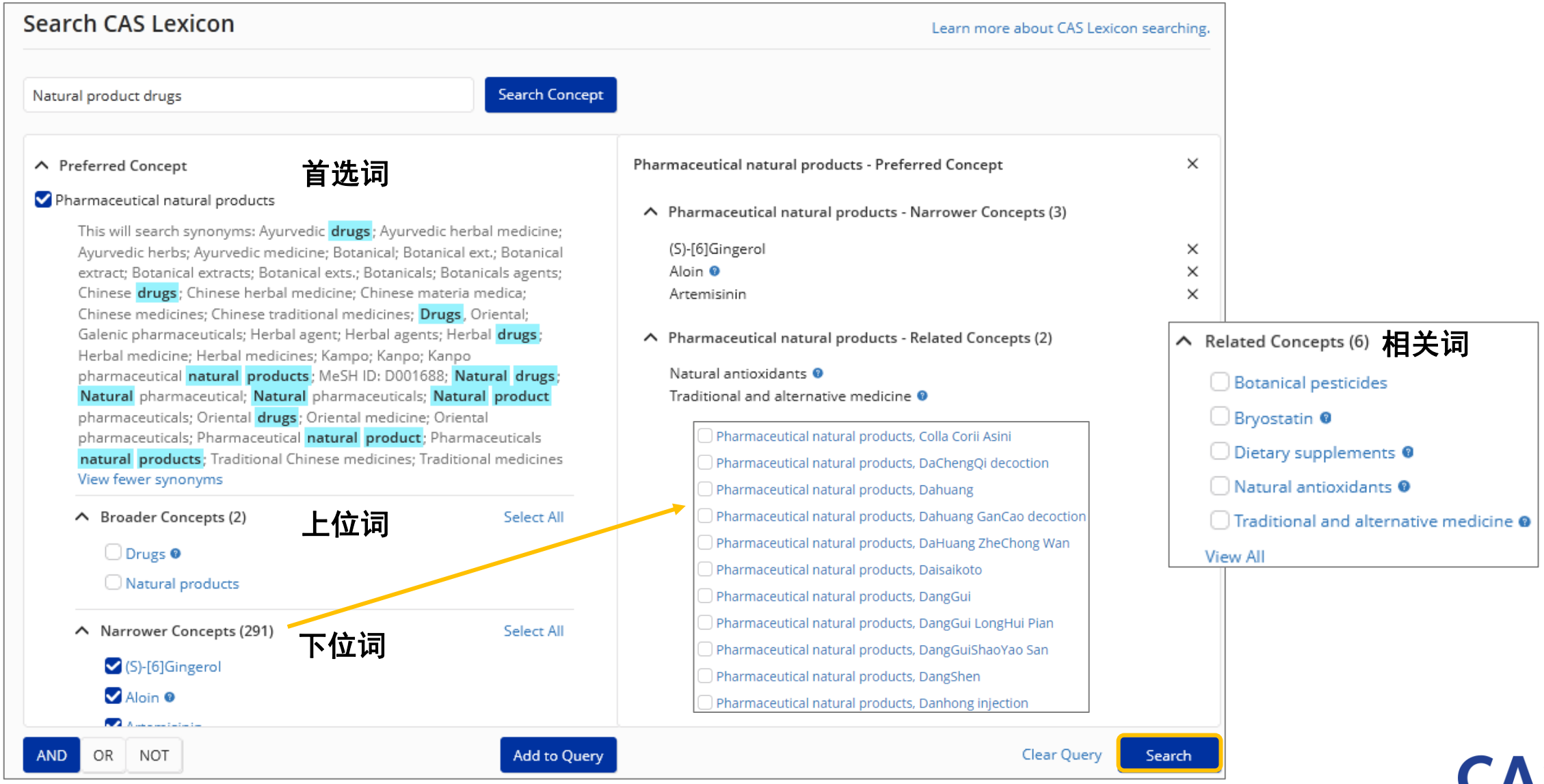
CAS Lexicon 词库检索近义词和相关技术术语



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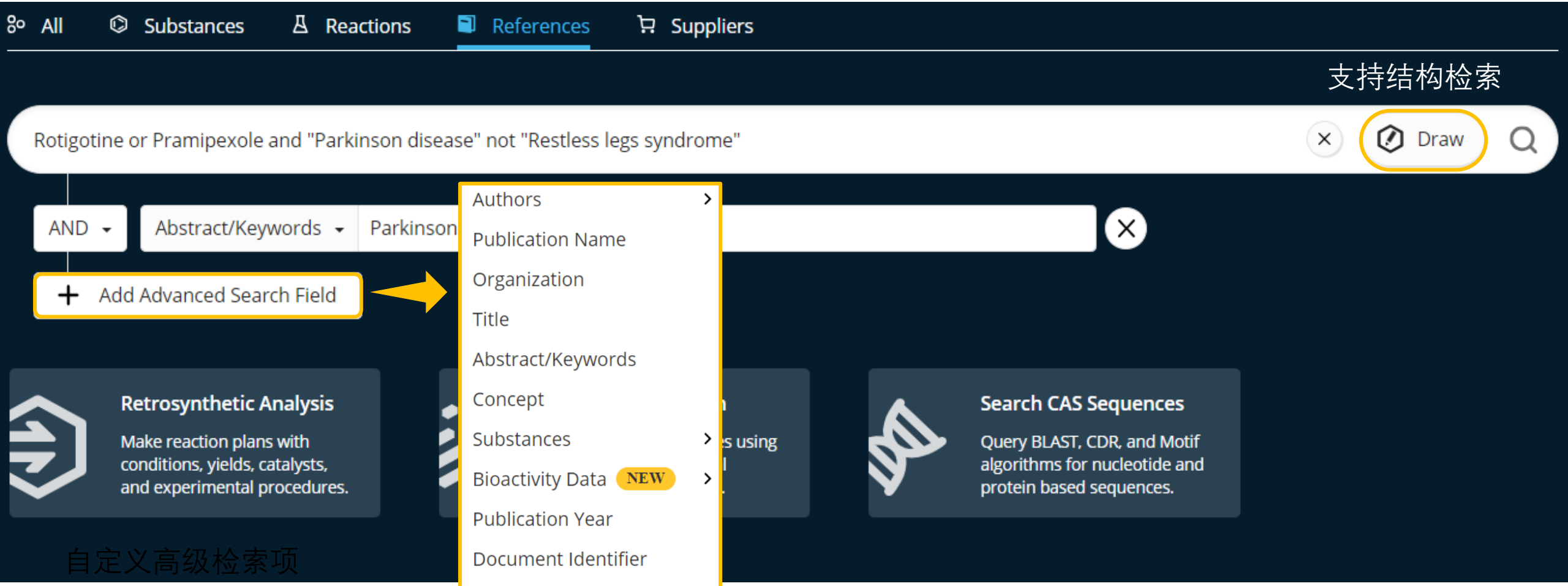

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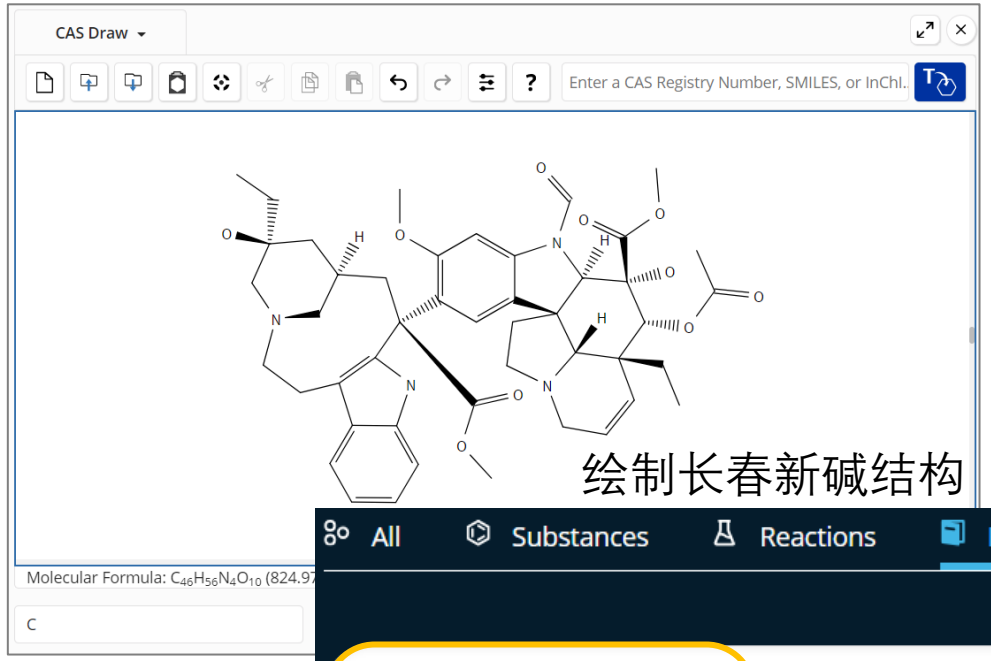
物质结构与关键词联合检索文献



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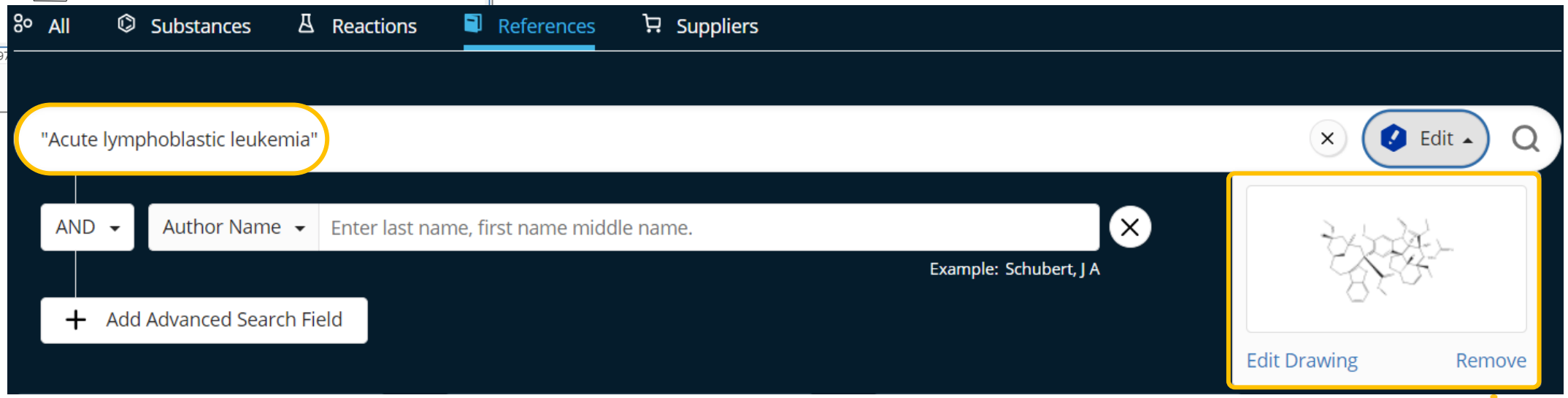

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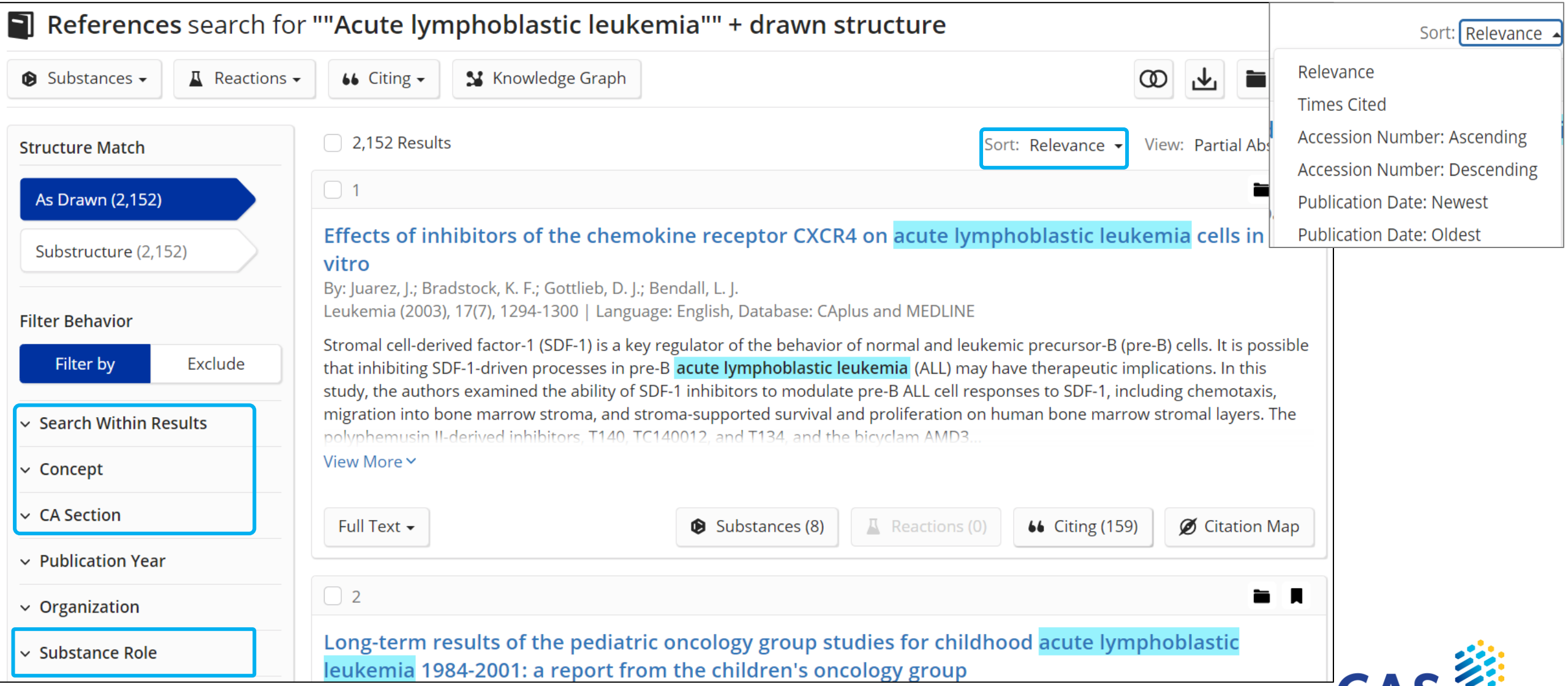
检索结果分析与筛选



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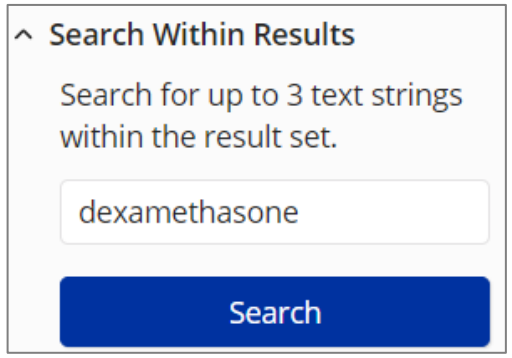

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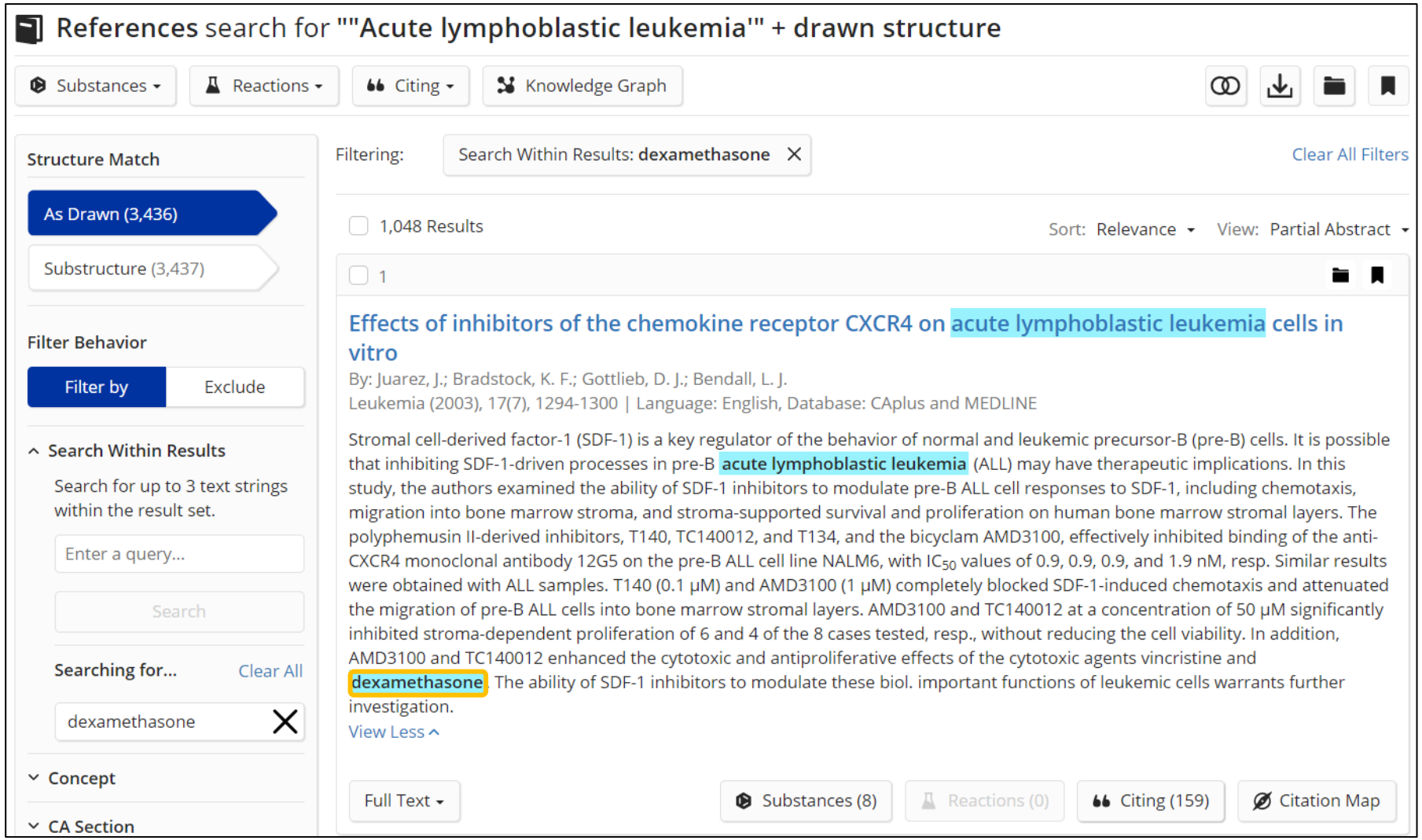

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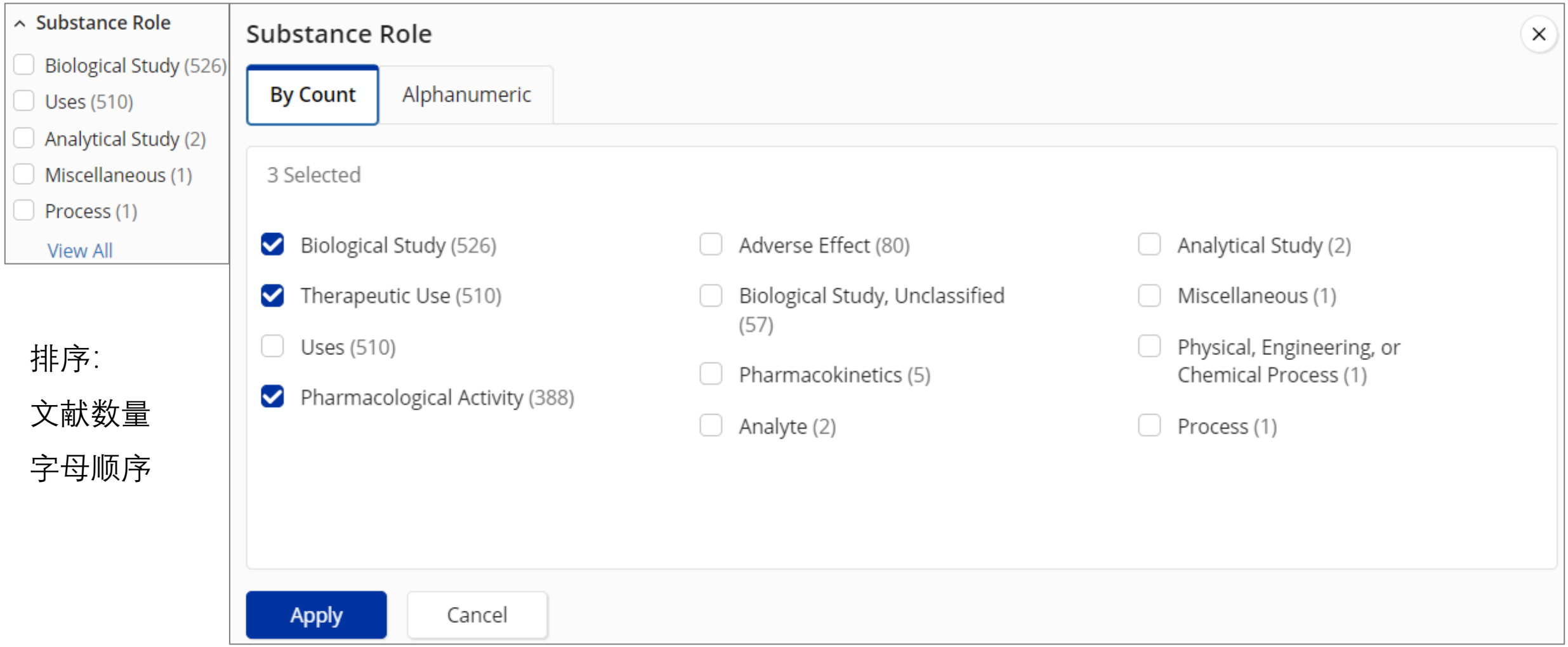
物质角色筛选文献：Substance Role



排序:

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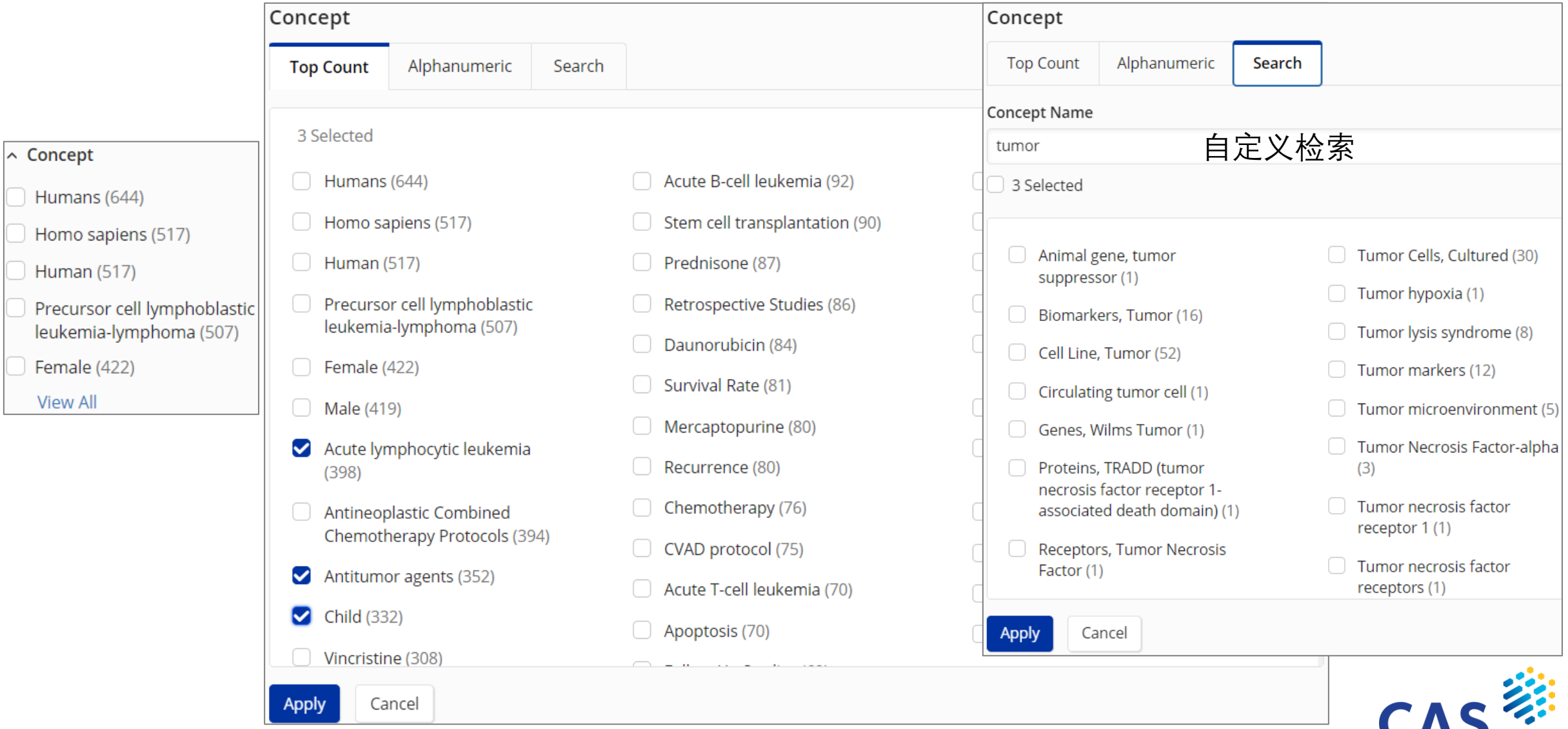
确定文献核心研究内容：Concept



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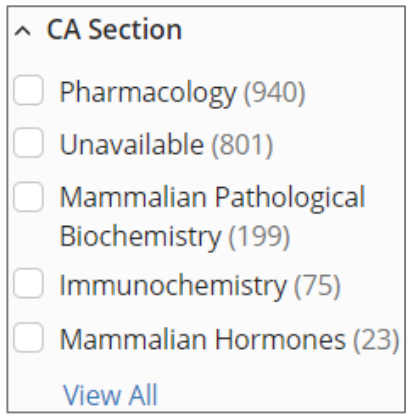
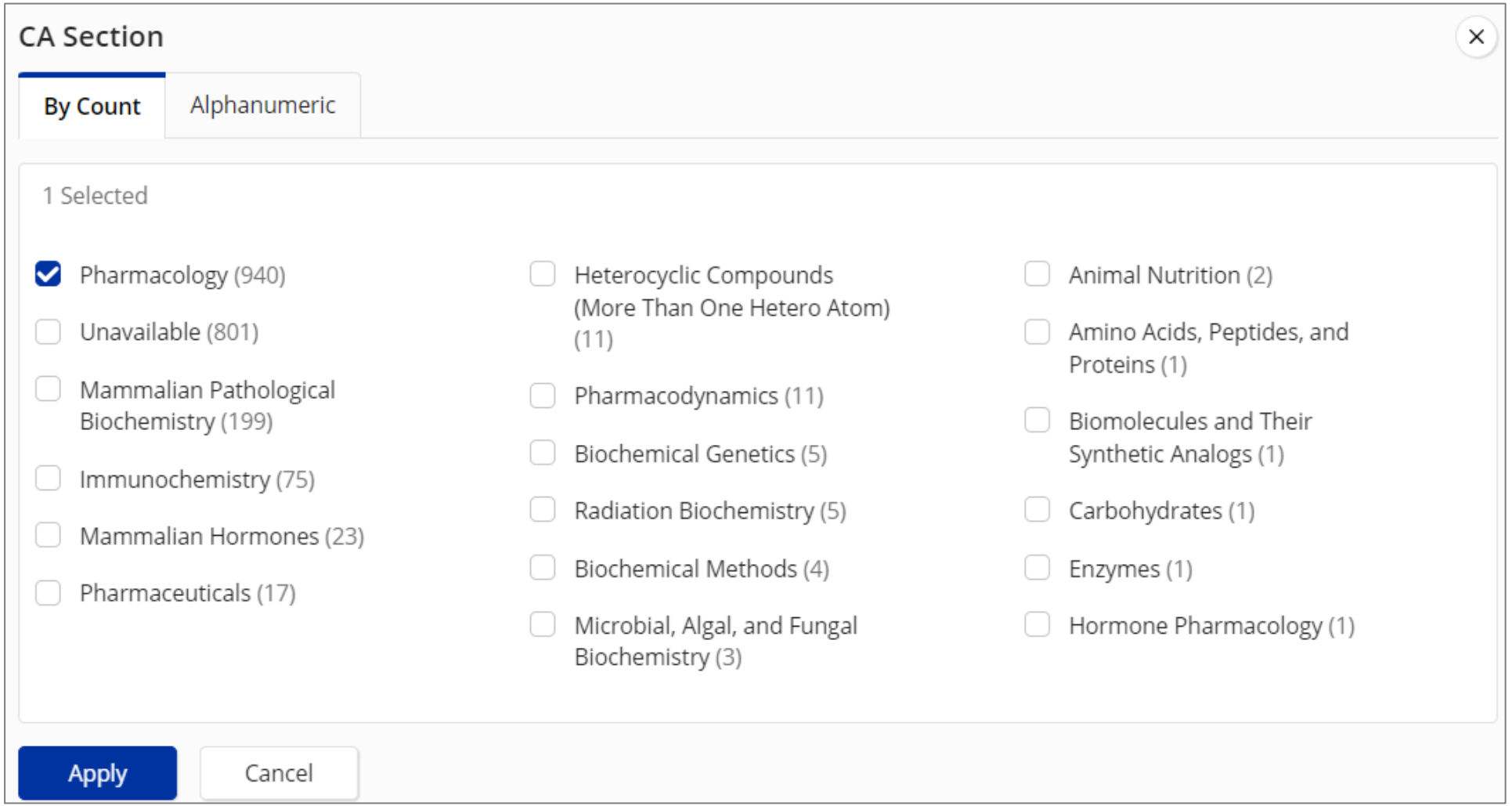
筛选不同研究领域文献：CA Section





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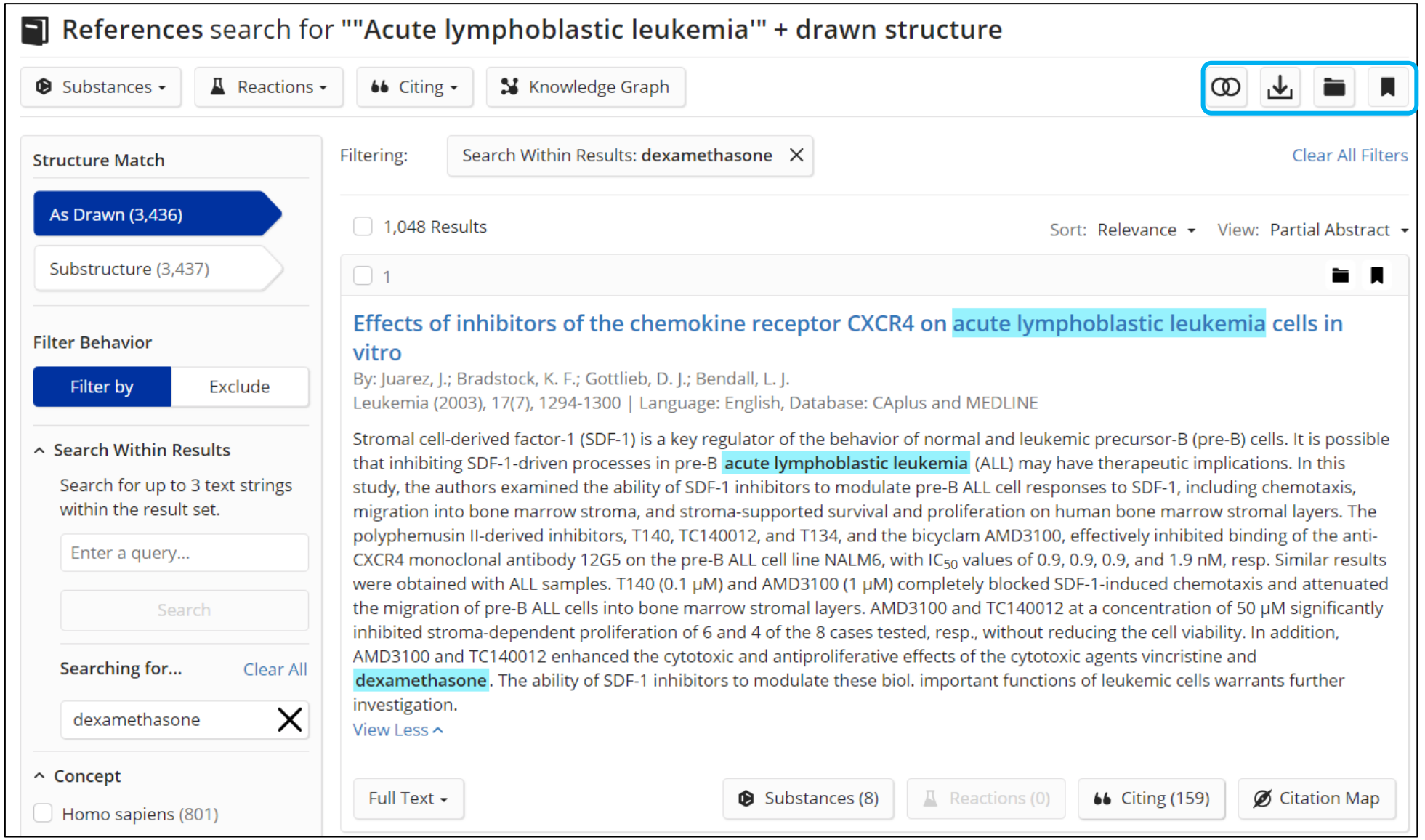

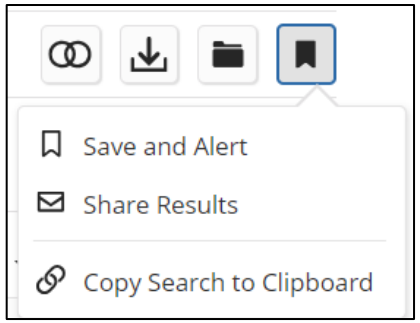

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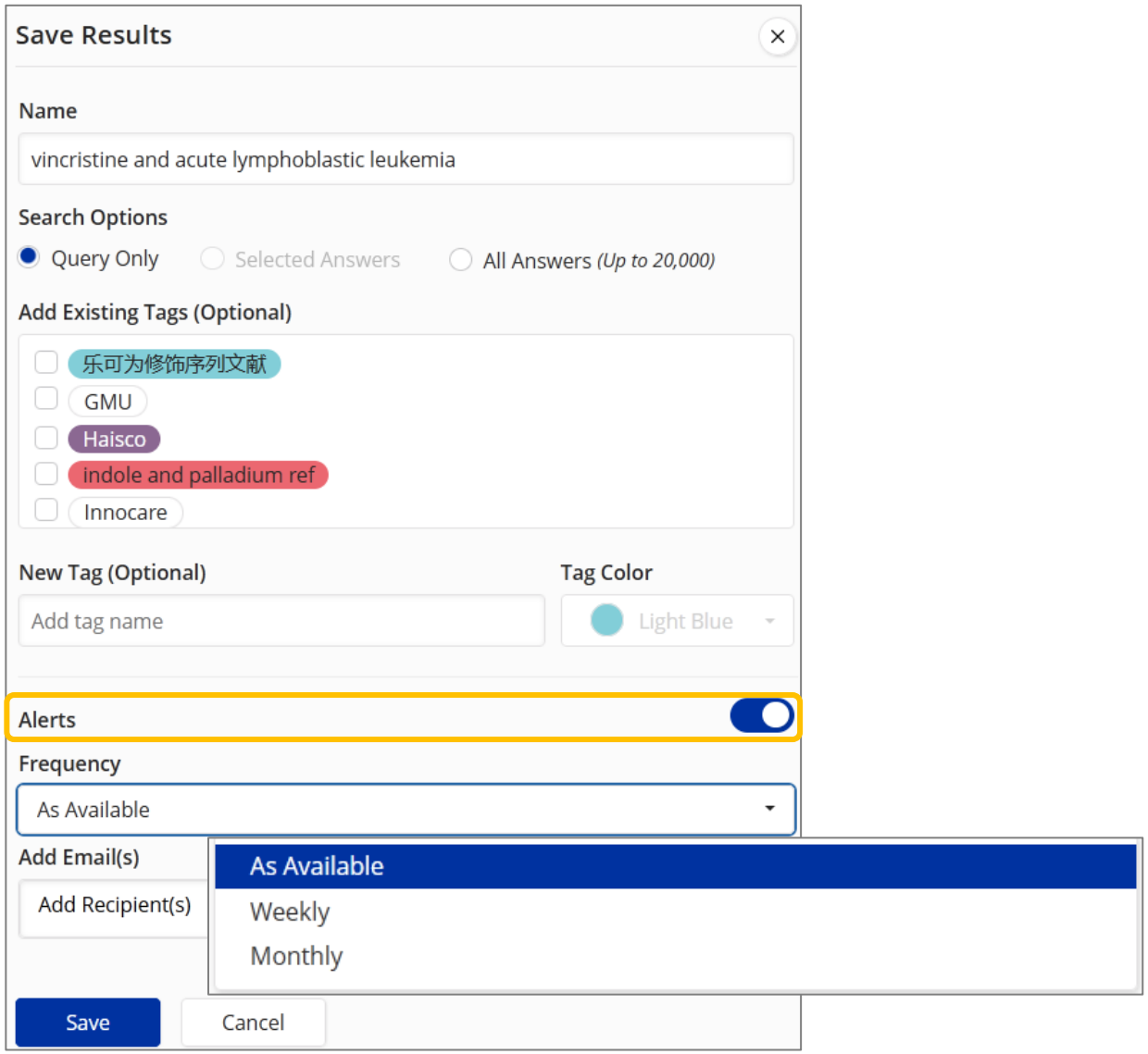

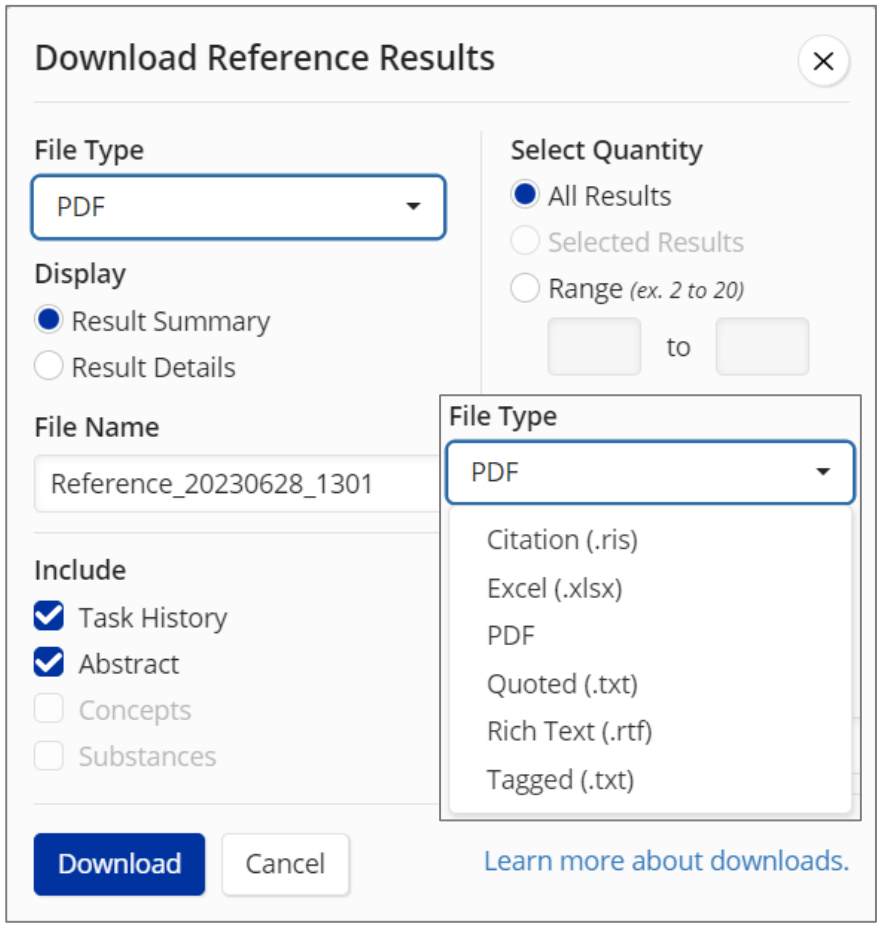

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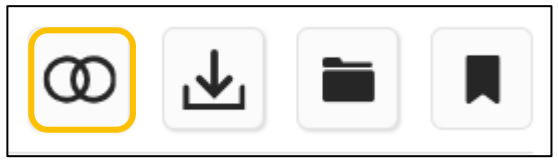

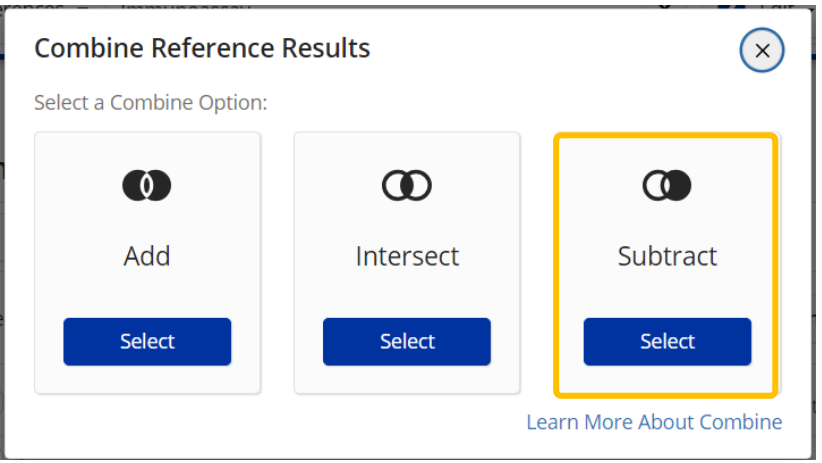

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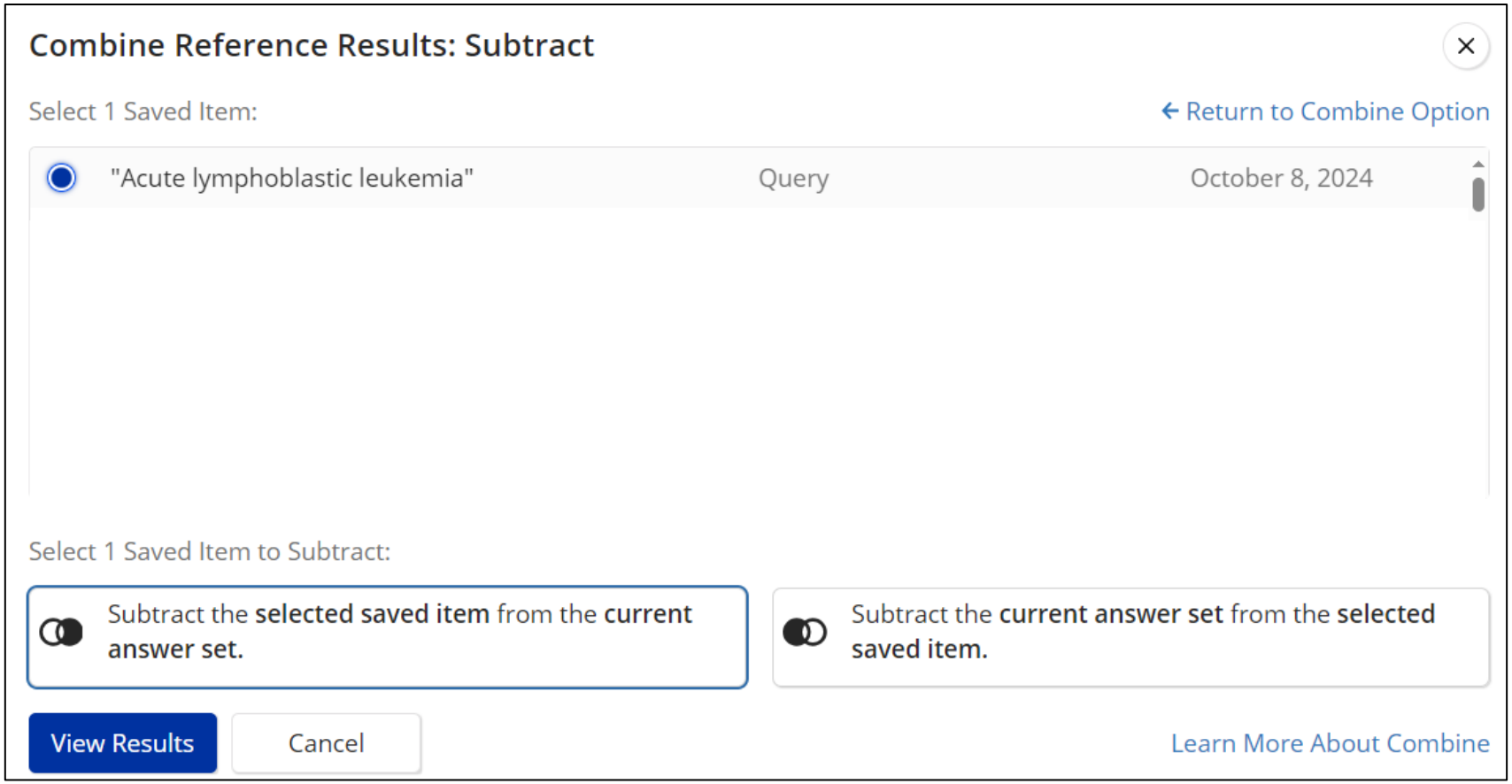

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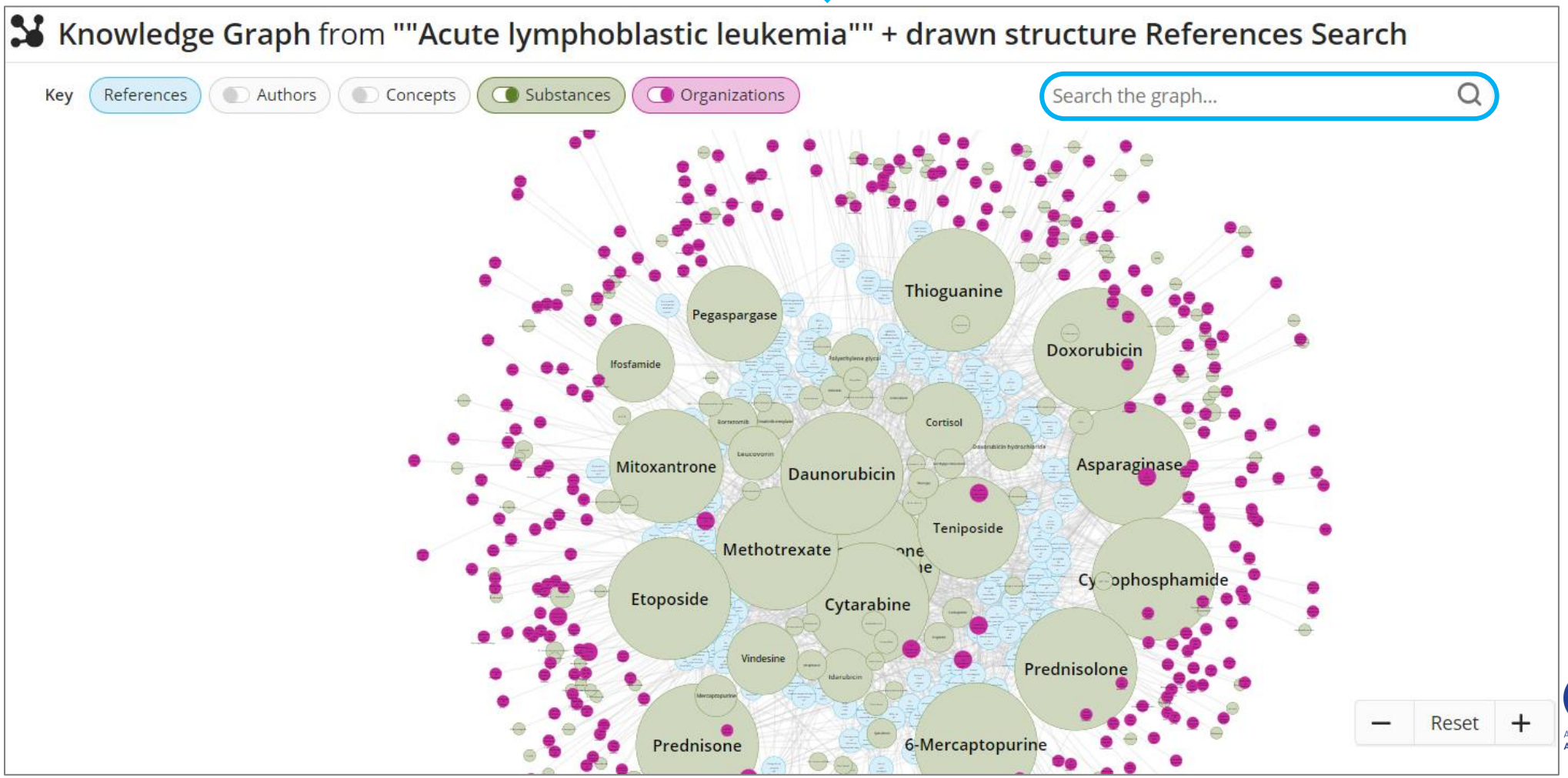
绘制知识谱图：Knowledge Graph

References search for ""Acute lymphoblastic leukemia"" + drawn structure

Substances | Reactions | Citing | Knowledge Graph | Save and Alert



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查看目标文献详情

Prospective study of hemostatic alterations in children with acute lymphoblastic leukemia

11 | 0 | 49 | Citation Map

In this Reference
- Concepts
- Substances
- Cited Documents

By: Giordano, Paola; Molinari, Angelo Claudio; Del Vecchio, Giovanni Carlo; Saracco, Paola; Russo, Giovanna; Altomar
Paolo; Crescenzio, Nicoletta; Santoro, Nicola; Marchetti, Marina; et al
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DOI: 10.1002/ajh.21665

In a group of newly diagnosed acute lymphocytic leukemia (ALL) children we evaluated a number of hemostatic an
markers at diagnosis and at different time points during chemotherapy for the remission induction to identify altera
levels of prothrombotic markers before and during the course of chemotherapy. The following plasma markers were evaluated: thrombin-
antithrombin complex (TAT), D-Dimer, plasminogen activator inhibitor 1 (PAI-1), antithrombin, fibrinogen, von Wil
antigen and high mol. weight VWF (HMW-VWF) multimers, P-selectin, tumor necrosis factor alpha (TNF-α), and int
samples were collected at the following time points: at TO (baseline) and T1 (+24 days of therapy), T2 (+36 days th
therapy). The results show that, at diagnosis, ALL children presented with laboratory signs of increased thrombin
formation (i.e. high TAT and D-dimer levels), fibrinolysis inhibition (i.e. high PAI-1 level), endothelial activation (i.e.,
soluble P-selectin levels) and inflammation (i.e. high TNF-alpha and IL-6 levels). After starting induction therapy, t
markers and inflammatory cytokines significantly decreased. To the opposite, PAI-1 and P-selectin significantly in
insult by chemotherapy on the vascular endothelium. These effects were more evident during steroid administra
venous thromboembolism (VTE) episodes developed in two cases during induction therapy, which did not allow t
predictive value for VTE of laboratory markers.

Keywords: hemostatic alteration child acute lymphoblastic leukemia

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Publication Information • Journal

Source	Database Information	Company/Organization	Publisher	Language
American Journal of	AN: 2010:674136	Pediatric Department	Wiley-Liss, Inc.	English

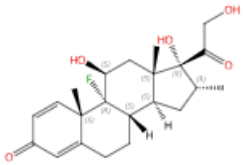
CAS Concepts — CAS 科学家提供的核心研究点

Acute lymphocytic leukemia	Fibrinogens Role: Biological Study, Unclassified
Biomarkers	Homo sapiens
Blood plasma	Human
Blood platelet	Inflammation
Child development	Interleukin 6 Role: Biological Study, Unclassified

Substances — 重点研究物质

Substances (11)

50-02-2

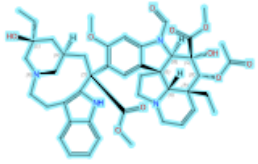


Absolute stereochemistry shown

$C_{22}H_{29}FO_5$
Dexamethasone

Role: Pharmacological Activity, Therapeutic Use, Biological Study, Uses

57-22-7



Absolute stereochemistry shown, Rotation (+)

$C_{46}H_{56}N_4O_{10}$
Vincaleukoblastine, 22-oxo-

Role: Pharmacological Activity, Therapeutic Use, Biological Study, Uses

物质角色

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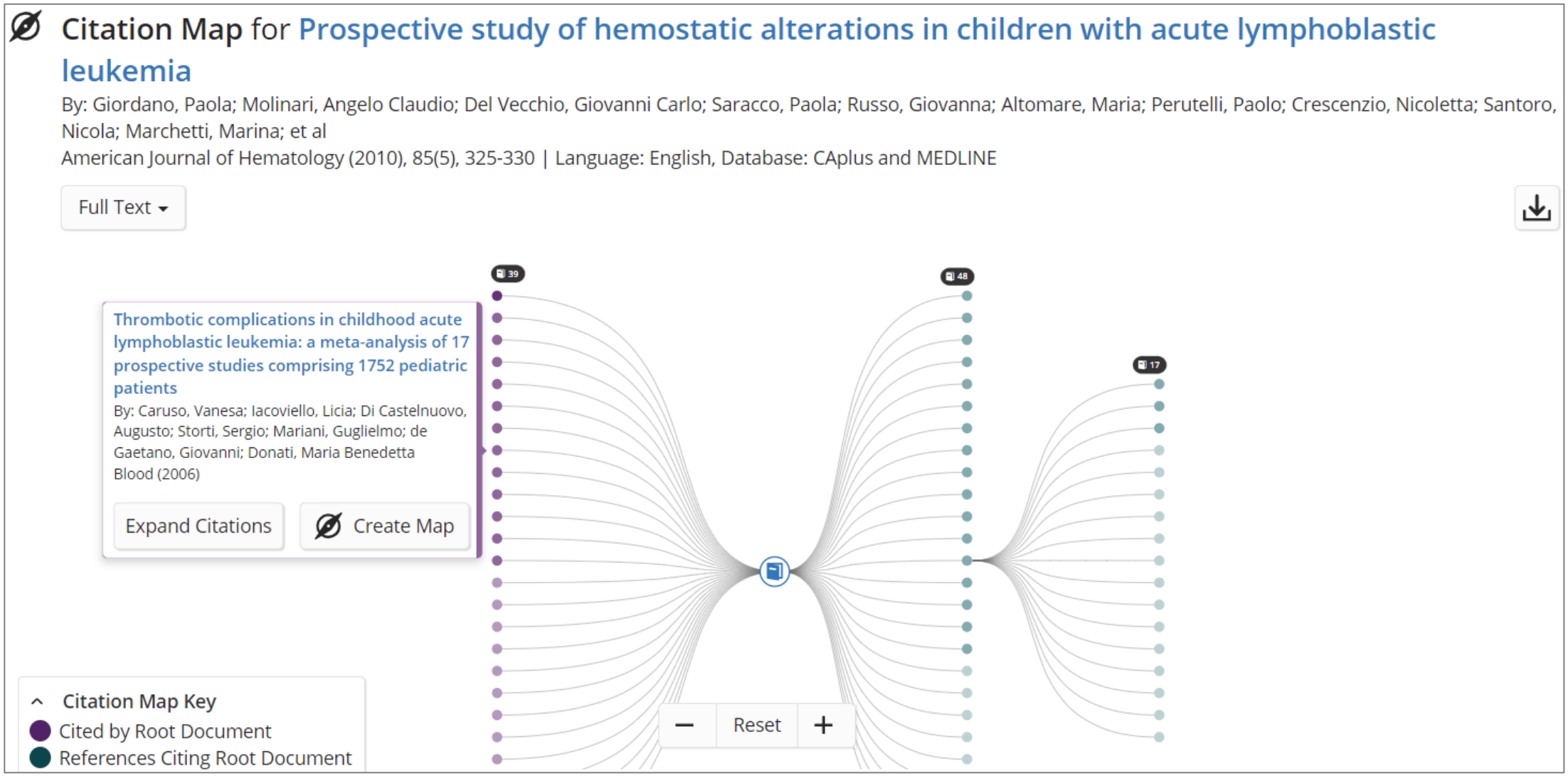

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查看专利详情

Rotigotine ionic liquid and compositions for use as dopamine D2 receptor agonists or antiparkinson agent

34 | 2 | 1 | Citation Map

In this Reference

- IPC Data
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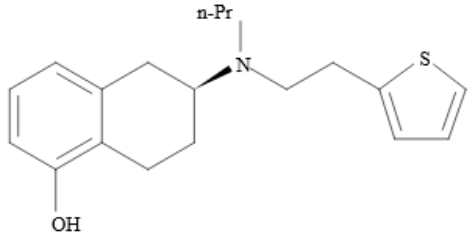
- Substances
- Reactions
- Formulations
- Cited Documents

By: Janssen, Christian

The present invention provides ionic liquids of rotigotine, pharmaceutical compositions comprising said ionic transdermal compositions and methods of preparing such ionic liquids An ionic liquid comprising at least one and at least one counter ion derived from an organic compound is used in the treatment, prevention, amelior disease susceptible to a dopamine D2 receptor agonist or an antiparkinson agent. The invention further provi compositions described herein to overcome problems arising from polymorphism, solubility and delivery, to c functionality, to enhance efficacy, and to improve ease of use and manufacture For example, an ionic liquid co and an octanoic anion was obtained in quant. yield using rotigotine and octanoic acid.



Keywords: rotigotine ionic liquid preparation antiparkinson dopamine D2 receptor agonist

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Publication Information • Patent — View Less

Patent Number	Publication Date	Application Number	Application Date	Kind Code
WO2012074988	2012-06-07	WO2011-US62364	2011-11-29	A1

Priority Application

Priority Application Number	Application Date
EP2010-15079	2010-11-29
US2010-61419070P	2010-12-02
WO2011-EP71321	2011-11-29
WO2011-US62364	2011-11-29

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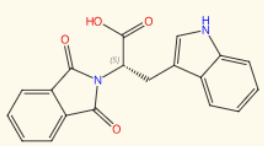
Key Substances in Patent

CAS RN
48208-26-0



Analyst Markup Locations (2)
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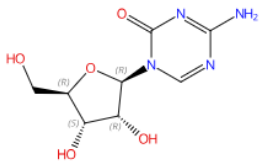
CAS RN
9037-42-7
DNA methyltransferase

Analyst Markup Locations (1)
Page 16

CAS RN
320-67-2



Analyst Markup Locations (2)
Page 16
Page 21

EP 1 574 499 A1

Fig. 3

[0060] The effect of RG108 on human cell lines. (a) Growth of HCT116 (left panel) and NALM-6 cells (right panel) in medium supplemented with 10 μM RG 108 (filled circles) or 10 μM 5-azacytidine (grey diamonds). Controls are shown as open squares. (b) Viability of HCT116 and NALM-6 cells under the same conditions as described in (a). (c) Genomic cytosine methylation levels of HCT116 (left panel) and NALM-6 cells (right panel)) in medium supplemented with 10 μM RG 108 (black bars) or 10 μM 5-azacytidine (grey bars). Controls are shown as white bars. DNA methylation levels were determined after 5 and 15 days, as indicated. DNA from NALM-6 cells incubated with 5-azacytidine for 15 days could not be analyzed due to degradation. All results were obtained from multiple experiments. Standard deviations for panels (a) and (b) were negligible.

Fig. 4

[0061] The carboxyl-group of RG108 is important for its interaction with DNA methyltransferases. (a) Structure of ΔC-RG108, a control compound that lacks the carboxyl-group of RG-108. (b) Calculated binding energies of ΔC-RG108 (grey bar) docked into the DNMT1 active site are compared to cytidine (white bar) and RG108 (black bar). (c) Genomic cytosine methylation levels of HCT116 cells incubated with ΔC-RG108 (black bar) are compared to methylation levels of corresponding cells incubated with no inhibitor (white bar) or RG108 (grey bar).

Fig. 5

[0062] RG108 causes complete demethylation of the human hMLH1 gene in cells treated with 10 micromolar RG108, while no demethylation was observed in control experiments without inhibitor or with 10 micromolar 5-azacytidine (Sigma), respectively (Fig. 5). M indicates amplification products from methylated templates, U indicates amplification

精准定位

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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

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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?

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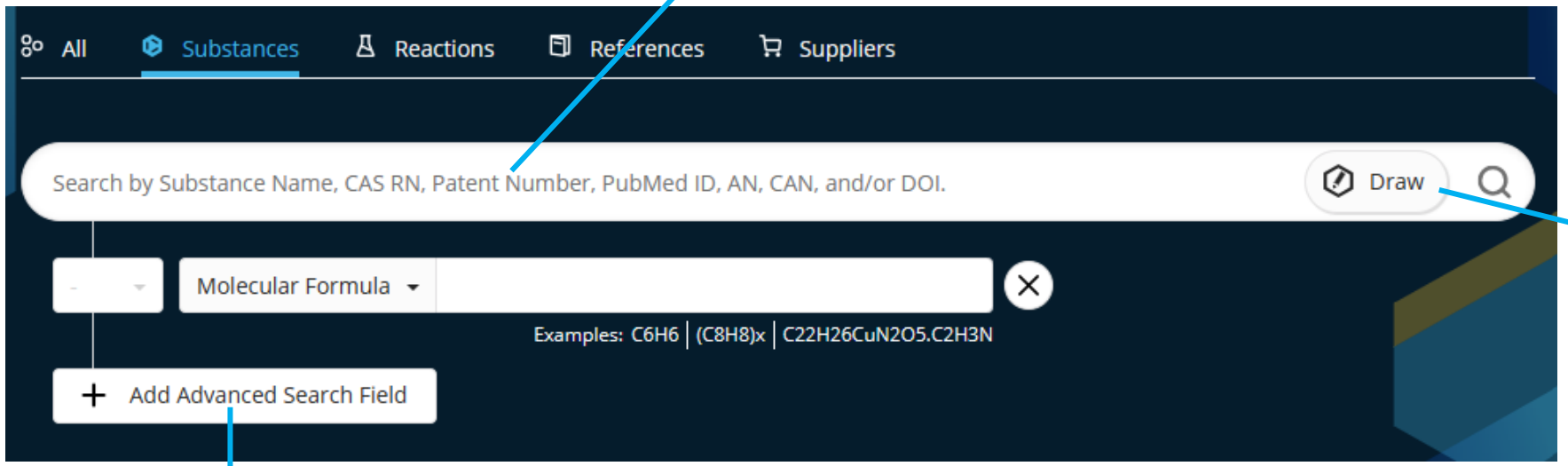
研究某种/某类物质?

- 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

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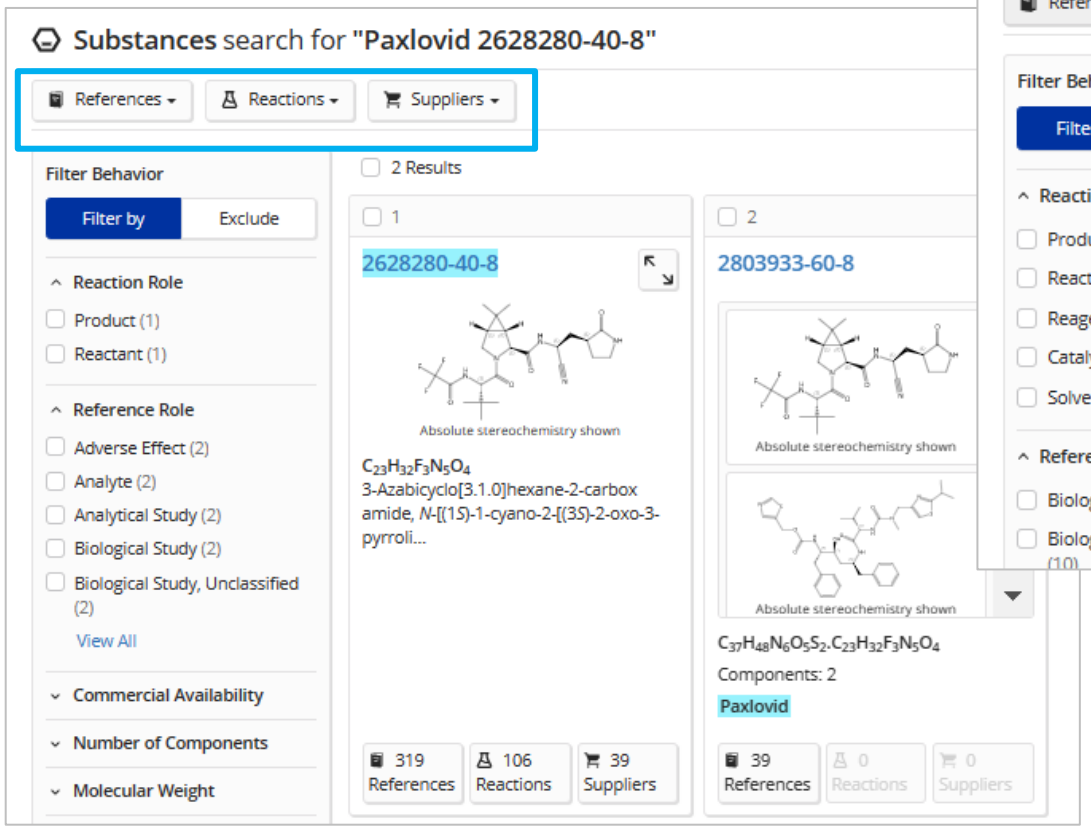
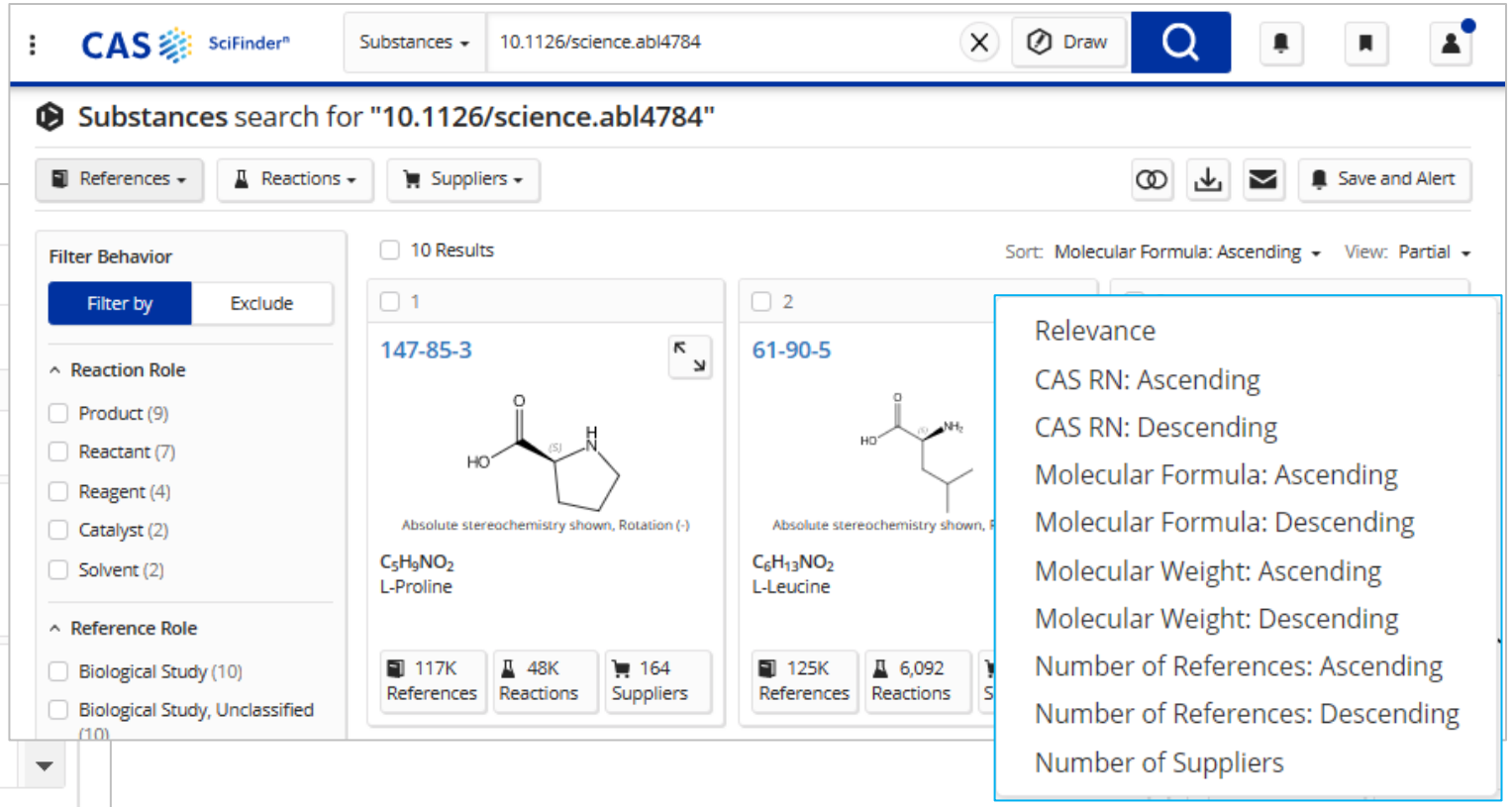
物质检索—物质/文献标识符

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

- 迅速获得关注文献中的物质信息





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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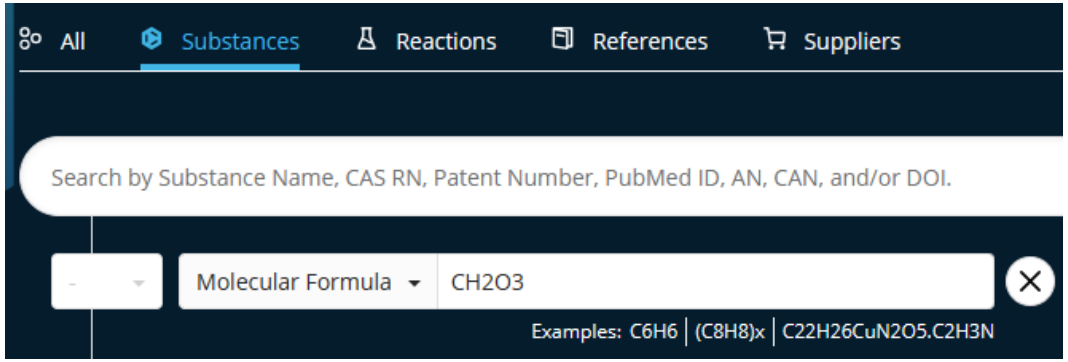
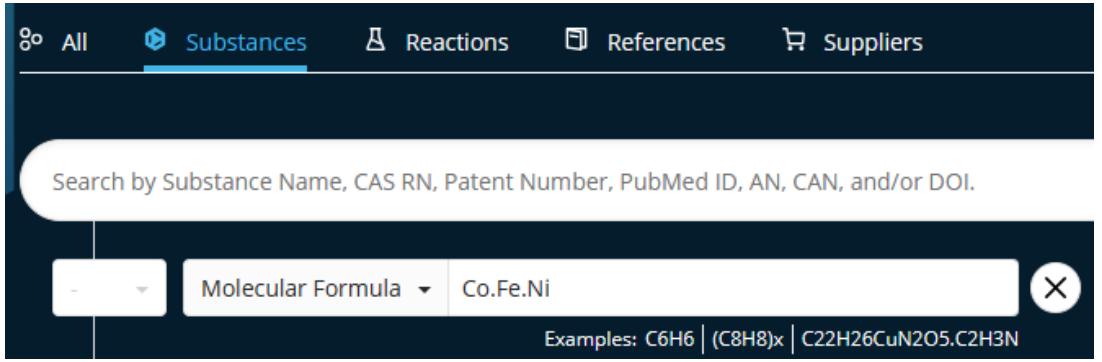
分子式检索：高效检索聚合物或无机化合物

- 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 Co.Fe.Ni
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性





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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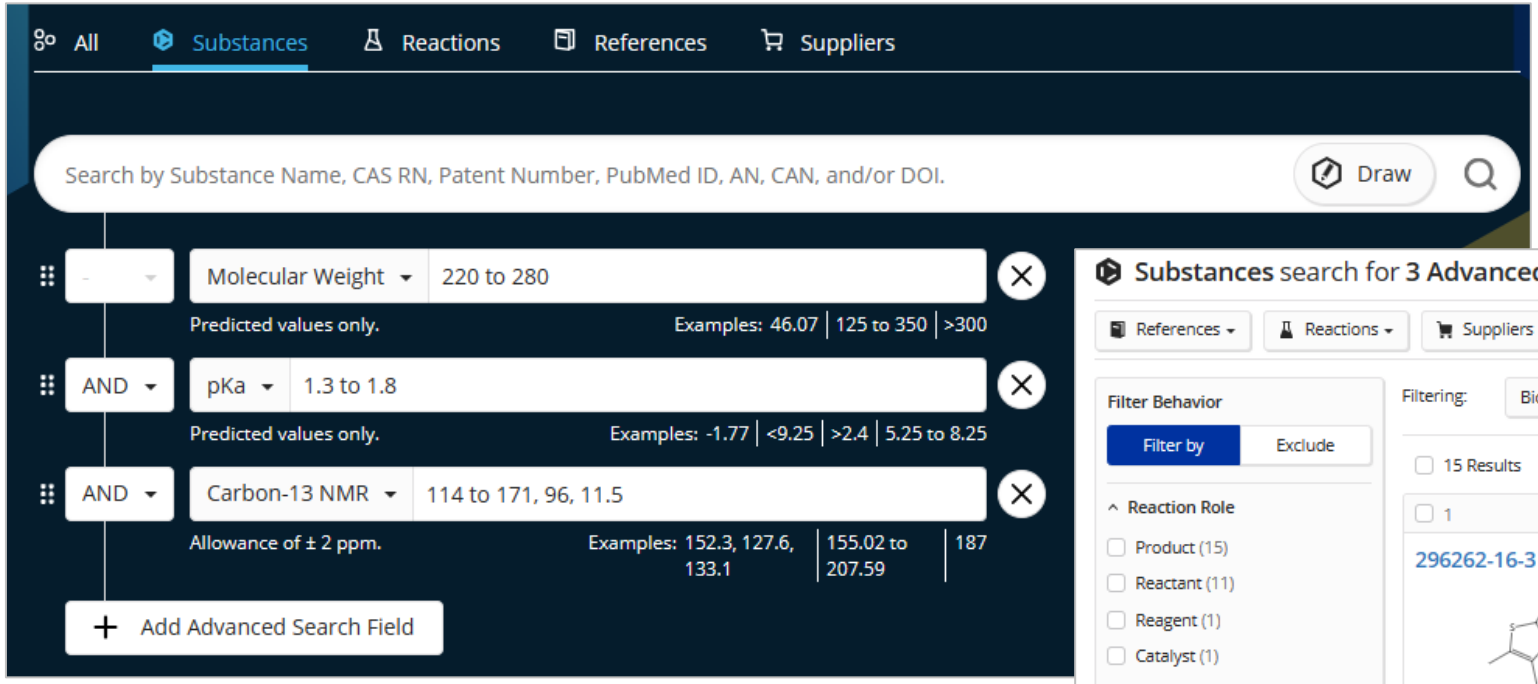
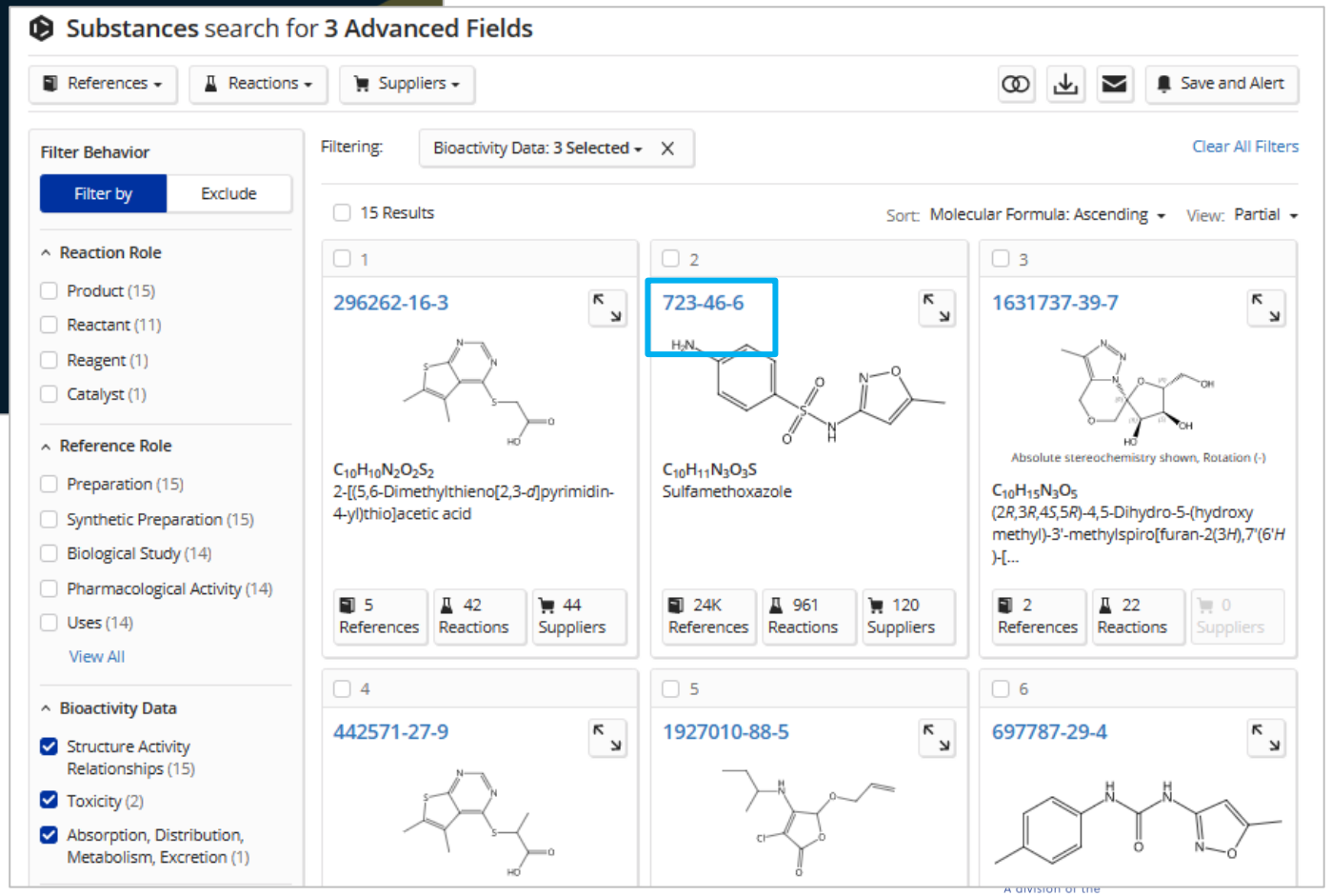
属性值、谱图数值联用检索物质





- 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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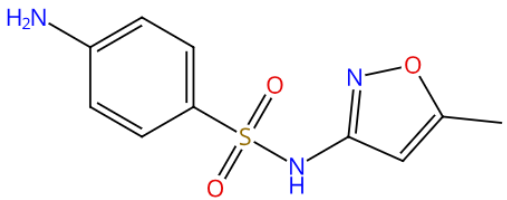
物质详情

- 折叠菜单显示物质各类信息

CAS Registry Number: 723-46-6

References (26K) | Reactions (995) | Suppliers (127) | Save



$C_{10}H_{11}N_3O_3S$

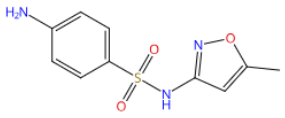
Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Key Physical Properties
Molecular Weight
Melting Point (Experimental)
Boiling Point (Predicted)
Density (Experimental)
pKa (Predicted)

Experimental Properties | Spectra

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Structure Activity Relationships
- Absorption, Distribution, Metabolism, and Excretion Data
- Toxicity
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements
- Additional Details

723-46-6



$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

Working Frequency
400 MHz

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

Temperature
20 °C

Spectrum Summary

Spectrum ID
F0175-0013

Source
Spectral data were obtained from Life Chemicals

Experimental Spectra

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

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

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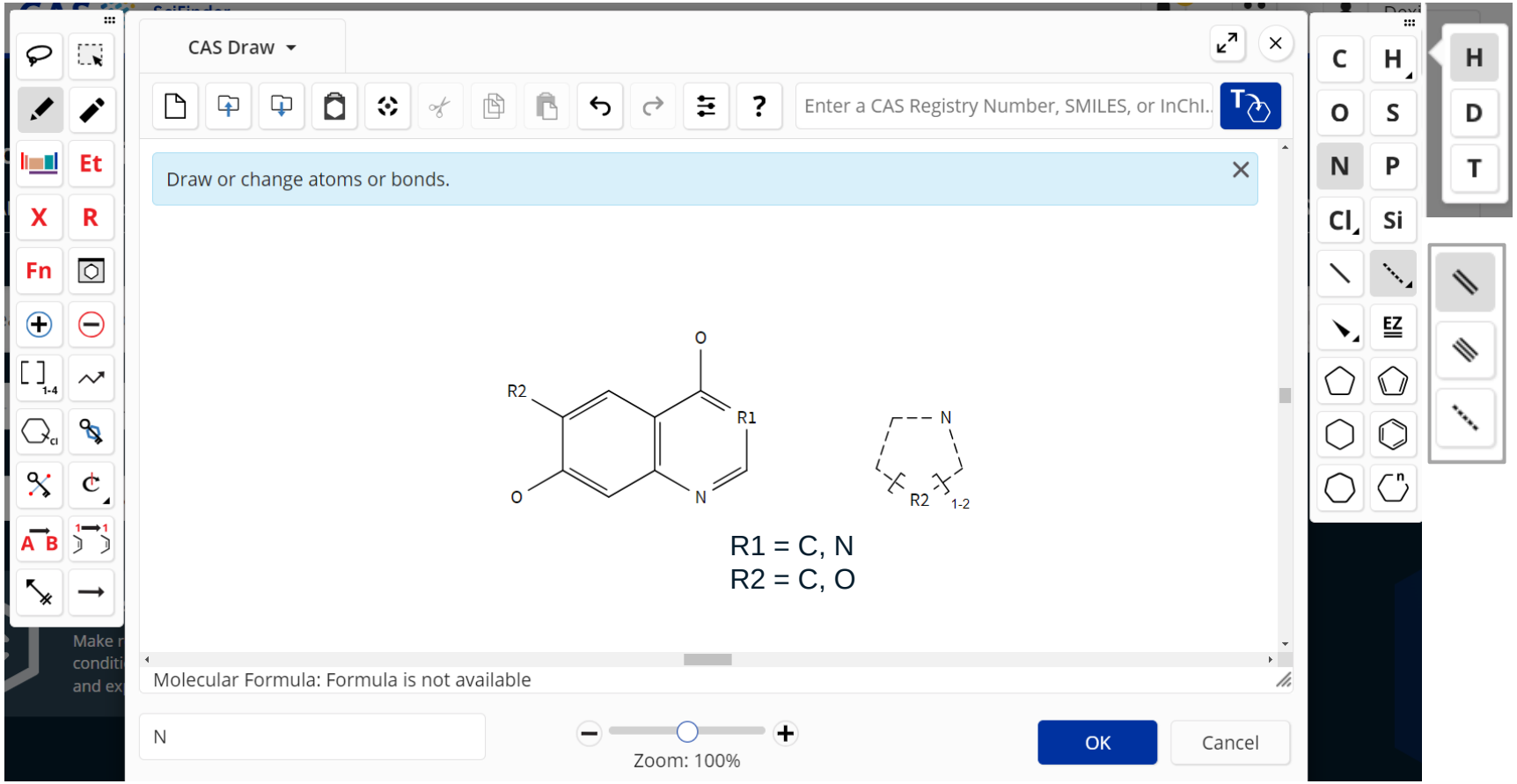
结构检索

灵活构建通式结构，提高物质/反应信息的检索效率

- 选择可变基团
- 自定义R基团
- 片段结构
- 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
3. 环系范围的定义

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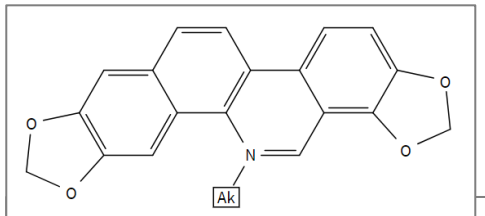
结构检索

例：已知结构片段的物质检索

结构检索时，无需分步进行，一次检索即可得到As Drawn, Substructure和Similarity结果



Substances search for drawn structure

References | Reactions | Suppliers | Save

Structure Match

As Drawn (81)

Substructure (148)

Similarity (38K)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.
Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by | Exclude

81 Results

Sort: Relevance View: Partial

1

2447-54-3

$C_{20}H_{14}NO_4$
Sanguinarine

2,605 References | 113 Reactions | 44 Suppliers

2

777808-75-0

$C_{20}H_{11}NO_4T_3$
[1,3]Benzodioxolo[5,6-*c*]-1,3-dioxolo[4,5-*i*]phenanthridinium, 13-(methyl-t_3)-

0 References | 0 Reactions | 0 Suppliers

3

117-00-0

$C_{20}H_{14}NO_4.HO$
Components: 2
Component RN: 2447-54-3
[1,3]Benzodioxolo[5,6-*c*]-1,3-dioxolo[4,5-*i*]phenanthridinium, 13-methyl-, hydroxi...

37 References | 0 Reactions | 0 Suppliers

Filter Behavior

Filter by | Exclude

- Search Within Results
- Substance Class
- Reaction Role
- Reference Role
- Number of Components
- Experimental Property
- Experimental Spectrum
- Bioactivity Data
- Bioactivity Indicator
- Target Indicator
- Regulatory Data by Country/Region
- GHS Hazard Statements

物质筛选类别：

二次检索

物质类别

反应角色

文献角色

组分数

实验物性数据

实验谱图

……

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物质检索结果的筛选

Search Within Results

Substance Class 物质类别

- Salt and Compound With (50)
- Mixture (20)
- Organic/Inorganic Small Molecule (7)
- Polymer (4)

Reaction Role 物质在反应中的角色

- Product (33)
- Reactant (2)

Reference Role

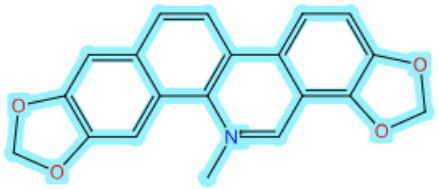
- Biological Study (53)
- Uses (46)
- Preparation (45)
- Synthetic Preparation (40)
- Therapeutic Use (36)

View All

物质在文献中的研究角色

4

693824-79-2



$C_{20}H_{14}NO_4.CN$

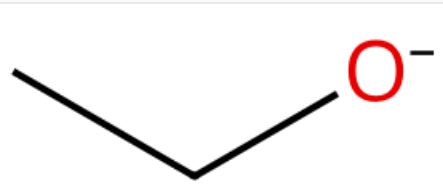
Components: 2

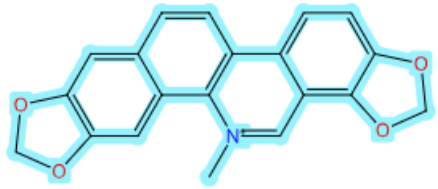
[1,3]Benzodioxolo[5,6-*c*]-1,3-dioxolo[4,5-*i*]phenanthridinium, 13-methyl-, cyanide

5 References | 0 Reactions | 0 Suppliers

5

117235-09-3





$C_{20}H_{14}NO_4.C_2H_5O$

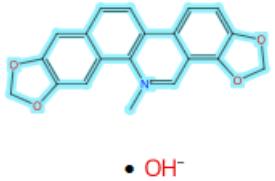
Components: 2

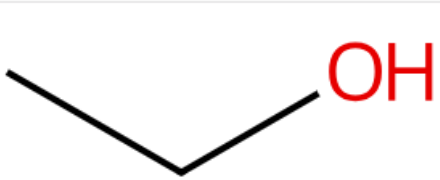
[1,3]Benzodioxolo[5,6-*c*]-1,3-dioxolo[4,5-*i*]phenanthridinium, 13-methyl-, salt wi...

1 Reference | 0 Reactions | 0 Suppliers

6

6533-66-0





$C_{20}H_{14}NO_4.C_2H_6O.HO$

Components: 3

[1,3]Benzodioxolo[5,6-*c*]-1,3-dioxolo[4,5-*i*]phenanthridinium, 13-methyl-, hydroxi...

0 References | 0 Reactions | 0 Suppliers

7 8 9

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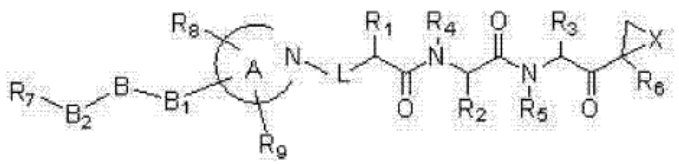
CAS Markush检索，助力结构查新

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



I

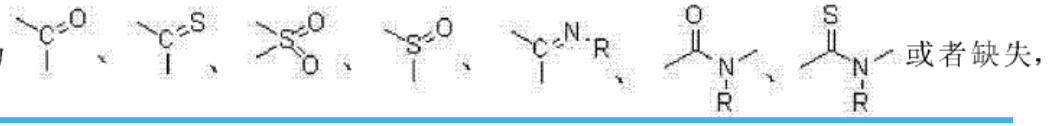
其中：

R_1，R_2，R_3 各自独立选自 H、C_{1-6} 烷基 -D、卤代的 C_{1-6} 烷基 -D、C_{1-6} 羟基烷基、C_{1-6} 巯基烷基、C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中 :D 为 N(R_a)(R_b) 或缺失，R_a，R_b 各自独立选自 H、OH、C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4，R_5 各自独立选自 H、OH、C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H，C_{1-6} 烷基，卤代的 C_{1-6} 烷基，C_{1-6} 羟基烷基，C_{1-6} 烷氧基，卤代的 C_{1-6} 烷氧基，C(O)O-C_{1-6} 烷基，C(O)NH-C_{1-6} 烷基，芳烷基；

X 为 O、S、NH、N-C_{1-6} 烷基或 N- 卤代的 C_{1-6} 烷基；

L 为  或者缺失，

其中 R 选自 H、C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

环 A 选自 5 ～ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ～ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ～ 3 个选自 O 、N 和 S 的杂原子并任选地被 R_8、R_9 和 B_1 基团取代；

R_8，R_9 分别独立选自 H、OH，C_{1-6} 烷基，C_{1-6} 烷氧基，C_{1-6} 羟基烷基，C_{1-6} 巯基烷基，C_{1-6} 烷

具体物质[Specific Substance]：以具体化学结构陈述的特定物质，会被分配CAS RN

预测性物质[Prophetic Substance]：

- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

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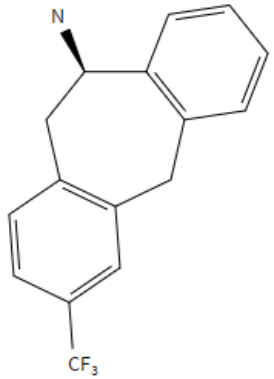
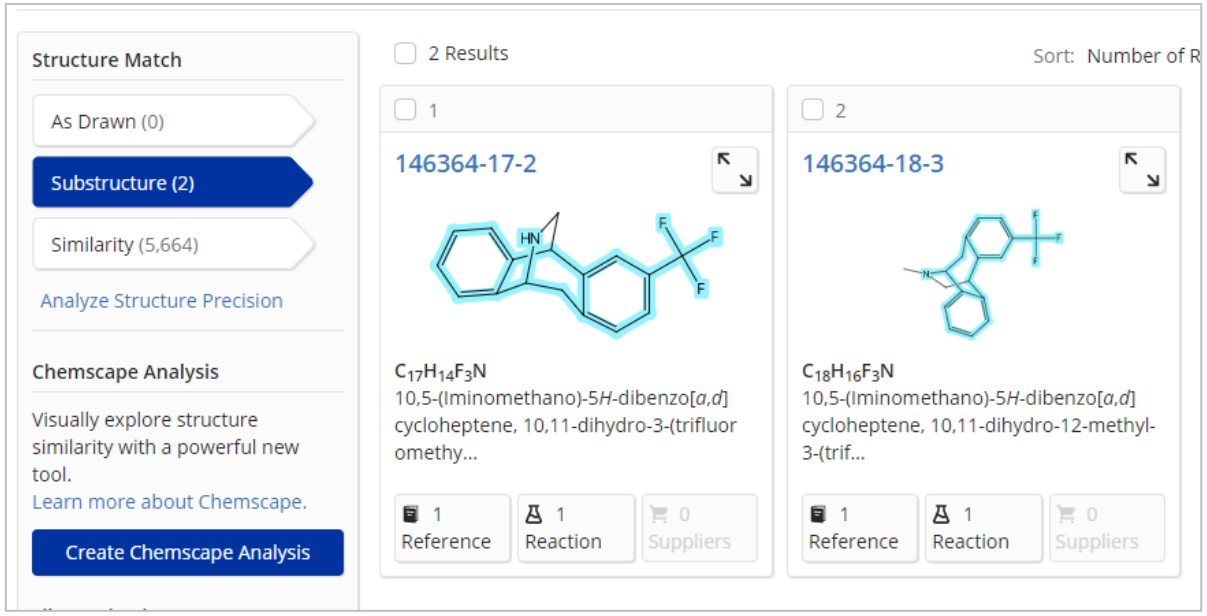
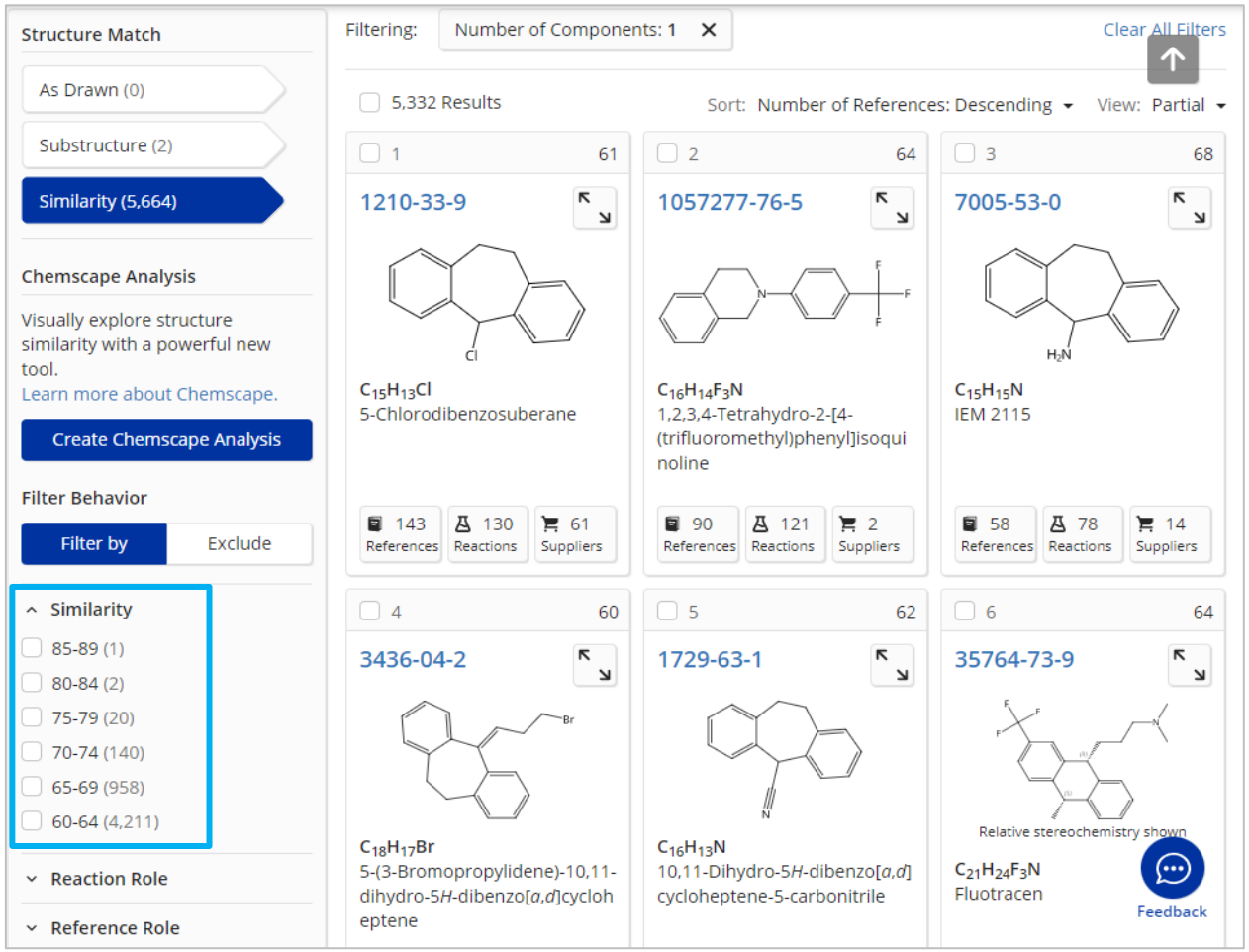
CAS Markush检索

第一步：物质结构检索

- As drawn结果为0
- Substructure结果为2
- Similarity相似度最高85-89%







为了尽可能完整地获得公开的结构信息，需要同时进行Substance和Markush结构检索

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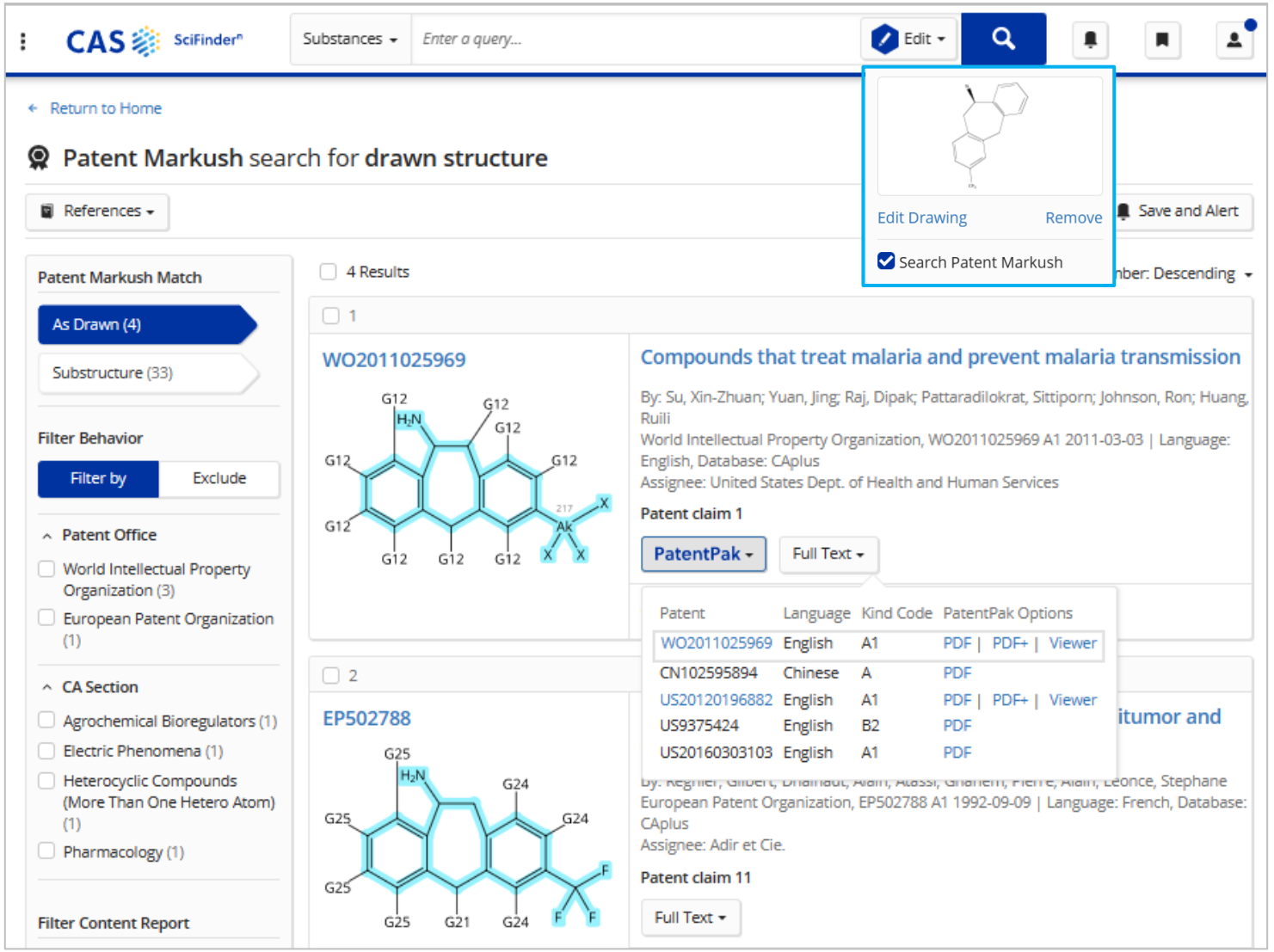
CAS Markush检索

第二步：Markush结构检索
获得四项专利文献

- 直观呈现检索结构与专利原文中Markush匹配部分的结构；
- 标引其在专利中出现的位置；
- 详细的结构取代信息描述



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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

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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?

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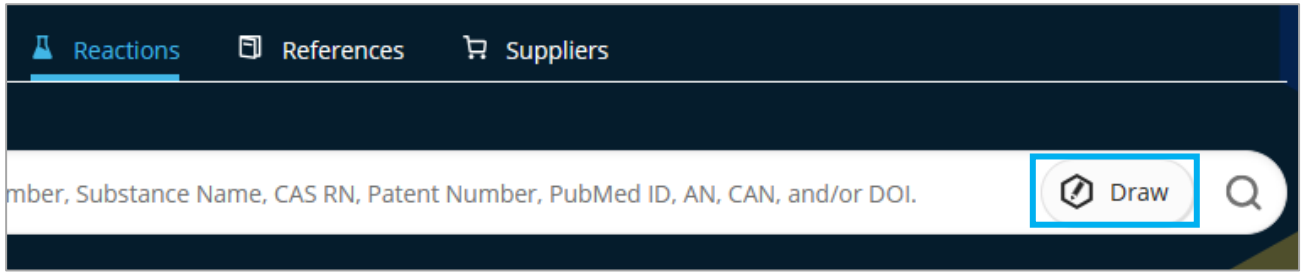
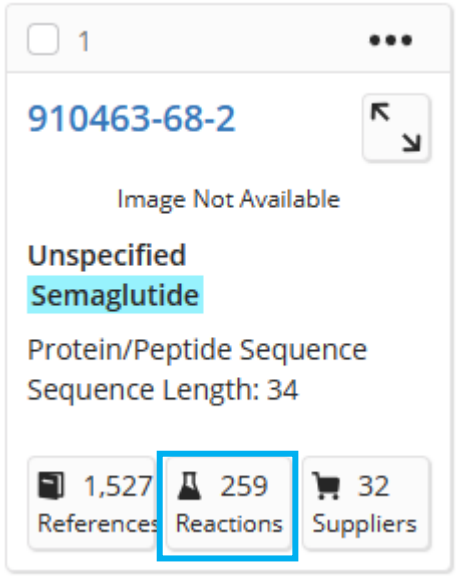
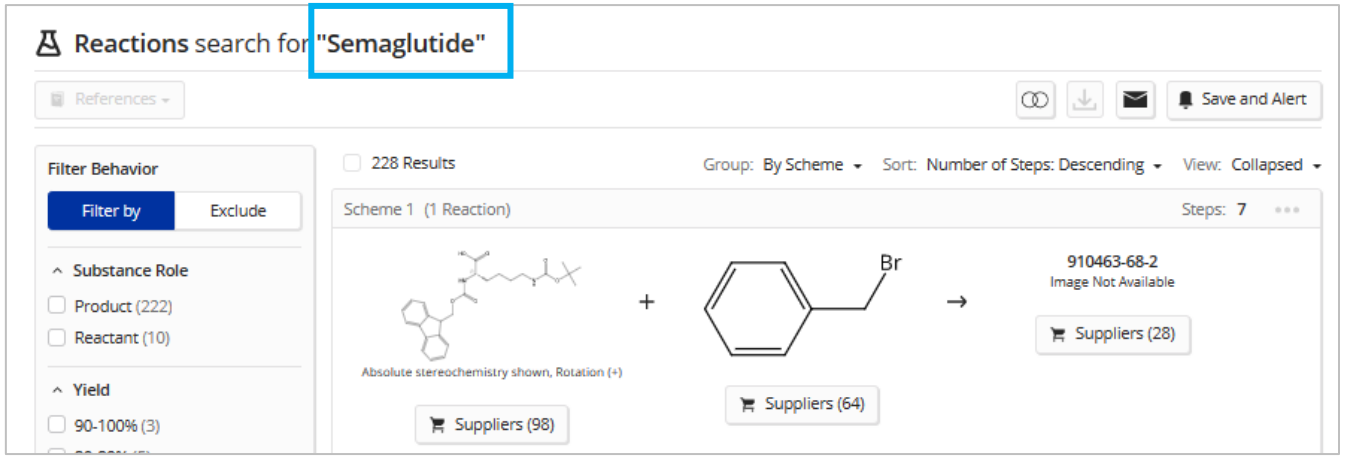
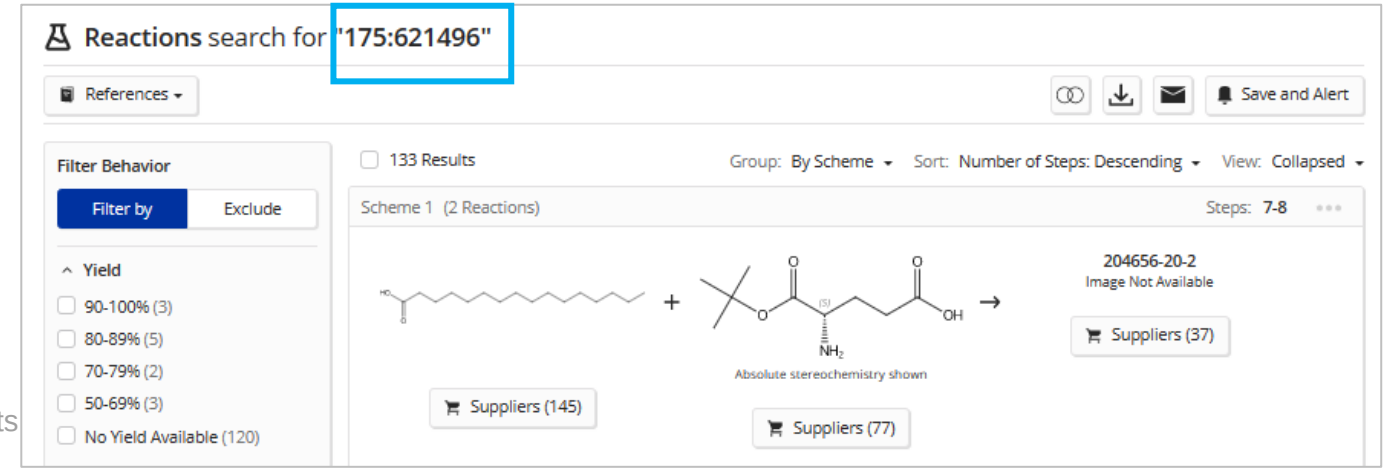
研究某种/某类反应?

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









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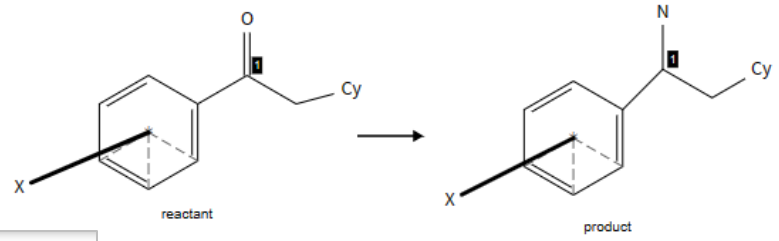
查找亚结构反应或相似反应



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)

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

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)

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

反应排序:
相关度
公布时间
产率
步数

反应分组:
按反应式
按文献
按转化类型

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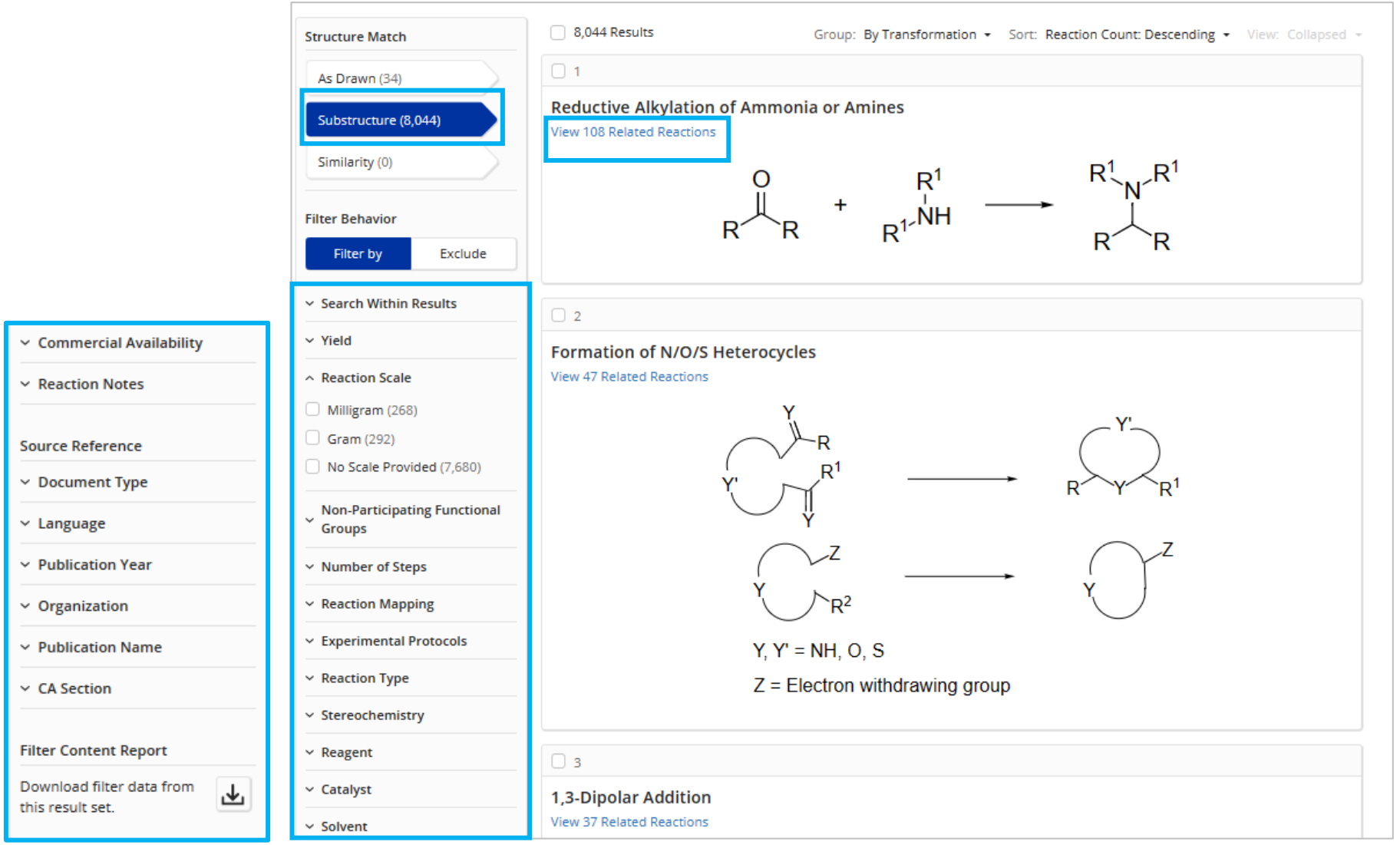
高效筛选目标反应

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



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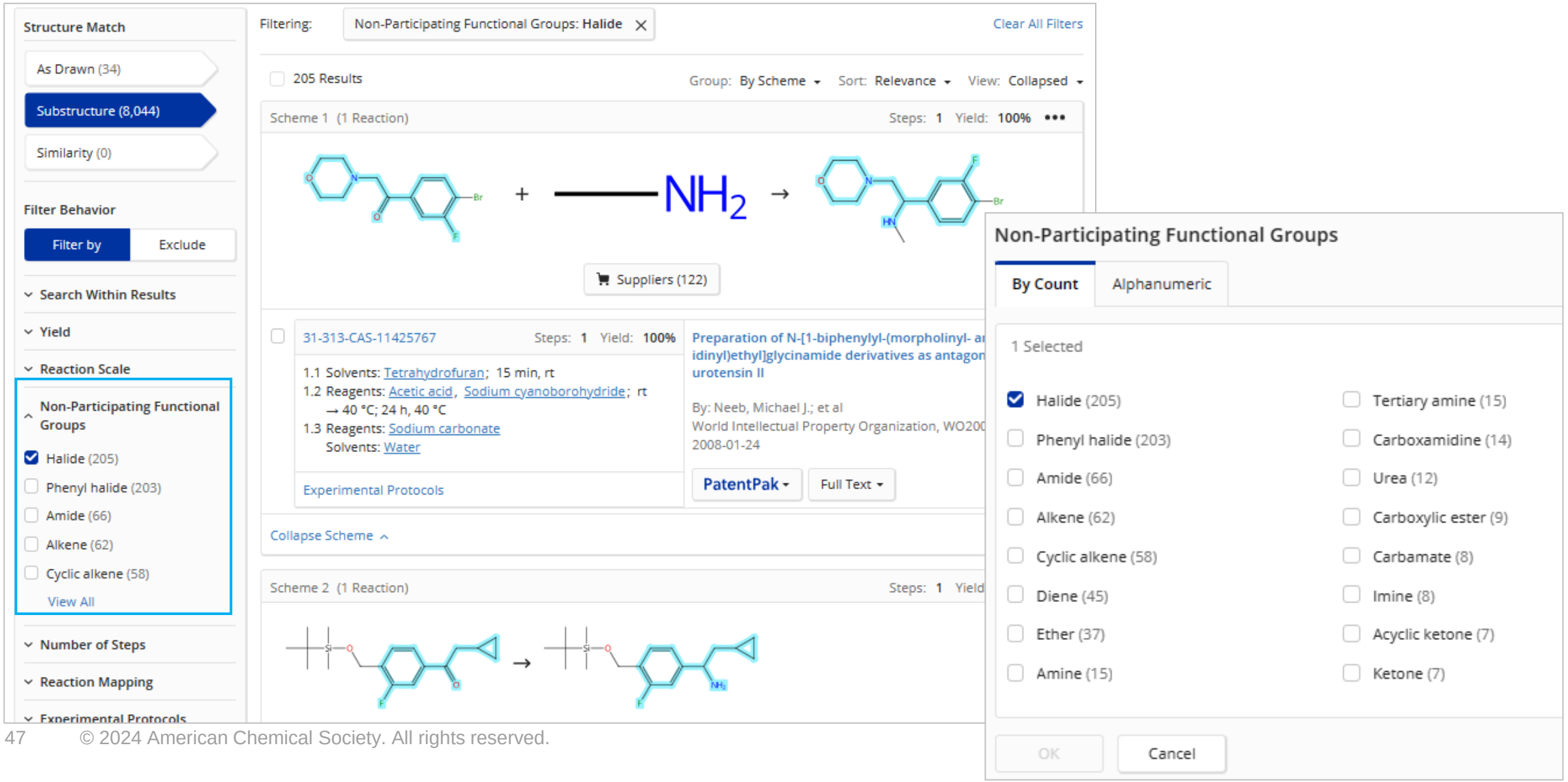
筛选工具：不参与反应官能团

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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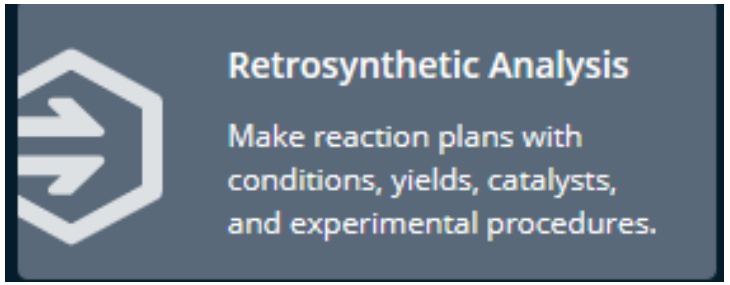
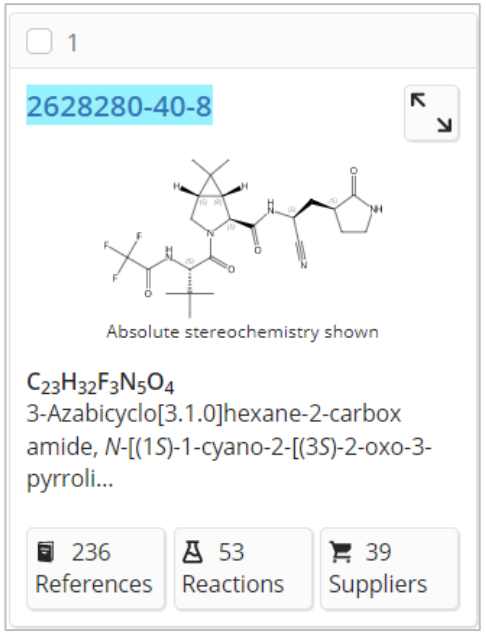
如何获得逆合成路线?

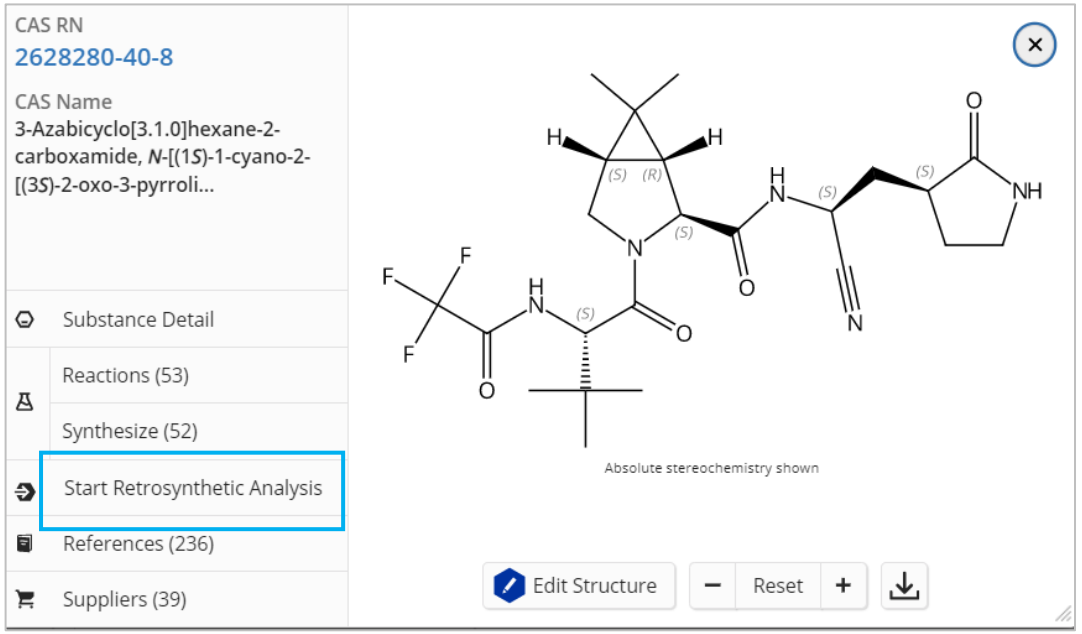
（1）已知/未知化合物：点击Retrosynthesis检索项，打开绘图板，绘制目标化合物，获得实验路线

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

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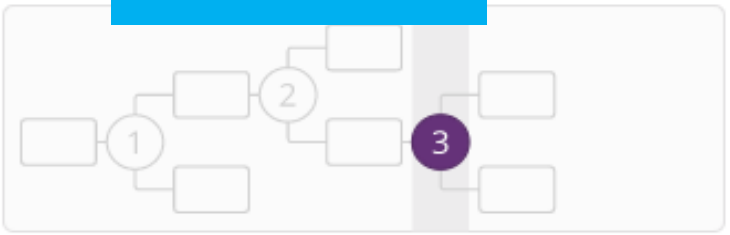
预设和调节参数

Retrosynthesis Plan Options for drawn structure

合成深度

Select Synthetic Depth Learn more.

- 1
- 2
- 3
- 4



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.

100 起始原料费用 USD/mol

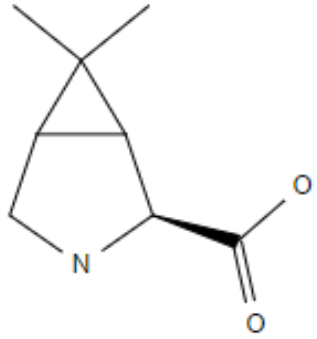
Email me when my plan is complete

Create Retrosynthesis Plan

Break and Protect Bonds

Break Bond | Protect Bond | Clear All Bond Selections

断裂键或保护键



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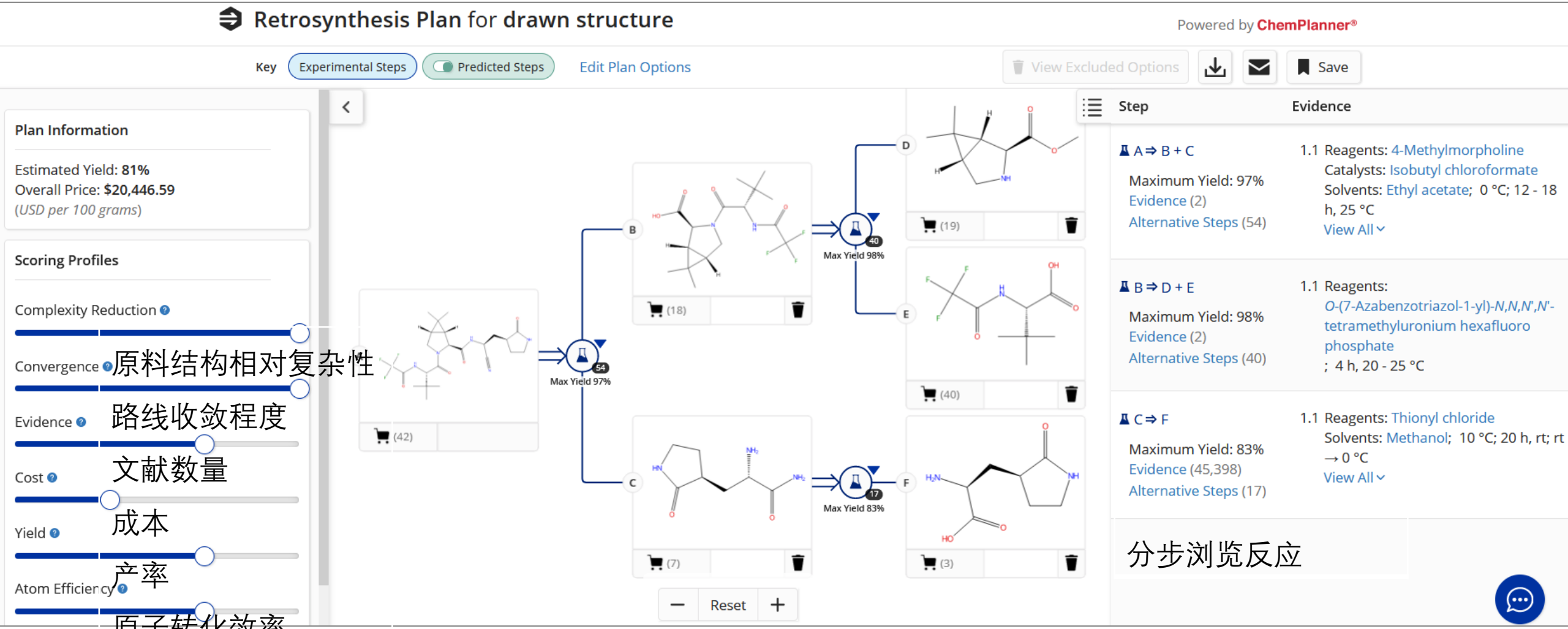
反应路线概览



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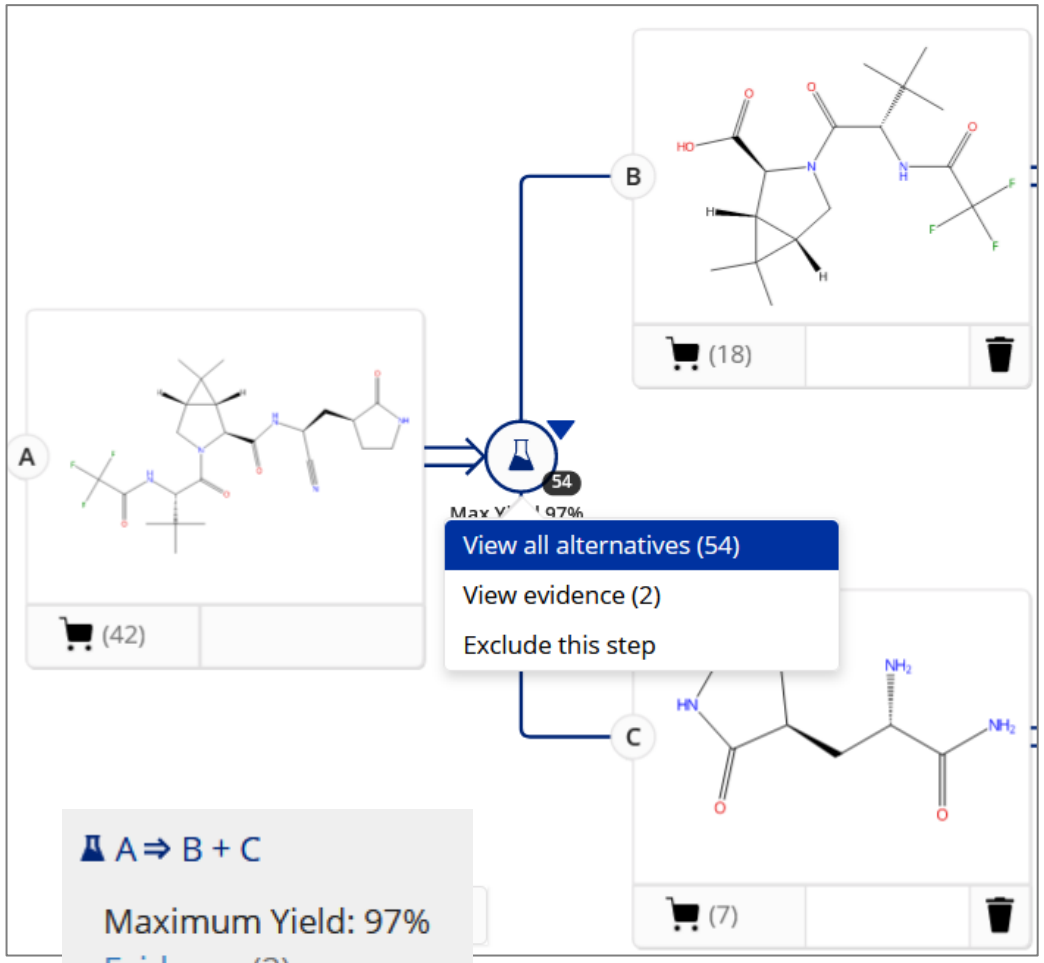
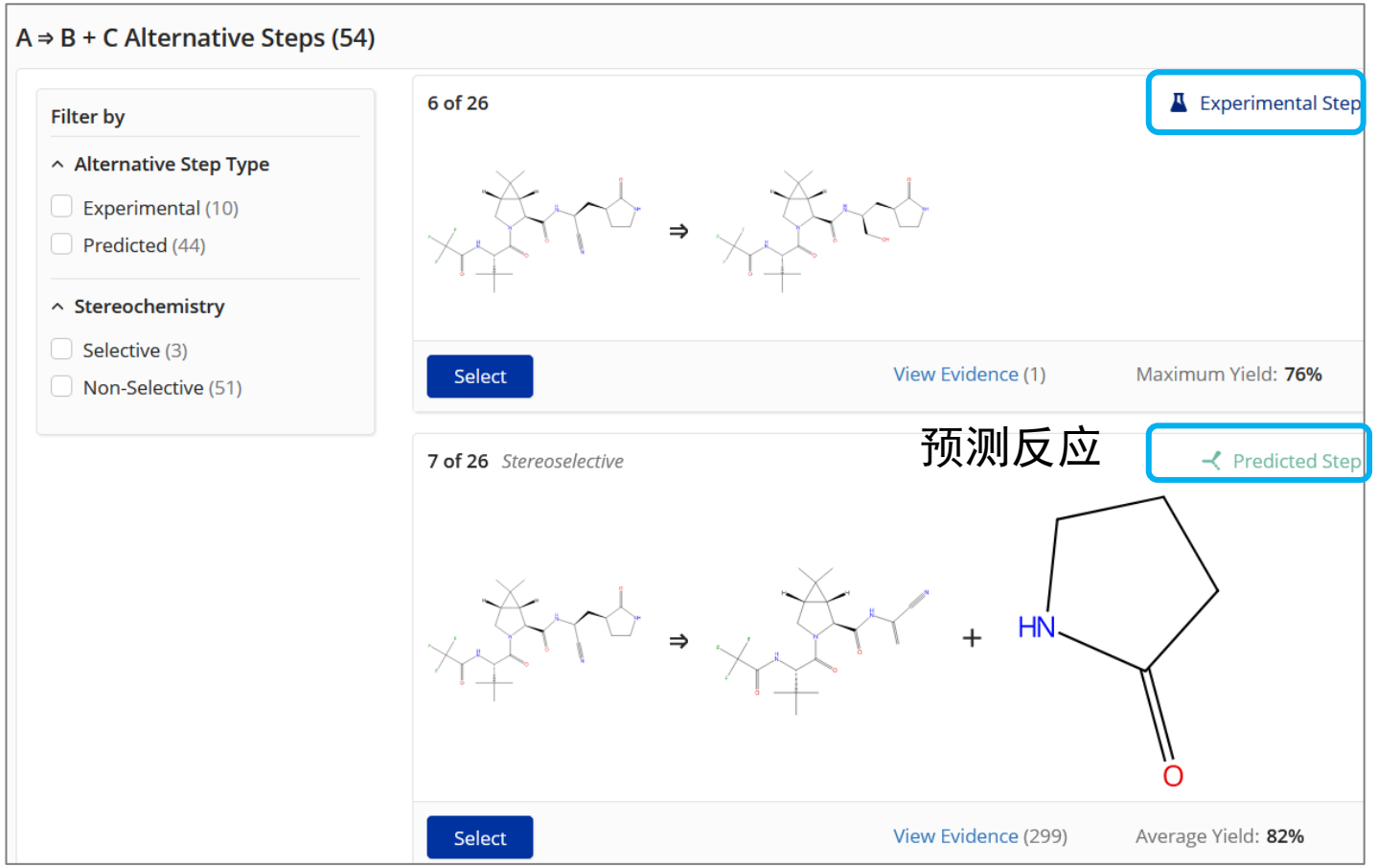
路线优化，考虑替换路线?



报道反应



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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. 关键词与反应式的联合检索
4. 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

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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?

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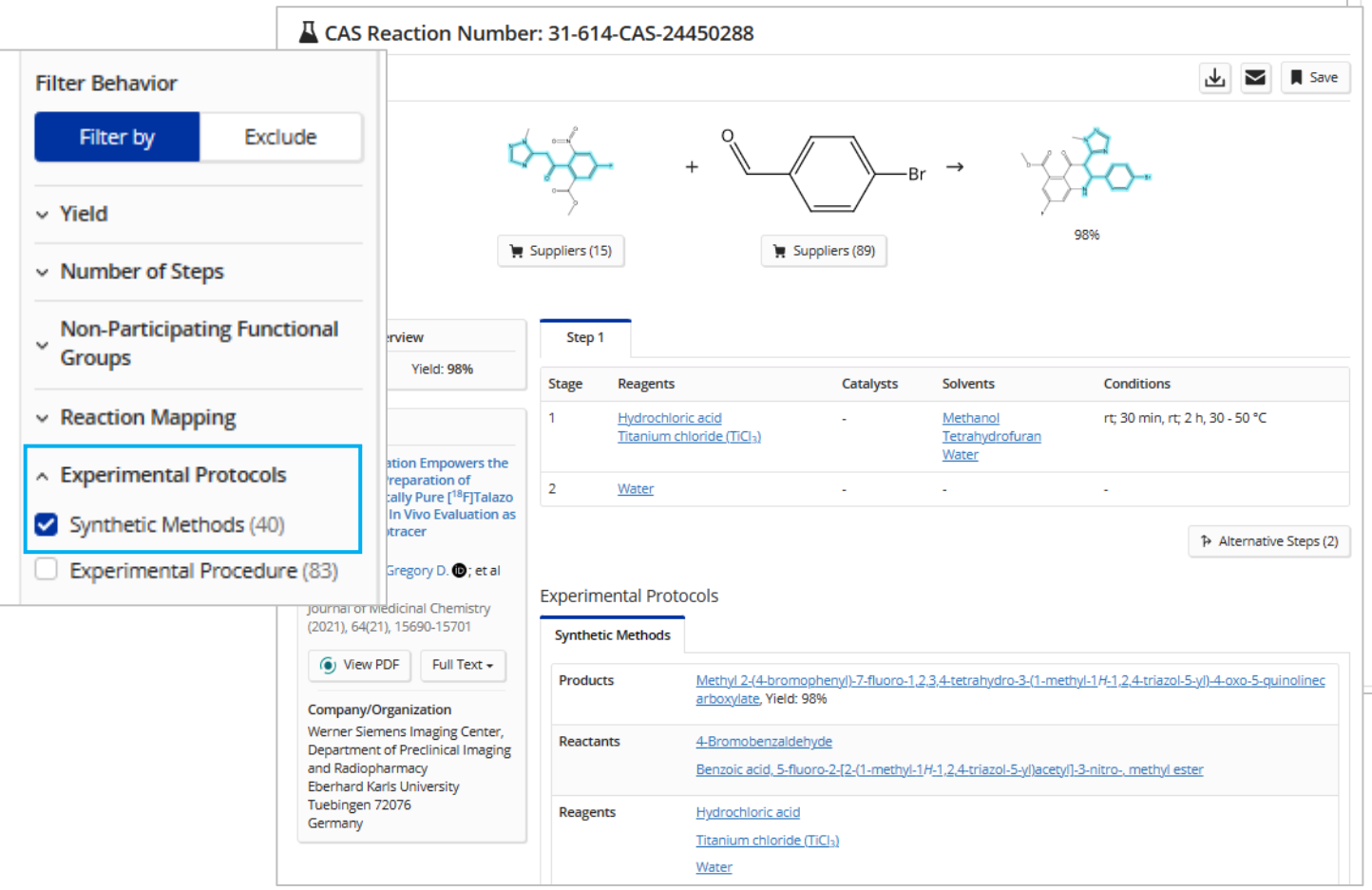
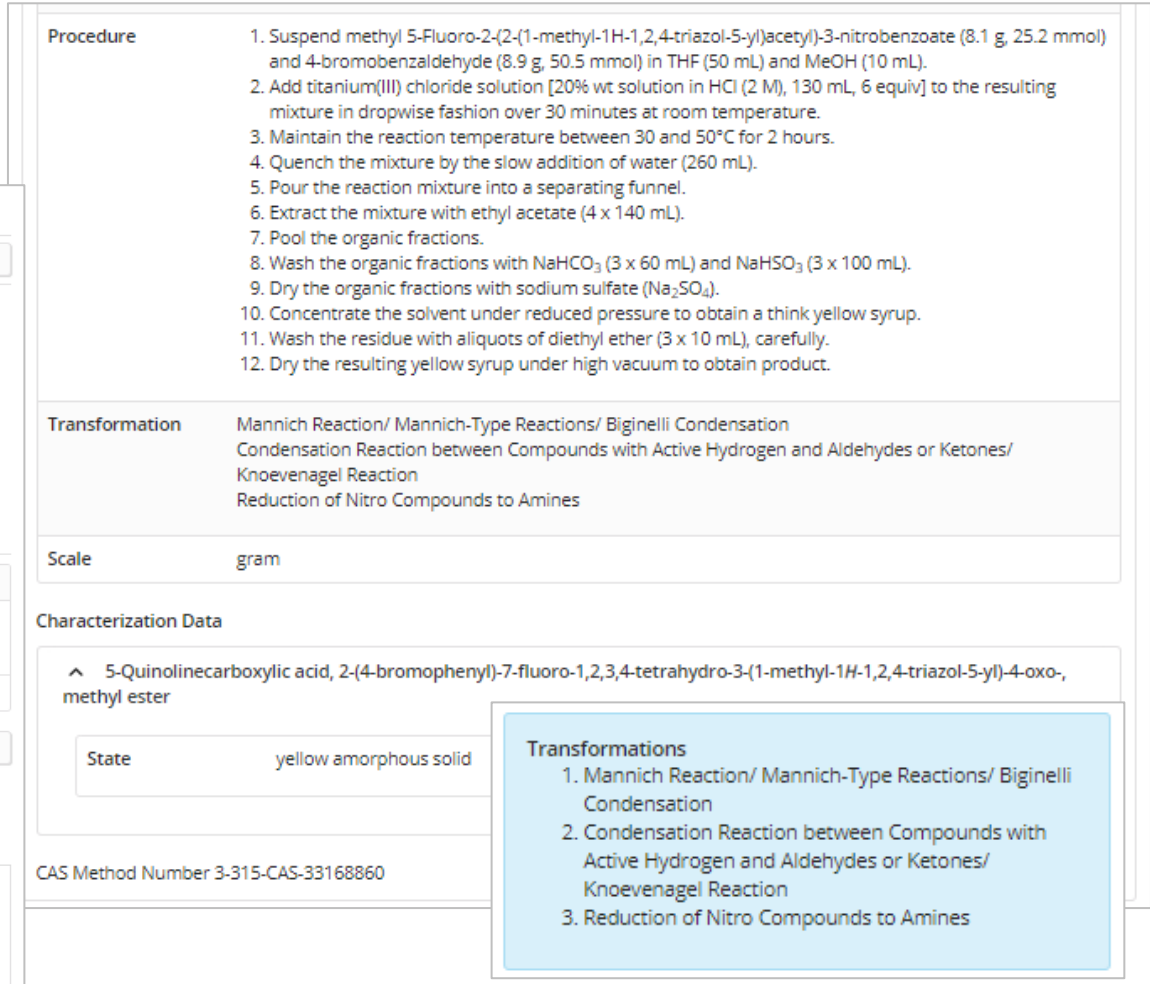
直观的合成实验详情 Synthetic Methods

- 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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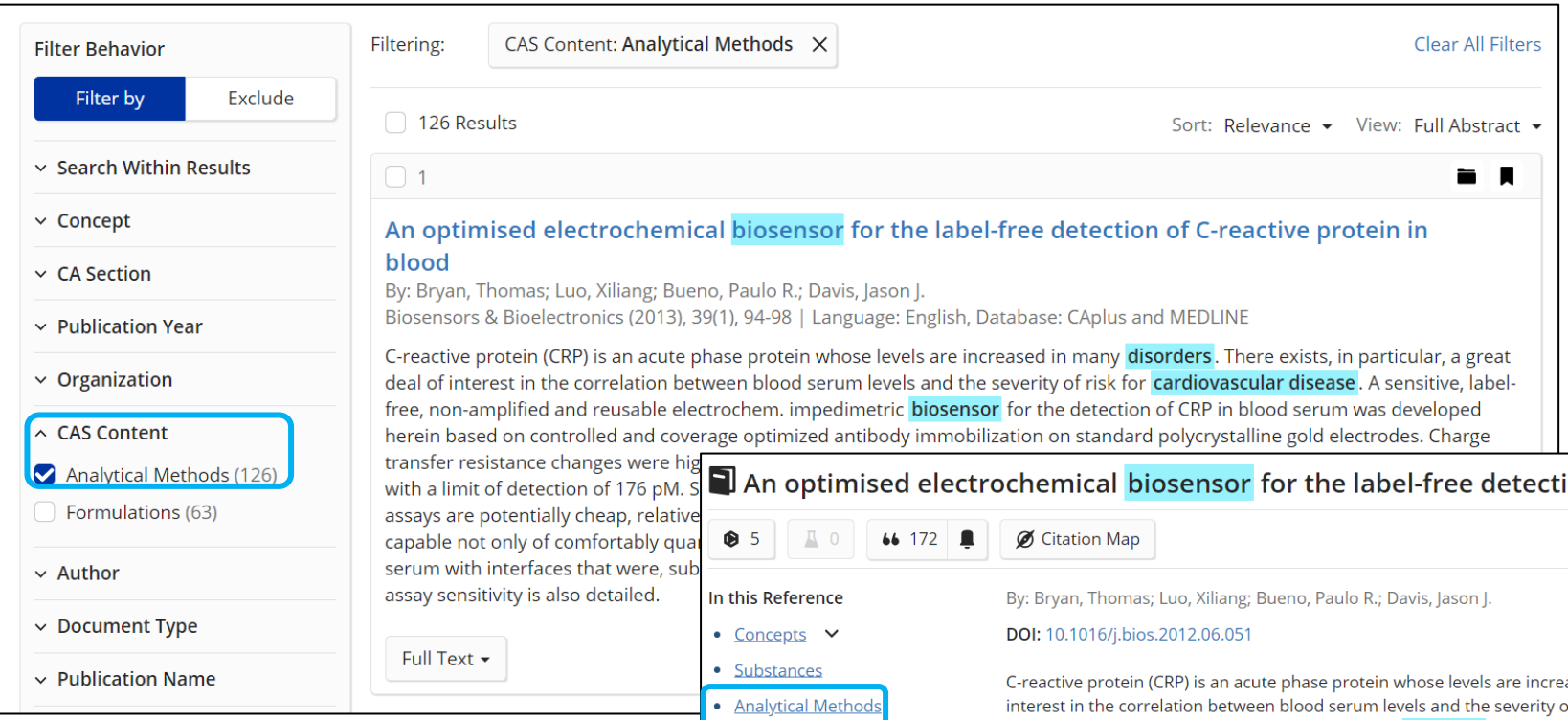
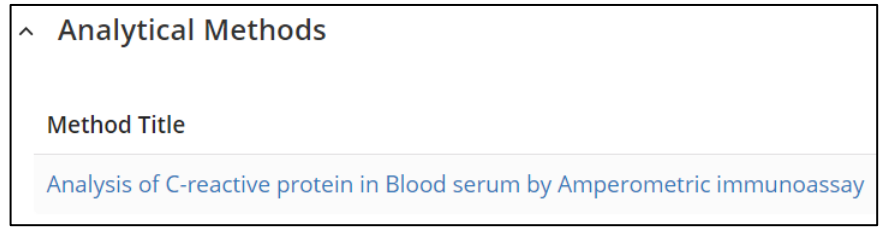
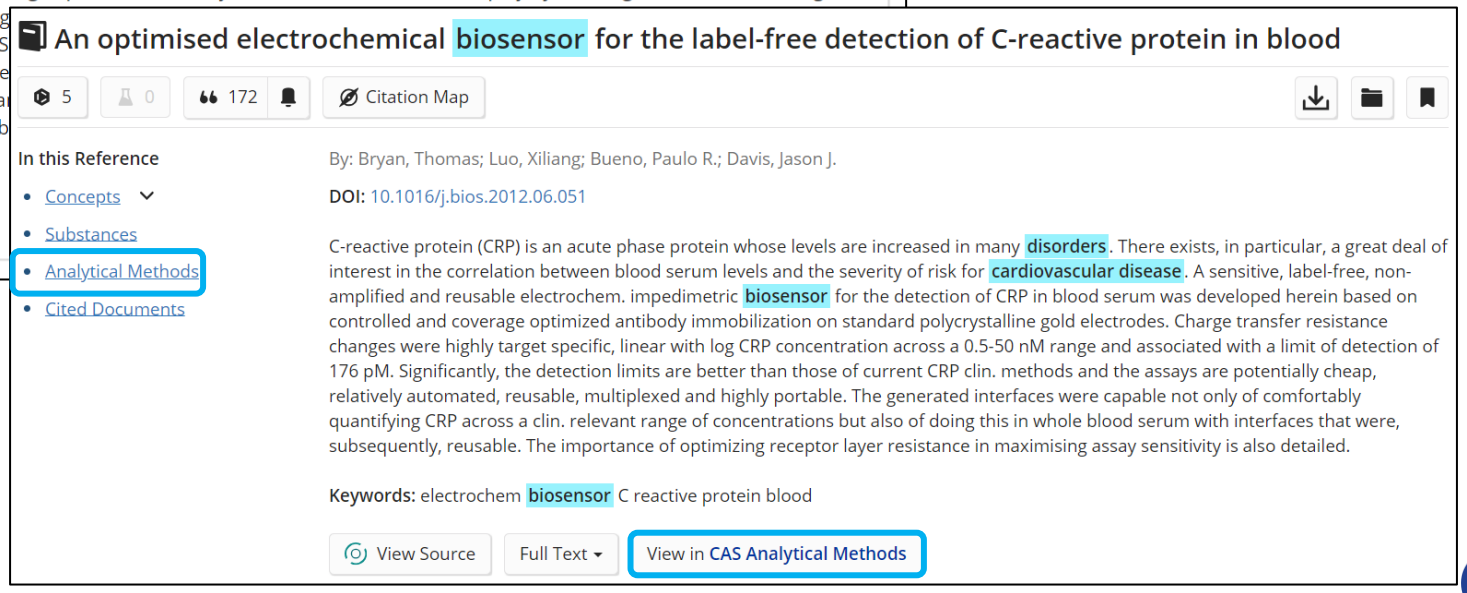
关注文献关联的分析方法?

方法一：点击CAS Content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







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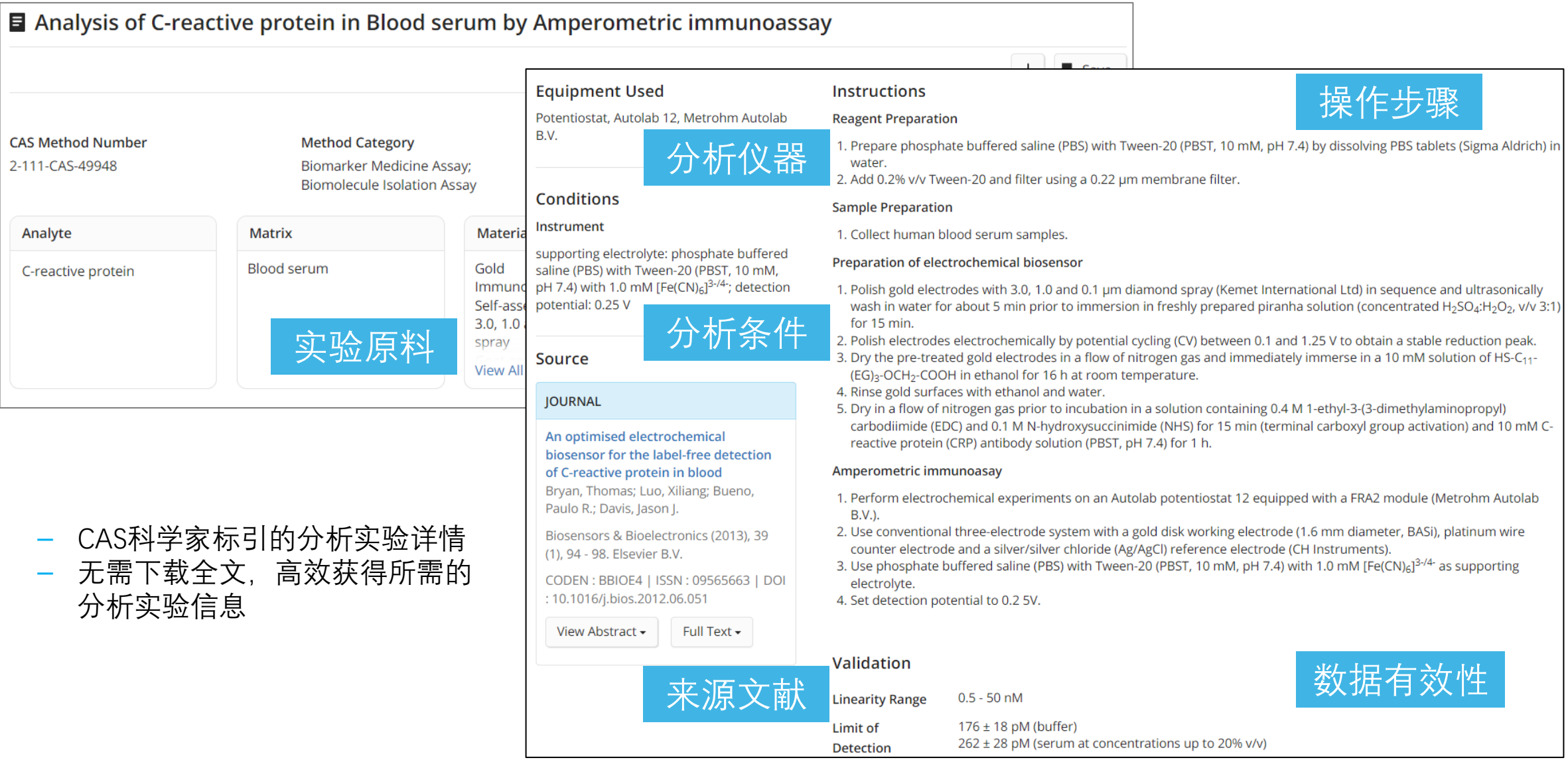
CAS 分析实验方法详情



Analysis of C-reactive protein in Blood serum by Amperometric immunoassay

CAS Method Number
2-111-CAS-49948

Method Category
Biomarker Medicine Assay;
Biomolecule Isolation Assay

Analyte	Matrix	Materia
C-reactive protein	Blood serum	Gold Immunc Self-ass 3.0, 1.0 spray View All

实验原料

Equipment Used

Potentiostat, Autolab 12, Metrohm Autolab B.V.

分析仪器

Conditions

Instrument

supporting electrolyte: phosphate buffered saline (PBS) with Tween-20 (PBST, 10 mM, pH 7.4) with 1.0 mM $[Fe(CN)_6]^{3-/4-}$; detection potential: 0.25 V

分析条件

Source

JOURNAL

An optimised electrochemical biosensor for the label-free detection of C-reactive protein in blood

Bryan, Thomas; Luo, Xiliang; Bueno, Paulo R.; Davis, Jason J.

Biosensors & Bioelectronics (2013), 39 (1), 94 - 98. Elsevier B.V.

CODEN : BBIOE4 | ISSN : 09565663 | DOI : 10.1016/j.bios.2012.06.051

View Abstract ▾ Full Text ▾

来源文献

Instructions

操作步骤

Reagent Preparation

1. Prepare phosphate buffered saline (PBS) with Tween-20 (PBST, 10 mM, pH 7.4) by dissolving PBS tablets (Sigma Aldrich) in water.
2. Add 0.2% v/v Tween-20 and filter using a 0.22 µm membrane filter.

Sample Preparation

1. Collect human blood serum samples.

Preparation of electrochemical biosensor

1. Polish gold electrodes with 3.0, 1.0 and 0.1 µm diamond spray (Kemet International Ltd) in sequence and ultrasonically wash in water for about 5 min prior to immersion in freshly prepared piranha solution (concentrated H_2SO_4:H_2O_2, v/v 3:1) for 15 min.
2. Polish electrodes electrochemically by potential cycling (CV) between 0.1 and 1.25 V to obtain a stable reduction peak.
3. Dry the pre-treated gold electrodes in a flow of nitrogen gas and immediately immerse in a 10 mM solution of HS-C_{11}-$(EG)_3$-OCH_2-COOH in ethanol for 16 h at room temperature.
4. Rinse gold surfaces with ethanol and water.
5. Dry in a flow of nitrogen gas prior to incubation in a solution containing 0.4 M 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) and 0.1 M N-hydroxysuccinimide (NHS) for 15 min (terminal carboxyl group activation) and 10 mM C-reactive protein (CRP) antibody solution (PBST, pH 7.4) for 1 h.

Amperometric immunoasay

1. Perform electrochemical experiments on an Autolab potentiostat 12 equipped with a FRA2 module (Metrohm Autolab B.V.).
2. Use conventional three-electrode system with a gold disk working electrode (1.6 mm diameter, BASi), platinum wire counter electrode and a silver/silver chloride (Ag/AgCl) reference electrode (CH Instruments).
3. Use phosphate buffered saline (PBS) with Tween-20 (PBST, 10 mM, pH 7.4) with 1.0 mM $[Fe(CN)_6]^{3-/4-}$ as supporting electrolyte.
4. Set detection potential to 0.2 5V.

Validation

数据有效性

Linearity Range	0.5 - 50 nM
Limit of Detection	176 ± 18 pM (buffer) 262 ± 28 pM (serum at concentrations up to 20% v/v)

- 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

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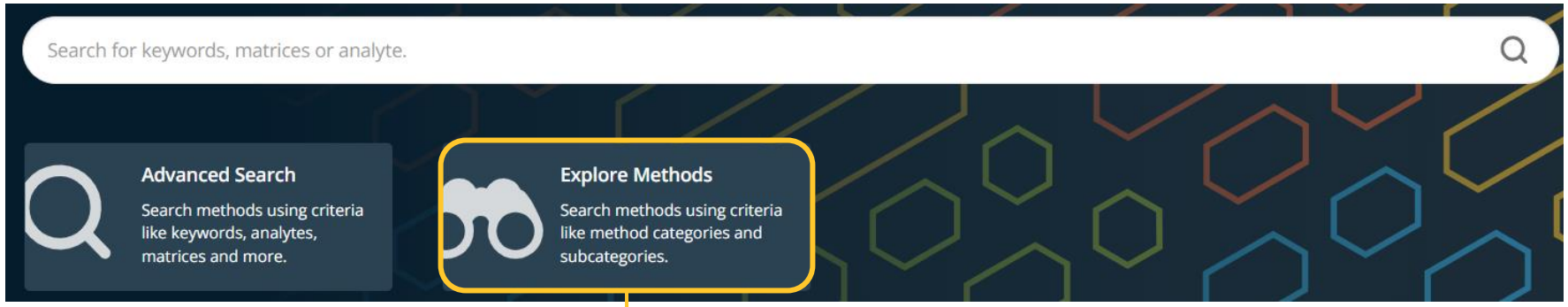
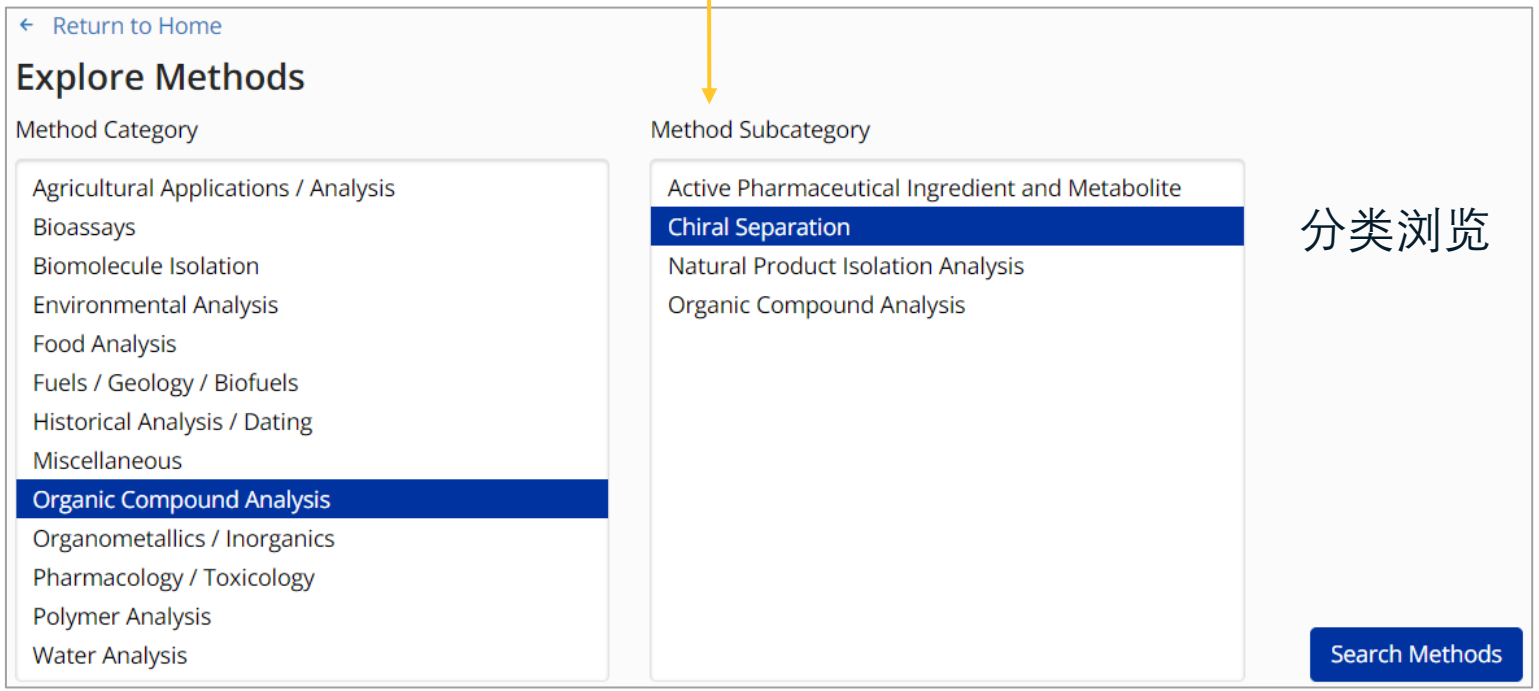
直接检索感兴趣的分析实验方法

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



直接输入主题检索



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、毒理学分析等

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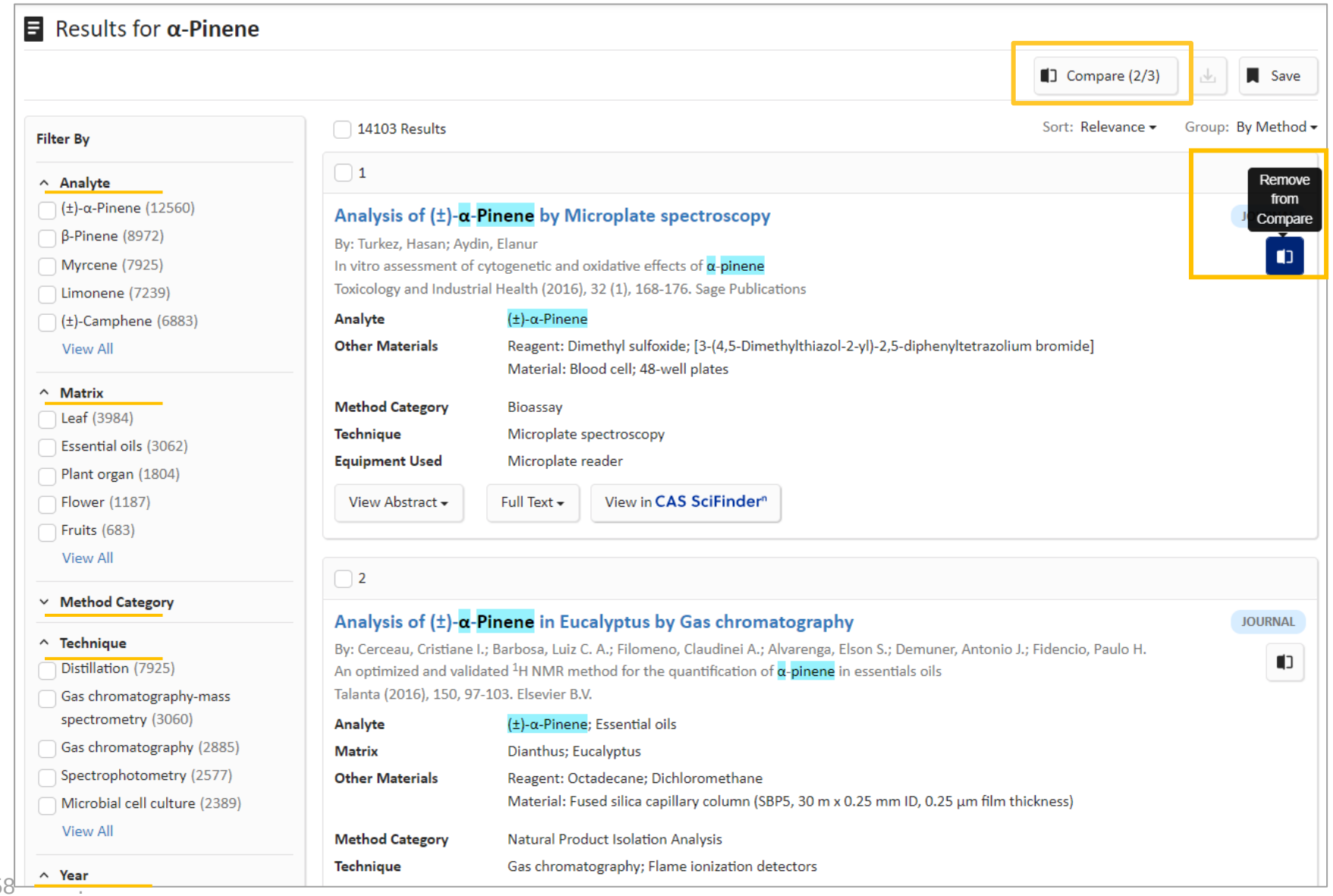
如何选择合适的分析方法？



- 分析目标物
- 介质
- 方法类别
- 分析技术
- 发表年份

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如何选择合适的分析实验方法？

	Method 1	Method 2	Method 3
	Analysis of (±)-α-Pinene by Microplate spectroscopy	Analysis of (±)-α-Pinene in Eucalyptus by Gas chromatography	Analysis of (±)-α-Pinene in Eucalyptus by
CAS Method Number	2-107-CAS-144805	1-131-CAS-295750	
Method Category	Bioassay	Natural Product Isolation Analysis	
Technique	Microplate spectroscopy	Gas chromatography; Flame ionization det	
Analyte	(±)-α-Pinene	(±)-α-Pinene; Essential oils	
Matrix	-	Dianthus; Eucalyptus	
Other Materials	Dimethyl sulfoxide; [3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide]; Blood cell; 48-well plates	Octadecane; Dichloromethane; Fused silica capillary column (SBP5, 30 m x 0.25 mm ID µm film thickness)	
Equipment Used	Microplate reader, Microquant	GC system, 17A, Shimadzu; Flame ionizatic detector (FID), Shimadzu	
Conditions	**Instrument:** Absorbance wavelength: 570 nm	**Instrument:** Column: fused silica capillary (SBP5, 30 m x 0.25 mm ID, 0.25 µm film	

详细的分析实验方法对比

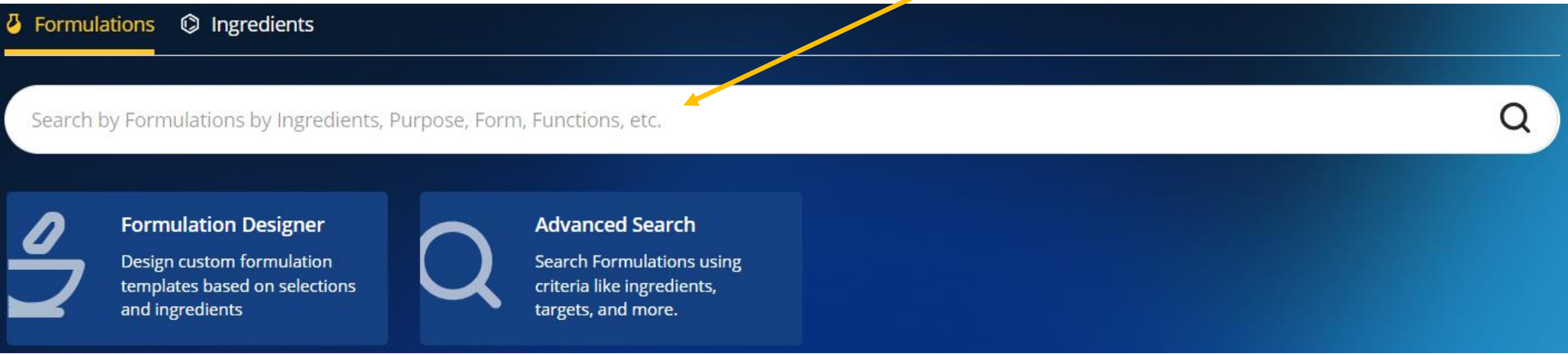
便捷对比实验方法和数据

Method	**Cell viability assay** 1. Seed human blood cells in 48-well plates. 2. Incubate the cells at 37 °C in a humidified 5% carbon dioxide and 95% air mixture. 3. Treat with α-pinene at different concentrations (0, 10, 25, 50, 75, 100, 150 and 200 mg/L) for 24 h. 4. Use the 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl tetrazolium bromide (MTT) substrate solution according to the manufacturer's instructions (Cayman Chemical Company, USA). 5. Add MTT to the cell cultures for 3 h. 6. Dissolve the formed formazan crystals in dimethyl sulfoxide. 7. Analyze the plates using Microquant reader at 570 nm wavelength. View Less	**Gas chromatography analysis with flame ionization detection using external standardization (GC-ES) method** 1. Analyze the samples using a Shimadzu equipment, model 17A, connected to a flame ionization detector (GC-FID), equipped with a fused silica capillary column (SBP5-Supelco, 30 m x 0.25 mm ID, 0.25 µm film thickness). 2. Perform separation with a fused silica capillary column (SBP5-Supelco, 30 m x 0.25 mm ID, 0.25 µm film thickness). 3. Program the column temperature as follows: from 40 °C (4 min) to 200 °C at a rate of 3 °C/min. 4. Use nitrogen as carrier gas. 5. Set the flow rate at 1.80 mL/min. 6. Set the injector temperature to 200 °C. 7. Inject 10 µL (1.0% w/v solution of the oil in dichloromethane) of the sample with a split ratio of 1:10. 8. Set the detector temperature to 240 °C. View Less	**Gas chromatography analysis with flame ionization detection using internal standardization (GC-IS) method** 1. Analyze the samples using a Shimadzu equipment, model 17A, connected to a flame ionization detector (GC-FID), equipped with a fused silica capillary column (SBP5-Supelco, 30 m x 0.25 mm ID, 0.25 µm film thickness). 2. Perform separation with a fused silica capillary column (SBP5-Supelco, 30 m x 0.25 mm ID, 0.25 µm film thickness). 3. Program the column temperature as follows: from 40 °C (4 min) to 200 °C at a rate of 3 °C/min. 4. Use nitrogen as carrier gas. 5. Set the flow rate at 1.80 mL/min. 6. Set the injector temperature to 200 °C. 7. Inject 10 µL (1.0% w/v solution of the oil in dichloromethane) of the sample with a split ratio of 1:10. 8. Set the detector temperature to 240 °C. View Less
Helpful Hints	interferent: safetyInfo: troubleshooting: View All	interferent: safetyInfo: troubleshooting: View All	interferent: safetyInfo: troubleshooting: View All
Bioactivity	90, 91, 91, 90, 92, 91 and 90% (Read from figure, cell viability) at 0, 10, 25, 50, 75, 100 and 150 mg/L added concentrations, respectively	-	-
Concentration	-	34% (read from figure, *E. saligna*), 15% (read from figure, pink pepper essential oils, *Schinus terebinthifolius*), 37% (read from figure, hybrid *E. urophylla* x *E. grandis*), 13% (read from figure, *E.*	34% (read from figure, *E. saligna*), 10.3% (read from figure, pink pepper essential oils, *Schinus terebinthifolius*), 33% (read from figure, hybrid *E. urophylla* x *E. grandis*), 10.3% (read from figure, *E.*

研究课题在产品中的应用？配方的检索与设计

方法一：登 https://formulus.cas.org 输入检索式

原料、用途、物理形态、功能或文献标识符



- 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

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配方结果集

Formulations search for "orthopedic and implant"

Get Additional References | Compare (0/3) | Save

256 Results Sort: Relevance

Filter by

Industry
- Cleaning & Surfactant Products
- Cosmetics & Personal Care
- Pharmaceutical
- Unclassified

Purpose
- Pharmaceutical formulations (256)
- Drug delivery systems (128)
- Analgesics (106)
- Pharmaceutical implants (87)
- Stabilizing agents (87)

View All

Physical Form
- Tablets (256)
- Capsules (230)
- Pharmaceutical implants (171)
- Powders (163)
- Solutions (124)

View All

1

Oral Solid Composition: Pharmaceutical Formulations

Location: Table 1, Comparative Example 1
Purpose: Pharmaceutical formulations
Target: Homo sapiens
Delivery Route: Oral drug delivery systems
Physical Form: Tablets

一次最多可以比较三种不同制剂或配方的信息详情

Add to Compare

Component	Function	Amount Reported
Levonorgestrel	-	1.5 mg
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?)	-	125.2 mg
Starch	additives	7 mg
Poly(vinylpyrrolidone)	additives	4.2 mg

Additional components reported

View Formulation Detail

PATENT

Oral solid composition comprising progestin and levonorgestrel, its manufacturing method, and method for manufacturing oral tablet

Assignee : Fuji Pharma Co., Ltd.
JP2020132640
Language: Japanese

Patent PDF | View in CAS SciFinder

76 Similar Formulations - View All (opens in a new window)

Delivery Route
- Oral drug delivery systems (166)
- Intramuscular injections (95)
- Intraperitoneal injections (93)
- Subcutaneous drug delivery systems (88)
- Buccal drug delivery systems (83)

View All

Information Included
- Component Amount (159)
- Process (120)
- Experimental Activity (91)
- Effective Dose (8)

Document Type
- Patent (256)
  - Claim (94)
  - Comparative Example (2)
  - Example (160)

Organization
- SSP Co., Ltd. (42)
- Coeruleus Ltd. (40)
- Biogen Idec, Inc. (27)
- Skyepharma, Inc. (27)
- Fuji Pharma Co., Ltd. (12)

View All

Publication Year

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配方的制备？实验评估？

Oral Solid Composition: Pharmaceutical Formulations

Save

Purpose	Target	Delivery Route	Physical Form	Source
Pharmaceutical formulations	Homo sapiens	Oral drug delivery systems	Tablets	View

Formulation Ingredients

Component	Function	Amount Reported	Optionality
Levonorgestrel	-	1.5 mg	Mandatory
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?)	-	125.2 mg	Mandatory
Starch	additives	7 mg	Mandatory
Poly(vinylpyrrolidone)	additives	4.2 mg	Mandatory
Silica	fluidizing agents	0.7 mg	Mandatory
Magnesium stearate	pharmaceutical lubricants	1.4 mg	Mandatory

More Formulations like this... NEW

- **Pharmaceutical Tablet Containing Entecavir: Antiviral Agents**
  Purpose: Antiviral agents
  Target: Hepatitis B, Homo sapiens
  Delivery Route: Oral drug delivery syst...
  Physical Form: Tablets
- **Oral Pharmaceutical Composition: Pharmaceutical Formulations**
  Purpose: Pharmaceutical formulations
  Target: Homo sapiens
  Delivery Route: Oral drug delivery syst...
  Physical Form: Capsules, Compression...
- **Fluconazole Tablet Composition: Drug Delivery Systems**
  Purpose: Drug delivery systems
  Target: fluconazole
  Delivery Route: -
  Physical Form: Tablets
- **Pharmaceutical Formulation for Treating Tumor: Antitumor Agents**
  Purpose: Antitumor agents
  Target: Homo sapiens, Neoplasm
  Delivery Route: -
  Physical Form: Capsules, Granular mat...

Process

production of tablets: (1) pre-mixing lactose hydrate (200 M), corn starch and povidone K-30 are mixed in a V-type mixer (5L, mixed at Tokuju Kosakusho Co., Ltd.). (2) granulation/drying the powder mixed by the premixing of (1) is put into a fluidized bed granulator (FD-MP-01 D, manufactured by Paulec Co., Ltd.), and 95% with levonorgestrel. An ethanol suspension composed of ethanol was sprayed at an air volume of 0.3 m/min, an air supply temperature of 60 °C., a spray volume of 14 g / min, and a spray air volume of 55 L/min, granulated, and then dried. levonorgestrel having a cumulative 10% particle diameter of 1 μm, a cumulative 50% particle diameter of 4 μm, and a cumulative 90% particle diameter of 7 μm was used. It was confirmed that the amount of residual ethanol in the dried powder was less than the concentration limit value described in the 17 th Revised Japanese Pharmacopoeia "residual solvent". (3) primary mixing the powder dried in (2), light anhydrous silicic acid were mixed with a locking mixer (RM-10-2, manufactured by Aichi electric Co., Ltd.). secondary mixing powder mixed in the primary mixing of (3) and Magnesium stearate were mixed with a locking mixer (RM-10-2, manufactured by Aichi electric Co., Ltd.). (5) locking the powder mixed by the secondary mixing of (4) is subjected to a locking machine (VIRGO 0512SS2AY, manufactured by Kikusuiseisakusho co. , Ltd.) at a locking pressure of 7 kN, a lock diameter of 7.0 mm, and a mass of 140 mg.

Experimental Activity

Descriptor	Notes	Details
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 15 minutes	45.2
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 30 minutes	56.4
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 45 minutes	62.3
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 60 minutes	66.2
dissolution rate	dissolution rate of the tablet was evaluated for 0 month at 90 minutes	70.6

Source Patent

Oral solid composition comprising progestin and levonorgestrel, its manufacturing method, and method for manufacturing oral tablet

Assignee : Fuji Pharma Co., Ltd.
JP2020132640
Language: Japanese
Location: Table 1, Comparative Example 1

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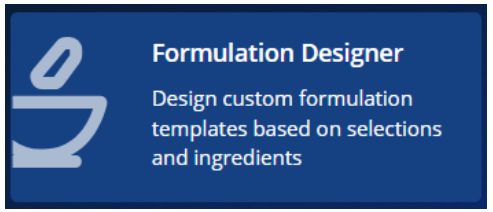

Formulation Designer

Clear All Selections

Industry

- Pharmaceutical
- Cosmetics & Personal Care
- Agrochemical
- Cleaning & Surfactant Products
- Food & Related
- Inks, Paints, & Coatings

Purpose

- Cosmetics and Personal care products
- Skin conditioners
- Sunscreens
- Hair dyes
- Hair preparations
- Antiperspirants
- Cleaning compositions
- Skin-lightening cosmetics
- Skin cleansers
- Oral hygiene products
- Skin care products
- - View More Purposes -

Physical Form

- Emulsions
- Cream preparations
- Cosmetic lotions
- Cosmetic packs
- Gels
- Liquids
- Solutions
- Nanospheres
- Pastes
- Capsules
- - View More Physical Forms -

Add up to 5 Ingredients

Vitamin A

Polyethylene glycol

+ Add Another Ingredient

Create Template

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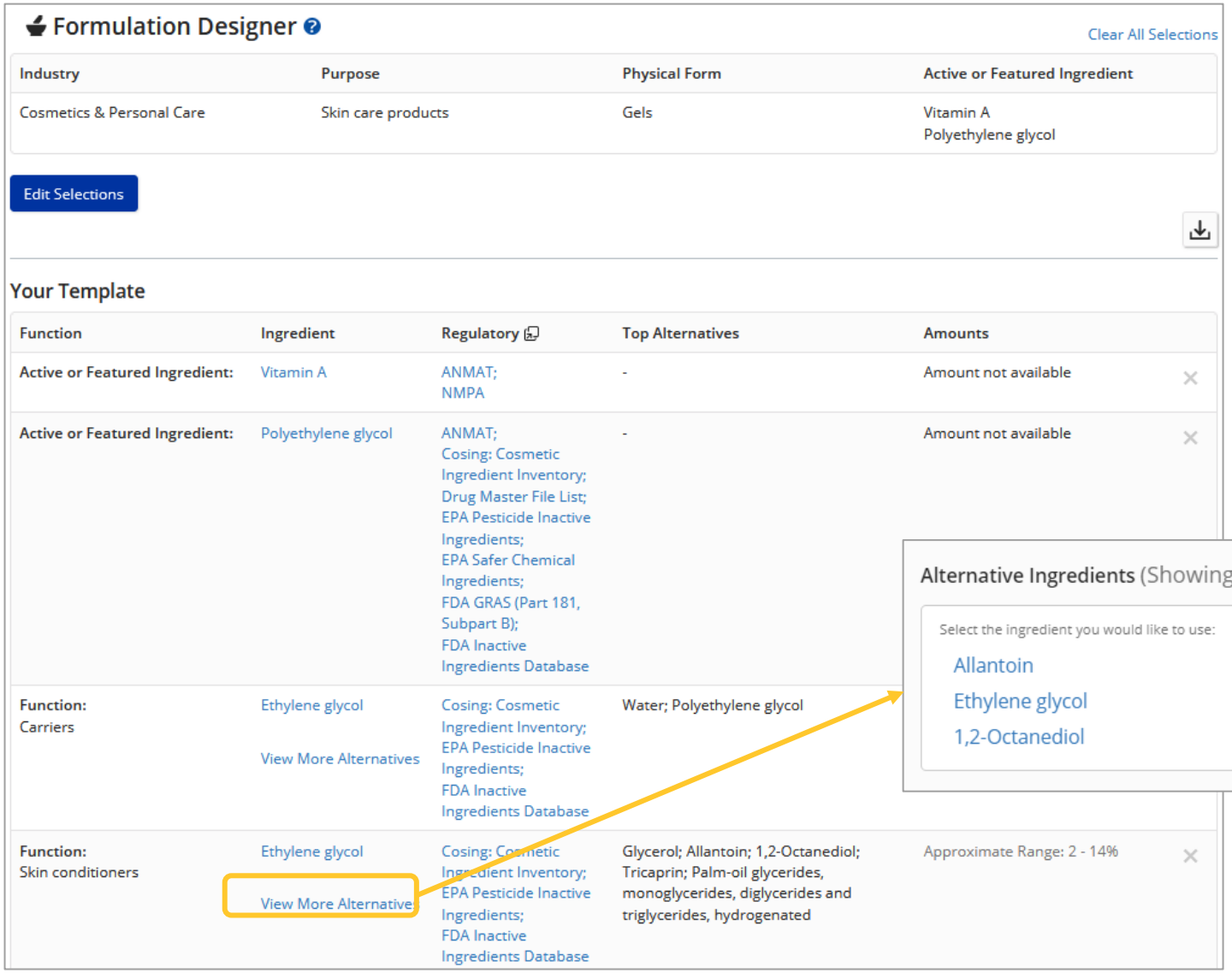

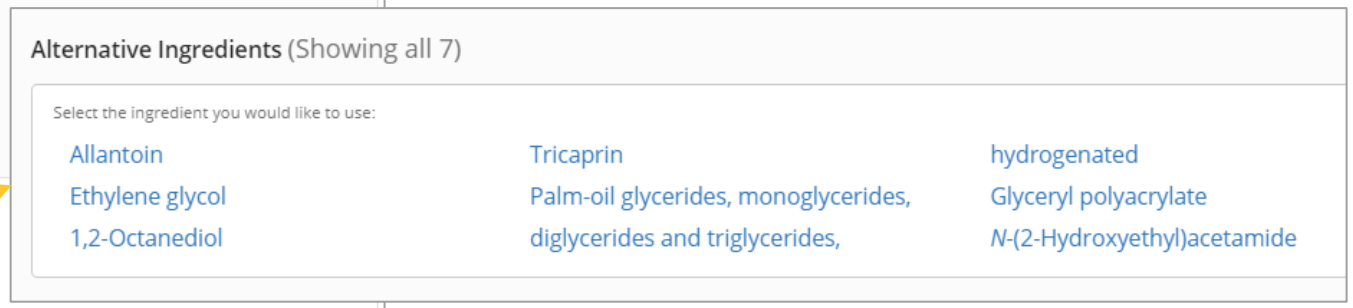

- 原料详情
- 原料管制信息
- 可替代的原料选项

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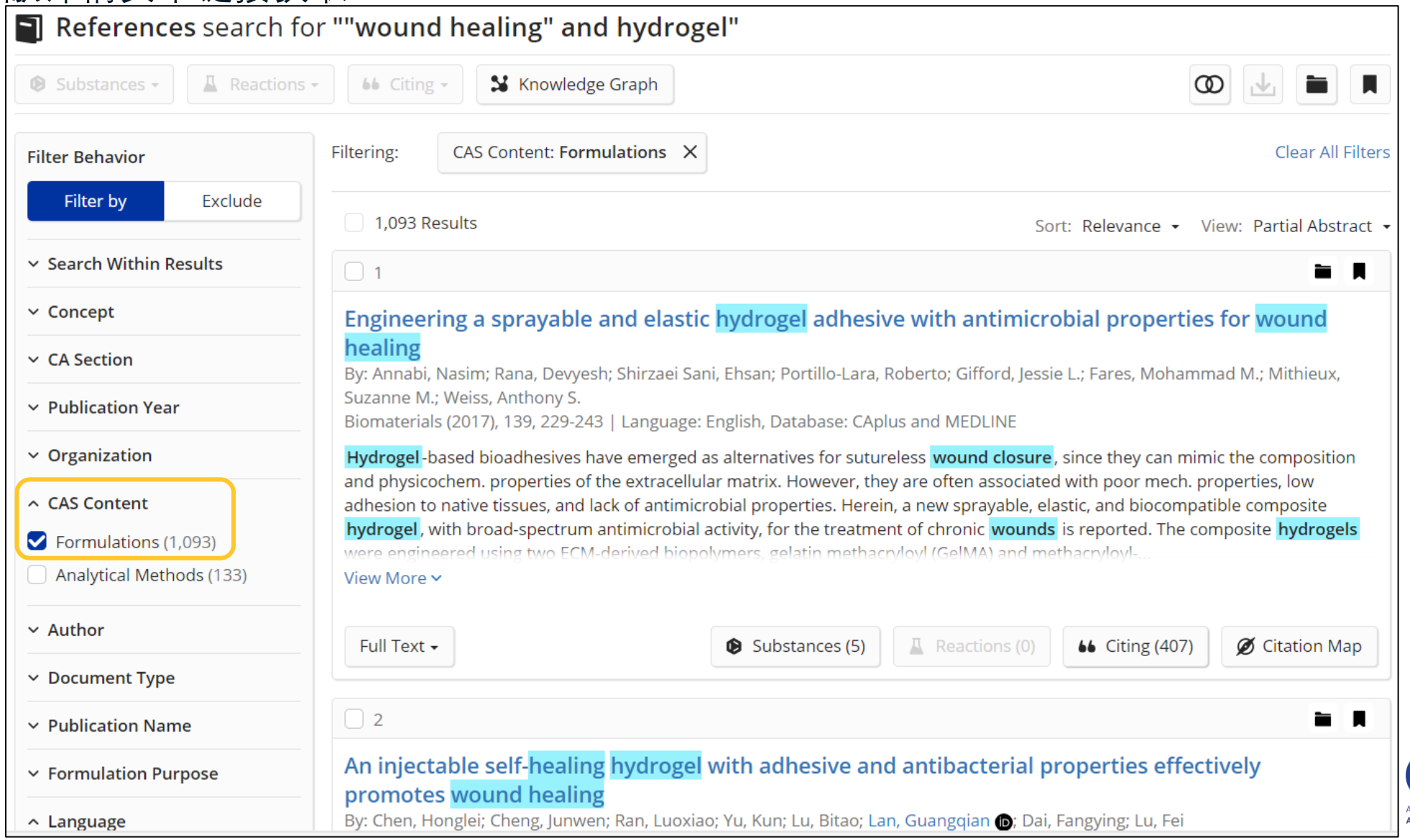

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文献关联的配方

Engineering a sprayable and elastic hydrogel adhesive with antimicrobial properties for wound healing

5 | 0 | 407 | Citation Map

In this Reference

- Concepts
- Substances
- Formulations
- Cited Documents

By: Annabi, Nasim; Rana, Devyesh; Shirzaei Sani, Ehsan; Portillo-Lara, Roberto; Gifford, Jessie L.; Fares, Mohammad M.; Mithieux, Suzanne M.; Weiss, Anthony S.

DOI: 10.1016/j.biomaterials.2017.05.011

Hydrogel-based bioadhesives have emerged as alternatives for sutureless wound closure, since they can mimic the composition and physicochem. properties of the extracellular matrix. However, they are often associated with poor mech. properties, low adhesion to native tissues, and lack of antimicrobial properties. Herein, a new sprayable, elastic, and biocompatible composite hydrogel, with broad-spectrum antimicrobial activity, for the treatment of chronic wounds is reported. The composite hydrogels were engineered using two ECM-derived biopolymers, gelatin methacryloyl (GelMA) and methacryloyl-substituted recombinant human tropoelastin (MeTro). MeTro/GelMA composite hydrogel adhesives were formed via visible light-induced crosslinking. Addnl., the antimicrobial peptide Tet213 was conjugated to the hydrogels, instilling antimicrobial activity against Gram (+) and (-) bacteria. The phys. properties (e.g. porosity, degradability, swellability, mech., and adhesive properties) of the engineered hydrogel could be fine-tuned by varying the ratio of MeTro/GelMA and the final polymer concentration The hydrogels supported in vitro mammalian cellular growth in both two-dimensional and three dimensional culture
vivo. The engineered MeTro/G
promote healing of chronic w

Keywords: hydrogel adhesive

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Formulations

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Formulation Title
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Antimicrobial Peptides Hydrogel: Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin-Zinc Oxide Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Composite Hydrogel: Antimicrobial or Wound Healing Promoters
Gelatin Methacryloyl and Methacryloyl-Substituted Recombinant Human Tropoelastin Antimicrobial Peptides Hydrogel: Wound Healing Promoters

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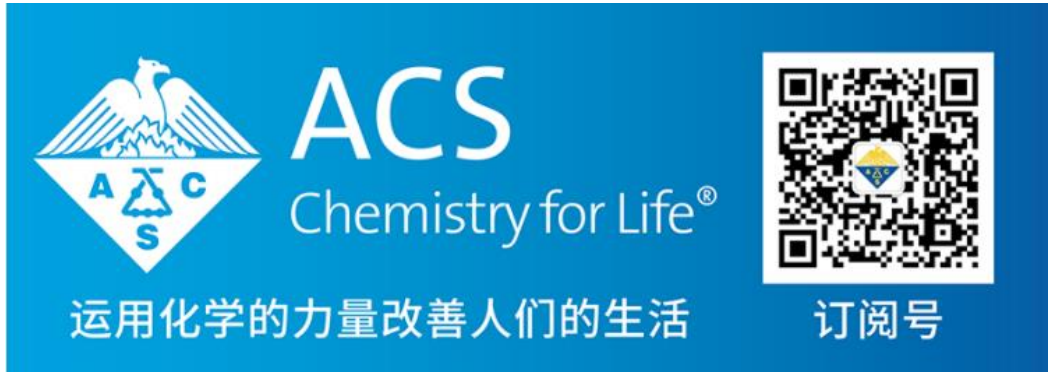

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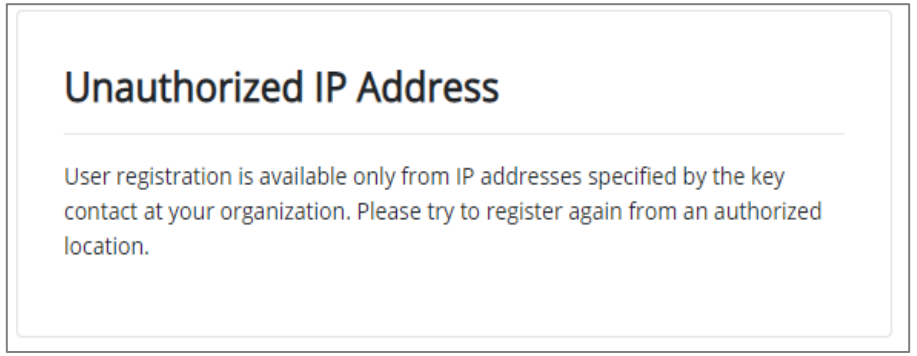

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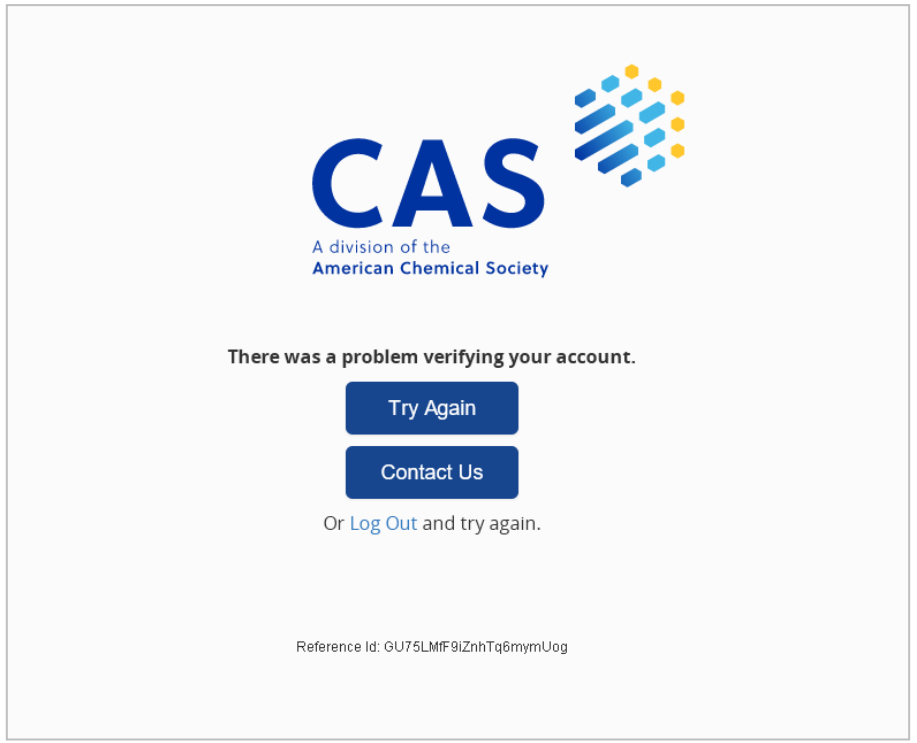

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