CAS SciFinder Discovery Platform (Academic)

全面高效获取医药信息

汤健钊　高级客户顾问　jtang@acs-i.org

CAS
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大纲

- CAS及CAS SciFinder Discovery Platform (Academic)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*)
  - 序列检索*
  - 分析实验方法（CAS Analytical Methods）
  - 配方/制剂信息检索（CAS Formulus*）
- 常见问题及解答

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

Connecting past discoveries
to build a better future

连接前人的发现，建设更美好的未来

INSIGHT

Revealing unseen relationships that spark ideas and speed discovery

揭示能激发想法和加速发现的，未预见的联系

FORESIGHT

Identifying trends and emerging opportunities to accelerate growth

确定加速增长的趋势和新机遇

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CAS 具有最全面的学科连接内容合集

Over
55K
scientific journals and documents

Over
274
million substances

Over
50
languages translated

Over
64
patent offices worldwide

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CAS独特的内容合集

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

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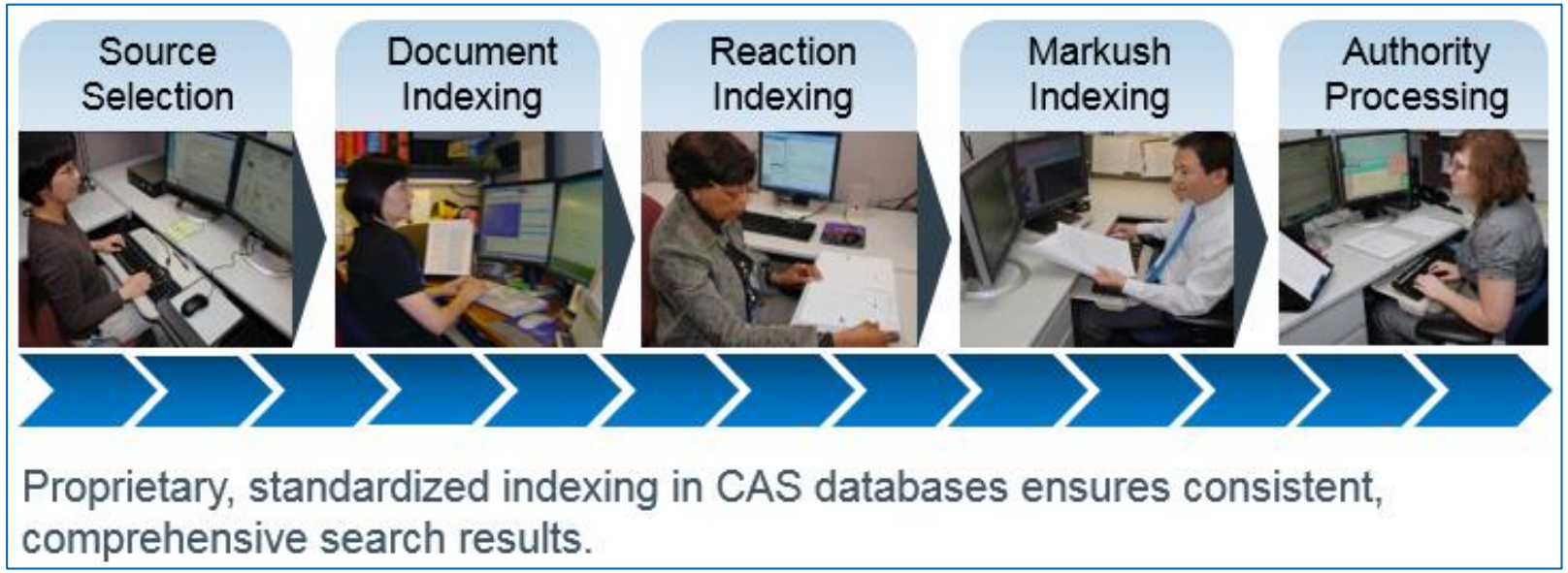
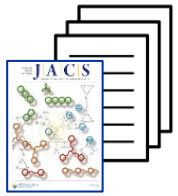
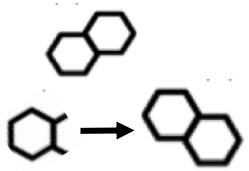
CAS科学家的智力标引

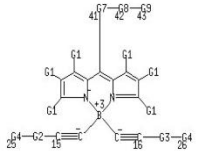


Data pre-repository



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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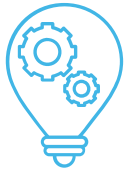
CAS解决方案与服务

Discovery

CAS SciFinder Discovery Platform™

Get discoveries to market faster and optimize margins by giving researchers the information they need



Intellectual Property

STN IP Protection Suite™

Ensure that your intellectual property is protected and find opportunities to extend into new markets

Custom Solutions

CAS Custom Services℠

Customized data, analytics and insights to maximize the value of information assets and fuel digitalization success

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CAS SciFinder Discovery Platform (Academic)平台解决方案

CAS SciFinder^n ——加速科学发现的业界领先的科学工具

业界最领先的相关性搜索引擎，提供和化学相关的各学科的文献、物质、反应和生物序列等检索内容，检索智能、高效、简单。可用于基金申请的文献准备、为新课题制定实验计划、寻求学术合作者、进行逆合成分析以及更多其他的教学和科研活动。

CAS Analytical Methods ——借助CAS科学家深度加工的科学方法，提升研究效率

分析方法解决方案涵盖来自期刊中的化学分析方法，提供检索和对比功能，可快速获得能直接在实验室操作的分析方法。可为法医学、食品科学、农学、制药、环境等学科的教学和实验提供帮助。

CAS Formulus ——助力开发安全、有效的产品

集成配方（制剂）数据与工作流程的解决方案，提供来自期刊、专利和产品说明中的配方详情。可检索制药、化妆品、食品、农化、油墨、涂料等众多领域中的配方，及其工艺、成分、目标成分的常见配伍成分、设计配方、和探索合规要求等。

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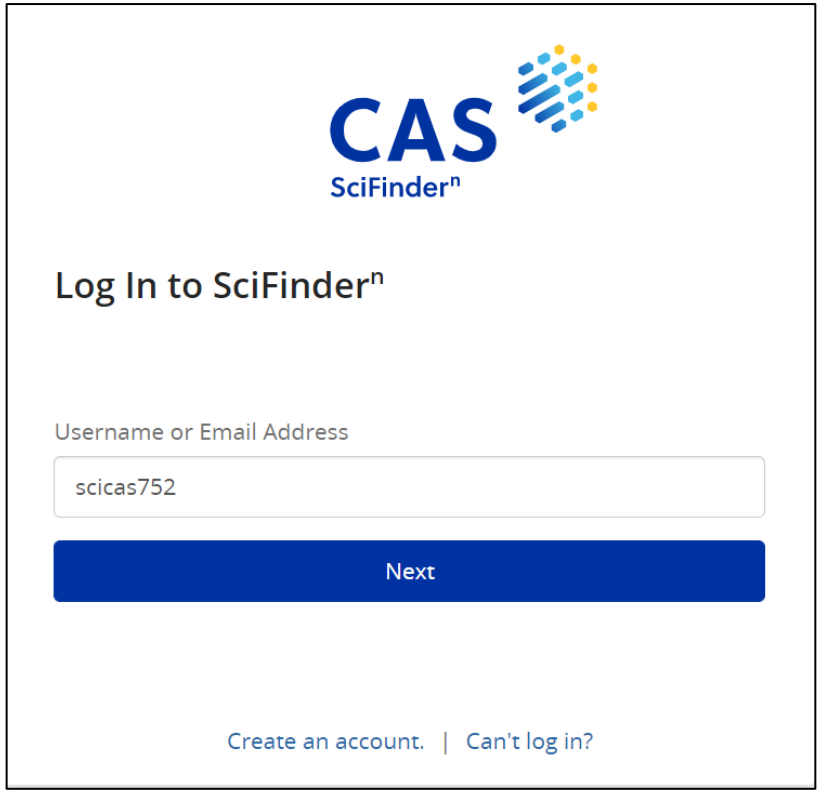
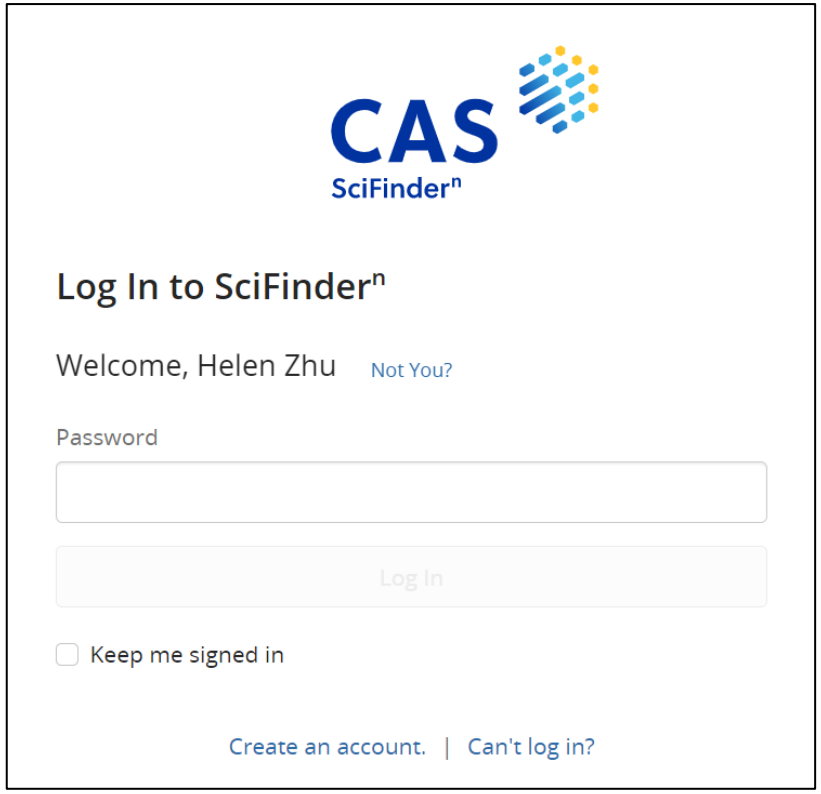
CAS SciFinder^{n}登录网址: https://SciFinder-n.cas.org





使用CAS SciFinder账号登录

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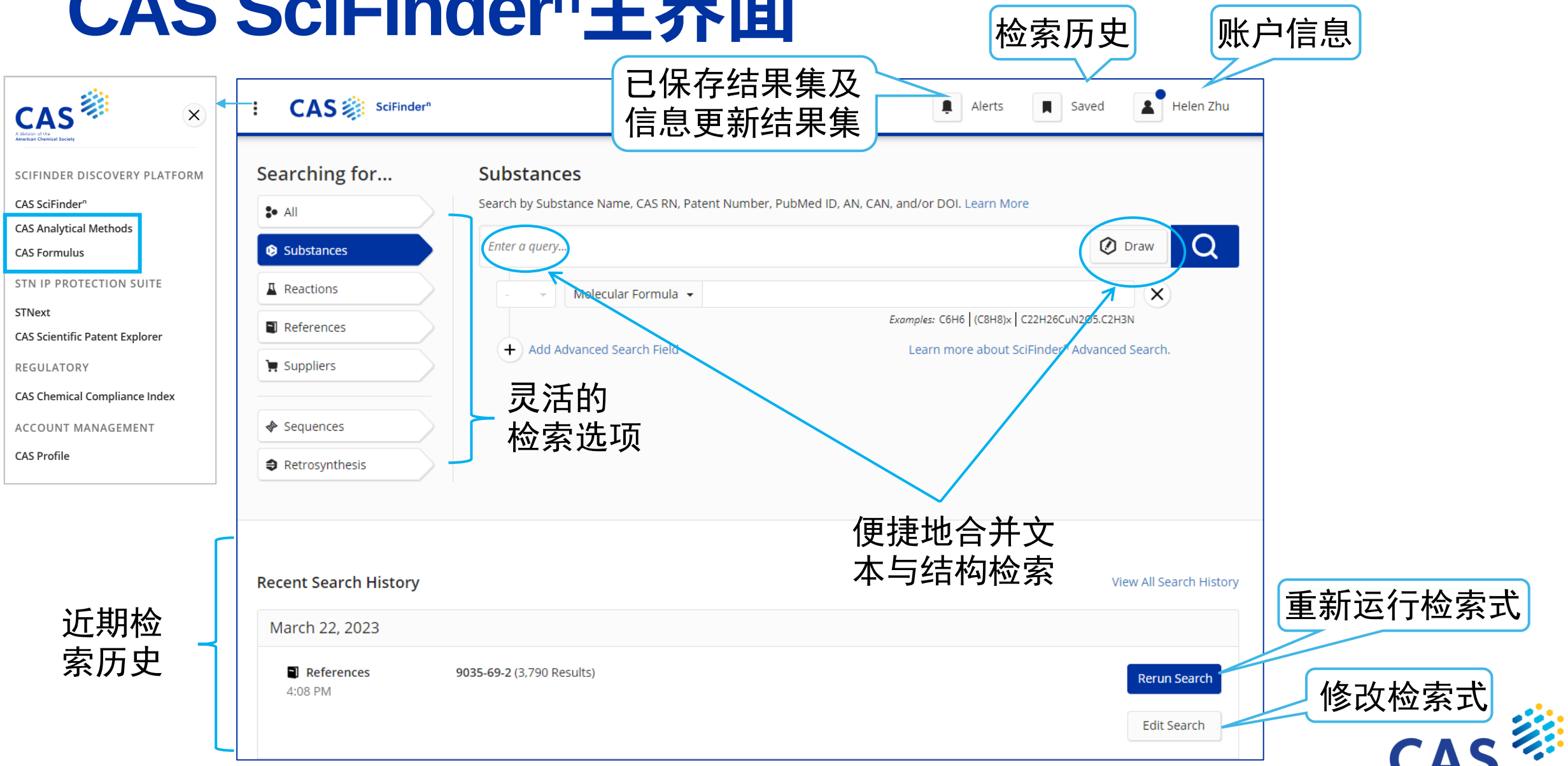
CAS SciFinder^{n}主界面



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*)
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  - 配方/制剂信息检索（CAS Formulus*）
- 常见问题及解答

大纲

- CAS SciFinder^{n}中的文献检索
  - 主题词检索及布尔逻辑算符的运用
  - 文献检索结果集的筛选
  - 引文地图的应用
  - 文献结果集的导出和检索历史管理
  - 定位专利原文中的重要信息
  - 利用ChemZent丰富化学历史知识

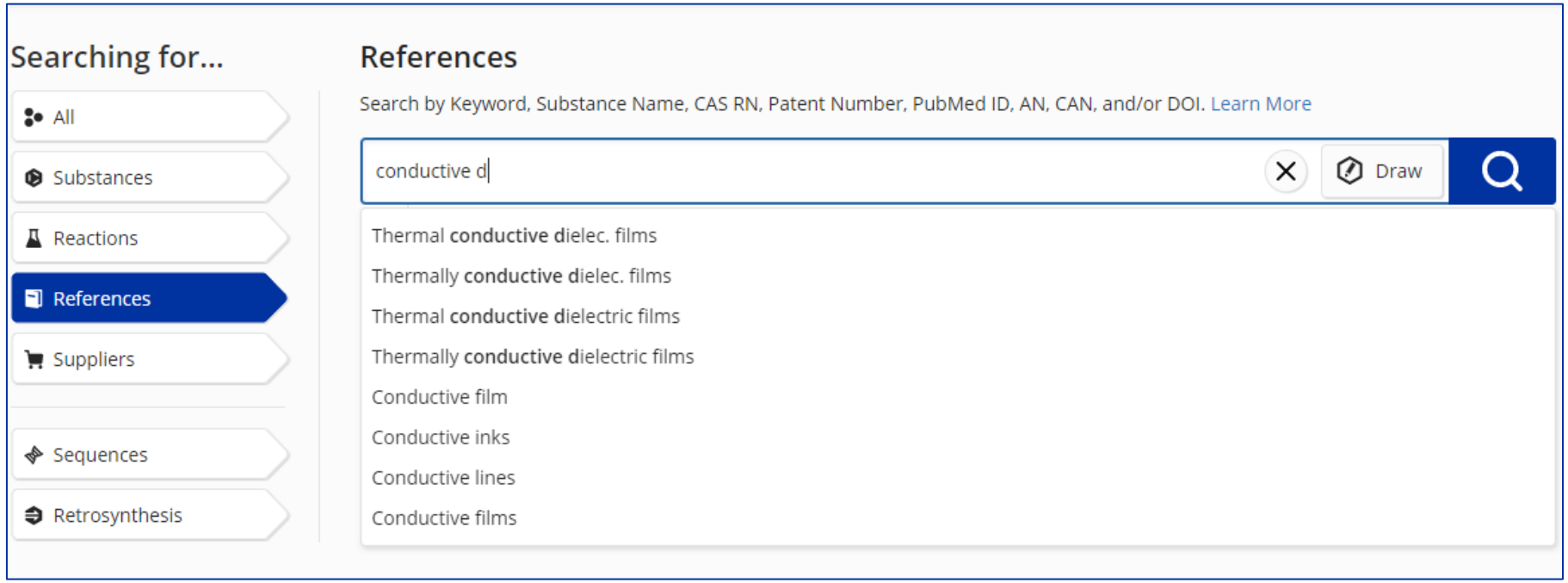
视频链接：
https://american-chemical-society.zoom.us/rec/share/9PrTtd4gKFB245SuJax26so0a4WAHC9MsgB74Bt3mPRK9TgcwZI753ROg4eHHseL.I_K0dQtNjGzGJK5y

文献检索

- 文献检索方法
  - 主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
  - 各种字段：作者名、期刊名、机构名、题目、摘要、概念词、物质标识符、出版商
  - 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

文献检索--主题词检索及布尔逻辑算符的使用

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



基于科学家创建的叙词表，充分利用自动提示检索词，启发检索思路

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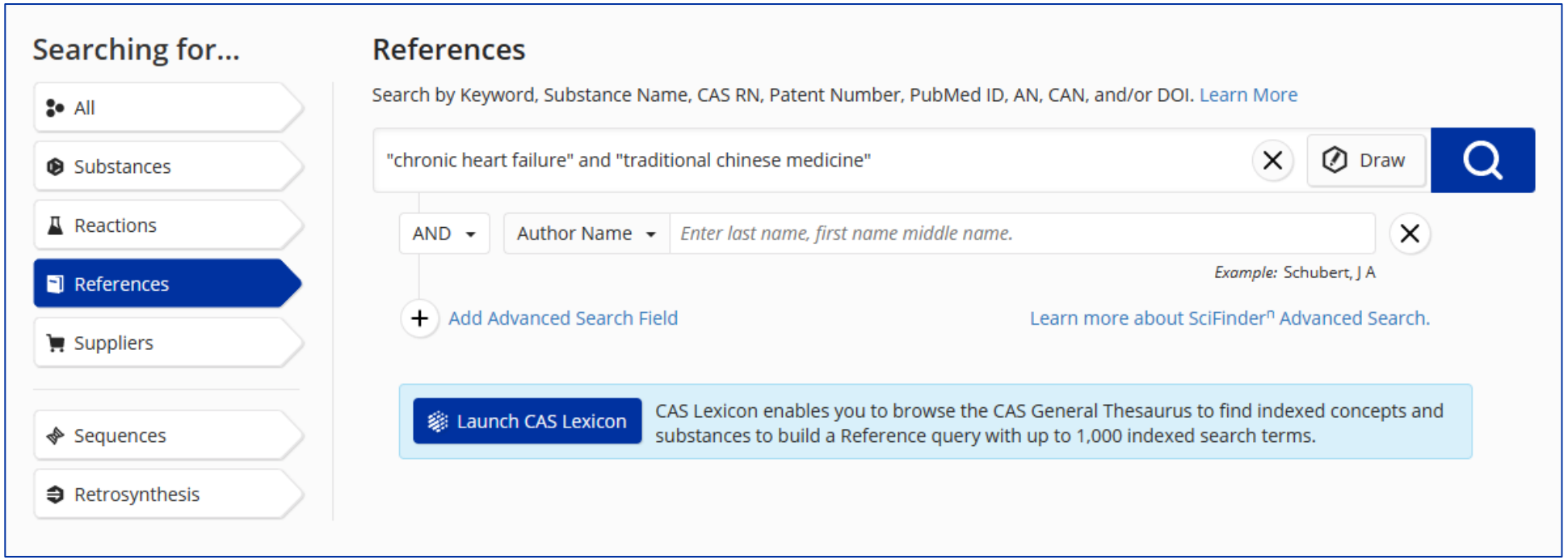
文献检索--主题词检索及布尔逻辑算符的使用



- 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 medic*可代表medical, medicine, medication, medicinal等（*代表0或多个字符；？代表0或1个字符）

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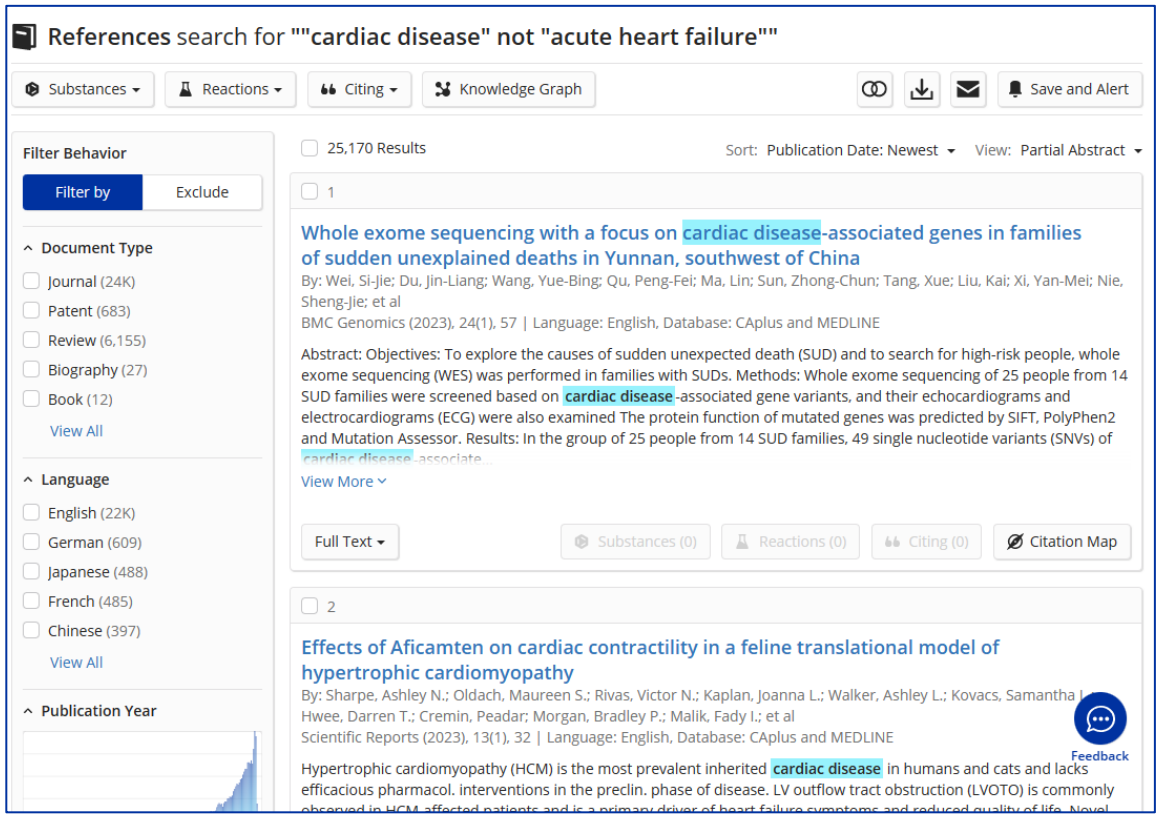
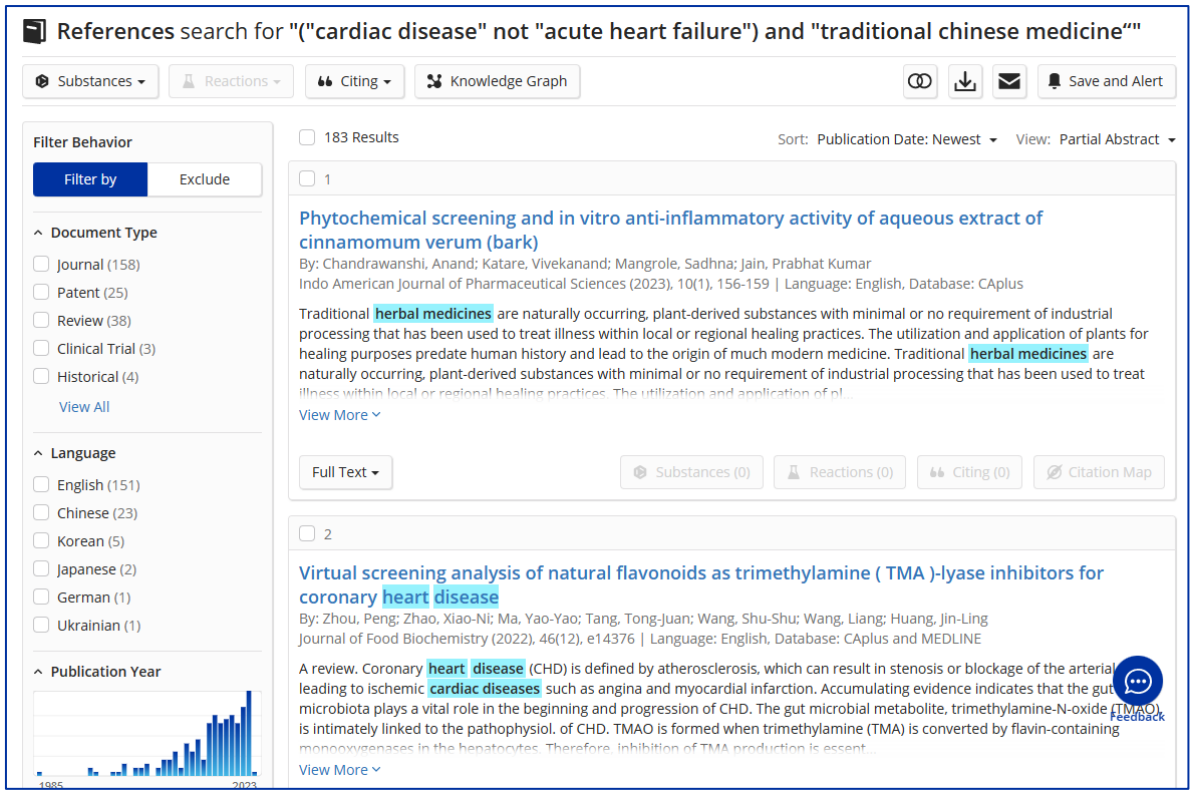
文献检索--主题词检索及布尔逻辑算符的使用

"cardiac disease" not “acute heart failure“
检索：心脏疾病，排除急性心衰



("cardiac disease" not “acute heart failure“) and "traditional chinese medicine”
检索：排除心衰的心脏疾病，且与中医药相关



使用布尔逻辑运算符，精准构建检索主题

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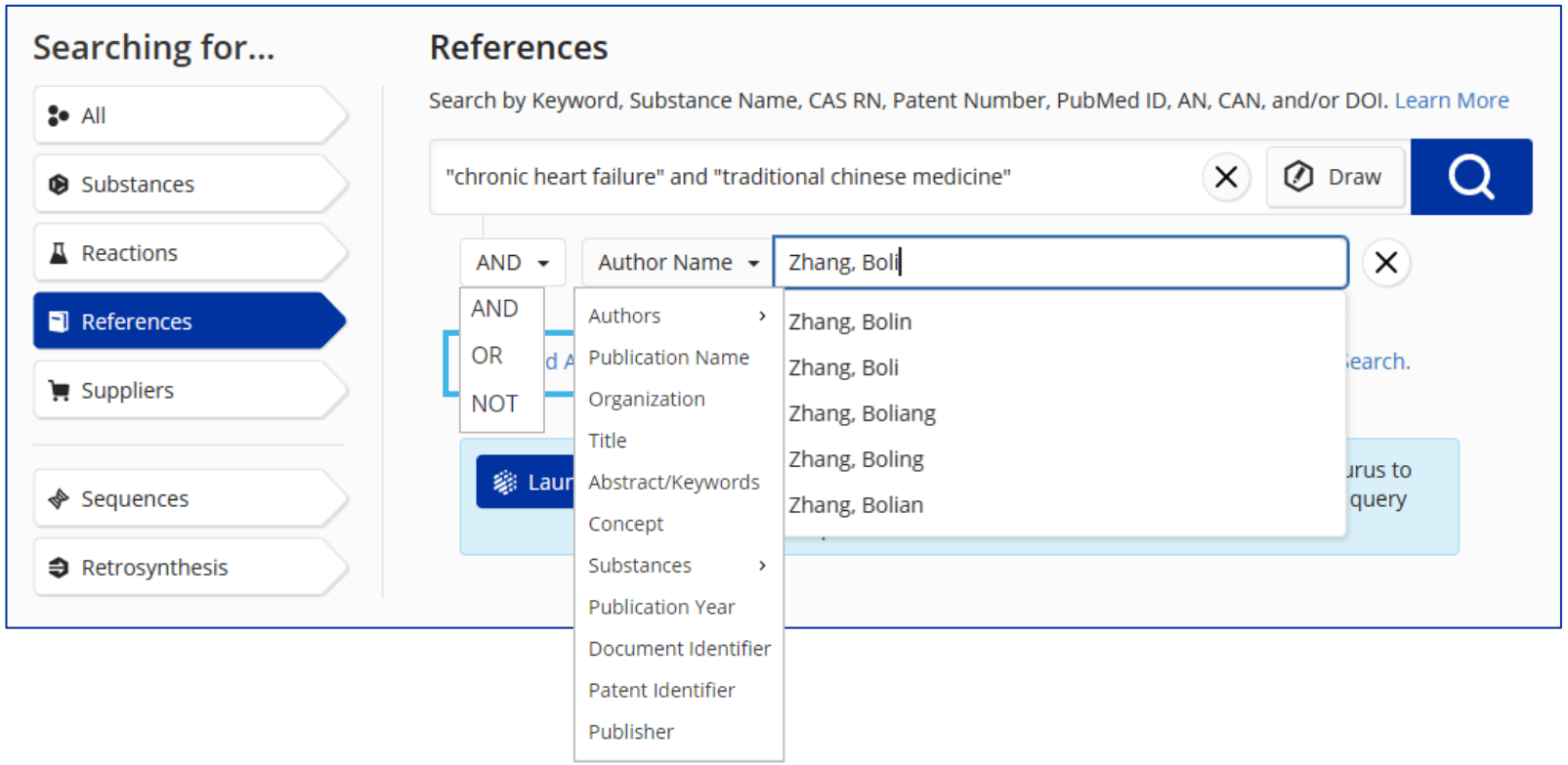
高级检索—高效实现多项自定义组合检索



* 检索方法可单独使用，也可联用

主检索框：关键词、物质名称、CAS RN、DOI等

高级检索字段：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

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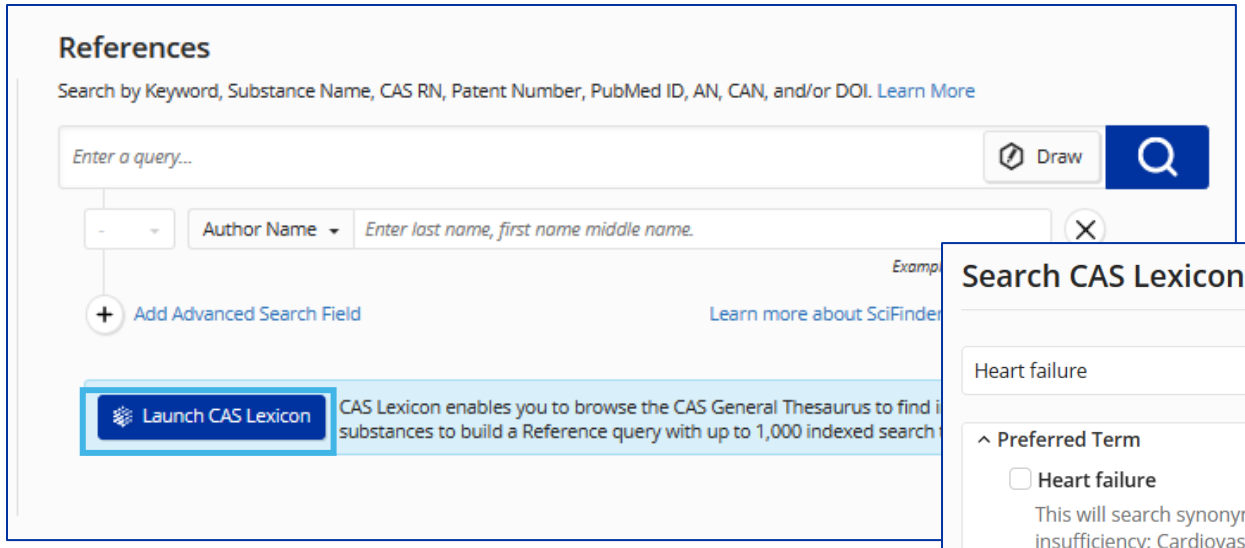
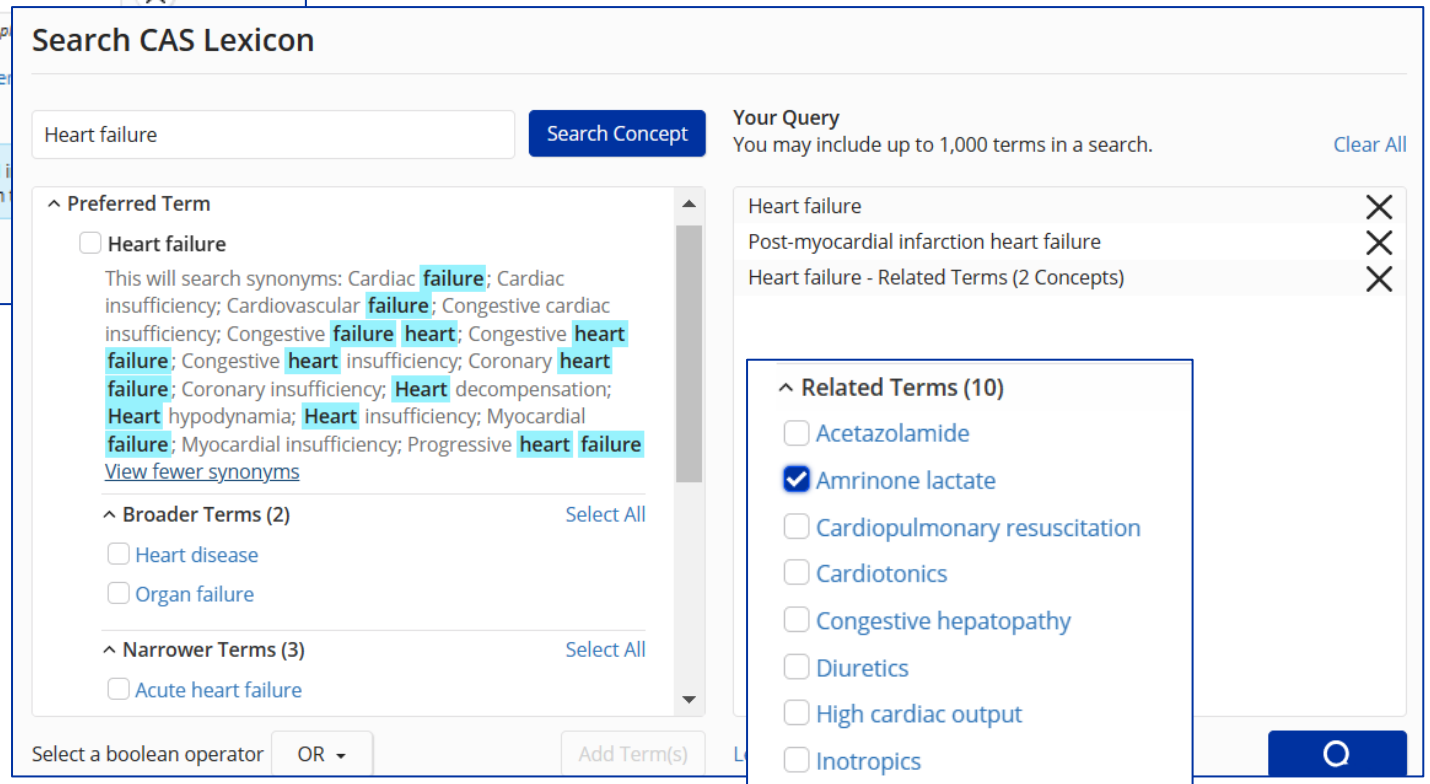
CAS Lexicon—利用词库选词获得准确结果



可在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（建立的检索式中最多可使用1000个词）



检索并浏览CAS Lexicon词库中的层级，勾选适合的主题词：

Preferred Term、Broader Terms、Narrower Terms、Related Terms

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文献结果集—排序与筛选

文献类型

文献语言

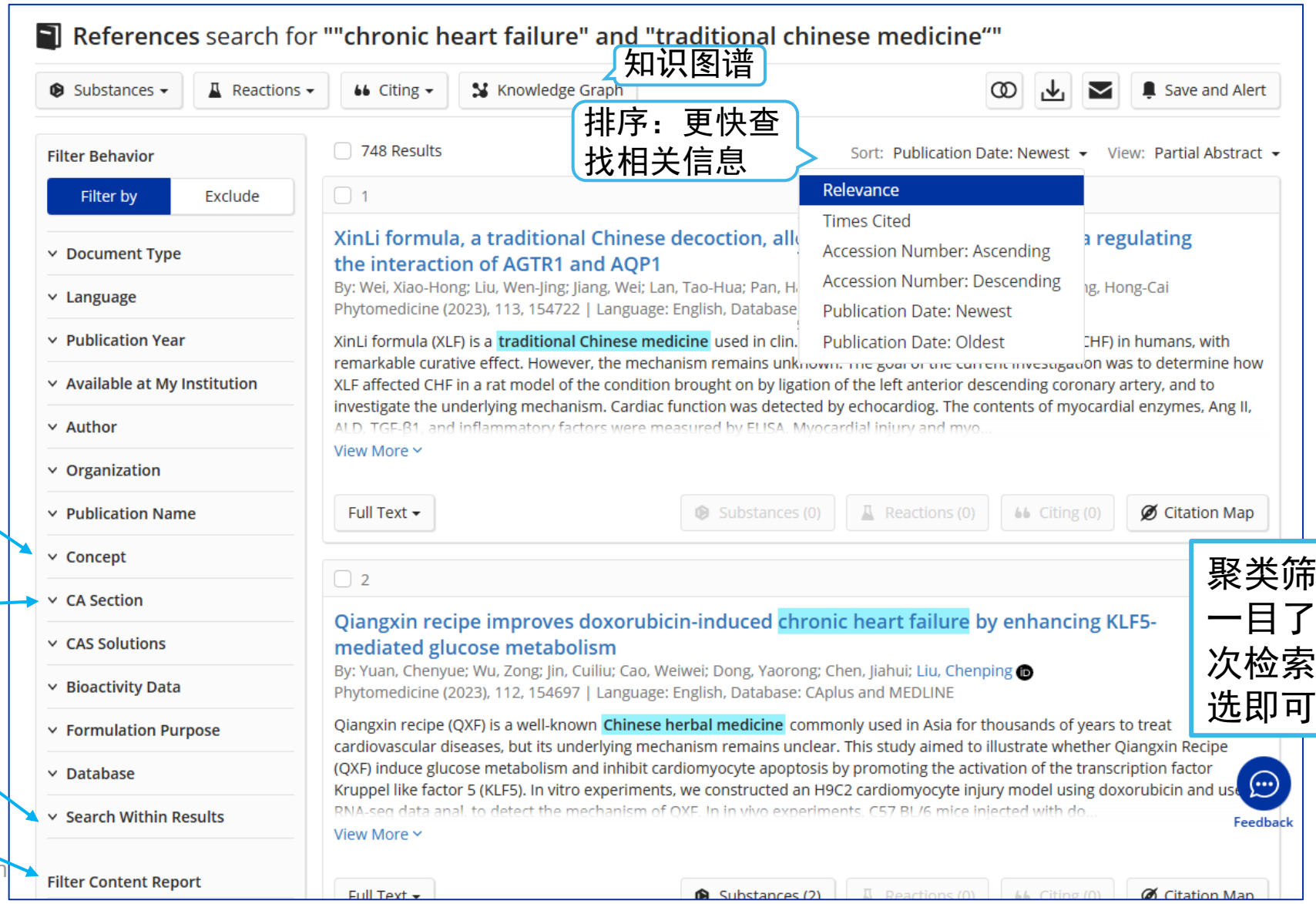
研究发展趋势

CAS标引的技术术语

CAS学科研究方向

二次检索

下载数据分析报告



聚类筛选项节省时间，一目了然。无需逐步二次检索和限定，直接勾选即可定位所需信息

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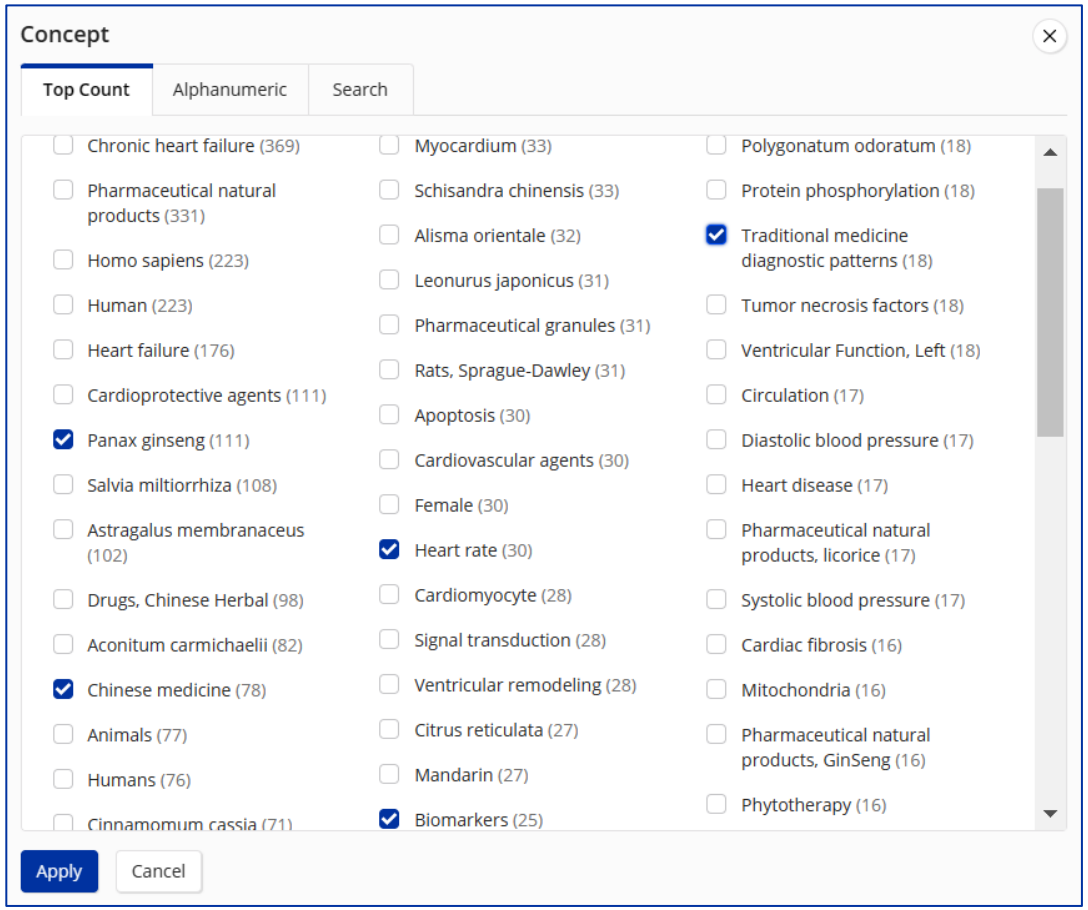
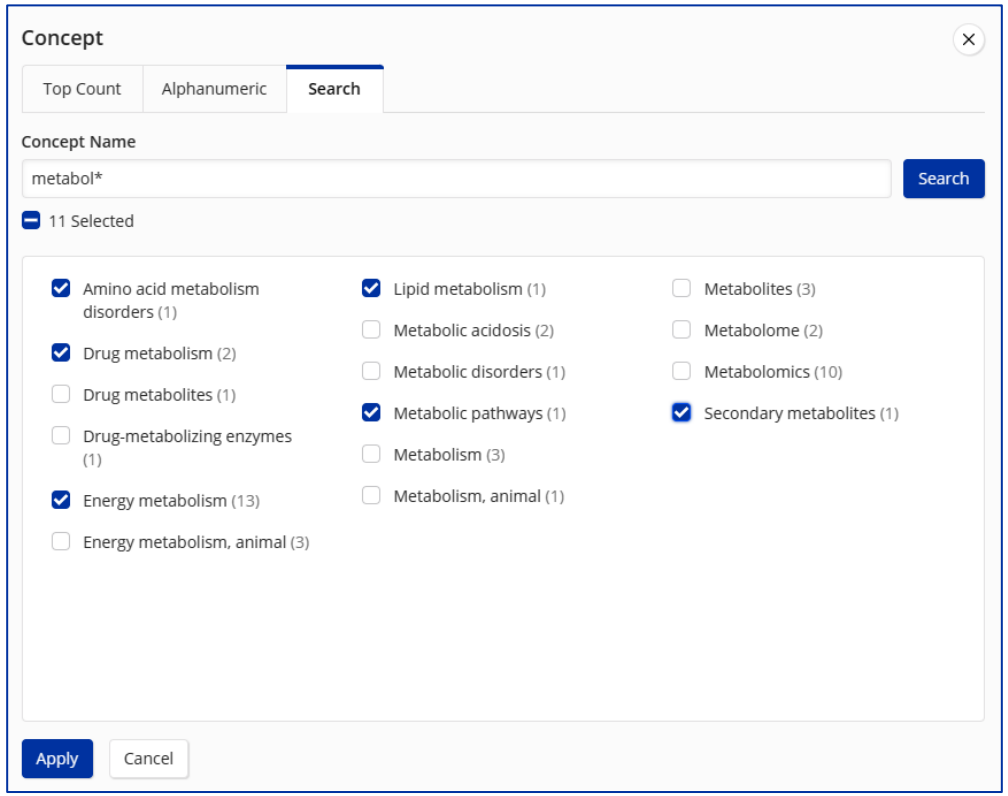
文献结果集—聚类筛选Concept





通过Concept纵览并精准定位感兴趣的核心研究点

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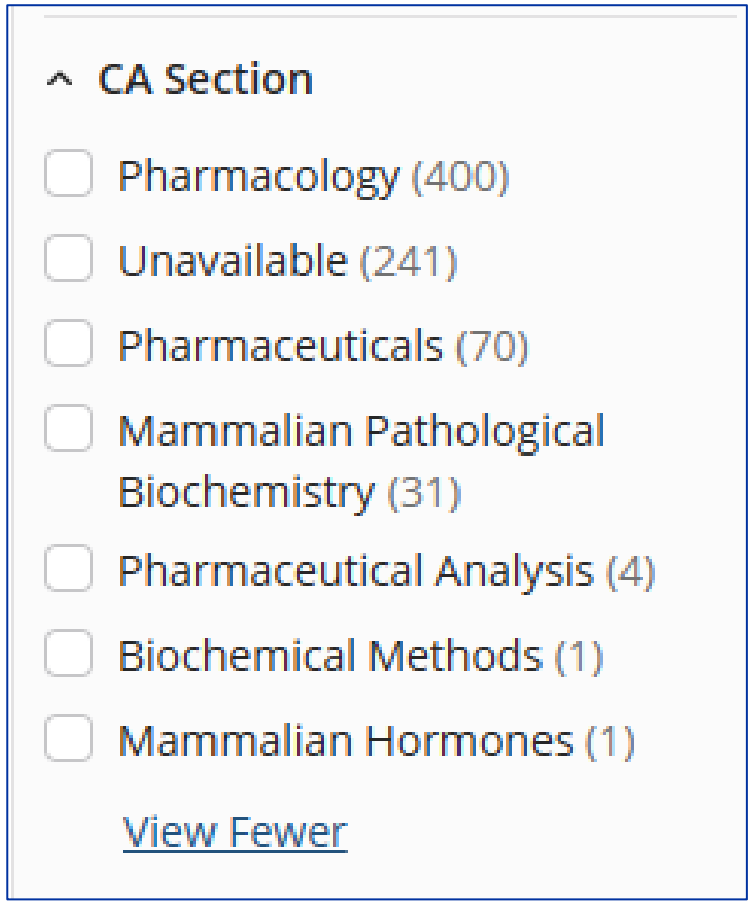
文献结果集—聚类筛选CA Section



通过CA Section快速锁定学科研究方向

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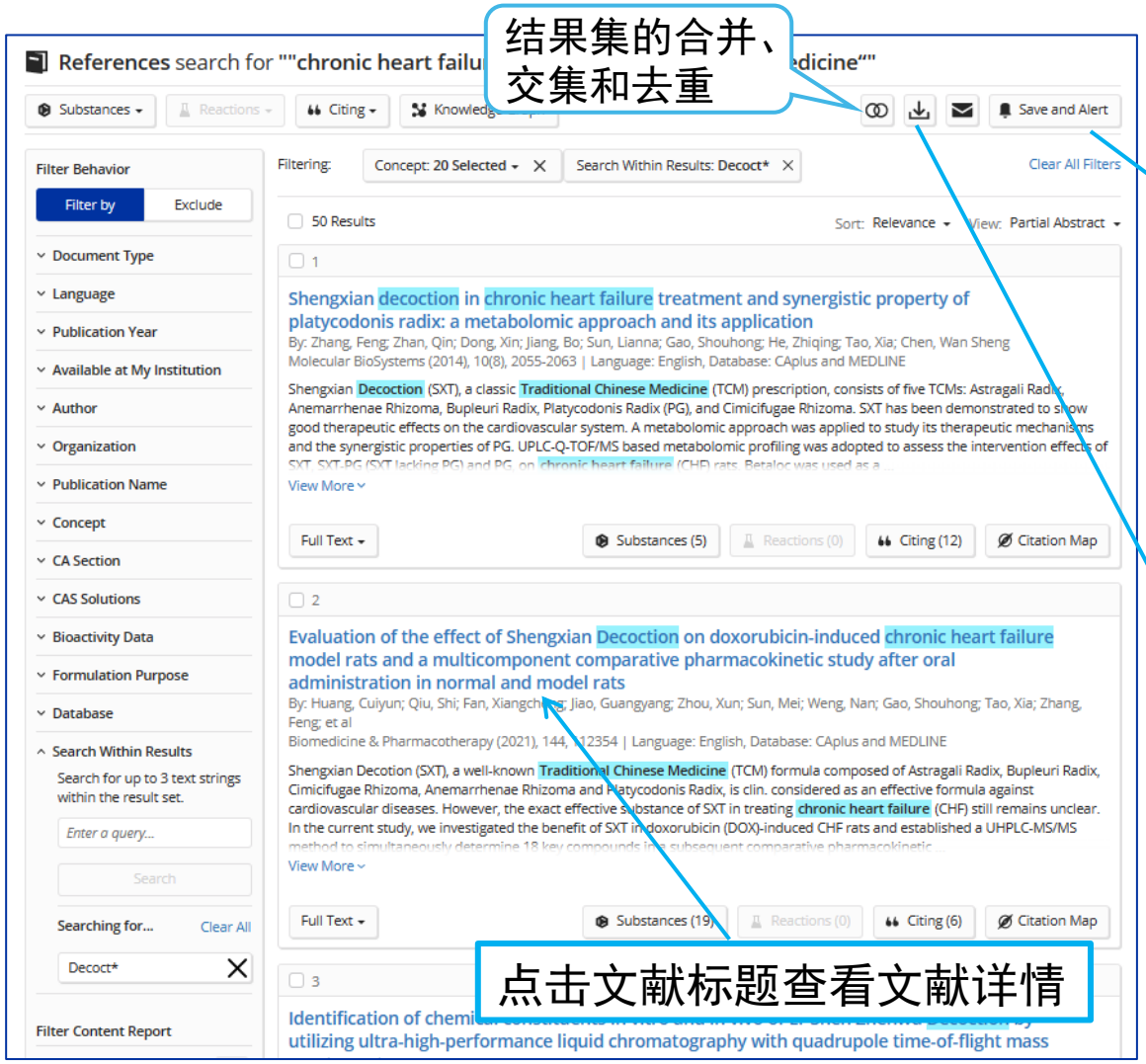
文献结果集—保存及下载



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文献详情

文献详情界面包括：

- 标题
- 摘要
- 文献中重要的技术术语（含Caplus、Medline的关键词）
- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
- 参考文献
- 链接原文
- 引文地图

科学家增值标引的信息

参考文献

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文献详情

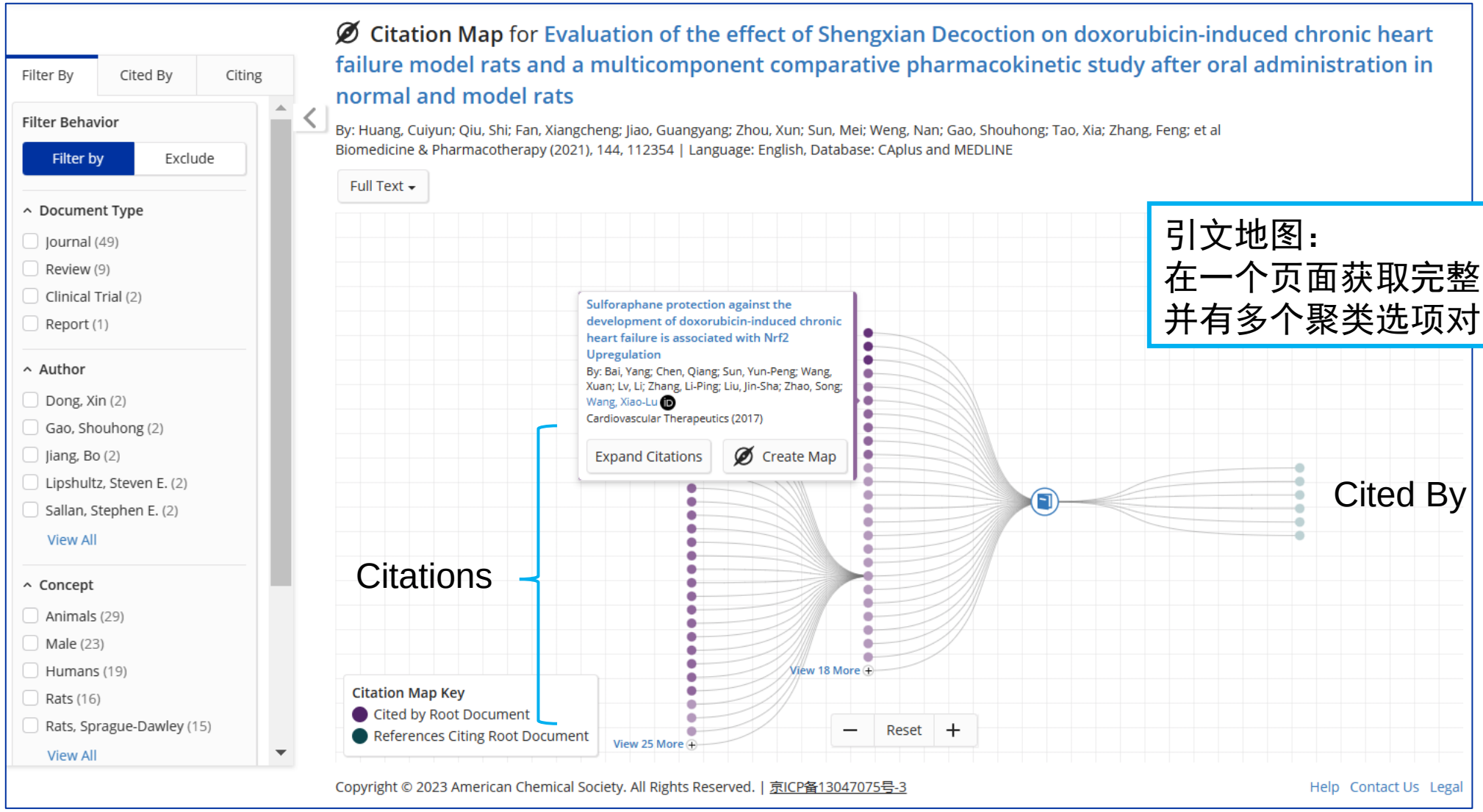
Concepts：
CAS科学家提供的标准技术术语，能更全面、更精准地检索。

Medline Subject Headings：
从不同的专业角度将文献研究核心点标出，更全面了解文献

Substances：
对原文中重点研究的物质信息一目了然；由Role了解文献对物质研究的学科方向

物质角色

文献详情—引文地图



引文地图：
在一个页面获取完整的前向、后向引文，并有多个聚类选项对引文进行筛选。

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专利文献

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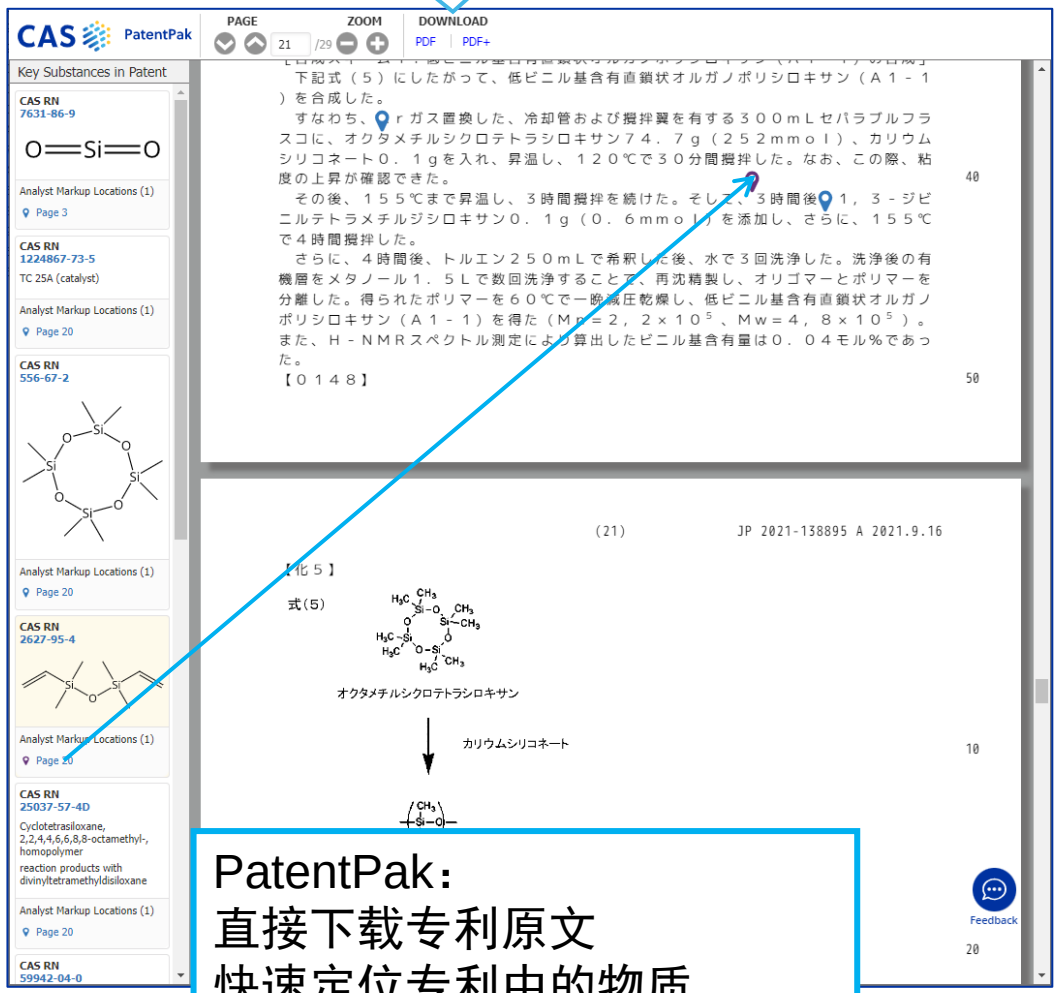

PatentPak：
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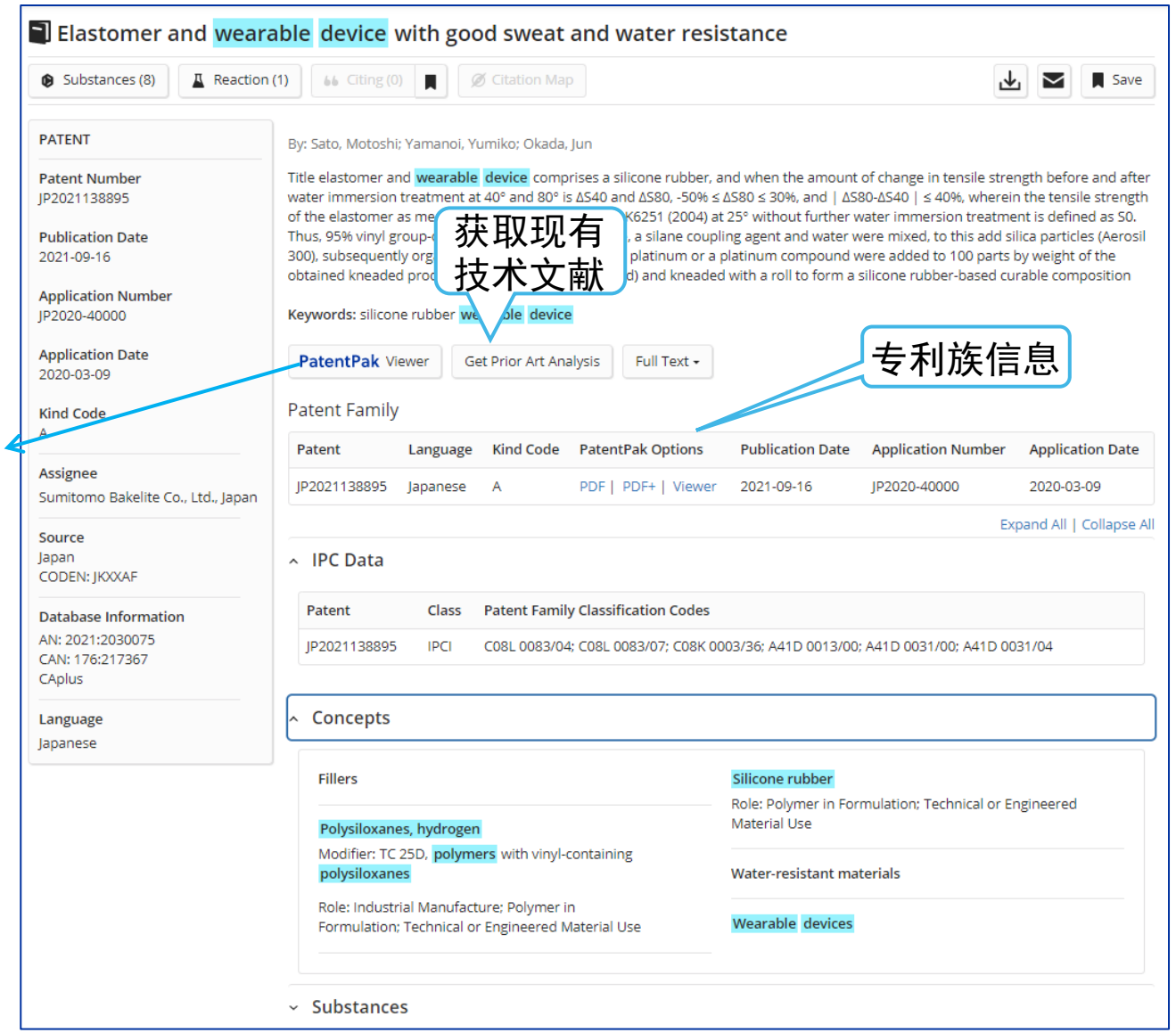
快速理解专利
阅读熟悉语言撰写的等同专利



查看ChemZent 来源的文献

References search for "enzyme and reduction" + drawn structure

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

Structure Match

As Drawn (0)

Substructure (8,881)

Filter Behavior

Filter by | Exclude

Document Type

Language

Publication Year

Available at My Institution

Author

Publication Name

Concept

Database

CAplus (8,605)

MEDLINE (6,814)

CHEMZENT (31)

Search Within Results

Filter Content Report

Download filter data from this result set.

Filtering: Database: CHEMZENT ×

Clear All Filters

31 Results

Sort: Relevance View: Partial Abstract

1

Fabric change of CARB azole in rats and rabbit

By: Johns, S. R.; Wright, S. E.

Chemisches Zentralblatt (1966), 137(5), 01578-01578 | Language: German, Database: CHEMZENT

Machine Translated: After administration of carbazoles is 3-hydroxy carbazole, conjugate with glucuronic acid in the urine separated Hauptstoffwechselprod. in rats and rabbits. The hydroxylation in 3-position is in accordance with the etching oxidizing enzymes at the position of greatest electron density. For the investigation of werden carbazole-14 C is used. Experiments: 14C-carbazole (I), Melting Point 242-244 ° (from benzene) by diazotization and reduction of 14C-aniline to 14C-phenylhydrazine (240-245 ° F.) with cyclohexanone in 14C-tetrahydrocarbazole is converted. Dehydrogenation to Pd-C gives I. Respect m...

View More

ChemZent | Full Text | Substances (14) | Reactions (0) | Citing (0) | Citation Map

2

Cobamide and ribo nucleotide reduction. 3. Part The content of the Cobamid-abhängigen Ribonucleosid-triphosphatreduktase in Lactobacillus leichmanii influencing factors

By: Ghambeer, R. K.; Blakley, R. L.

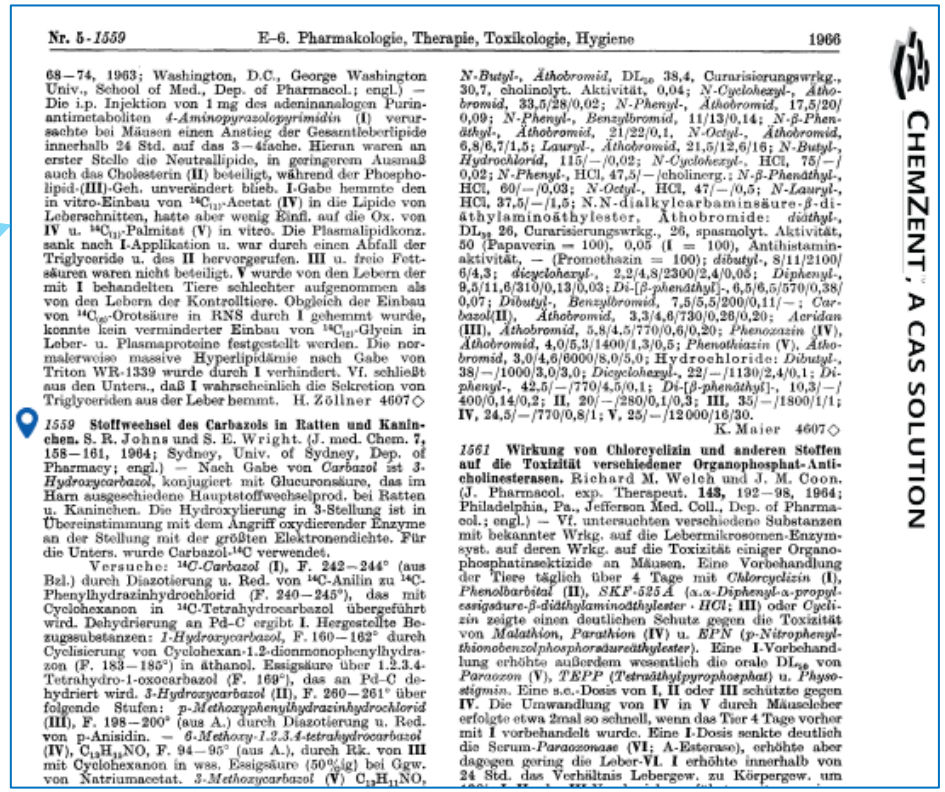
Chemisches Zentralblatt (1968), 139(28), 160-160 | Language: German, Database: CHEMZENT

Machine Translated: Hysic. Res. common. 20 (1965) 20. — the content of ribo nucleoside triphosphate reductase (I) in extracts of L. leichmanii depends on the age of the culture. During the linear growth if I-Geh. with increasing age up to the end of the linear phase on and falls then. Extracts from stationary cells exhibit no significant I-Aktivität. The rapid I-Synth. during the linear growth by chloramphenicol and ActinomycinD inhibited. The decrease of I-Geh. after completion of the linear growth is based not on the presence one increased amount proteolyt. Enzymes nor on incomplete release of said enzyme. The...

View More

ChemZent | Full Text | Substances (3) | Reactions (0) | Citing (0)

3



Nr. 5 - 1559 E–6. Pharmakologie, Therapie, Toxikologie, Hygiene 1966

68—74, 1963; Washington, D.C., George Washington Univ., School of Med., Dep. of Pharmacol.; engl.) — Die i.p. Injektion von 1 mg des adeninanalogen Purin-antimetaboliten *4-Aminopyrazolopyrimidin* (I) verursachte bei Mäusen einen Anstieg der Gesamtleberlipide innerhalb 24 Std. auf das 3—4fache. Hierun waren an erster Stelle die Neutrallipide, in geringerem Ausmaß auch das Cholesterin (II) beteiligt, während der Phospholipid-(III)-Geh. unverändert blieb. I-Gabe hemmte den in vitro-Einbau von $^{14}C_{(1)}$-Acetat (IV) in die Lipide von Leberschnitten, hatte aber wenig Einfl. auf die Ox. von IV u. $^{14}C_{(1)}$-Palmitat (V) in vitro. Die Plasmalipidkonz. sank nach I-Applikation u. war durch einen Abfall der Triglyceride u. des II hervorgerufen. III u. freie Fettsäuren waren nicht beteiligt. V wurde von den Lebern der mit I behandelten Tiere schlechter aufgenommen als von den Lebern der Kontrolltiere. Obgleich der Einbau von $^{14}C_{(6)}$-Orotsäure in RNS durch I gehemmt wurde, konnte kein verminderter Einbau von $^{14}C_{(2)}$-Glycin in Leber- u. Plasmaproteine festgestellt werden. Die normalerweise massive Hyperlipidämie nach Gabe von Triton WR-1339 wurde durch I verhindert. Vf. schließt aus den Unters., daß I wahrscheinlich die Sekretion von Triglyceriden aus der Leber hemmt. H. Zöllner 4607◇

1559 **Stoffwechsel des Carbazols in Ratten und Kaninchen.** S. R. Johns und S. E. Wright. (J. med. Chem. **7**, 158—161, 1964; Sydney, Univ. of Sydney, Dep. of Pharmacy; engl.) — Nach Gabe von *Carbazol* ist *3-Hydroxycarbazol*, konjugiert mit Glucuronsäure, das im Harn ausgeschiedene Hauptstoffwechselprod. bei Ratten u. Kaninchen. Die Hydroxylierung in 3-Stellung ist in Übereinstimmung mit dem Angriff oxydierender Enzyme an der Stellung mit der größten Elektronendichte. Für die Unters. wurde Carbazol-^{14}C verwendet.

Versuche: *^{14}C-Carbazol* (I), F. 242—244° (aus Bzl.) durch Diazotierung u. Red. von ^{14}C-Anilin zu ^{14}C-Phenylhydrazinhydrochlorid (F. 240—245°), das mit Cyclohexanon in ^{14}C-Tetrahydrocarbazol übergeführt wird. Dehydrierung an Pd-C ergibt I. Hergestellte Bezugssubstanzen: *1-Hydroxycarbazol*, F. 160—162° durch Cyclisierung von Cyclohexan-1.2-dionmonophenylhydrazon (F. 183—185°) in äthanol. Essigsäure über 1.2.3.4-Tetrahydro-1-oxocarbazol (F. 169°), das an Pd-C dehydriert wird. *3-Hydroxycarbazol* (II), F. 260—261° über folgende Stufen: *p-Methoxyphenylhydrazinhydrochlorid* (III), F. 198—200° (aus A.) durch Diazotierung u. Red. von p-Anisidin. — *6-Methoxy-1.2.3.4-tetrahydrocarbazol* (IV), $C_{13}H_{15}NO$, F. 94—95° (aus A.), durch Rk. von III mit Cyclohexanon in wss. Essigsäure (50%ig) bei Ggw. von Natriumacetat. *3-Methoxycarbazol* (V) $C_{13}H_{11}NO$,

N-Butyl-, Äthobromid, DL_{50} 38,4, Curarisierungswrkg., 30,7, cholinolyt. Aktivität, 0,04; *N-Cyclohexyl-, Äthobromid*, 33,5/28/0,02; *N-Phenyl-, Äthobromid*, 17,5/20/0,09; *N-Phenyl-, Benzylbromid*, 11/13/0,14; *N-β-Phenäthyl-, Äthobromid*, 21/22/0,1, *N-Octyl-, Äthobromid*, 6,8/6,7/1,5; *Lauryl-, Äthobromid*, 21,5/12,6/16; *N-Butyl-, Hydrochlorid*, 115/—/0,02; *N-Cyclohexyl-*, HCl, 75/—/0,02; *N-Phenyl-*, HCl, 47,5/—/cholinerg.; *N-β-Phenäthyl-*, HCl, 60/—/0,03; *N-Octyl-*, HCl, 47/—/0,5; *N-Lauryl-*, HCl, 37,5/—/1,5; N.N-dialkylcarbaminsäure-β-diäthylaminoäthylester, Äthobromide: *diäthyl-*, DL_{50} 26, Curarisierungswrkg., 26, spasmolyt. Aktivität, 50 (Papaverin = 100), 0,05 (I = 100), Antihistaminaktivität, — (Promethazin = 100); *dibutyl-*, 8/11/2100/6/4,3; *dicyclohexyl-*, 2,2/4,8/2300/2,4/0,05; *Diphenyl-*, 9,5/11,6/310/0,13/0,03; *Di-[β-phenäthyl]-*, 6,5/6,5/570/0,38/0,07; *Dibutyl-, Benzylbromid*, 7,5/5,5/200/0,11/—; *Carbazol*(II), *Äthobromid*, 3,3/4,6/730/0,28/0,20; *Acridan* (III), *Äthobromid*, 5,8/4,5/770/0,6/0,20; *Phenoxazin* (IV), *Äthobromid*, 4,0/5,3/1400/1,3/0,5; *Phenothiazin* (V), *Äthobromid*, 3,0/4,6/6000/8,0/5,0; Hydrochloride: *Dibutyl-*, 38/—/1000/3,0/3,0; *Dicyclohexyl-*, 22/—/1130/2,4/0,1; *Diphenyl-*, 42,5/—/770/4,5/0,1; *Di-[β-phenäthyl]-*, 10,3/—/400/0,14/0,2; II, 20/—/280/0,1/0,3; III, 35/—/1800/1/1; IV, 24,5/—/770/0,8/1; V, 25/—/12000/16/30.

K. Maier 4607◇

1561 **Wirkung von Chlorcyclizin und anderen Stoffen auf die Toxizität verschiedener Organophosphat-Anticholinesterasen.** Richard M. Welch und J. M. Coon. (J. Pharmacol. exp. Therapeut. **143**, 192—98, 1964; Philadelphia, Pa., Jefferson Med. Coll., Dep. of Pharmacol.; engl.) — Vf. untersuchten verschiedene Substanzen mit bekannter Wrkg. auf die Lebermikrosomen-Enzymsyst. auf deren Wrkg. auf die Toxizität einiger Organophosphatinsektizide an Mäusen. Eine Vorbehandlung der Tiere täglich über 4 Tage mit *Chlorcyclizin* (I), *Phenolbarbital* (II), *SKF-525 A* (α.α-*Diphenyl-α-propylessigsäure-β-diäthylaminoäthylester · HCl*; III) oder *Cyclizin* zeigte einen deutlichen Schutz gegen die Toxizität von *Malathion*, *Parathion* (IV) u. *EPN* (*p-Nitrophenylthionobenzolphosphorsaureäthylester*). Eine I-Vorbehandlung erhöhte außerdem wesentlich die orale DL_{50} von *Paraoxon* (V), *TEPP* (*Tetraäthylpyrophosphat*) u. *Physostigmin*. Eine s.c.-Dosis von I, II oder III schützte gegen IV. Die Umwandlung von IV in V durch Mäuseleber erfolgte etwa 2mal so schnell, wenn das Tier 4 Tage vorher mit I vorbehandelt wurde. Eine I-Dosis senkte deutlich die Serum-*Paraoxonase* (VI; A-Esterase), erhöhte aber dagegen gering die Leber-VI. I erhöhte innerhalb von 24 Std. das Verhältnis Lebergew. zu Körpergew. um

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- 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

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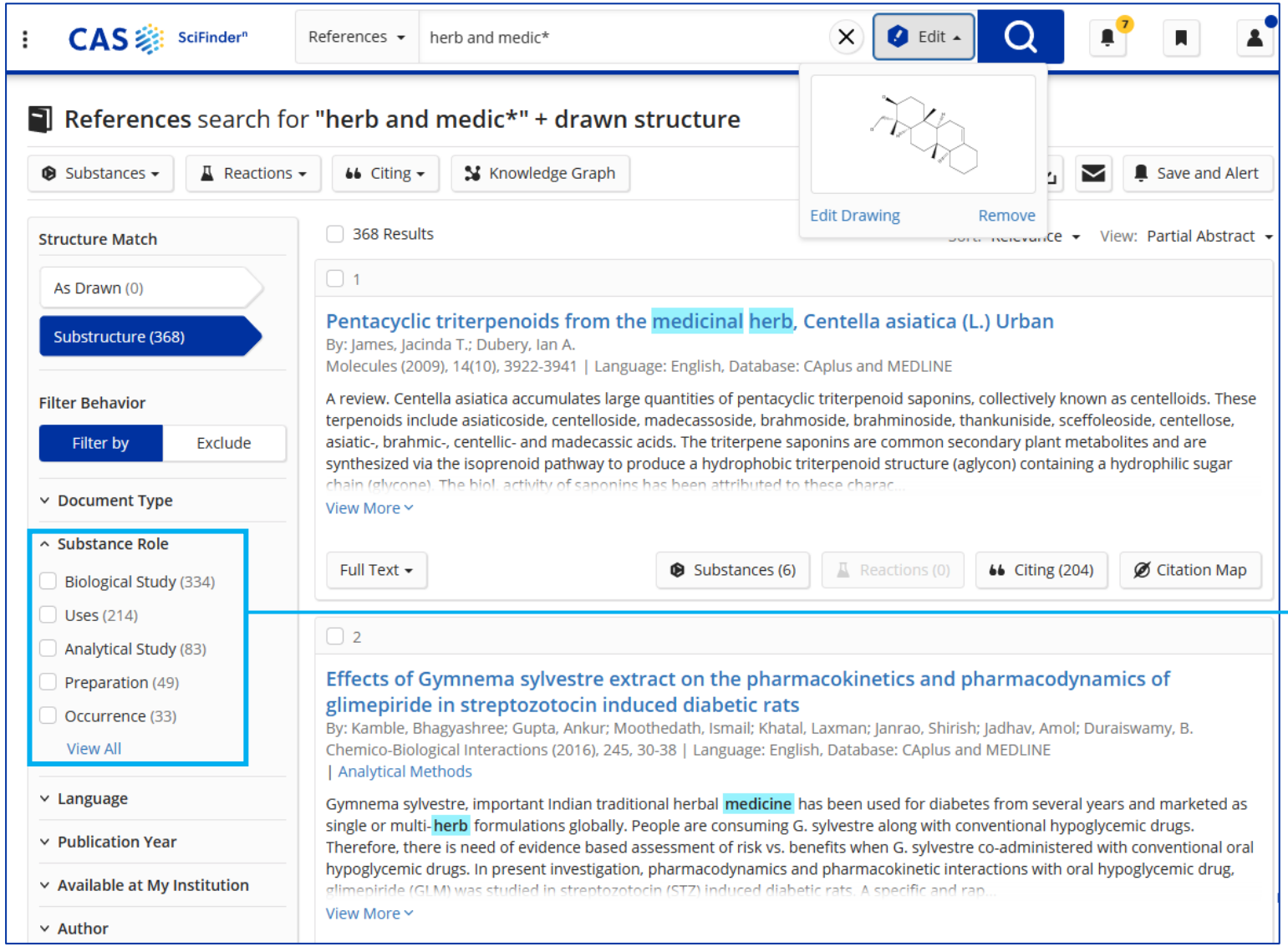
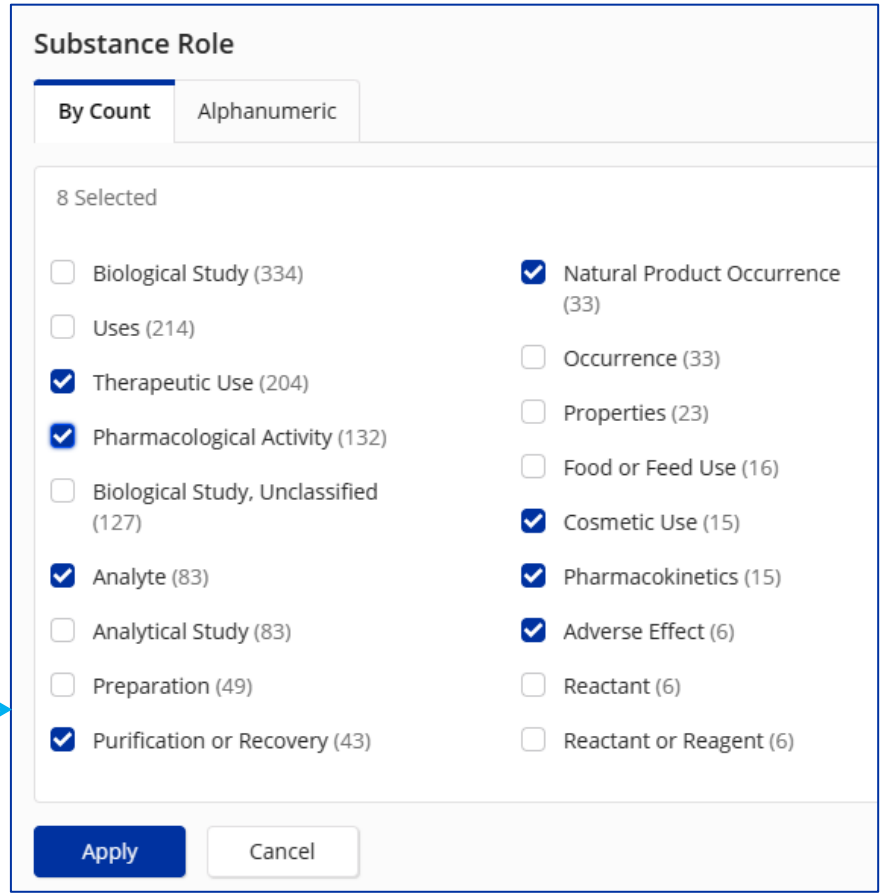
文献检索—主题词+结构联合检索





物质在文献中的研究角色

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文献检索小结

1. 使用布尔逻辑算符and、or、not连接主题词
2. 利用CAS Lexicon选词精准检索文献
3. 通过聚类筛选工具快速获得目标文献
4. 从引文地图拓展检索，获得更多灵感
5. 用PatentPak提高专利阅读效率
6. 主题词+结构联合检索快速获得文献

物质检索

- 物质检索方法
  - 物质标识符：化学名称，CAS RN
  - 文献标识符：专利号、文献号、PubMed ID、DOI
  - 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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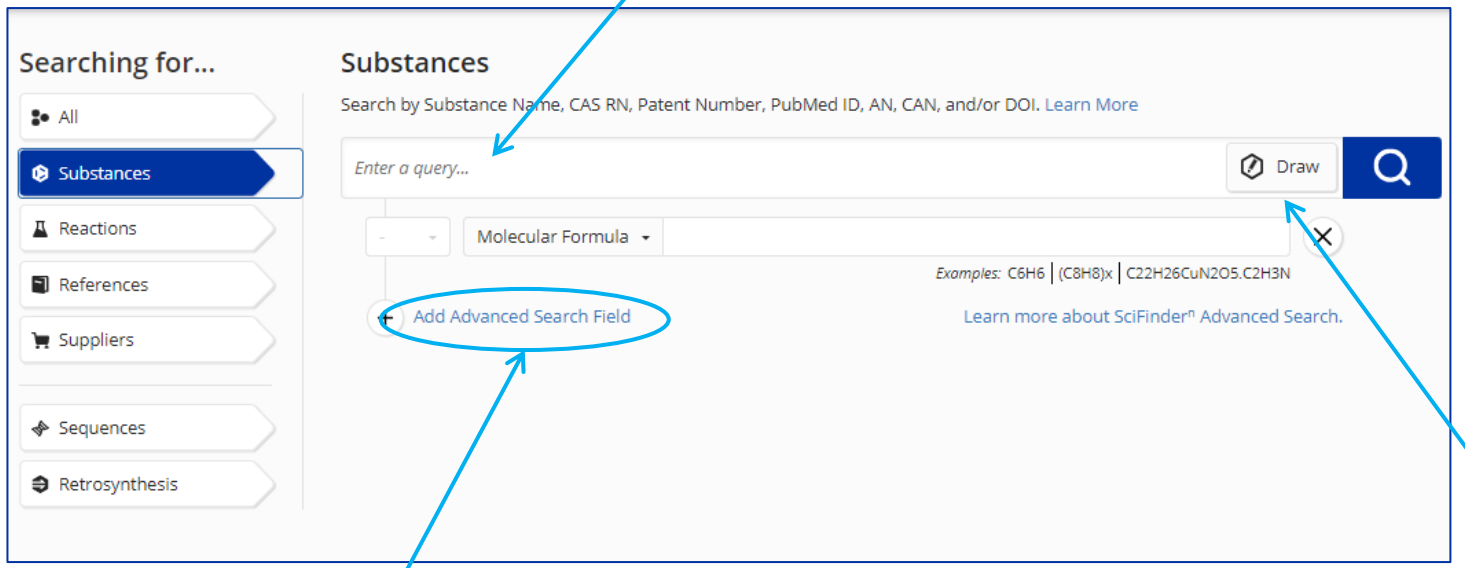
物质检索

通过物质名称、CAS RN，文献标识符检索物质



通过分子式、物性参数、谱图数据检索物质

打开结构绘制面板进行结构检索

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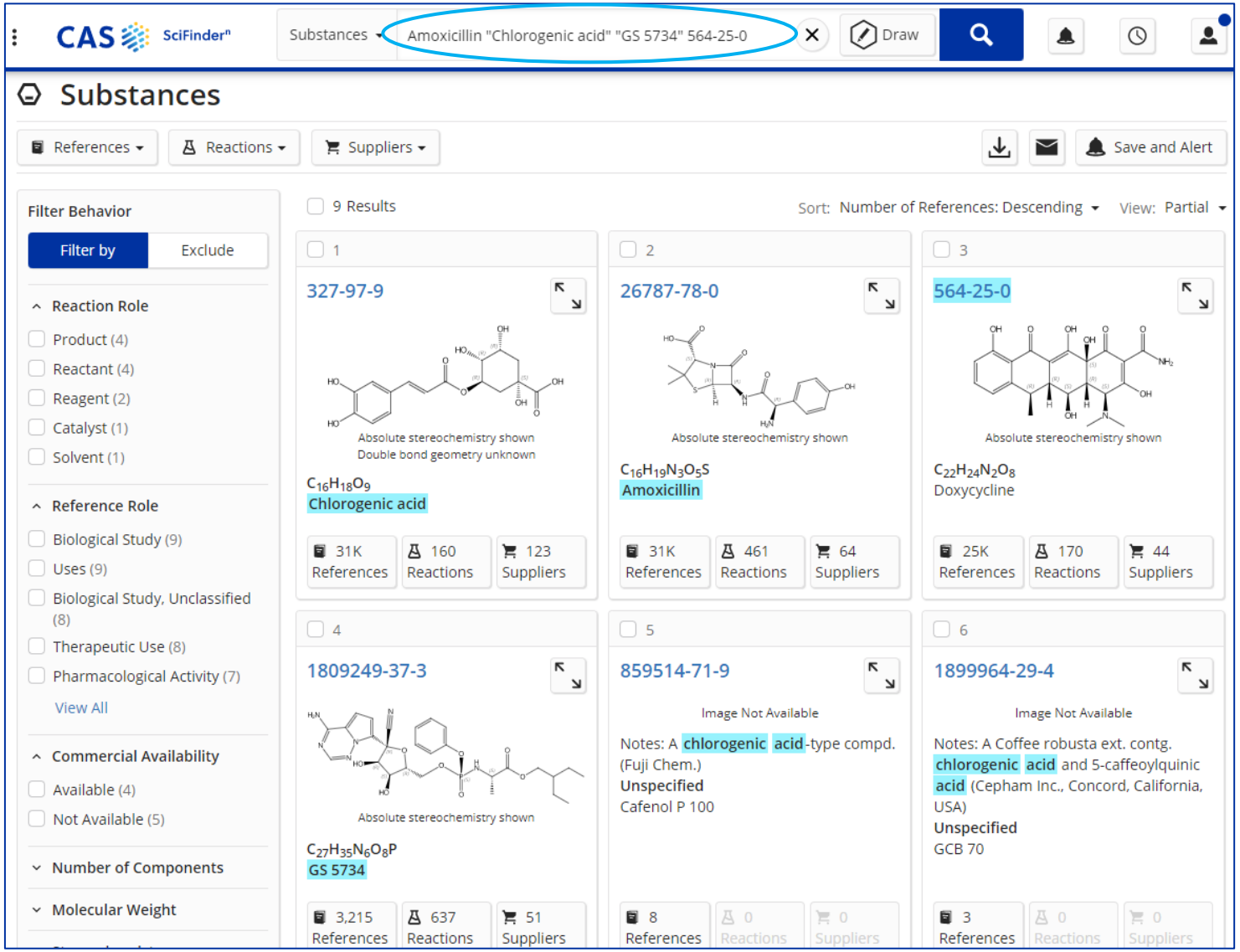
物质检索—物质名称、CAS RN、代码



- 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）；
- 双引号“ ”可精准识别物质识别符；
- 不同的物质使用空格隔开，支持高达2000个字符

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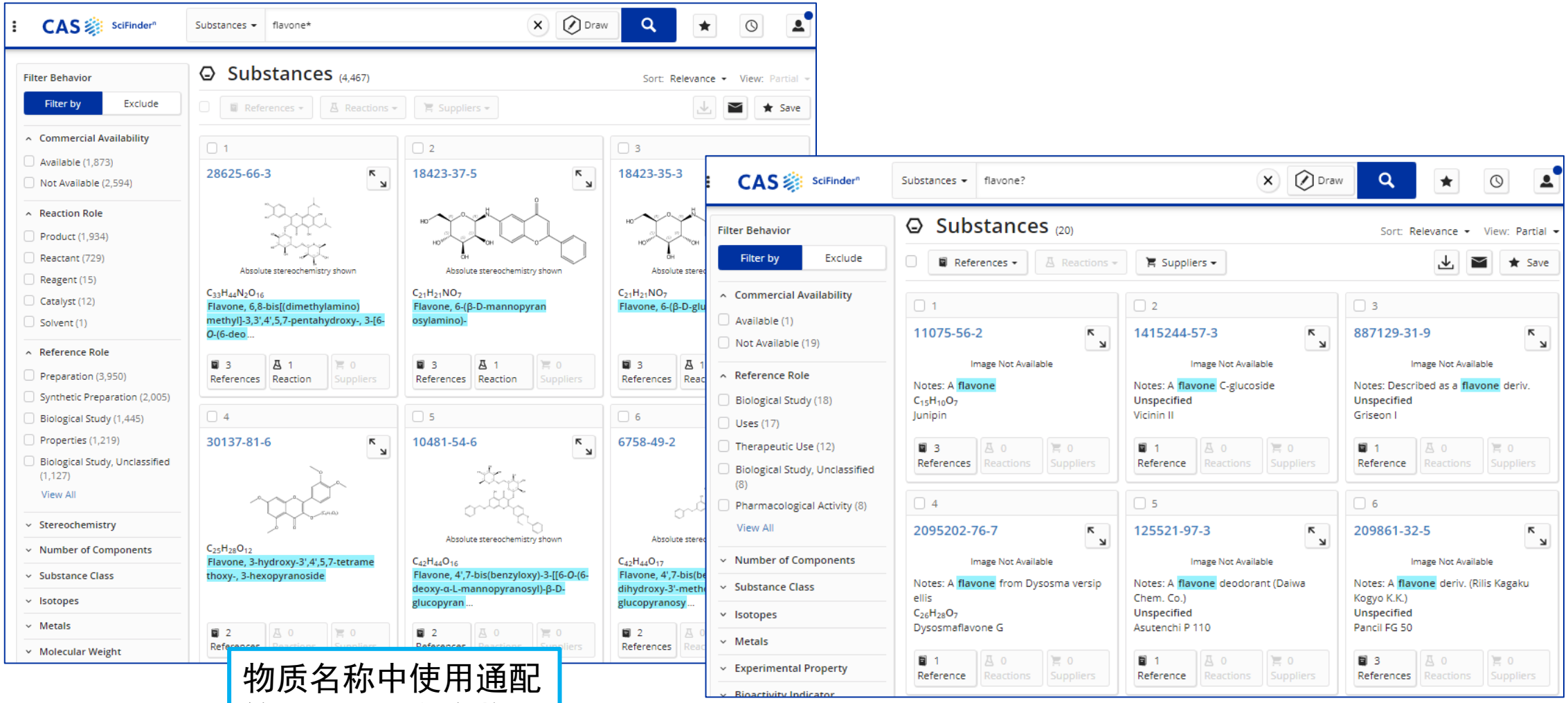
物质检索—物质名称中间或词尾使用通配符*或？



物质名称中使用通配符可以检索多个物质

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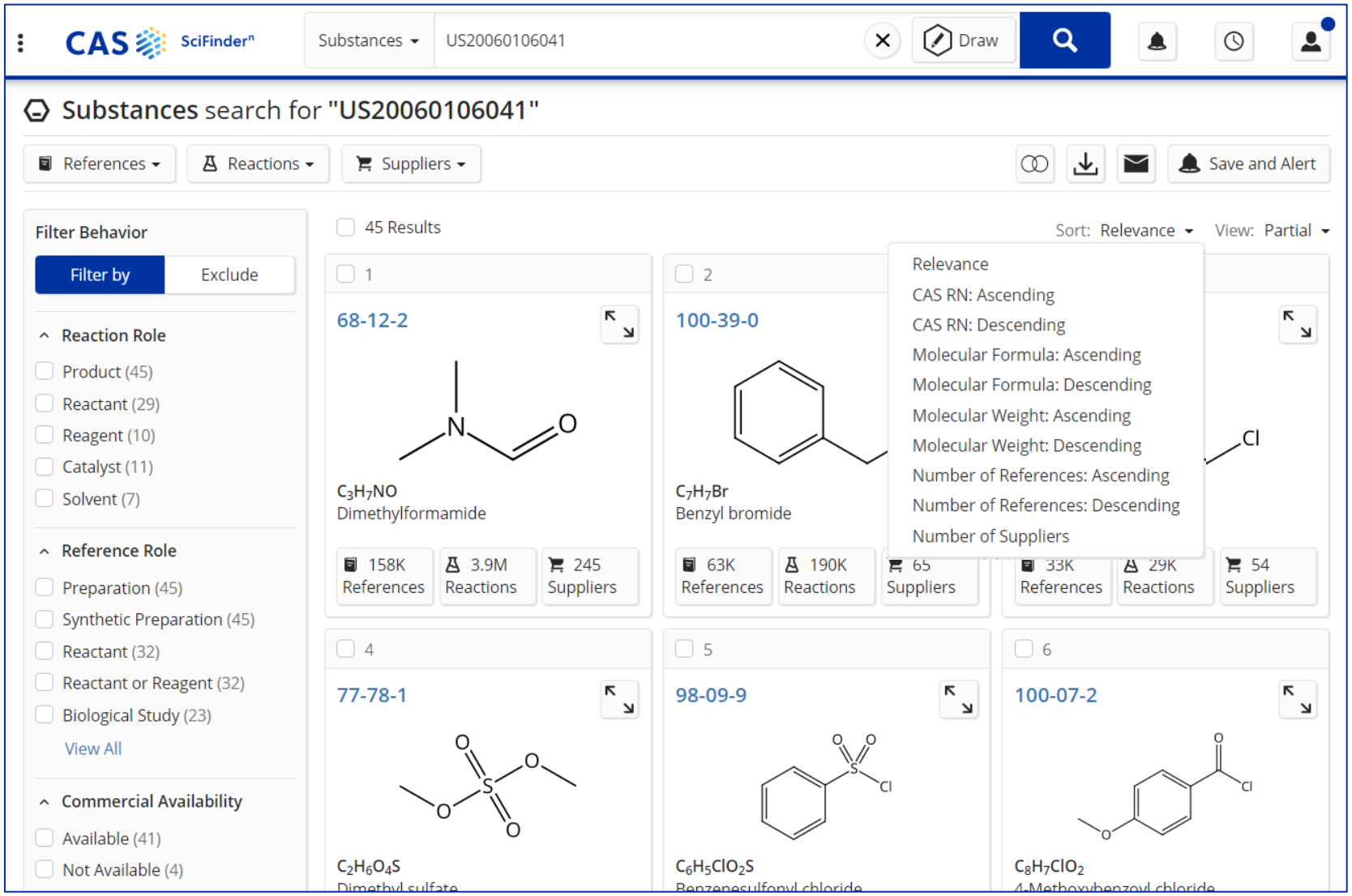
物质检索—文献标识符及结果集排序



利用物质排序快速查找目标物质：
相关度
CAS RN
分子式
分子量
文献量
供应商数量

帮助用户迅速获得关注文献中的物质信息

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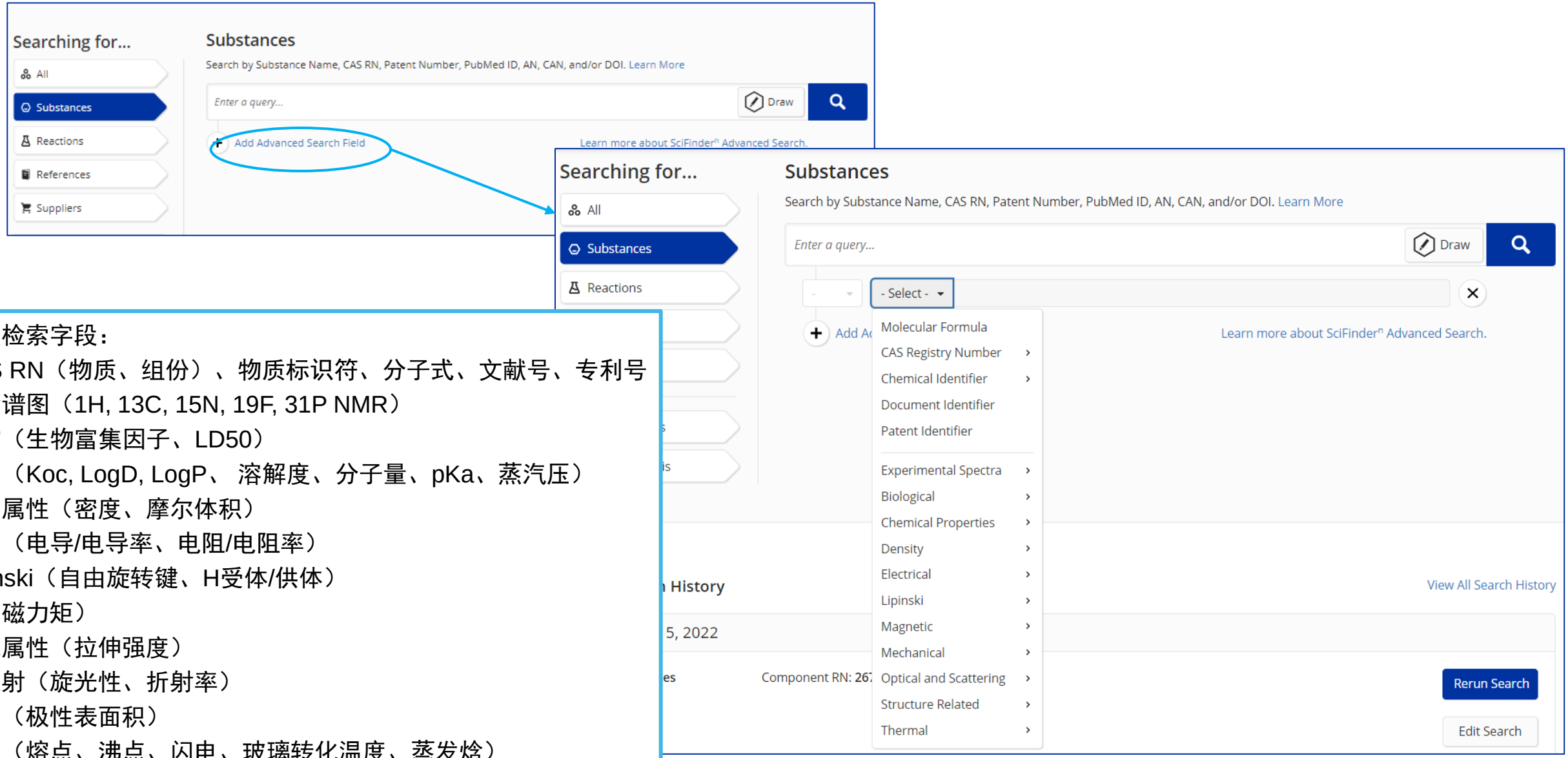
物质检索—Advanced Search



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（1H, 13C, 15N, 19F, 31P NMR）

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）

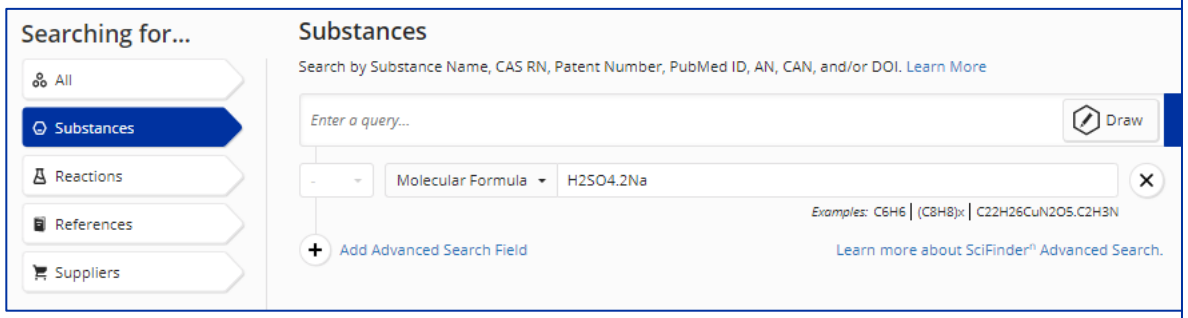
光散射（旋光性、折射率）

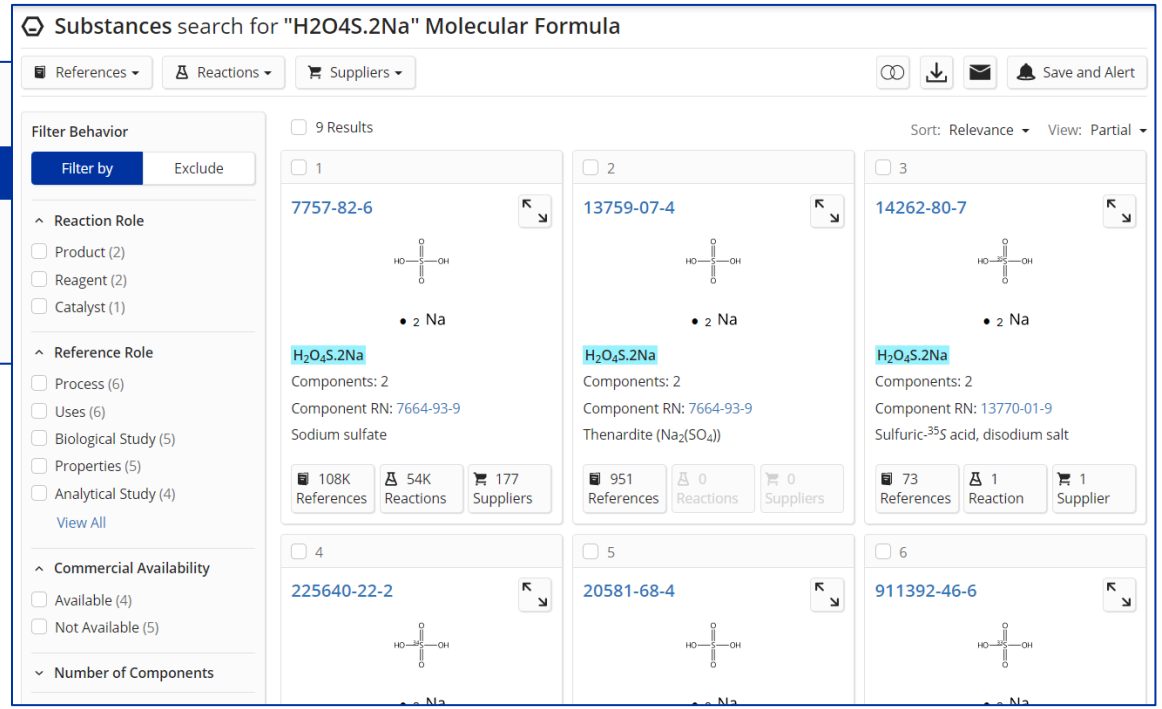
结构（极性表面积）

热学（熔点、沸点、闪电、玻璃转化温度、蒸发焓）

物质检索—分子式

Na2SO4：H2O4S.2Na





- 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

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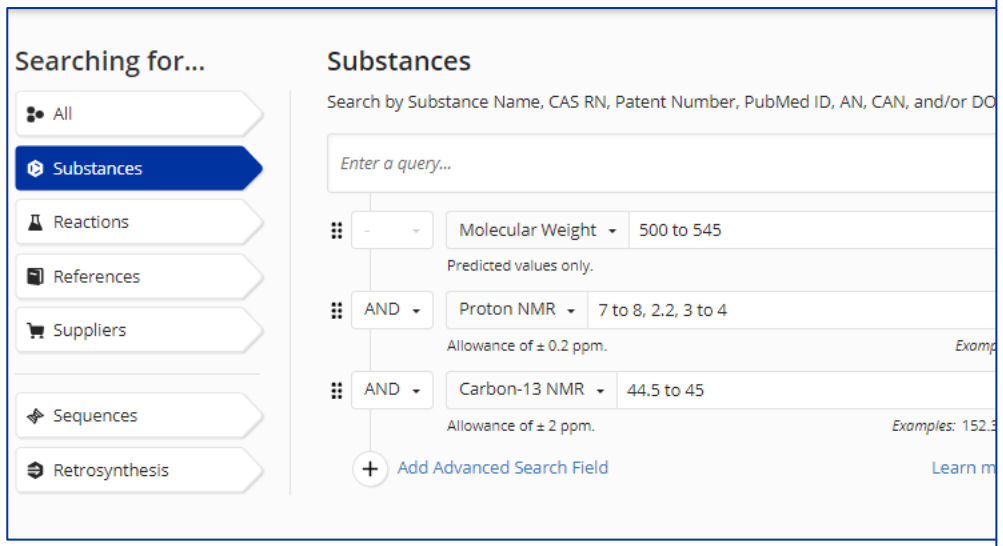
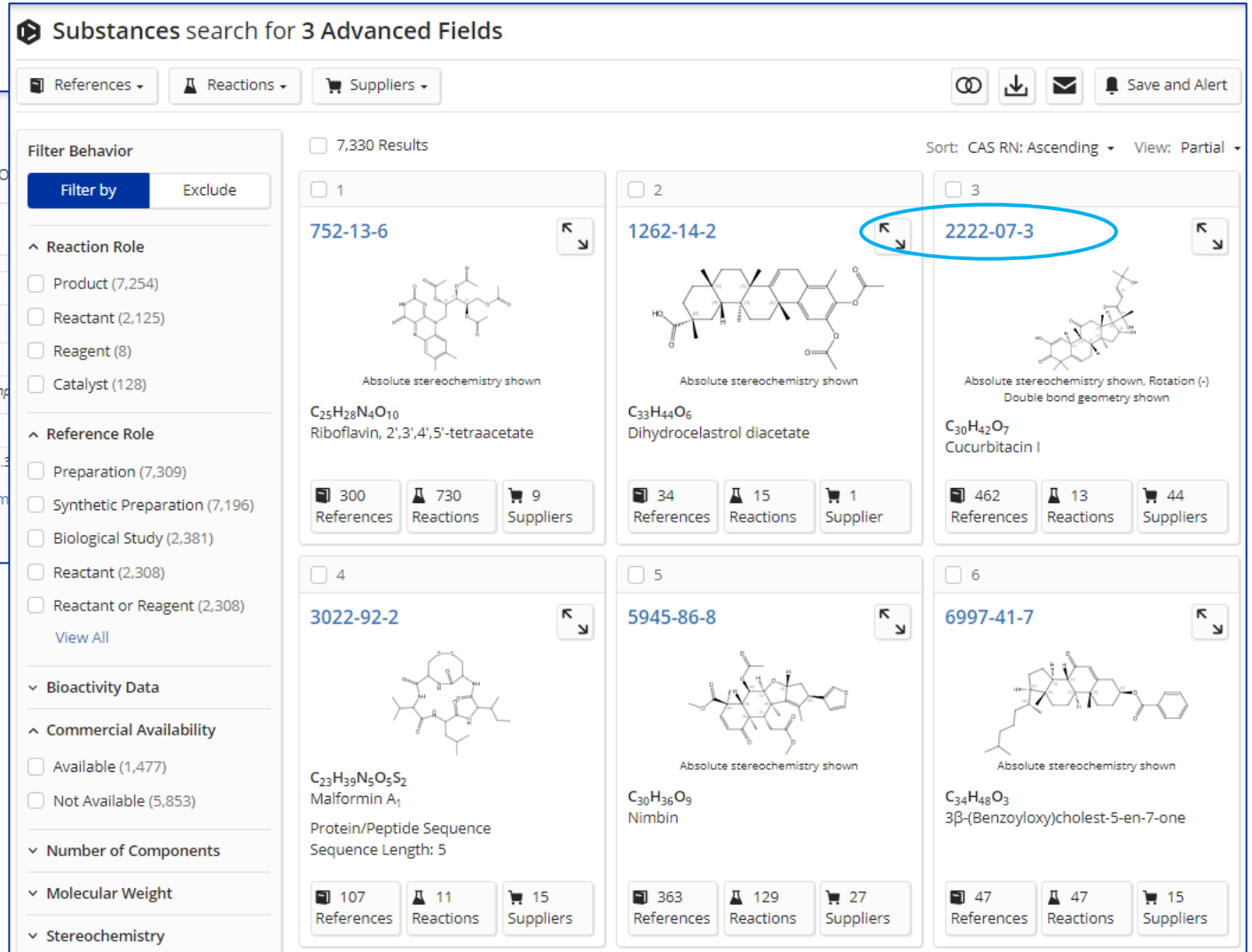
物质检索—联合检索

H谱特征峰化学位移数据：7 to 8, 2.2, 3 to 4

C谱特征峰化学位移数据：44.5 to 45

分子量：500--545之间

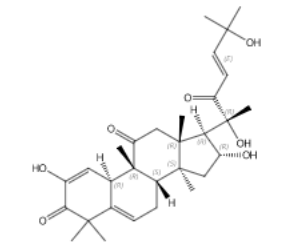




物质详情

CAS Registry Number: 2222-07-3

References (462) | Reactions (13) | Suppliers (44) | Save



Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown

$C_{30}H_{42}O_7$

19-Norlanosta-1,5,23-triene-3,11,22-trione, 2,16,20,25-tetrahydroxy-9-methyl-, (9β,10α,16α,23*E*)- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	514.65	-
Boiling Point (Predicted)	698.3±55.0 °C	Press: 760 Torr
Density (Predicted)	1.26±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	8.51±0.70	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
- Toxicity — CAS LIFE SCIENCES
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- Additional Details

折叠菜单显示物质各类信息

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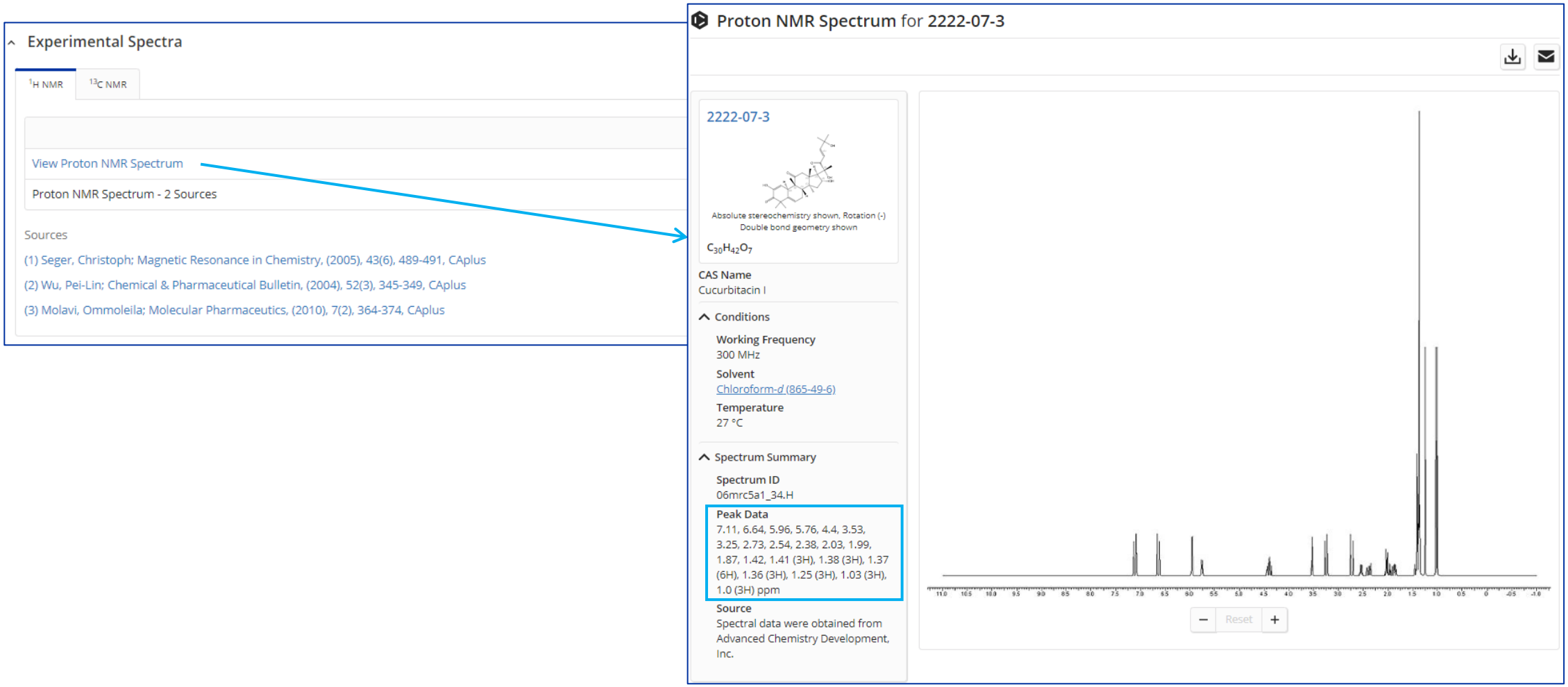
物质详情



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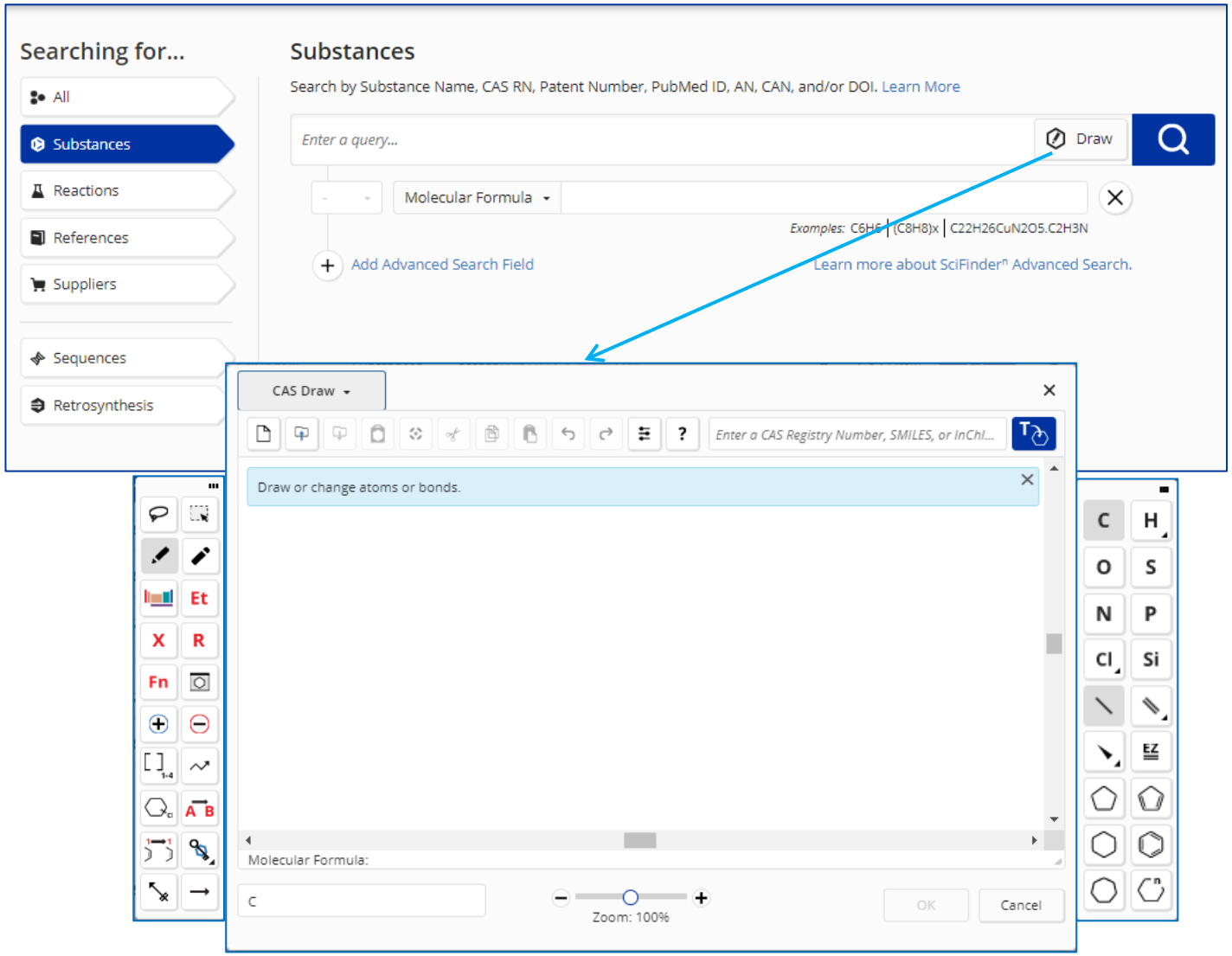
物质检索—结构检索



选择可变基团

自定义R基团

片段定义工具

重复片段工具

取代位点可变

锁工具

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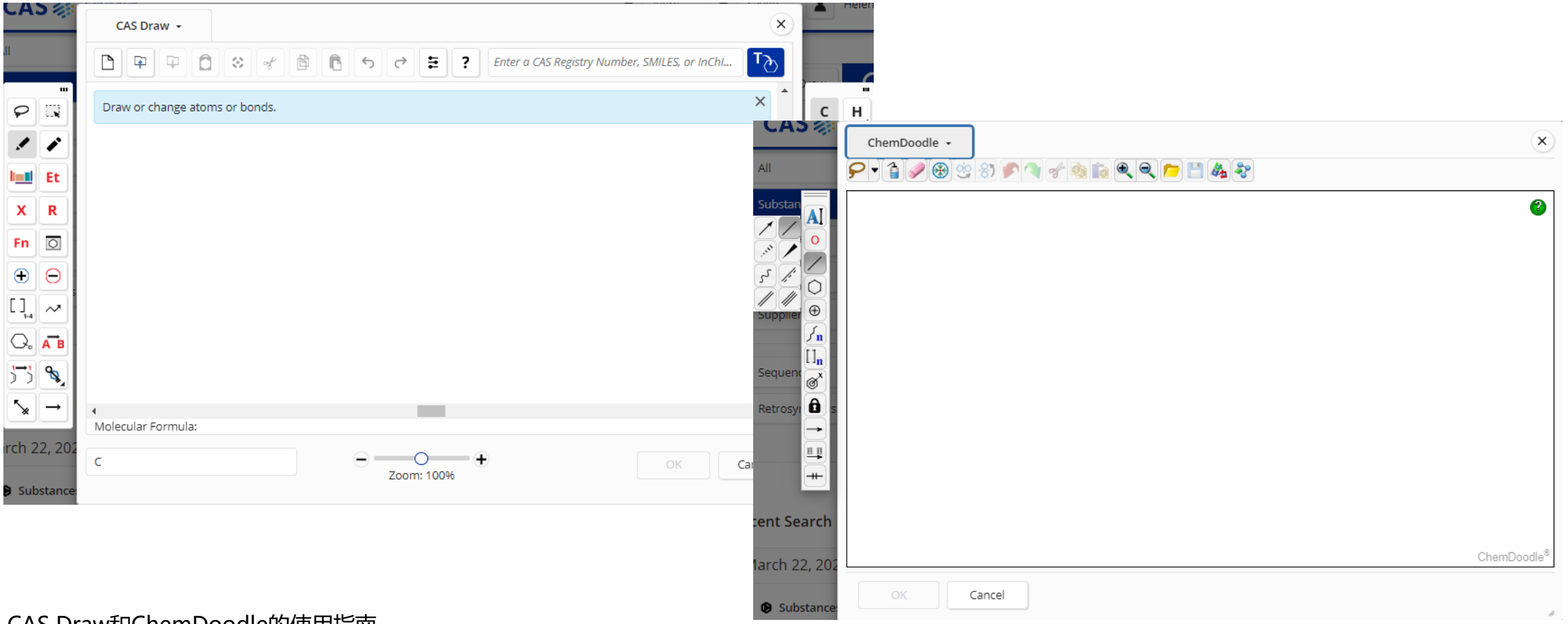
物质检索—结构绘图板



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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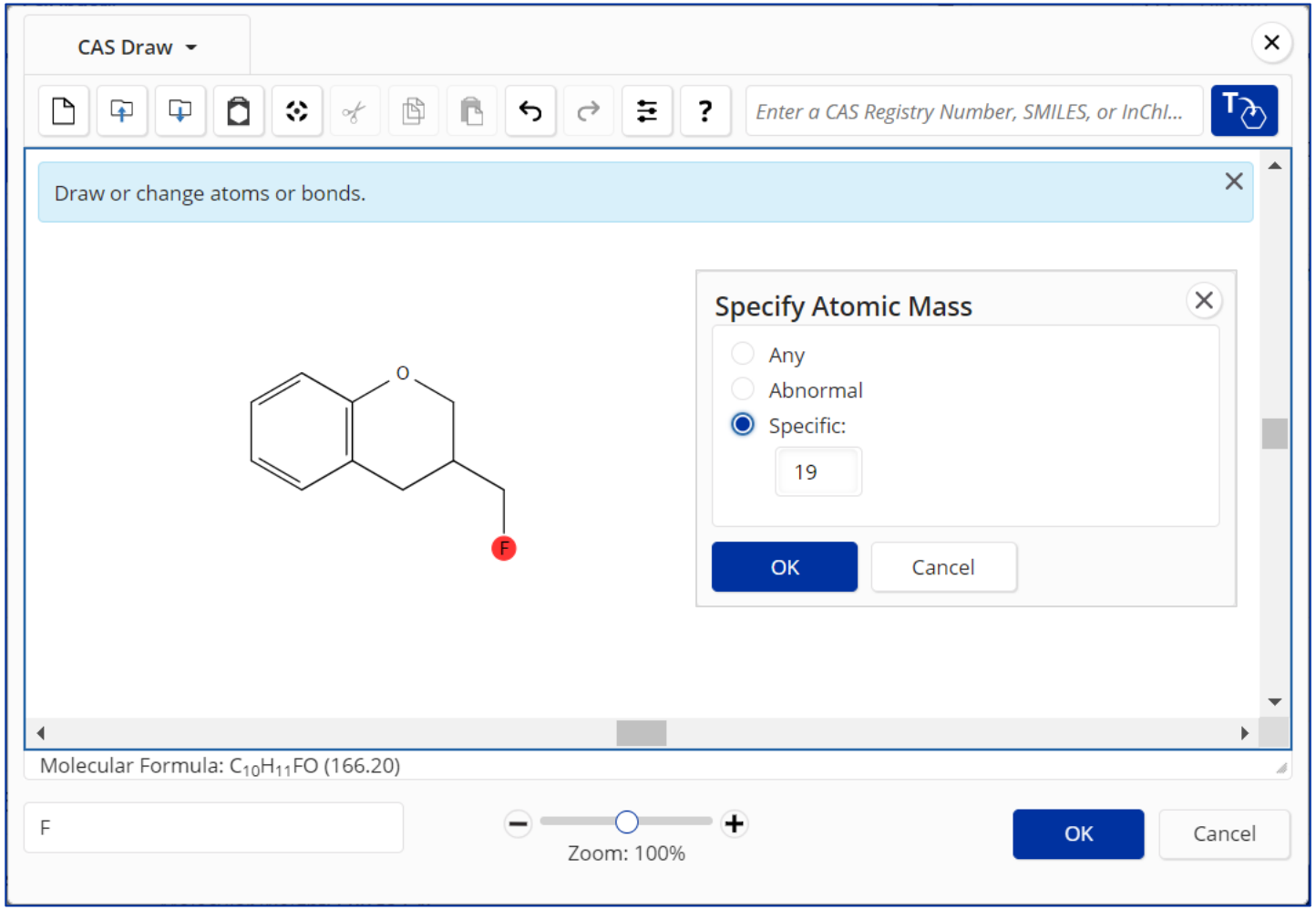
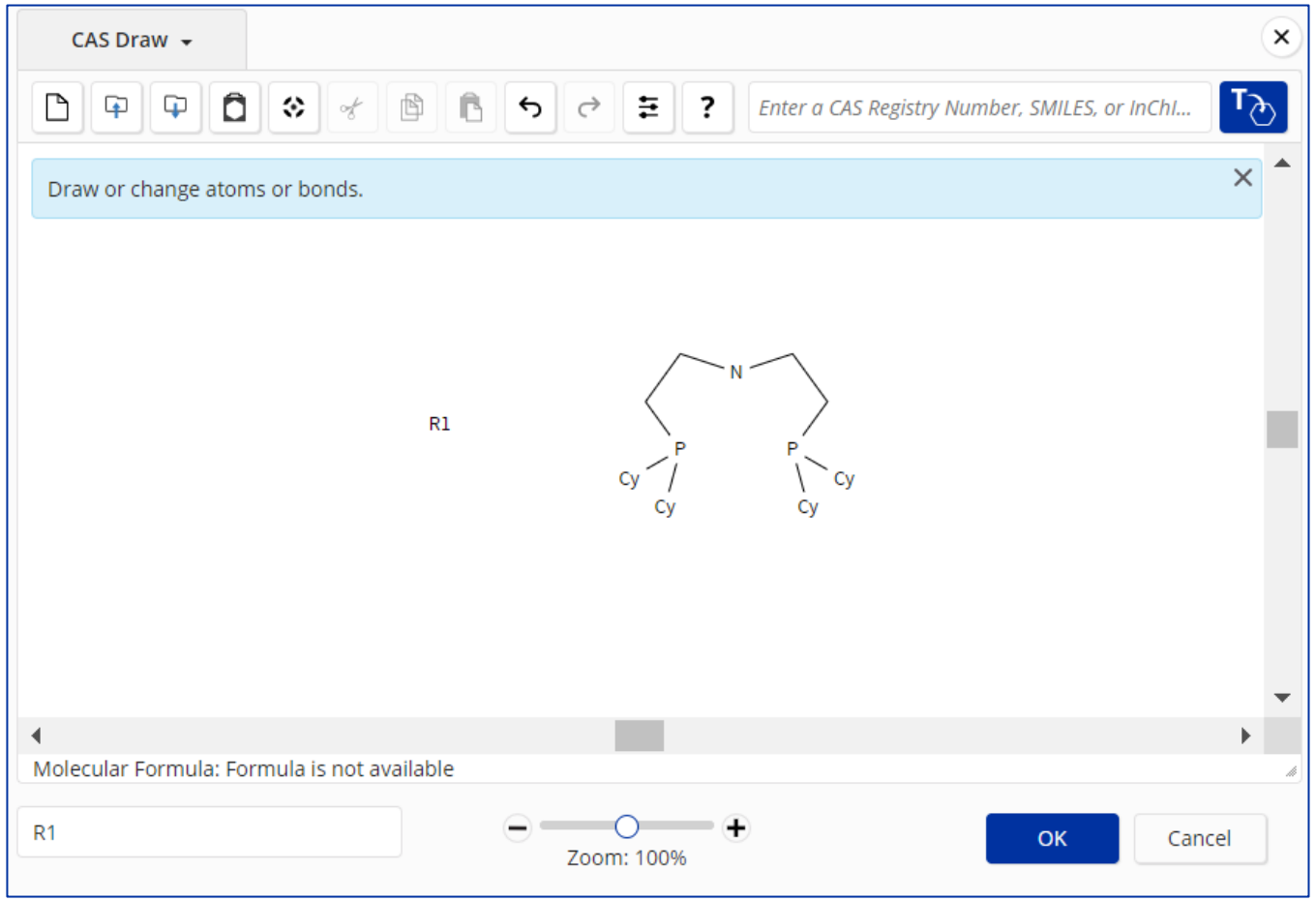
结构绘图工具的使用—同位素原子的绘制

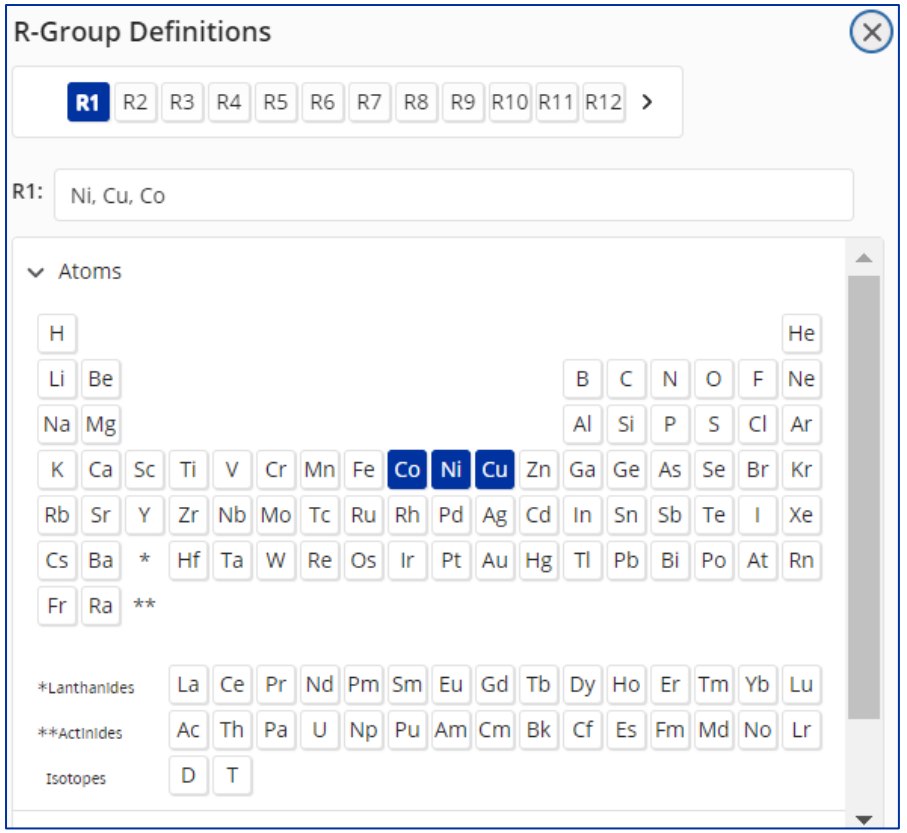


鼠标右键点击某原子，在弹出窗口中对F原子进行设置：
Any：获取所有F的同位素和非同位素标记物;
Abnormal：获取F的所有同位素标记物;
Specific：可输入具体的同位素质量数，点击OK, 精准检索特定的F同位素标记物。

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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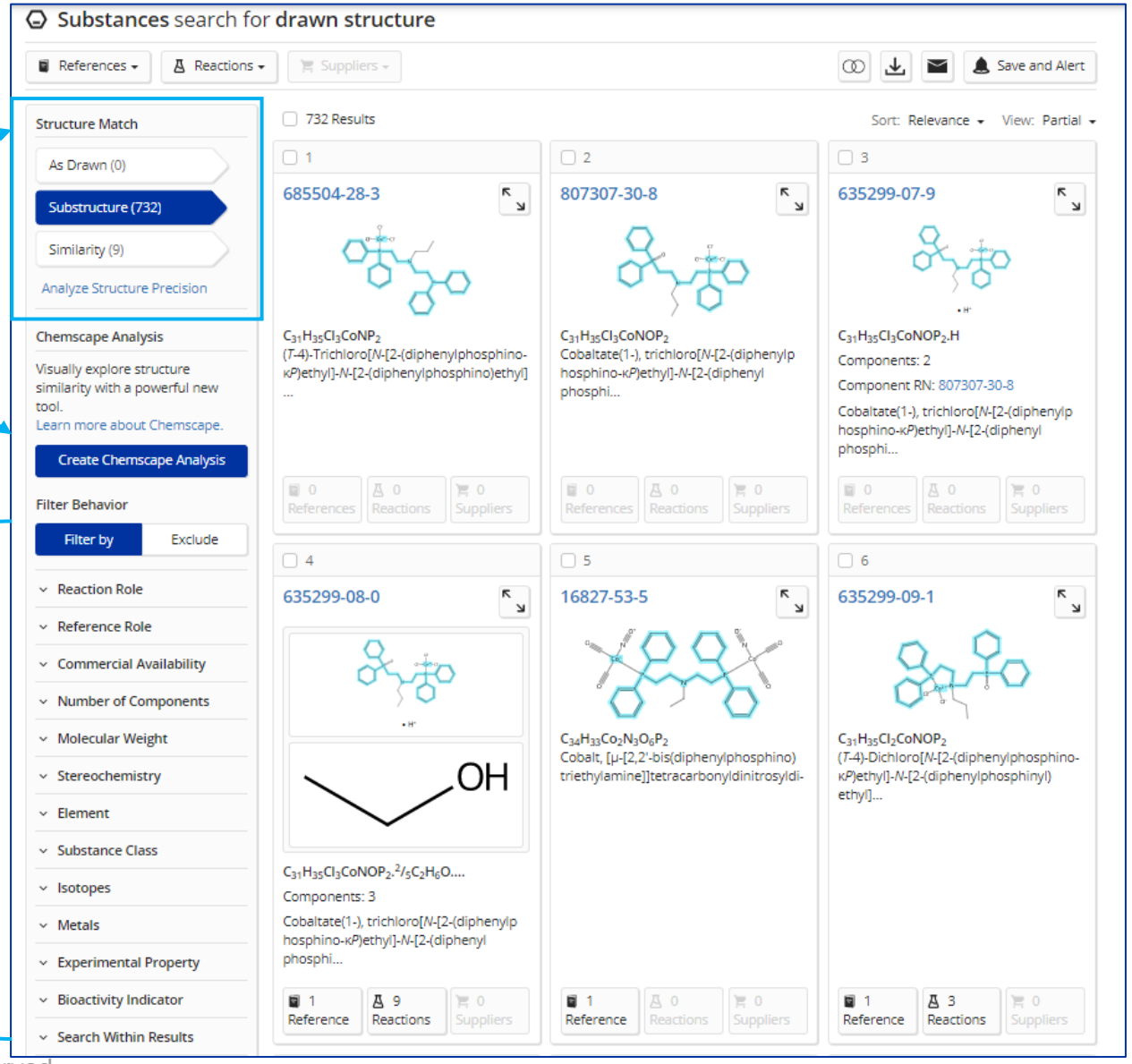
物质检索—检索结果集筛选

结构检索类别：
As Drawn
亚结构
相似结构
结构精准度筛选

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……



物质检索--结构检索

结构检索类别：

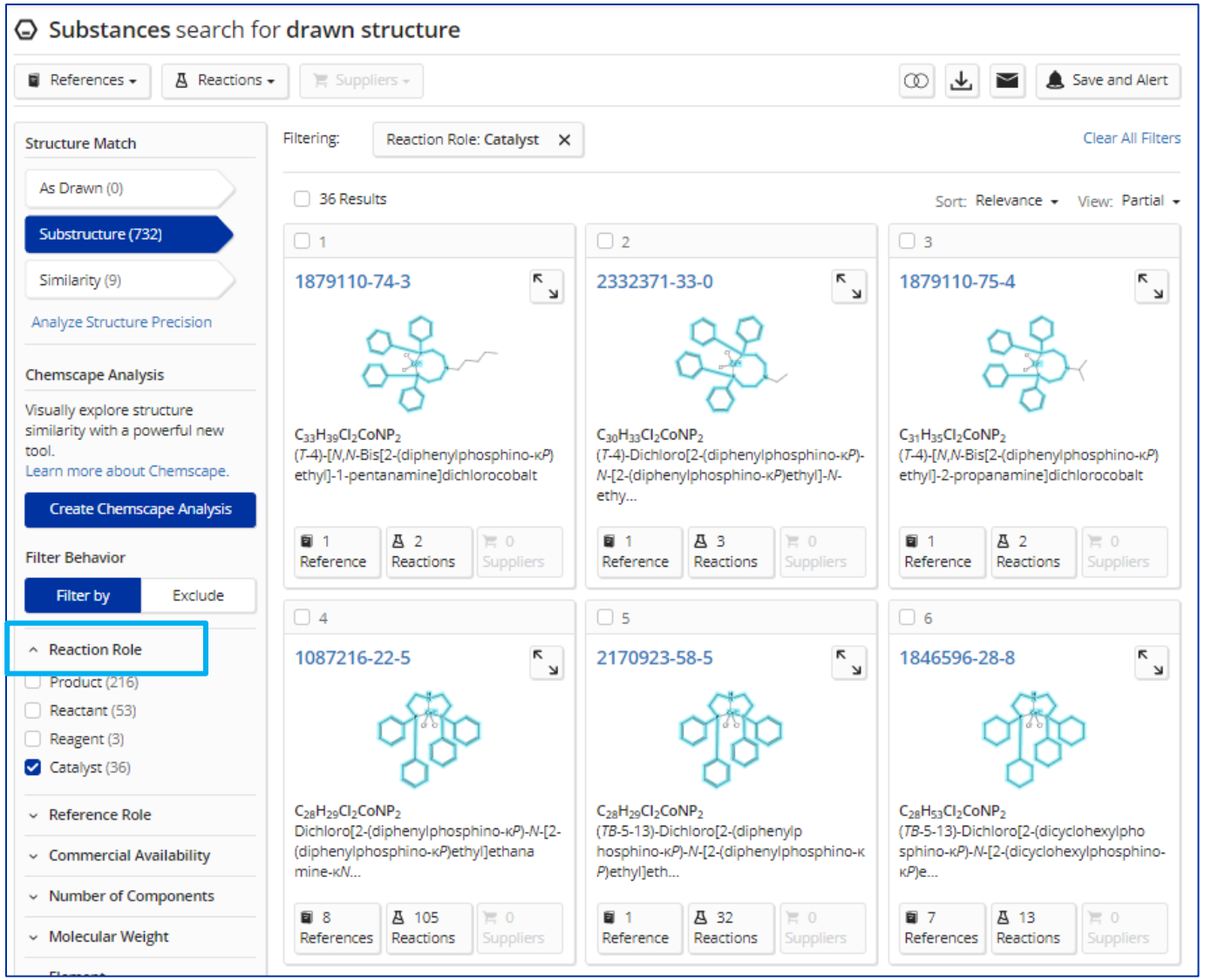
- As Drawn
  可用可变基团X或R基团等可变工具定义，其他位点默认为原子锁定，环系默认为环锁定

- 亚结构
  包括As Drawn检索结果，及被检索结构的修饰结构。位点默认为开放，环系未被环锁定

- 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

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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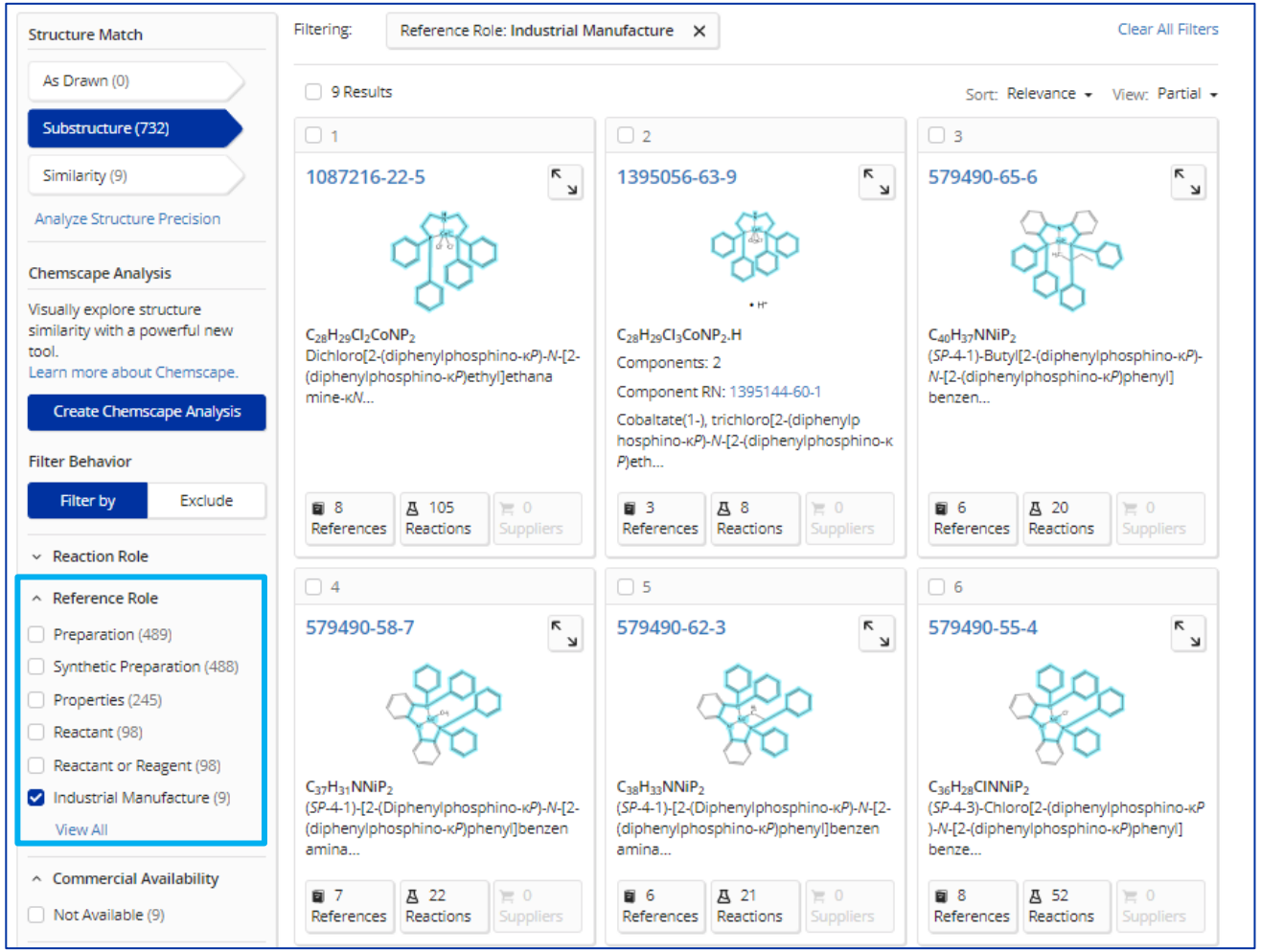
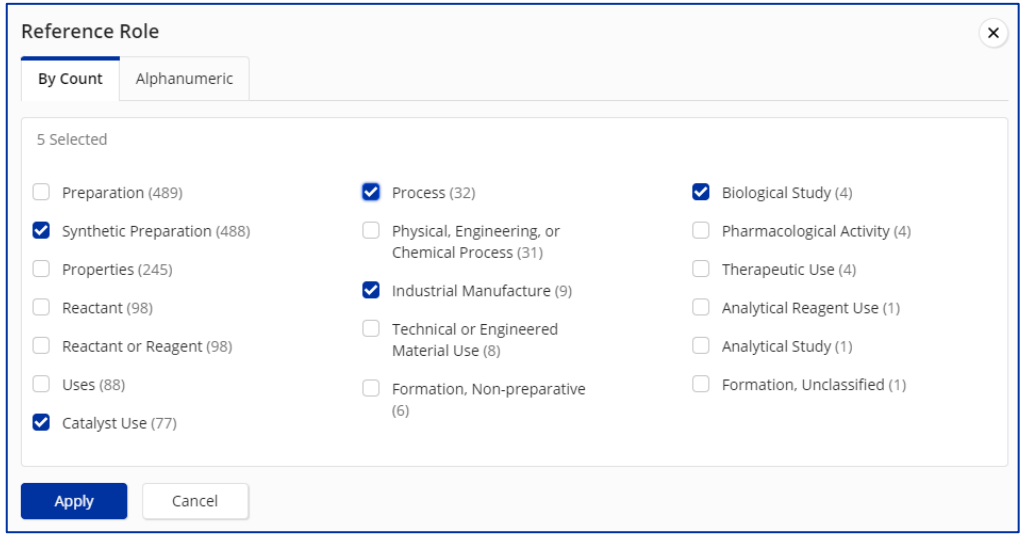
物质检索—检索结果集筛选：Reference Role





利用Reference Role（物质的研究方向）精准定位相应的物质

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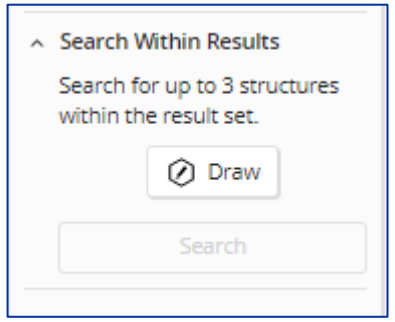
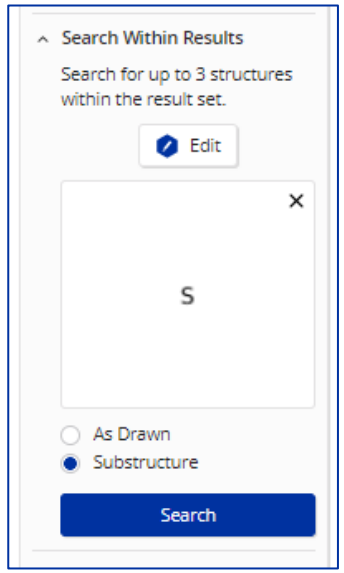
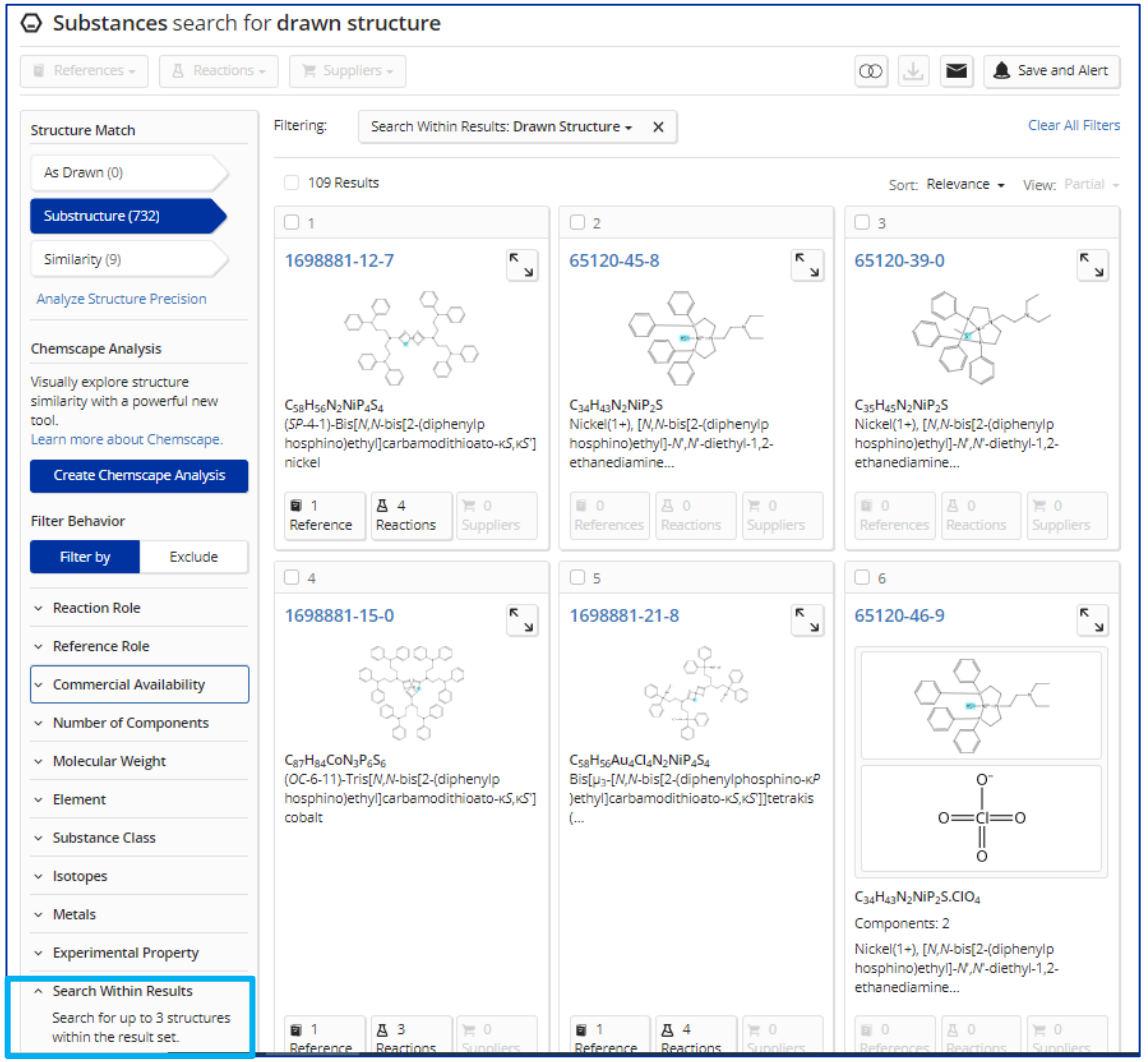
物质检索—检索结果集筛选：结构







利用物质筛选工具
快速锁定目标物质

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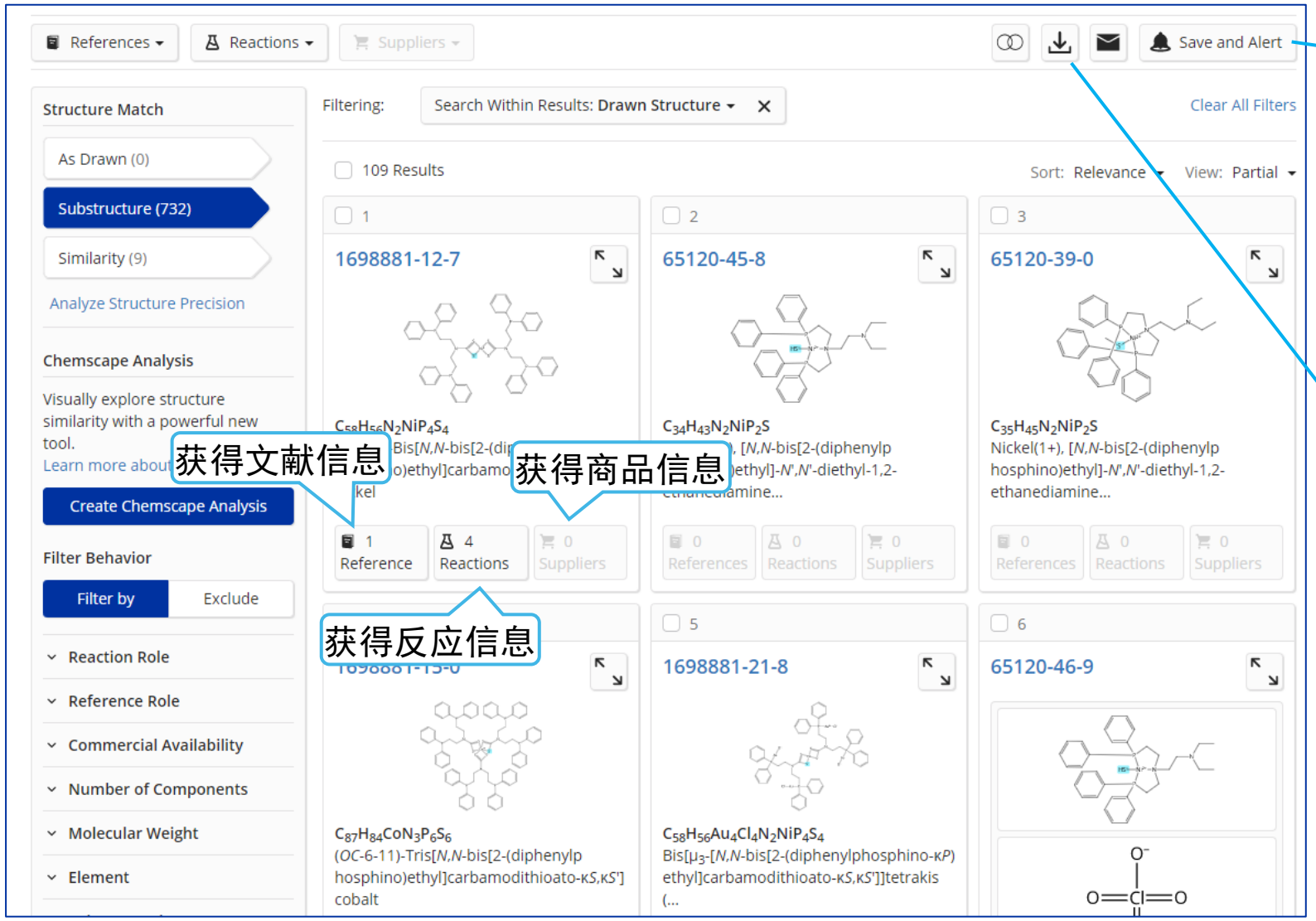
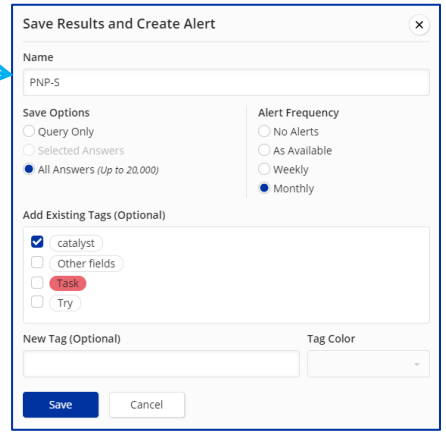
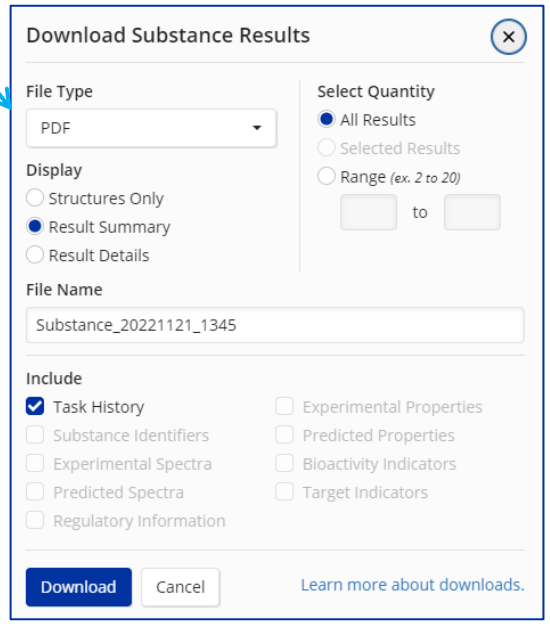
物质检索—检索结果集的保存







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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

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(74)专利代理机构 杭州求是专利事务所有限公司 33200
代理人 张法高 赵杭丽
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A61P 35/00(2006.01)
A61P 35/02(2006.01)
A61P 25/28(2006.01)
A61P 37/02(2006.01)

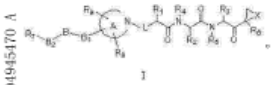
权利要求书3页 说明书24页 附图4页

(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：



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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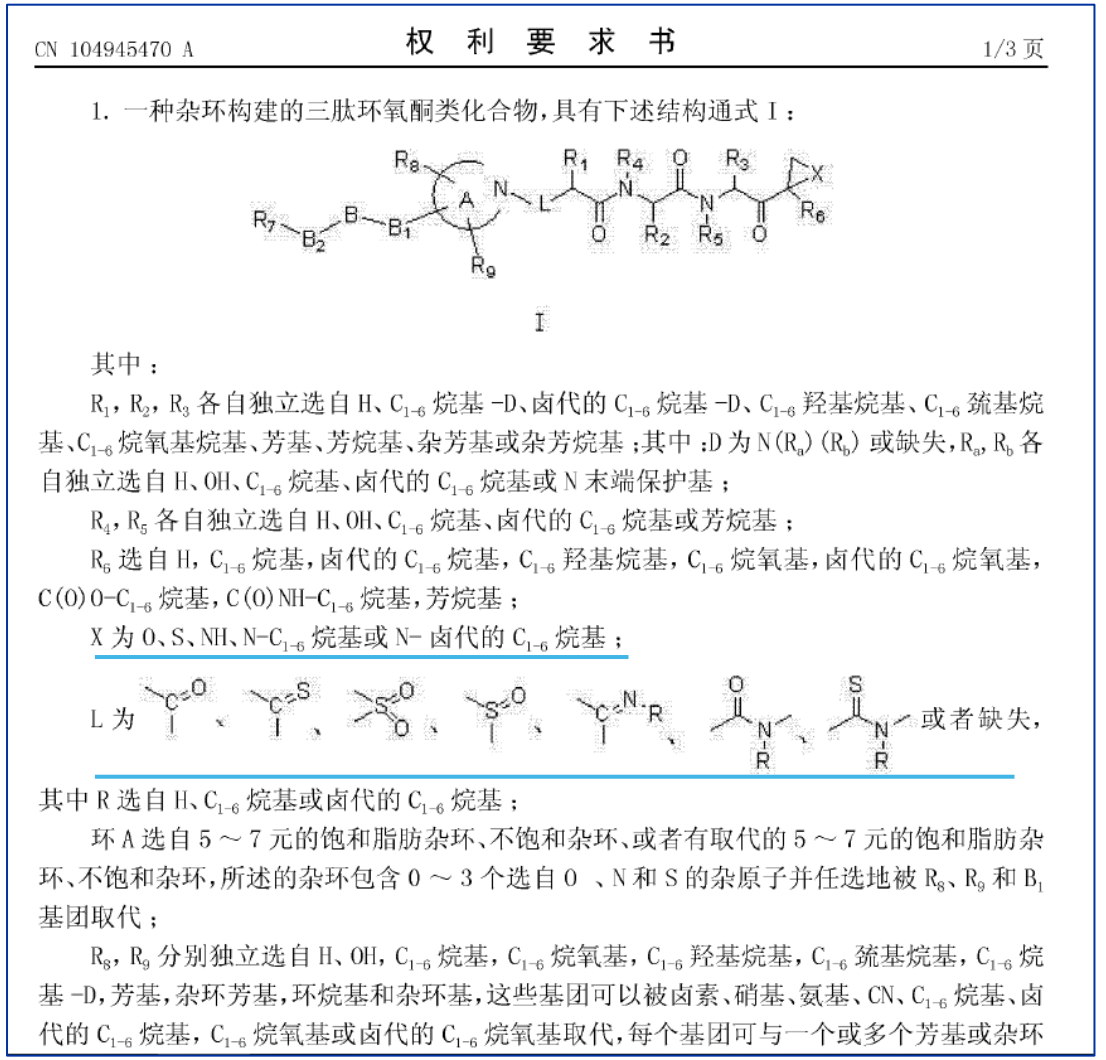
CAS Markush检索

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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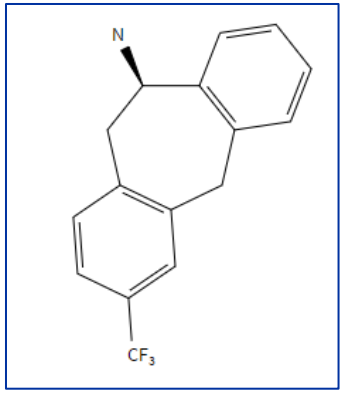
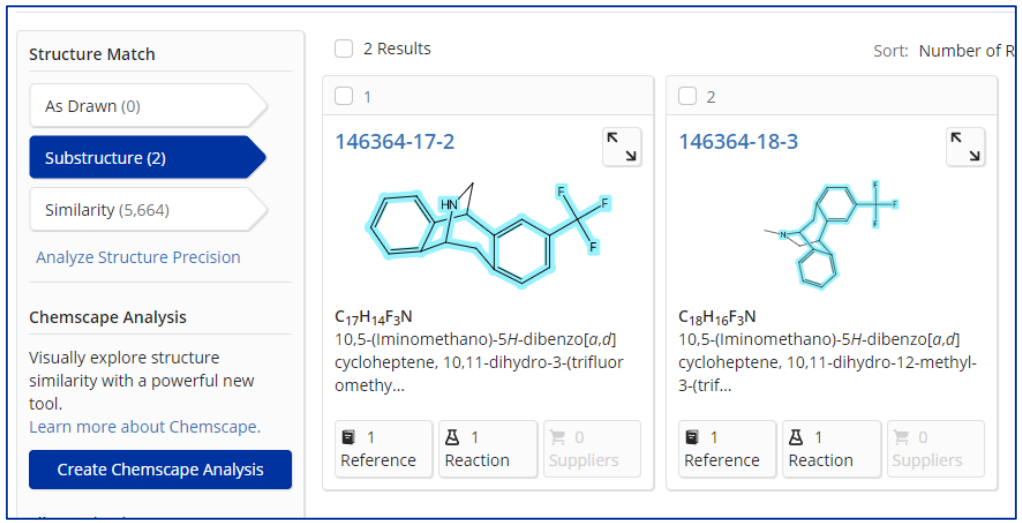
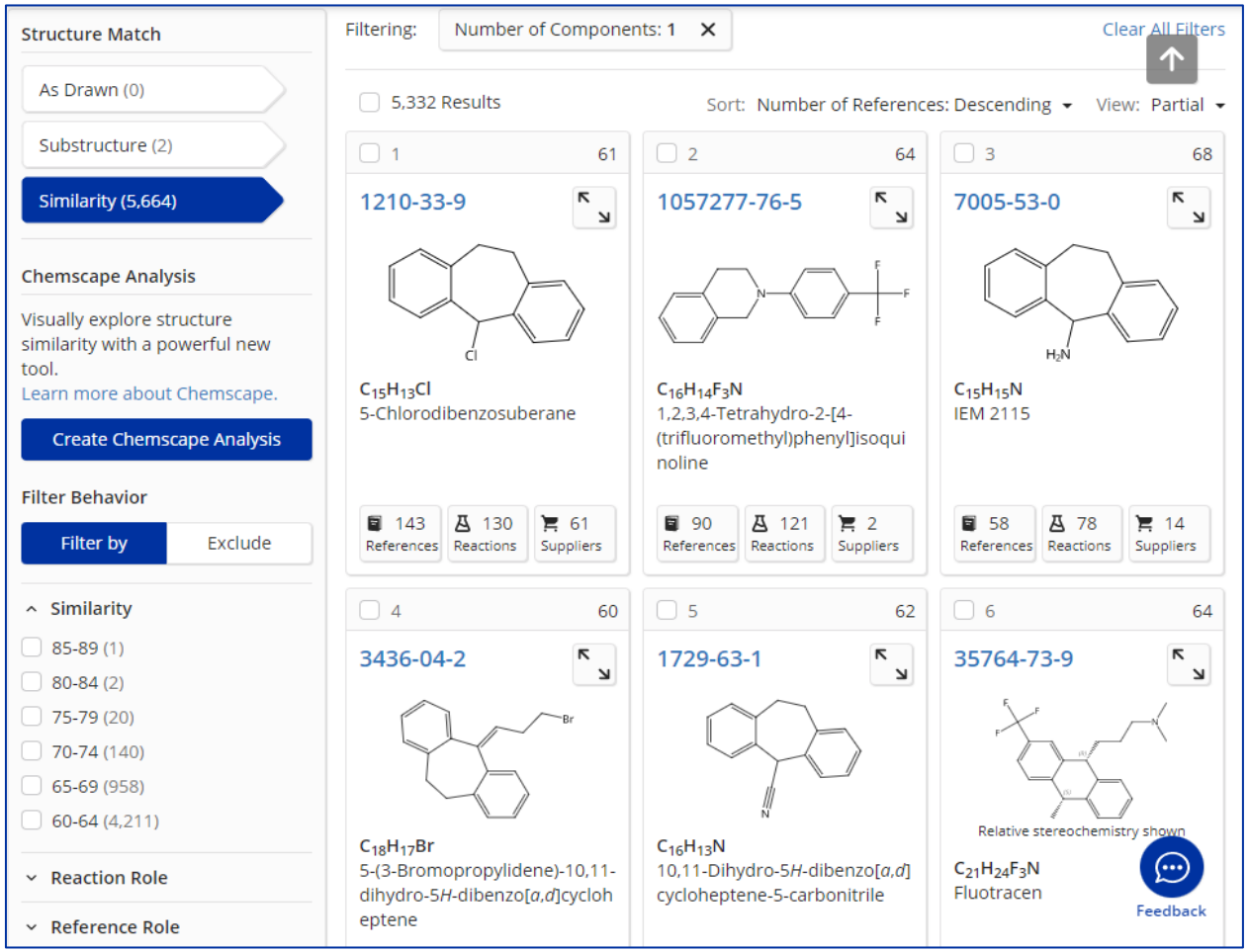
CAS Markush检索

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%







为了尽可能全面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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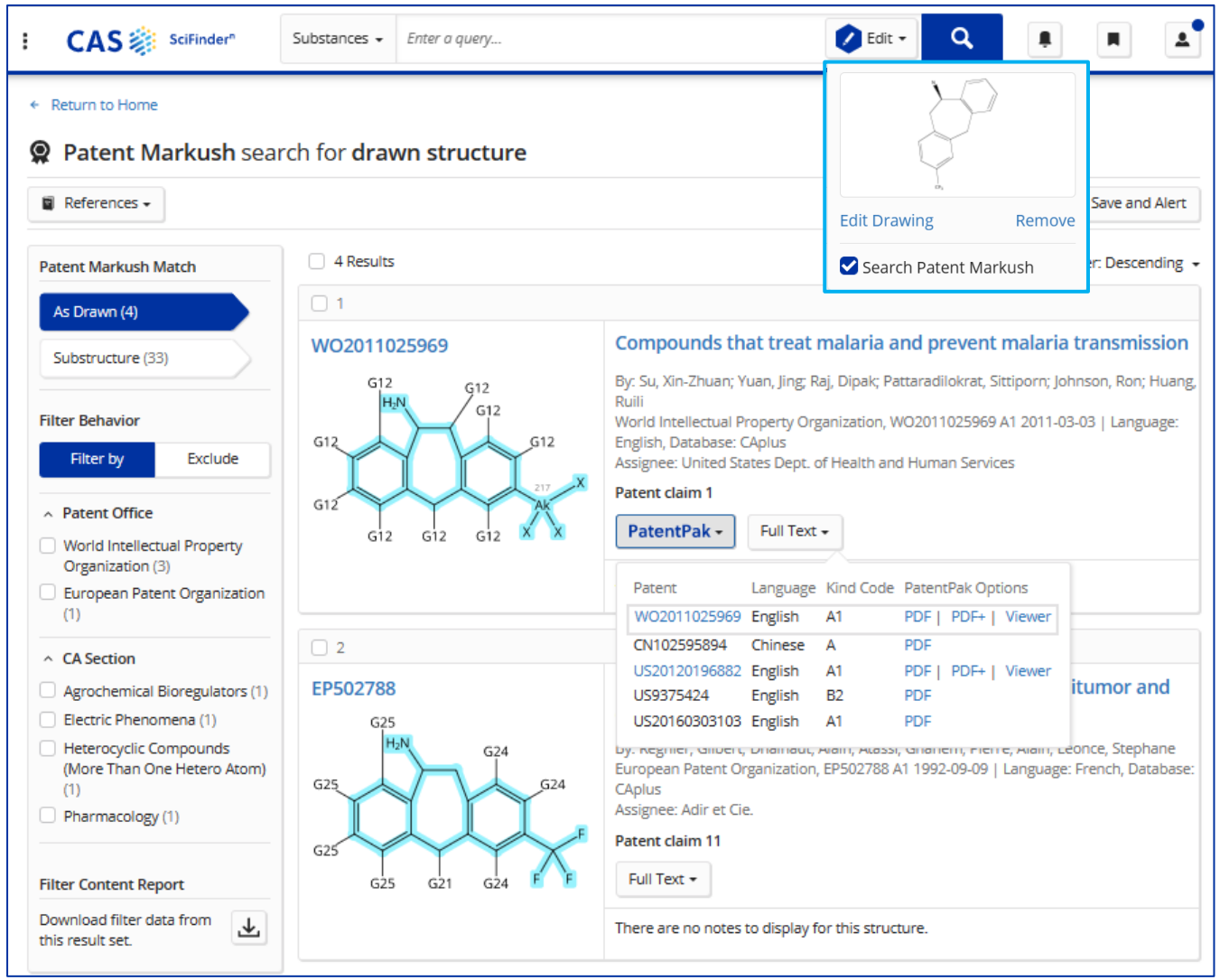
CAS Markush检索

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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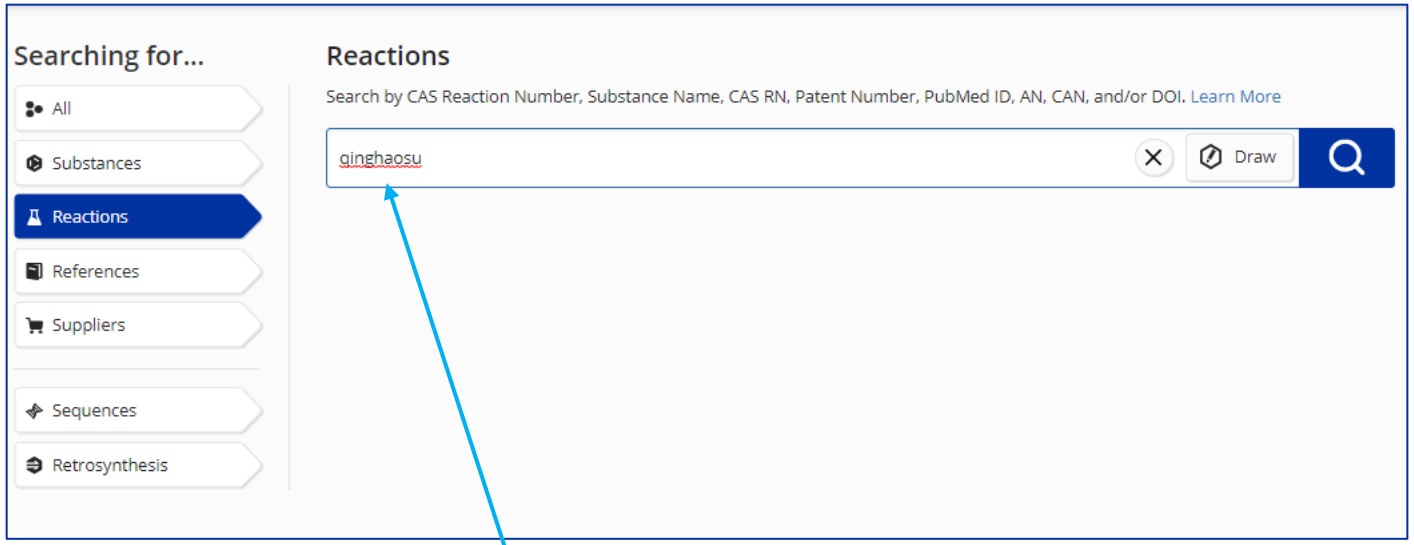
物质检索小结

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Structure Precision快速查找互变异构体/内盐
6. 利用CAS Markush检索尽可能全面的获得结构的公开信息

反应检索

- 反应检索方法
  - 结构式
  - 关键词
  - 物质名称、登记号
  - 文献标识符：专利号、收录号、DOI
- 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

反应检索



通过物质标识符、文献标识符进行检索

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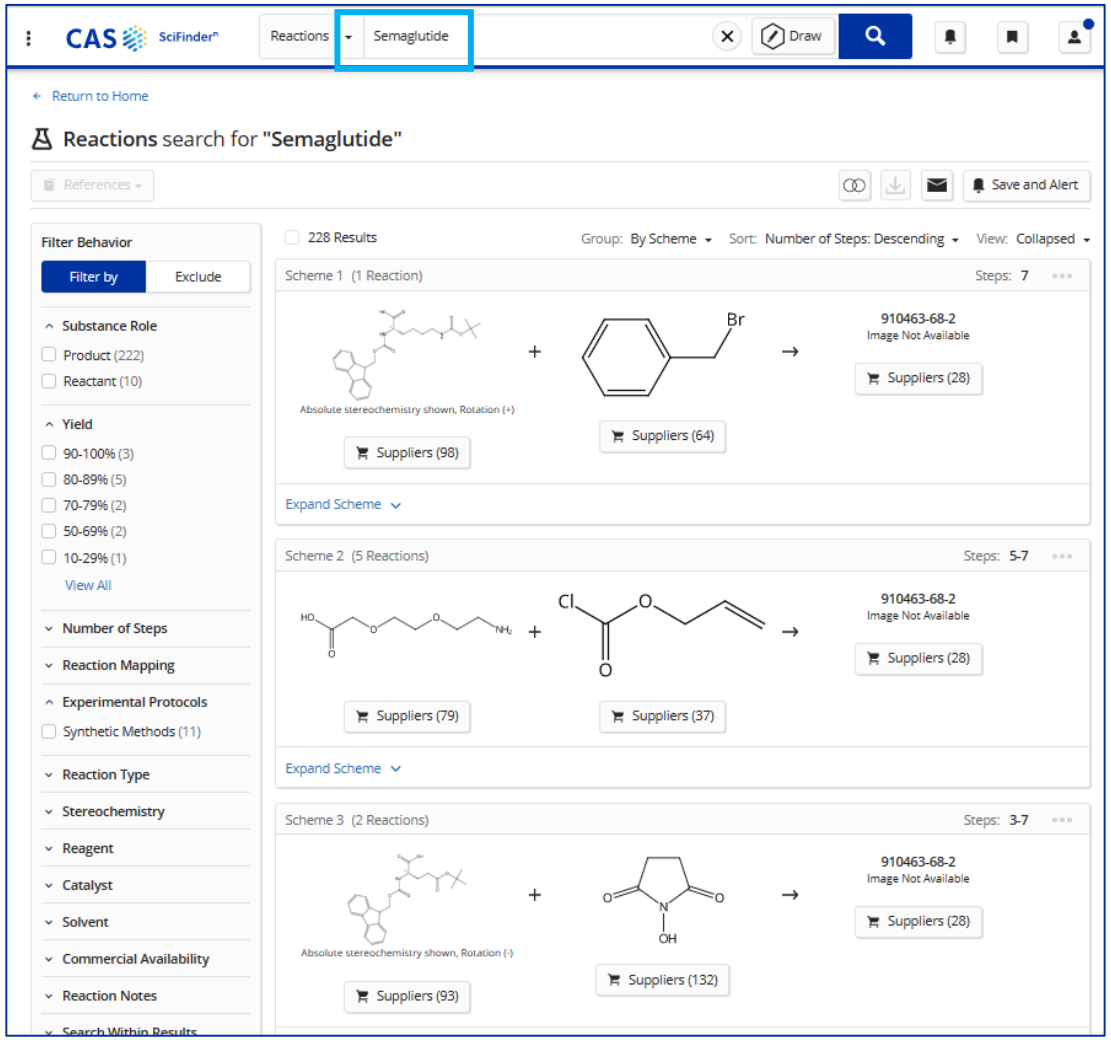
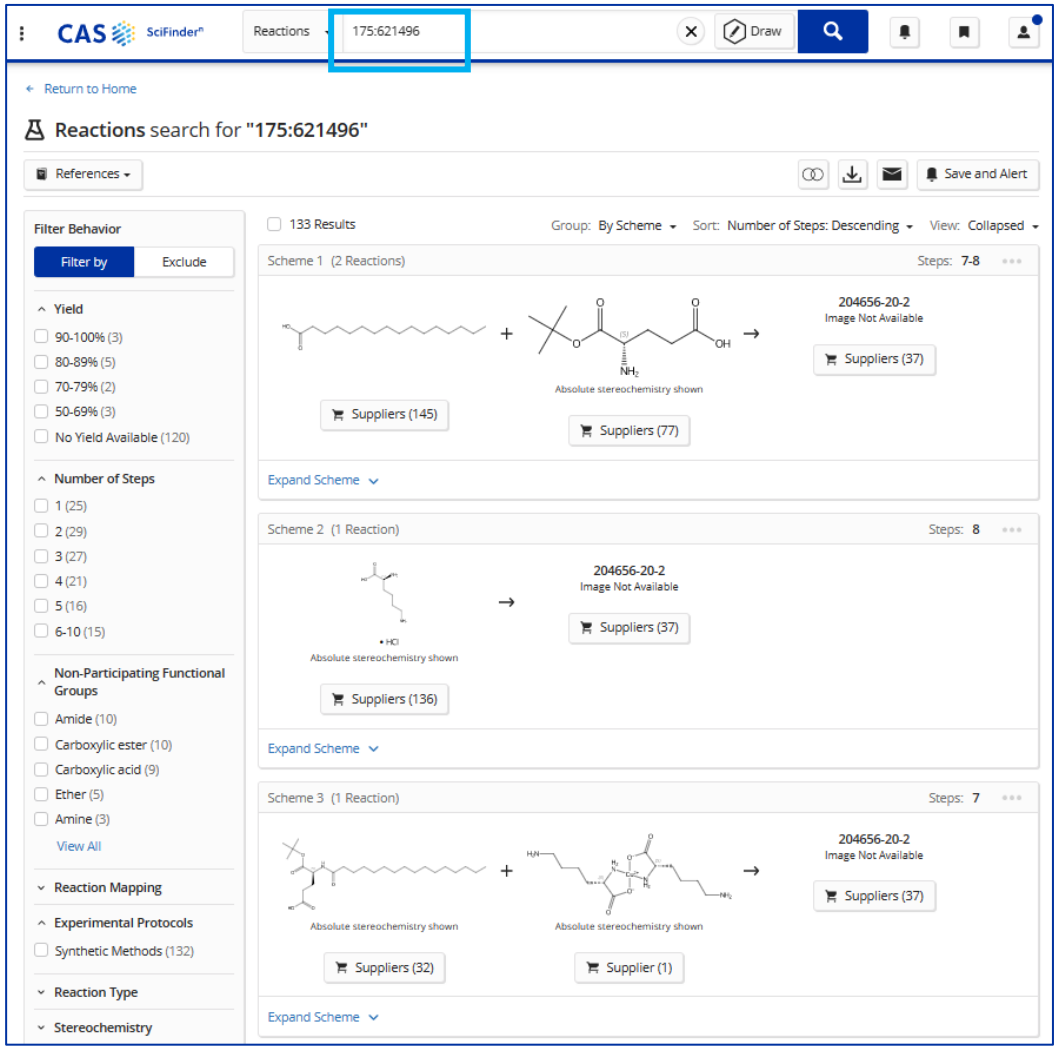
反应检索





通过物质或文献标识符进行检索

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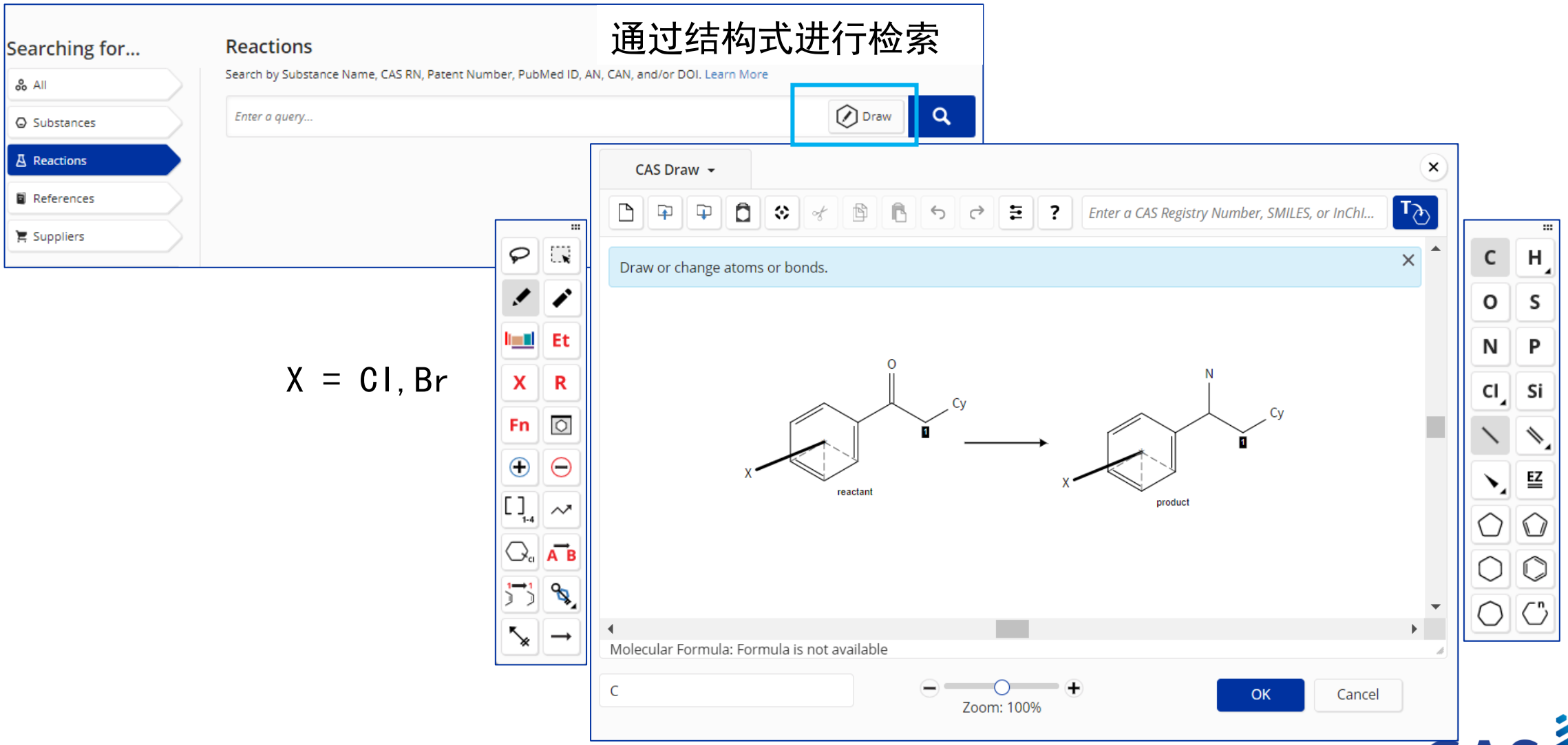
反应检索



X = Cl, Br

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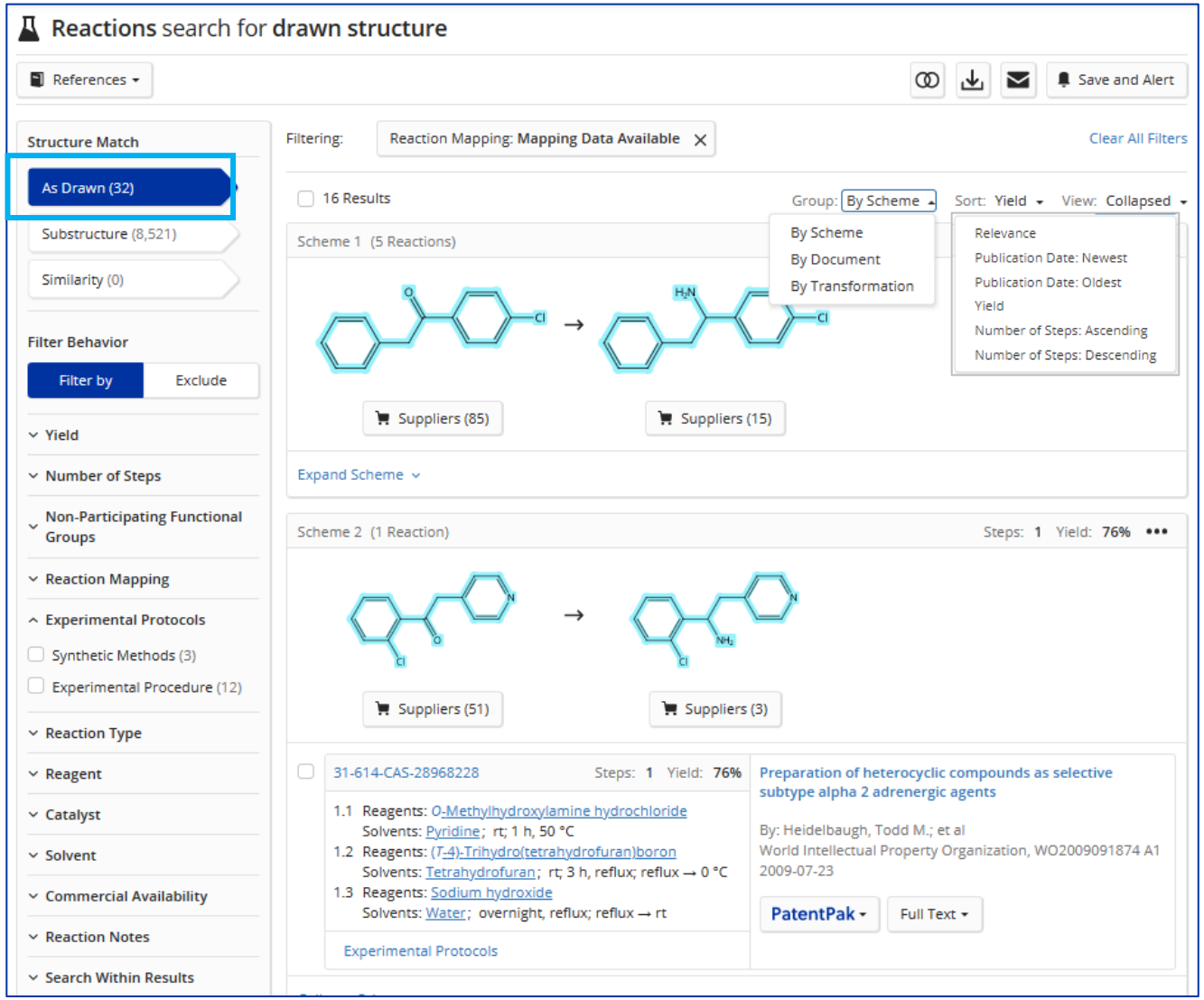
反应检索—结果集的分组与排序



反应分组Group:
按类型分组
按文献分组
按单步反应转化类型

反应排序Sort:
相关度
公布时间
产率
步数

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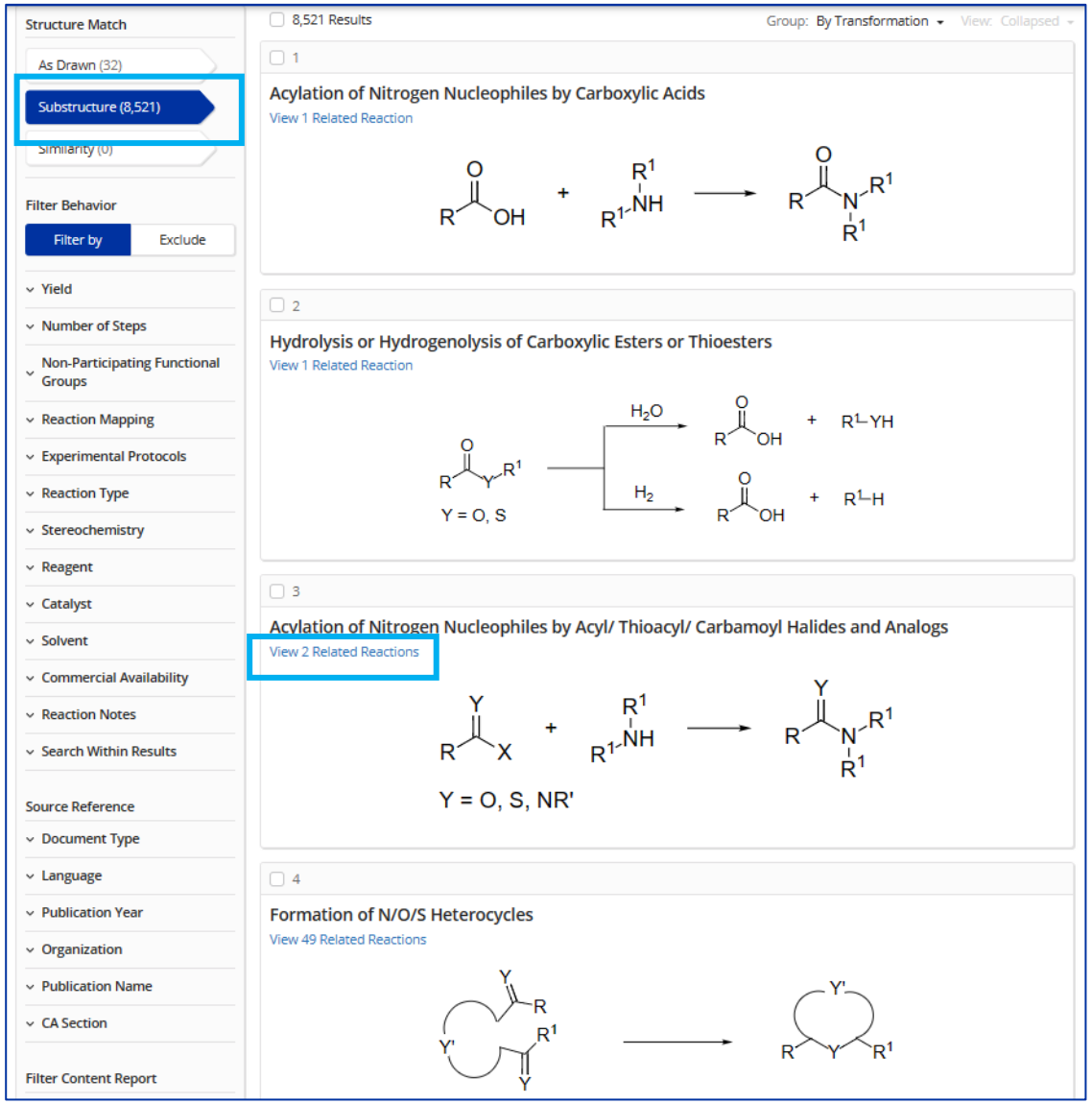
反应检索—结果集筛选

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
商业来源……

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放在一个菜单里，方便阅读和筛选

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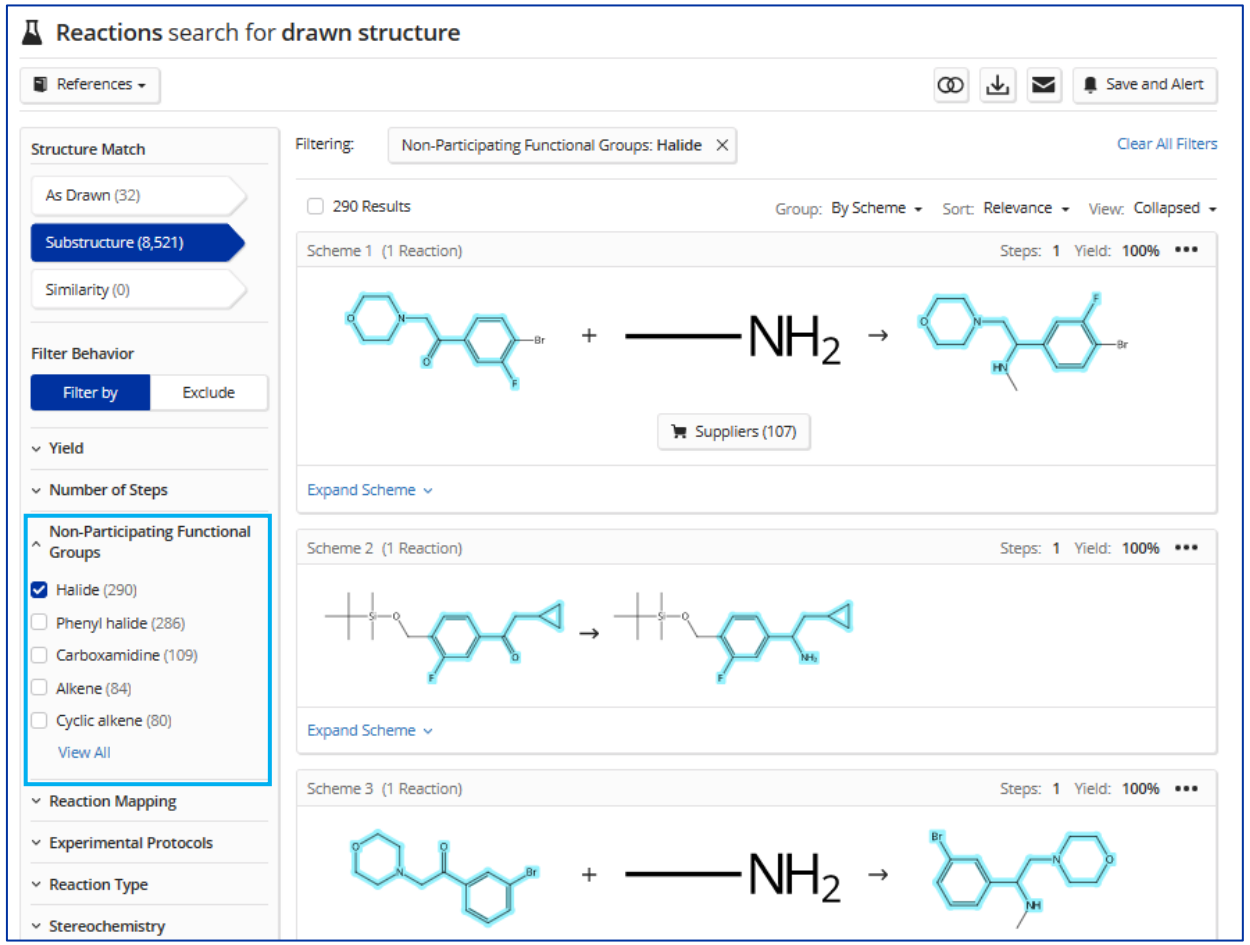
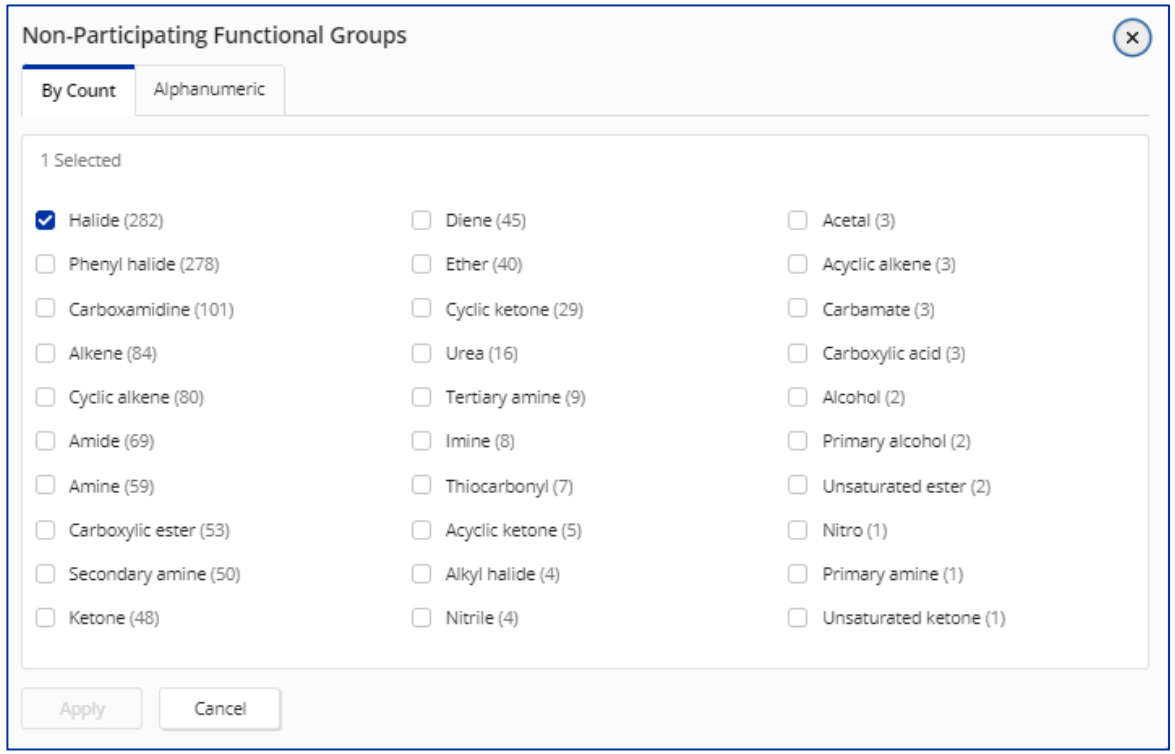
反应检索—结果集筛选：不参与反应官能团





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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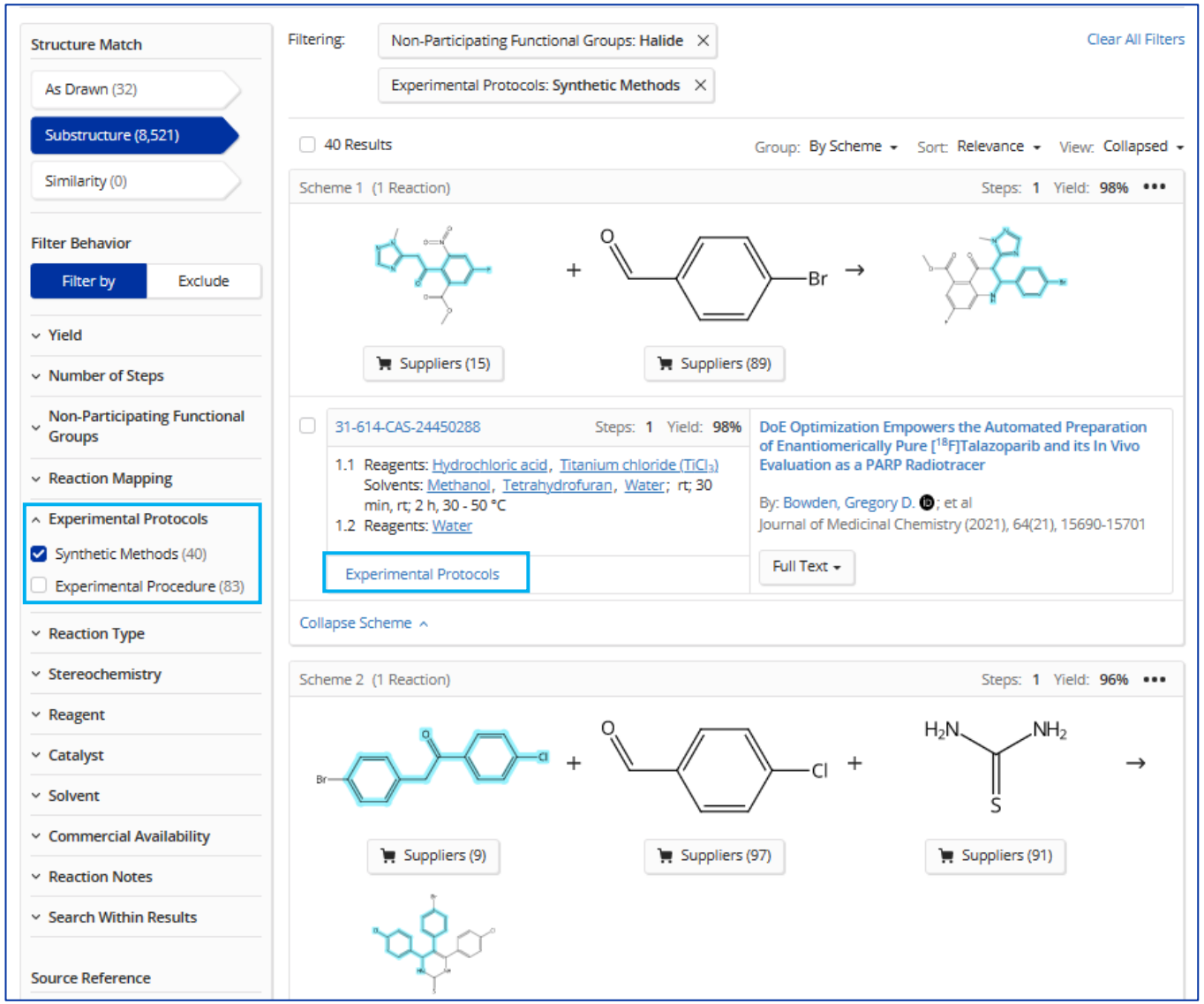
反应检索—结果集筛选：Synthetic Methods™



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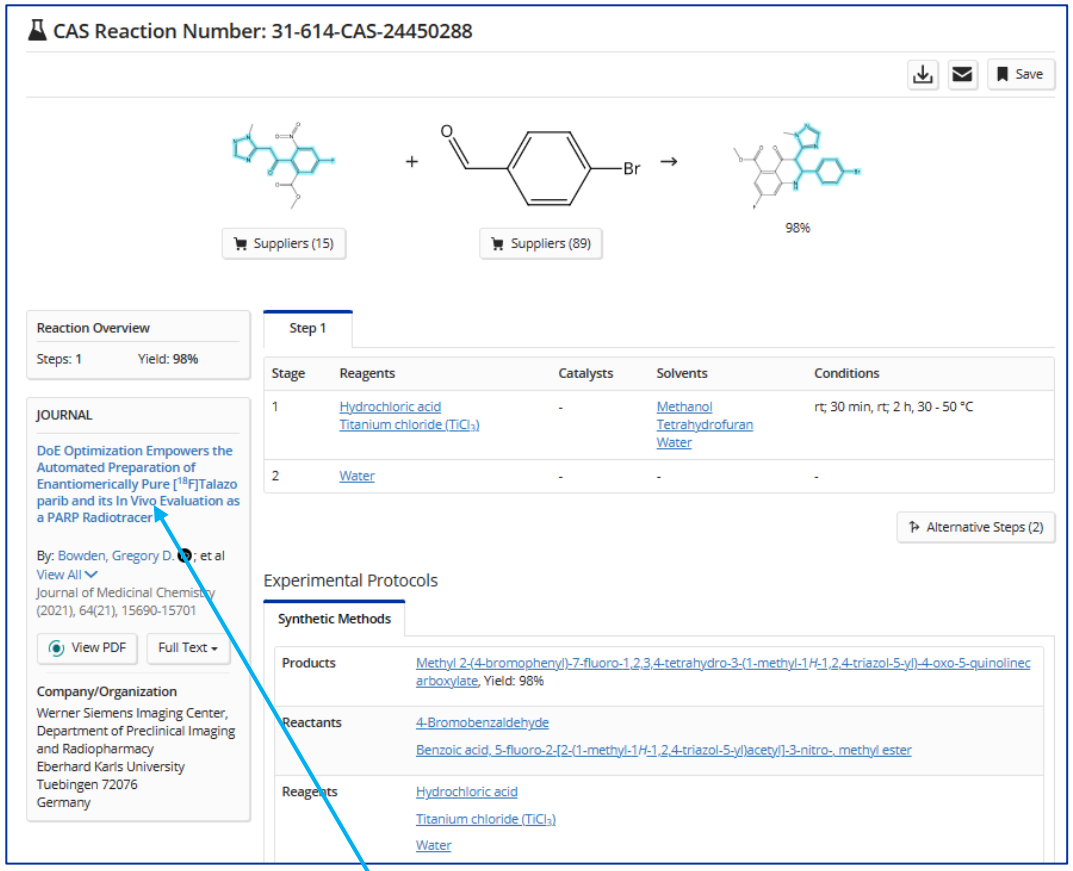
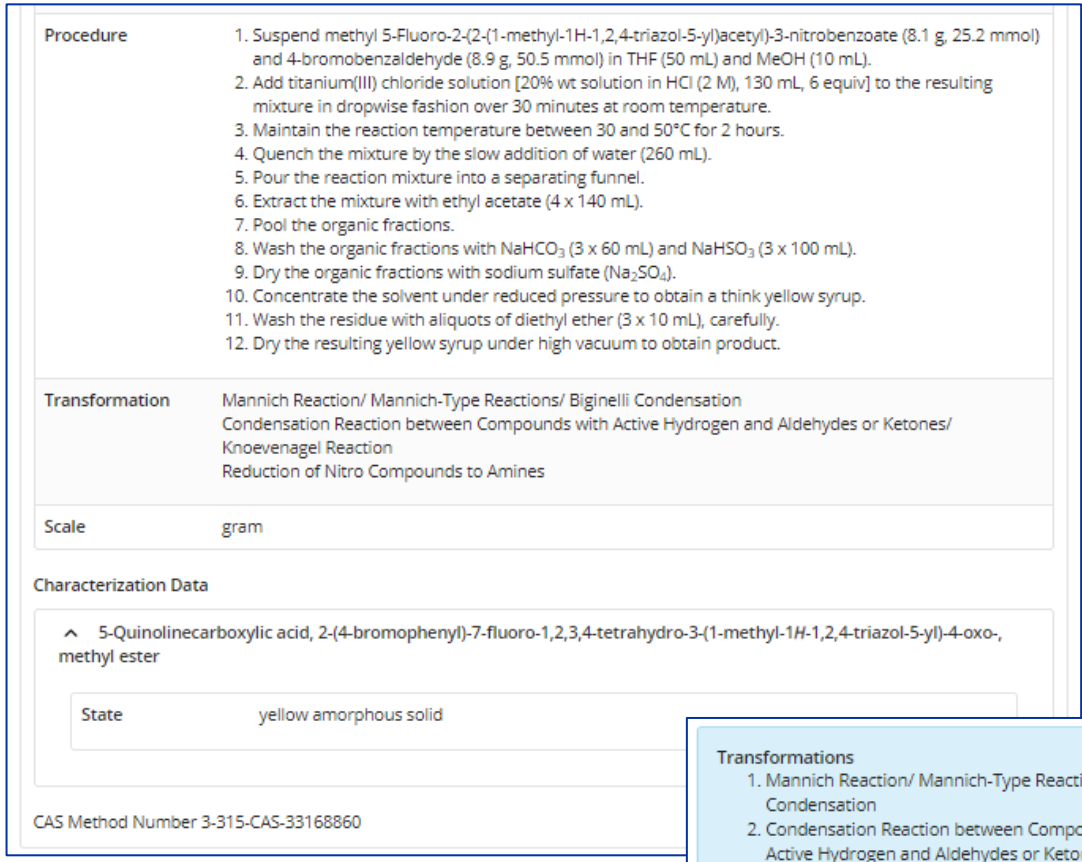
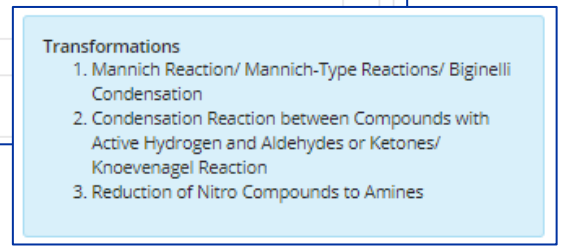
反应检索—结果集筛选：Synthetic Methods™







查看文献详情

Synthetic Methods™：
分类显示详尽信息，方便操作

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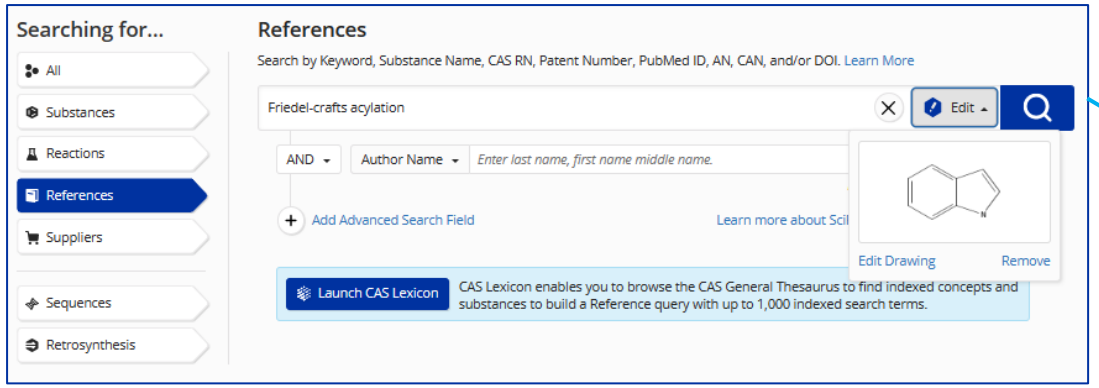
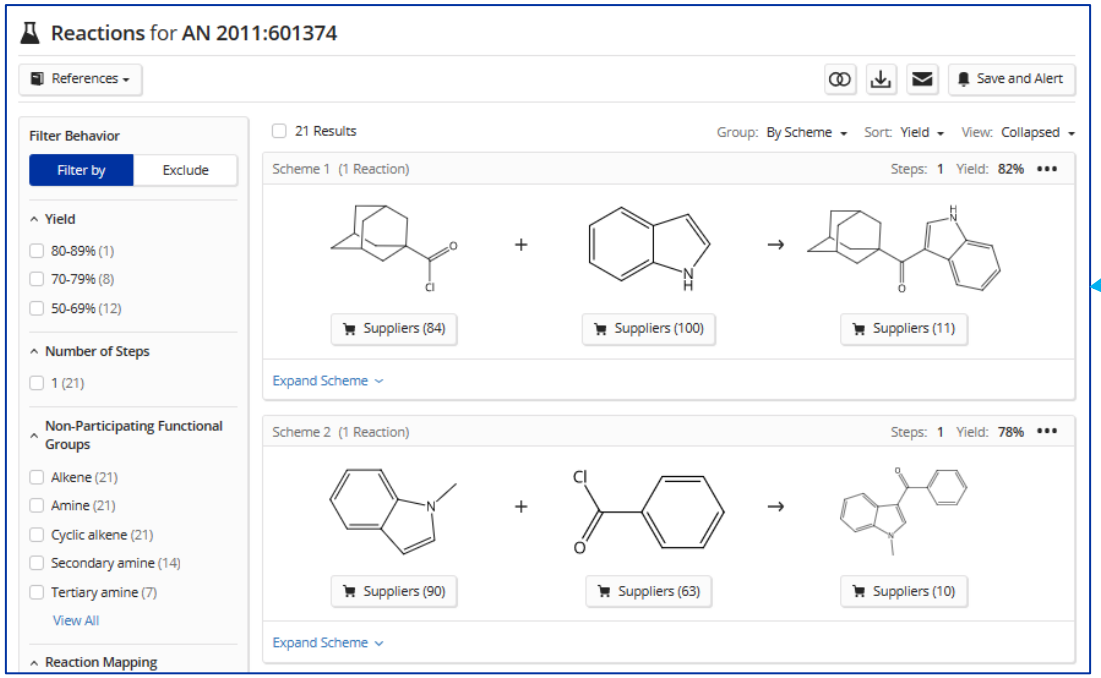
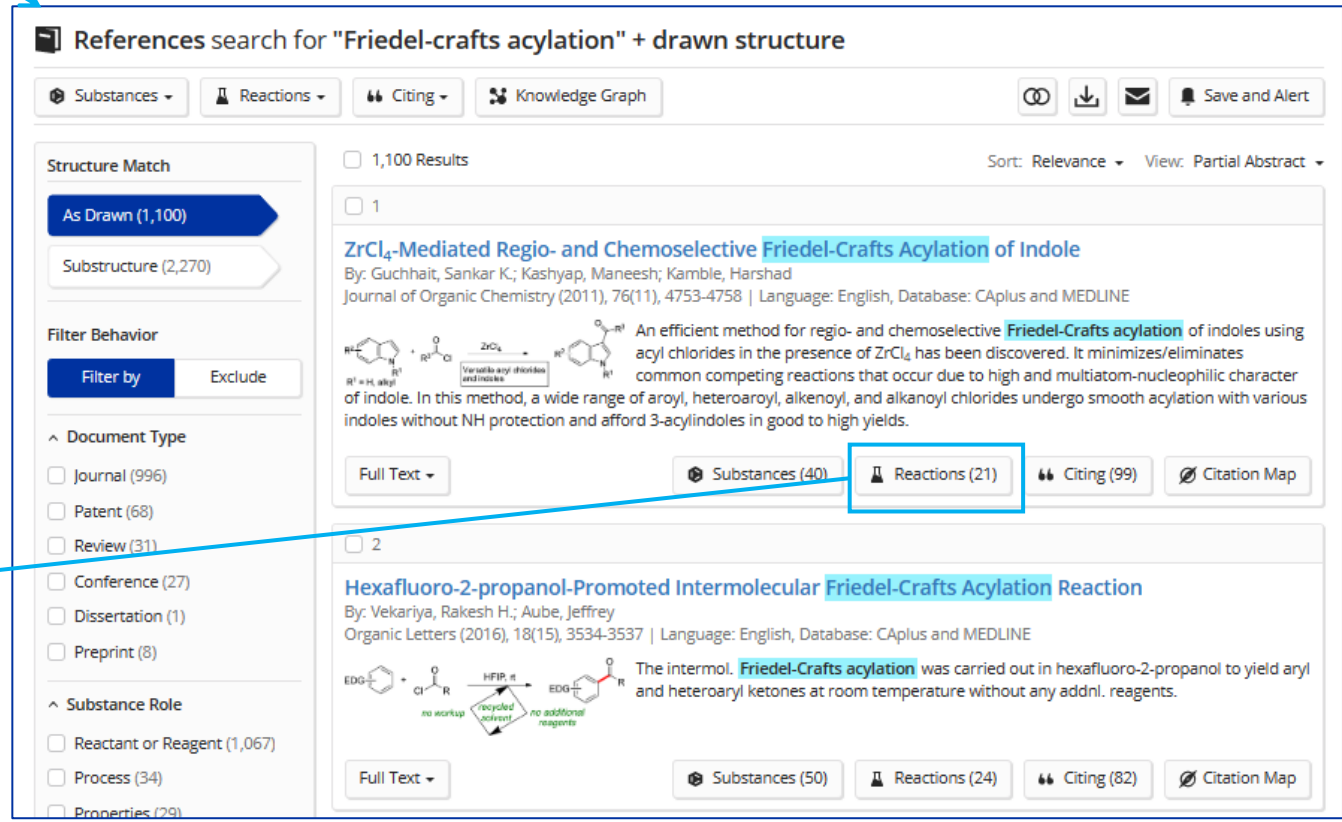
联合检索—结构与关键词







联合检索提高了检索速度

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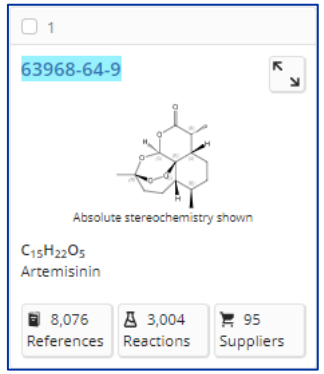
反应检索小结

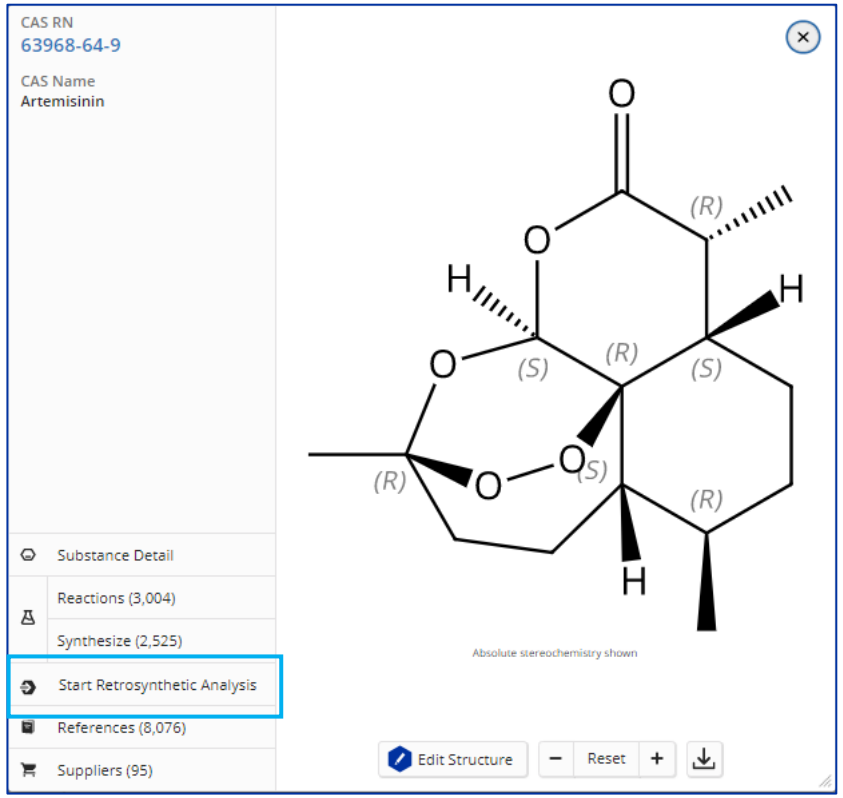
1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 利用Synthetic Methods™查看文献中合成方法详情
4. 关键词与反应式的联合检索

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

CAS Retrosynthesis Tool--由物质获得





从已知化合物获得逆合成路线：

点击物质结构，弹出的物质菜单中点击Create Retrosynthesis

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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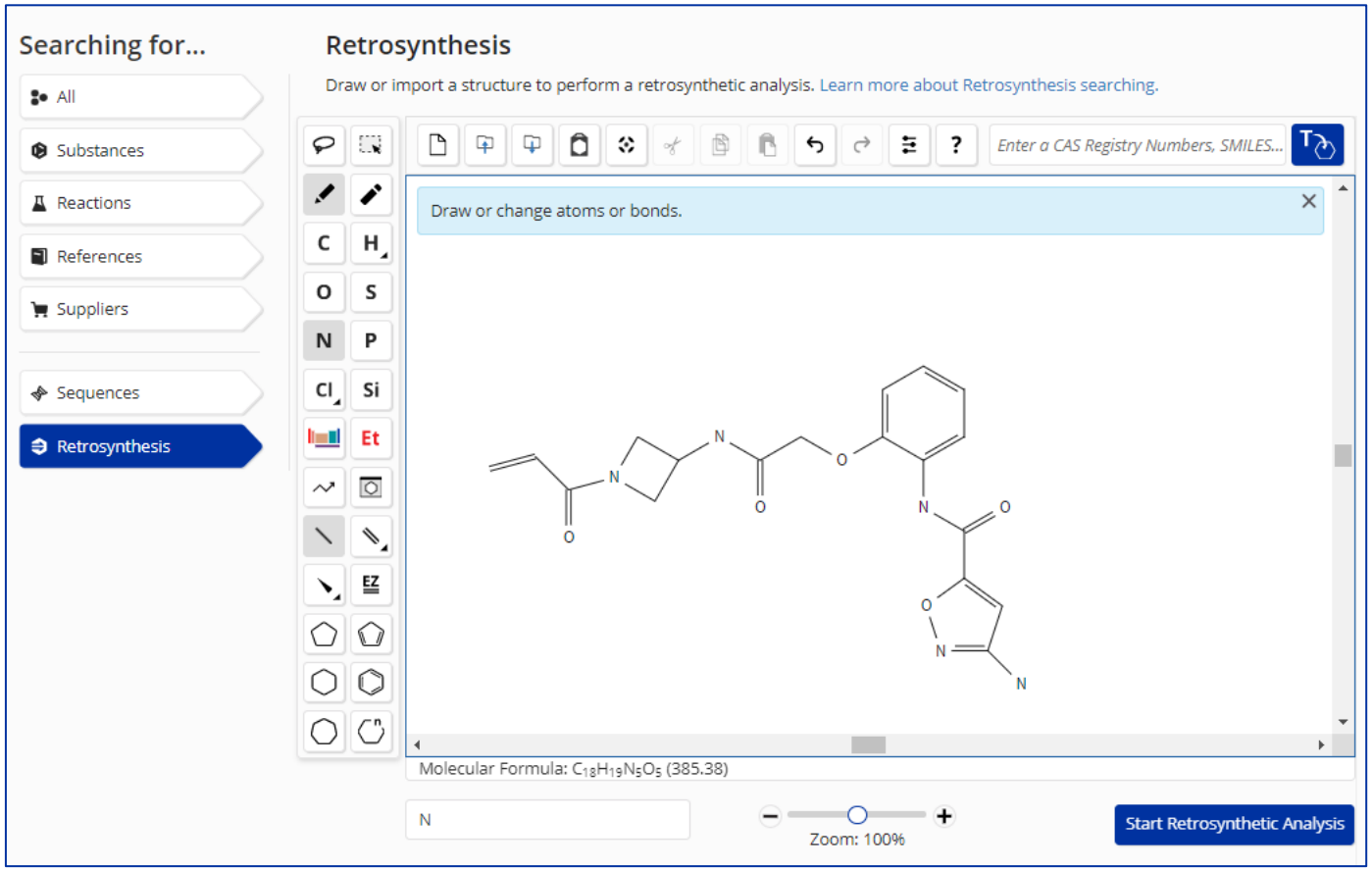
CAS Retrosynthesis Tool—直接绘制



绘制目标化合物：

从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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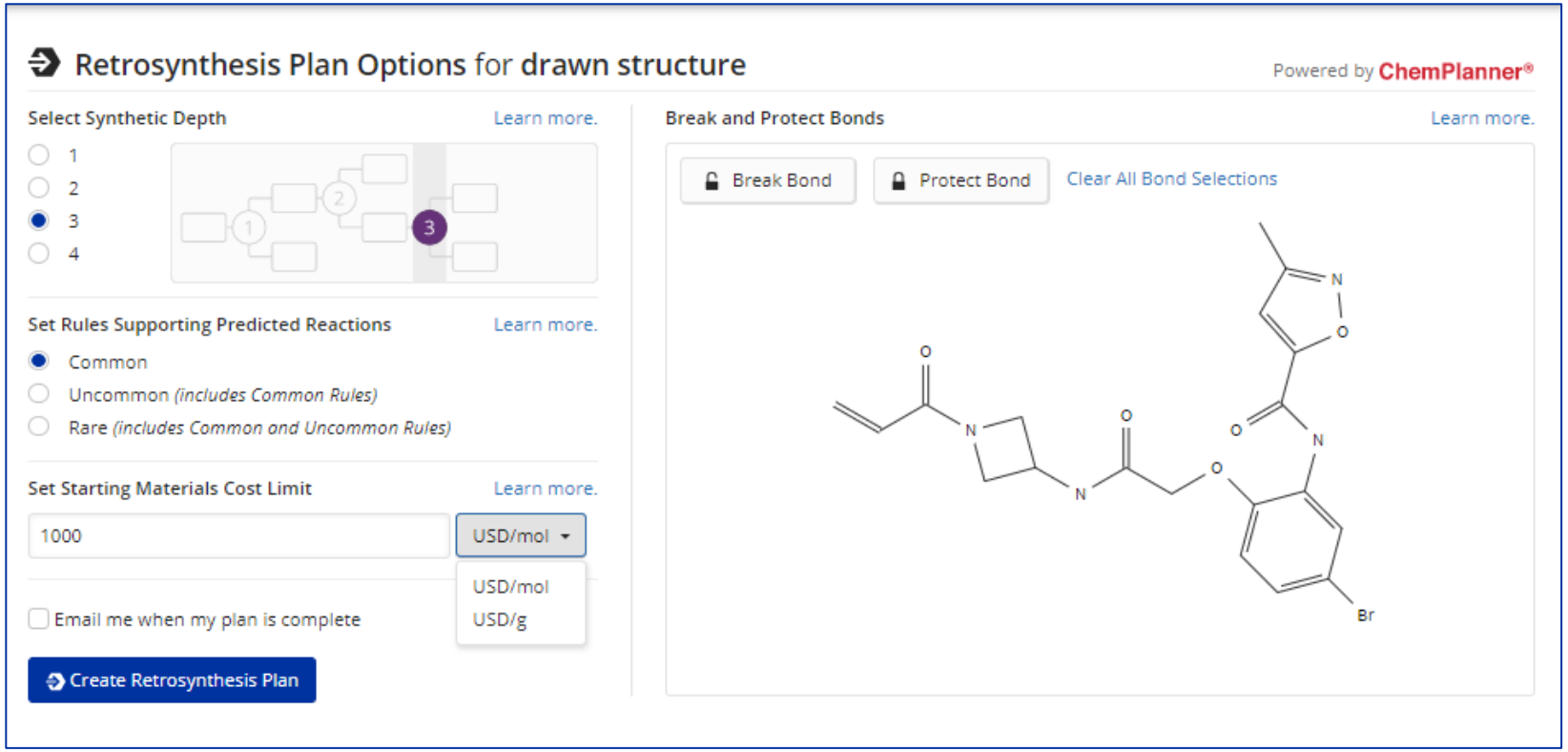
CAS Retrosynthesis Tool—预设参数



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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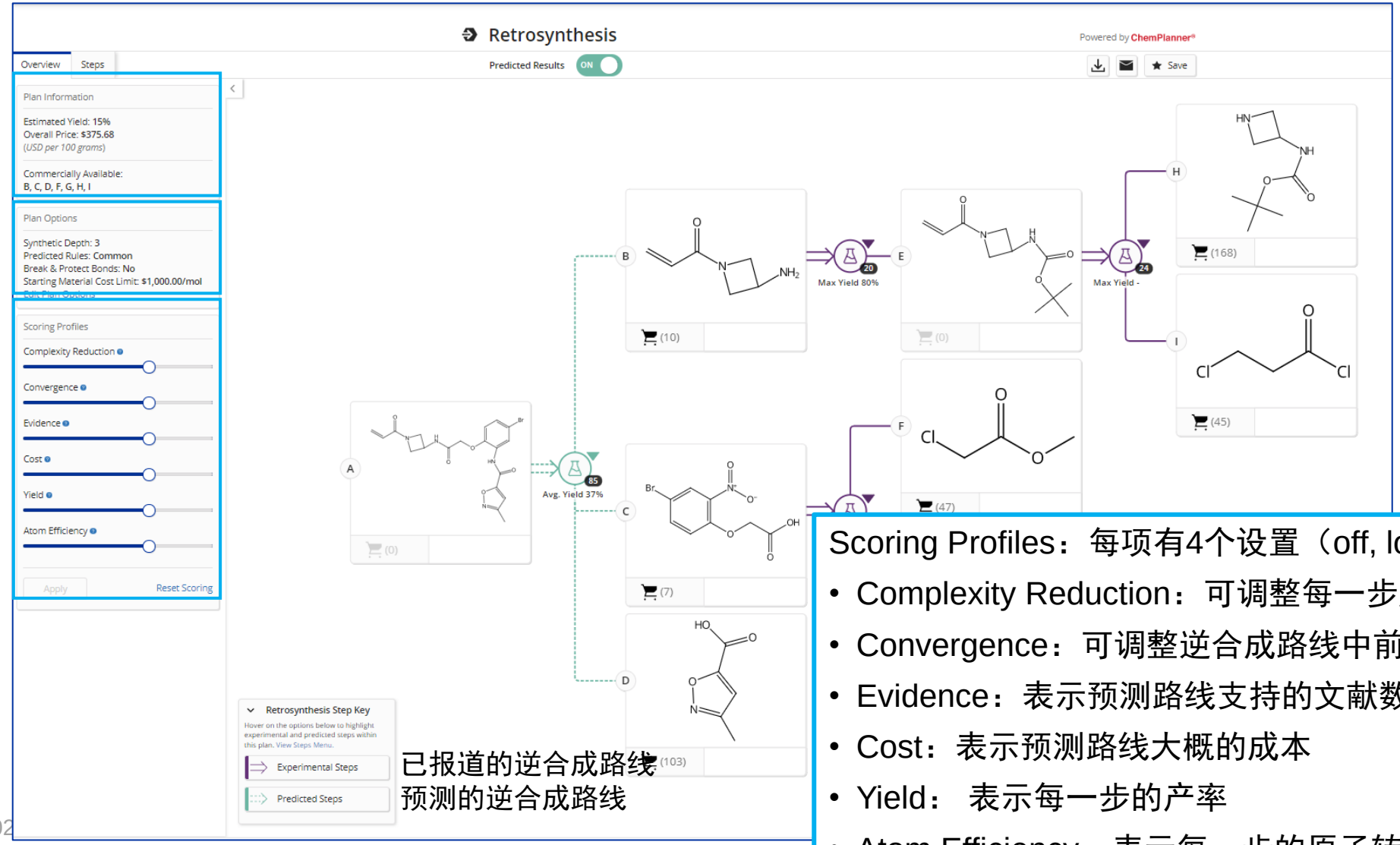
CAS Retrosynthesis Tool—路线概览

路线概览

重设参数

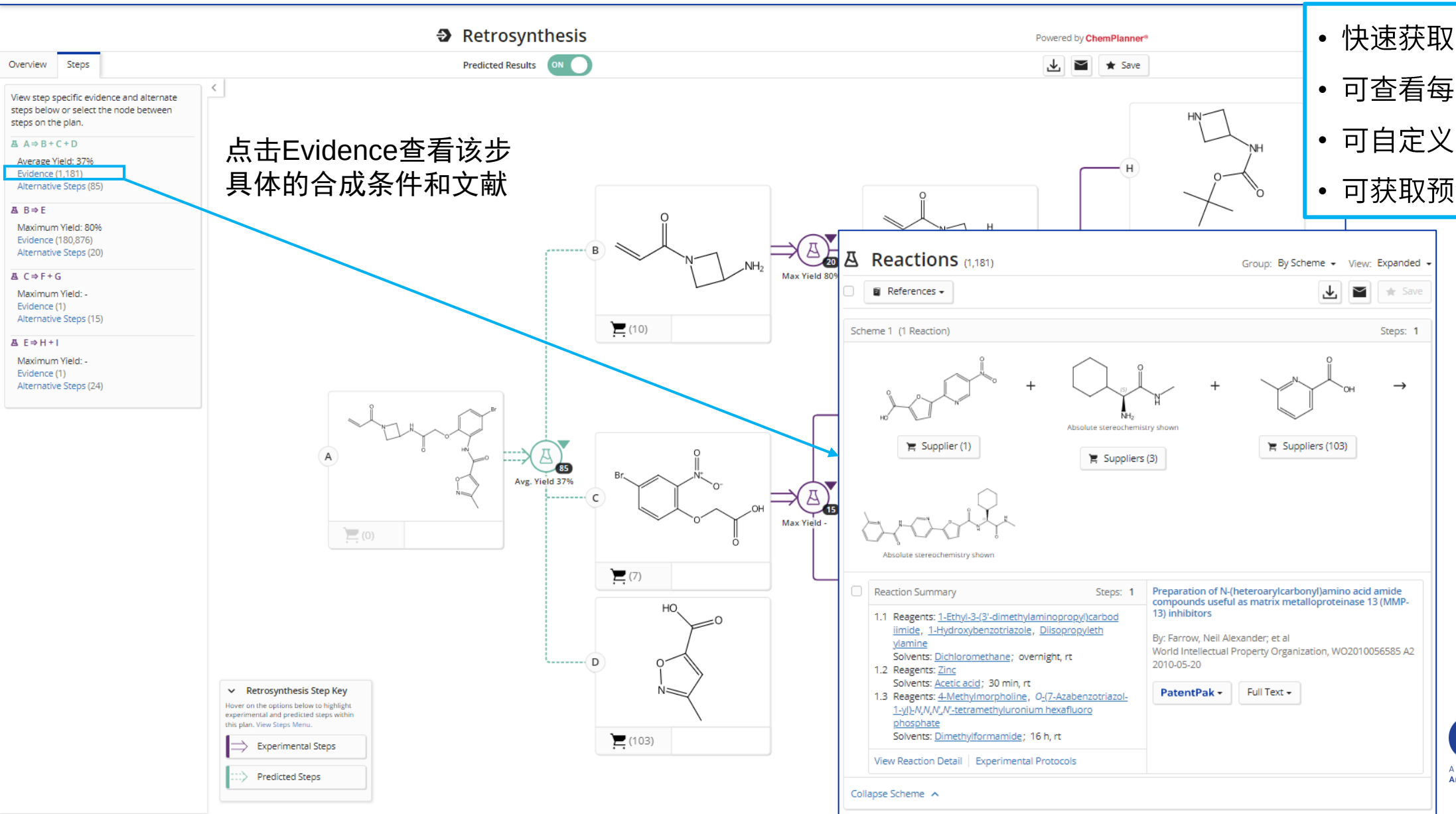


已报道的逆合成路线
预测的逆合成路线

Scoring Profiles：每项有4个设置（off, low, medium, high）

- Complexity Reduction：可调整每一步原料结构的复杂性
- Convergence：可调整逆合成路线中前体的数量
- Evidence：表示预测路线支持的文献数量多少
- Cost：表示预测路线大概的成本
- Yield： 表示每一步的产率
- Atom Efficiency：表示每一步的原子转化效率

CAS Retrosynthesis Tool—路线详情



- 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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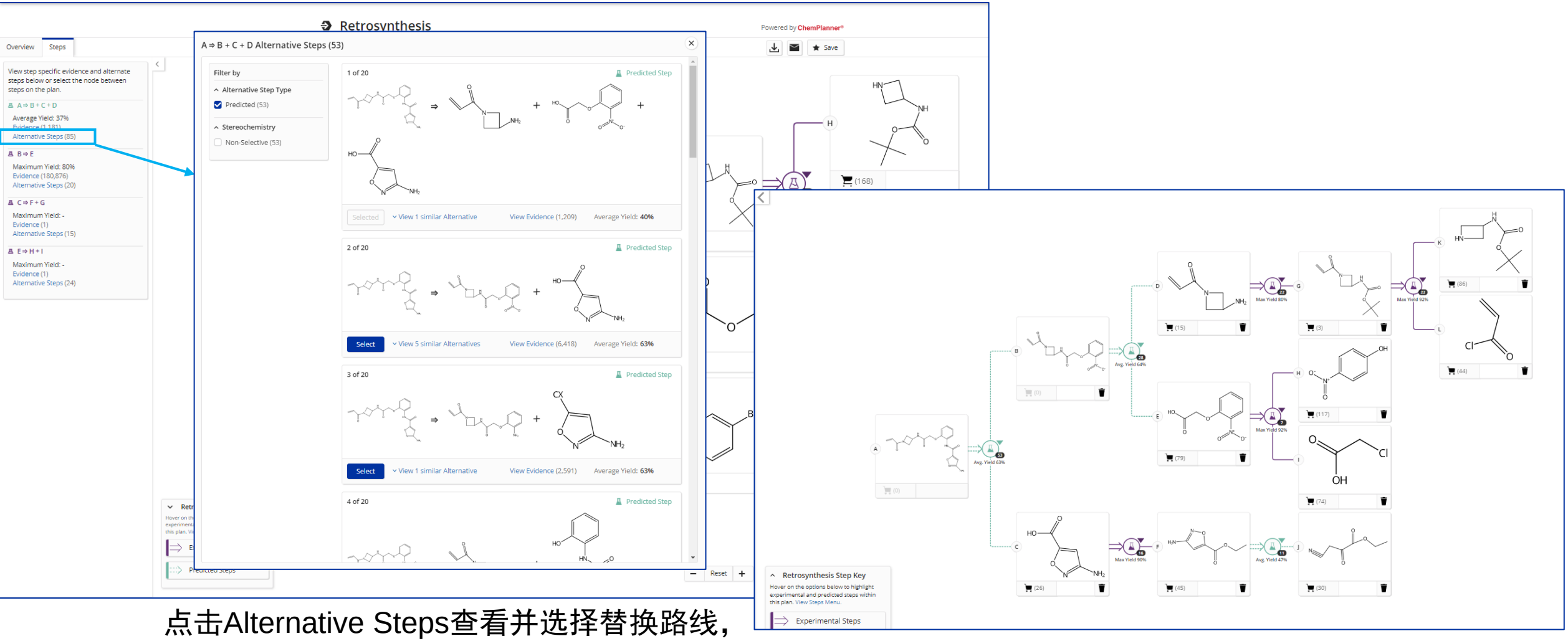
CAS Retrosynthesis Tool—路线详情



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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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

大纲

- CAS SciFinder^{n}中的序列检索
  - BLAST
  - CDR
  - Motif

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

下一节：分析实验方法

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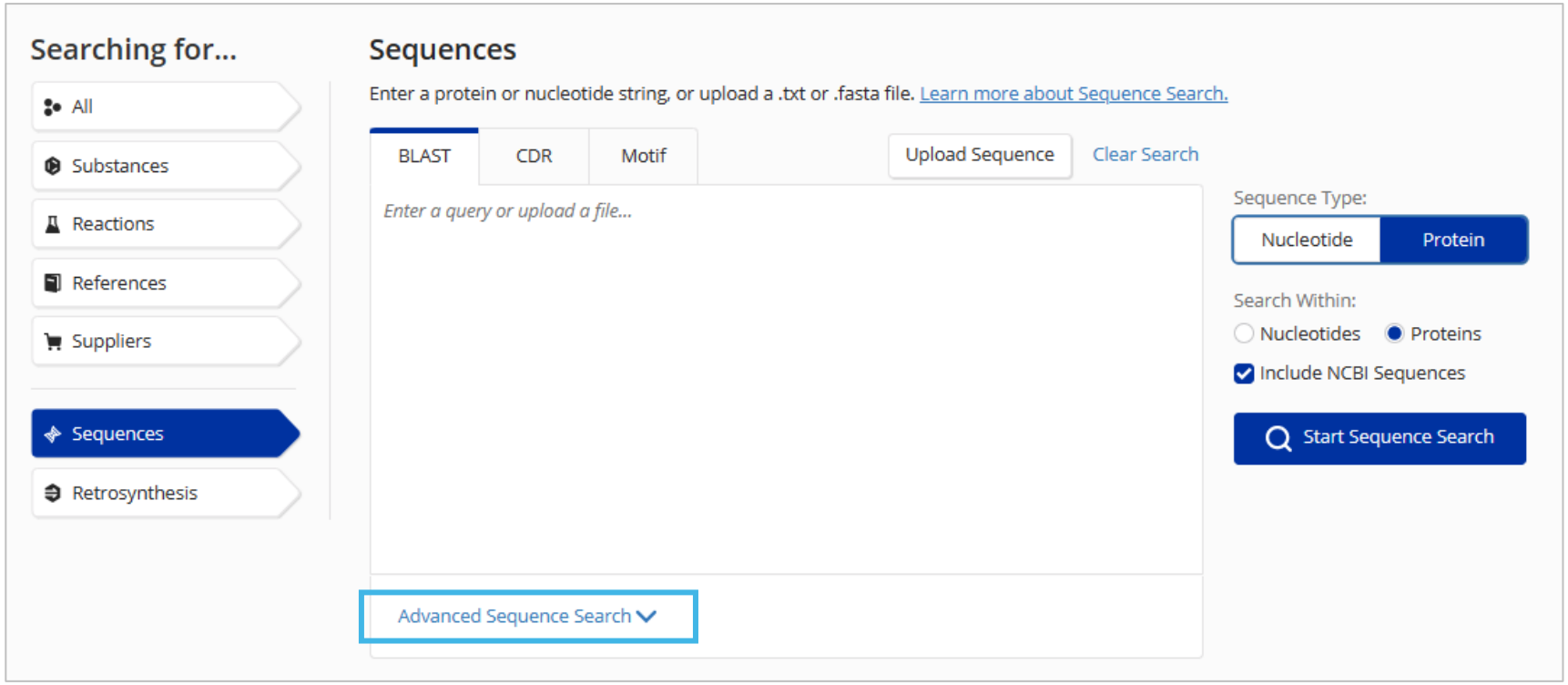
Sequences Search™ — Blast检索



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

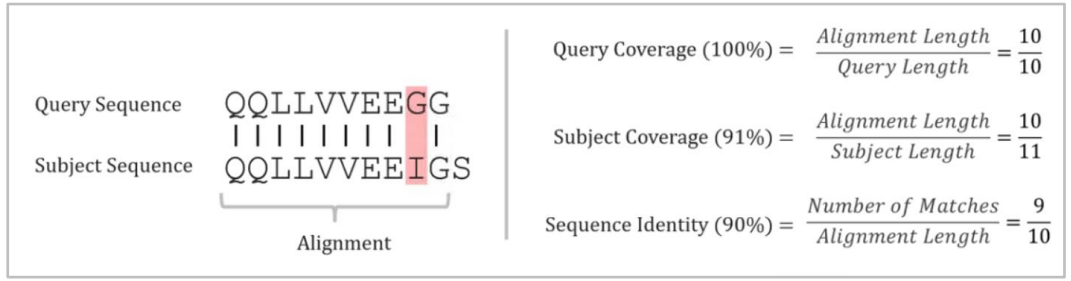
Search Within: Nucleotides | Proteins

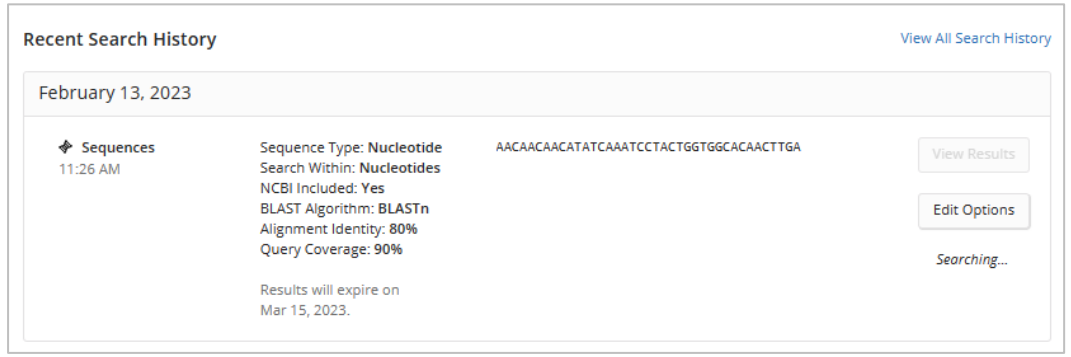
Include NCBI Sequences

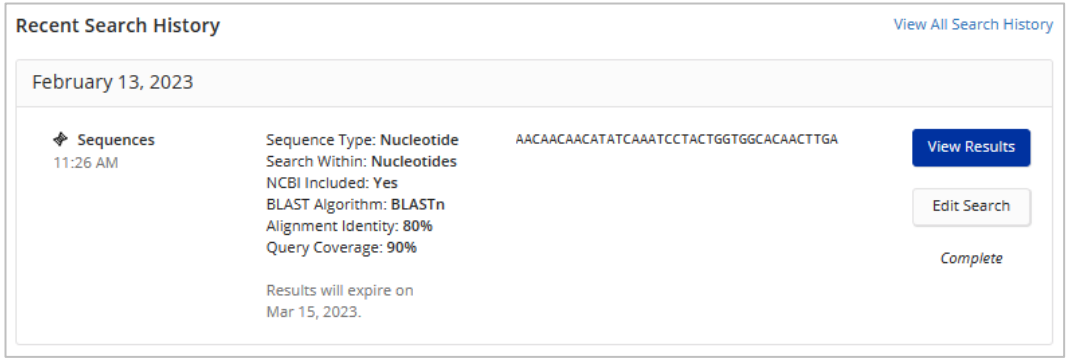
Start Sequence Search

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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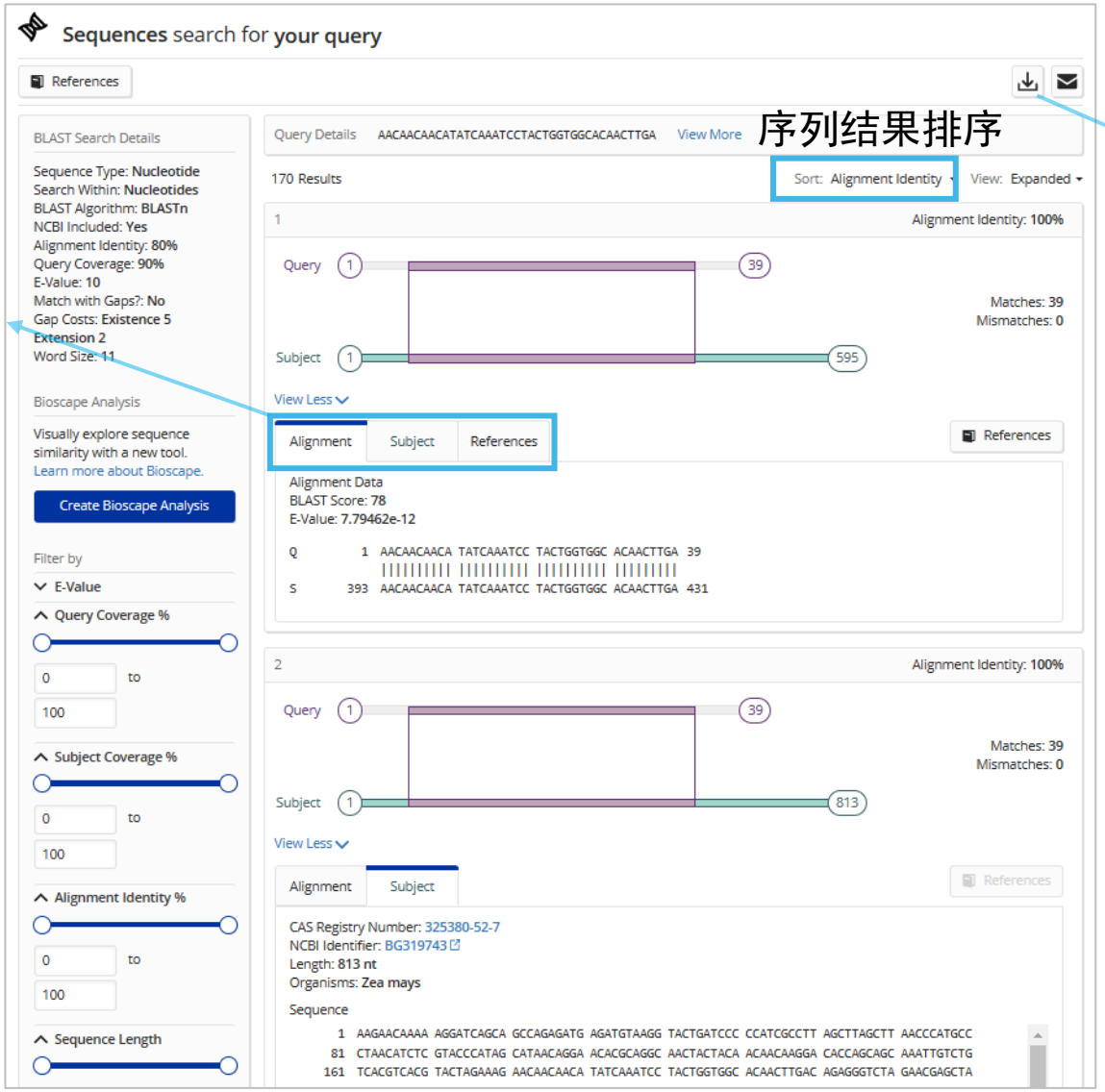
BLAST检索结果

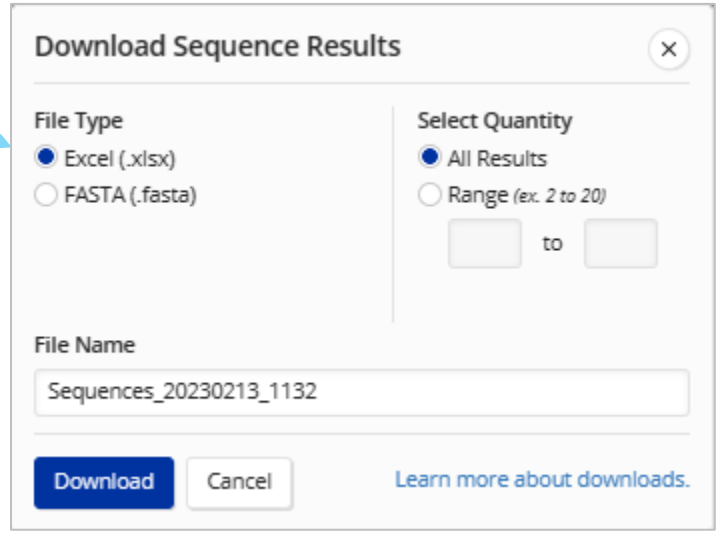
- 序列一致性详情
- 目标序列
- 披露序列的专利文献

- 可视化地图

- 结果筛选



序列结果排序



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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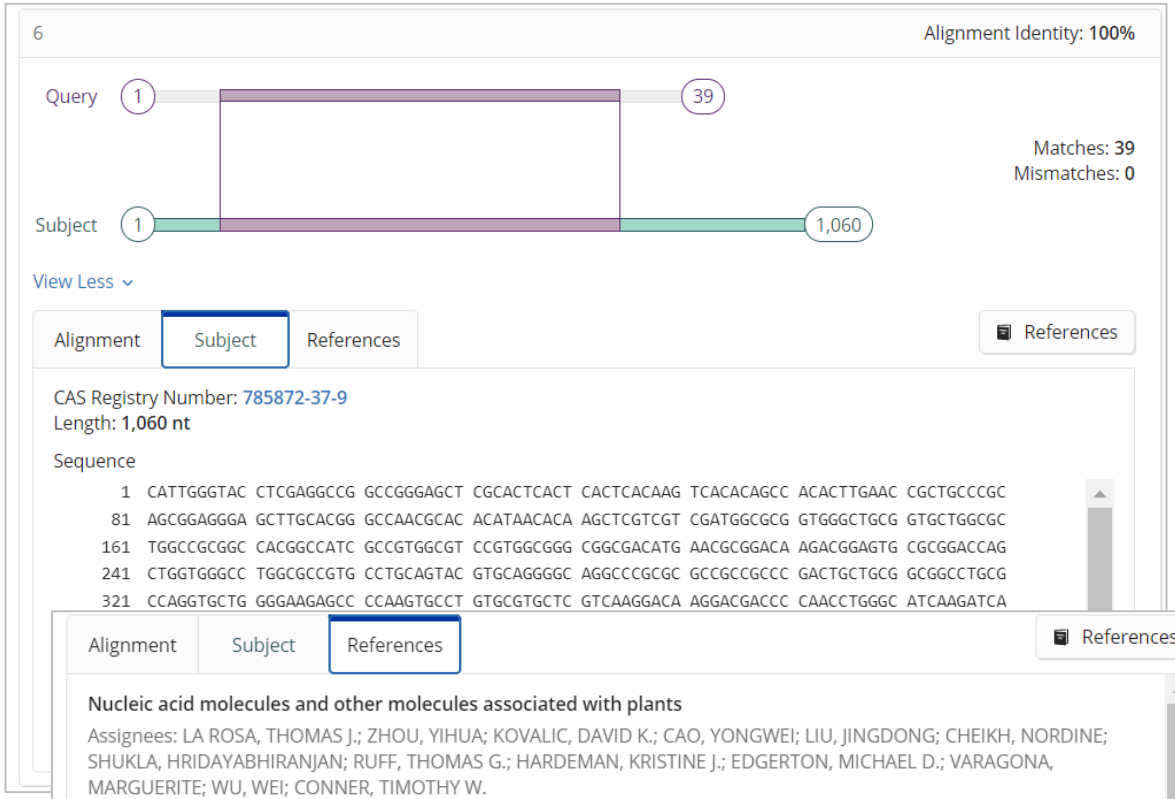
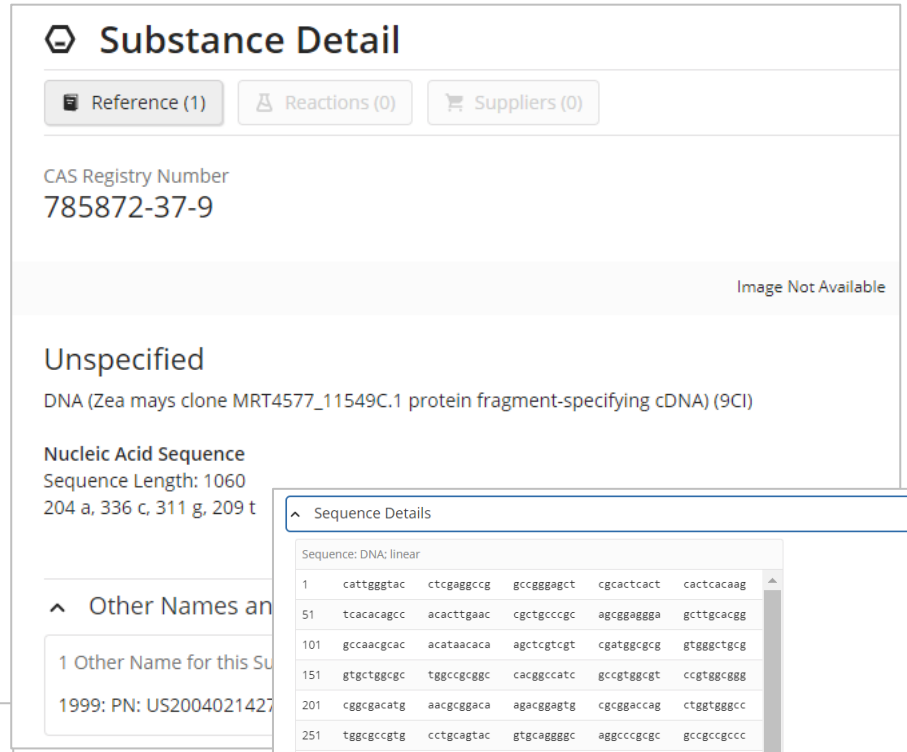
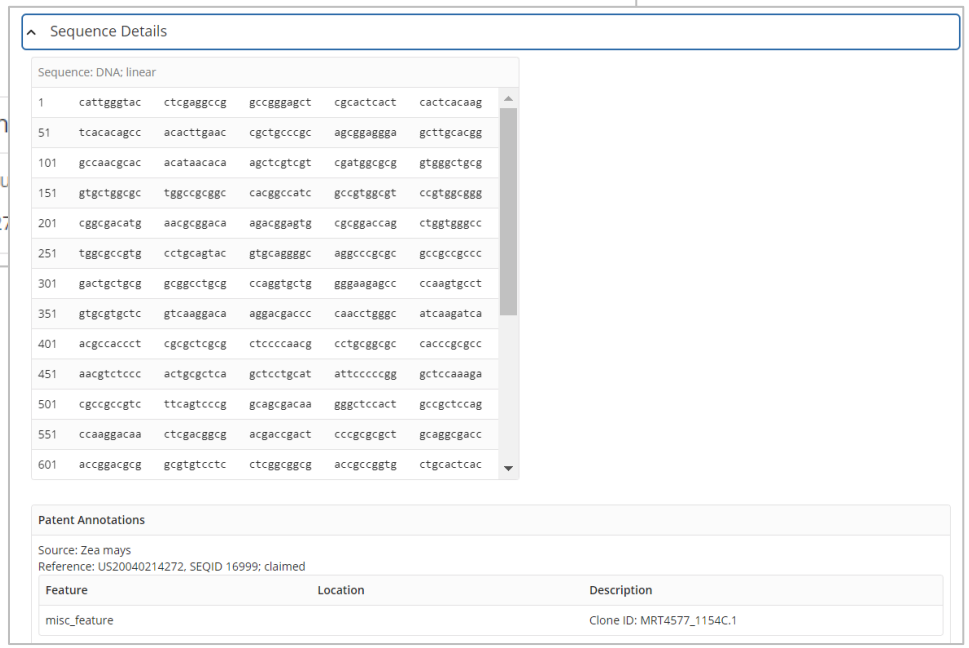
BLAST检索结果







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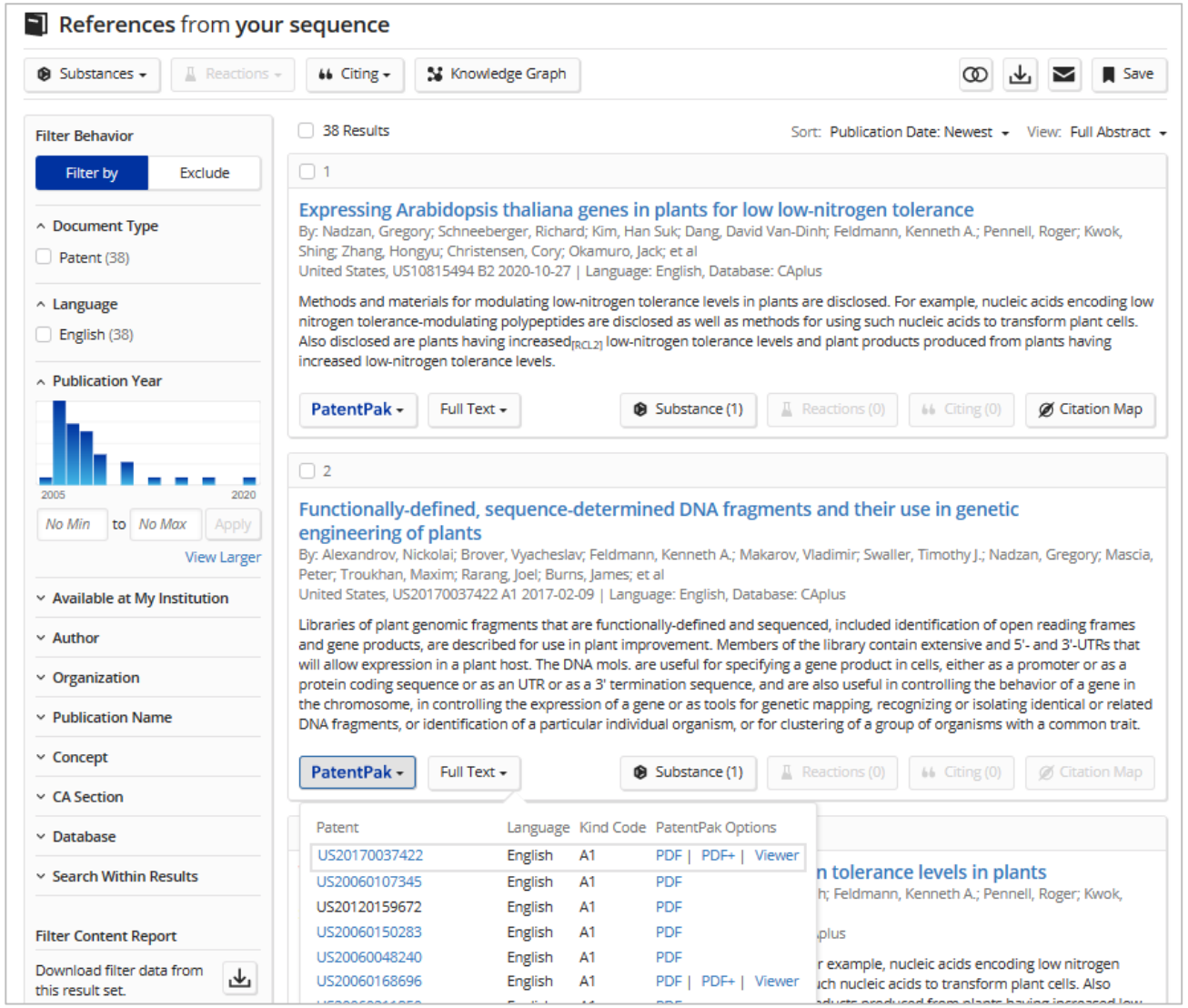
序列详情及相关的专利文献结果



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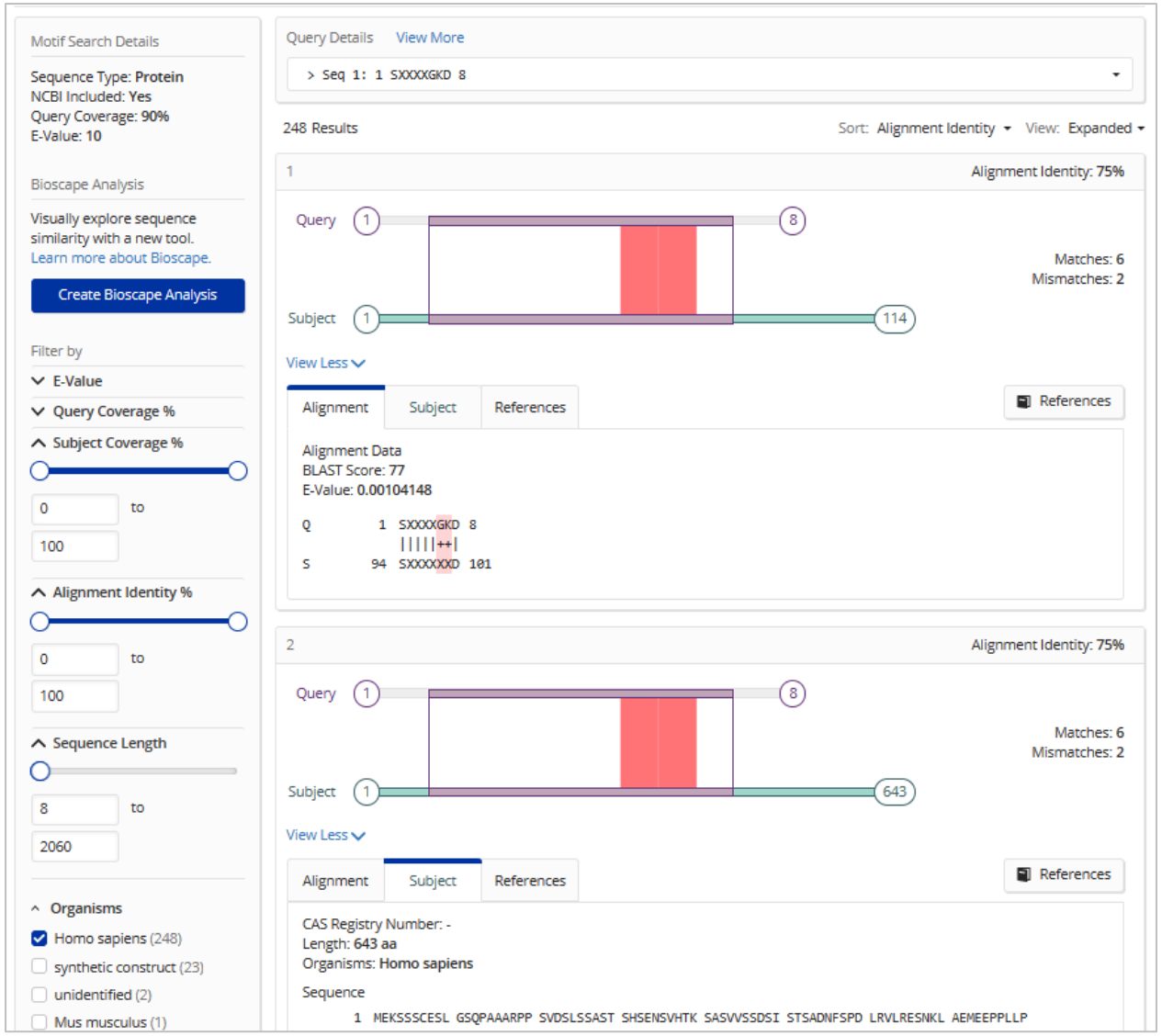
Sequences Search™—Motif检索

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

Motif检索结果



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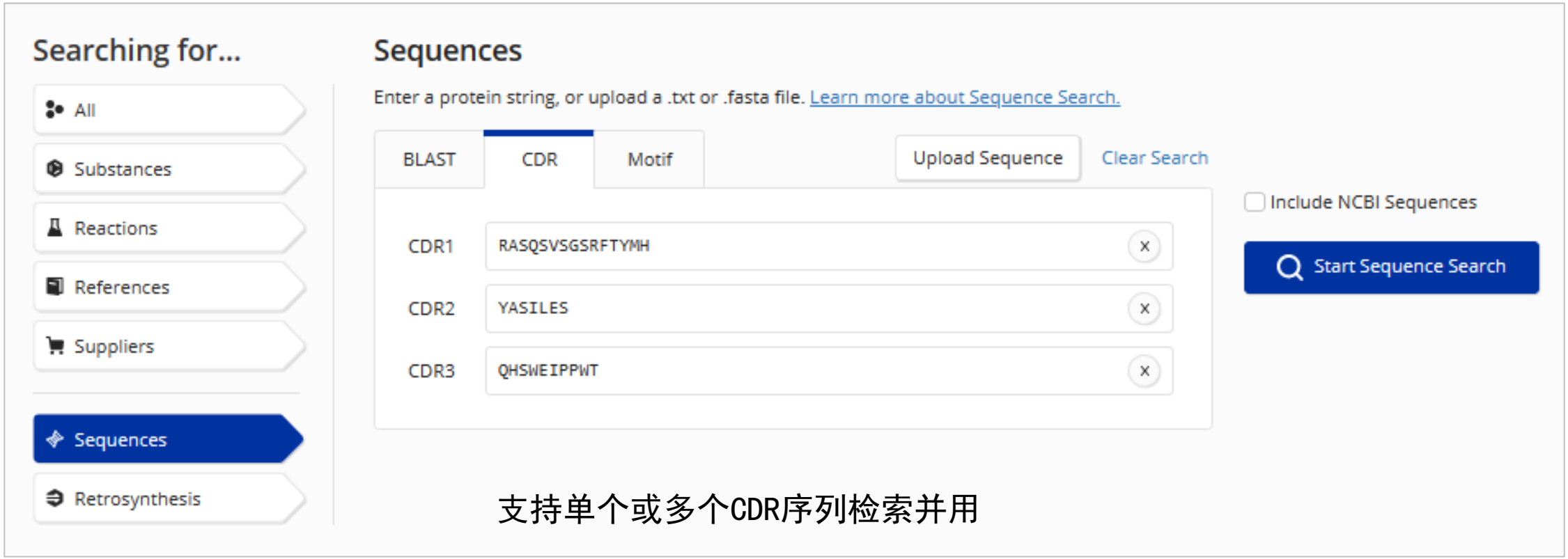
Sequences Search™—CDR检索

CDR（complementarity－determining regions）：抗体或细胞中的互补决定区



支持单个或多个CDR序列检索并用

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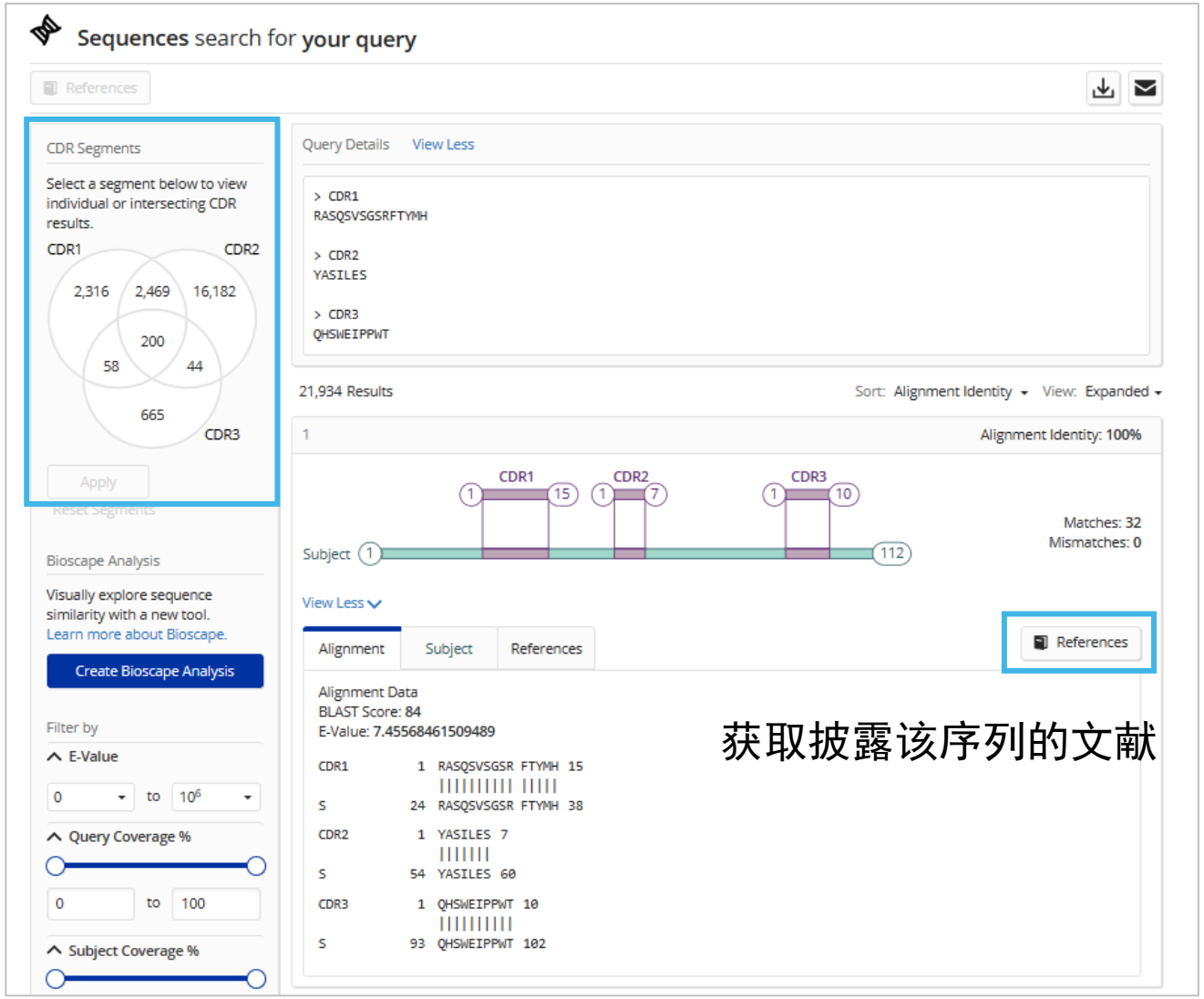
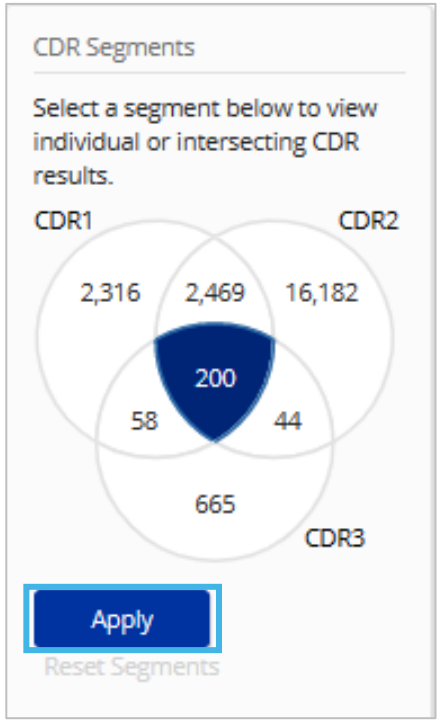
CDR检索结果



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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序列检索小结

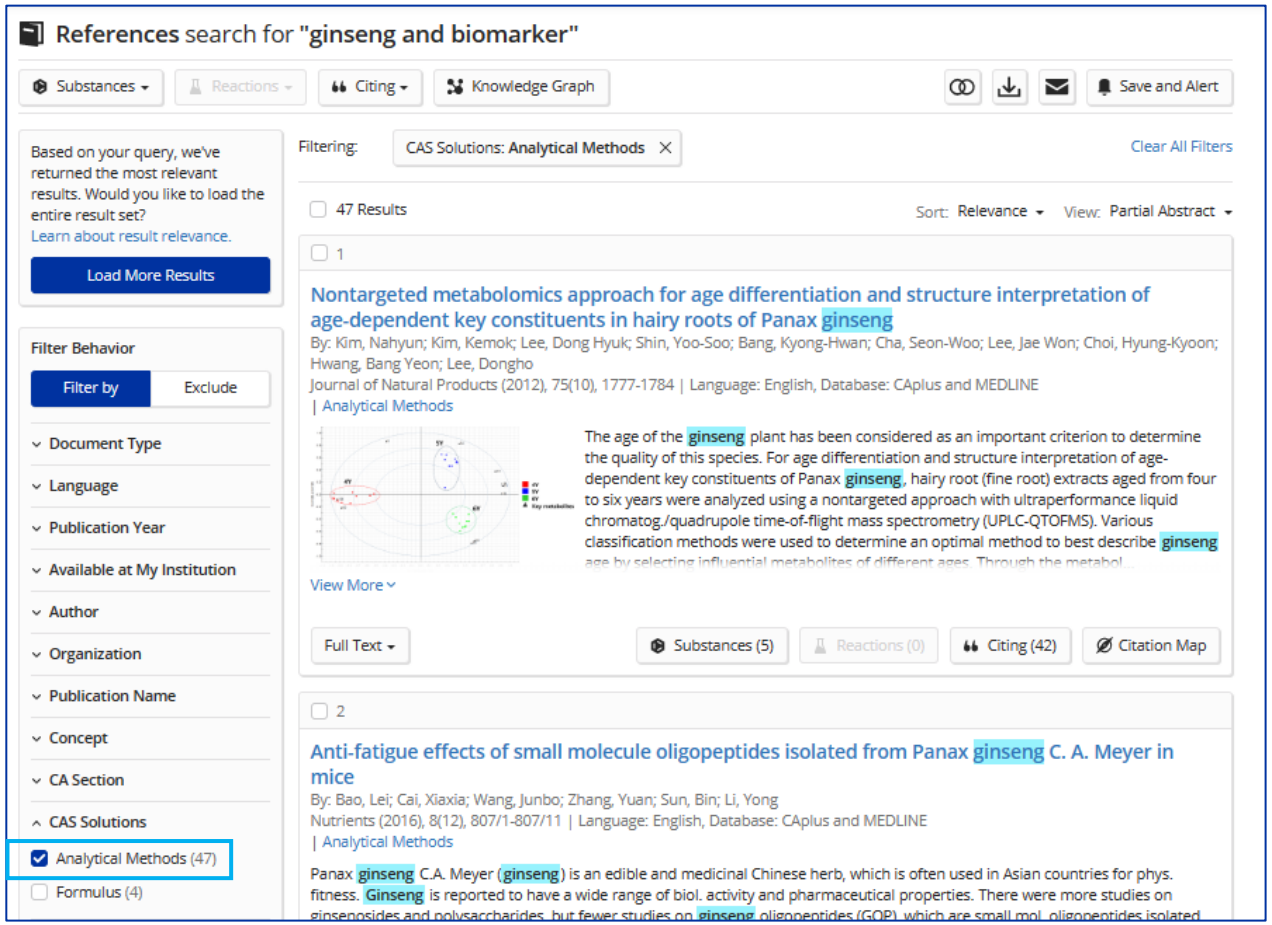
- Sequences涵盖期刊、专利、NCBI当中的序列信息
- Sequences可以针对DNA/RNA的核苷酸序列、肽/蛋白的氨基酸序列进行检索
- 生物序列的获取方法：Sequences检索、物质名称/代码/结构式、关键词及文献-物质的数据关联
- Motif适合检索短序列，并支持可变部分输入
  - ✓ X代表未指定氨基酸，N代表未指定核苷酸
  - ✓ [ ]表示出现在该位置的序列是括号里氨基酸/核苷酸中的任意一个
  - ✓ { } 代表氨基酸/核苷酸的重复次数，如重复次数是范围，用逗号将数字隔开，如{2,6}

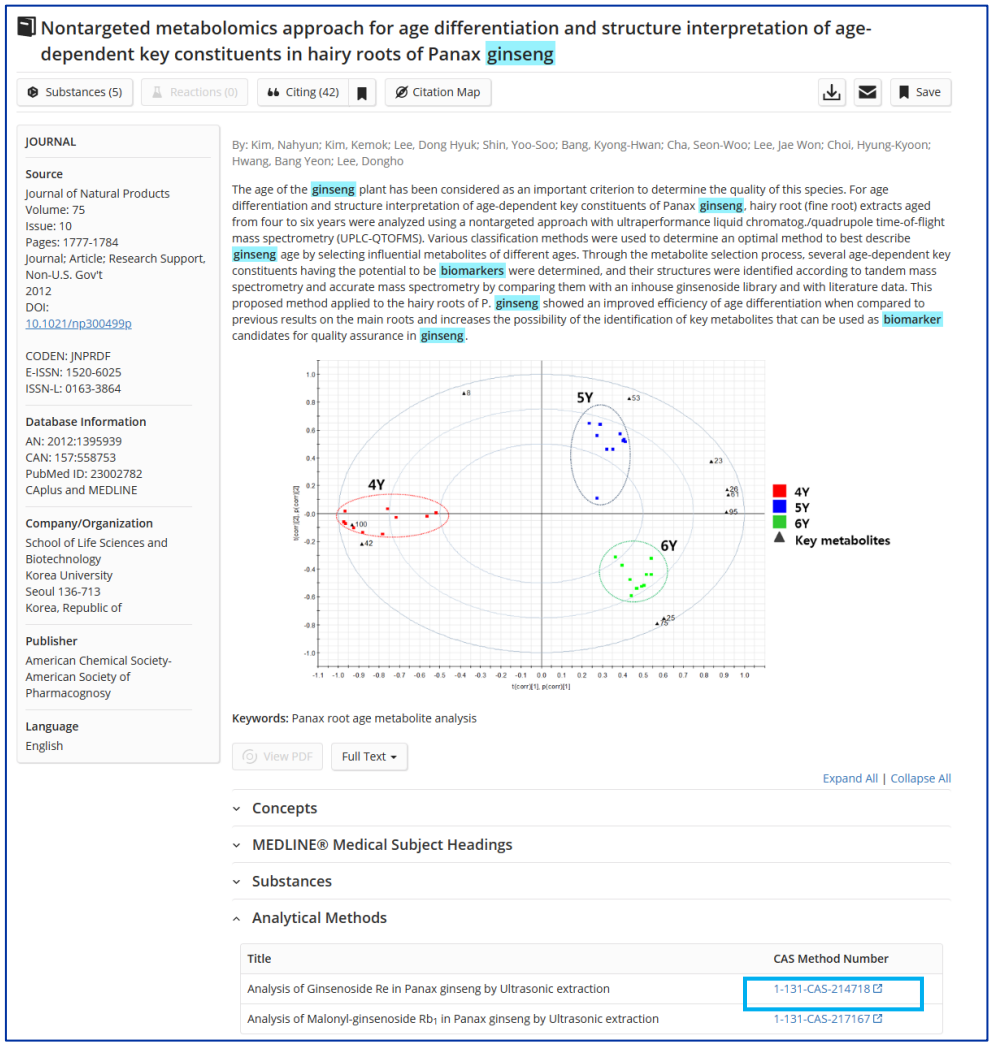
大纲

- 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

分析实验方法的获取 –从CAS SciFinder n结果集链接

方法一：在CAS SciFinder^{n}的文献结果集页面，点击CAS solutions中的 Analytical Methods获得有具体分析实验方法的文献，从文献详情页中链接至分析实验方法。





分析实验方法详情

Analysis of Ginsenoside Re in Panax ginseng by Ultrasonic extraction

CAS MN: 1-131-CAS-214718

实验原料

Method Category: Natural Product Isolation Analysis

Technique: Ultra-performance liquid chromatography; Ultrasonic extraction; Quadrupole mass spectrometry; Time-of-flight mass spectrometry

Materials	Role	Image	CAS RN
Ginsenoside Re	analyte	View Structure	52286-59-6
Ginsenoside Rg_2	analyte	View Structure	52286-74-5
Ginsenoside Rb_1	analyte	View Structure	41753-43-9
Ginsenoside Rd	analyte	View Structure	52705-93-8
Panax ginseng	matrix		
0.2 µm membrane filter	material		
Acquity UPLC BEH C18 column (i.d., 2.1 × 100 mm; particle size, 1.7 µm)	material		
Methanol	reagent	View Structure	67-56-1

Source

文献详情

Nontargeted metabolomics approach for age differentiation and structure interpretation of age-dependent key constituents in hairy roots of Panax ginseng

Kim, Nahyun; Kim, Kemok; Lee, Dong Hyuk; Shin, Yoo-Soo; Bang, Kyong-Hwan; Cha, Seon-Woo; Lee, Jae Won; Choi, Hyung-Kyoon; Hwang, Bang Yeon; Lee, Dongho

Journal of Natural Products (2012), 75 (10), 1777 - 1784. American Chemical Society-American Society of Pharmacognosy

CODEN: JNPRDF | ISSN: 01633864 | DOI: 10.1021/np300499p

Full Text | View in CAS SciFinder

Abstract

The age of the ginseng plant has been considered as an important criterion to determine the quality of this species. For age differentiation and structure interpretation of age-dependent key constituents of Panax ginseng, hairy root (fine root) extracts aged from four to six years were analyzed using a nontargeted approach with ultraperformance liquid chromatog./quadrupole time-of-flight mass spectrometry (UPLC-QTOFMS). Various classification methods were used to determine an optimal method to best describe ginseng age by selecting influential metabolites of different ages. Through the metabolite selection process, several age-dependent key constituents having the potential to be biomarkers were determined, and their structures were identified according to tandem mass spectrometry and accurate mass spectrometry by comparing them with an inhouse ginsenoside library and with literature data. This proposed method applied to the hairy roots of P. ginseng showed an improved efficiency of age differentiation when compared to previous results on the main roots and increases the possibility of the identification of key metabolites that can be used as biomarker candidates for quality assurance in ginseng.

Equipment Used

Freeze drier, Eyela, Tokyo, Japan

UPLC system, Acquity, Waters, Milford, MA, USA

Mass spectrometer, QTOF Micromass, Waters, Milford, MA, USA

Conditions

分析仪器

Instrument

Mobile phase: 0.1% formic acid in water (A) and 0.1% formic acid in acetonitrile (B); flow rate: 350 µL/min

分析条件

capillary voltage: 2800 V; cone voltage: 35 V; collision energy: 5 eV; source temperature: 100 °C; desolvation temperature: 250 °C; desolvation gas flow: 600 L/h; cone voltage and collision energy: 35-55 V and 30-50 eV, respectively.

Instructions

操作步骤

Collection of samples

1. Prepare *P. ginseng* samples and subject to analysis.

Preparation of standard solution

1. Prepare each ginsenoside standard in 50% methanol.
2. Store all the stock and working solutions at -20 °C before use.
3. Prepare stock solutions of ginsenosides and dilute to 0.08, 0.4, 2.0, 10.0 and 50.0 µg/mL to prepare the five-point calibration curves using the least-squares method.

Ultrasonic extraction

1. Cut and powder the hairy roots of *P. ginseng*.
2. Freeze dry (Eyela, Tokyo, Japan).
3. Powder.
4. Extract the samples ultrasonically with 70% methanol.
5. Centrifuge at 12000 rpm for 20 min.
6. Filter the supernatant through a 0.2 µm membrane filter.
7. Evaporate the solvent to dryness *in vacuo*.
8. Dilute the residue with 50% methanol to obtain a final concentration of 2 mg/mL.

Ultra-performance liquid chromatography quadrupole time of flight mass spectrometry (UPLC-QTOFMS) for the analysis of ginsenosides Rb1, Rd, Re and Rg2

1. Perform analysis using Acquity UPLC system (Waters, Milford, MA, USA) and a QTOF Micromass spectrometer (Waters, Manchester, UK).
2. Separate the analytes using Acquity UPLC BEH C18 column (i.d., 2.1 × 100 mm; particle size, 1.7 µm).
3. Use mobile phase consisting of 0.1% formic acid in water (A) and 0.1% formic acid in acetonitrile (B).
4. Maintain the following gradient elution program: 0.5 min 10% B, 3.0 min 25% B, 10.0 min 30% B, 16.0 min 35% B, 18.0 min 50% B, 21.0 min 65% B, 23.0 min 100% B for washing and 25.0 min 10% B to re-equilibrate the column with a flow rate of 350 µL/min.
5. Maintain the column and sample managers at 40 and 15 °C, respectively.
6. Inject 5 µL sample solution onto a column.
7. Perform mass spectral analysis in the negative-ion mode by scanning the m/z range of 200–1500.
8. Maintain the following mass spectral parameters: capillary voltage: 2800 V; cone voltage: 35 V; collision energy: 5 eV; source temperature: 100 °C; desolvation temperature: 250 °C; desolvation gas flow: 600 L/h; cone voltage and collision energy: 35-55 V and 30-50 eV, respectively.

Validation

数据有效性

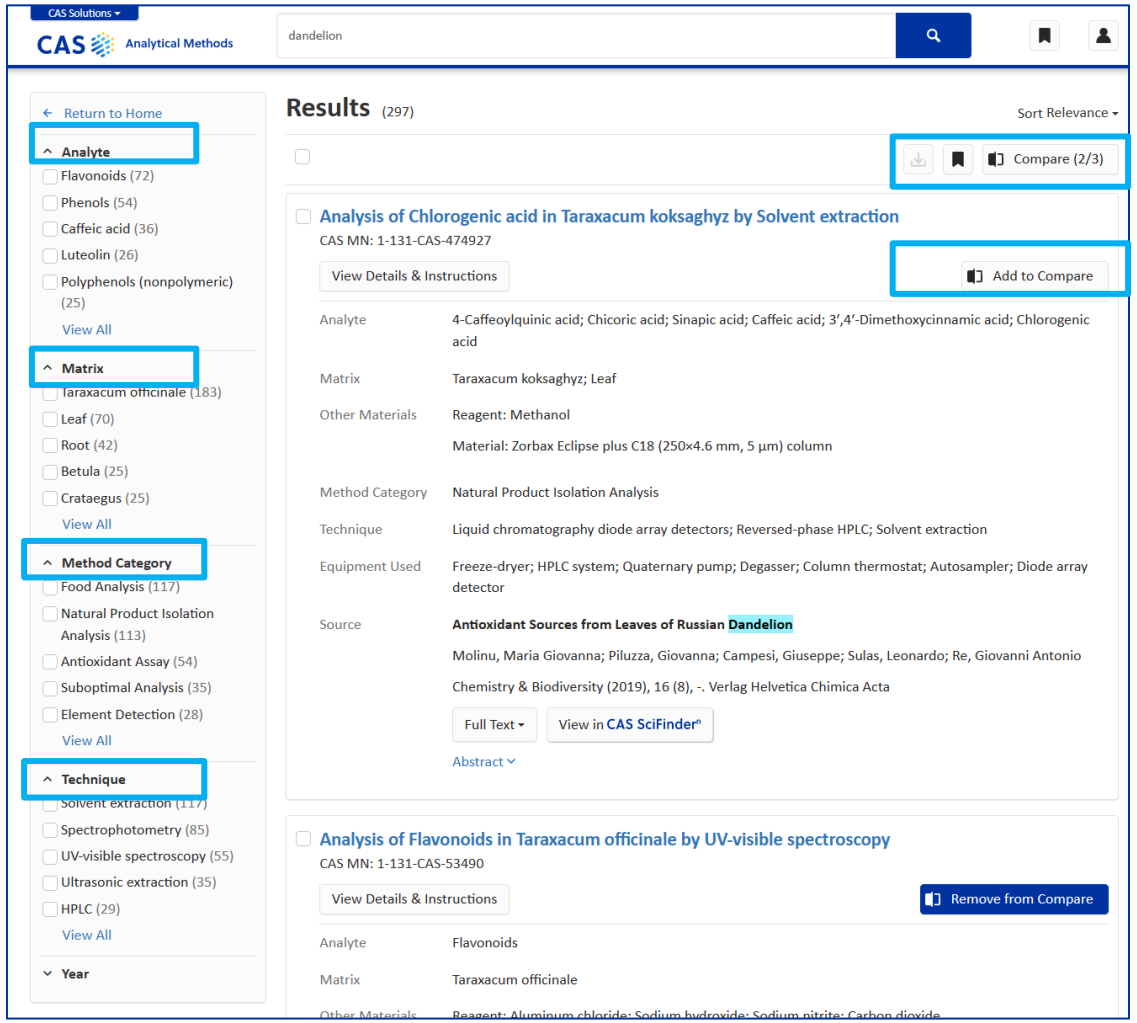
Retention Time	3.76 min, Ginsenoside Re
	13.71 min, Ginsenoside Rd
	8.7 min, Ginsenoside Rg2
	3.43 min, Ginsenoside Re
	17.3 min, Ginsenoside derivative
	9.89 min, Ginsenoside derivative
Concentration	6.719 ± 0.491 mg/g (sample data), Ginsenoside Rb1
	0.060 ± 0.026 mg/g (sample data), Ginsenoside Rd
	8.338 ± 1.464 mg/g (sample data), Ginsenoside Re
	0.197 ± 0.098 mg/g (sample data), Ginsenoside Rg2

分析实验方法的获取 -- https://methods.cas.org

方法二：登录Analytical Methods主页
- 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

Compare Methods

Expand All | Collapse All

	1	2
Title	**Analysis of Flavonoids in Taraxacum officinale by UV-visible spectroscopy**	**Analysis of Flavonoids in Taraxacum officinale by UV-visible spectroscopy**
CAS Method Number	1-131-CAS-78532	1-131-CAS-44155
Method Category	Natural Product Isolation Analysis	Natural Product Isolation Analysis; Suboptimal Analysis
Technique	UV-visible spectroscopy	UV-visible spectroscopy
Analyte	Flavonoids	Flavonoids
Matrix	Taraxacum officinale	Taraxacum officinale
Other Materials	Aluminum chloride; Carbon dioxide; Sodium hydroxide; Sodium nitrite	Sodium nitrite; Carbon dioxide; Sodium hydroxide; Aluminum chloride
Equipment Used	Double-beam UV-Vis spectrophotometer, Shanghai Precision Scientific Instrument Co. Ltd.; High-speed grinder, Shanghai Precision Scientific Instrument Co. Ltd.; Ultrasonic View All	Double-beam UV-Vis spectrophotometer, Shanghai Precision Scientific Instrument Co. Ltd.; High-speed grinder, Shanghai Precision Scientific Instrument Co. Ltd.; Ultrasonic View All
Conditions	**Instrument:** detection wavelength-510 nm	**Instrument:** detection wavelength-510 nm
Source	**Supercritical fluid extraction of flavonoids from dandelion** Wu, Jun; Luqiun; Rong, Shao View All	**Supercritical fluid extraction of flavonoids from dandelion** Wu, Jun; Luqiun; Rong, Shao View All
Method	**UV-VIS spectroscopy (Orthogonal experiments)** 1. Obtain dandelion (*Taraxacum officinale*) herb for the study. 2. Pulverize the dried dandelion (baked at 45 °C for 12 h) in a high-speed mixer-grinder and sieve the powders over a 60-mesh screen. 3. Pack the 2 L extractor in with the dried dandelion powders. 4. Use CO_2 as the solvent. 5. Determined the flavonoids content in the extract using nitritealuminum nitrate method. 6. Use rutin to prepare a standard curve. 7. Add rutin samples of 1.0, 2.0, 3.0, 4.0, 5.0, 6.0 mL, respectively to 25 mL volumetric flasks and dilute with 1 mL 5% $NaNO_2$, 1 mL 10% $AlCl_3$, 10 mL 4% NaOH and proper amount of water. 8. Dilute the parallel sample with the above chemicals but use containing no rutin for comparison. 9. Set the conditions for orthogonal experiment as follows: (a) pressure-35 MPa (b) temperature-50 °C (c) entrainer amount-4.0 mL/g (d) time-80 min. 10. Measure the absorbance at 510 nm using a double-beam UV-Vis spectrophotometer. 11. Calculate the concentration and the yield of flavonoids by the following equation: yield (mass of extract/mass of dry leaves,%) = c × v/m × 100, where c (g/mL)-the mass concentration of flavonoids, m (g)-the mass of dandelion, v (mL)-the volume of the extract. View Less	**UV-VIS spectroscopy (Orthogonal experiments)** 1. Obtain dandelion (*Taraxacum officinale*) herb for the study. 2. Pulverize the dried dandelion (baked at 45 °C for 12 h) in a high-speed mixer-grinder and sieve the powders over a 60-mesh screen. 3. Pack the 2 L extractor in with the dried dandelion powders. 4. Use CO_2 as the solvent. 5. Determined the flavonoids content in the extract using nitritealuminum nitrate method. 6. Use rutin to prepare a standard curve. 7. Add rutin samples of 1.0, 2.0, 3.0, 4.0, 5.0, 6.0 mL, respectively to 25 mL volumetric flasks and dilute with 1 mL 5% $NaNO_2$, 1 mL 10% $AlCl_3$, 10 mL 4% NaOH and proper amount of water. 8. Dilute the parallel sample with the above chemicals but use containing no rutin for comparison. 9. Set the conditions for orthogonal experiment as follows: (a) pressure-35 MPa (b) temperature-45 °C (c) entrainer amount-3.50 mL/g (d) time-100 min. 10. Measure the absorbance at 510 nm using a double-beam UV-Vis spectrophotometer. 11. Calculate the concentration and the yield of flavonoids by the following equation: yield (mass of extract/mass of dry leaves,%) = c × v/m × 100, where c (g/mL)-the mass concentration of flavonoids, m (g)-the mass of dandelion, v (mL)-the volume of the extract. View Less
Concentration	4.974%	4.45%

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分析实验方法小结

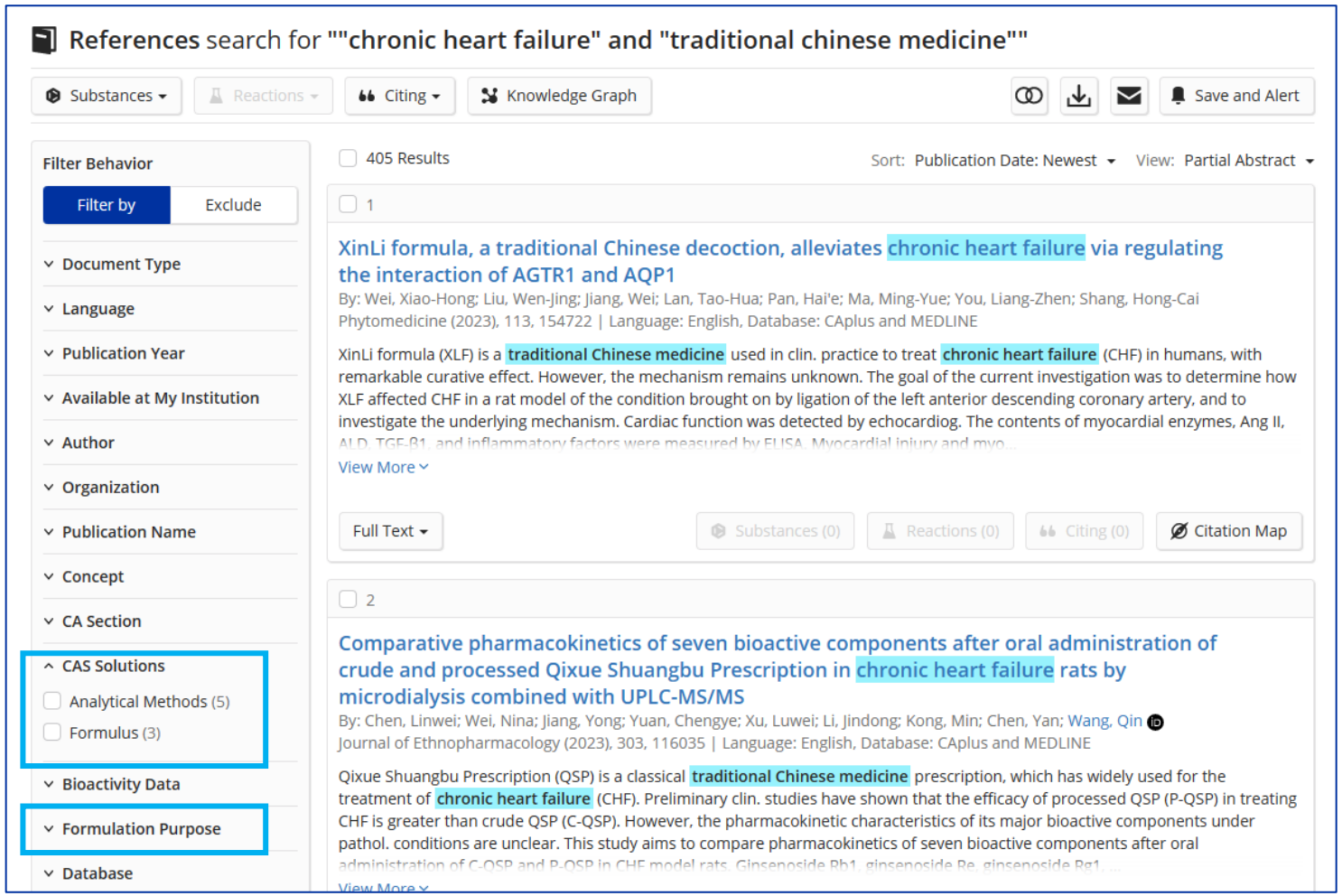
1. 通过CAS SciFinder^{n}中的文献结果集获得关联的分析方法
2. 在Analytical Methods平台中，直接通过主题检索或分类浏览获取分析实验方法
3. 查看分析实验方法操作详情，筛选分析目标物、介质、分析方法

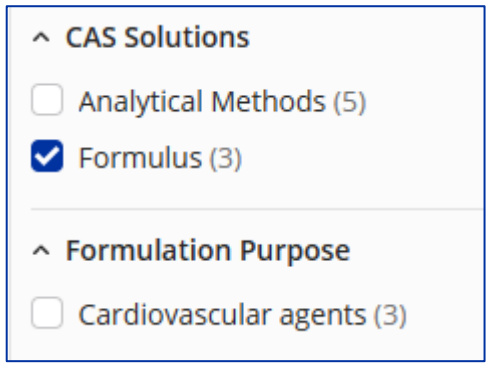
大纲

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

获取配方或制剂 -- 从CAS SciFinder n结果集链接

方法一：在CAS SciFinder^{n}的文献结果集页面，点击CAS solutions中的 Formulus 或勾选 Formulation Purpose选项，获得有具体配方或制剂信息的文献，从文献详情页中链接获取





定位配方或制剂的功能目标

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获取制剂或配方相关信息

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

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

PATENT

Patent Number
CN112190652

Publication Date
2021-01-08

Application Number
CN2020-11207191

Application Date
2020-11-03

Kind Code
A

Assignee
Capital Medical University, China

Source
China
CODEN: CNXXEV

Database Information
AN: 2021:56481
CAN: 176:120018
CAplus

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder^{n} users. View content from CAS Formulus® in this document. Learn more about Formulus®.

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

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

Keywords: myocardial hypertrophy prevention traditional Chinese medicine composition

PatentPak PDF | Get Prior Art Analysis | Full Text

Patent Family

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

Expand All | Collapse All

- IPC Data
- Concepts
- Formulations

Formulations

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

View CAS Formulus® Detail

Location: Claim 1, 2, 3, 4, 5, 6, 7, 8, 9
Purpose: Cardiovascular agents
Target: myocardial hypertrophy, human

成份 功能 用量

Component	Function	Amount Reported
Panax ginseng	-	175-225 wt. parts
Ophiopogon japonicus	-	175-225 wt. parts
Schisandra chinensis	-	100-150 wt. parts
Astragalus membranaceus	-	175-225 wt. parts

Additional Components Reported in Full Text

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

View CAS Formulus® Detail

Location: Example
Purpose: Cardiovascular agents
Target: myocardial hypertrophy, human

Component	Function	Amount Reported
Panax ginseng	-	200 wt. parts

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配方/制剂详情

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

Purpose	Target	Delivery Route	Physical Form	Source
Cardiovascular agents	ACTN2 protein level, ACTN2 protein level abnormal increase, Cardiac hypertrophy, Homo sapiens, TNNT2 protein level, TNNT2 protein level abnormal increase, interventricular septum thickness, interventricular septum thickness abnormal increase, left ventricle volume abnormal increase, left ventricular hypertrophy index, left ventricular hypertrophy index abnormal increase, left ventricular volume, malignant heart disease, myocardial cytoskeleton-related protein level, myocardial cytoskeleton-related protein level abnormal increase, posterior left ventricular wall thickness, posterior left ventricular wall thickness abnormal increase, stress-induced chronic heart failure	-	Capsules	View

制剂/配方的用途、靶点、递送途径及物理形式

制剂/配方的成分、功能及用量

Formulation Ingredients

Component	Function	Amount Reported	Optionality
Panax ginseng	-	200 wt. parts	Mandatory
Ophiopogon japonicus	-	200 wt. parts	Mandatory
Schisandra chinensis	-	133 wt. parts	Mandatory
Astragalus membranaceus	-	200 wt. parts	Mandatory
Salvia miltiorrhiza	-	267 wt. parts	Mandatory
Ligusticum striatum	-	133 wt. parts	Mandatory
Crataegus pinnatifida	-	200 wt. parts	Mandatory

More Formulations like this... NEW

相似的制剂/配方

- Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy:... — Purpose: Cardiovascular agents; Target: ACTN2 protein level, ACTN2 pr...; Delivery Route: -; Physical Form: Capsules
- Pharmaceutical Composition: Cardioprotective Agents or Cardiovascular Agents — Purpose: Cardioprotective agents, Car...; Target: Homo sapiens; Delivery Route: -; Physical Form: -
- Pharmaceutical Composition Containing Alantolactone: Angiogenesis Inhibitors or... — Purpose: Antiangiogenic agents, Antitu...; Target: Angiogenesis, Homo sapiens, ...; Delivery Route: Oral drug delivery syst...; Physical Form: Capsules, Pharmaceutic...
- Antifungal Composition: Antifungal Agents — Purpose: Fungicides; Target: Aspergillosis, Aspergillus clavat...; Delivery Route: -; Physical Form: -

Effective Dose

有效剂量

Descriptor	Solvent	Details
rate of administration of the capsules	-	0.16 g/kg/day

Experimental Activity

Descriptor	Notes	Details
cardioprotective effect	cardioprotective effect of the composition on SPF SD rats with myocardial hypertrophy was assessed after 8 weeks of administration.	the composition has the protective effect on cardiac function in the rats.

Descriptor	Solvent	Details
rate of administration of the capsules	-	0.32 g/kg/day

Experimental Activity

Descriptor	Notes	Details
cardioprotective effect	cardioprotective effect of the composition on SPF SD rats with myocardial hypertrophy was assessed after 8 weeks of administration.	the composition has the protective effect on cardiac function in the rats.

Descriptor	Solvent	Details
rate of administration of the capsules	-	0.64 g/kg/day

Experimental Activity

Descriptor	Notes	Details
cardioprotective effect	cardioprotective effect of the composition on SPF SD rats with myocardial hypertrophy was assessed after 8 weeks of administration.	the composition has the protective effect on cardiac function in the rats.

Source Patent

查看或下载专利全文

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

Assignee : Capital Medical University
CN112190652
Language: Chinese
Location: **Example**

Patent PDF | View

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- 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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检索配方或制剂 -- https://formulus.cas.org

方法二：

- 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

- 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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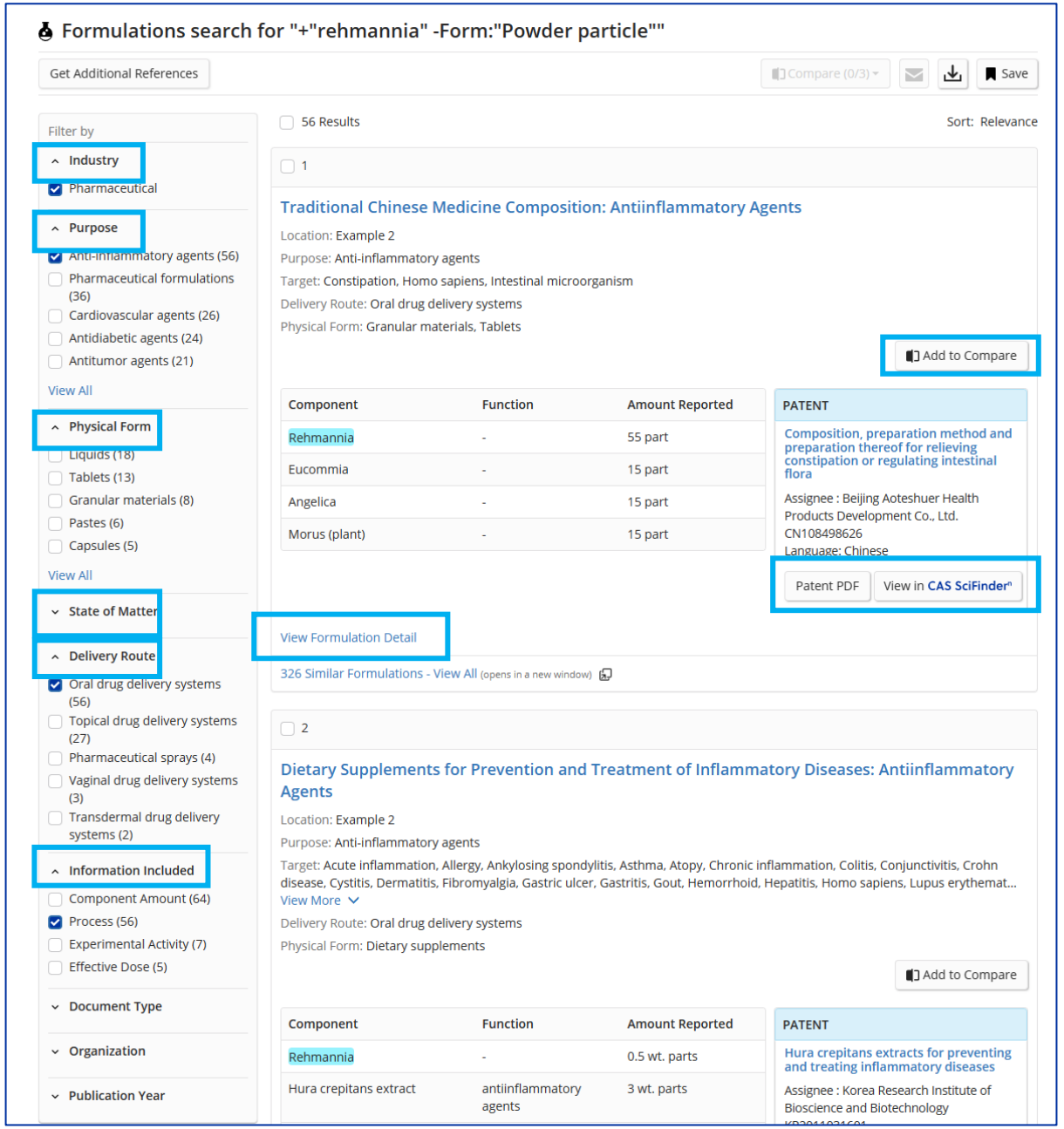
配方/制剂结果集

- 利用聚类项筛选结果：

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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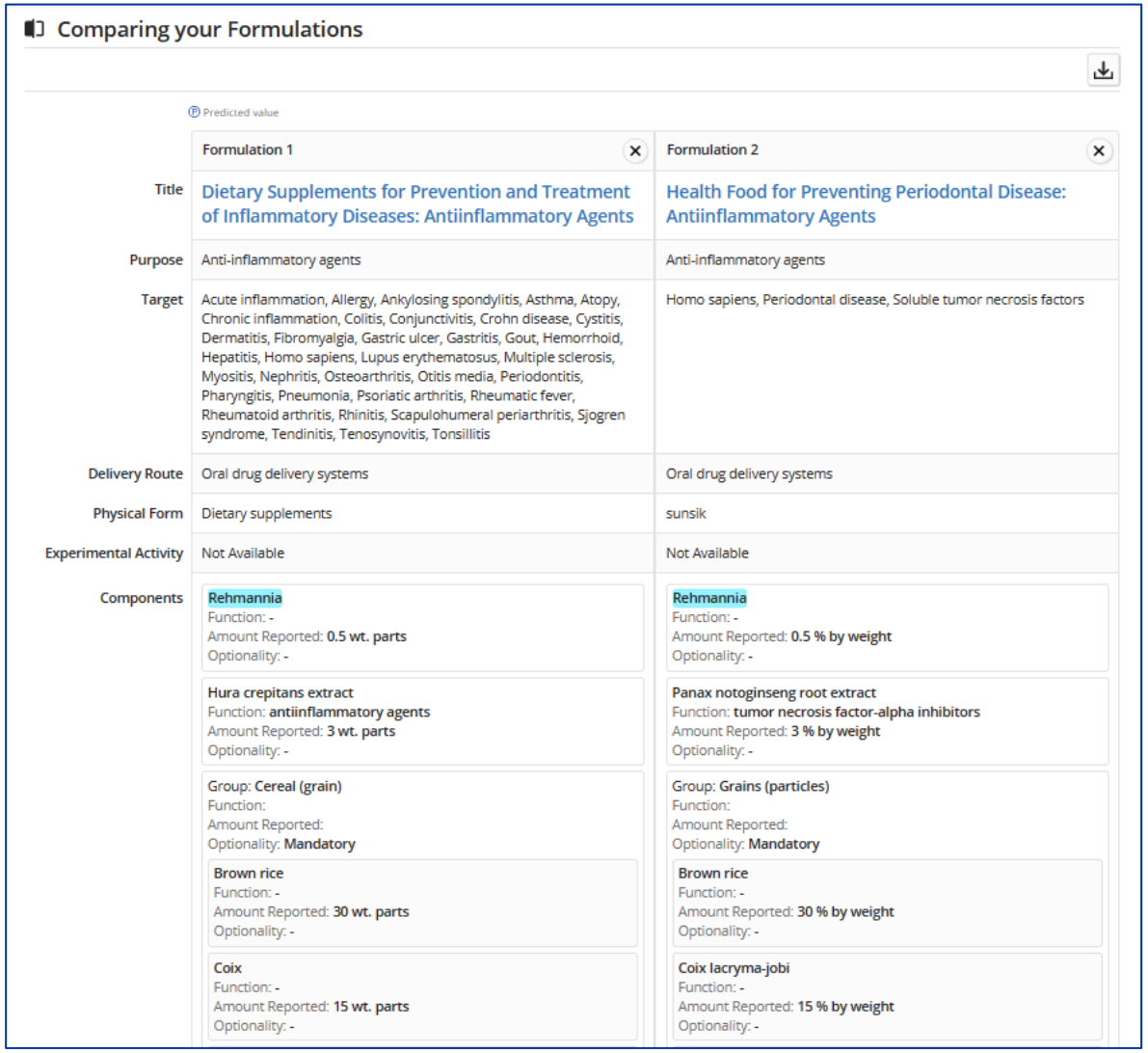
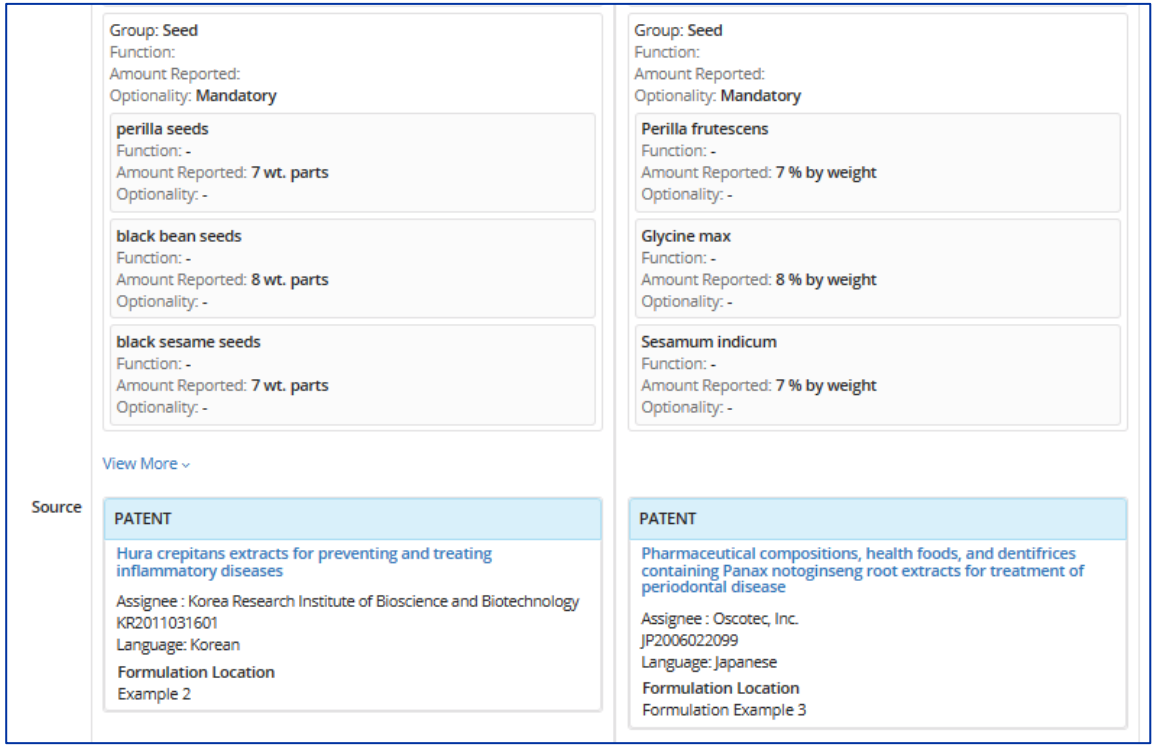
不同制剂或配方信息的对比



- 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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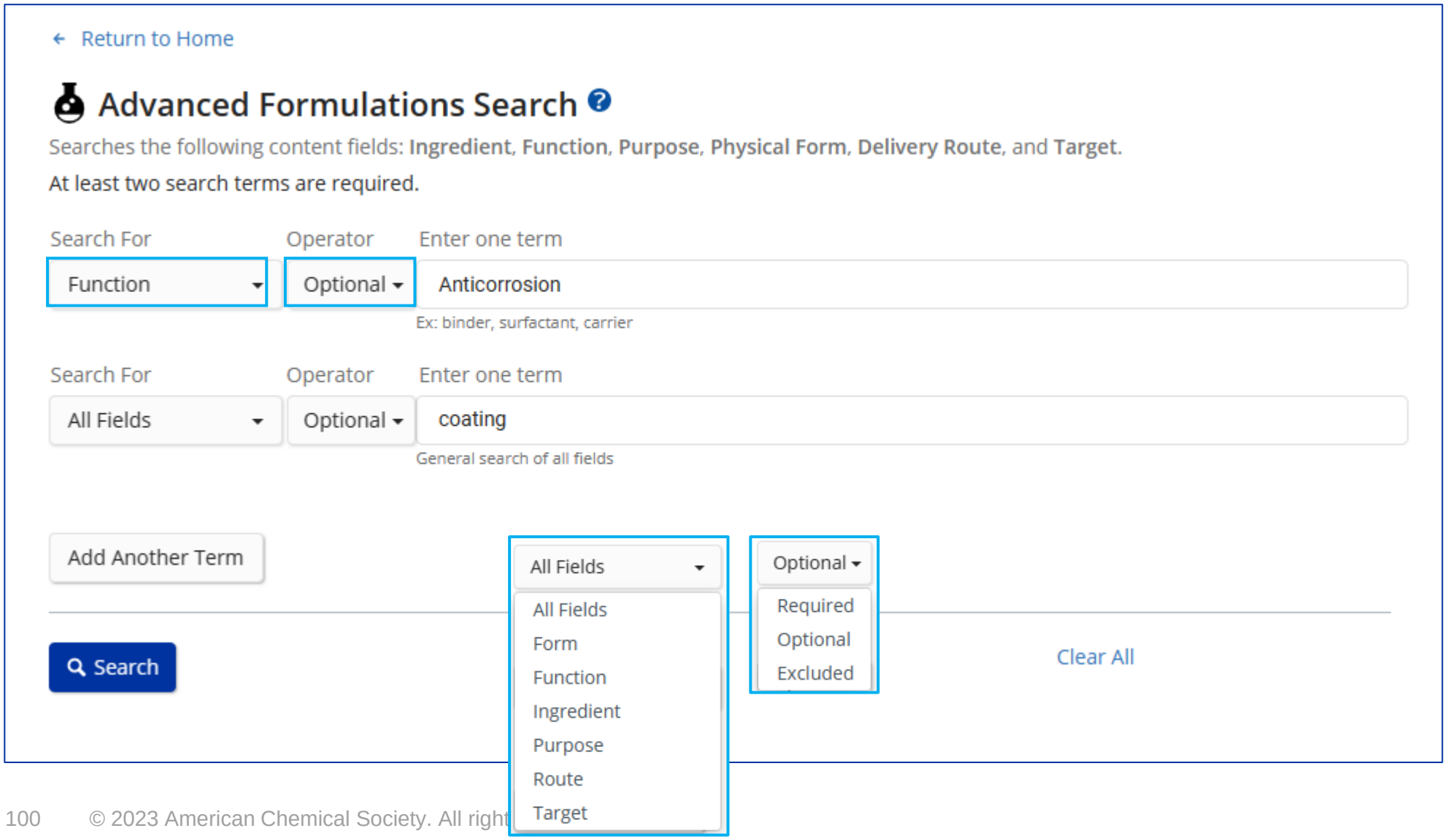
高级检索



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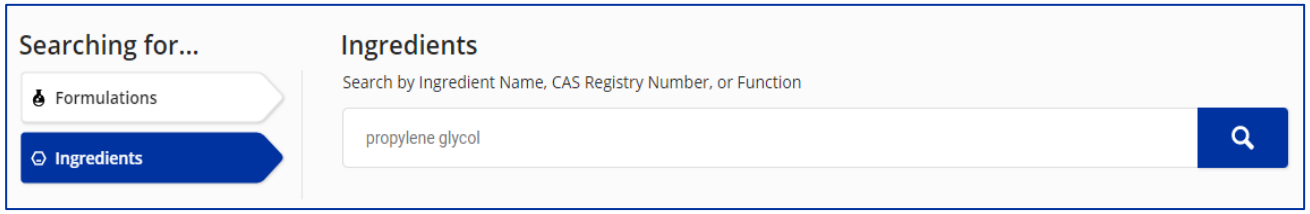
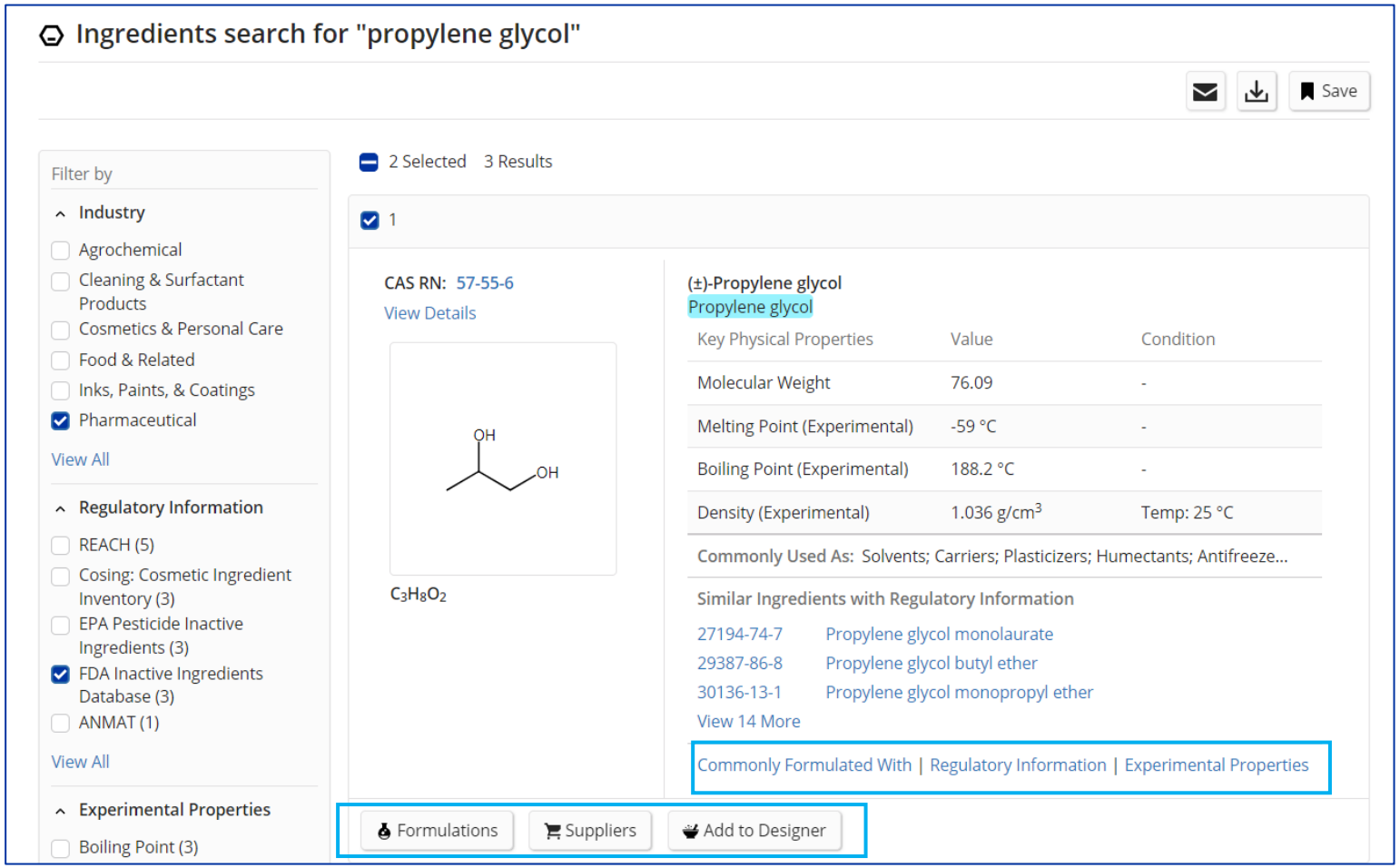
检索原料





- 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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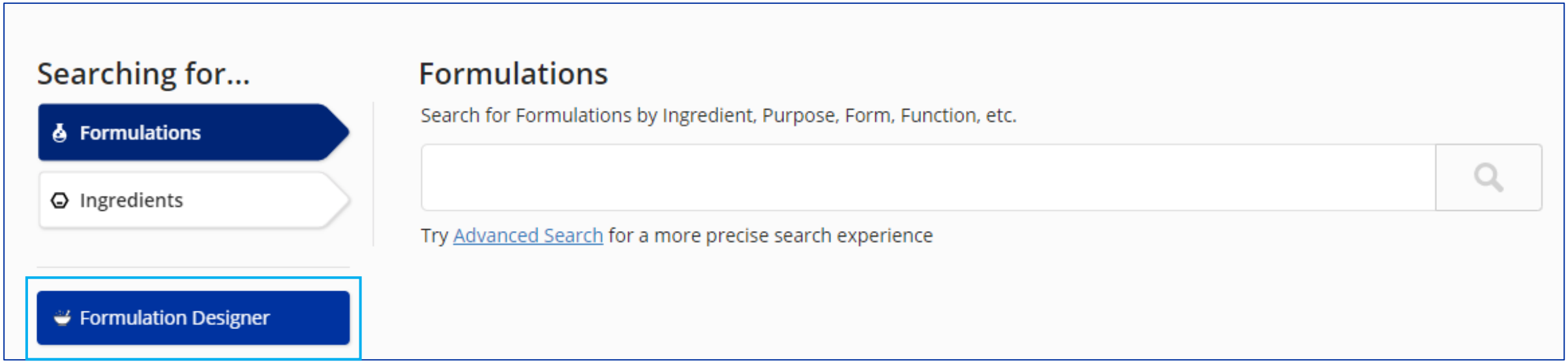
设计制剂或配方



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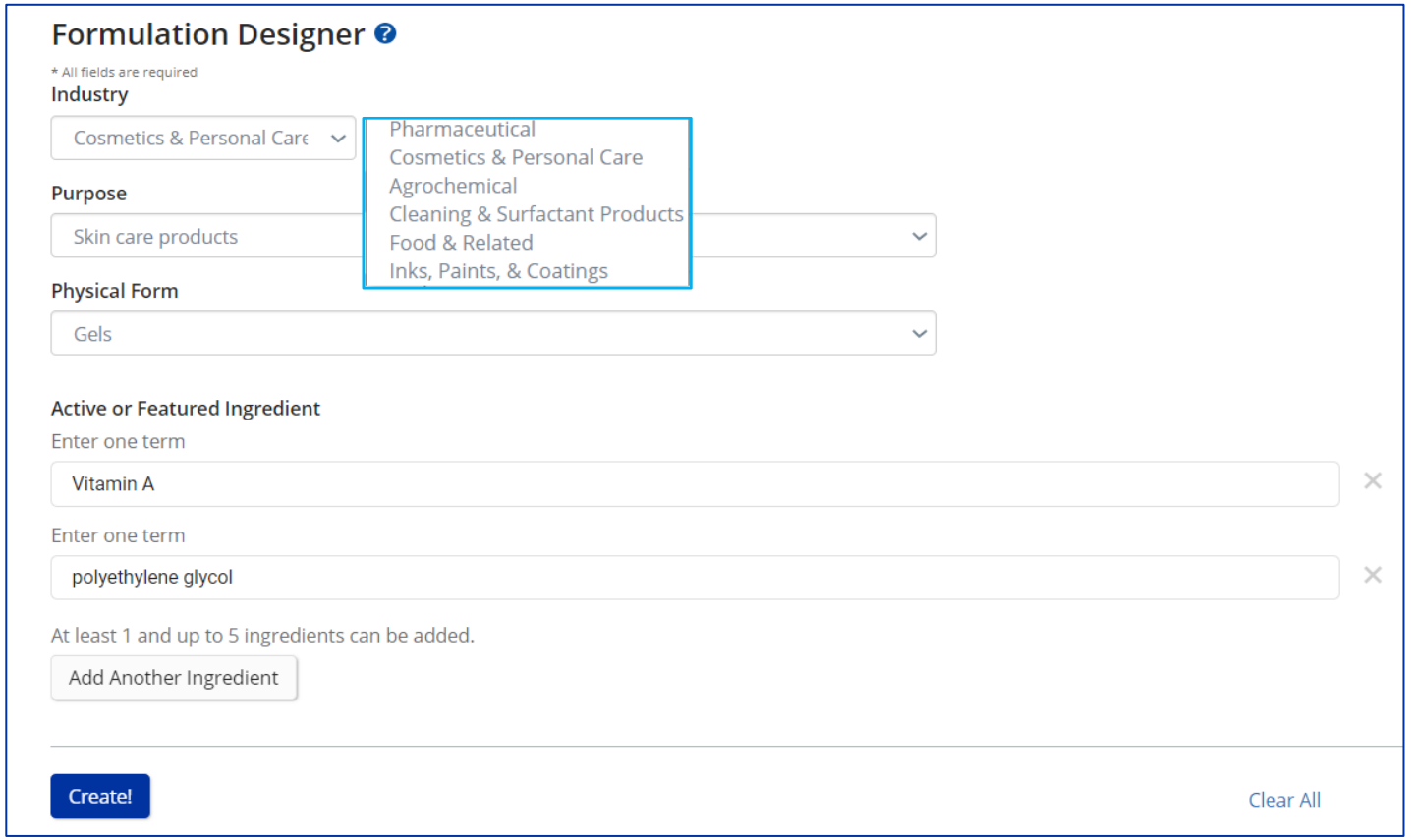
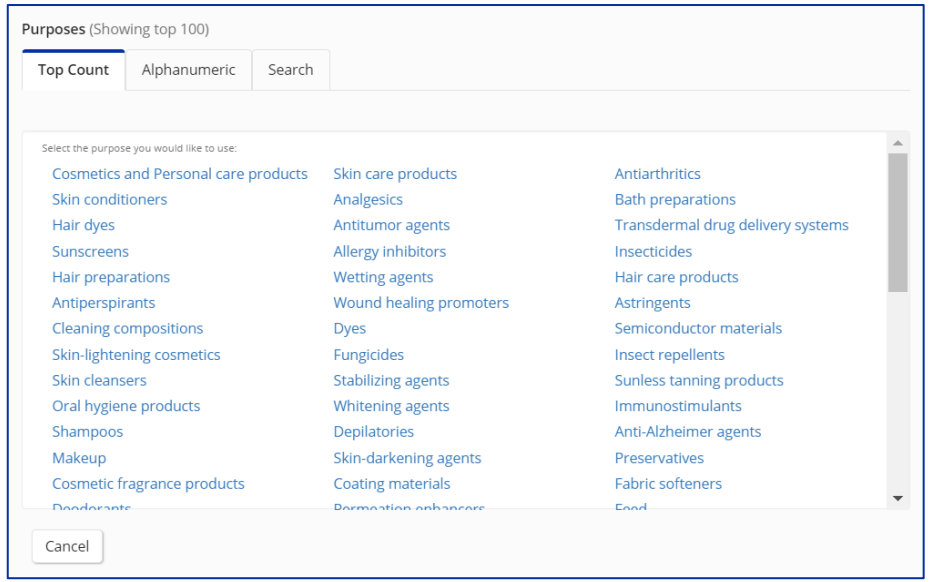
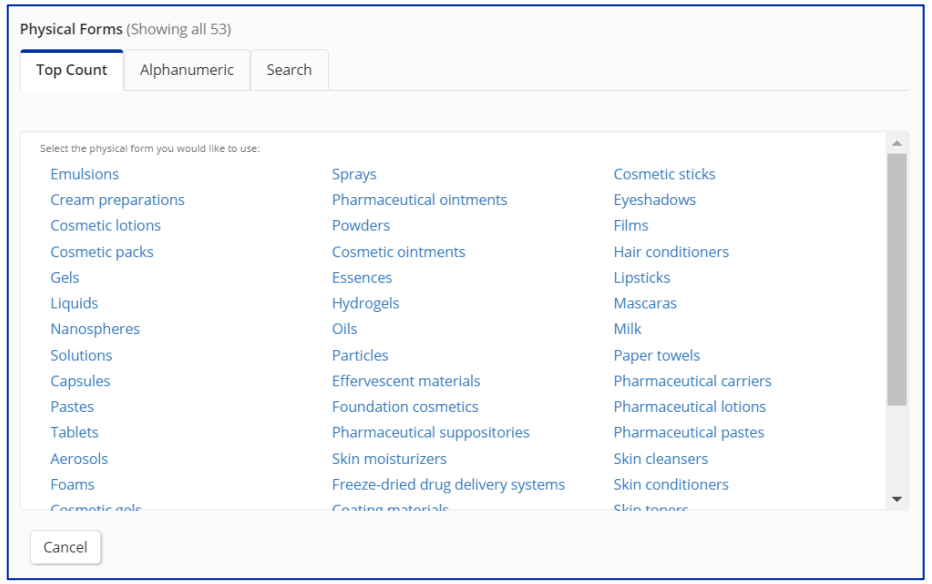
设计配方制剂







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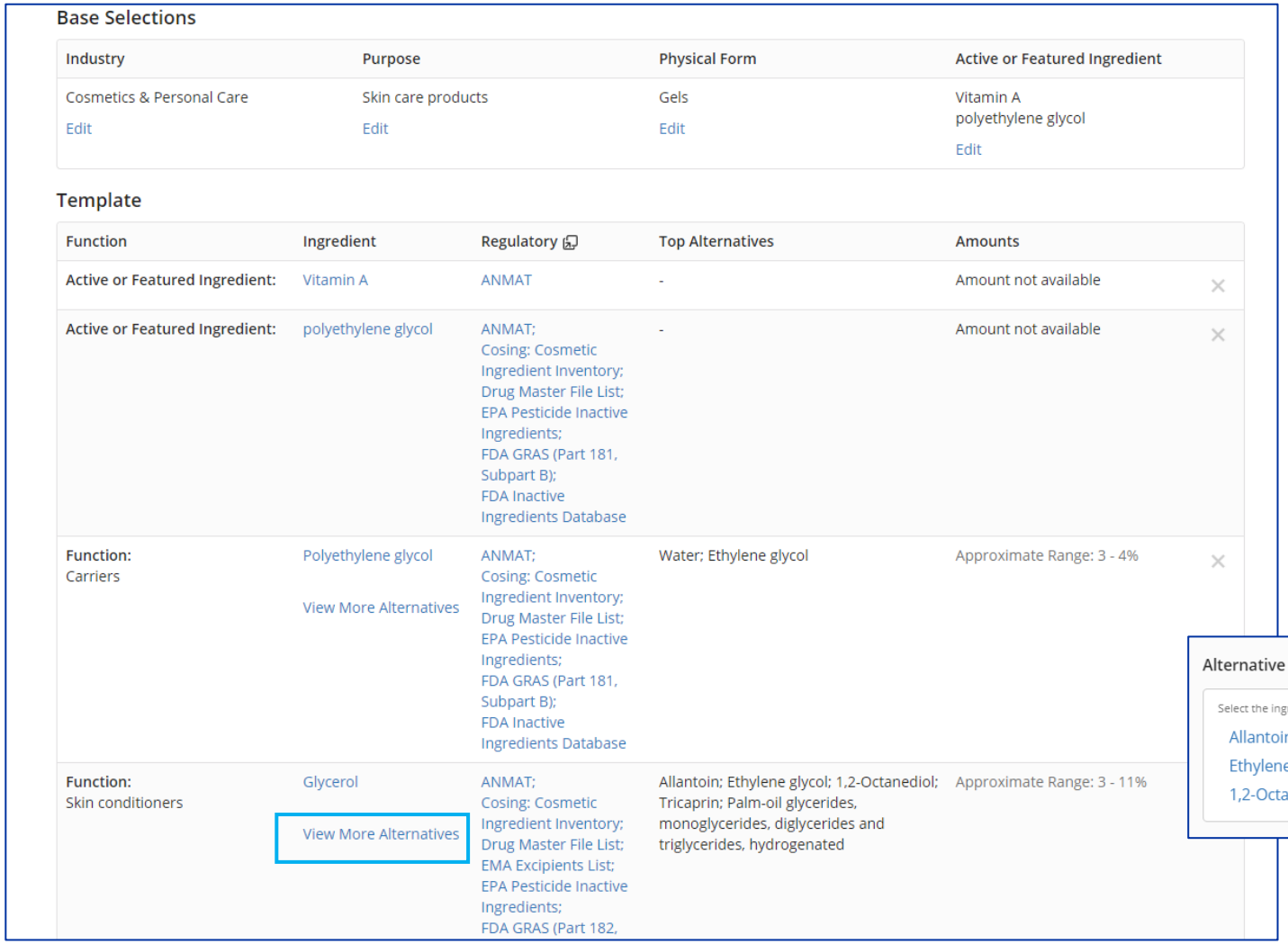
查看制剂或配方设计结果详情

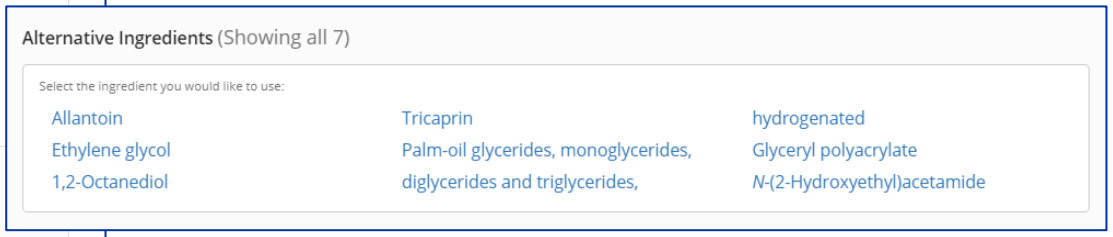


Base Selections

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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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

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
  - 生物序列检索*
  - 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*）
- 常见问题及解答

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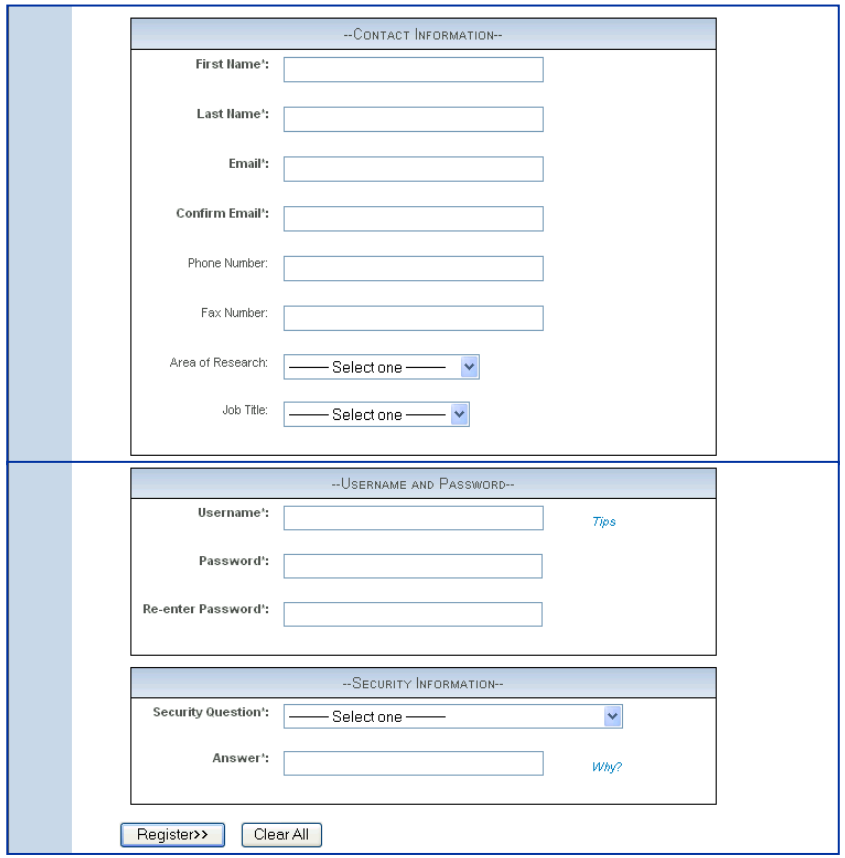
如何获取CAS SciFinder^{n}账号



请注意：
1.必须输入真实姓名和邮箱。
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）。

填写个人信息后注册成功；之后直接点击https://SciFinder-n.cas.org访问。

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检索浏览器推荐

浏览器推荐：

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

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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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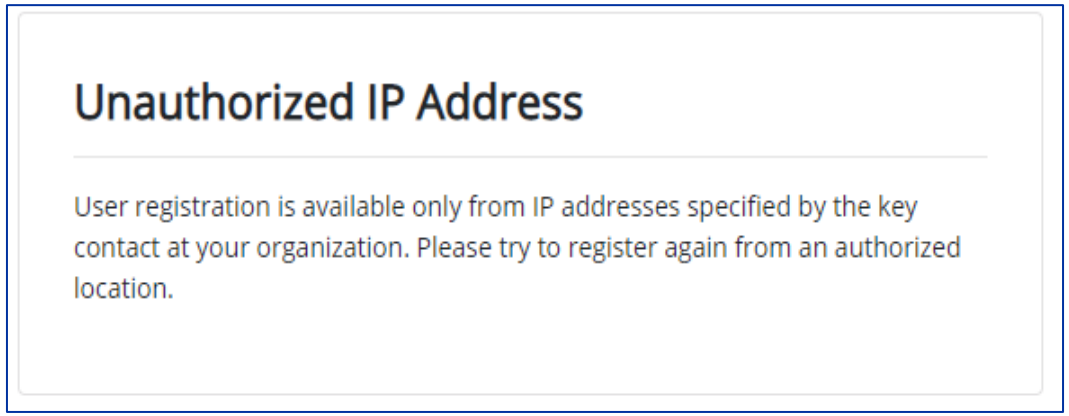
常见问题



- 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

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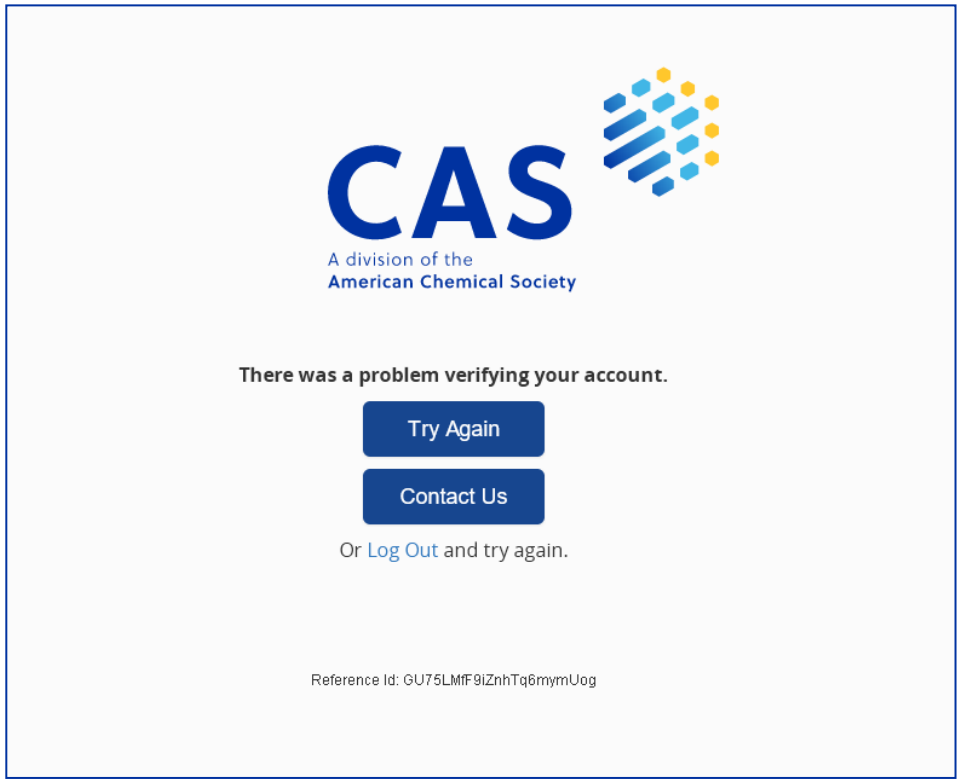
常见问题



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

学习资源

CAS SciFinderⁿ学习中心

预告：2023 CAS SciFinder Discovery Platform 论坛

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

回顾：2022 CAS SciFinderⁿ论坛合集

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2023 CAS 论坛直播时间表

3月1日 收看回放	解锁CAS SciFinder Discovery Platform新功能 主讲人：钱欣
3月8日 收看回放	巧用CAS SciFinder Discovery Platform文献检索快速进阶 主讲人：刘萌萌
3月15日 收看回放	万物互联｜CAS SciFinder Discovery Platform物质检索更高效 主讲人：钱欣
3月22日 18:00-19:00	CAS SciFinder Discovery Platform反应检索，不止A to B 主讲人：刘子露
4月4日 18:00-19:00	不止化学：CAS SciFinder Discovery Platform序列检索技巧 主讲人：刘萌萌
4月12日 18:00-19:00	新手入门开题和文献综述?巧用CAS SciFinder Discovery Platform事半功倍 主讲人：刘子露
4月19日 18:00-19:00	实验进展太慢?巧用CAS SciFinder Discovery Platform寻找启发 主讲人：钱欣
5月10日 18:00-19:00	毕业季｜CAS SciFinder Discovery Platform助力论文写作及答辩准备 主讲人：刘子露
5月24日 18:00-19:00	毕业季｜巧用CAS SciFinder Discovery Platform做足升学与择业准备 主讲人：钱欣

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