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china@acs-i.org
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大纲

- CAS及CAS SciFinder^{n}简介
- 常见检索方式
  - 文献检索
  - 物质检索 (CAS Markush*)
  - 反应检索
  - 逆合成反应路线设计 (CAS Retrosynthesis*)
  - 分析实验方法（CAS Analytical Methods）
  - 配方/制剂信息检索（CAS Formulus）
  - 生物序列检索*
- 常见问题及解答

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CAS 致力于提高创新效率

CAS的数据和服务是基于对以往知识经验的回顾，对当代前沿研究的洞察，以及对未来发展趋势的前瞻

HINDSIGHT

连接前人的发现，建设更美好的未来

INSIGHT

揭示能激发想法和加速发现的，未预见的联系

FORESIGHT

确定加速增长的趋势和新机遇

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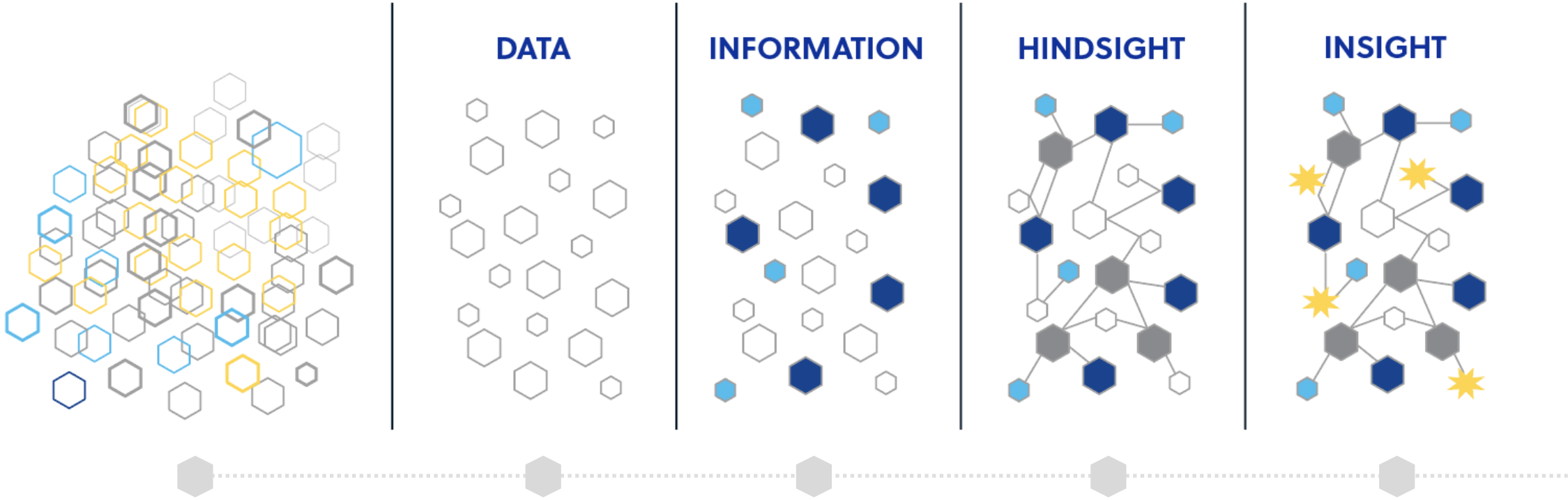
CAS科学家标引、关联和分析科学信息



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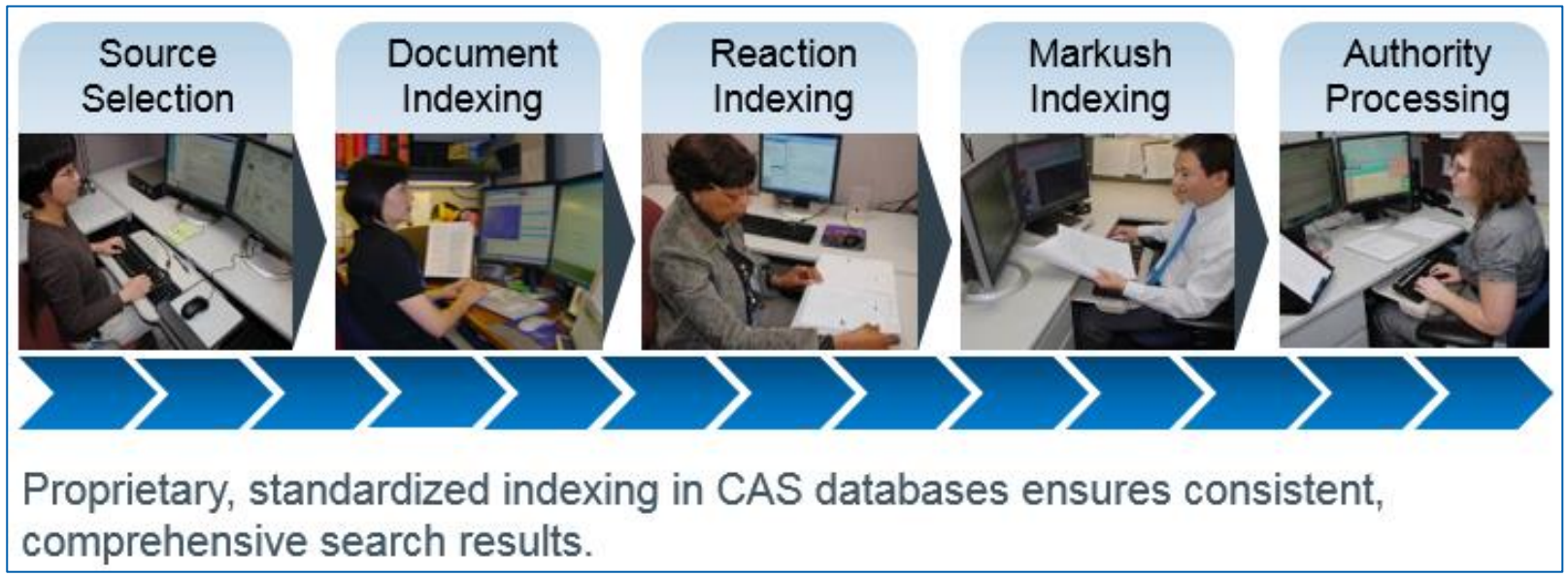
CAS科学家的智力标引



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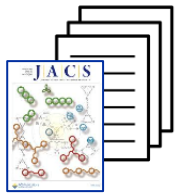
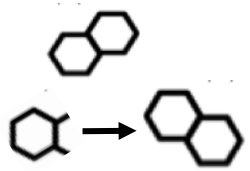
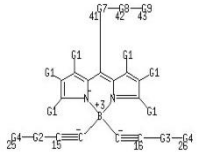


1990
Smith, M.
anthracene





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

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CAS解决方案与服务

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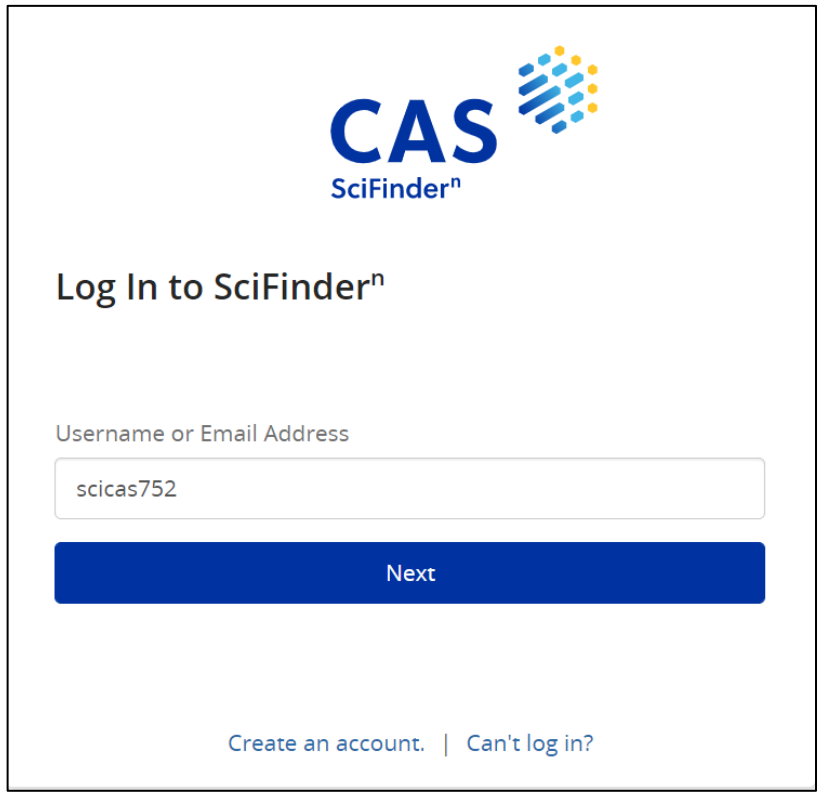

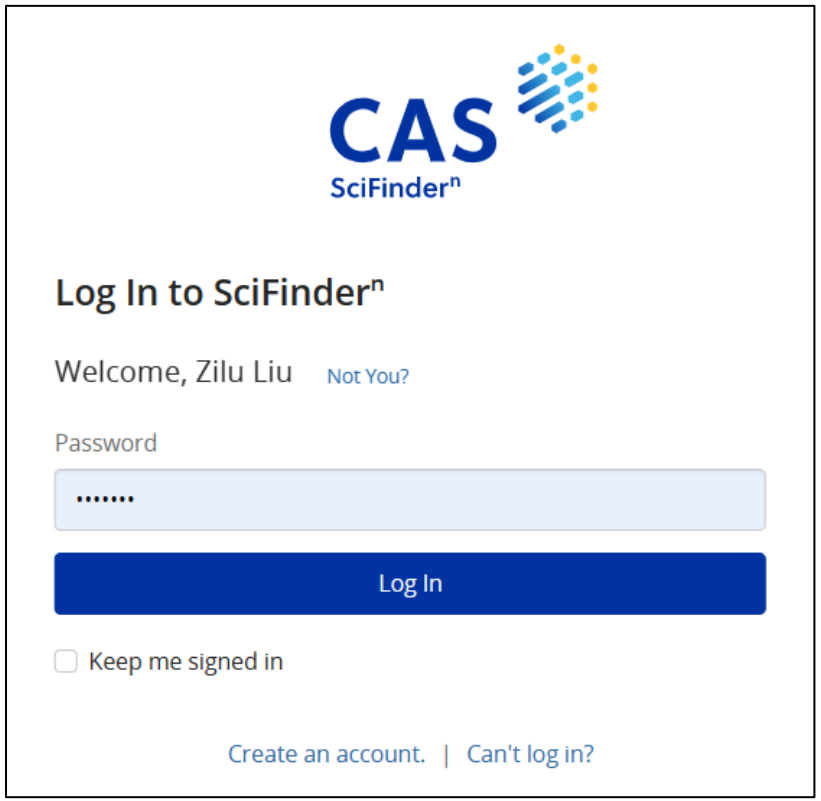

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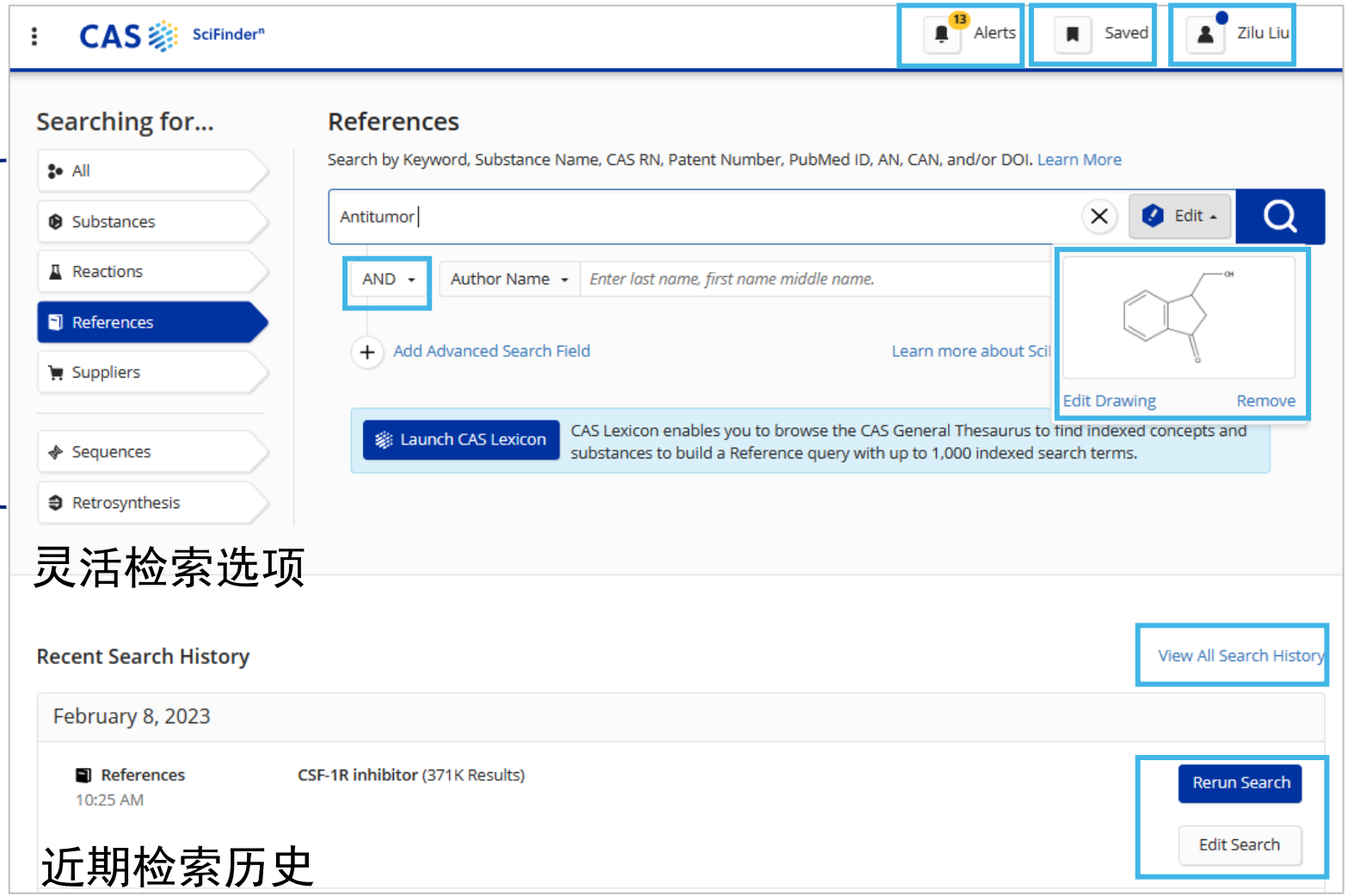
CAS SciFinder^{n}主界面



灵活检索选项

近期检索历史

提醒更新的结果
已保存的检索和结果集
账户信息

检索项逻辑关系
文本与结构检索便捷联用

查看全部检索历史

重新运行检索式
修改检索式

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- CAS及CAS SciFinder^{n}简介
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  - 反应检索
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  - 生物序列检索*
- 常见问题及解答

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文献检索

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

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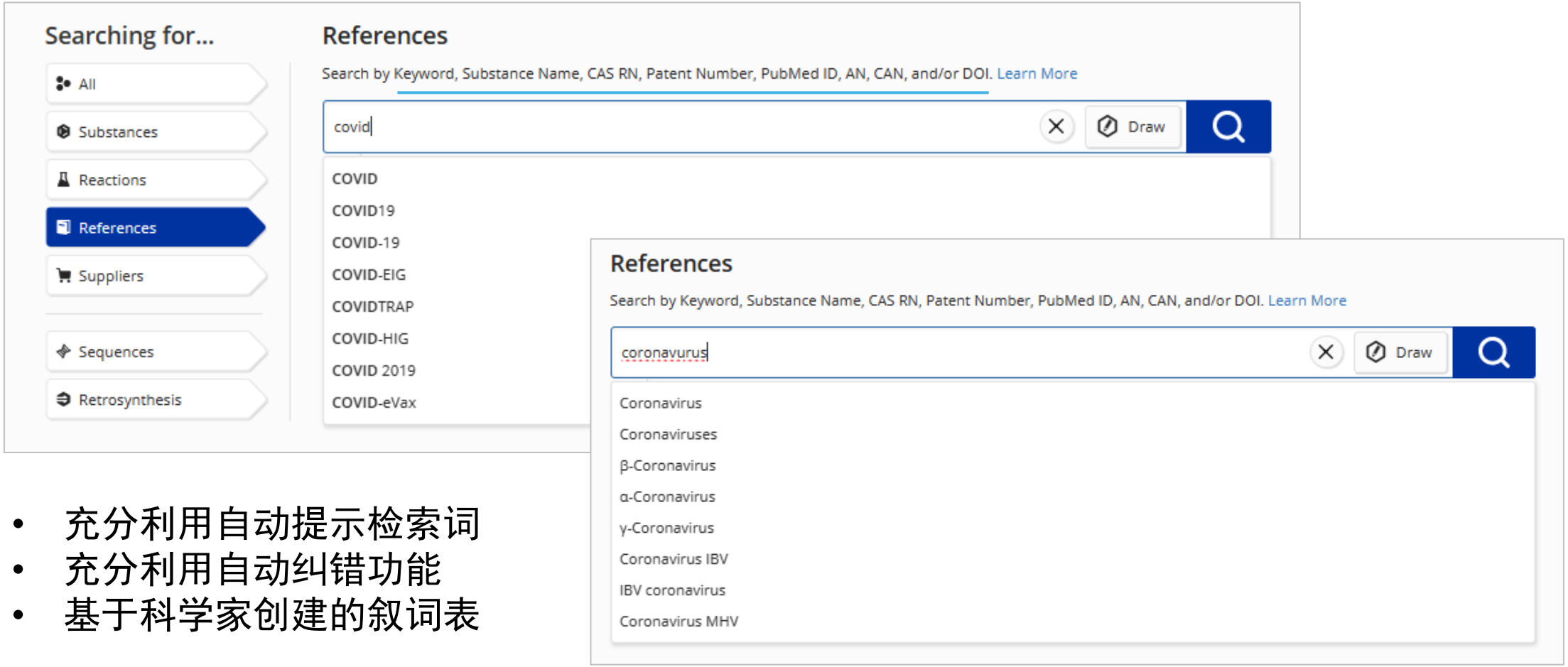
主题词检索

文本检索：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI



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

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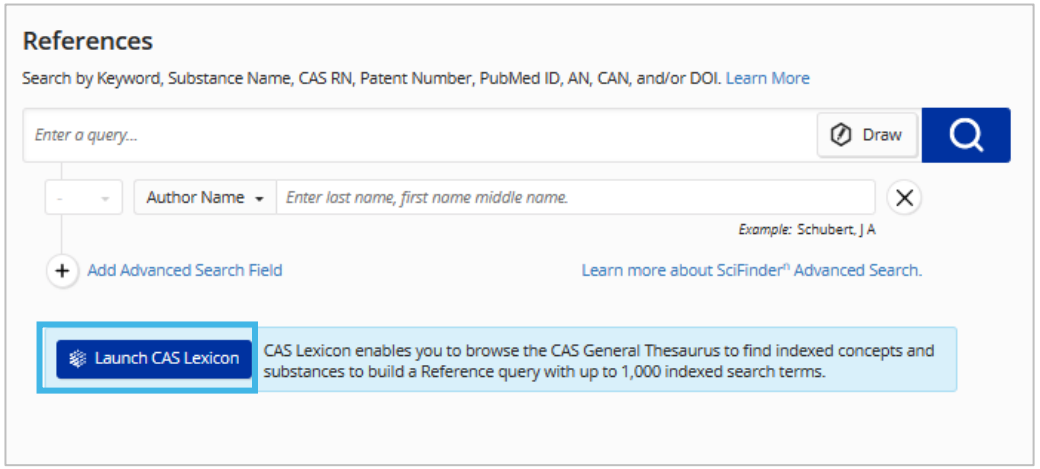
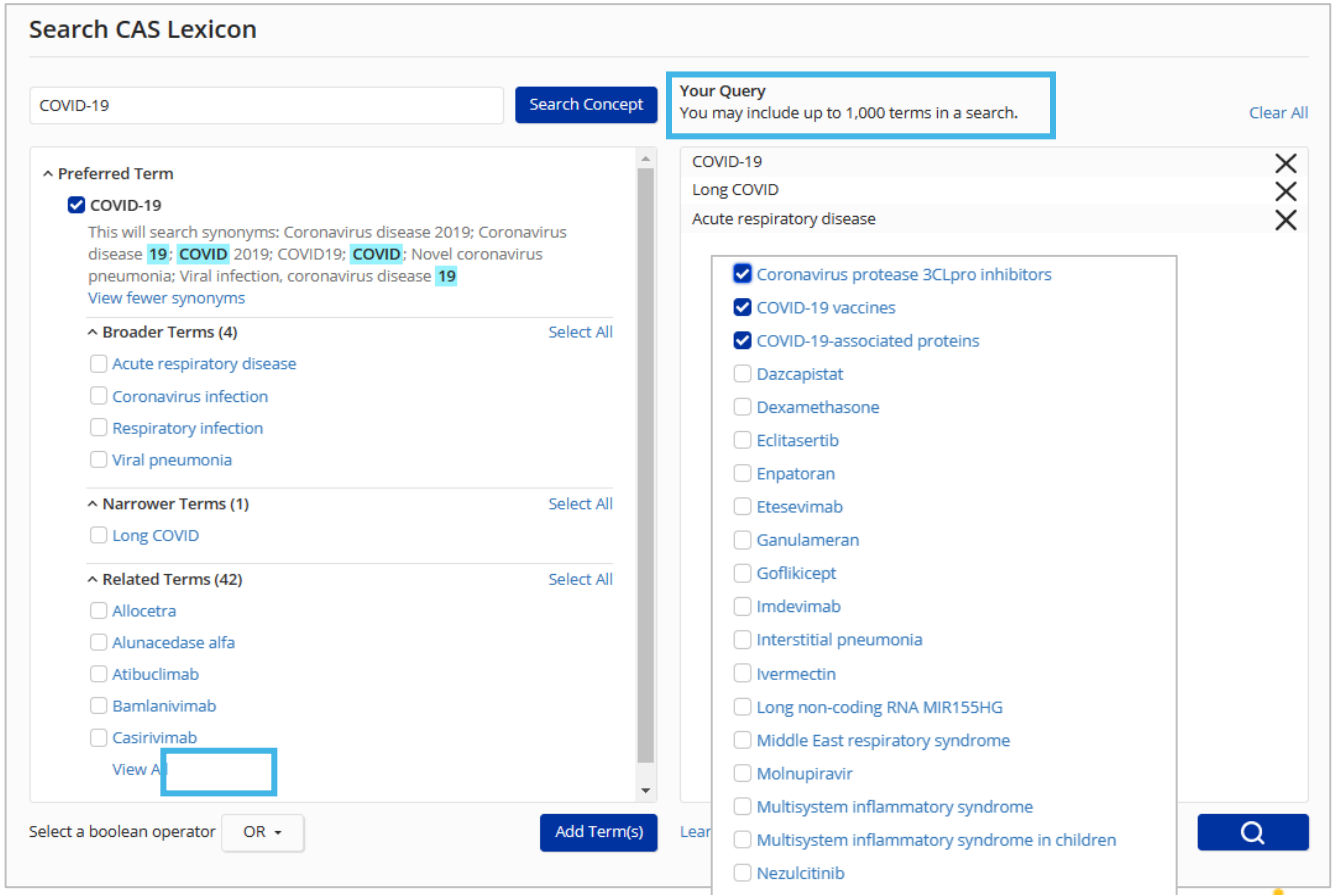
CAS Lexicon—利用词库选词启发检索

- 在CAS词库层级中浏览CAS标引的概念词（Concepts）和物质
- 建立用于检索文献的检索式（最多可用1000个词）





在CAS Lexicon词库层级中选择适合的主题词：

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

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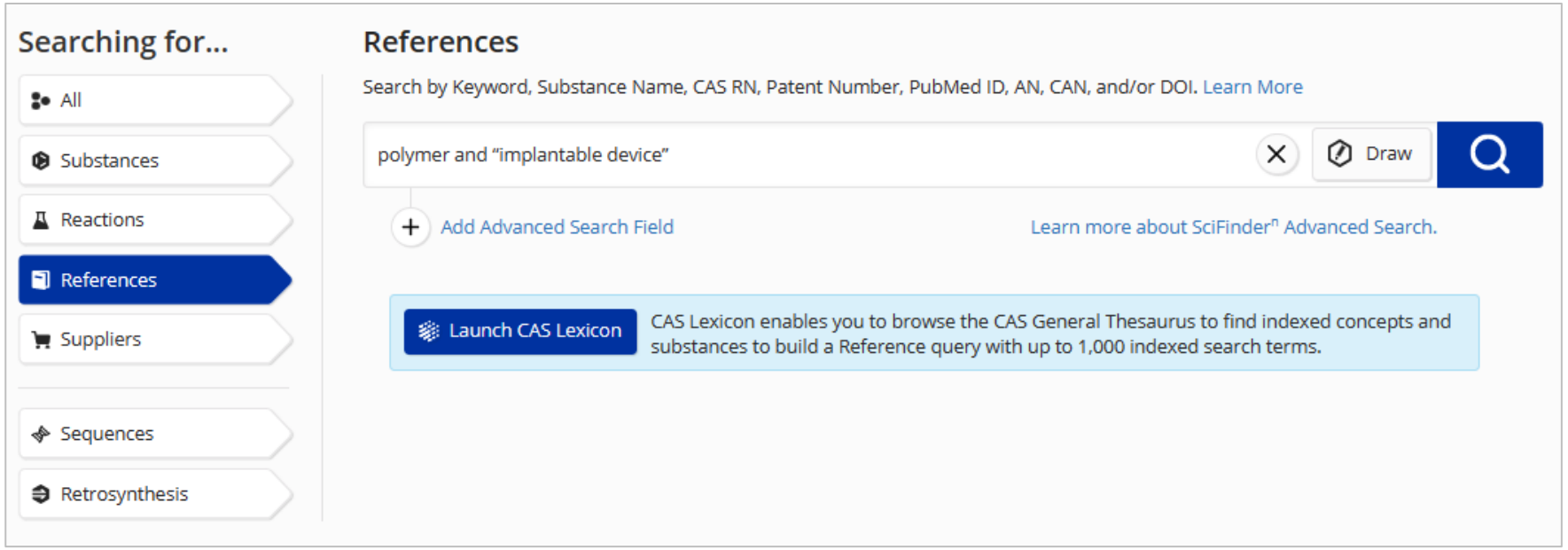
使用布尔逻辑运算符，精准构建检索主题

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



CAS SciFinder-n Help

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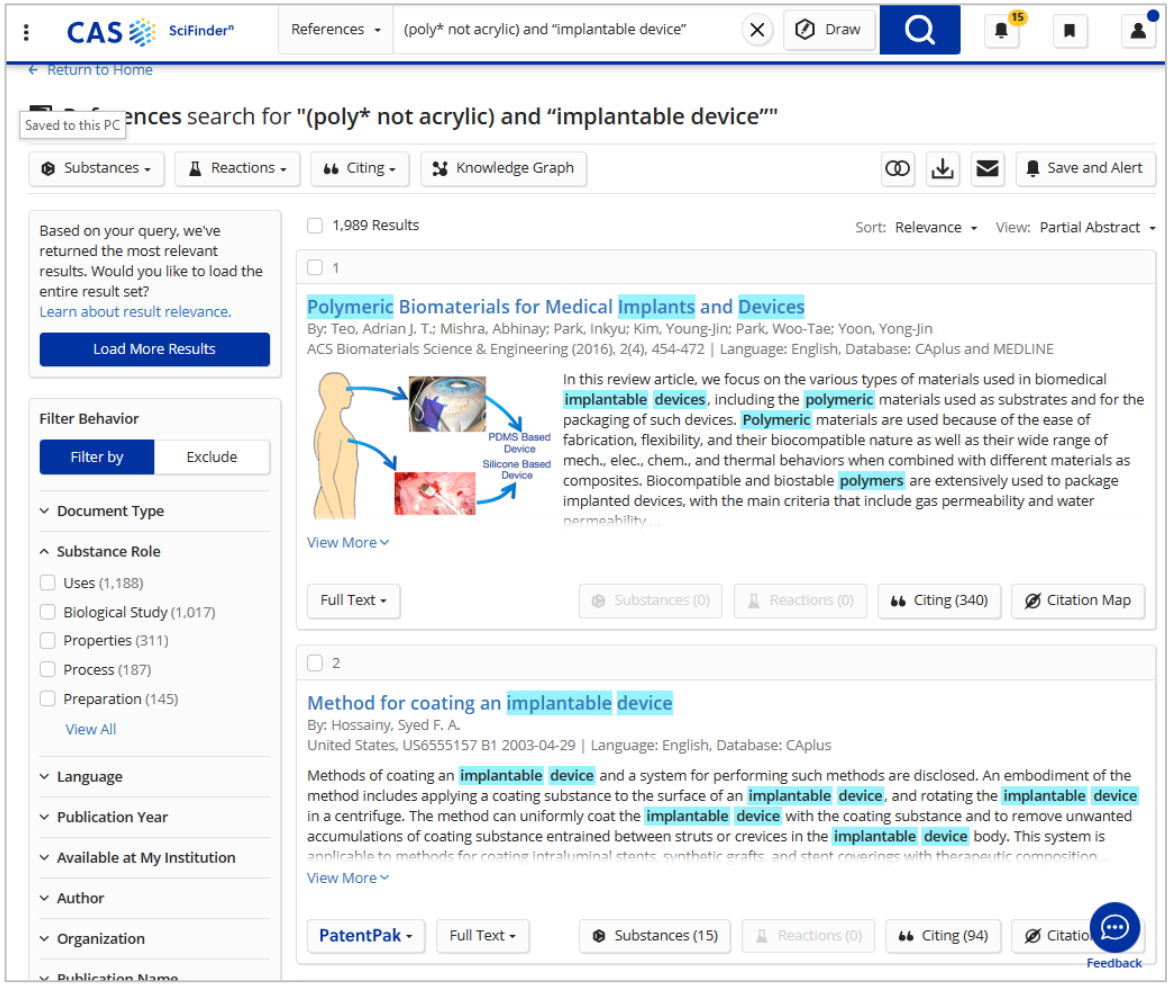
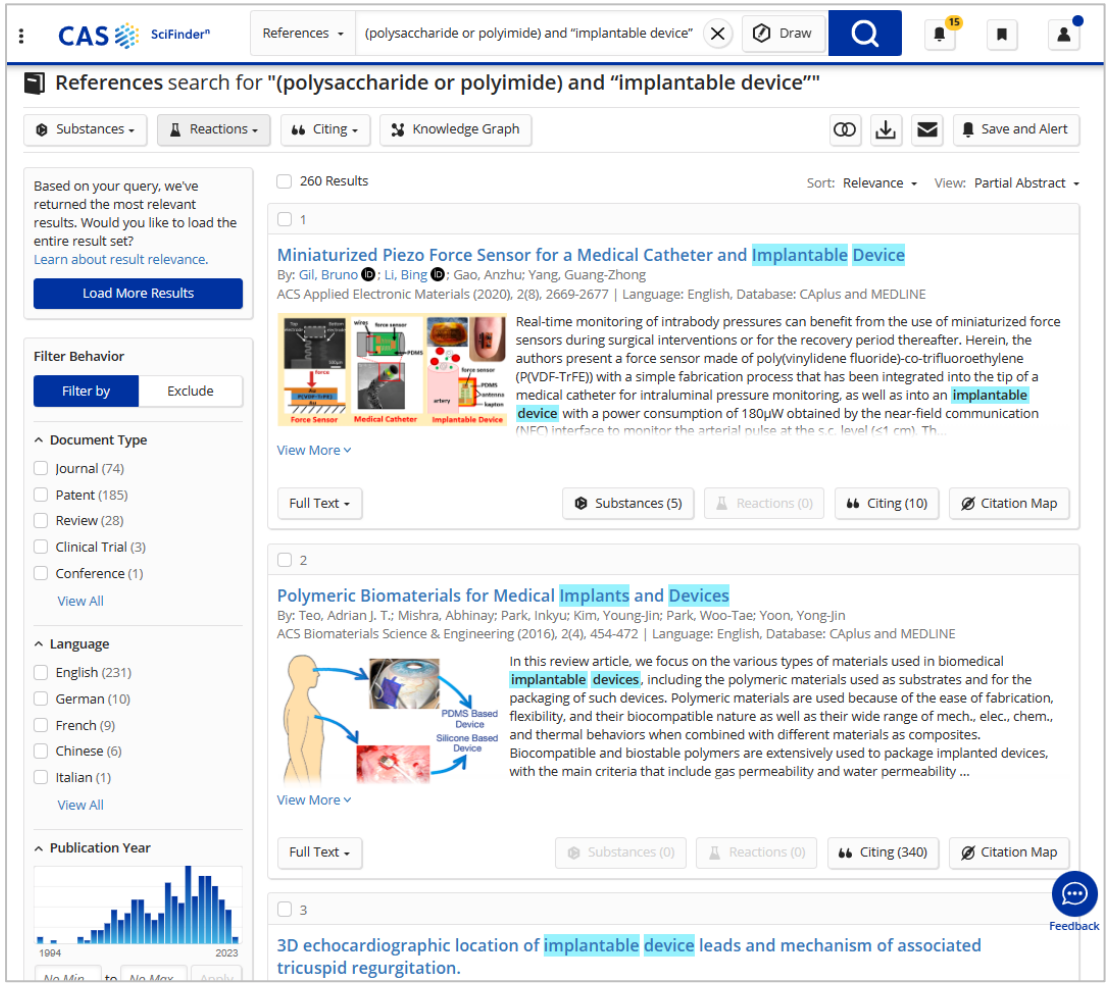
使用布尔逻辑运算符，精准构建检索主题

(poly* not acrylic) and “implantable device”
检索：非亚克力聚合物，作可植入器件



(polysaccharide or polyimide) and “implantable device”
检索：多聚糖或聚酰亚胺，作可植入器件



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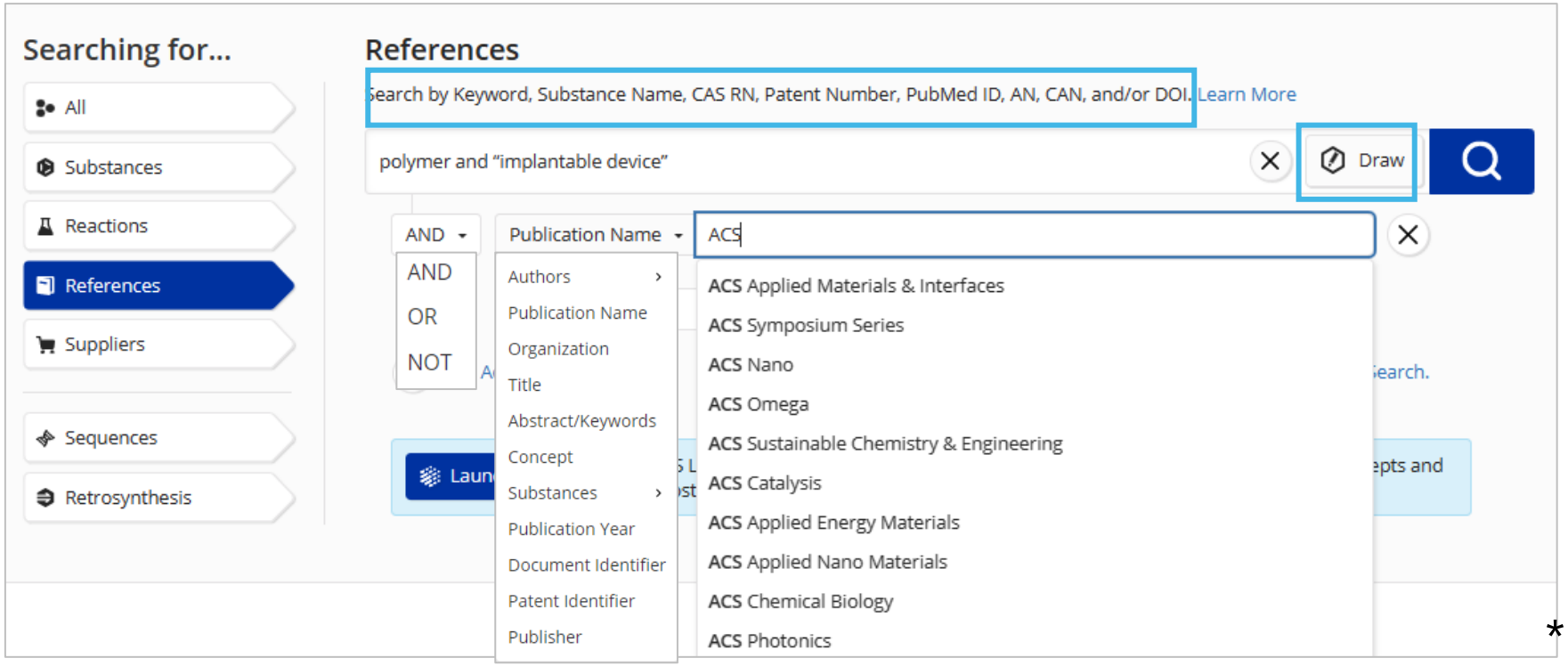
高级检索—高效实现多项自定义组合检索



文本检索：
关键词、物质名称、CAS RN、DOI等

高级检索：
作者名、期刊名、机构名、题目、摘要、概念词、物质标识符、出版商

结构检索

* 检索方法可单独使用，也可联用

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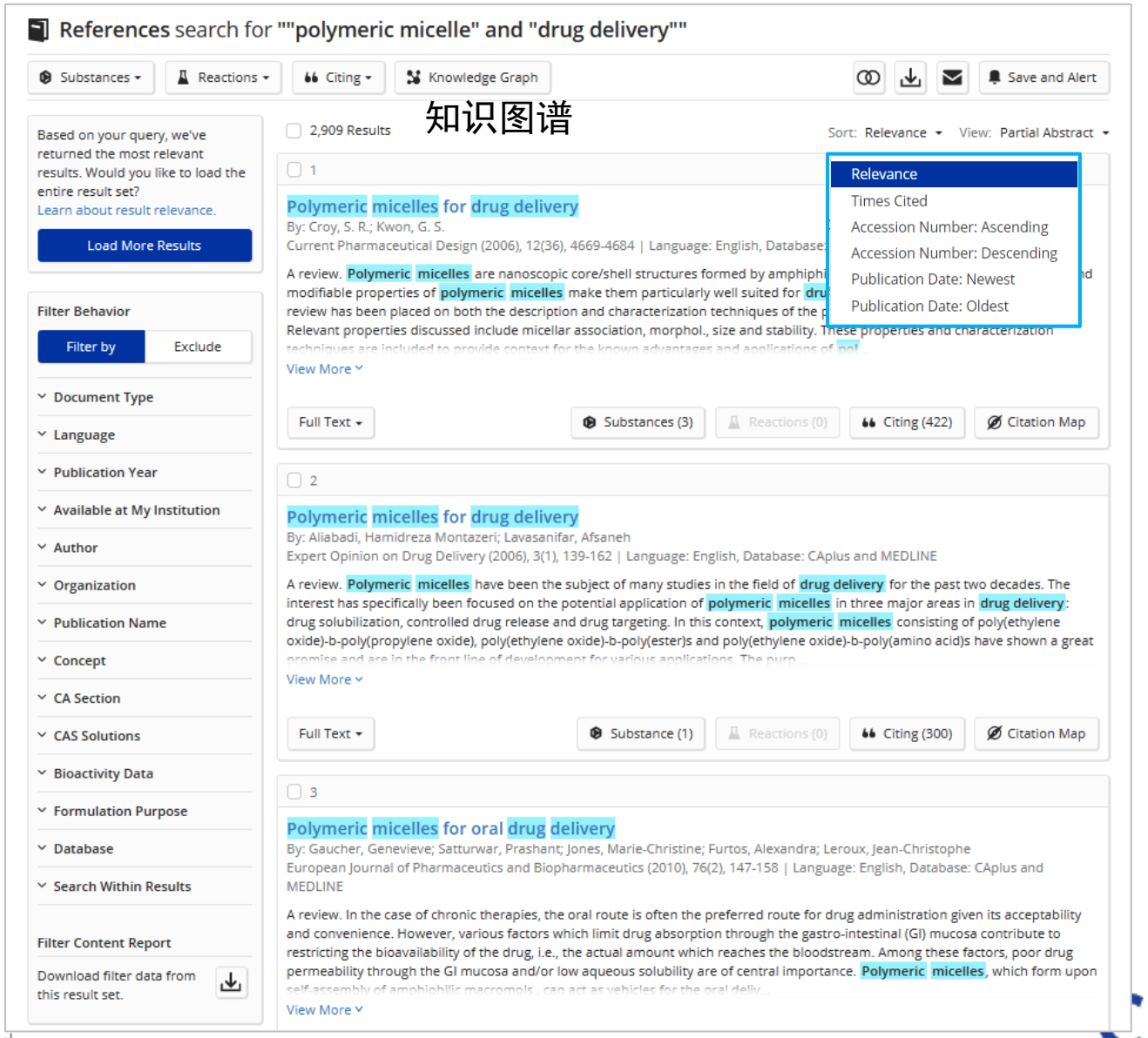
文献结果集—排序与筛选

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



排序方式：
相关性
引用次数
收录号
发表时间

文献类型
文献语言
研究发展趋势
作者
发表机构
发表年份

CAS标引的技术术语
CAS标引的学科研究方向

生物活性
制剂/配方目标

二次检索

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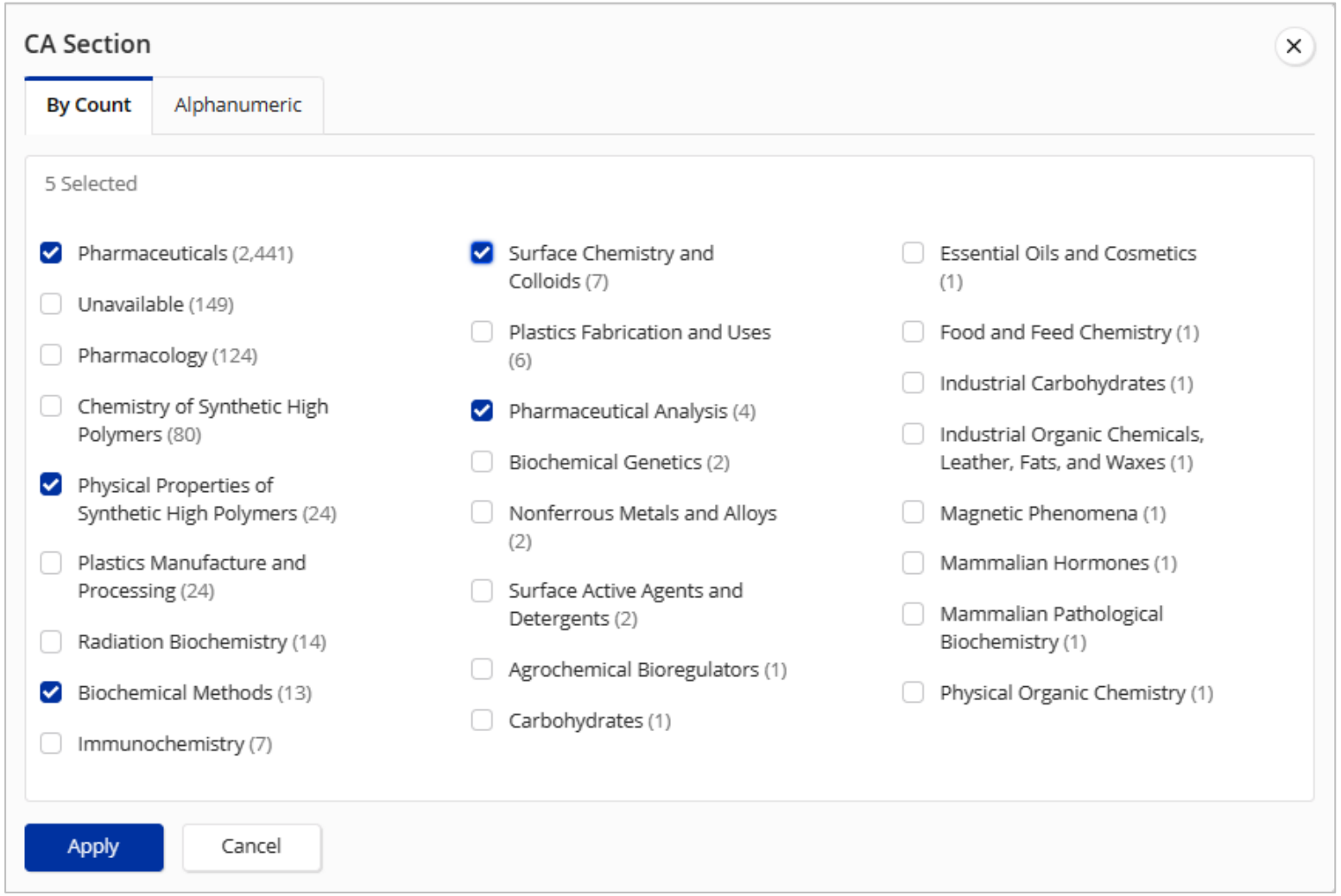
文献结果集—聚类筛选CA Section



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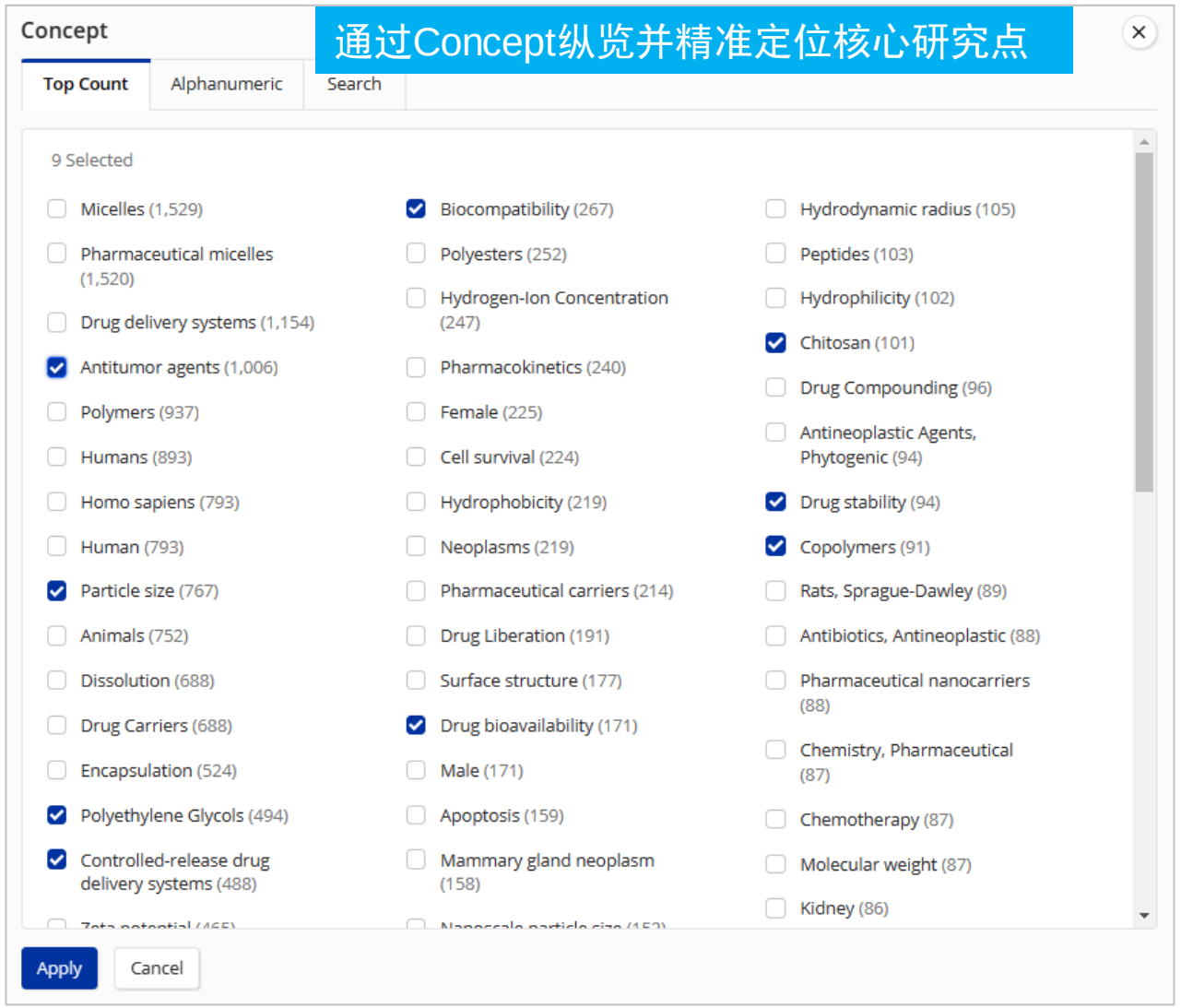
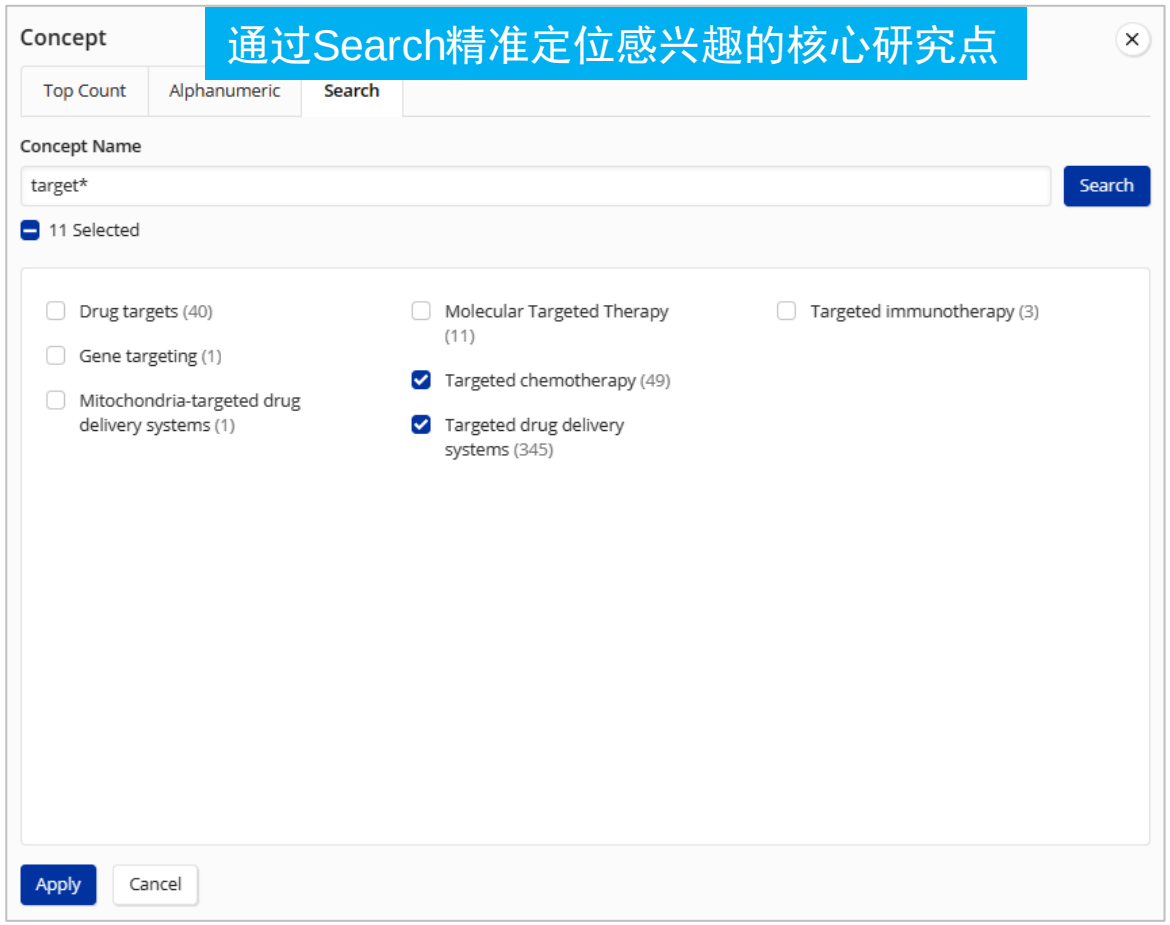
文献结果集—聚类筛选Concept





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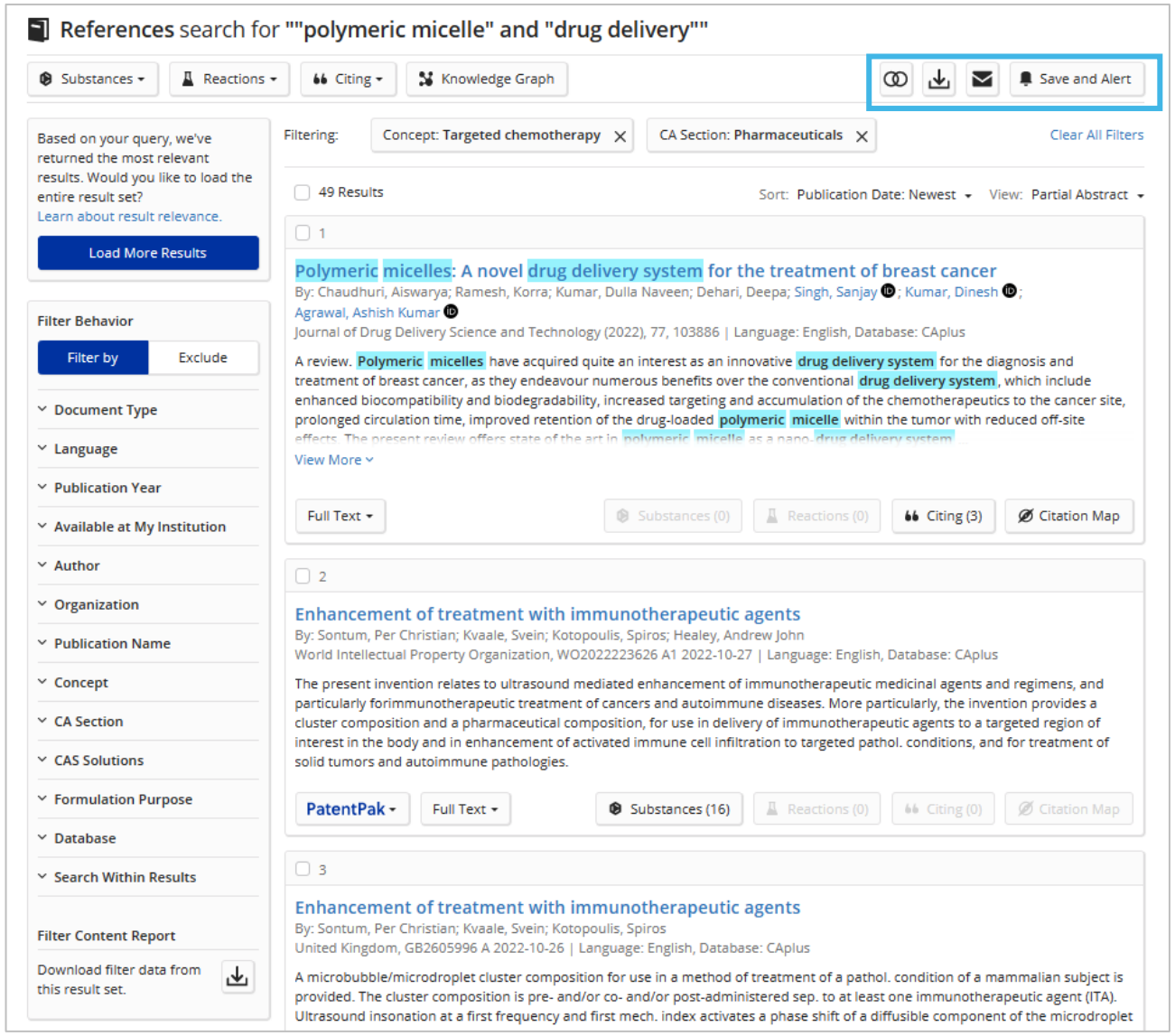

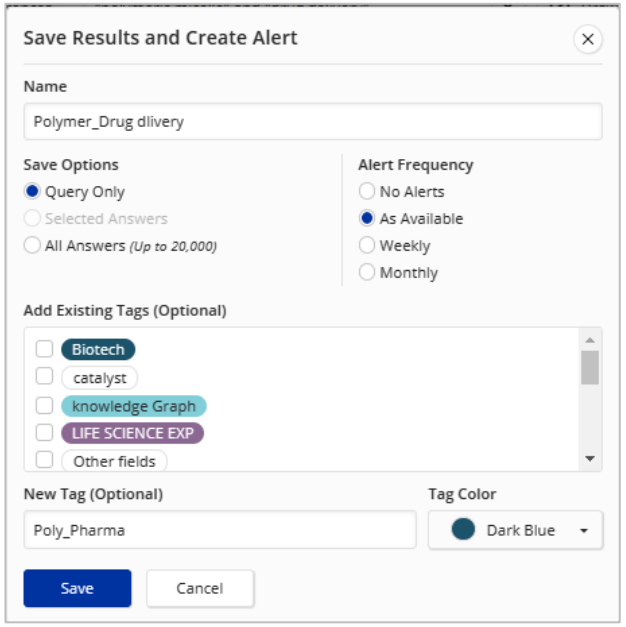

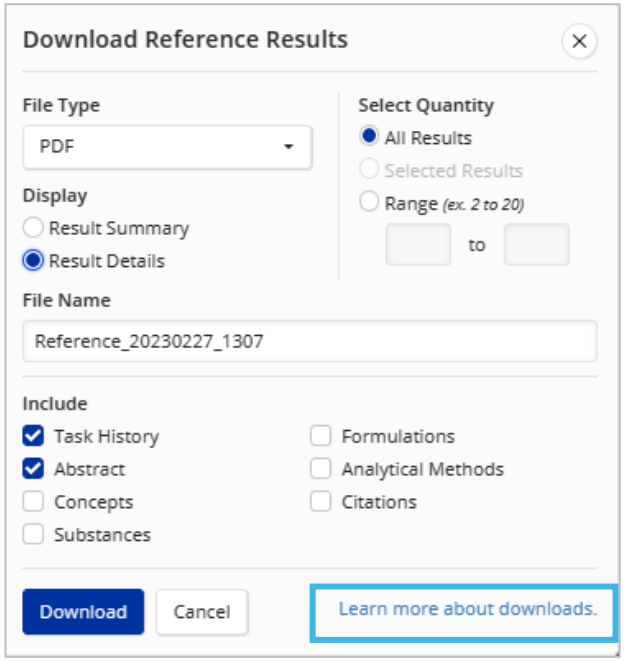

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文献详情

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

EGFR-Targeted Nanobody Functionalized Polymeric Micelles Loaded with mTHPC for Selective Photodynamic Therapy

Substances (16) | Reactions (11) | Citing (28) | Citation Map | Save

JOURNAL

Source
Molecular Pharmaceutics
Volume: 17
Issue: 4
Pages: 1276-1292
Journal; Article; Research Support, Non-U.S. Gov't
2020
DOI:
10.1021/acs.molpharmaceut.9b01280

CODEN: MPOHBP
E-ISSN: 1543-8392
ISSN-L: 1543-8384

Database Information
AN: 2020:437343
CAN: 176:347527
PubMed ID: 32142290
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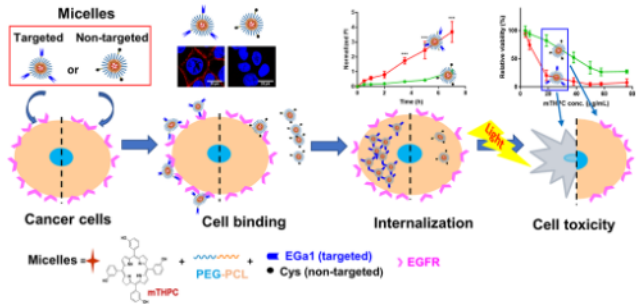
Department of Pharmaceutics, Utrecht Institute for Pharmaceutical Sciences
Utrecht University
Utrecht 3584 CS
Netherlands

Publisher
American Chemical Society

Language
English

By: Liu, Yanna; Scrivano, Luca; Peterson, Julia Denise; Fens, Marcel H. A. M.; Hernandez, Irati Beltran; Mesquita, Barbara; Torano, Javier Sastre; Hennink, Wim E.; van Nostrum, Cornelus F.; Oliveira, Sabrina

Meta-Tetra(hydroxyphenyl)chlorin (mTHPC) is one of the most potent second-generation photosensitizers, clin. used for photodynamic therapy (PDT) of head and neck squamous cell carcinomas. However, improvements are still required concerning its present formulation (i.e., Foscan, a solution of mTHPC in ethanol/propylene glycol (40:60 weight/weight)), as mTHPC has the tendency to aggregate in aqueous media, e.g., biol. fluids, and it has limited tumor specificity. In the present study, polymeric micelles with three different diameters (17, 24, and 45 nm) based on benzyl-poly(ε-caprolactone)-b-poly(ethylene glycol) (PCL_n-PEG; n = 9, 15, or 23) were prepared with mTHPC loadings ranging from 0.5 to 10 weight % using a film-hydration method as advanced nanoformulations for this photosensitizer. To favor the uptake of the micelles by cancer cells that overexpress the epidermal growth factor receptor (EGFR), the micelles were decorated with an EGFR-targeted nanobody (named EGa1) through maleimide-thiol chem. The enhanced binding of the EGFR-targeted micelles at 4°C to EGFR-overexpressing A431 cells, compared to low-EGFR-expressing HeLa cells, confirmed the specificity of the micelles. In addition, an enhanced uptake of mTHPC-loaded micelles by A431 cells was observed when these were decorated with the EGa1 nanobody, compared to nontargeted micelles. Both binding and uptake of targeted micelles were blocked by an excess of free EGa1 nanobody, demonstrating that these processes occur through EGFR. In line with this, mTHPC loaded in EGa1-conjugated PCL_{23}-PEG (EGa1-P_{23}) micelles demonstrated 4 times higher photocytotoxicity on A431 cells, compared to micelles lacking the nanobody. Importantly, EGa1-P_{23} micelles also showed selective PDT against A431 cells compared to the low-EGFR-expressing HeLa cells. Finally, an in vivo pharmacokinetic study shows that after i.v. injection, mTHPC incorporated in the P_{23} micelles displayed prolonged blood circulation kinetics, compared to free mTHPC, independently of the presence of EGa1. Thus, these results make these micelles a promising nanomedicine formulation for selective therapy.



Keywords: EGFR targeted nanobody polymer micelle mTHPC photodynamic therapy; EGFR; nanobody; photodynamic therapy; polymeric micelles; selectivity; targeting

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技术术语

Medline医学主题词表

重要物质

参考文献

CAS科学家提供的标准技术术语

Concepts

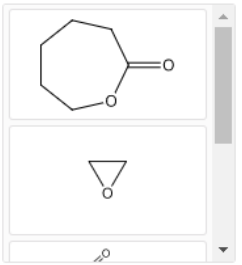
Antitumor agents	Photodynamic therapy
Biological transport, internalization	Polyesters, polyoxyalkylene-, block Modifier: diblock, nanobody conjugates
Epidermal growth factor receptors Role: Biological Study, Unclassified	Role: Physical, Engineering or Chemical Process; Properties; Synthetic Preparation; Therapeutic Use
Head and neck squamous cell carcinoma	Polyoxyalkylenes, polyester-, block Modifier: diblock, nanobody conjugates
Homo sapiens	Role: Physical, Engineering or Chemical Process; Properties; Synthetic Preparation; Therapeutic Use
Human	Single-domain antibodies Modifier: Nanobody, Ega1
Pharmaceutical micelles	Role: Properties; Therapeutic Use
Pharmaceutical photosensitizers	Targeted chemotherapy

原文中重点研究的物质信息

Substances

Substances (16)

2715003-31-7

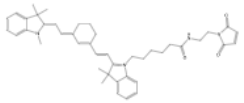


$C_7H_8O.(C_6H_{10}O_2.C_2H_4O)_x.C_6H_7NO_3$

Role: Physical, Engineering or Chemical Process, Properties, Reactant, Synthetic Preparation, Therapeutic Use, Process, Reactant or Reagent, Preparation, Biological Study, Uses

Notes: micelles; Ega1 nanobody conjugates

2120392-49-4

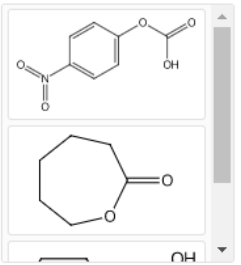


$C_{43}H_{51}N_4O_3$
1-[6-[[2-(2,5-Dihydro-2,5-dioxo-1*H*-pyrrol-1-yl)ethyl]amino]-6-oxohexyl]-2-[2-[3-...

Role: Reactant, Reactant or Reagent

Notes: reaction products with PCL-DTC-PEG

1827666-85-2

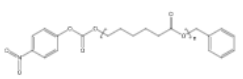


$C_7H_8O.C_7H_5NO_5.(C_6H_{10}O_2)_x$
2-Oxepanone, homopolymer, phenylmethyl ester, 4-nitrophenyl carbonate

Role: Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

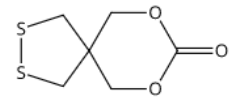
物质角色

1825357-84-3



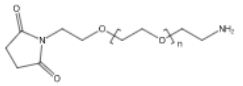
$(C_6H_{10}O_2)_nC_{14}H_{11}NO_5$

1627110-33-1



$C_6H_8O_3S_2$

1620962-19-7



$(C_2H_4O)_nC_8H_{14}N_2O_3$

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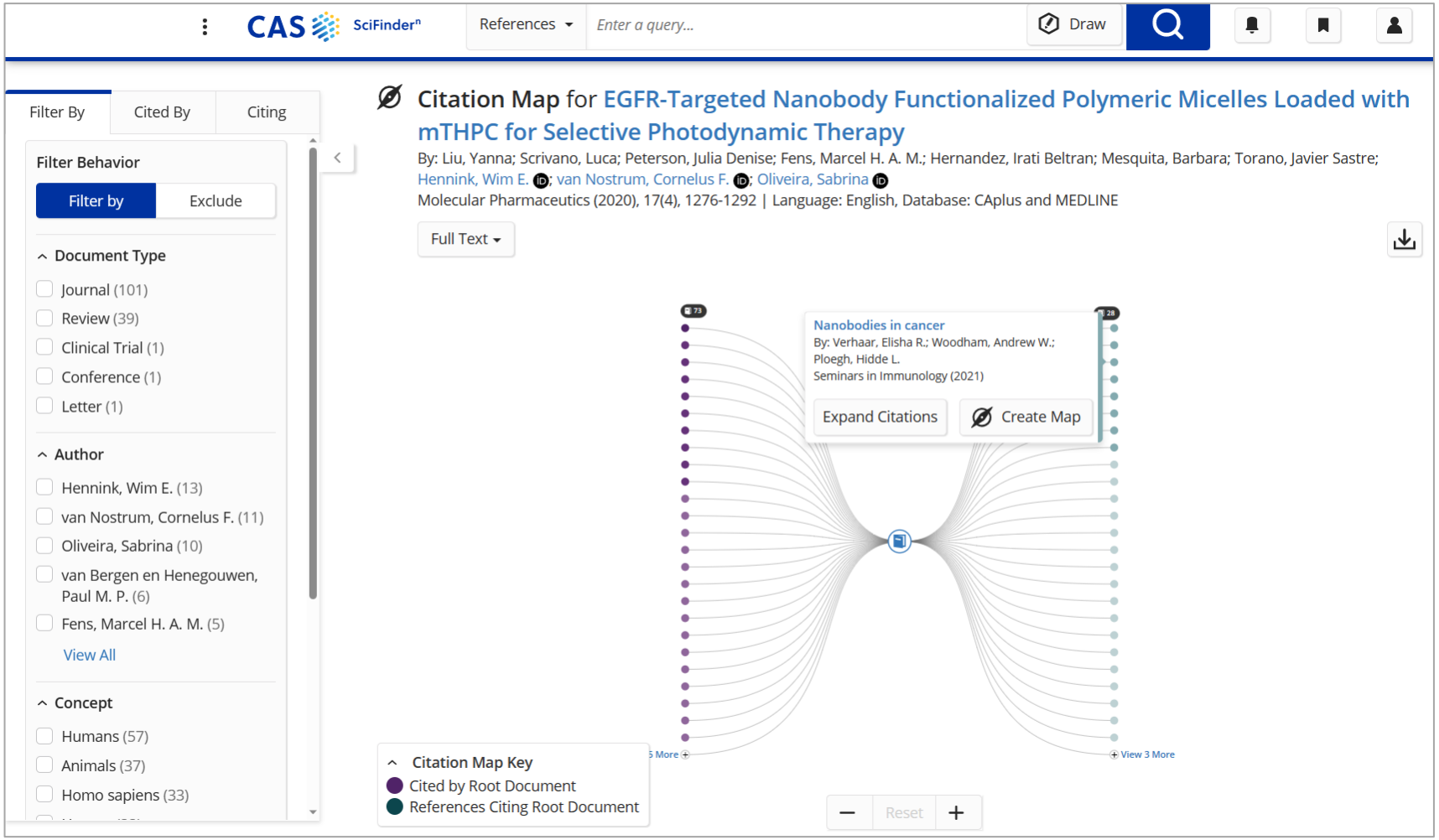
文献详情—引文地图



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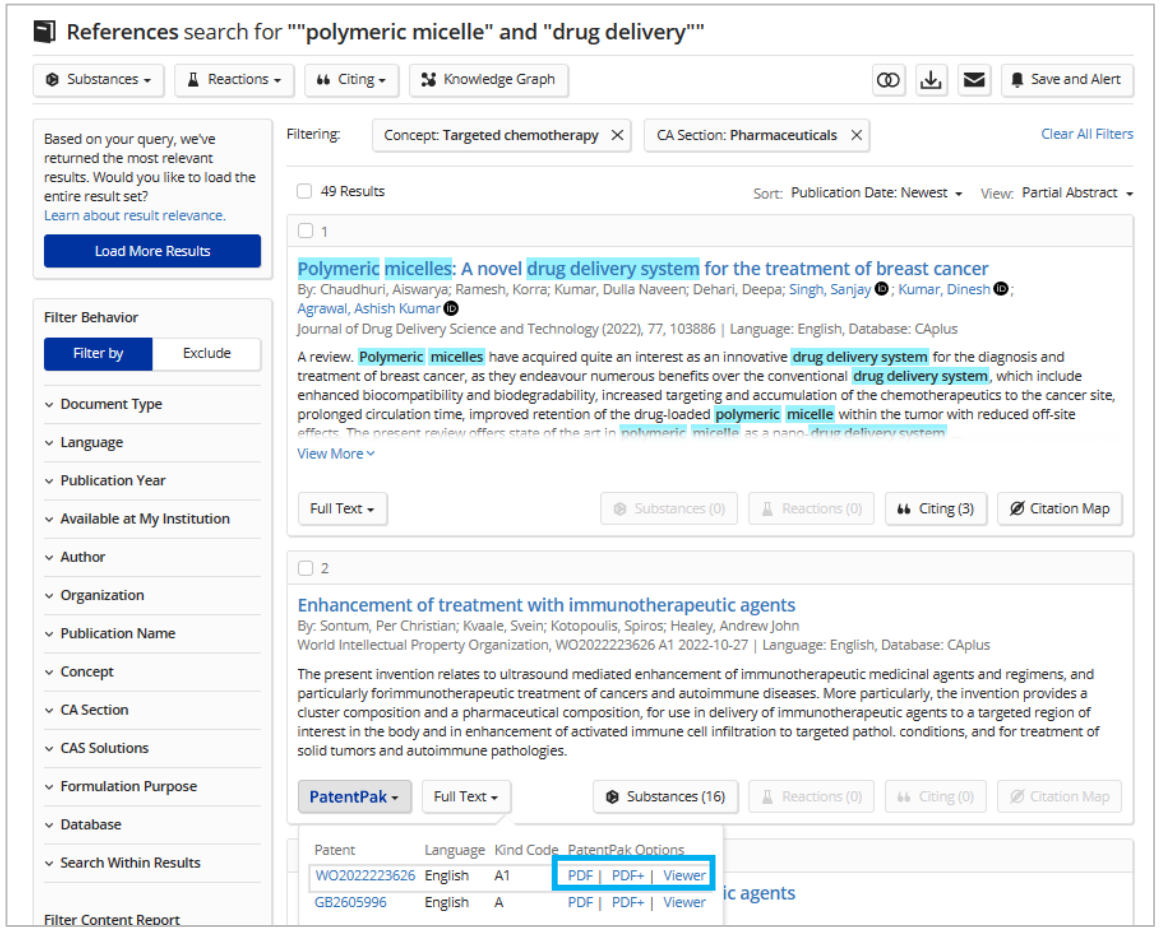

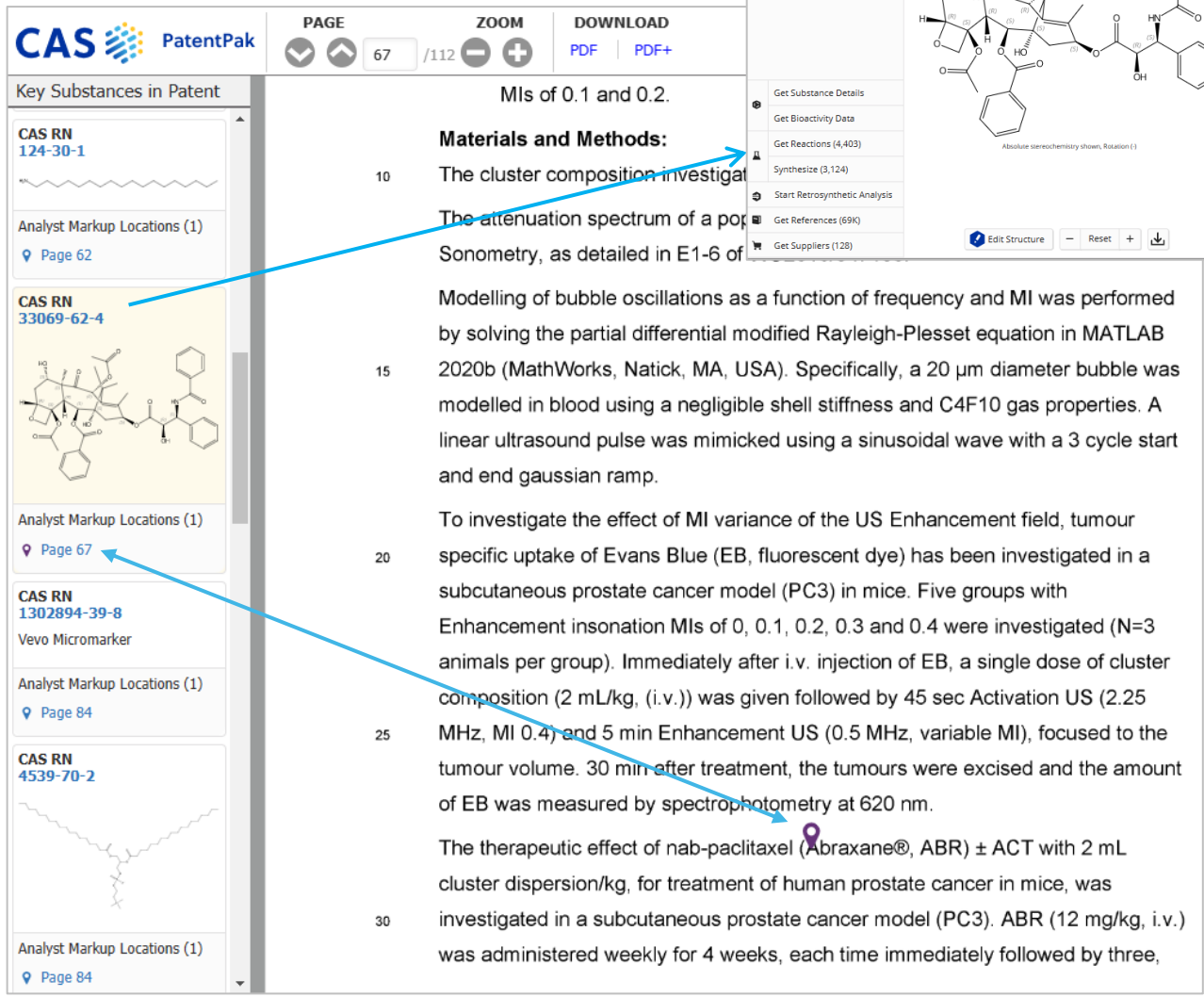

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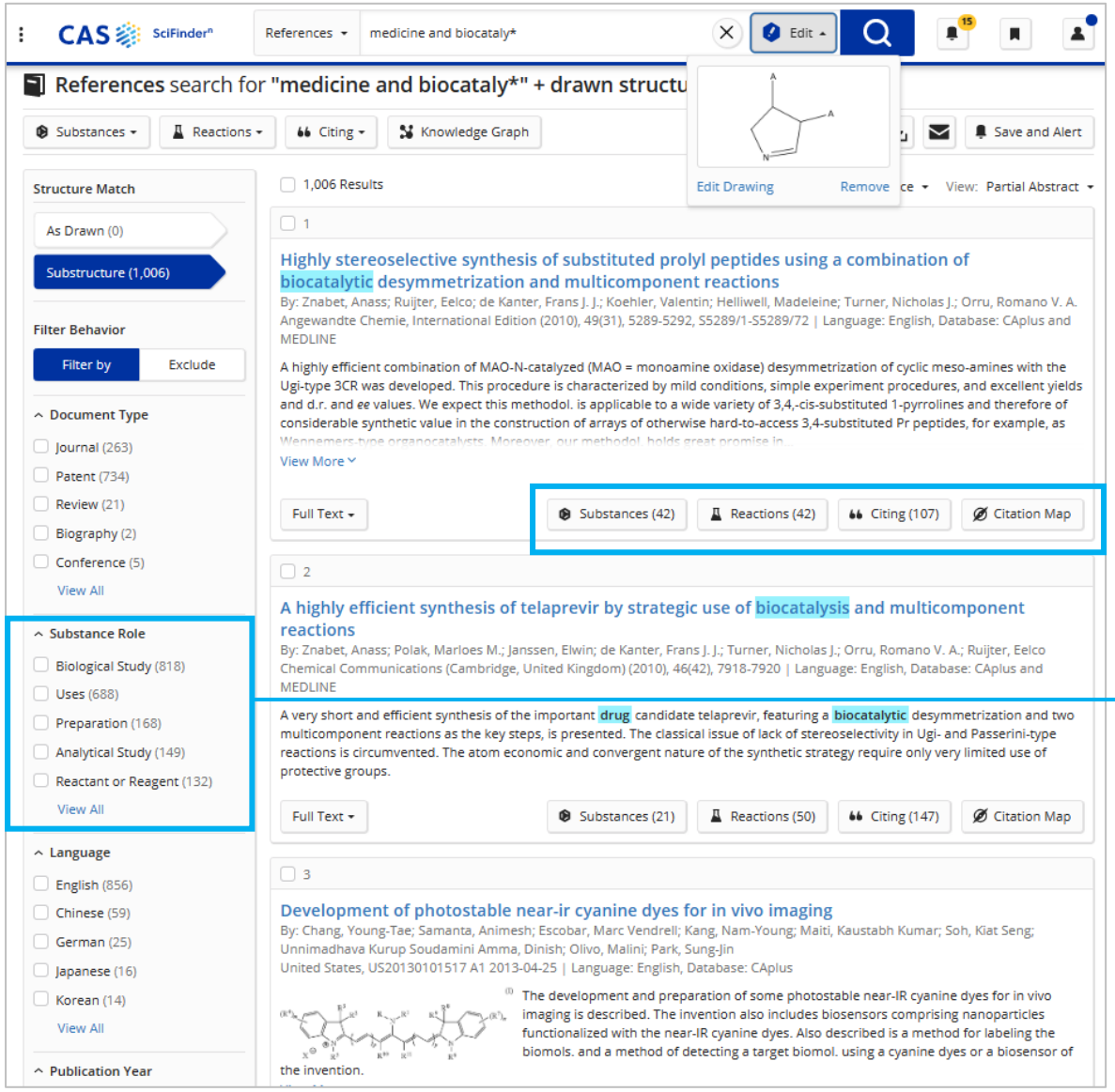
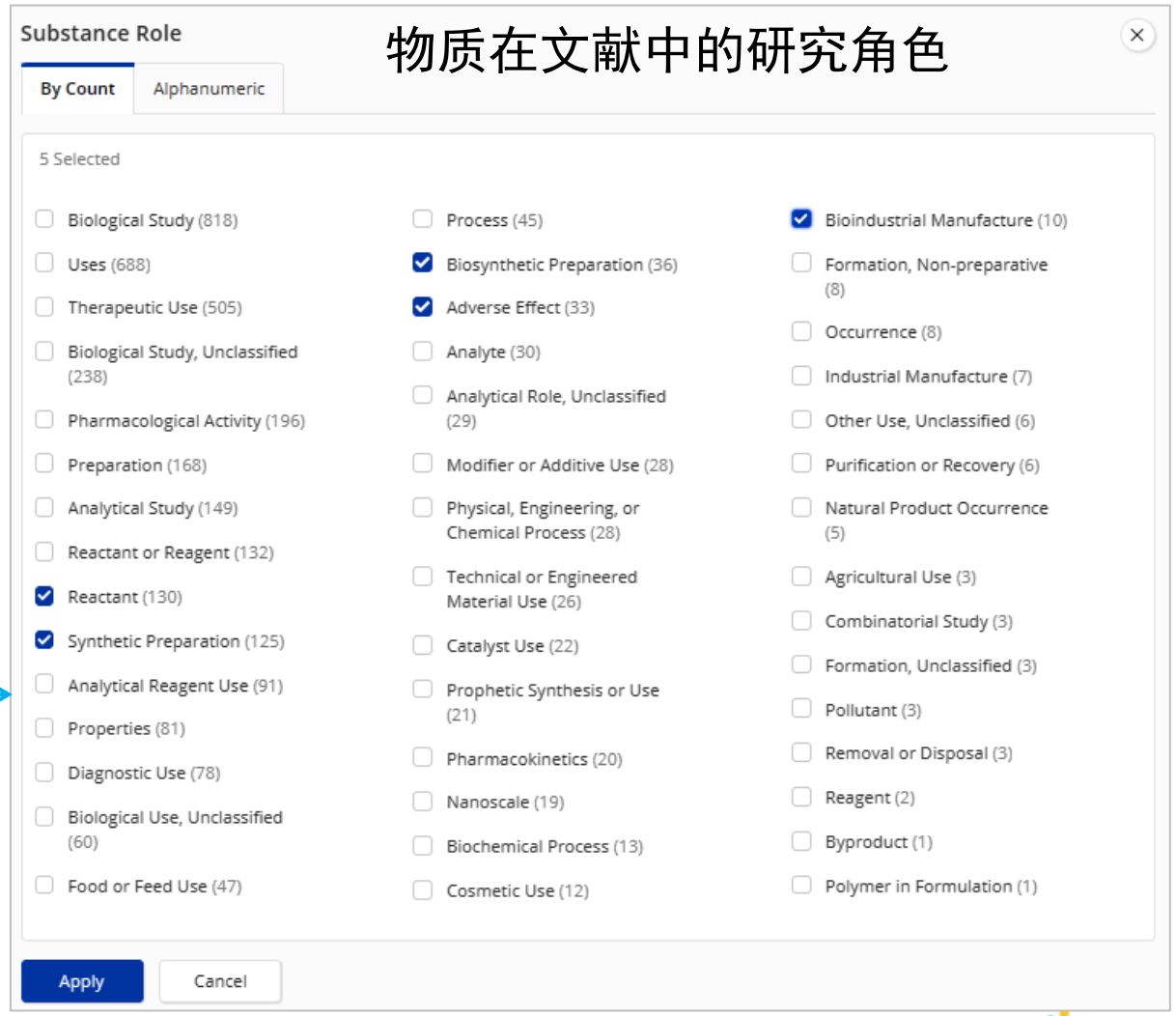
文献检索—主题词+结构联合检索





物质在文献中的研究角色

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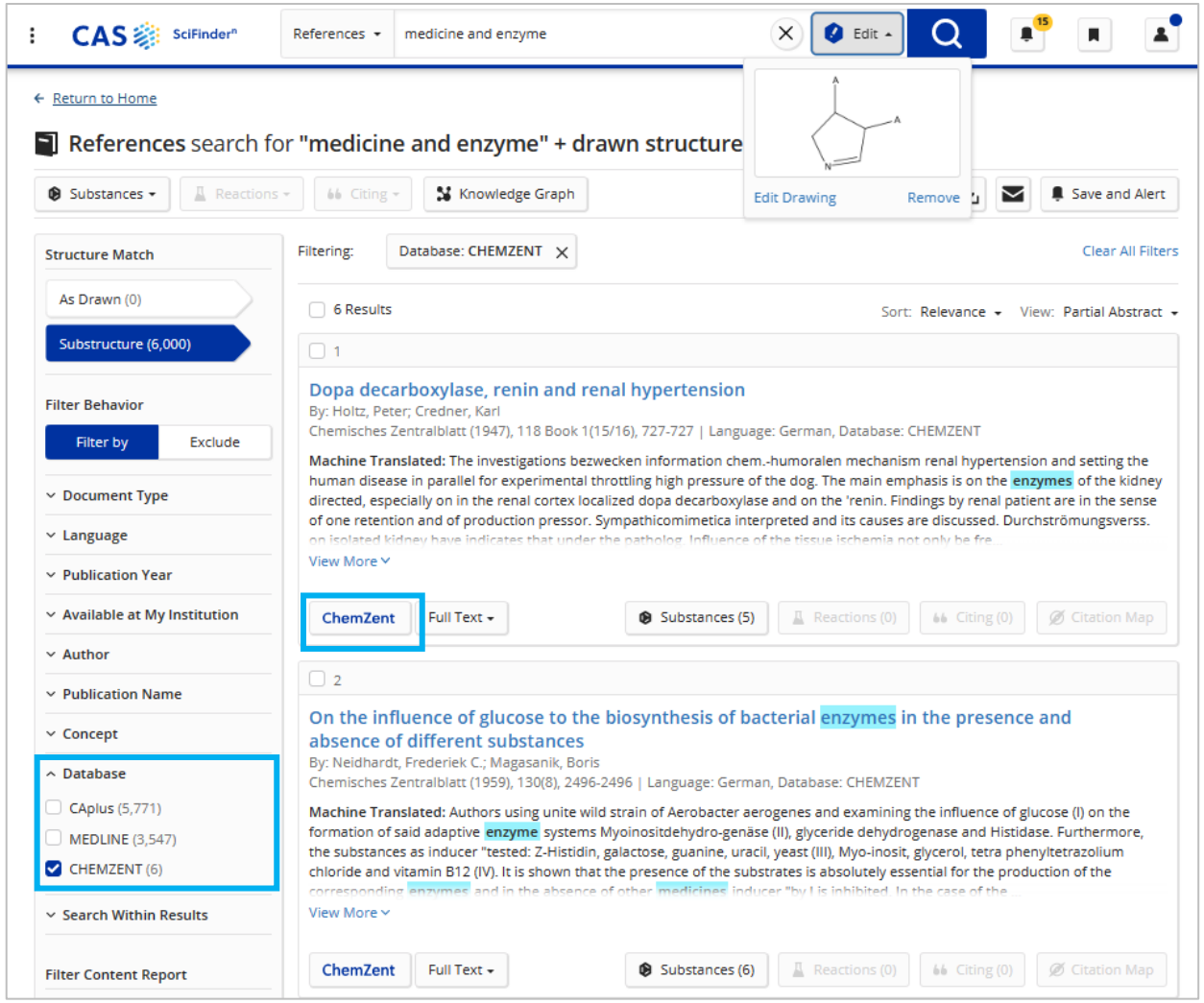
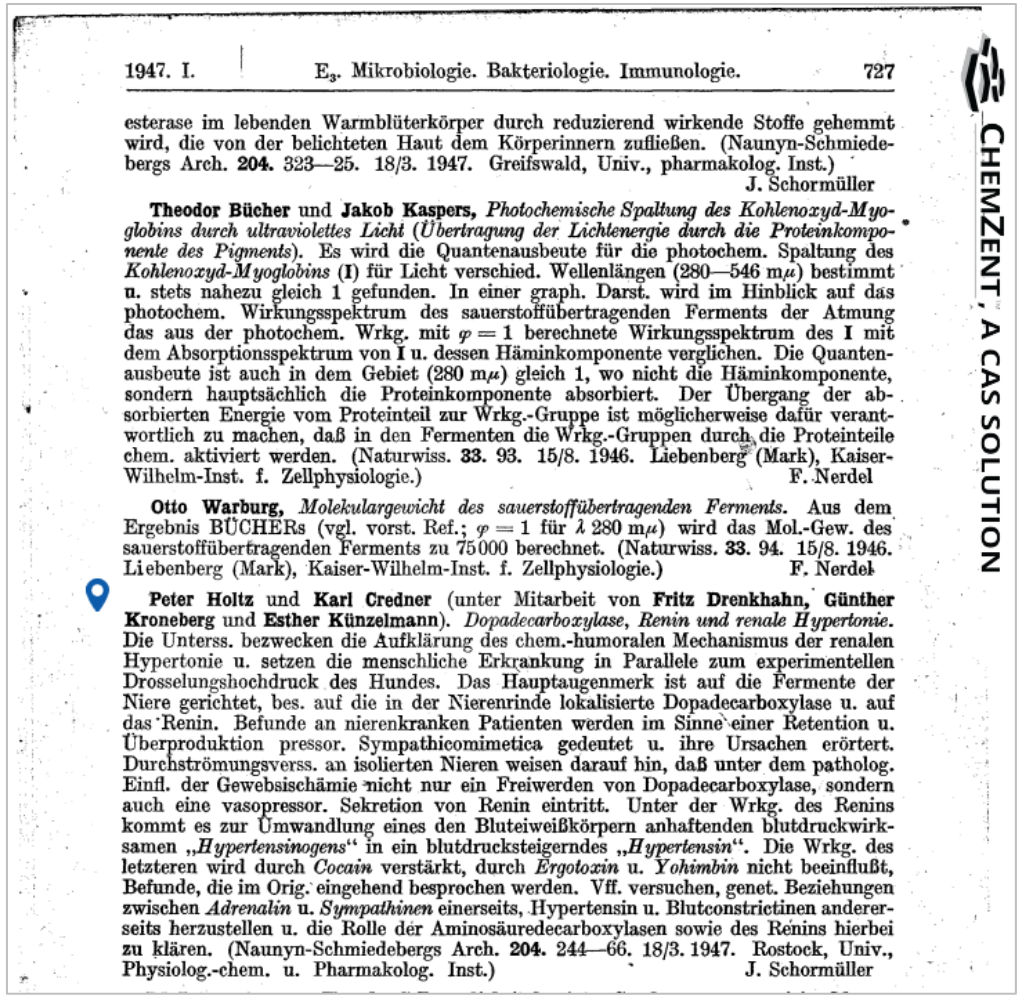
查看Chemzent 来源的文献

- ChemZent是最古老的德国化学文摘的英文版，唯一提供可用英文获取德国化学文摘的解决方案
- 化学研究相关文献可回溯至1830年，可用于追溯化学科学起源时期的研究，丰富化学历史知识





1947. I. E_3. Mikrobiologie. Bakteriologie. Immunologie. 727

esterase im lebenden Warmblüterkörper durch reduzierend wirkende Stoffe gehemmt wird, die von der belichteten Haut dem Körperinnern zufließen. (Naunyn-Schmiedebergs Arch. **204.** 323—25. 18/3. 1947. Greifswald, Univ., pharmakolog. Inst.) J. Schormüller

Theodor Bücher und **Jakob Kaspers,** *Photochemische Spaltung des Kohlenoxyd-Myoglobins durch ultraviolettes Licht (Übertragung der Lichtenergie durch die Proteinkomponente des Pigments).* Es wird die Quantenausbeute für die photochem. Spaltung des *Kohlenoxyd-Myoglobins* (**I**) für Licht verschied. Wellenlängen (280—546 mμ) bestimmt u. stets nahezu gleich 1 gefunden. In einer graph. Darst. wird im Hinblick auf das photochem. Wirkungsspektrum des sauerstoffübertragenden Ferments der Atmung das aus der photochem. Wrkg. mit $\varphi = 1$ berechnete Wirkungsspektrum des **I** mit dem Absorptionsspektrum von **I** u. dessen Häminkomponente verglichen. Die Quantenausbeute ist auch in dem Gebiet (280 mμ) gleich 1, wo nicht die Häminkomponente, sondern hauptsächlich die Proteinkomponente absorbiert. Der Übergang der absorbierten Energie vom Proteinteil zur Wrkg.-Gruppe ist möglicherweise dafür verantwortlich zu machen, daß in den Fermenten die Wrkg.-Gruppen durch die Proteinteile chem. aktiviert werden. (Naturwiss. **33.** 93. 15/8. 1946. Liebenberg (Mark), Kaiser-Wilhelm-Inst. f. Zellphysiologie.) F. Nerdel

Otto Warburg, *Molekulargewicht des sauerstoffübertragenden Ferments.* Aus dem Ergebnis BÜCHERs (vgl. vorst. Ref.; $\varphi = 1$ für λ 280 mμ) wird das Mol.-Gew. des sauerstoffübertragenden Ferments zu 75000 berechnet. (Naturwiss. **33.** 94. 15/8. 1946. Liebenberg (Mark), Kaiser-Wilhelm-Inst. f. Zellphysiologie.) F. Nerdel

Peter Holtz und **Karl Credner** (unter Mitarbeit von **Fritz Drenkhahn, Günther Kroneberg** und **Esther Künzelmann**). *Dopadecarboxylase, Renin und renale Hypertonie.* Die Unterss. bezwecken die Aufklärung des chem.-humoralen Mechanismus der renalen Hypertonie u. setzen die menschliche Erkrankung in Parallele zum experimentellen Drosselungshochdruck des Hundes. Das Hauptaugenmerk ist auf die Fermente der Niere gerichtet, bes. auf die in der Nierenrinde lokalisierte Dopadecarboxylase u. auf das Renin. Befunde an nierenkranken Patienten werden im Sinne einer Retention u. Überproduktion pressor. Sympathicomimetica gedeutet u. ihre Ursachen erörtert. Durchströmungsverss. an isolierten Nieren weisen darauf hin, daß unter dem patholog. Einfl. der Gewebsischämie nicht nur ein Freiwerden von Dopadecarboxylase, sondern auch eine vasopressor. Sekretion von Renin eintritt. Unter der Wrkg. des Renins kommt es zur Umwandlung eines den Bluteiweißkörpern anhaftenden blutdruckwirksamen „*Hypertensinogens*“ in ein blutdrucksteigerndes „*Hypertensin*“. Die Wrkg. des letzteren wird durch *Cocain* verstärkt, durch *Ergotoxin* u. *Yohimbin* nicht beeinflußt. Befunde, die im Orig. eingehend besprochen werden. Vff. versuchen, genet. Beziehungen zwischen *Adrenalin* u. *Sympathinen* einerseits, Hypertensin u. Blutconstrictinen andererseits herzustellen u. die Rolle der Aminosäuredecarboxylasen sowie des Renins hierbei zu klären. (Naunyn-Schmiedebergs Arch. **204.** 244—66. 18/3. 1947. Rostock, Univ., Physiolog.-chem. u. Pharmakolog. Inst.) J. Schormüller

CHEMZENT, A CAS SOLUTION

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文献检索小结

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

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大纲

- CAS SciFinder^{n}中的物质检索
  - 物质检索的常用方法
  - 物质详情解读
  - 结构绘图板的使用
  - 物质结果集的分析及筛选
  - Markush检索与结果解读

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物质检索

- 物质检索方法
  - 基础检索：物质标识符、文献标识符
  - 高级检索：分子式、物性参数、谱图数据
  - 结构式
- 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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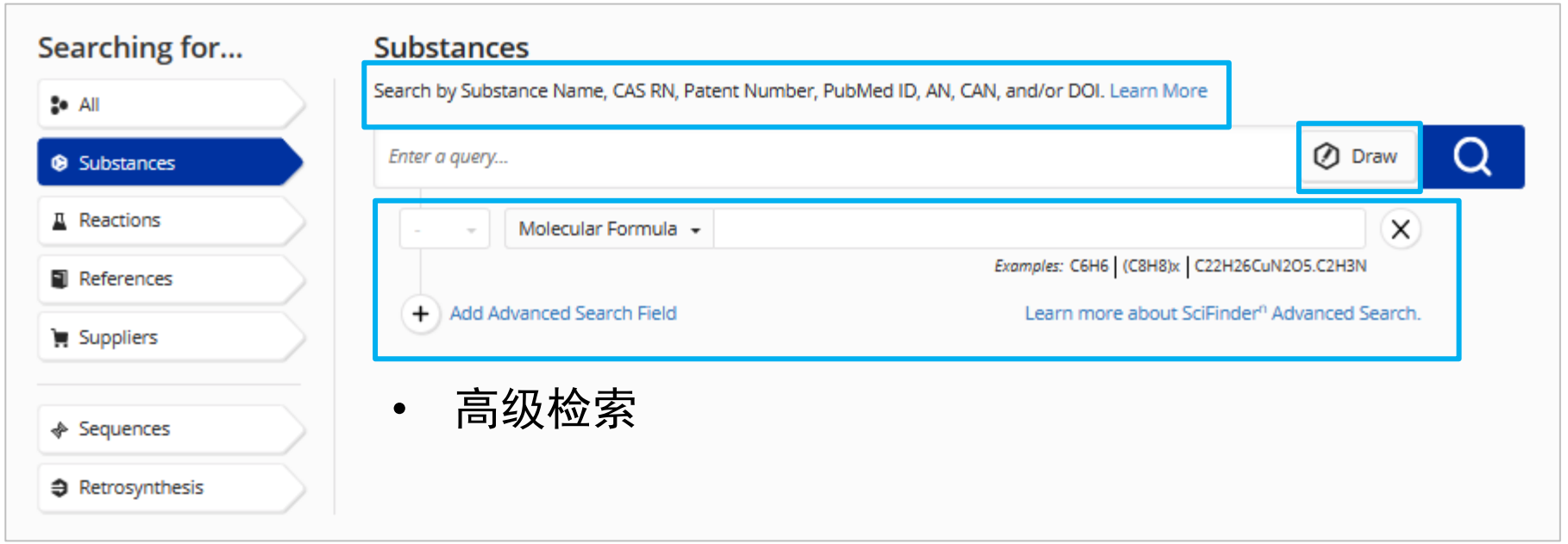
物质检索

- 通过物质标识符、文献标识符检索物质



- 高级检索

- 使用结构绘制面板进行结构检索

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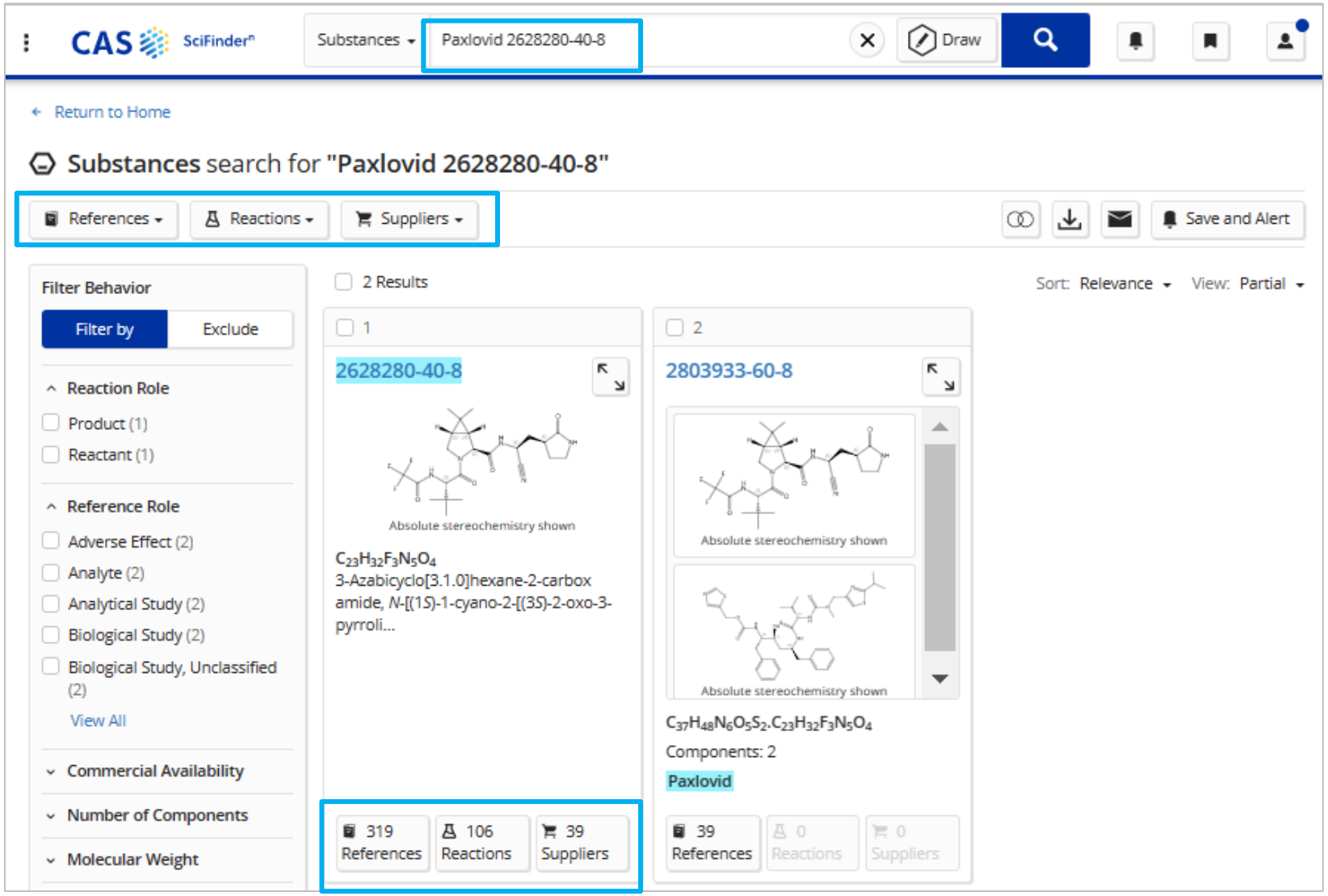
物质检索—物质名称、CAS RN、代码



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

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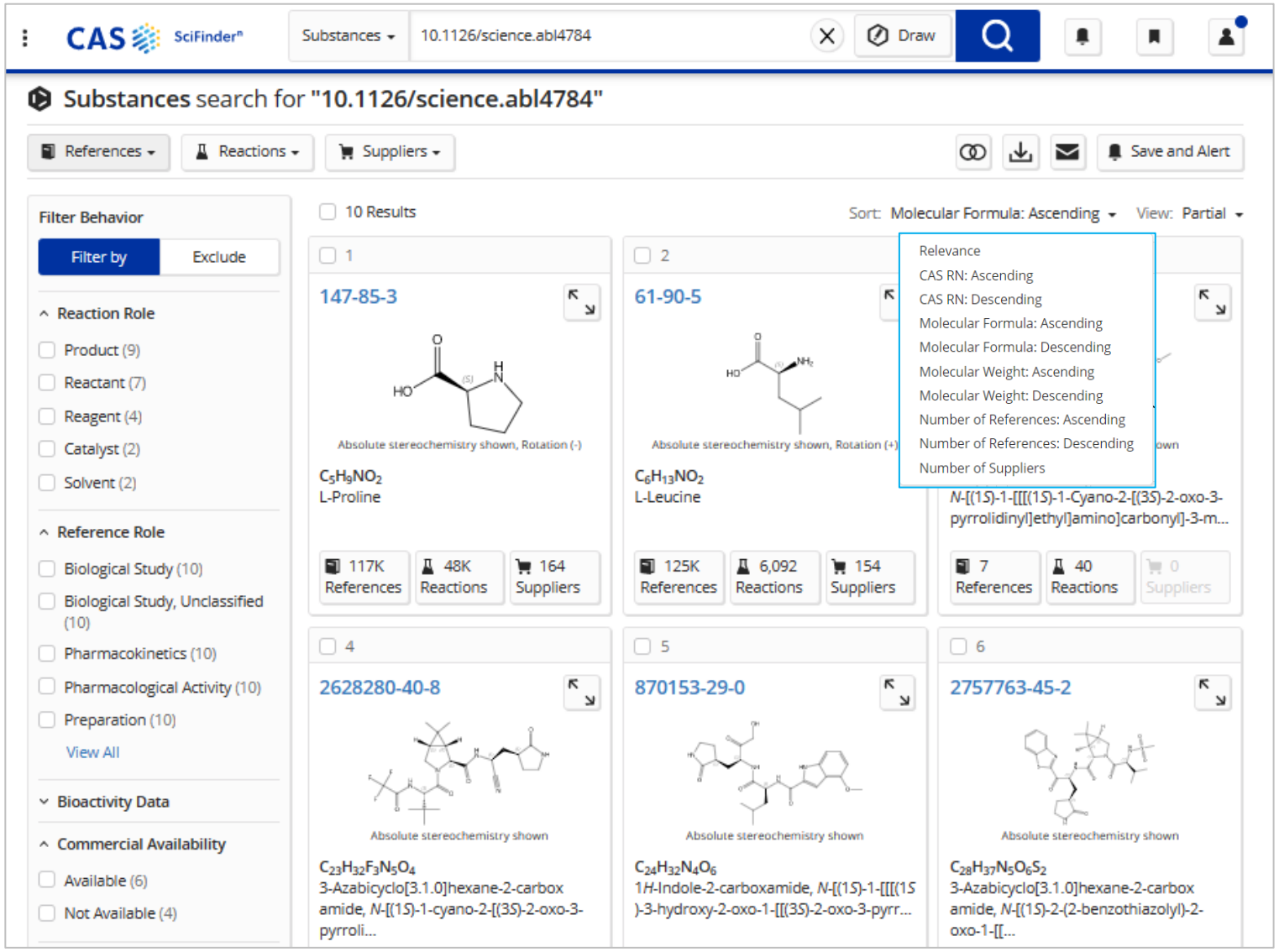
物质检索—文献标识符及结果集排序



使用文献标识符，迅速获得关注文献中的物质信息

不同物质排序：

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

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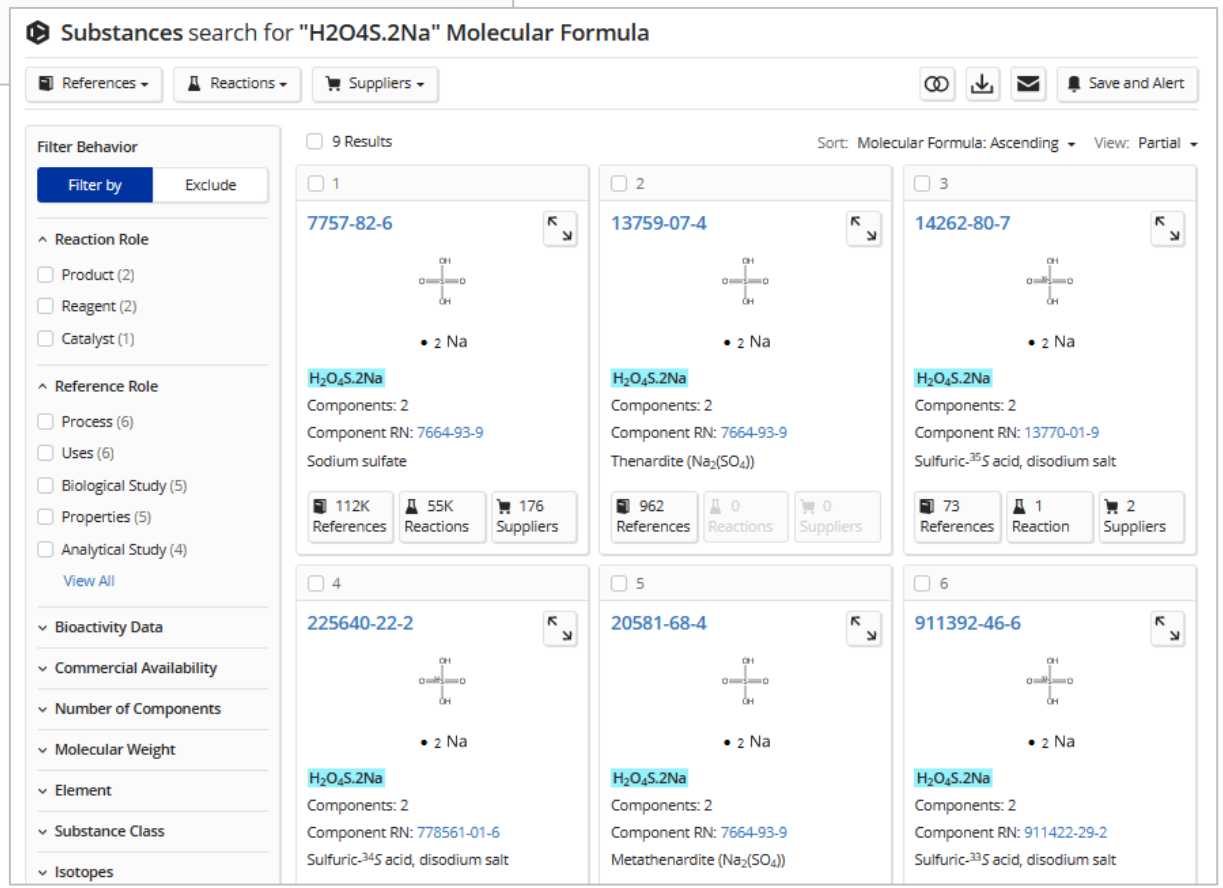
物质检索—分子式

Na2SO4：H2O4S.2Na



金属盐：

- 金属离子和阴离子间用点（.）分开
- 不同组份之间用点（.）分开

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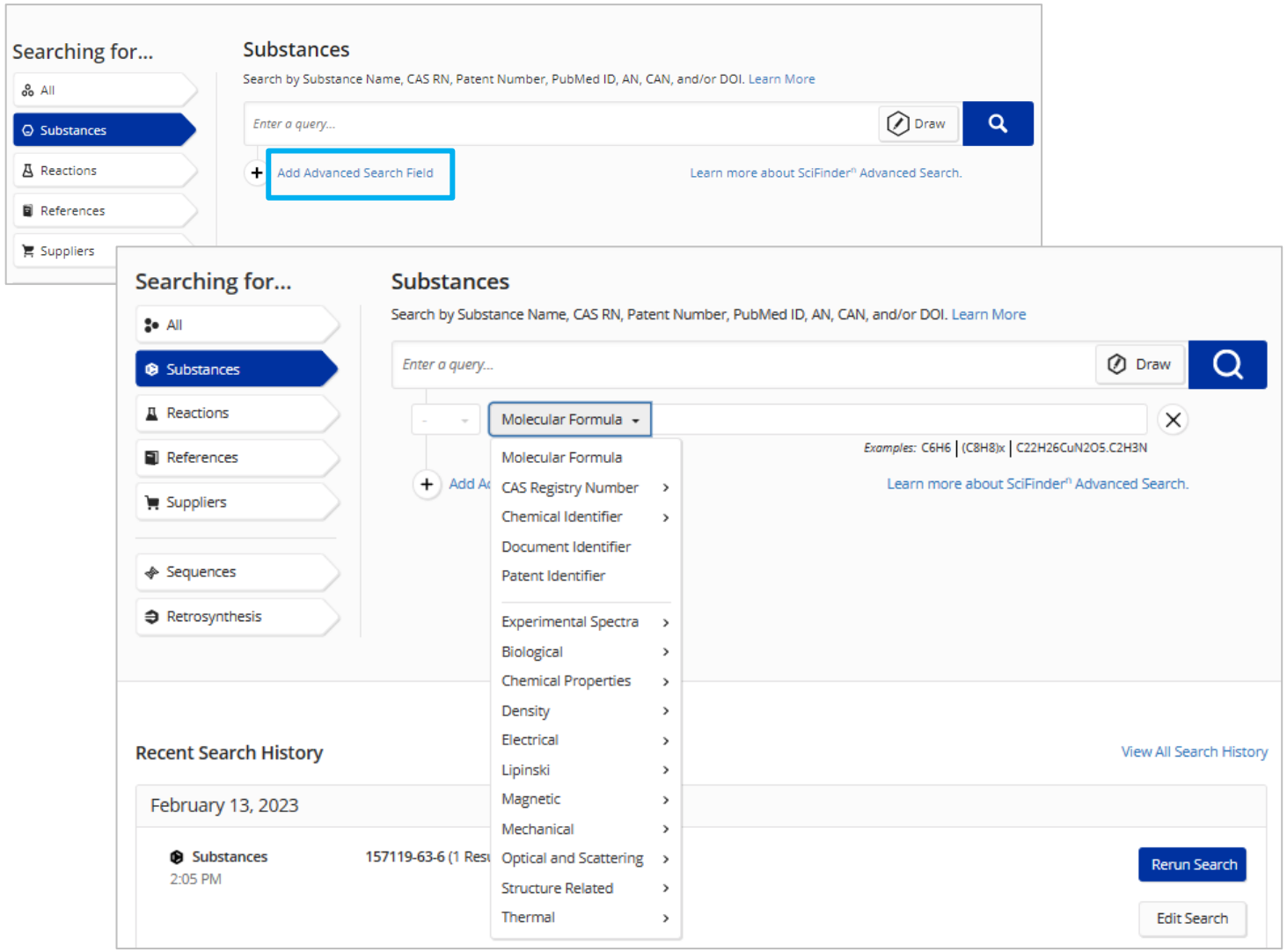
物质检索—Advanced Search



高级检索字段：

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

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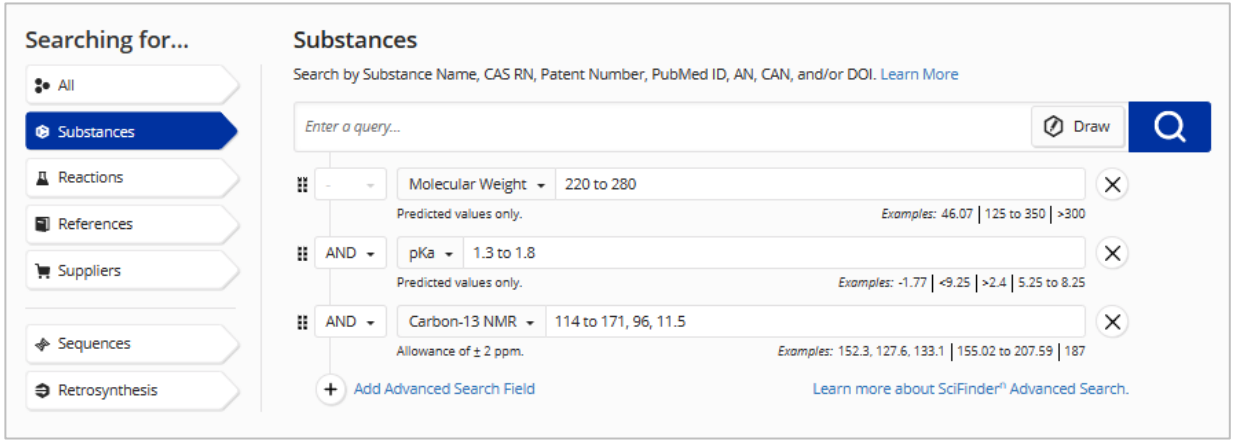
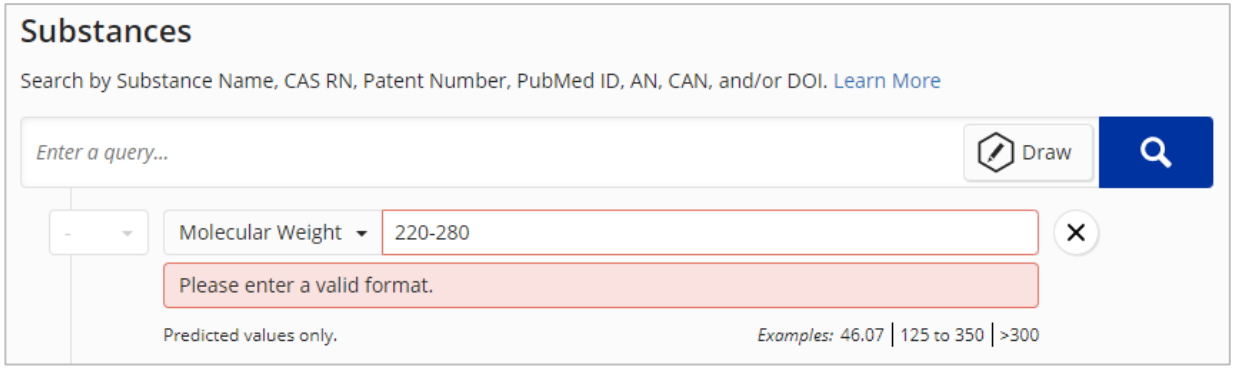
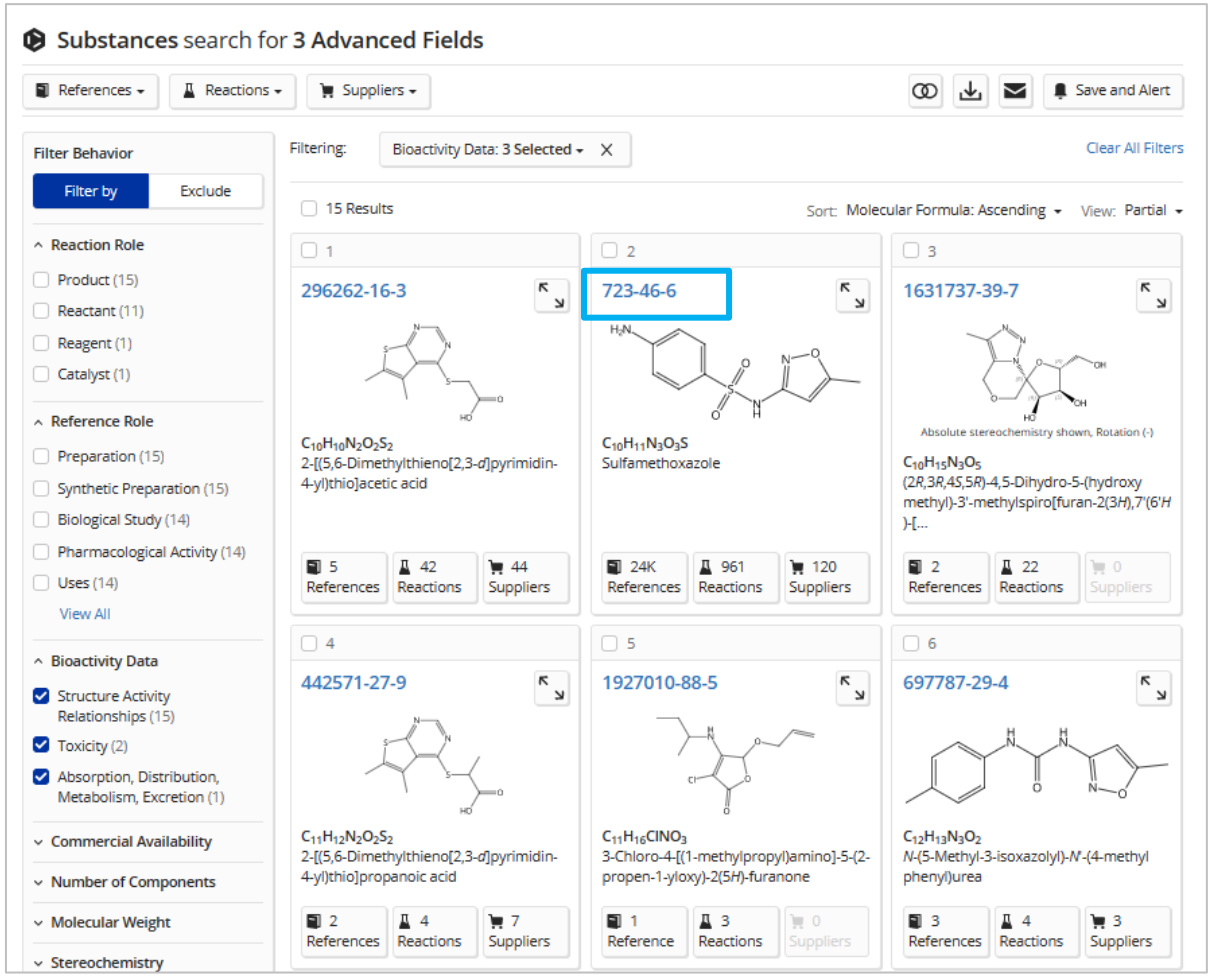
物质检索—联用检索

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







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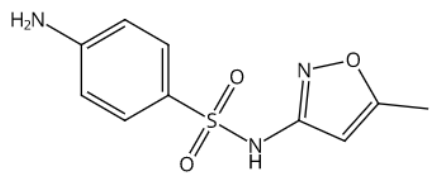
物质详情

CAS Registry Number: 723-46-6

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



$C_{10}H_{11}N_3O_3S$

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

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point (Predicted)	482.1±55.0 °C	Press: 760 Torr
Density (Experimental)	1.4895 g/cm^3	-
pKa (Predicted)	5.81±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Structure Activity Relationships (CAS LIFE SCIENCES)
- Absorption, Distribution, Metabolism, and Excretion Data (CAS LIFE SCIENCES)
- Toxicity (CAS LIFE SCIENCES)
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators

折叠菜单显示物质各类信息

Experimental Spectra

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

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

Sources

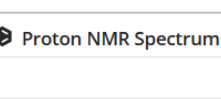
(1) Spectral data were obtained from Life Chemicals

(2) Spectral data were obtained from Enamine Ltd.

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

Proton NMR Spectrum for 723-46-6

723-46-6



$C_{10}H_{11}N_3O_3S$

CAS Name
Sulfamethoxazole

Conditions

Working Frequency
400 MHz

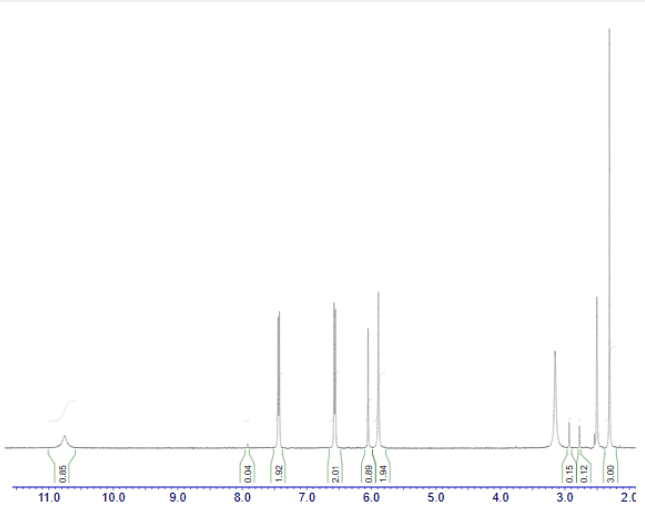
Solvent
Dimethyl sulfoxide (67-68-5)
Carbon tetrachloride (56-23-5)

Temperature
20 °C

Spectrum Summary

Spectrum ID
F0175-0013

Source
Spectral data were obtained from Life Chemicals



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物质详情

Structure Activity Relationships

CAS LIFE SCIENCES

Target | Function | Parameter | Disease | Organism

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

Apply | Clear All

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

Absorption, Distribution, Metabolism, and Excretion Data

CAS LIFE SCIENCES

Target | Function | Parameter | Disease

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

Apply | Clear All

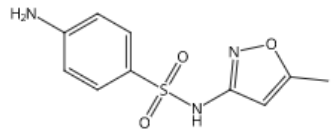
Target	Func	Value	Disease	Organism	Assay	Source
Methicillin-resistant Staphylococcus aureus	-	217.5 mg x h/L	Bacterial infections	-	View Detail	(1) CAS
Methicillin-resistant Staphylococcus aureus	-	13 mg/L	Bacterial infections	-	View Detail	(1) CAS
Methicillin-resistant Staphylococcus aureus	-	10 h	Bacterial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

Assay Data

CAS LIFE SCIENCES

← Prev (2 of 1,031) Next →

Ligand
723-46-6



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

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

Toxicity

CAS LIFE SCIENCES

Parameter

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

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

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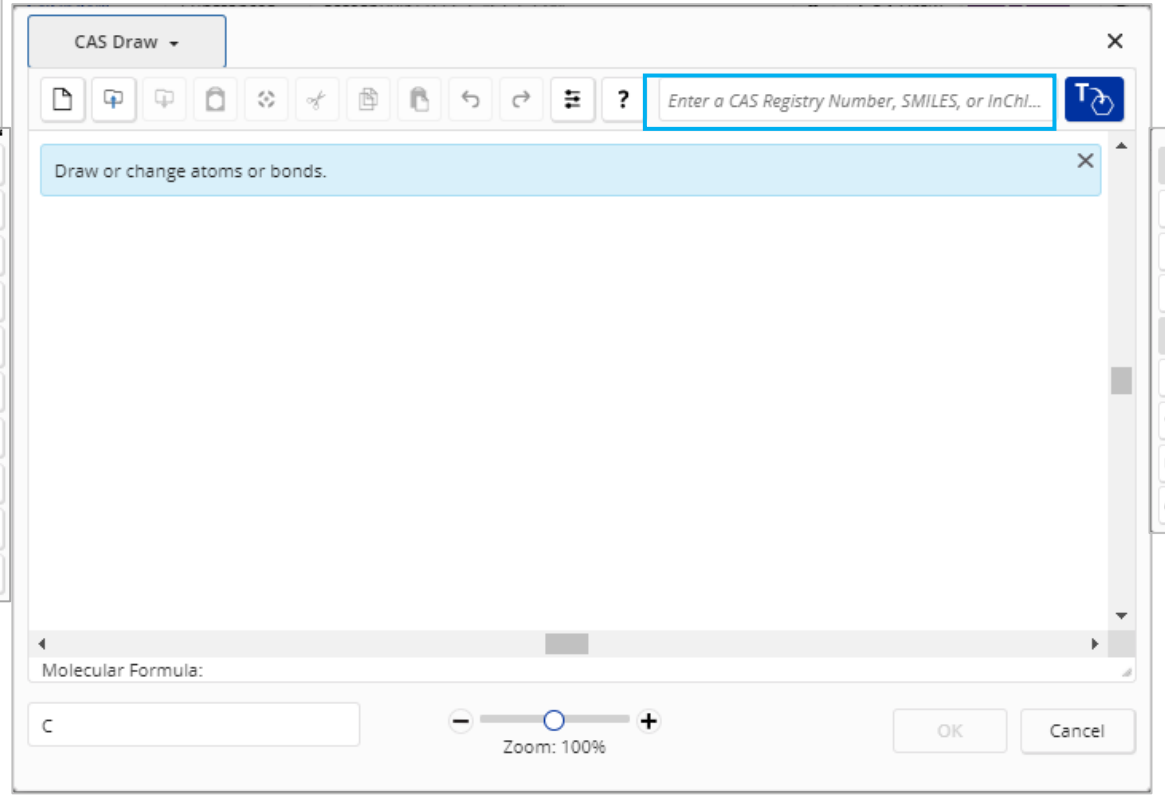
物质检索—结构检索



X 选择可变基团

Q 取代位点可变

R 自定义R基团

锁工具

重复片段工具

Fn 片段结构

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

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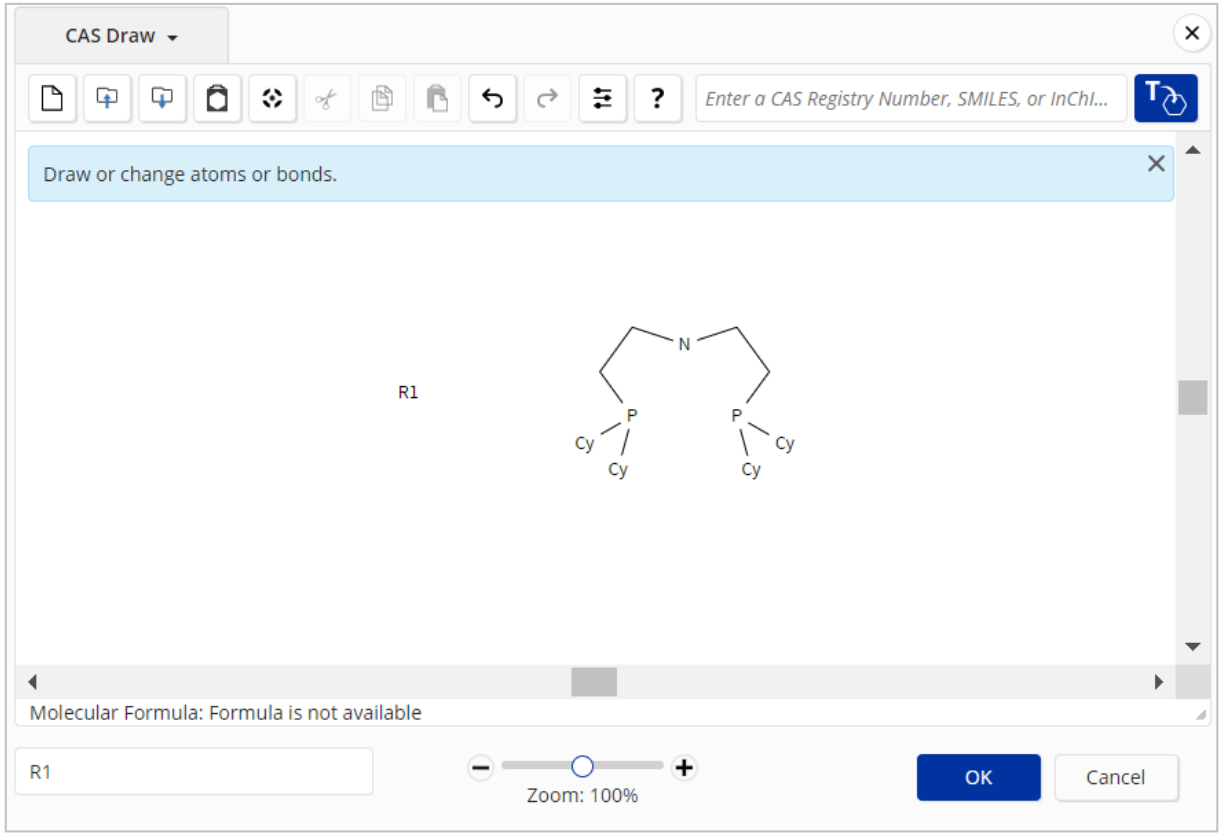
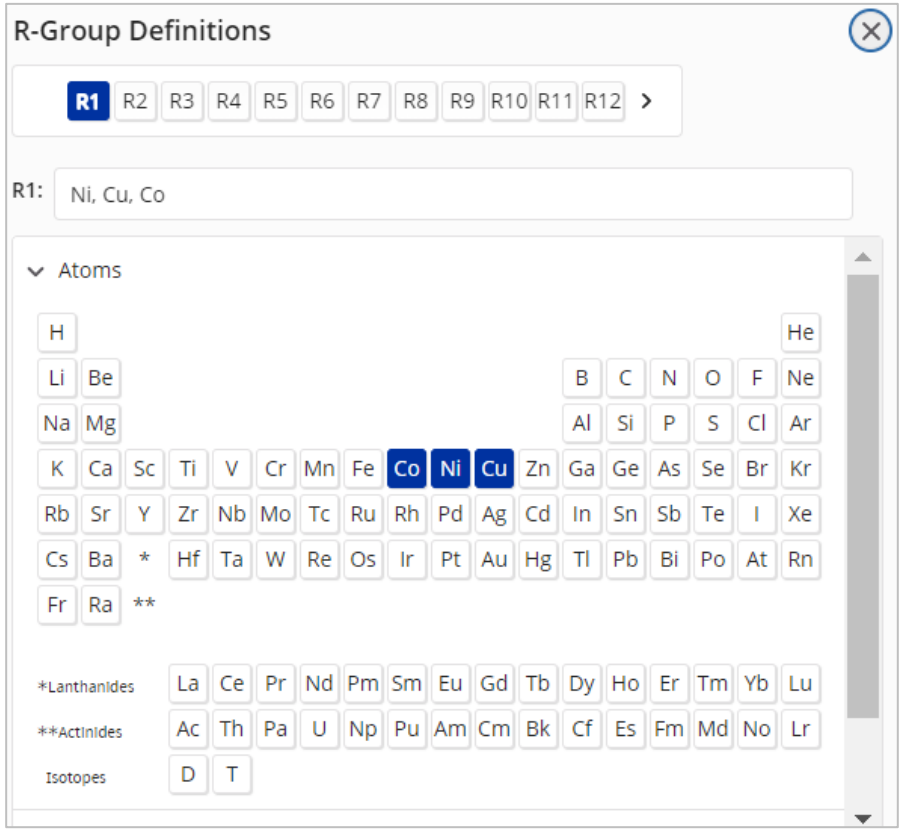
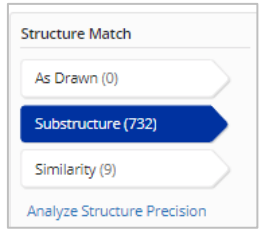
物质检索—结构检索

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







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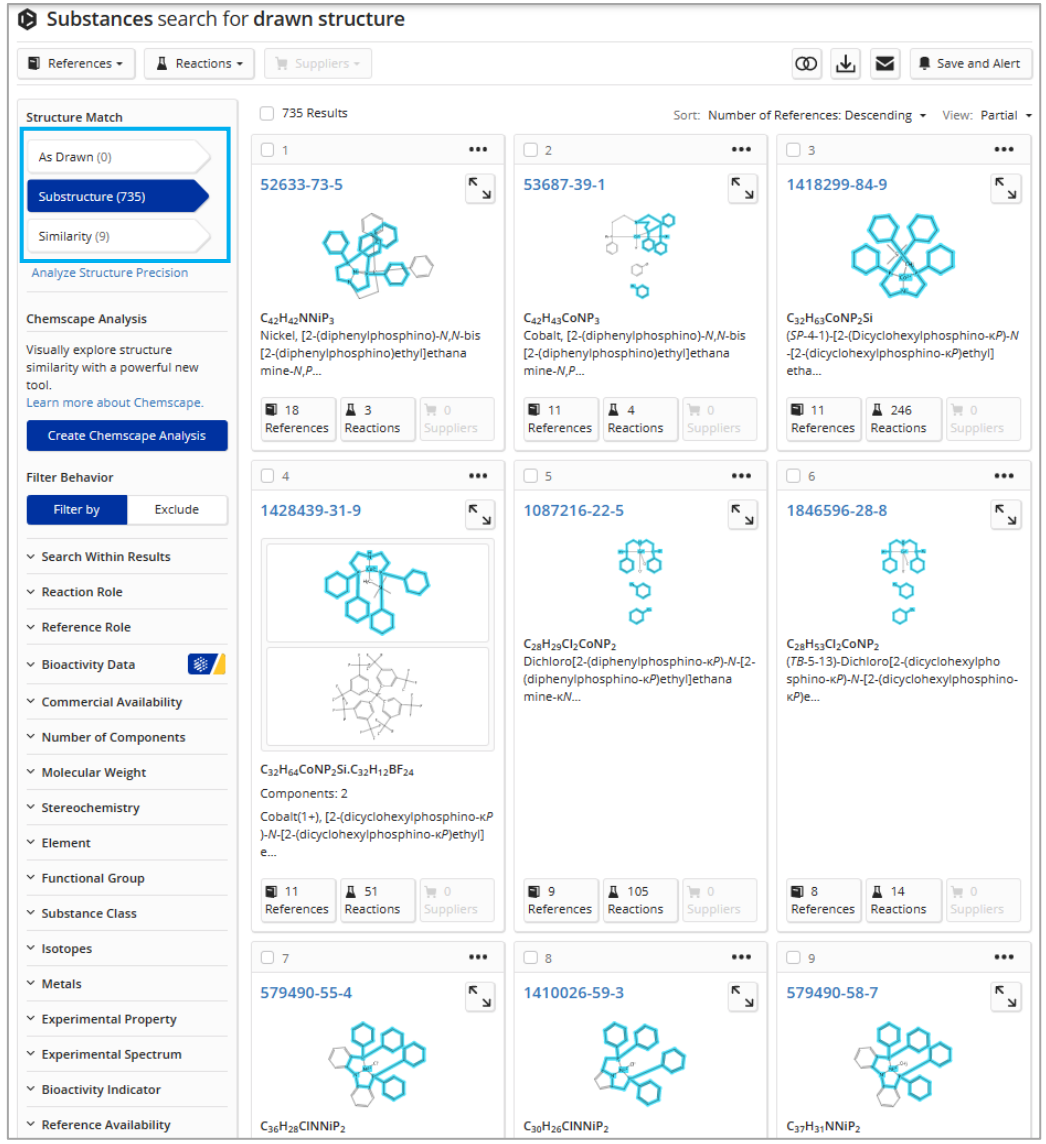
物质检索—检索结果集筛选

结构检索类别：
As Drawn
亚结构
相似结构

Chemscape分析

Filter by & Exclude

物质筛选类别：
反应角色
文献角色
立体化学
物质类别
同位素
金属包含
实验物性数据
二次检索……



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物质检索—结构检索

结构检索类别：

- As Drawn

  绘制结构中可出现R基团、可变基团；绘制结构中价态未达饱和的原子只能接氢；如有环系，不与其他环稠合或成桥环

- Substructure 亚结构

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

- Similarity 相似结构

  获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

  注：如果关注相似结构检索结果，请不要绘制通式结构

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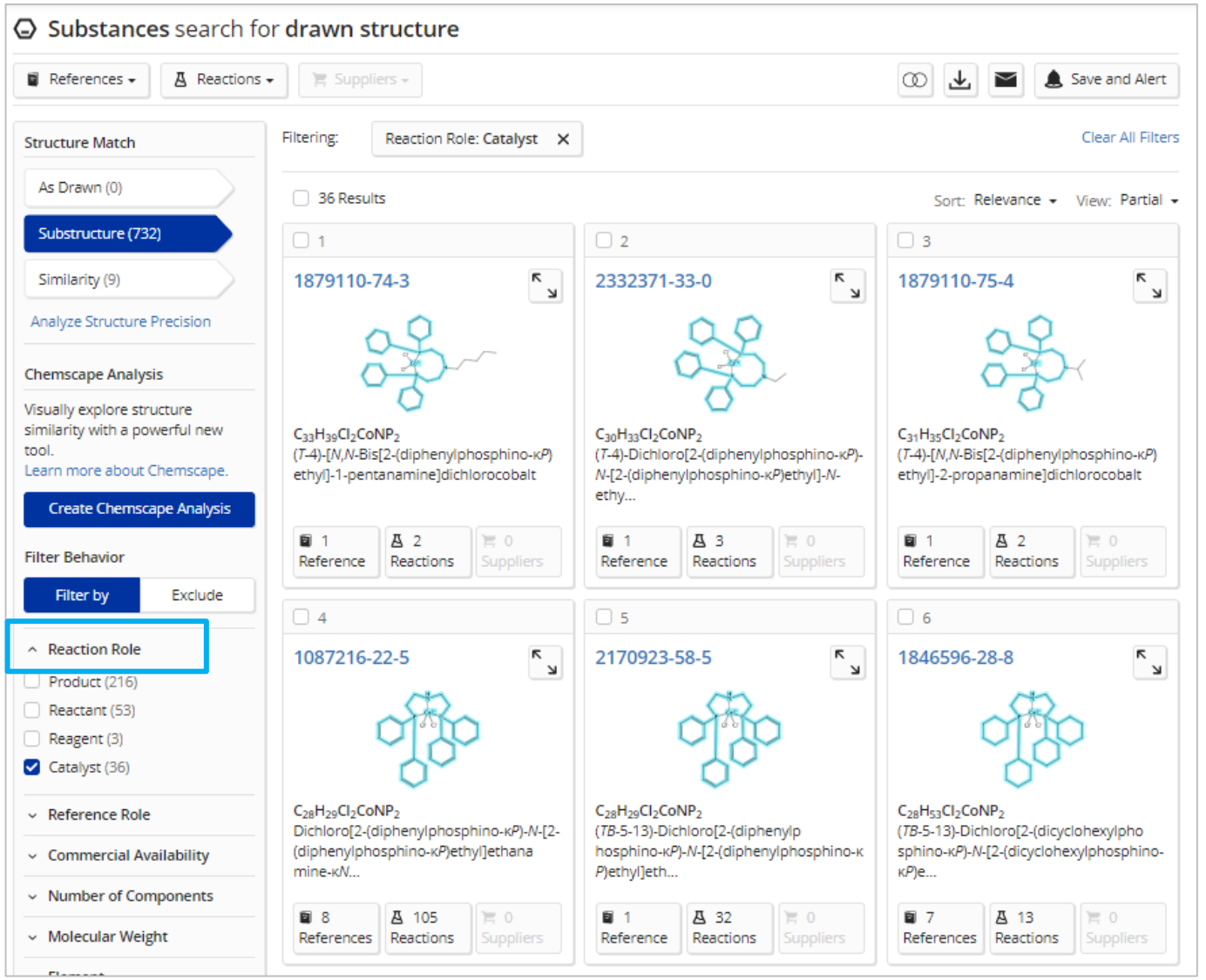
物质检索--检索结果集筛选：Reaction Role

利用物质在反应中的角色精准定位相应的物质



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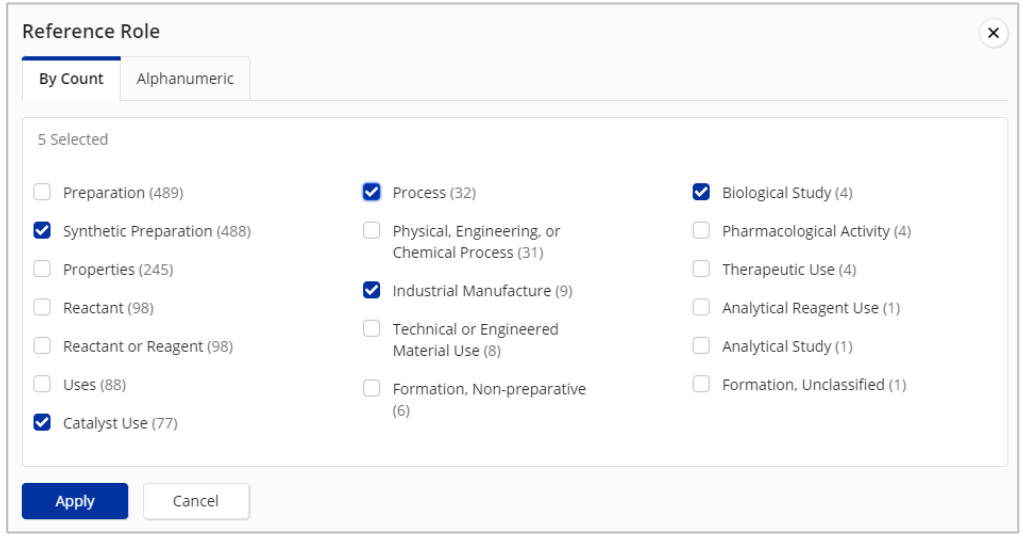
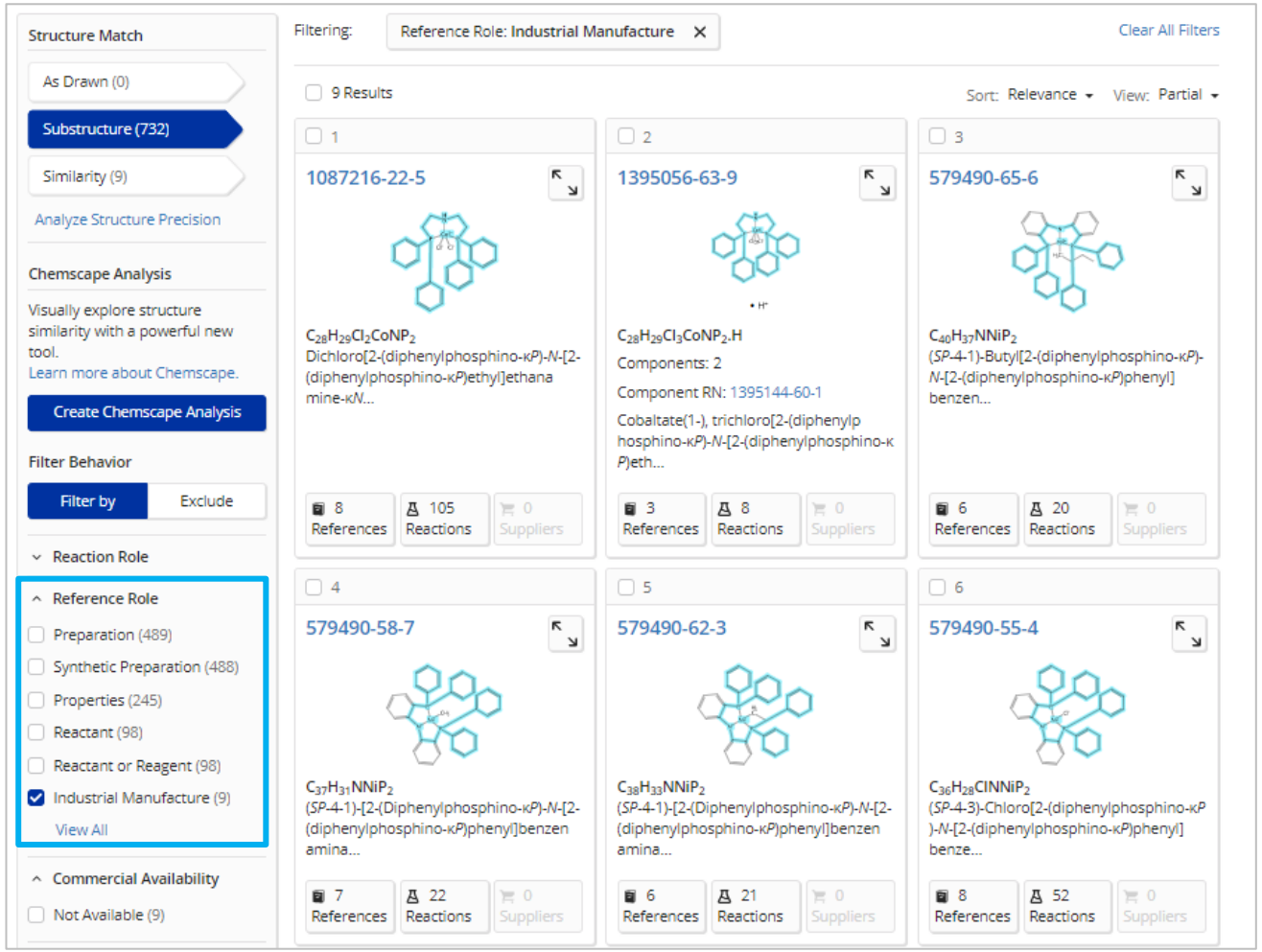
物质检索—检索结果集筛选：Reference Role

利用物质的研究角色精准定位相应的物质





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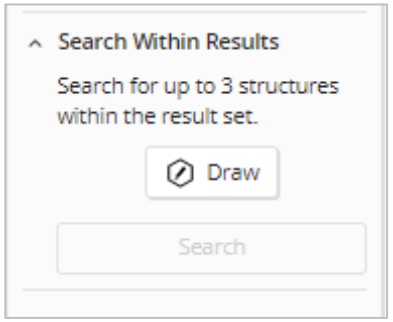
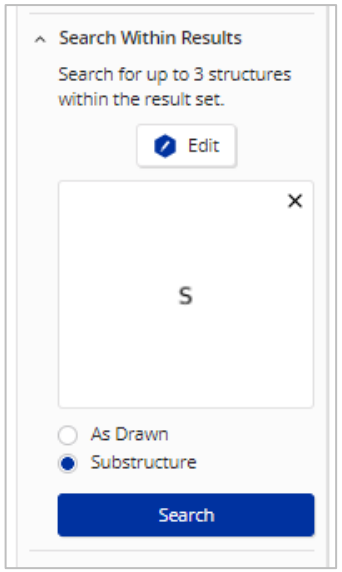
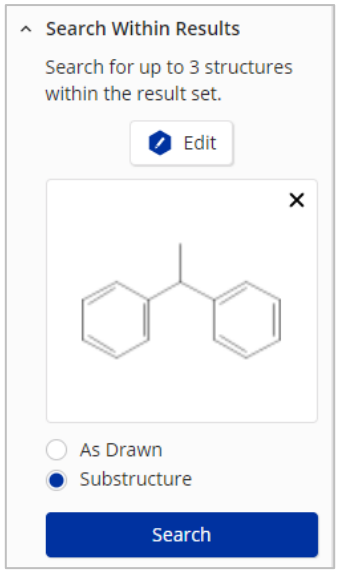
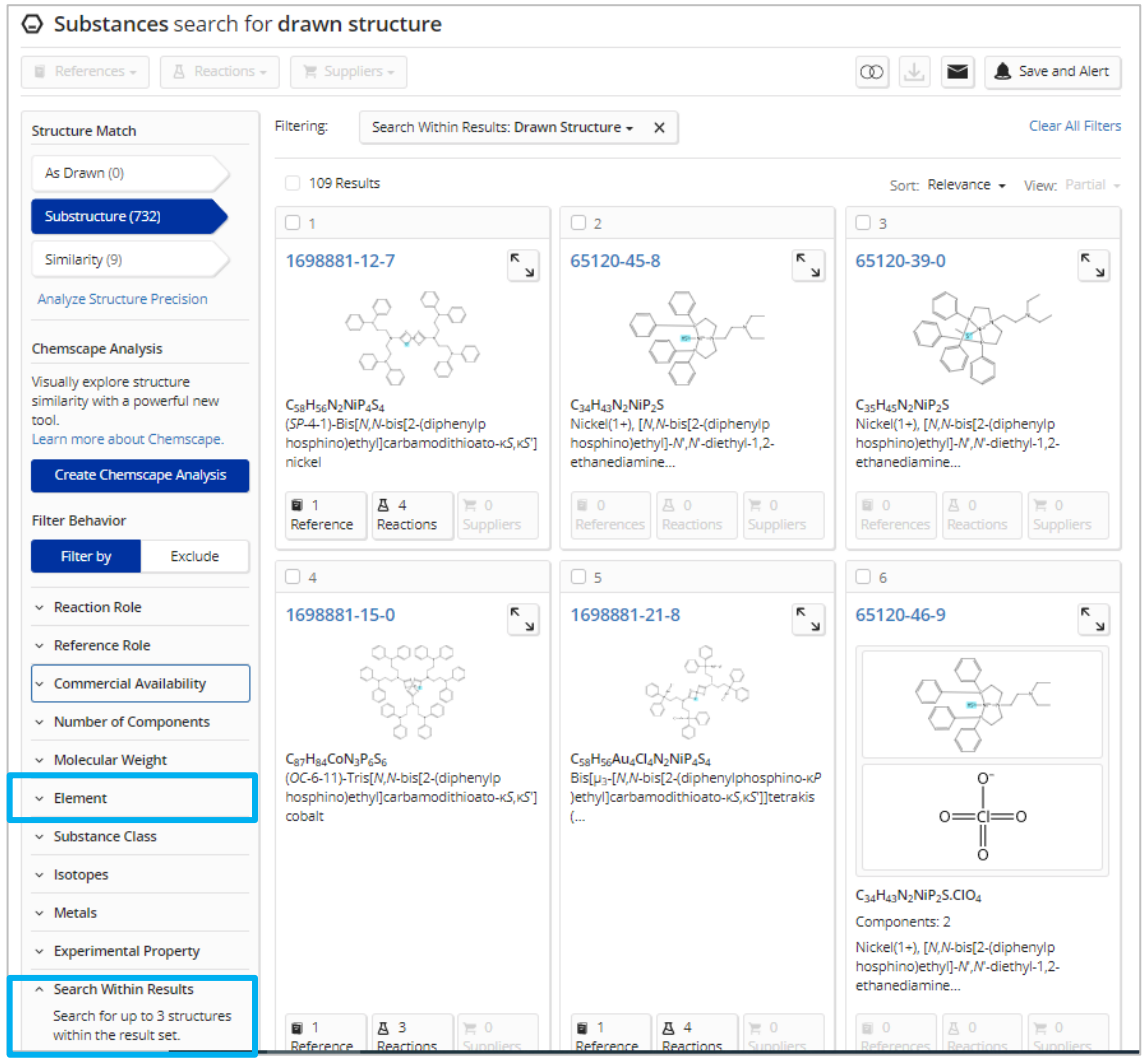
物质检索—检索结果集筛选：结构

利用物质筛选工具快速锁定目标物质









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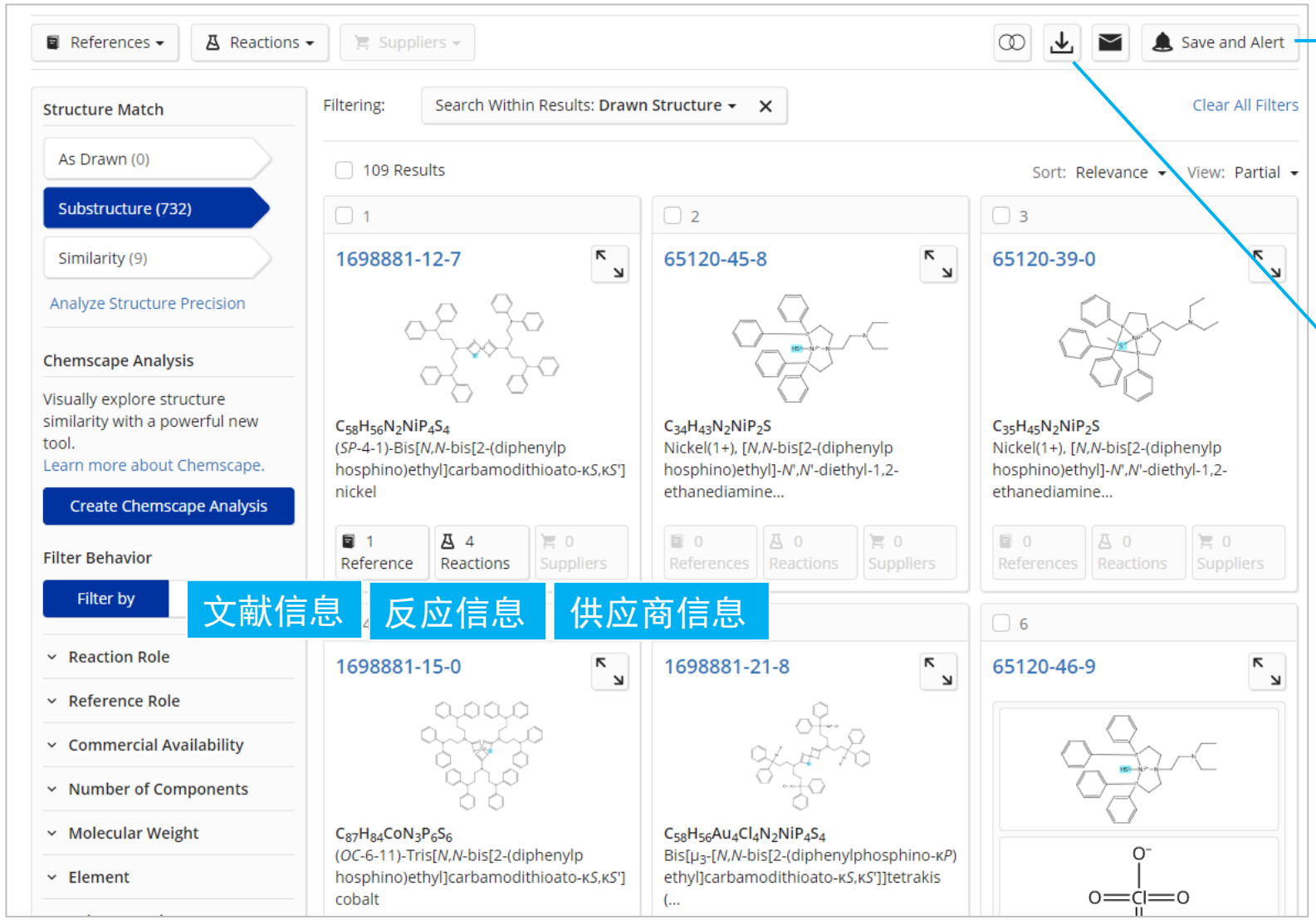
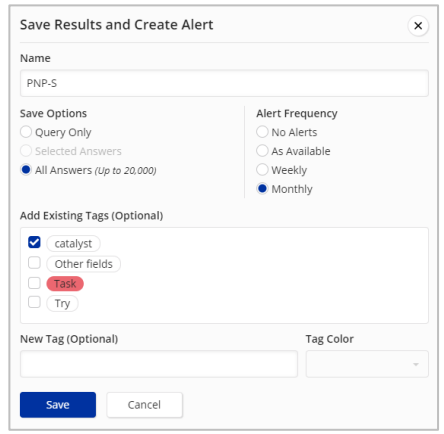
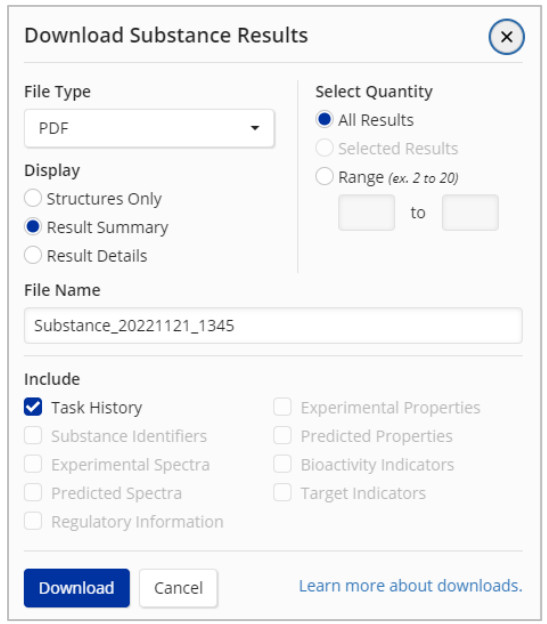
物质检索—检索结果集的保存







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CAS Markush检索

(19)中华人民共和国国家知识产权局

(12)发明专利申请

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

(21)申请号 201410122313.4
(22)申请日 2014.03.30
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代理人 张法高 赵杭丽
(51)Int.Cl.
C07K 5/087(2006.01)
C07K 5/083(2006.01)
C07K 1/16(2006.01)
C07K 1/06(2006.01)
A61K 38/06(2006.01)
A61P 35/00(2006.01)
A61P 35/02(2006.01)
A61P 25/28(2006.01)
A61P 37/02(2006.01)

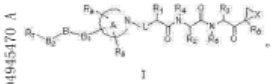
权利要求书3页 说明书24页 附图4页

(54)发明名称

杂环构建的三肽环氧酮类化合物及制备和应用

(57)摘要

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



I

CN 104945470 A

具体物质[Specific Substance]：

以具体化学结构陈述的特定物质，会被分配CAS RN

具体实施方式

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

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

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

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

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

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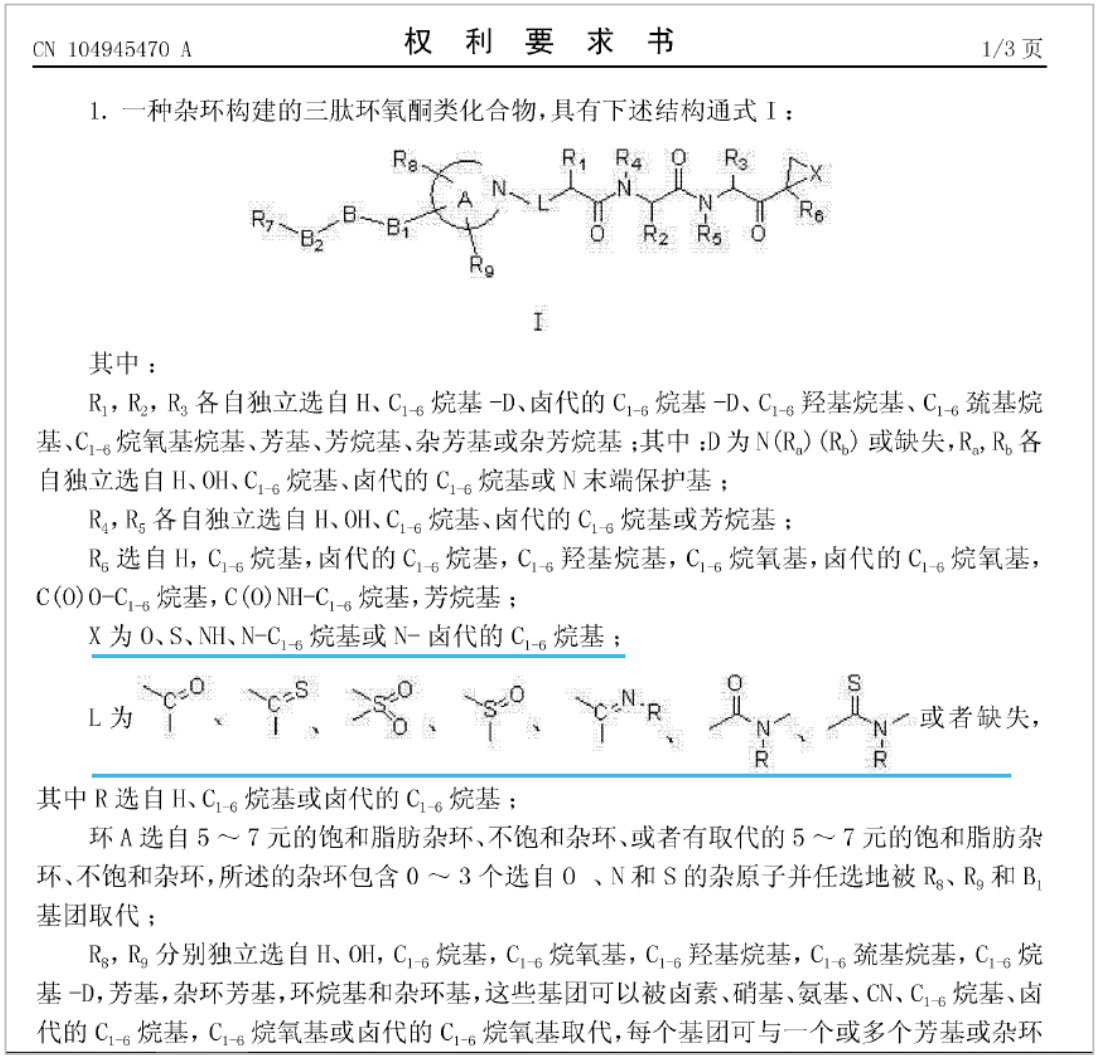
CAS Markush检索

预测性物质[Prophetic Substance]：

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



CN 104945470 A　　权 利 要 求 书　　1/3 页

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：

I

其中：

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

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

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

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

L 为 或者缺失，

其中 R 选自 H、C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

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

R_8，R_9 分别独立选自 H、OH，C_{1-6} 烷基，C_{1-6} 烷氧基，C_{1-6} 羟基烷基，C_{1-6} 巯基烷基，C_{1-6} 烷基 -D，芳基，杂环芳基，环烷基和杂环基，这些基团可以被卤素、硝基、氨基、CN、C_{1-6} 烷基、卤代的 C_{1-6} 烷基，C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代，每个基团可与一个或多个芳基或杂环

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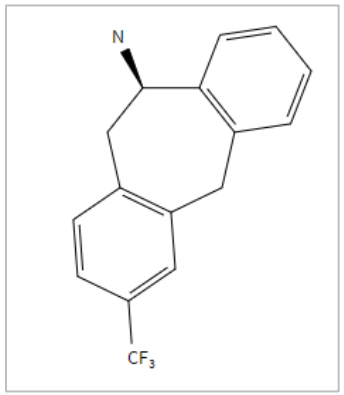
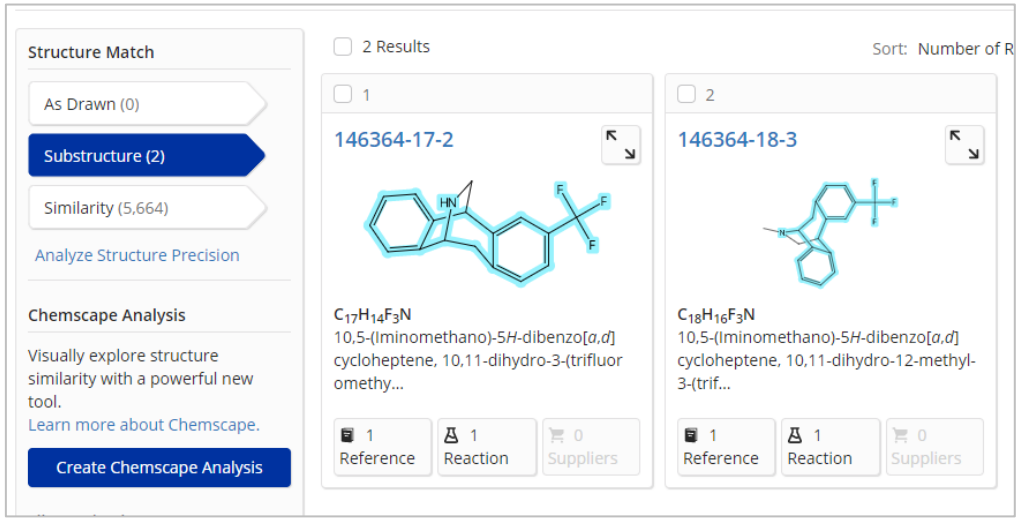
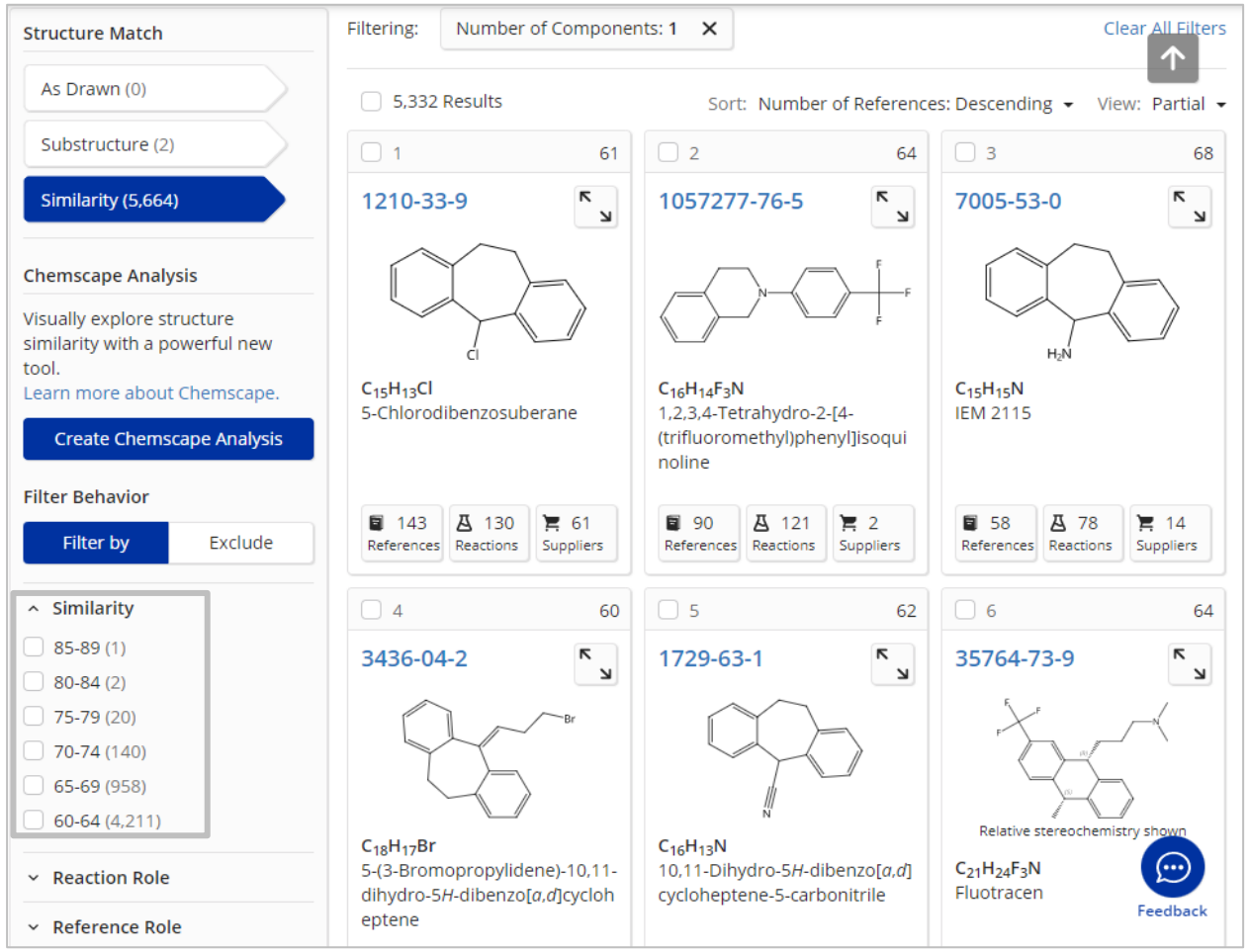
CAS Markush检索

第一步：物质结构检索

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







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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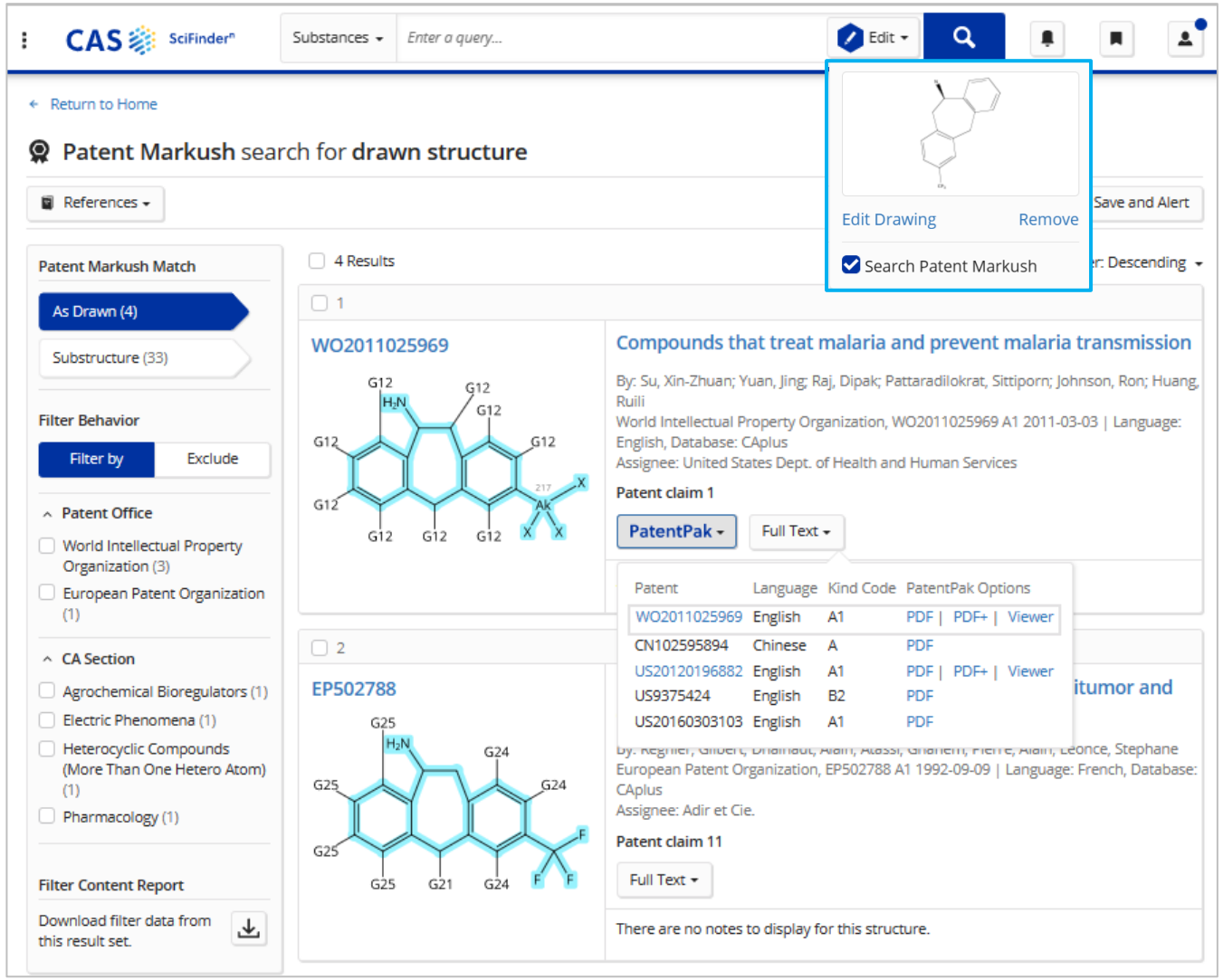
CAS Markush检索

第二步：Markush结构检索
获得四件专利文献

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



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物质检索小结

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

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大纲

- CAS SciFinder^{n}中的反应检索
  - 反应检索的常用方法
  - 反应结果集的浏览与筛选
  - Synthetic Methods™的使用
  - 关键词与反应式的联合检索

视频链接：
https://american-chemical-society.zoom.us/rec/share/eheXjH8iLM3q7tT2flBtPm-c-_IMCDEF8qCgXmSngeTk7DtculPYx1IZZn83BYc.cAuZdpJTknUmPvaK?startTime=1647338414000

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反应检索

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

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

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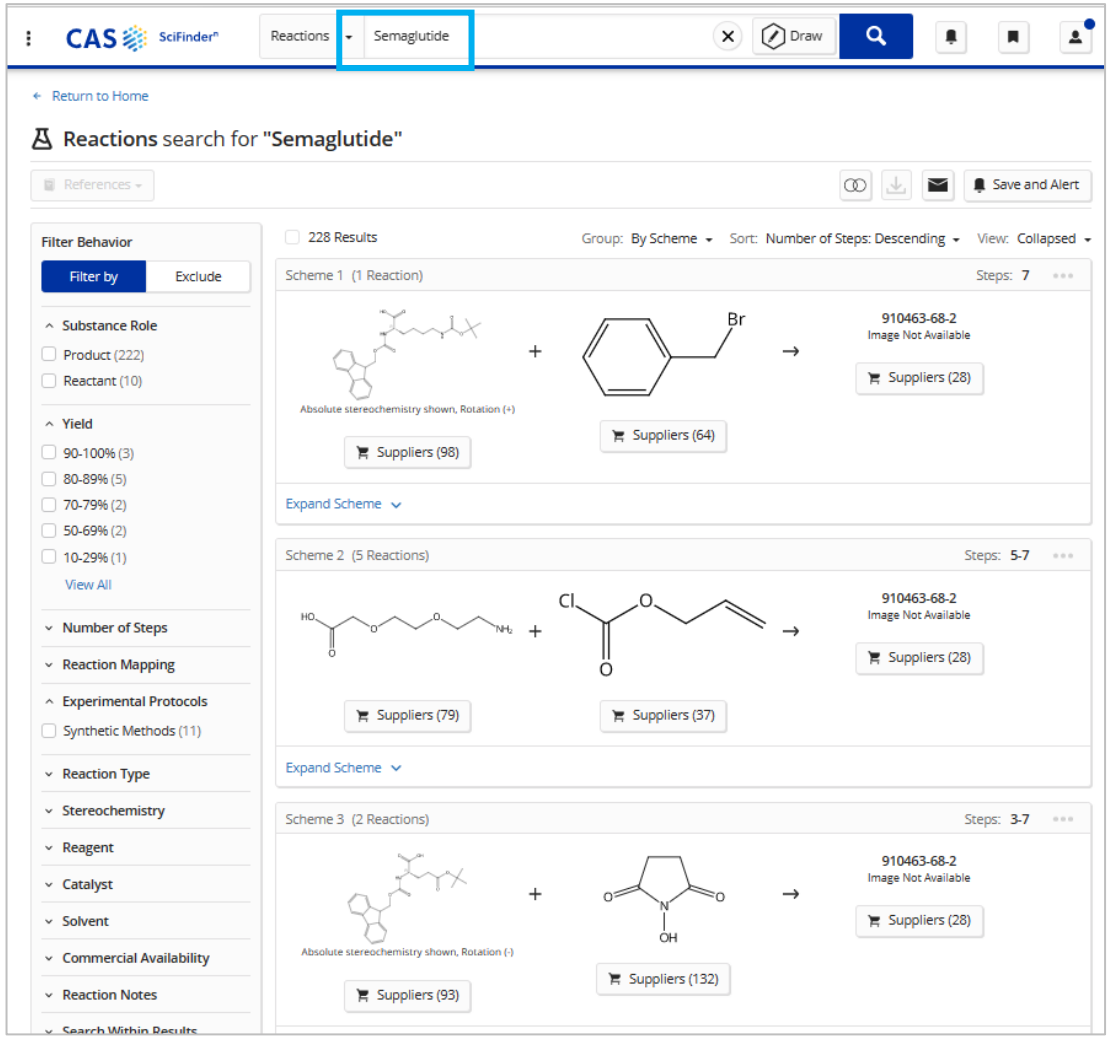
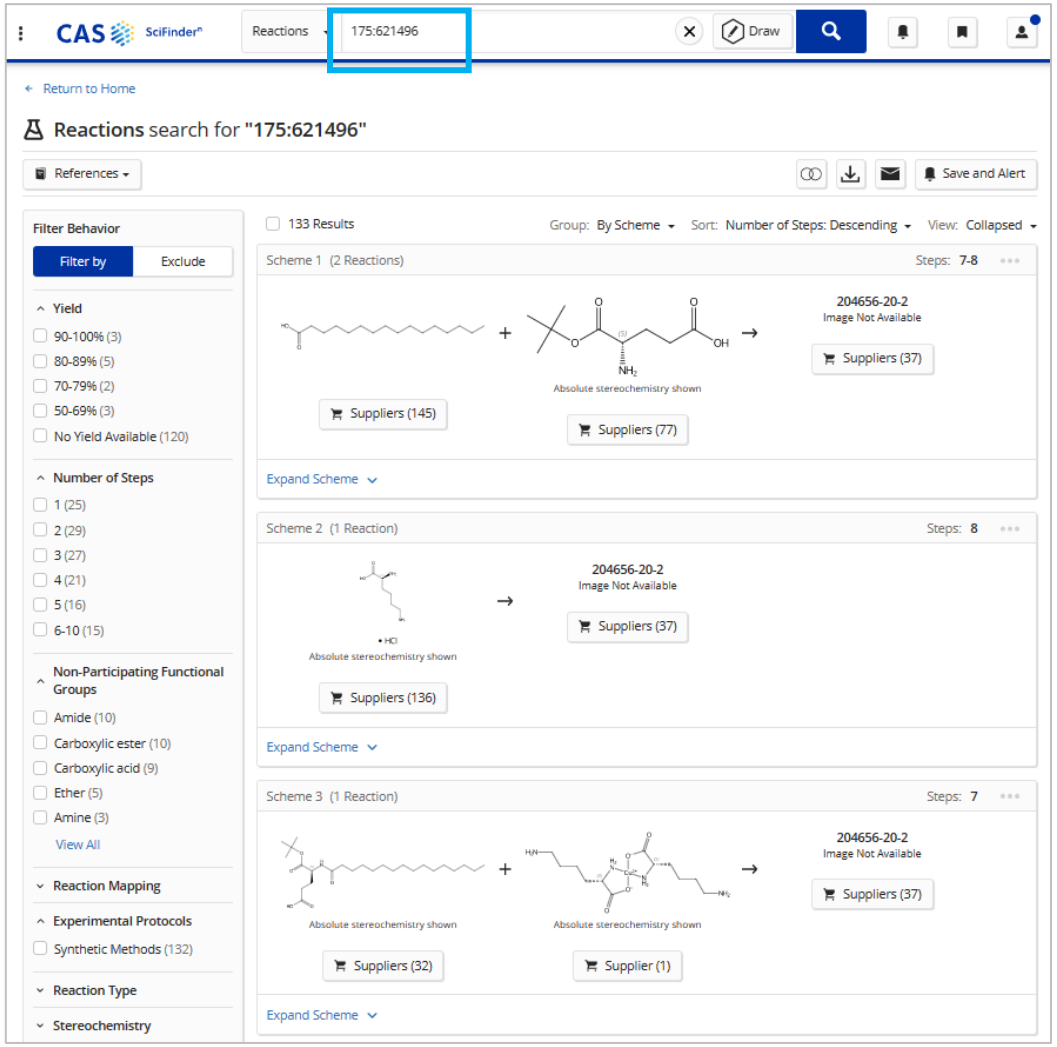
反应检索

通过物质或文献标识符进行检索





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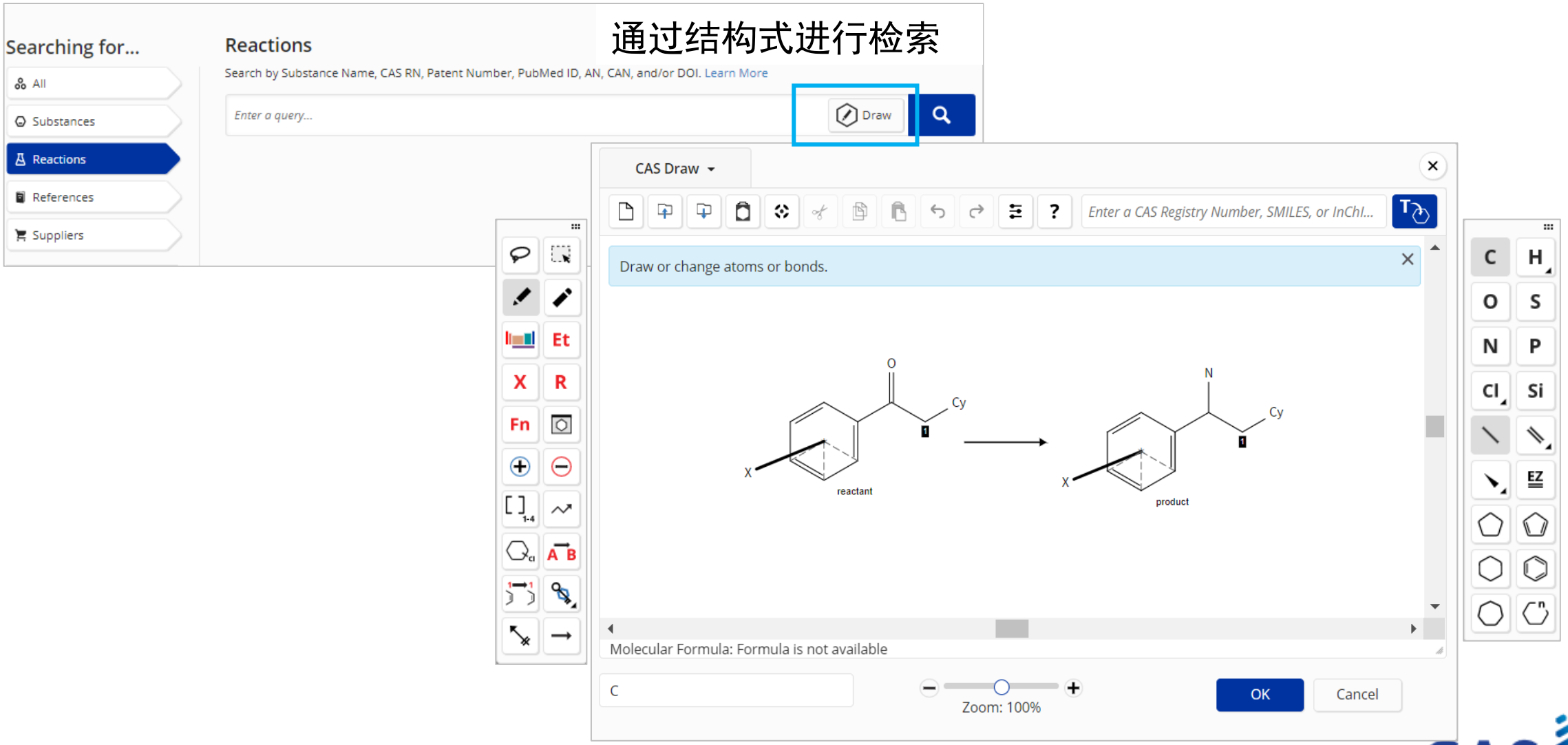
反应检索



X = Cl, Br

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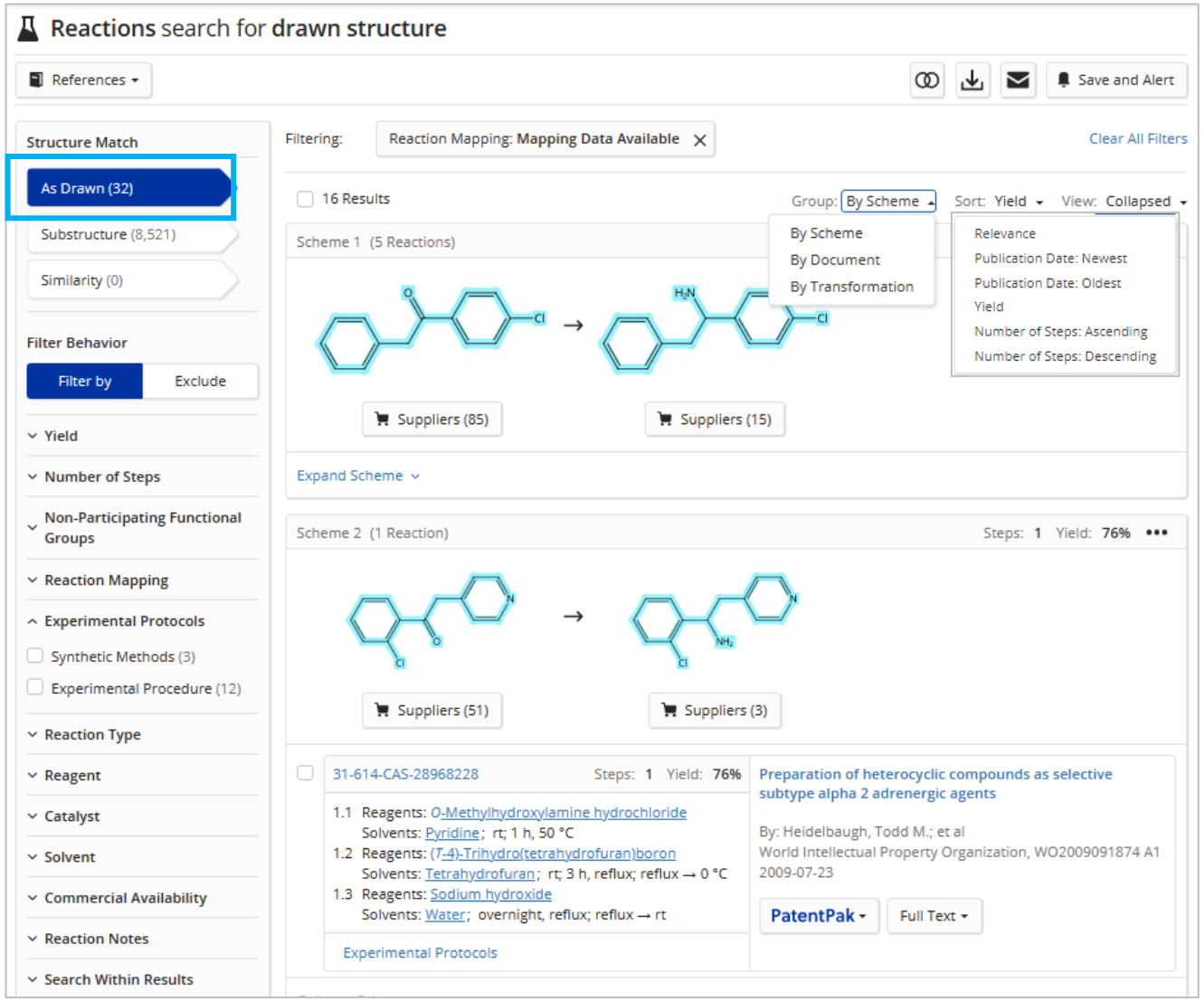
反应检索—结果集的分组与排序



反应分组：
按类型分组
按文献分组

反应排序：
相关度
公布时间
产率
步数

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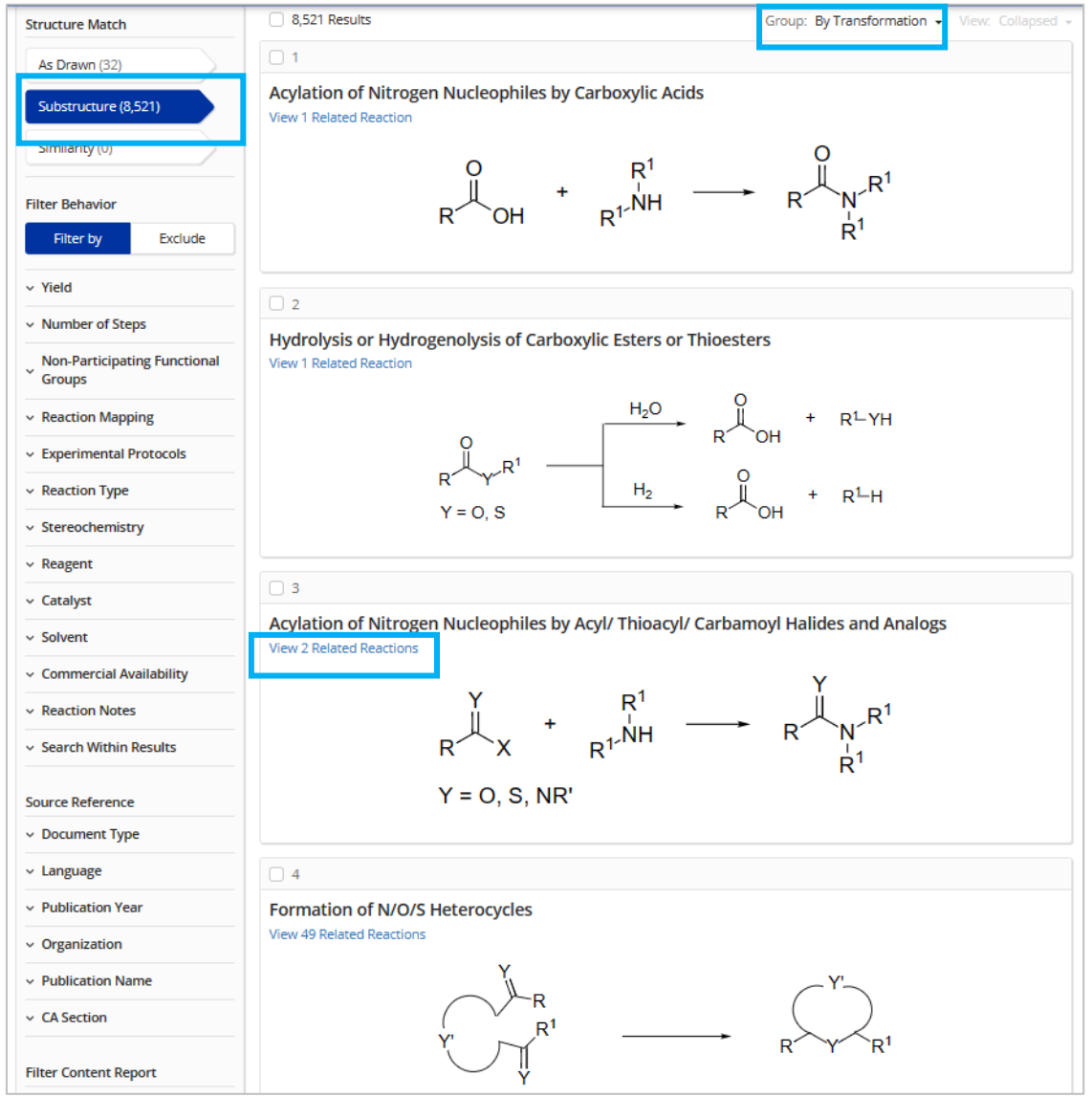
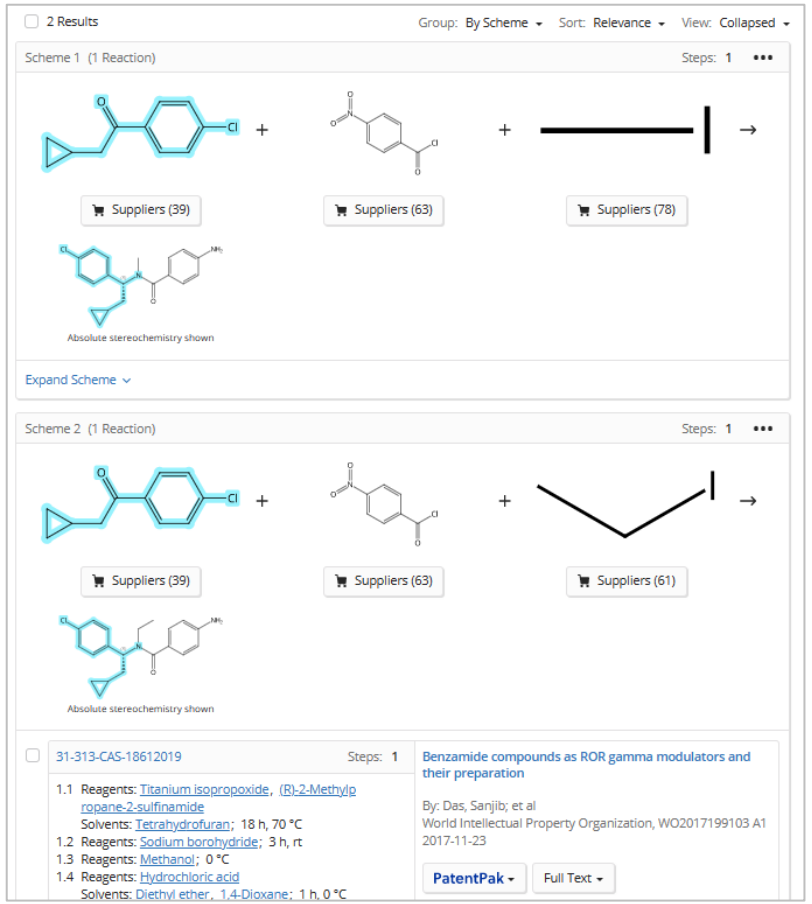
反应检索—结果集筛选

As Drawn反应检索
亚结构反应检索
相似反应检索

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

文献筛选类别：
文献类型、语言
出版年份、刊物名





折叠菜单显示：相同反应类型的反应在同一菜单里，方便阅读和筛选

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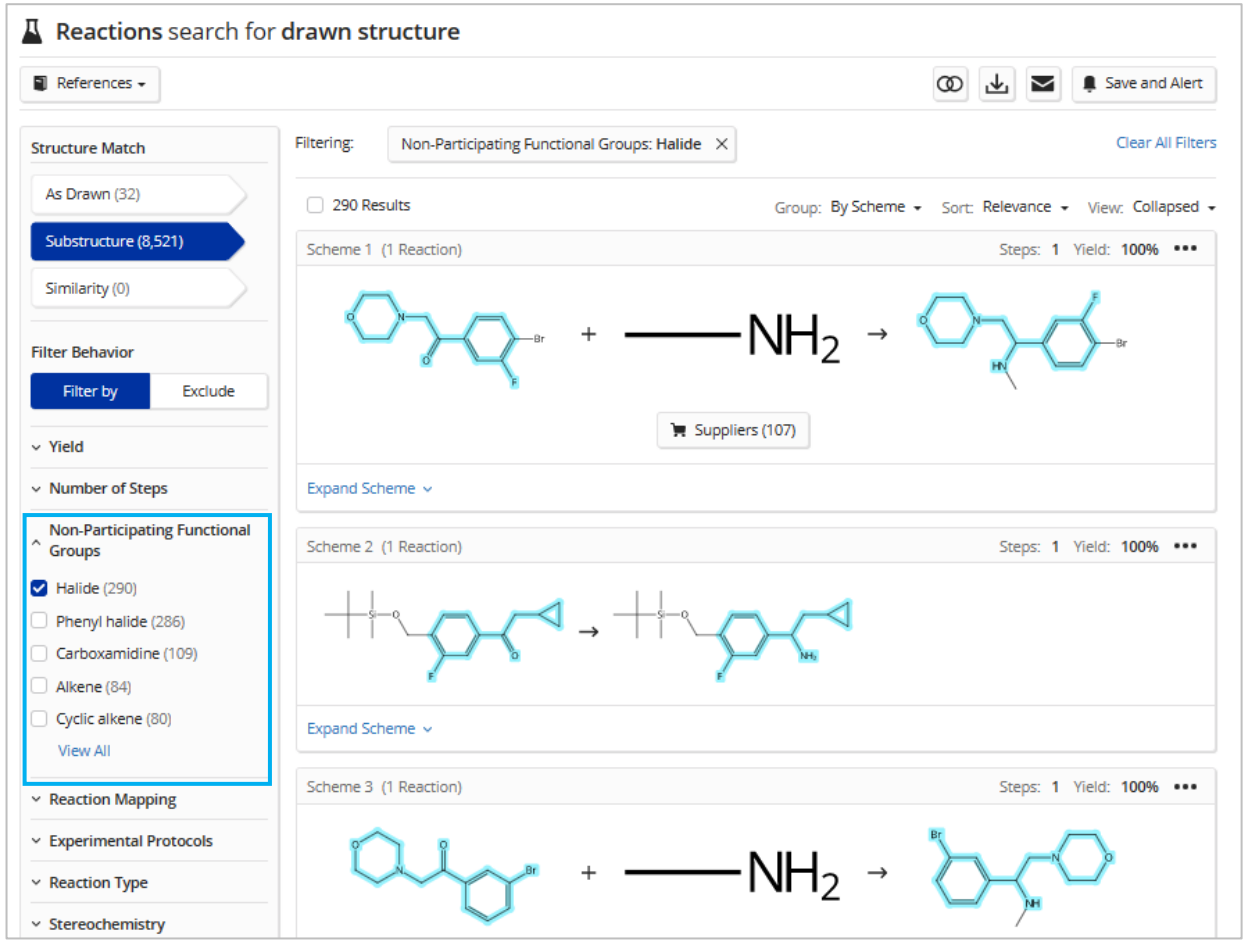
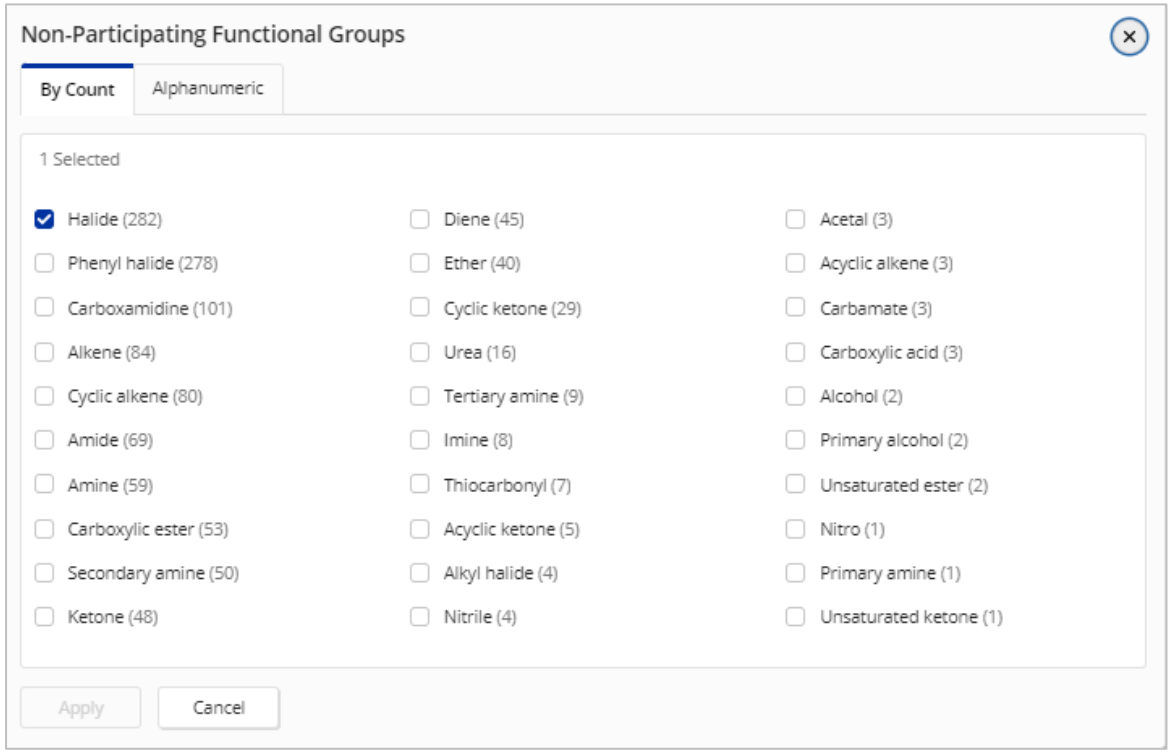
反应检索—结果集筛选：不参与反应官能团



不参与反应官能团：

出现在反应前后，但未发生变化的官能团



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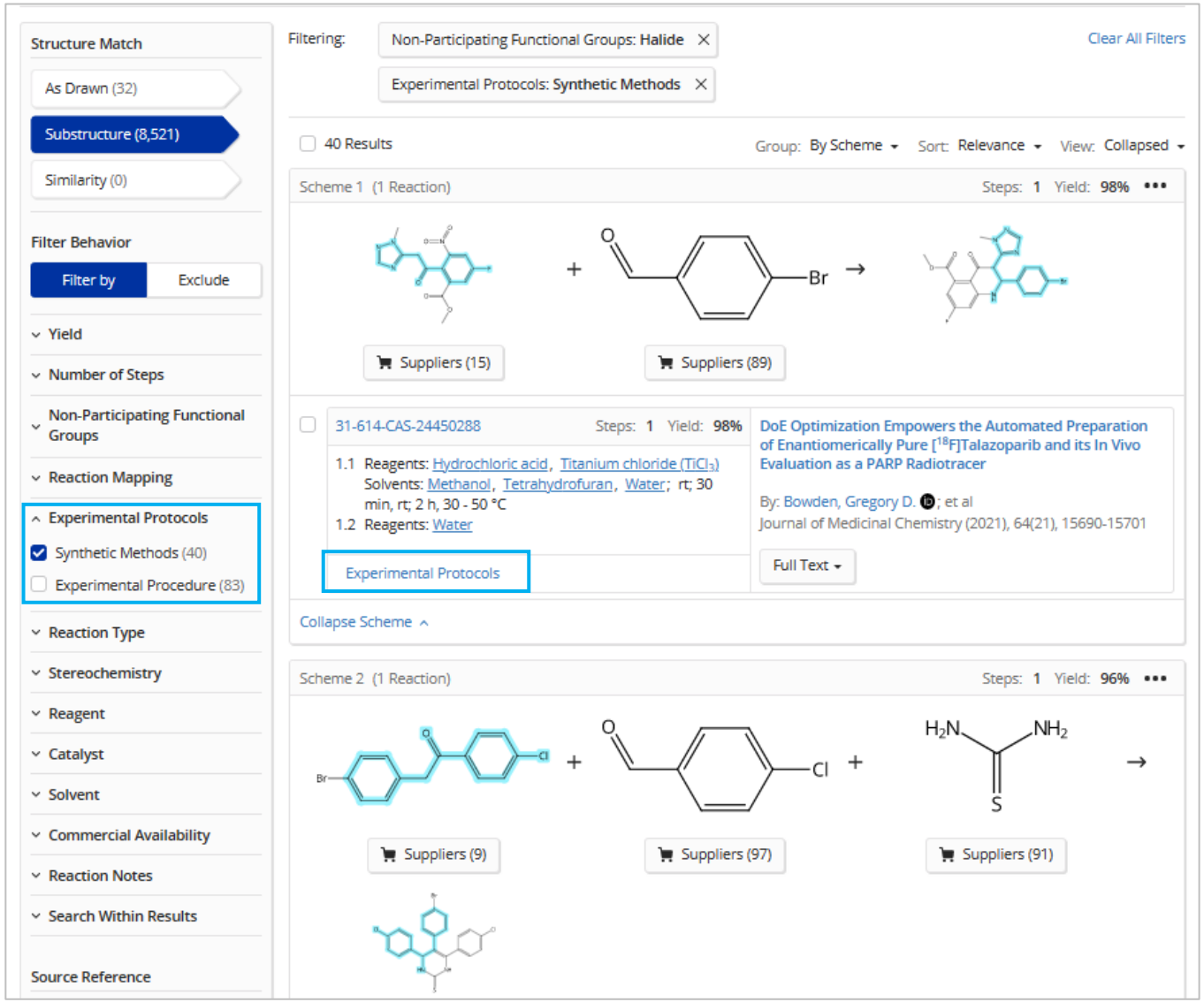
反应检索—结果集筛选：Synthetic Methods™



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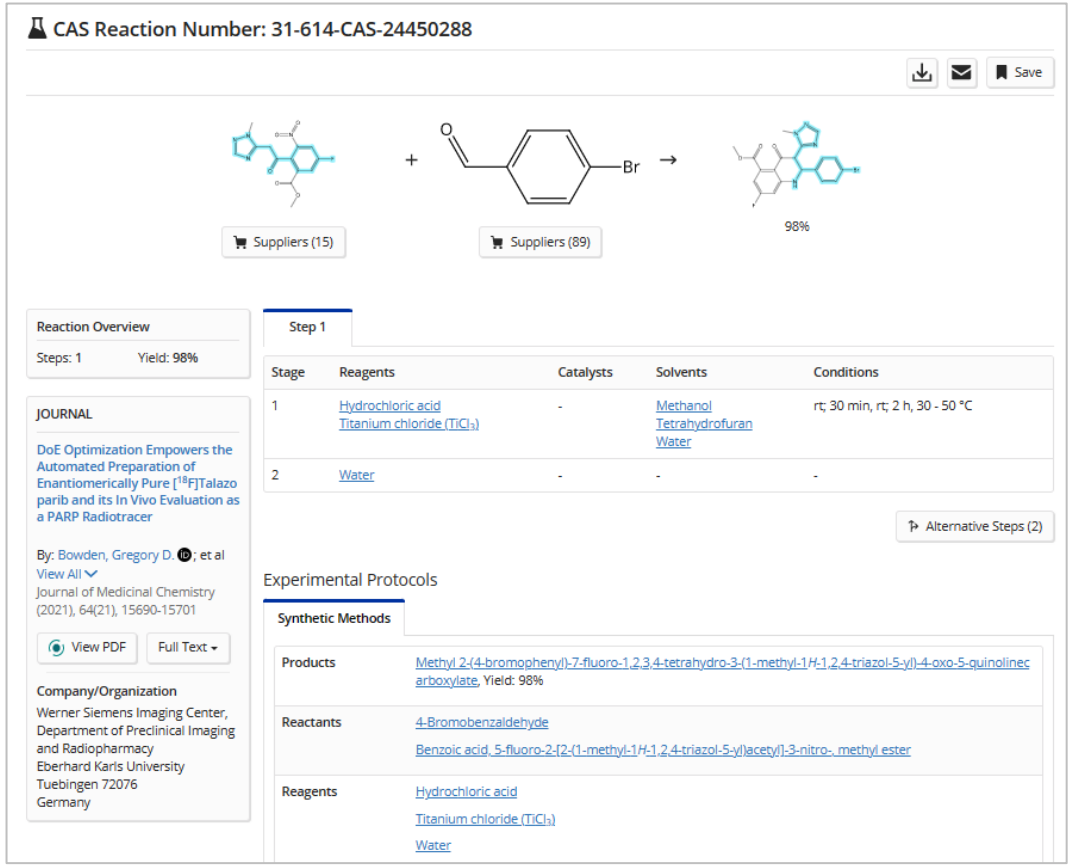
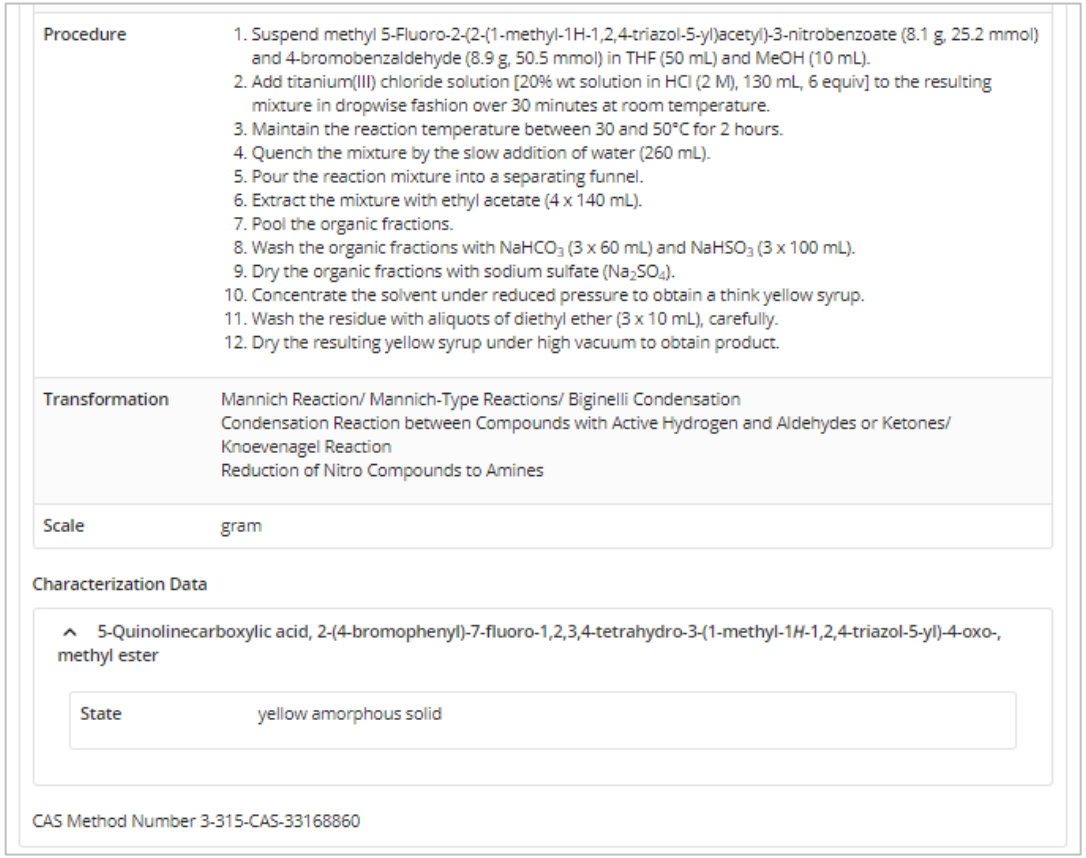
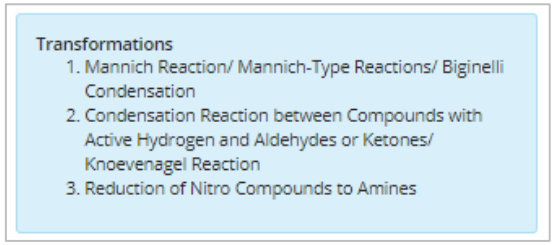
反应检索—结果集筛选：Synthetic Methods™

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







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反应检索小结

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

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大纲

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

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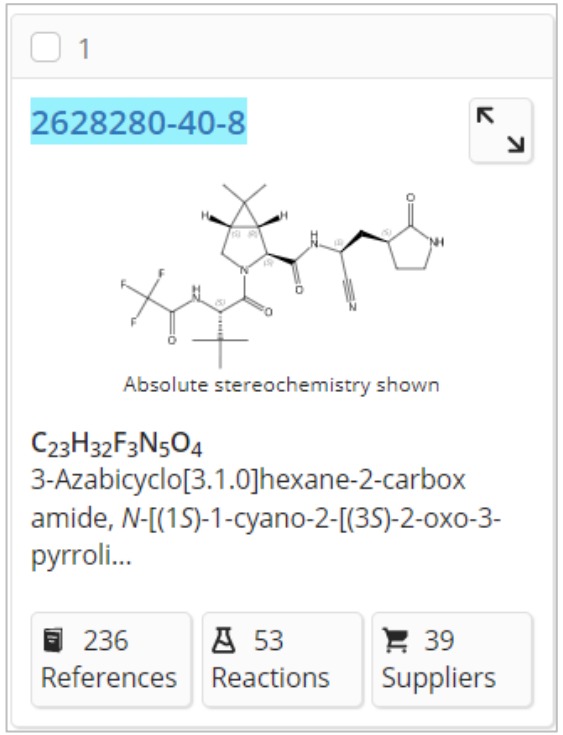
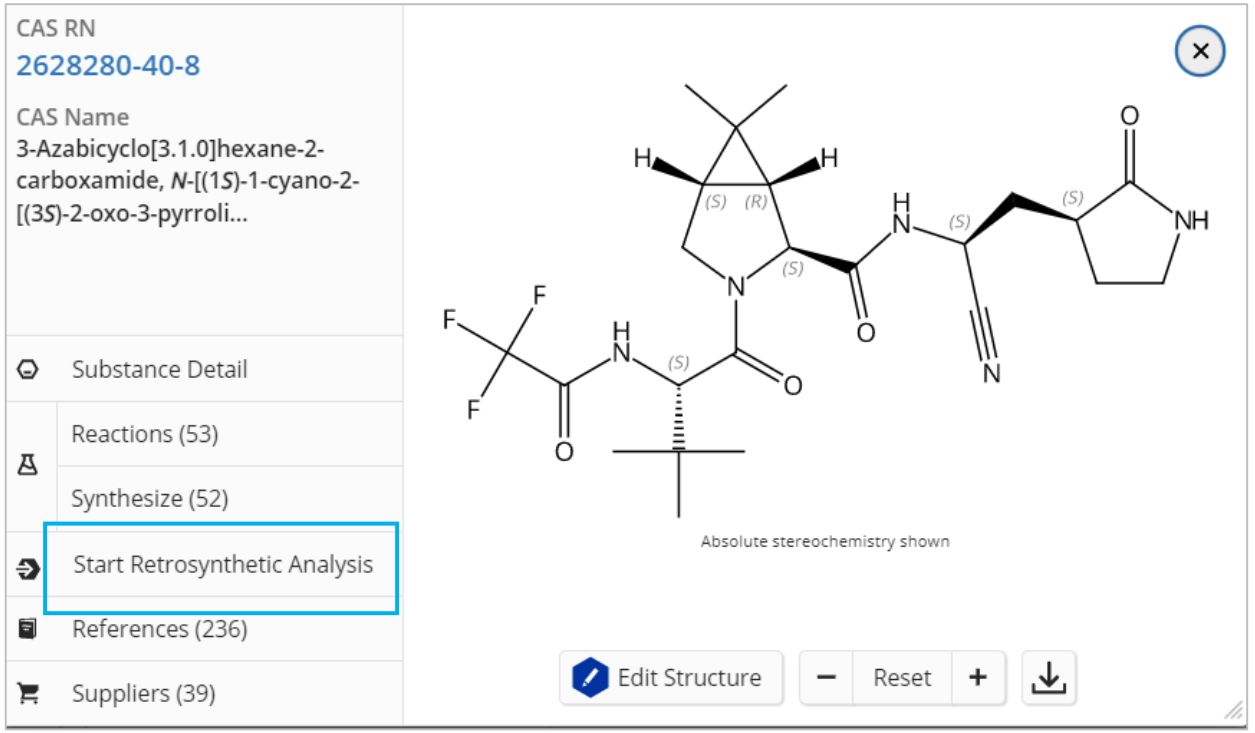
CAS Retrosynthesis Tool--由物质获得

获得已知化合物的逆合成路线（1）：
点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis





CAS Retrosynthesis Tool：

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

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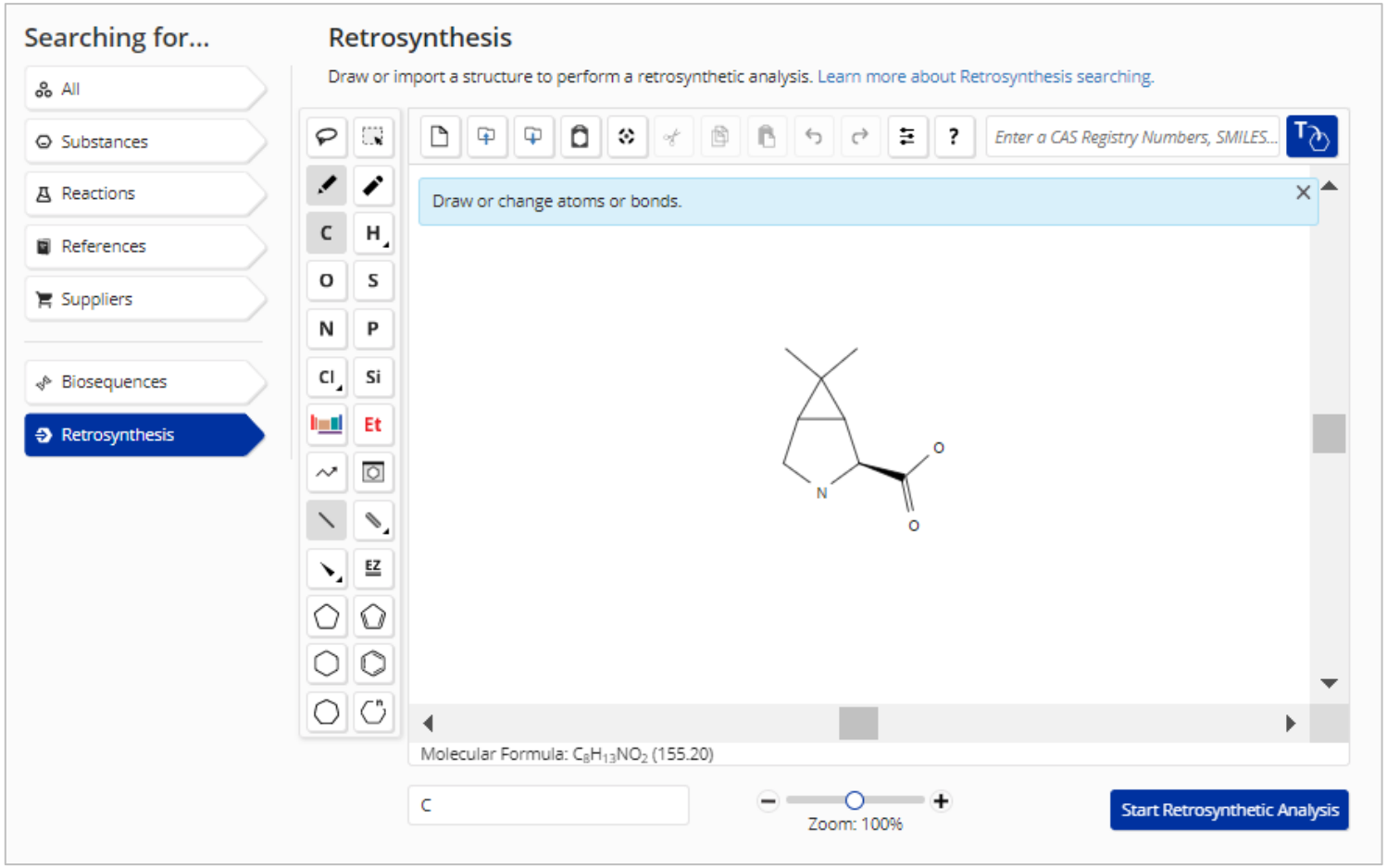
CAS Retrosynthesis Tool—直接绘制

获得已知化合物的逆合成路线（2）：
点击Retrosynthesis检索项，打开绘图板，绘制目标化合物，获得实验路线



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CAS Retrosynthesis Tool—预设参数

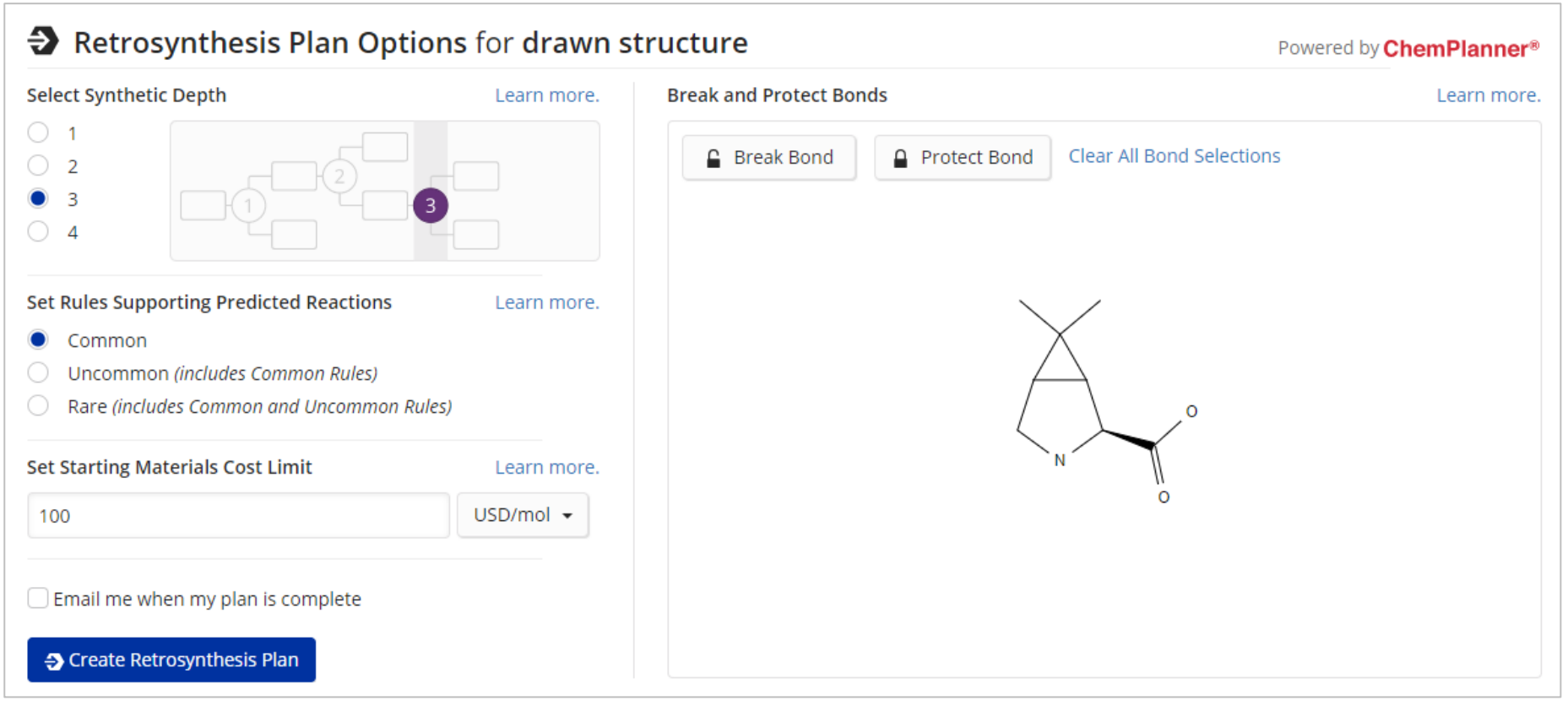
预设反应路线参数：

反应深度

反应规则常见性

起始原料费用

设置断裂键或保护键



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CAS Retrosynthesis Tool—路线概览

Off Low Medium High

Scoring Profiles：

降低每步原料结构的复杂性

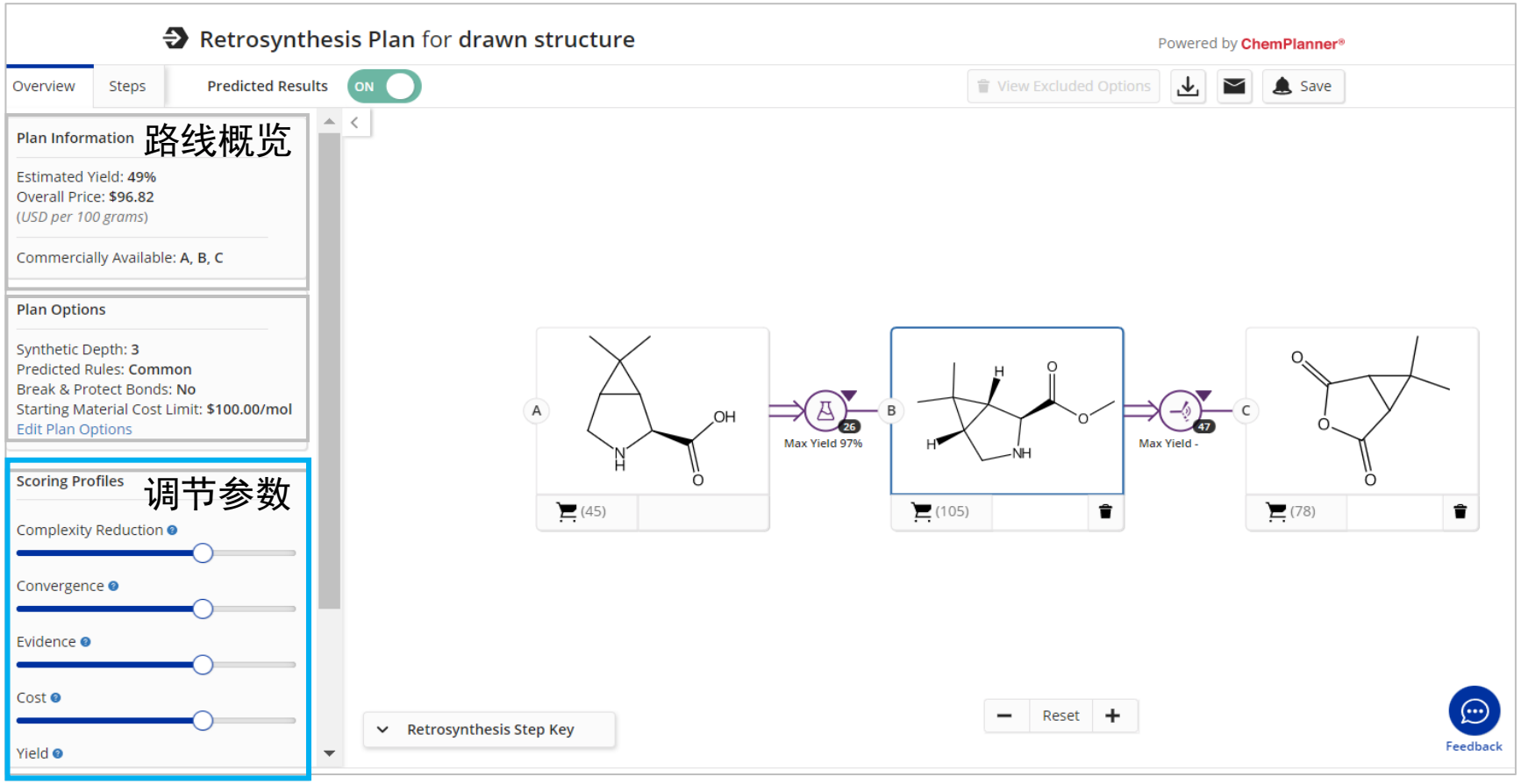
逆合成路线中前体的数量

支持预测路线的文献数量多少

预测路线大概成本

每步的产率

每步的原子转化效率



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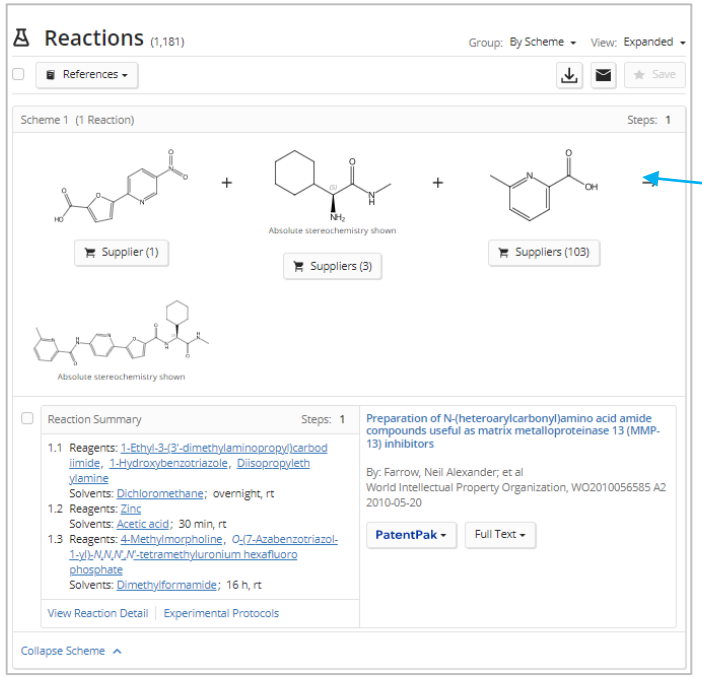
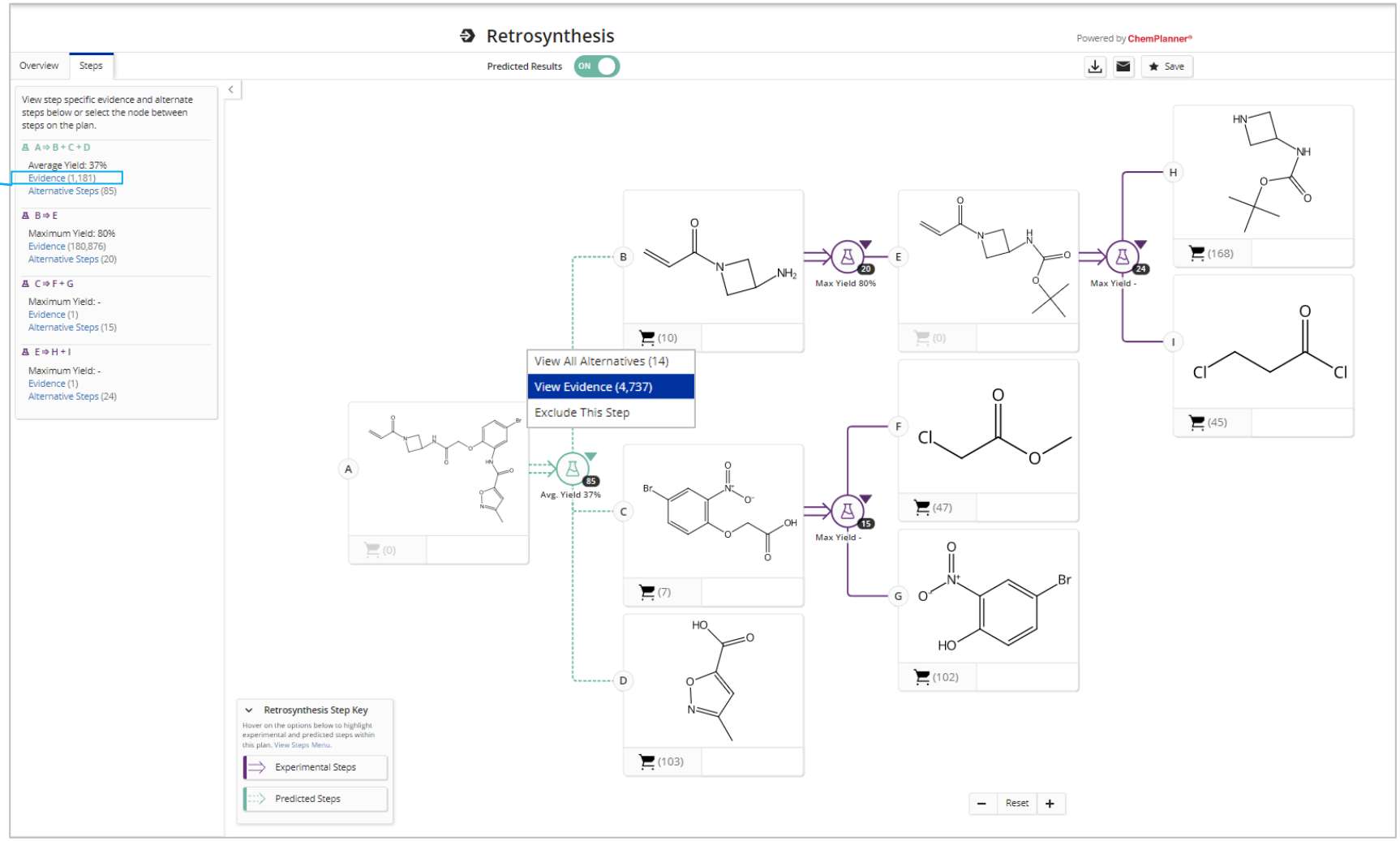
CAS Retrosynthesis Tool—路线详情

获得预测的逆合成路线





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

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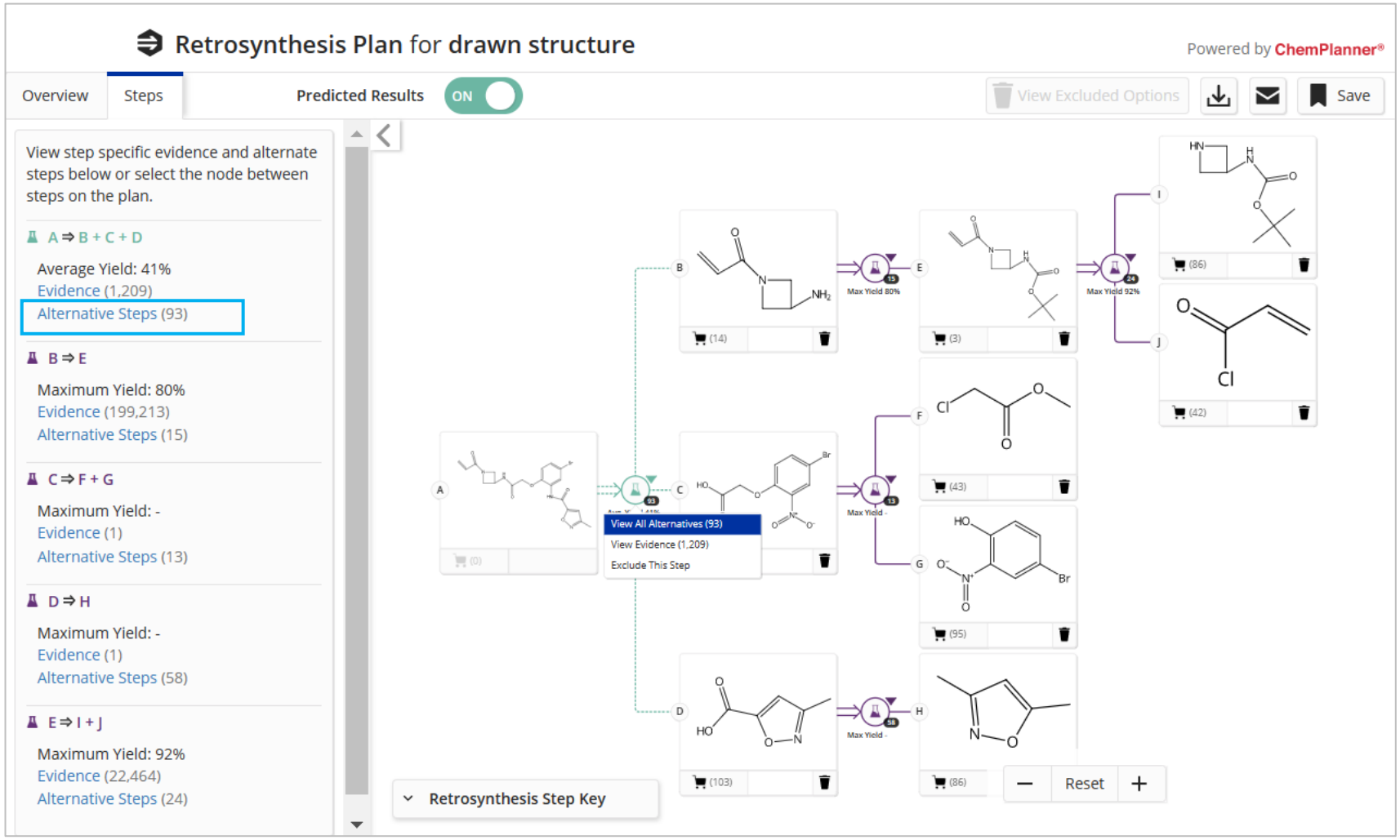
CAS Retrosynthesis Tool—路线详情

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



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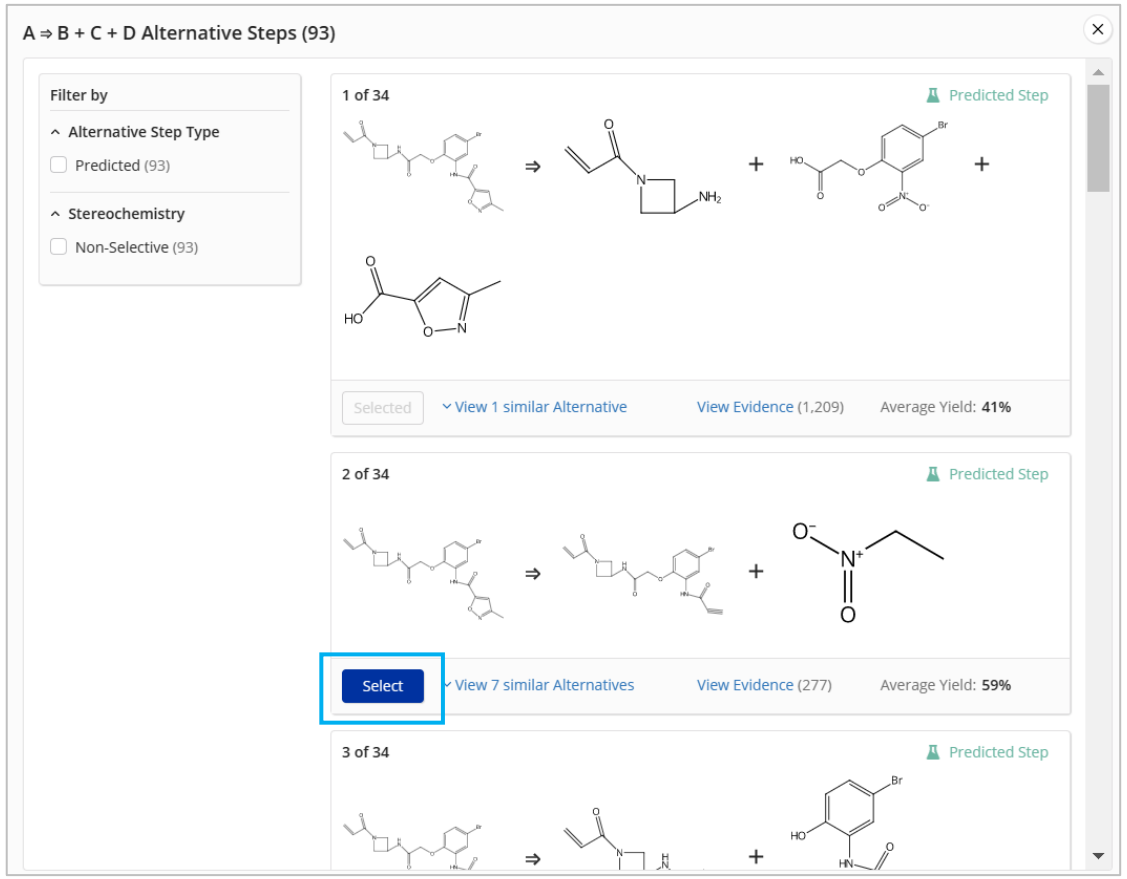
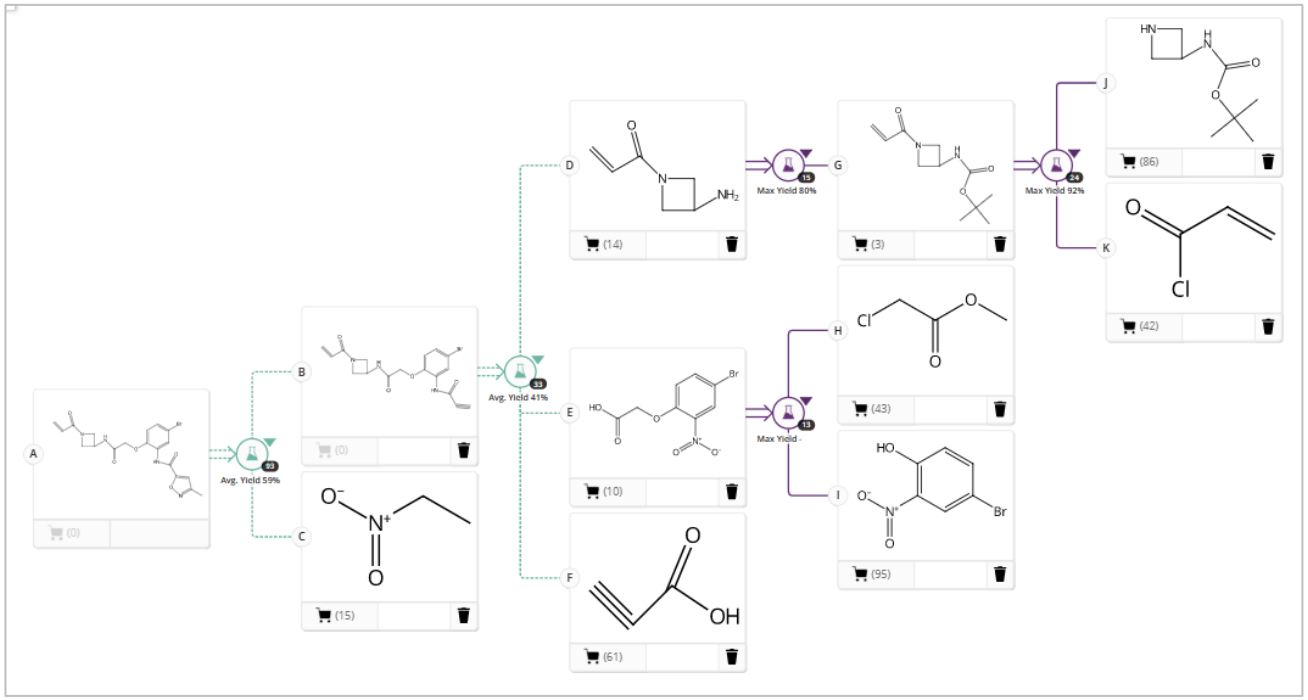
获取替代路线





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逆合成路线小结

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

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大纲

- 分析实验方法
  - 通过文献获得分析方法
  - 主题检索或分类浏览

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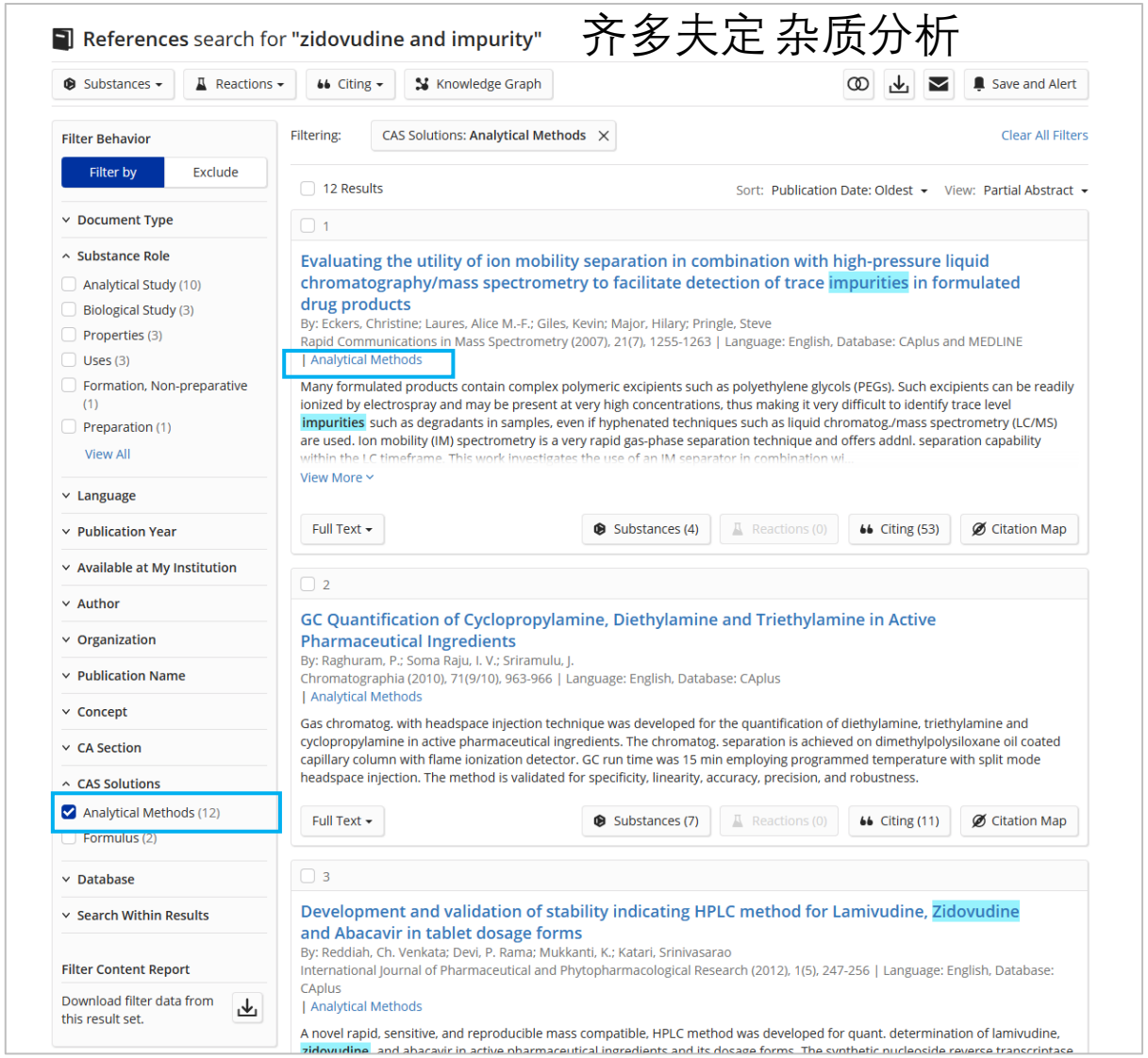
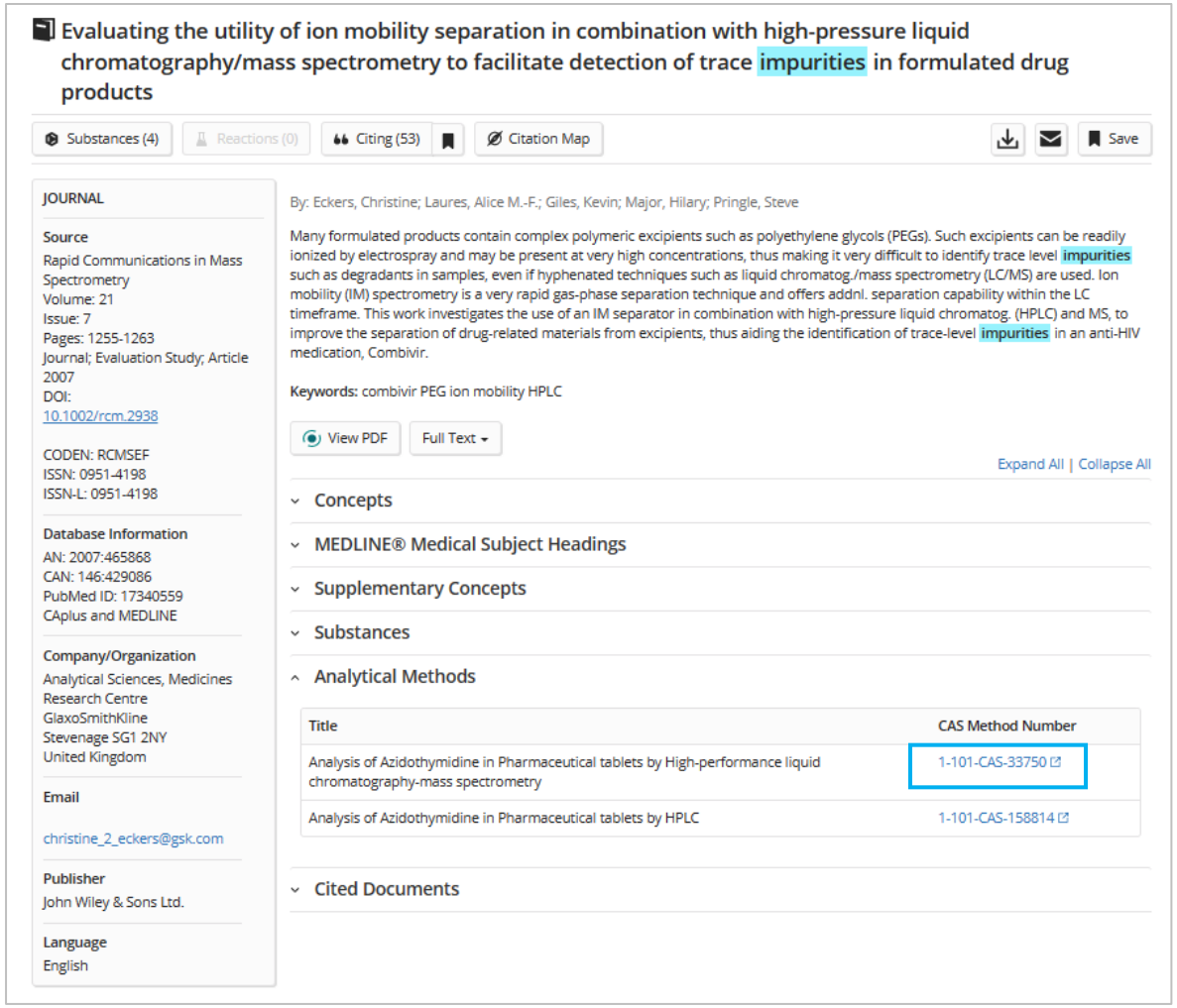
分析实验方法的获取 (1)

方法一：在文献结果页面，点击CAS solutions中的 Analytical Methods查看分析方法

齐多夫定 杂质分析





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分析实验方法详情

Method Detail (1 of 1)

← Prev Next →

Analysis of Azidothymidine in Pharmaceutical tablets by High-performance liquid chromatography-mass spectrometry

CAS MN: 1-101-CAS-33750

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: High-performance liquid chromatography-mass spectrometry

实验原料

Materials	Role	Image	CAS RN
Azidothymidine	analyte	View Structure	30516-87-1
Lamivudine	analyte	View Structure	134678-17-4
Pharmaceutical tablets	matrix		
Luna 3 µm C18(2), 100 × 4.6 mm column	material		
Acetonitrile	reagent	View Structure	75-05-8

文献详情

Source

Evaluating the utility of ion mobility separation in combination with high-pressure liquid chromatography/mass spectrometry to facilitate detection of trace impurities in formulated drug products

Eckers, Christine; Laures, Alice M.-F.; Giles, Kevin; Major, Hilary; Pringle, Steve

Rapid Communications in Mass Spectrometry (2007), 21 (7), 1255 - 1263. John Wiley & Sons Ltd.

CODEN: RCMSEF | ISSN: 09514198 | DOI: 10.1002/rcm.2938

Full Text | View in CAS SciFinder

Abstract

Many formulated products contain complex polymeric excipients such as polyethylene glycols (PEGs). Such excipients can be readily ionized by electrospray and may be present at very high concentrations, thus making it very difficult to identify trace level impurities such as degradants in samples, even if hyphenated techniques such as liquid chromatog./mass spectrometry (LC/MS) are used. Ion mobility (IM) spectrometry is a very rapid gas-phase separation technique and offers addnl. separation capability within the LC timeframe. This work investigates the use of an IM separator in combination with high-pressure liquid chromatog. (HPLC) and MS, to improve the separation of drug-related materials from excipients, thus aiding the identification of trace-level impurities in an anti-HIV medication, Combivir.

Equipment Used

分析仪器

Chromatography system, 1100, Agilent Technologies, Stockport, UK

Q-ToF Ultima quadrupole orthogonal acceleration (oa) ToF mass spectrometer, Waters Corp., Milford, MA, USA

Conditions

分析条件

Instrument

column: Luna 3 µm C18(2), 100 × 4.6 mm; mobile phase: eluent (A) 0.025 M ammonium acetate in water, pH adjusted to 4.5 with glacial acetic acid and eluent (B) 0.025 M ammonium acetate in methanol; elution program: 25% volume fraction of B increased to 50% over 9 min; flow rate: 1 mL/min

positive electrospray ionization (+ve ESI) mode; electrospray probe held at 3 kV; nitrogen desolvation and nebuliser gas flow rates: 400 and 90 L/h; source temperature: 100 °C; desolvation temperature: 300 °C; cone voltage: 30 V

Instructions

操作步骤

Preparation of tablet

1. Prepare tablet samples (containing 150 mg of active ingredient in approximately 750 mg of tablet) by taking a weight of tablet material containing an equivalent of 10 mg of zidovudine.
2. Shake with 2 mL of 75/25 water/acetonitrile and centrifuge at 13, 000 rpm for 1 min.
3. Use supernatant for the analysis.

Preparation of standard samples

1. Prepare standard samples at a concentration of 1 mg/ mL in 75/25 v/v water/acetonitrile and serially dilute in the same solvent to give the required concentration of 100 ng/mL.
2. Prepare polyethylene glycol (PEG-400) at a concentration of 0.1 mg/mL and mix 1:1 with the standards for the infusion experiments.

Liquid chromatography-mass spectrometry (LC/MS) analysis

1. Analyze the sample using Agilent 1100 chromatography system (Agilent Technologies, Stockport, UK) for LC/MS on the Q-ToF Ultima and a Waters ACQUITY UPLC system, operating at HPLC pressures.
2. Perform separation with Luna 3 µm C18(2), 100 × 4.6 mm column at room temperature.
3. Use eluent (A) 0.025 M ammonium acetate in water, pH adjusted to 4.5 with glacial acetic acid and eluent (B) 0.025 M ammonium acetate in methanol as mobile phase.
4. Set the elution program as: 25% volume fraction of B increased to 50% over 9 min.
5. Set the flow rate at 1 mL/min.
6. Operate Q-ToF Ultima quadrupole orthogonal acceleration (oa) ToF mass spectrometer (Waters Corp., Milford, MA, USA) in positive electrospray ionization (+ve ESI) mode.
7. Set the parameters as: electrospray probe held at 3 kV; nitrogen desolvation and nebuliser gas flow rates: 400 and 90 L/h; source temperature: 100 °C; desolvation temperature: 300 °C; cone voltage: 30 V.
8. Detect at 245 - 285 nm using spectrometer.

数据有效性

Validation

Retention Time	1.89 min, Lamivudine
	4.55 min, Zidovudine

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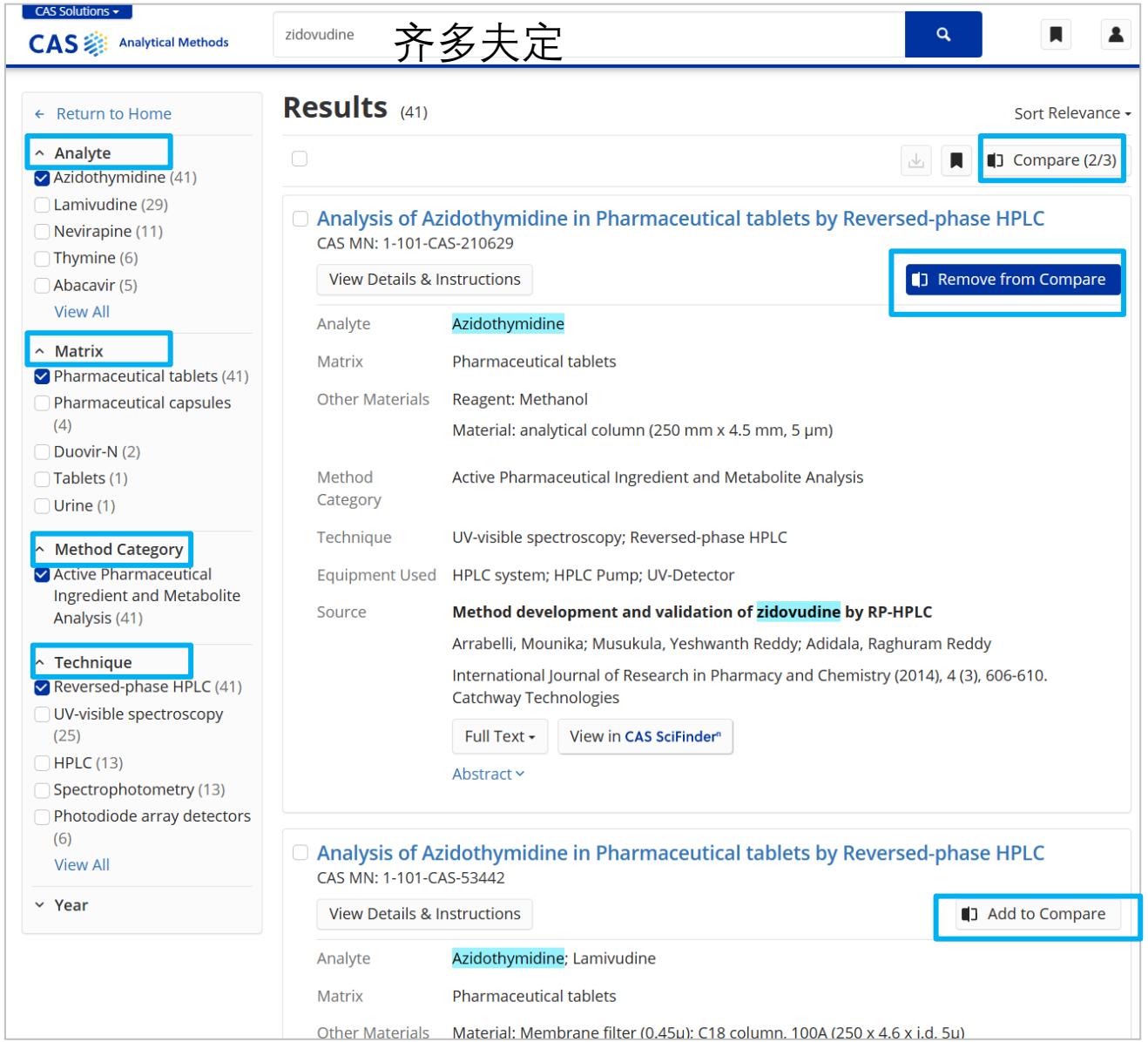
分析实验方法的获取 (2)

方法二：登录https://methods.cas.org

- 主题检索或分类浏览；
- 筛选分析目标物、介质、方法类别、分析技术等

方法分类: 13大类，45小类

农业应用、生物鉴定、生物分子分离、环境、食品、考古、有机物、药学、毒理学等



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分析方法的对比

方法名称、CAS方法登记号、方法类别、分析技术、分析目标物、介质、相关材料、分析仪器、条件、文献来源、样品制备、分析方法详情、检测限、分析精度、滞留时间等

Compare Methods

Expand All | Collapse All

	1	2
Title	**Analysis of Azidothymidine in Pharmaceutical tablets by Reversed-phase HPLC**	**Analysis of Lamivudine in Pharmaceutical tablets by Reversed-phase HPLC**
CAS Method Number	1-101-CAS-210629	1-101-CAS-102694
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	UV-visible spectroscopy; Reversed-phase HPLC	Liquid chromatography spectrometric detectors; Reversed-phase HPLC
Analyte	Azidothymidine	Efavirenz; Azidothymidine; Lamivudine
Matrix	Pharmaceutical tablets	Pharmaceutical tablets
Other Materials	Methanol; analytical column (250 mm x 4.5 mm, 5 µm)	C_{18} column (250 × 4.6 mm, ø 5 µm); Filter paper (0.28 µm); 0.45 µm Filter
Equipment Used	HPLC system, Shimadzu; HPLC Pump, LC10AD, Shimadzu; UV-Detector, SPD-10A, Shimadzu	HPLC system, 110, HP/Agilent; Quaternary pump, G1311A, HP/Agilent; Diode array detector, G1315A, HP/Agilent; Autoinjector, G1367A, HP/Agilent; Column oven, G1322A, View All
Conditions	**Instrument:** Mobile phase- methanol:water (80:20 v/v); folw rate- 1 mL/min; injection volume- 20 µL; temperature- room temperature; Detection wavelength- 267 nm	**Instrument:** mobile phase A: acetonitrile; mobile phaseB: water; injection volume:10 µL; detection wavelength, 278 nm
Source	**Method development and validation of zidovudine by RP-HPLC** Arrabelli. Mounika: Musukula. Yeshwanth Reddv: Adidala. View All	**Simultaneous determination of antiretroviral zidovudine, lamivudine and efavirenz by RP HPLC-DAD** Soares. Monica F. de L. R.: Soares-Sobrinho. Iose L.: da Silva. View All
Preparation	**Sample Preparation** 1. Powder 10 tablets of zidovudine using motor and pestle View All	**Processing of pharmaceutical tablets** 1. Collect the DFC tablets, weigh, crush and pulverize. 2. Weigh analytically an equivalent of 12.50 mg of View All
Method	1. Analyze the samples using Shimadzu HPLC model with LC10AD Pump and SPD-10A UV-Detector. 2. Separate the analytes using an analytical Inspire C_{18} View All	**High performance liquid chromatography analysis** 1. Analyze the sample using HP/Agilent HPLC 110 equipment consisting of quaternary G1311A pumps View All
Limit of Quantitation	0.025 µg/mL	
Accuracy	91.76 - 98.79% (intra-day), 91.71 - 98.23% (inter-day), for 40 - 4000 ng/mL spiked	
Precision	1.323 - 7.254% (CV, intra-day), 1.30 - 7.83% (CV, inter-day), for 40 - 4000 ng/mL spiked	1.20% (RSD), Zidovudine, 0.47% (RSD), Lamivudine, 0.69% (RSD), Efavirenz
Retention Time	10.2 min	2.84 min, Zidovudine, 2.28 min, Lamivudine, 8.30 min, Efavirenz

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分析实验方法小结

1. 通过文献结果集获得关联的分析方法
2. 直接通过主题检索或分类浏览获取分析实验方法
3. 查看分析实验方法操作详情，筛选分析目标物、介质、分析方法

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大纲

- 配方/制剂信息检索
  - 通过检索式检索配方/制剂
  - 通过文献获得配方/制剂信息

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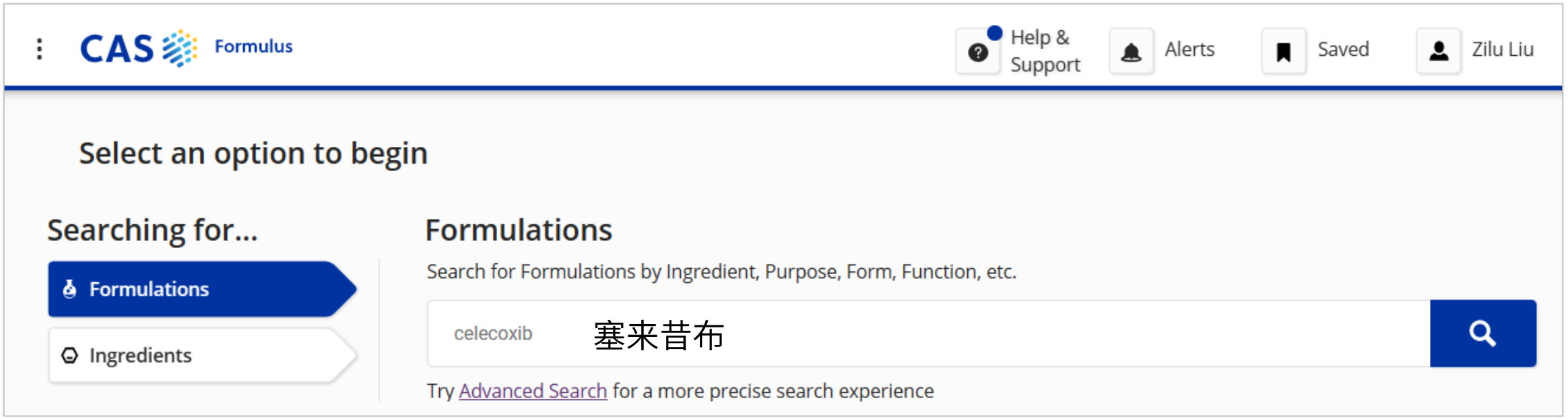
检索配方或制剂 https://formulus.cas.org

方法（1）：

- 登录CAS Formulus主页
- 在检索框输入检索式，如制剂或配方的原料、用途、物理形态、功能或文献识别符（包括专利号、DOI号和CA入库号）进行检索
- 支持高级检索



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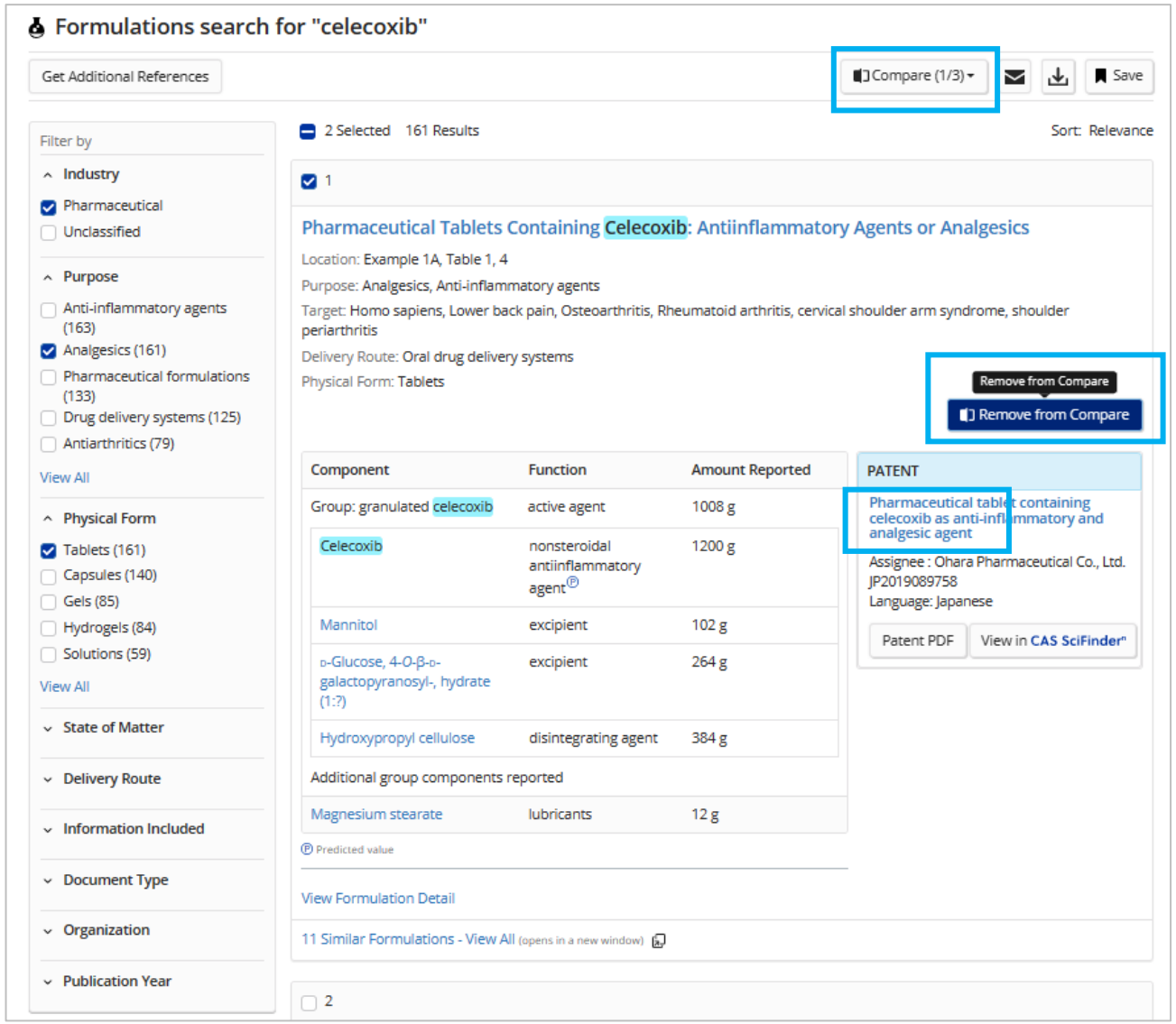
配方/制剂结果集



- 利用聚类项精简结果：

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

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

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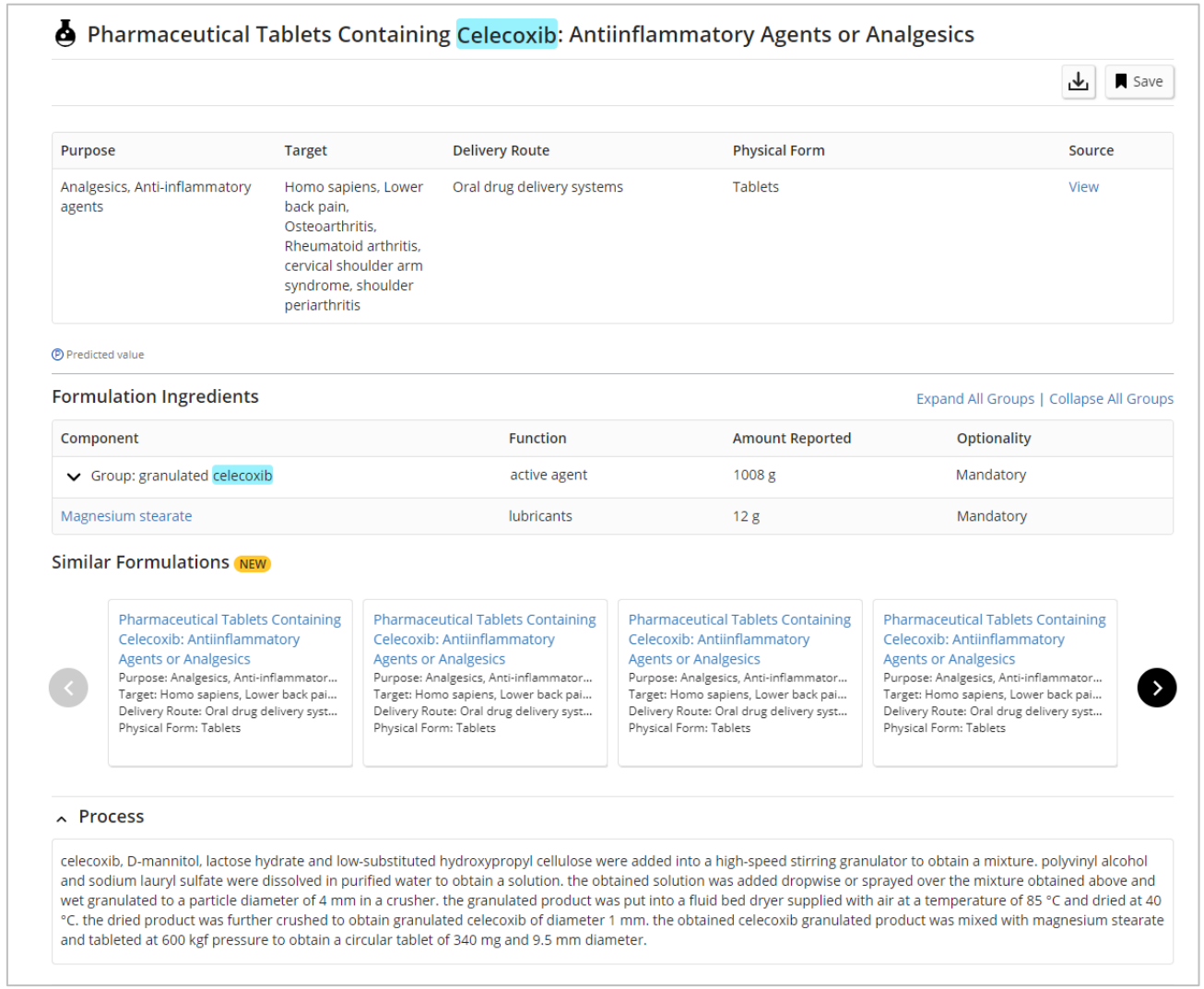
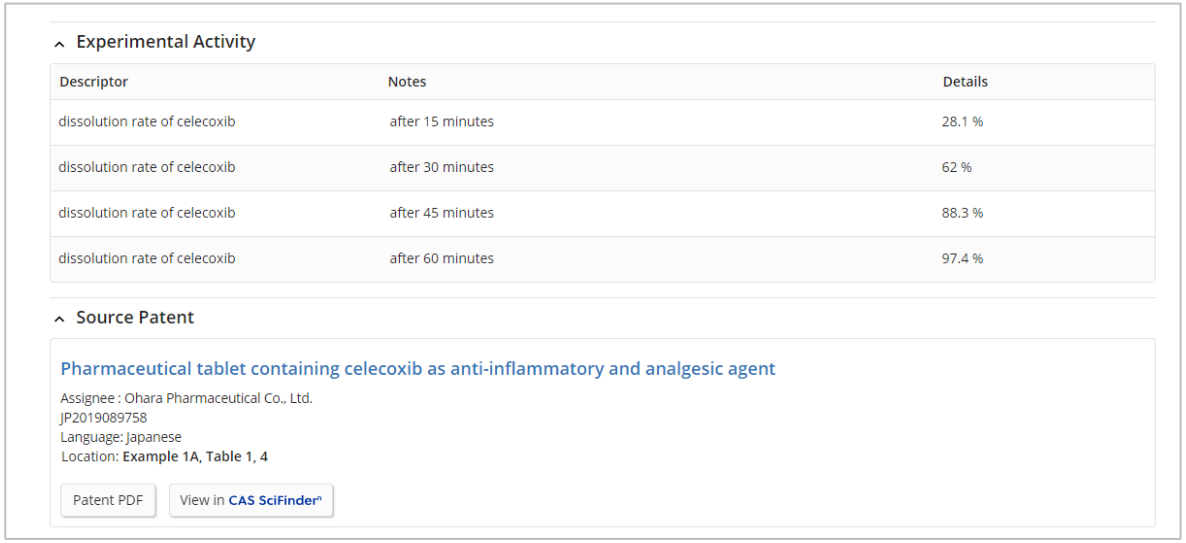
查看制剂或配方详情





- 制剂或配方原料
- 相似的制剂或配方
- 制备工艺
- 制剂或配方实验评估
- 专利来源

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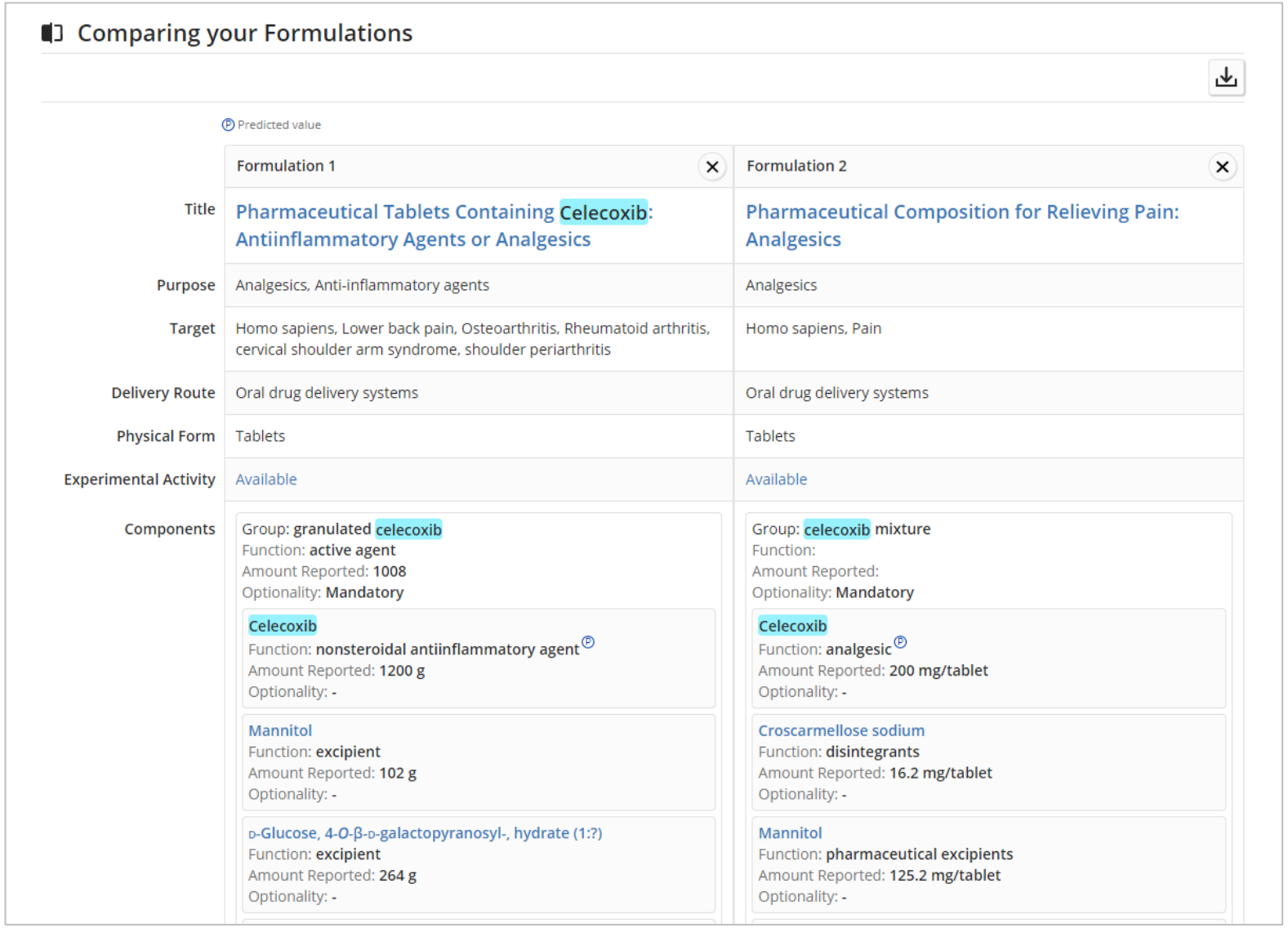
不同制剂或配方信息的对比



Comparing your Formulations

Predicted value

	Formulation 1	Formulation 2
Title	Pharmaceutical Tablets Containing Celecoxib: Antiinflammatory Agents or Analgesics	Pharmaceutical Composition for Relieving Pain: Analgesics
Purpose	Analgesics, Anti-inflammatory agents	Analgesics
Target	Homo sapiens, Lower back pain, Osteoarthritis, Rheumatoid arthritis, cervical shoulder arm syndrome, shoulder periarthritis	Homo sapiens, Pain
Delivery Route	Oral drug delivery systems	Oral drug delivery systems
Physical Form	Tablets	Tablets
Experimental Activity	Available	Available
Components	Group: granulated celecoxib Function: active agent Amount Reported: 1008 Optionality: Mandatory Celecoxib Function: nonsteroidal antiinflammatory agent (P) Amount Reported: 1200 g Optionality: - Mannitol Function: excipient Amount Reported: 102 g Optionality: - D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?) Function: excipient Amount Reported: 264 g Optionality: -	Group: celecoxib mixture Function: Amount Reported: Optionality: Mandatory Celecoxib Function: analgesic (P) Amount Reported: 200 mg/tablet Optionality: - Croscarmellose sodium Function: disintegrants Amount Reported: 16.2 mg/tablet Optionality: - Mannitol Function: pharmaceutical excipients Amount Reported: 125.2 mg/tablet Optionality: -

- 选择感兴趣的制剂或配方进行对比
- 一次最多可以比较三种不同制剂或配方的信息详情

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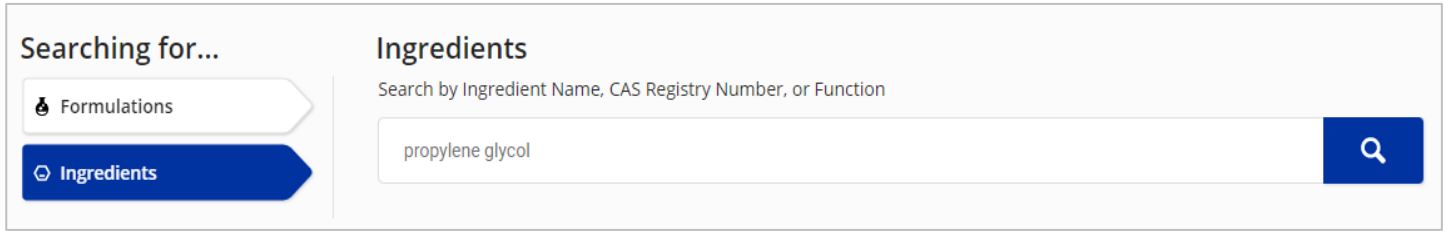
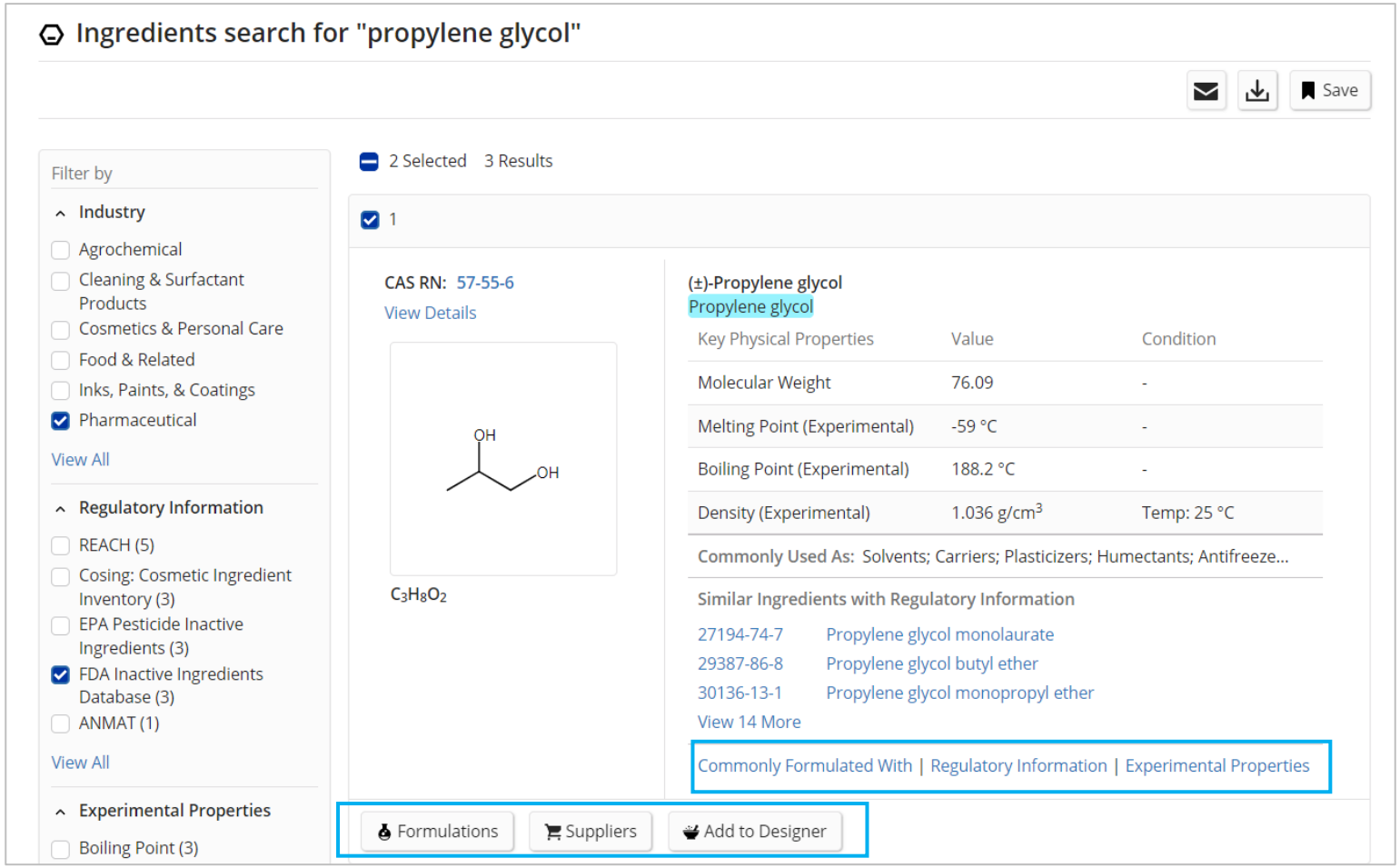
检索原料





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

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

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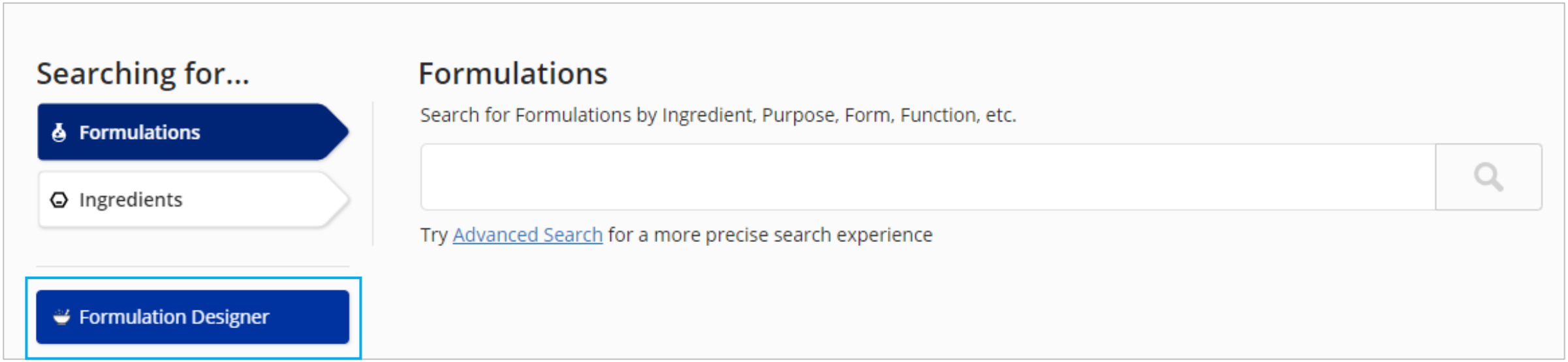
设计制剂或配方



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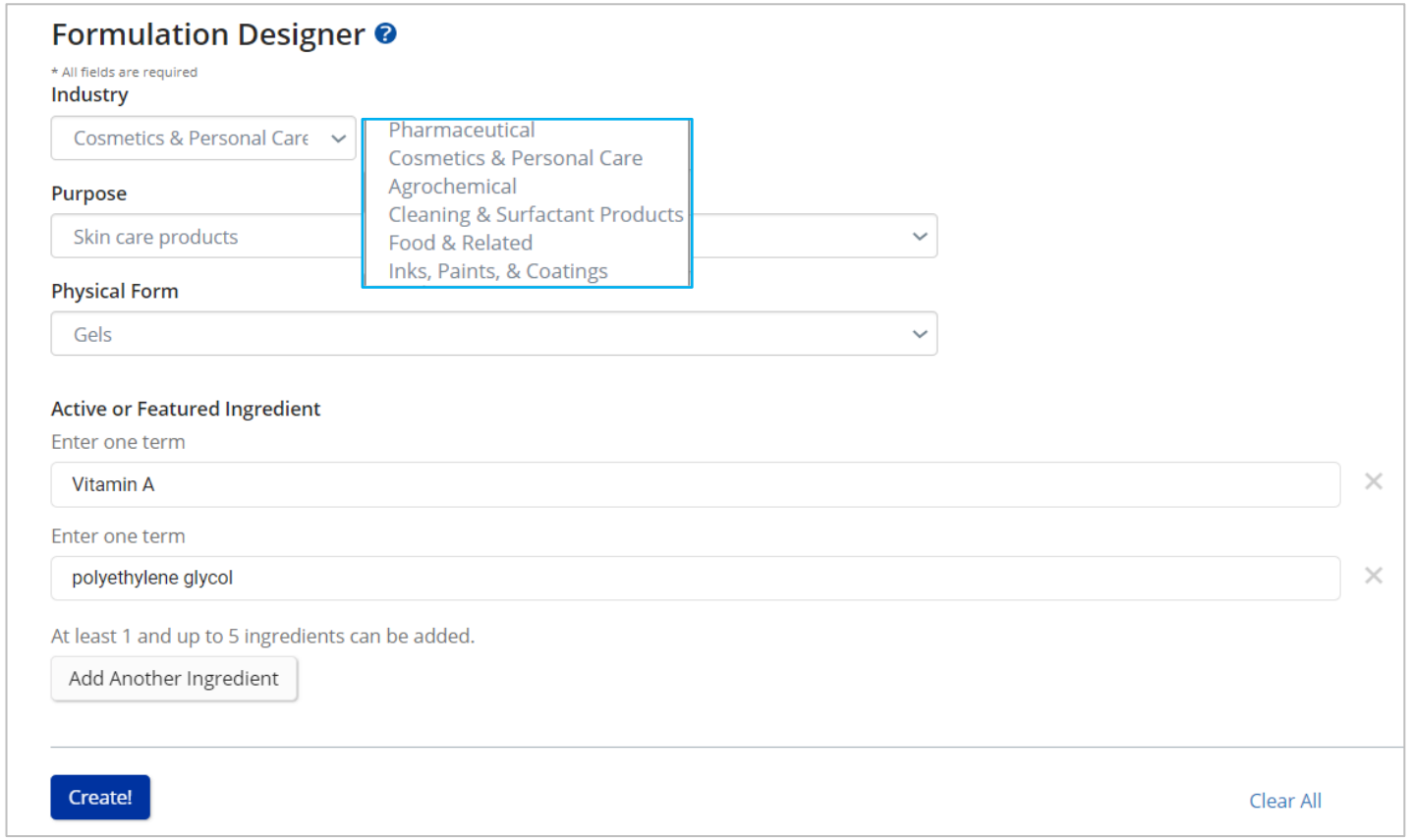
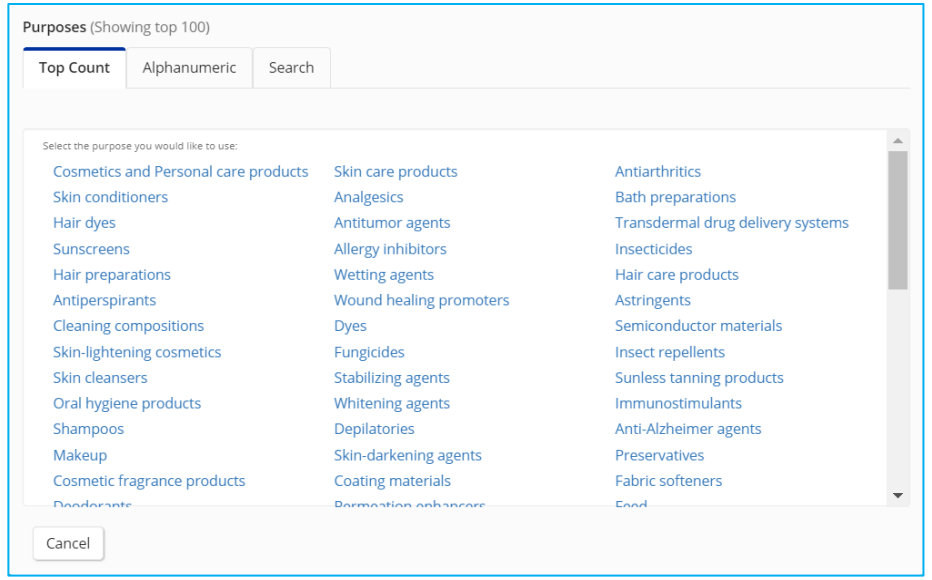
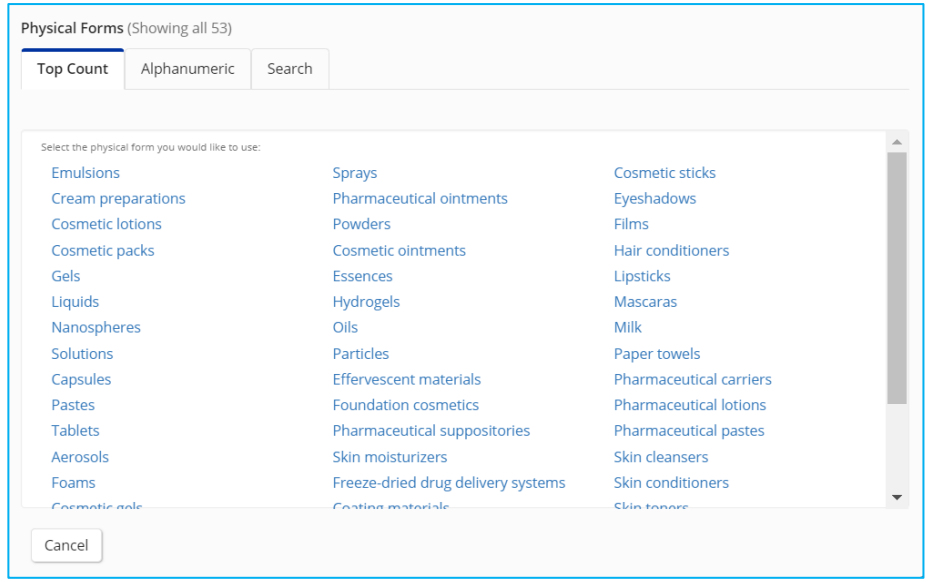
设计配方制剂







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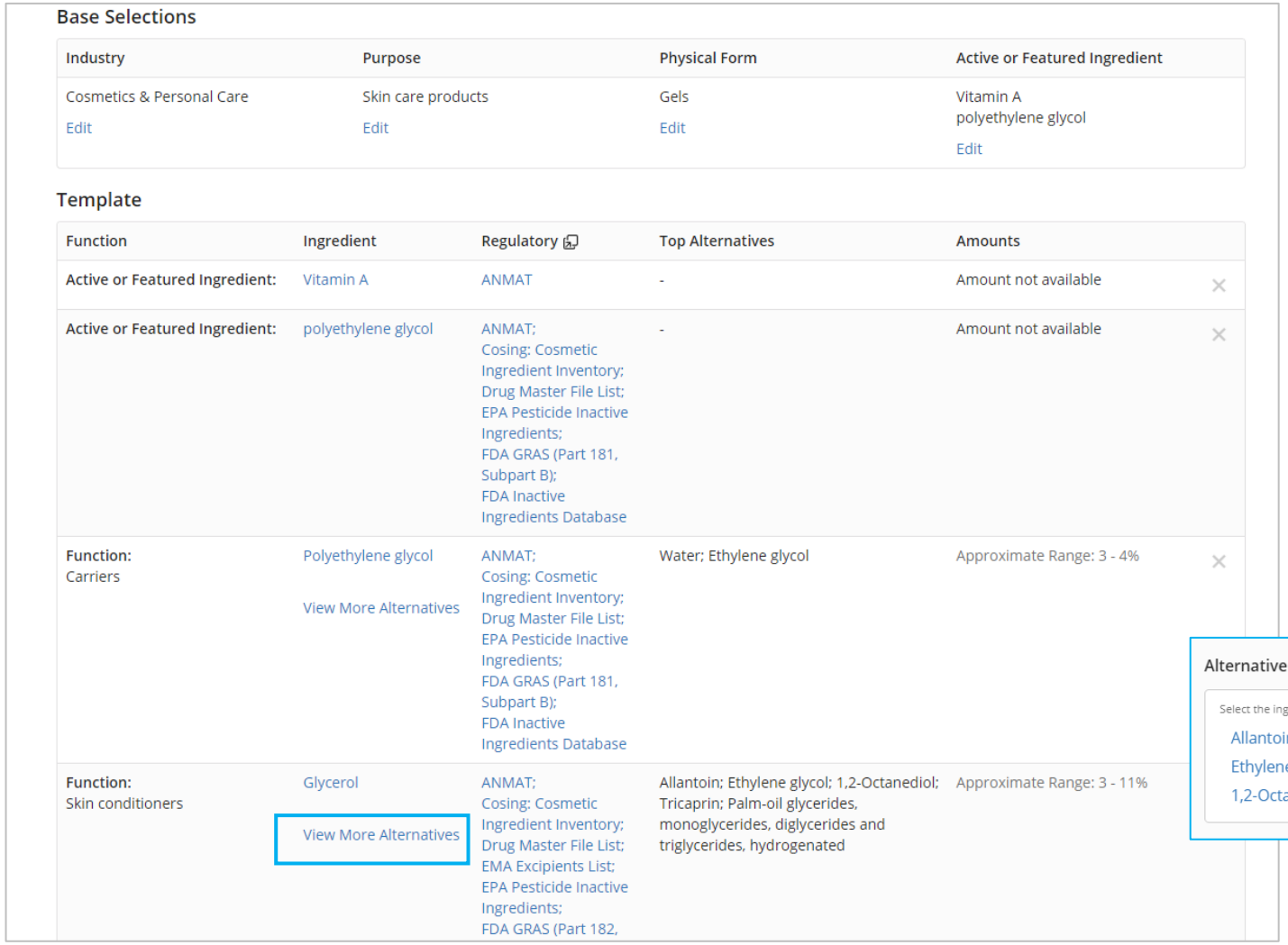
查看制剂或配方设计结果详情



Base Selections

Industry	Purpose	Physical Form	Active or Featured Ingredient
Cosmetics & Personal Care Edit	Skin care products Edit	Gels Edit	Vitamin A polyethylene glycol Edit

Template

Function	Ingredient	Regulatory	Top Alternatives	Amounts
Active or Featured Ingredient:	Vitamin A	ANMAT	-	Amount not available
Active or Featured Ingredient:	polyethylene glycol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available
Function: Carriers	Polyethylene glycol View More Alternatives	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	Water; Ethylene glycol	Approximate Range: 3 - 4%
Function: Skin conditioners	Glycerol View More Alternatives	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 182,	Allantoin; Ethylene glycol; 1,2-Octanediol; Tricaprin; Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated	Approximate Range: 3 - 11%

Alternative Ingredients (Showing all 7)

Select the ingredient you would like to use:

Allantoin	Tricaprin	hydrogenated
Ethylene glycol	Palm-oil glycerides, monoglycerides,	Glyceryl polyacrylate
1,2-Octanediol	diglycerides and triglycerides,	*N*-(2-Hydroxyethyl)acetamide

- 原料详情
- 原料管制信息
- 可替代的原料选项

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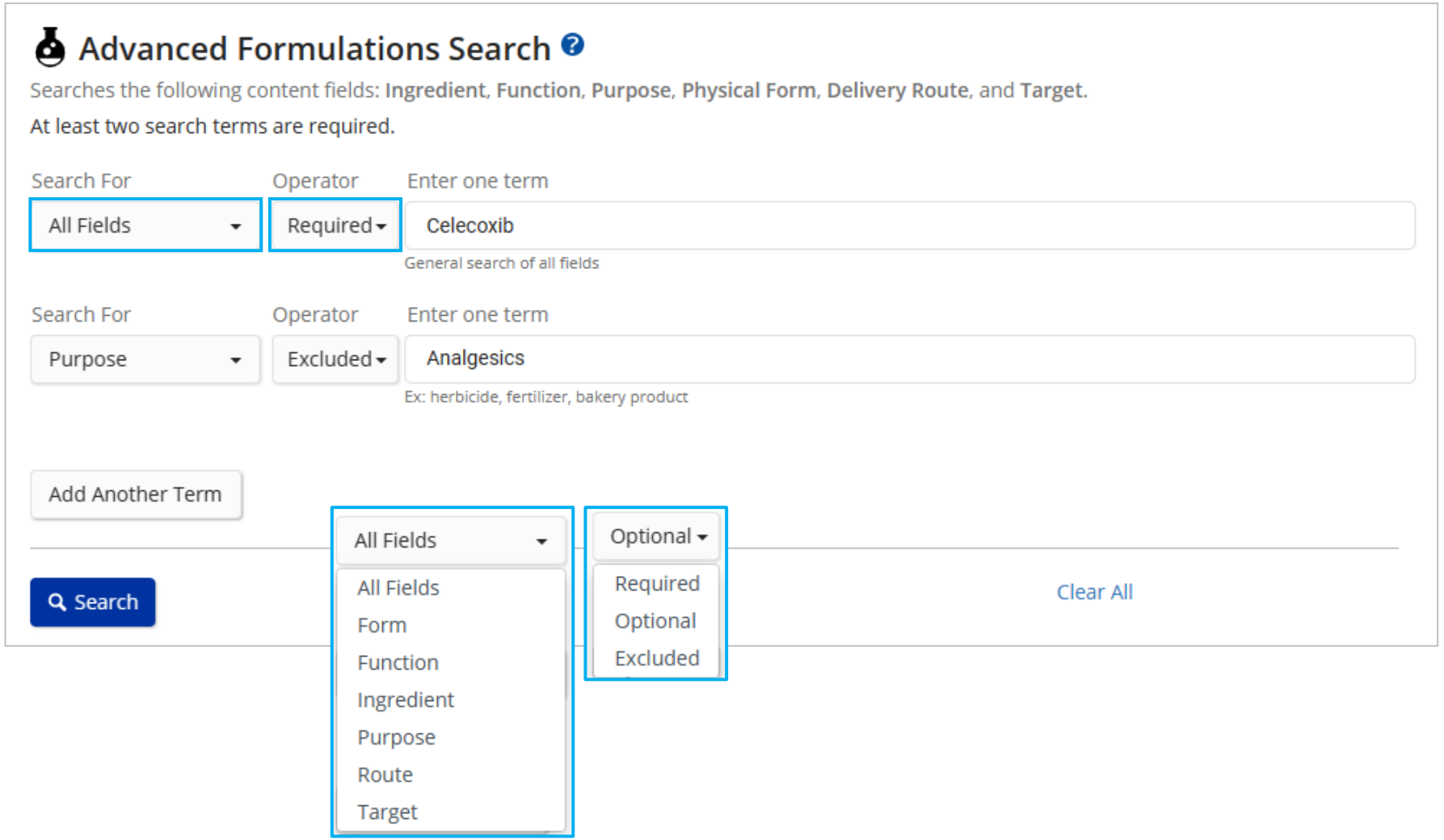
高级检索



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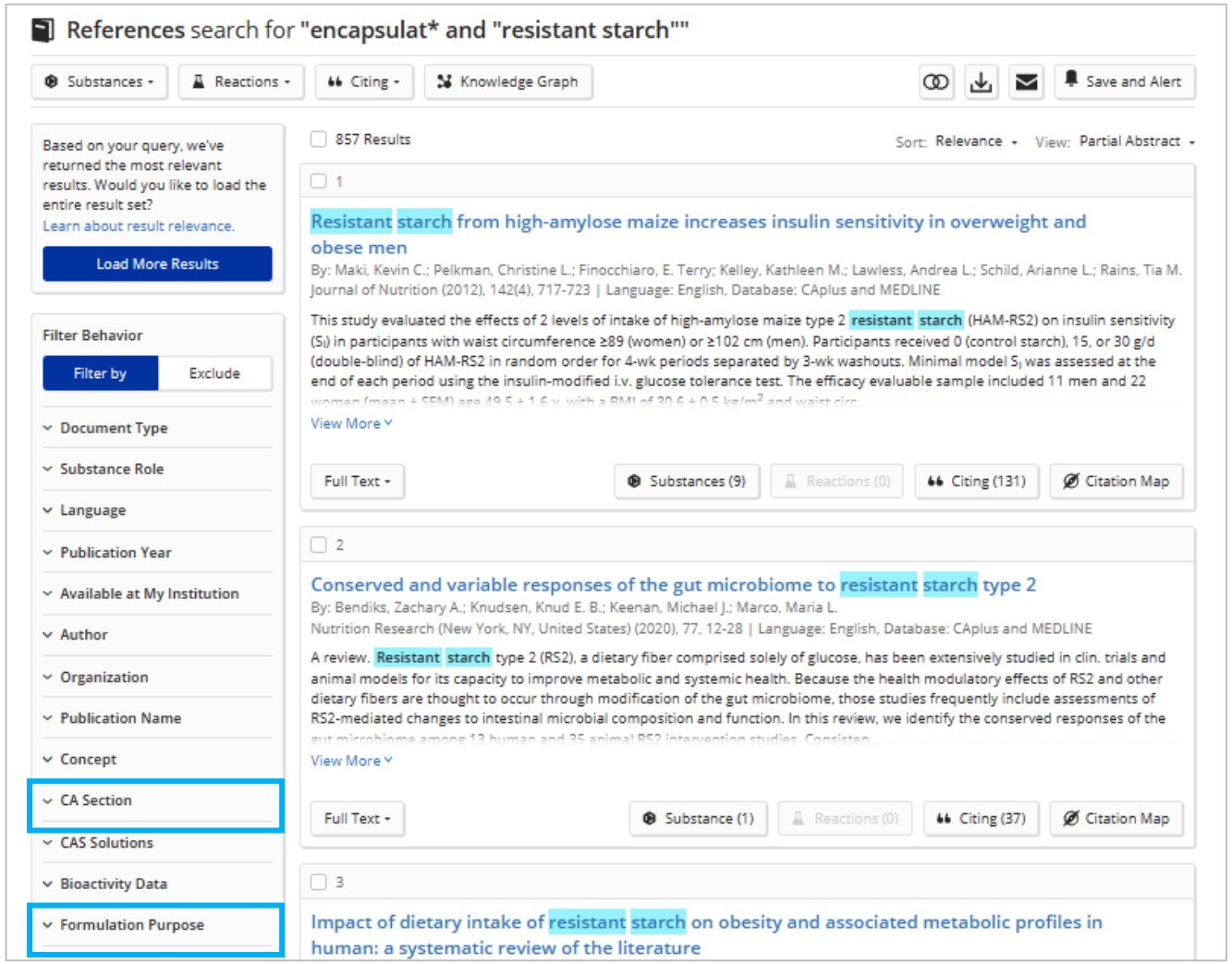
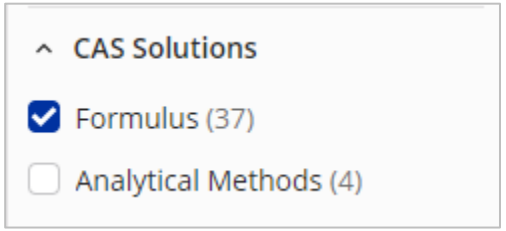
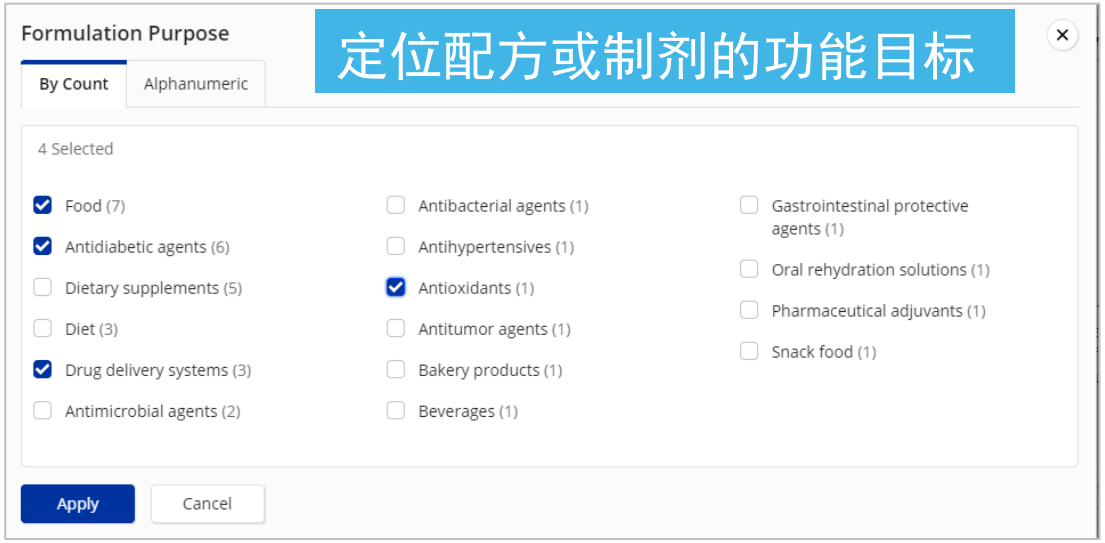
获取配方或制剂

方法（2）：在文献结果页面中，点击CAS Solutions中的Formulus 浏览相关的配方或制剂信息







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获取制剂或配方相关信息

Resistant Starch Film-Coated Microparticles for an Oral Colon-Specific Polypeptide Delivery System and Its Release Behaviors

Substances (3) | Reactions (0) | Citing (42) | Citation Map | Save

JOURNAL

Source
Journal of Agricultural and Food Chemistry
Volume: 62
Issue: 16
Pages: 3599-3609
Journal; Evaluation Study; Article; Research Support, Non-U.S. Gov't
2014
DOI:
10.1021/jf500472b

CODEN: JAFCAU
E-ISSN: 1520-5118
ISSN-L: 0021-8561

Database Information
AN: 2014:519911
CAN: 160:534190
PubMed ID: 24684664
CAplus and MEDLINE

Company/Organization
Ministry of Education Engineering Research Centre of Starch and Protein Processing, Guangdong Province Key Laboratory for Green Processing of Natural Products and Product Safety
South China University of Technology
Guangzhou 510640
China

Publisher
American Chemical Society

Language
English

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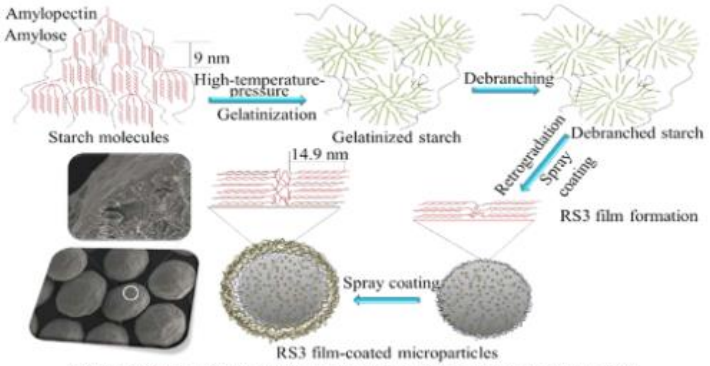
By: Situ, Wenbei; Chen, Ling; Wang, Xueyu; Li, Xiaoxi

For the delivery of bioactive components to the colon, an oral colon-specific controlled release system coated with a resistant starch-based film through aqueous dispersion coating process was developed. Starch was modified by a high-temperature-pressure reaction, enzymic debranching, and retrogradation, resulting in a dramatic increase in the resistibility against enzymic digestion (meaning the formation of resistant starch, specifically RS3). This increase could be associated with an increase in the relative crystallinity, a greater amount of starch mol. aggregation structure, and the formation of a compact mass fractal structure, resulting from the treatment. The microparticles coated with this RS3 film showed an excellent controlled release property. In streptozotocin (STZ)-induced type II diabetic rats, the RS3 film-coated insulin-loaded microparticles exhibited the ability to steadily decrease the plasma glucose level initially and then maintain the plasma glucose level within the normal range for total 14-22 h with different insulin dosages after oral administration; no glycopenia or glycemic fluctuation was observed Therefore, the potential of this new RS3 film-coated microparticle system has been demonstrated for the accurate delivery of bioactive polypeptides or protein to the colon.



Formation of the RS3 film coating layer and the RS3 film-coated microparticles

Keywords: starch film coated microparticle colon polypeptide delivery insulin

View PDF | Full Text

Expand All | Collapse All

- Concepts
- MEDLINE® Medical Subject Headings
- Substances
- Formulations

Formulations

Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

View CAS Formulus® Detail

Location: SI Page 3 Article Page 2 Figure 1S
Purpose: Drug delivery systems
Target: 5-aminosalicylic acid

Component 成分	Function 功能	Amount Reported 用量
Group: bioactive component-loaded microparticle core	model active agent	-
5-Aminosalicylic acid	-	20 %
Cellulose	additives	Ratio: 3
Starch	excipients	Ratio: 1
Group: RS3-based aqueous coating dispersion	coating materials	-
Starch	release control agent	-
(±)-Propylene glycol	plasticizers	10 %
Water	Solvents	-

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配方/制剂信息检索小结

1. 通过检索原料、用途、物理形态、功能或文献识别符获得配方/制剂信息
2. 检索原料
3. 配方或制剂的设计
4. 通过文献结果集获得关联的配方/制剂信息
5. 查看配方/制剂详情
6. 对比不同配方/制剂信息

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大纲

- CAS SciFinder^{n}中的生物序列检索
  - BLAST
  - CDR
  - Motif

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

下一节：反应检索

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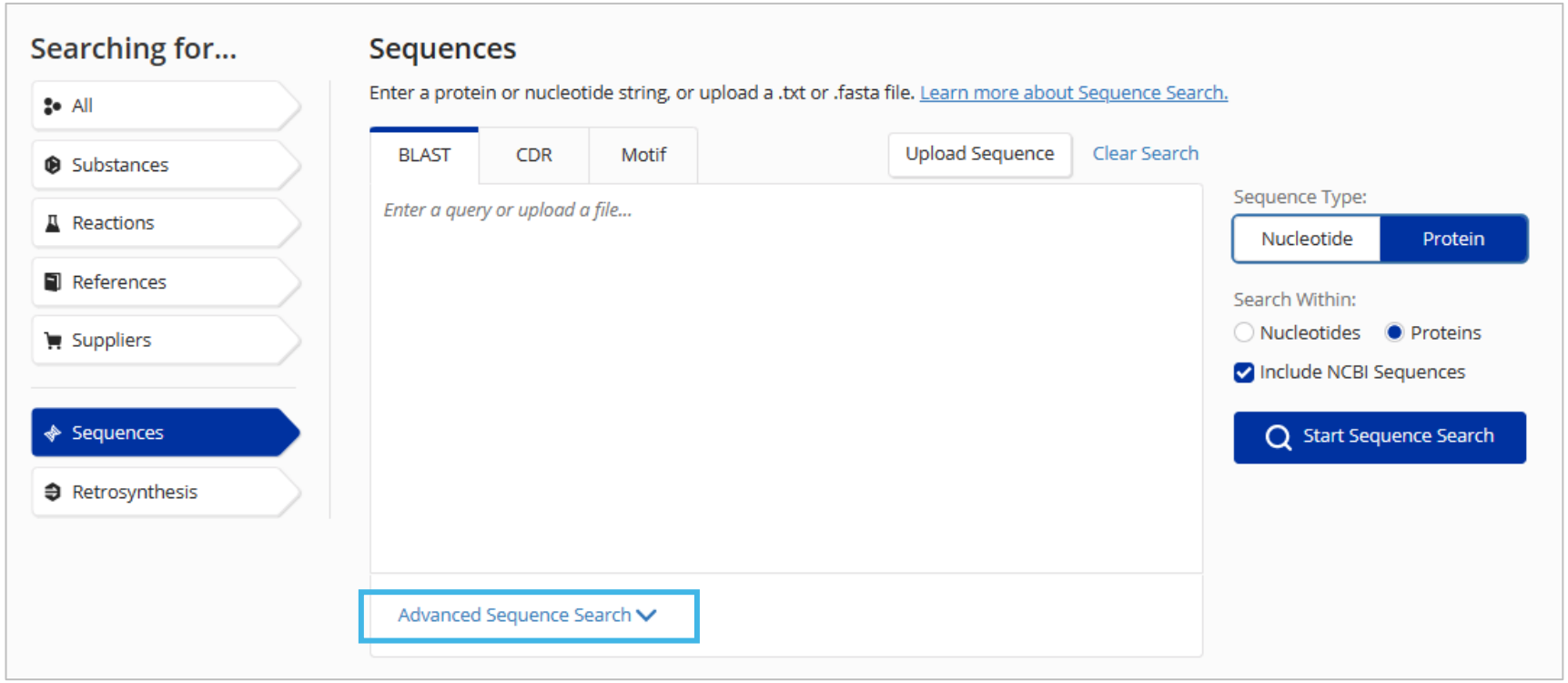
Sequences Search™ — Blast检索



可选择是否包含NCBI中的序列

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

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高级检索—设置相关参数

Sequences

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

BLAST | CDR | Motif

Upload Sequence | Clear Search

AACAACAACATATCAAATCCTACTGGTGGCACAACTTGA

Sequence Type: Nucleotide | Protein

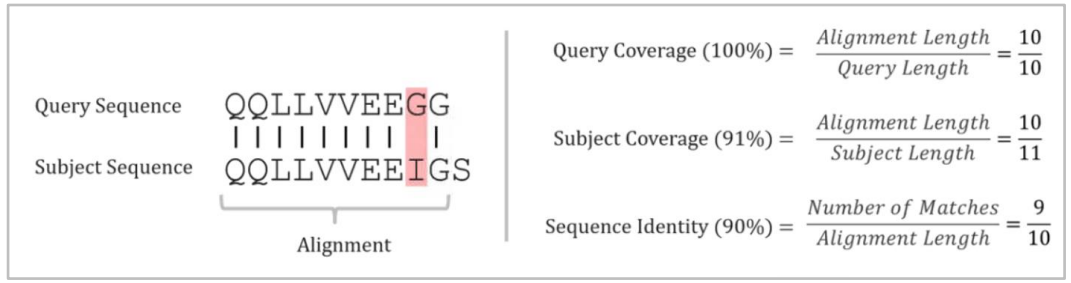
Search Within: Nucleotides | Proteins

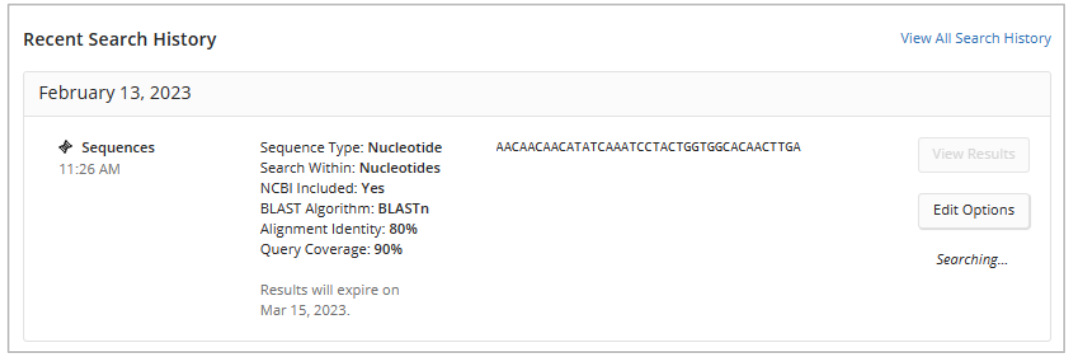
Include NCBI Sequences

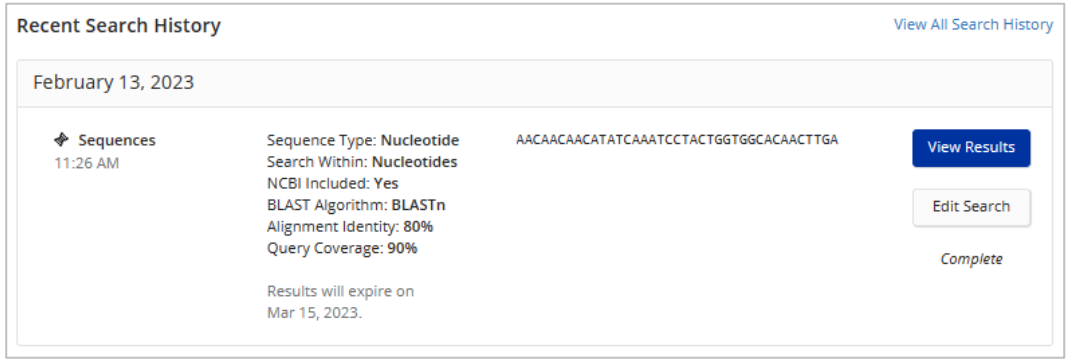
Start Sequence Search

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

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







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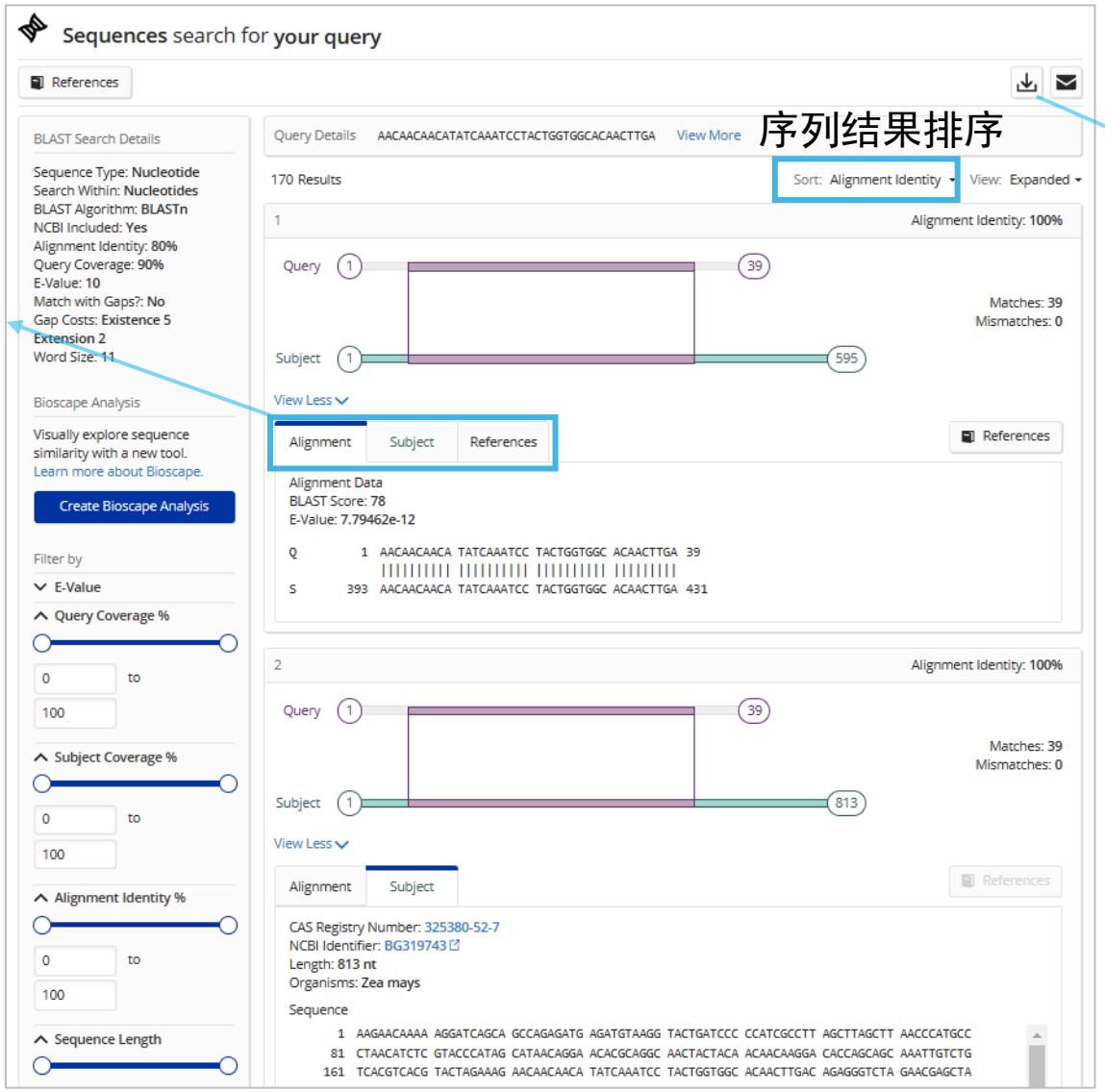
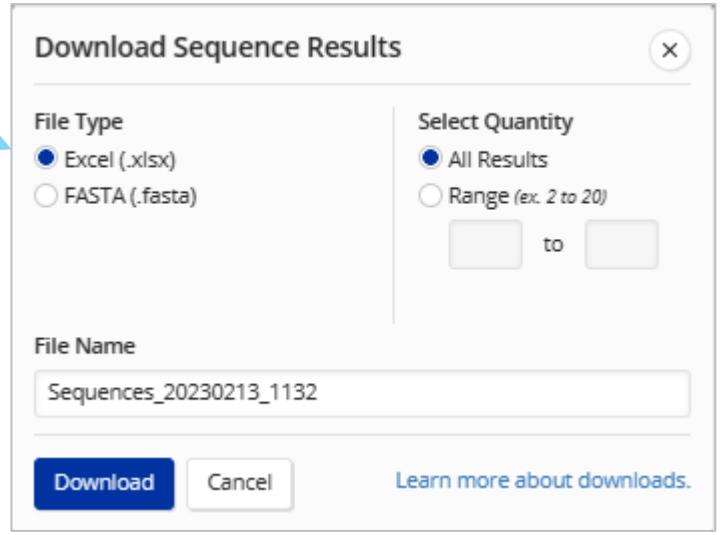
BLAST检索结果

- 序列一致性详情
- 目标序列
- 披露序列的专利文献

- 可视化地图

- 结果筛选





下载结果:

- 比对详情
- 序列长度参数
- 相关专利号
- 专利中的序列编号等

（Excel或FASTA格式）

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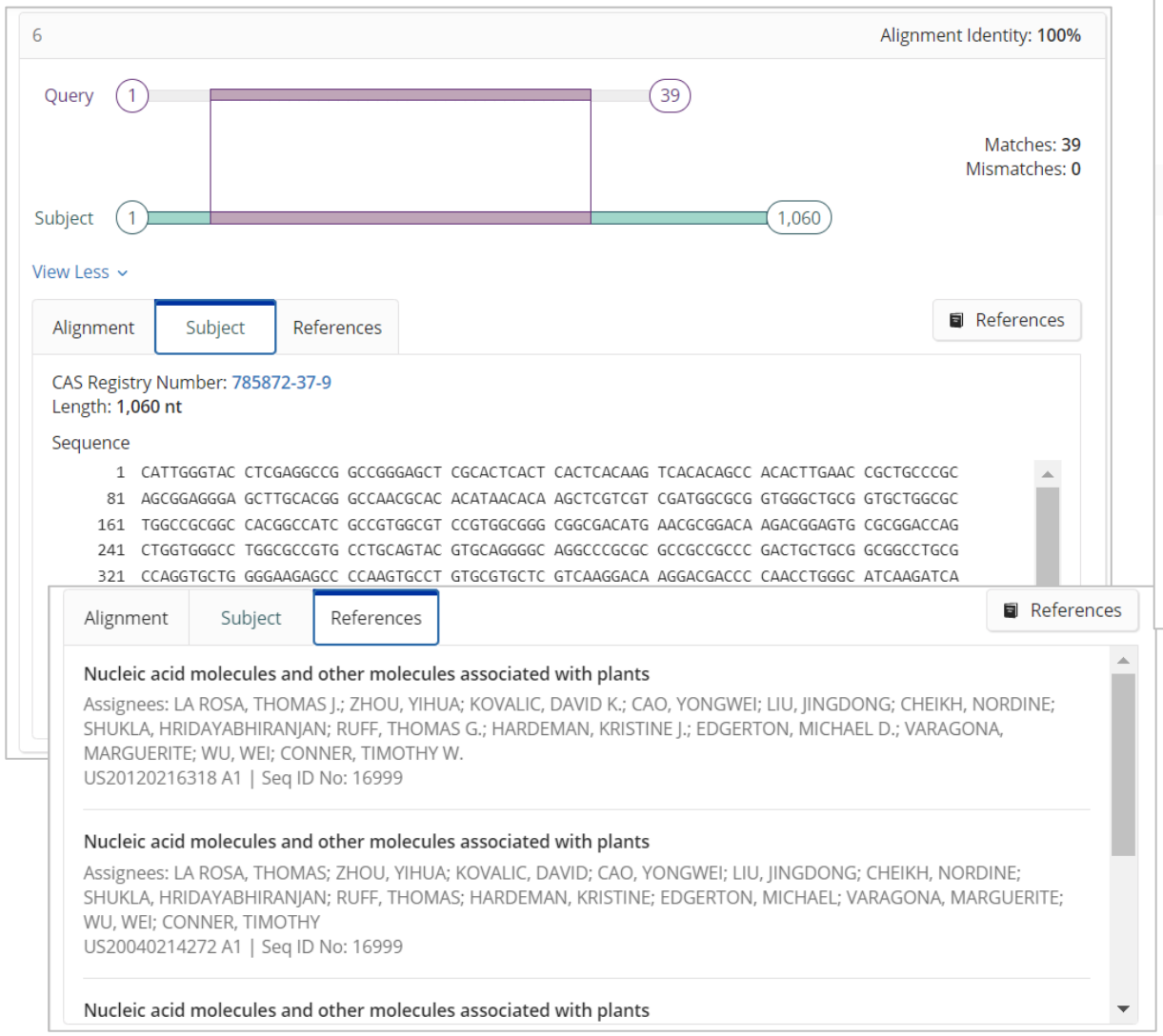
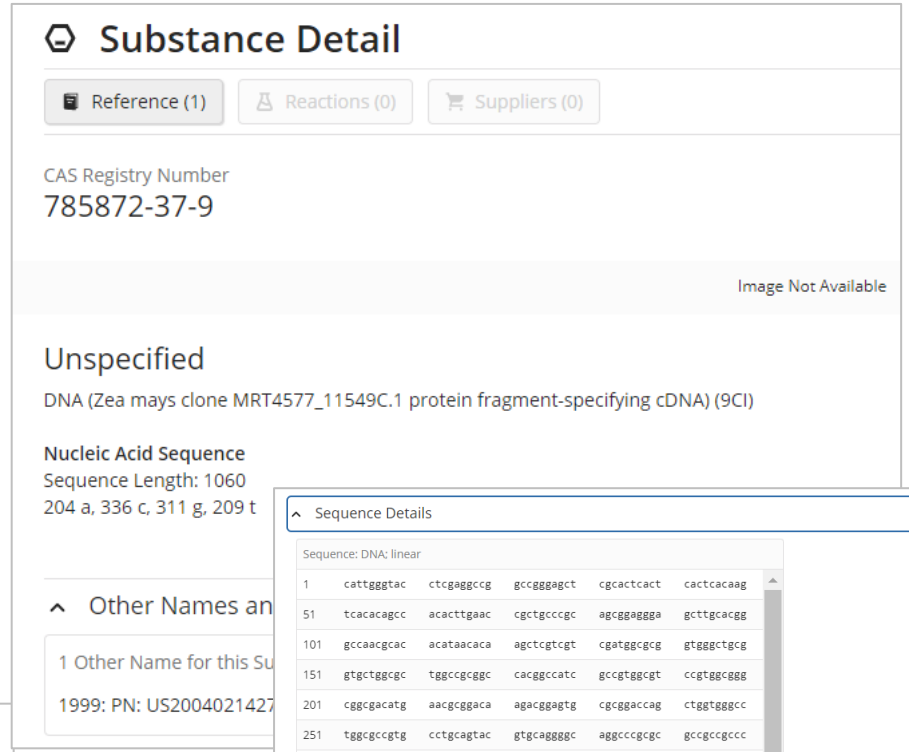
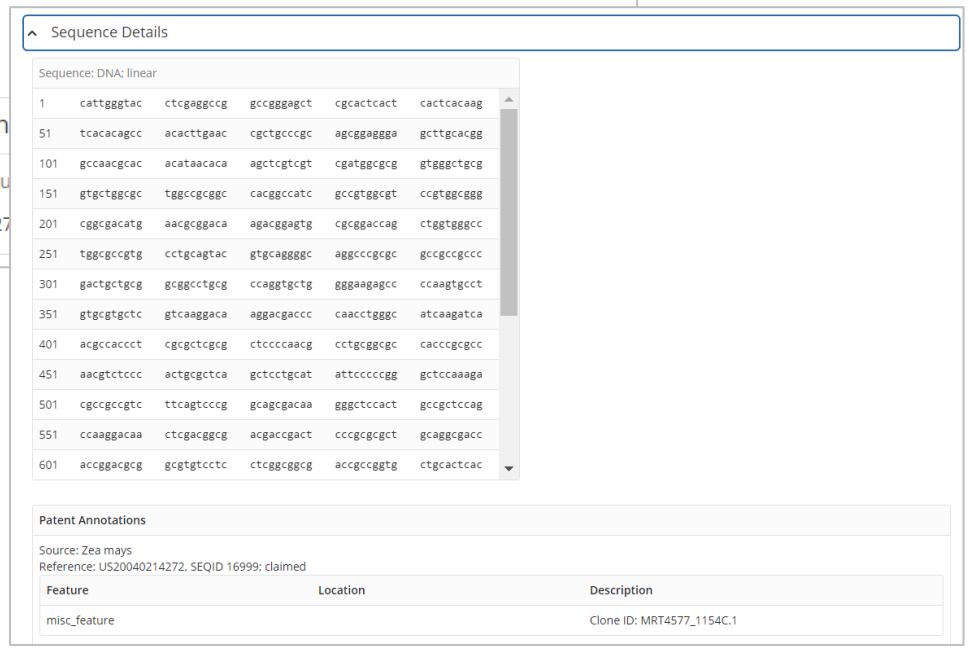
BLAST检索结果







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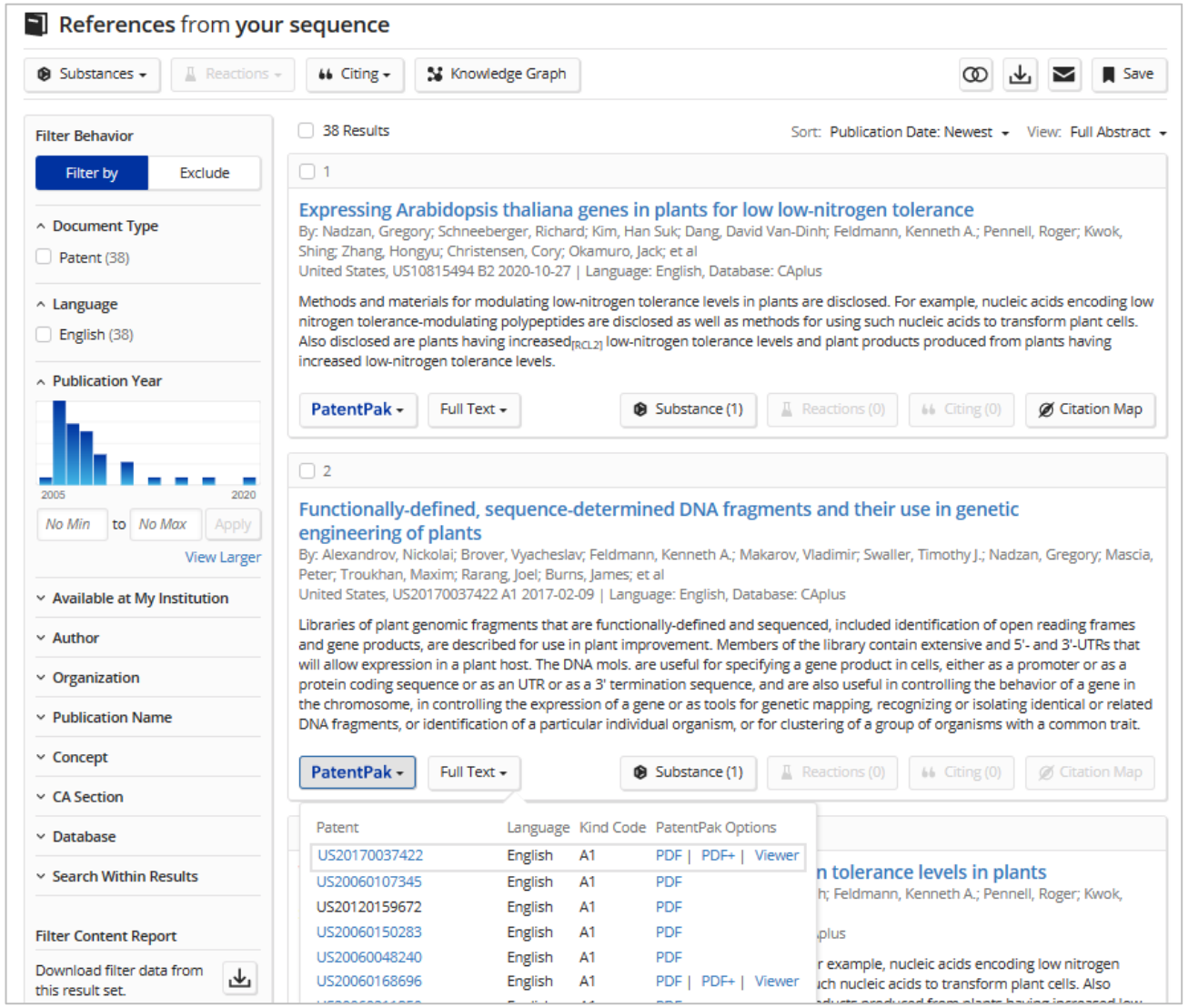
序列详情及相关的专利文献结果



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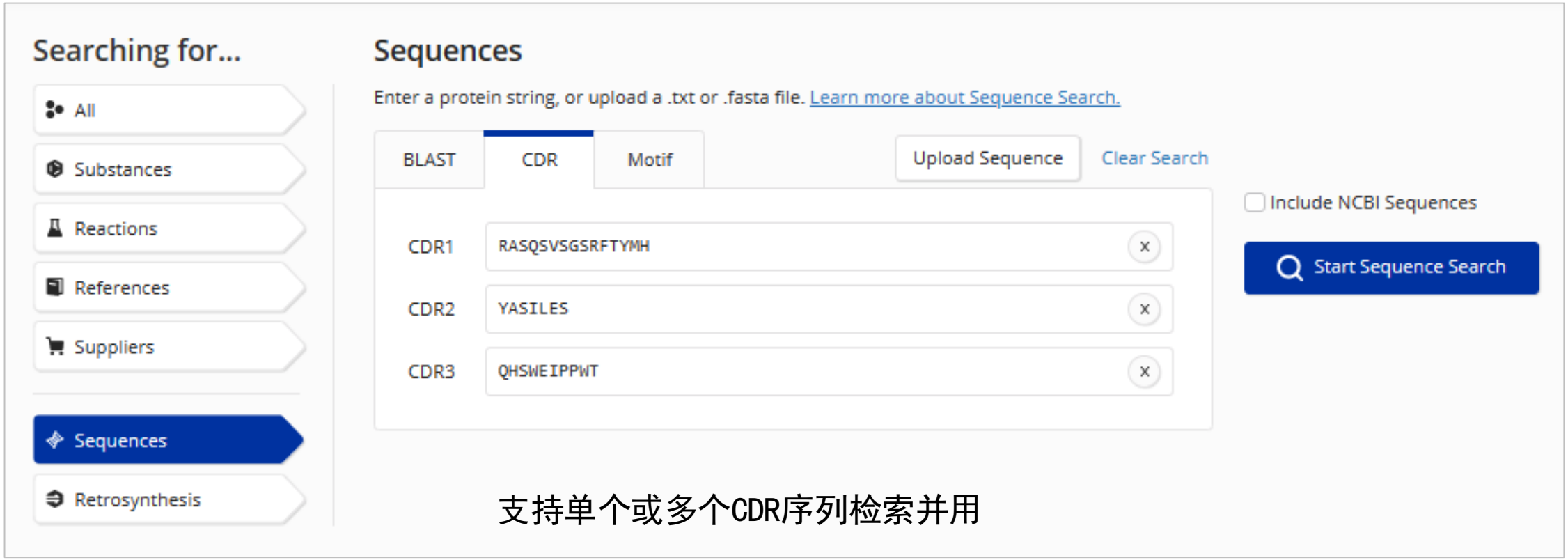
Sequences Search™—CDR检索



支持单个或多个CDR序列检索并用

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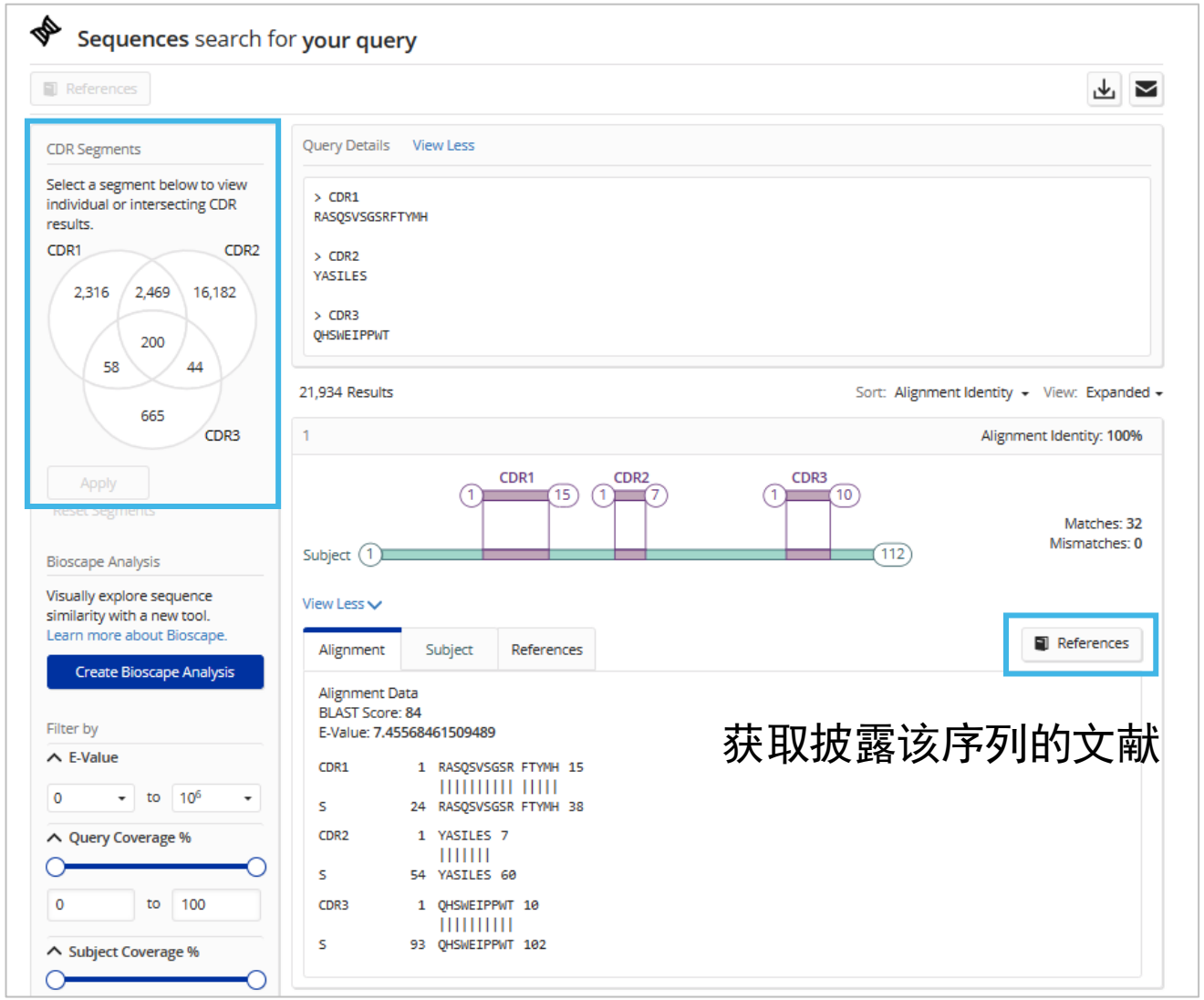
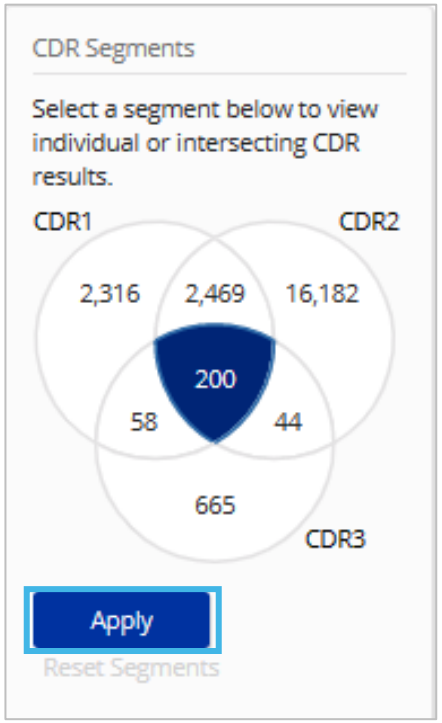
CDR检索结果



获取披露该序列的文献



CDR Segments：

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

Reset segments：

- 重新选择查看匹配的序列结果

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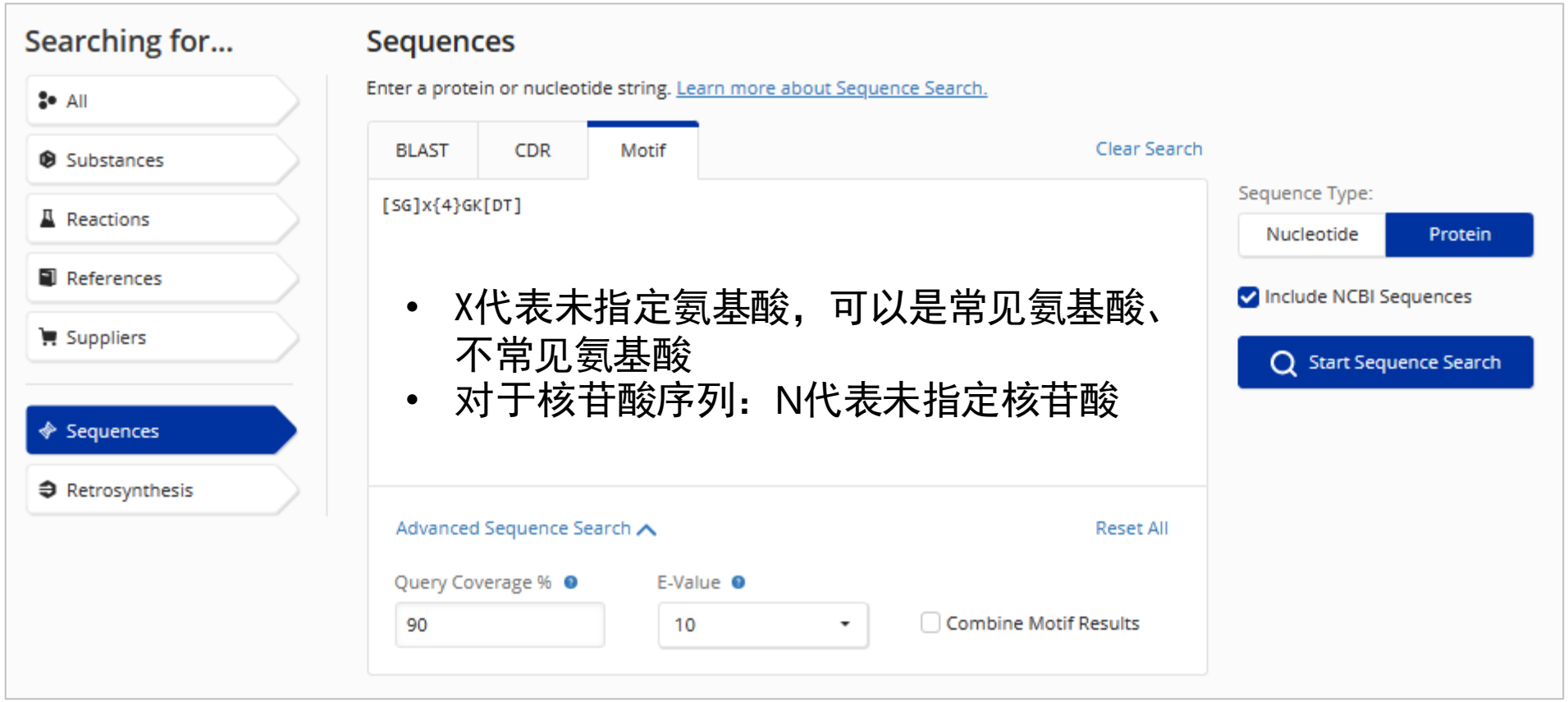
Sequences Search™—Motif检索

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



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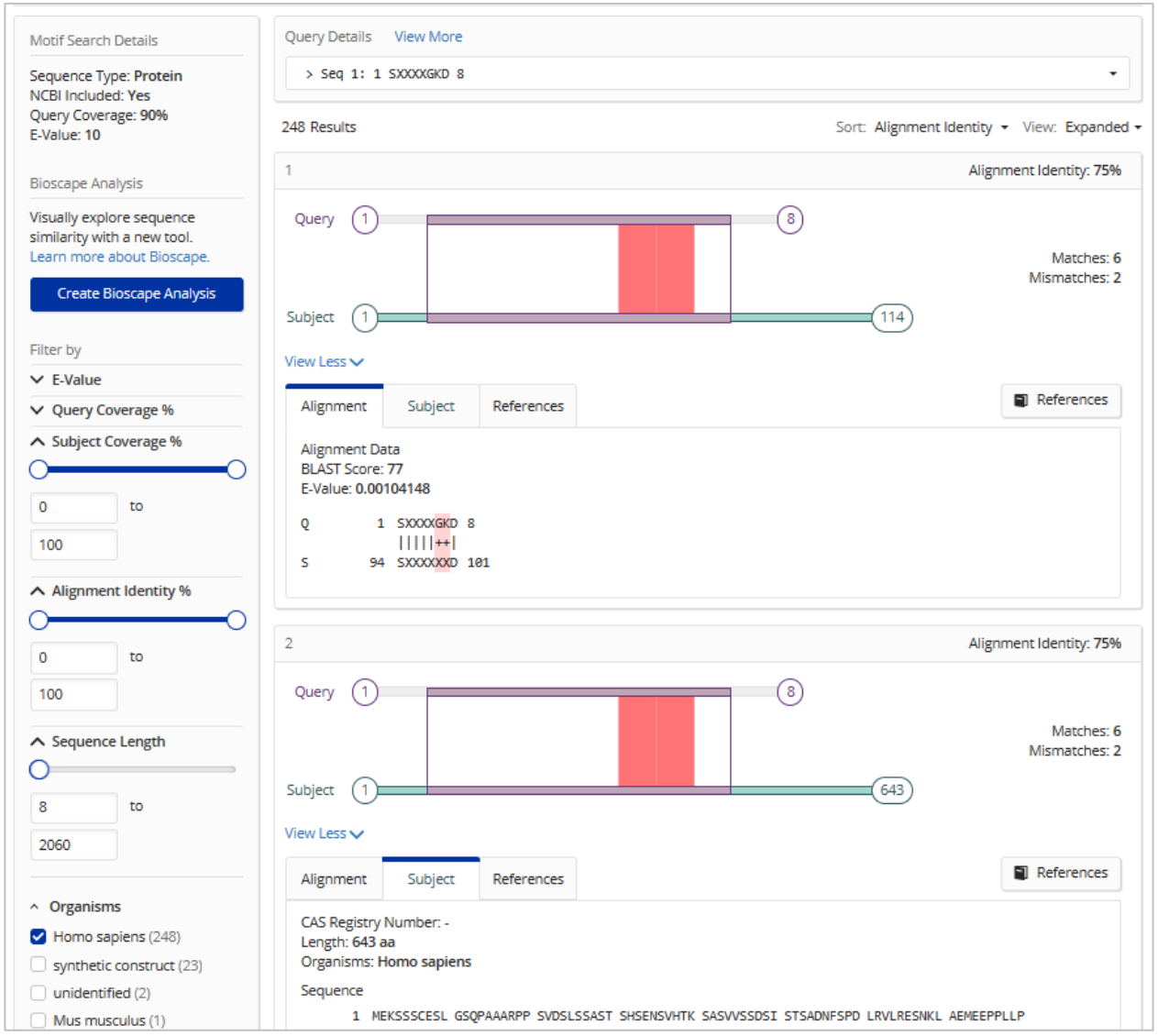
Motif检索结果



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序列检索小结

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

思考题：在SciFinder^{n}中检索获得目标序列，是否能获得披露该序列的专利或文献信息？

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大纲

- CAS及CAS SciFinder^{n}简介
- 常见检索方式
  - 文献检索
  - 物质检索 (CAS Markush*)
  - 反应检索
  - 逆合成反应路线设计 (CAS Retrosynthesis*)
  - 分析实验方法（CAS Analytical Methods）
  - 配方/制剂信息检索（CAS Formulus）
  - 生物序列检索*
- 常见问题及解答

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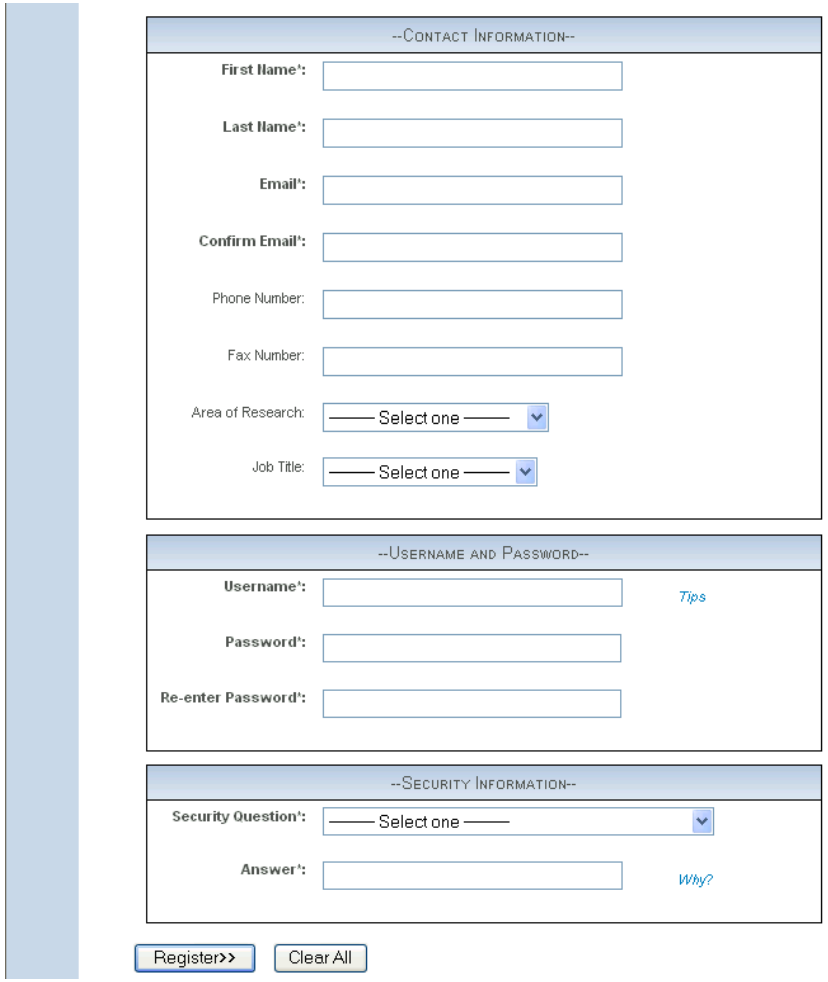
如何获取CAS SciFinder^{n}账号

- 登录https://SciFinder-n.cas.org进行注册
- 可登录贵校图书馆网站，查看注册相关的链接和说明



请注意：
1.必须输入真实姓名和学校邮箱。
2.用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：
- -（破折号）
- _（下划线）
- .(句点）
- @（表示“at”的符号）

3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

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

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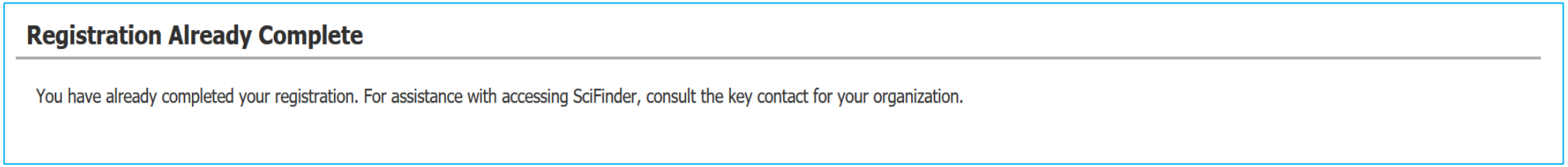
CAS SciFinder^{n}检索浏览器推荐

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



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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使用注意事项

- 一人注册一个帐号
- 实名注册，请提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（https://www.cas.org/legal/infopolicy）
- 不得账号分享
- 不得将账号用于非学术研究

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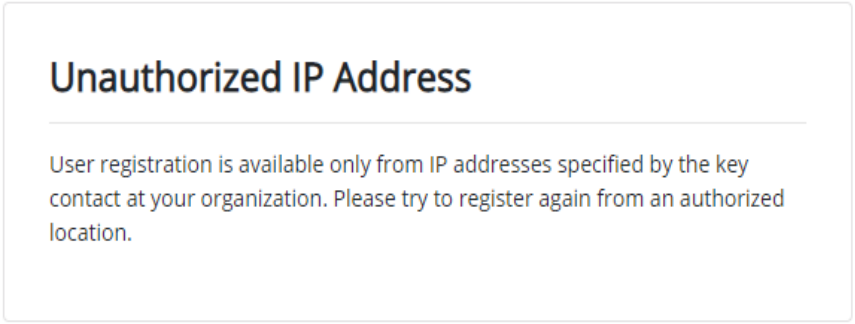
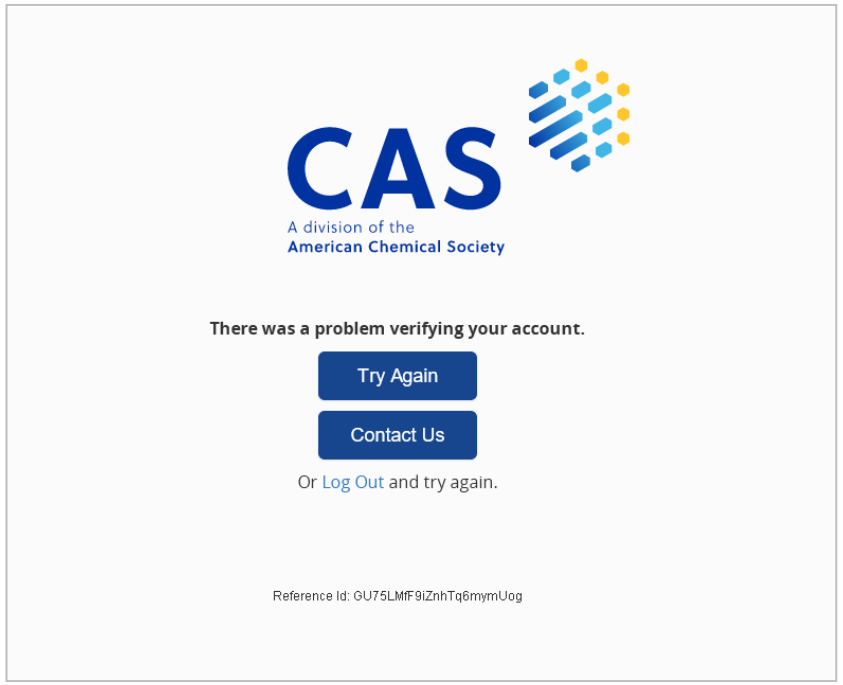
常见问题



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



- 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

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学习资源

CAS SciFinder^{n}学习中心

预告：2023 CAS SciFinder Discovery Platform 论坛

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

回顾：2022 CAS SciFinder^{n}论坛合集

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