CAS SciFinder Discovery Platform™ (Academic)

驱动科研创新与学科发展

刘子露
ZLiu@acs-i.org
美国化学文摘社(CAS)北京代表处

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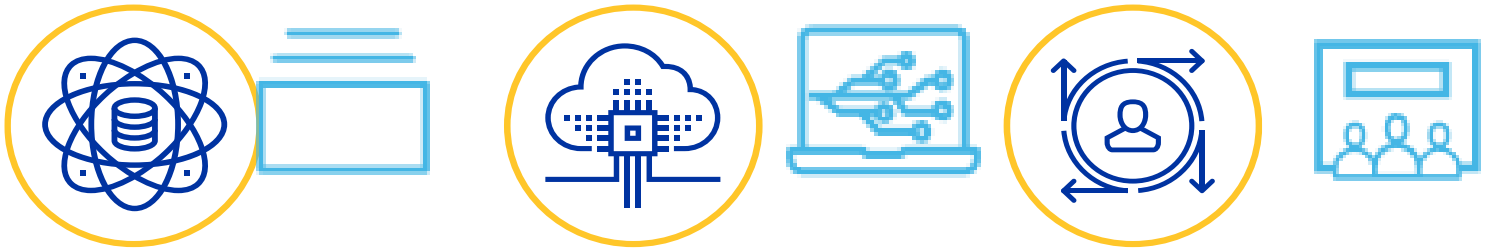
大纲

- CAS（美国化学文摘社）及CAS SciFinder Discovery Platform简介
- 新一代科研创新信息工具CAS SciFinder®
- 分析方法解决方案CAS Analytical Methods™
- 配方/制剂解决方案CAS Formulus®

美国化学文摘社 (CAS) 隶属美国化学会 (ACS)

- 拥有超过110年的经验；创立权威化学索引《化学文摘》 (CA)
- 密切追踪、标引和提炼全球化学相关的文献（包括专利）
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新，助力于解决科研方面的难题与挑战



UNPARALLELED
SCIENTIFIC CONTENT

SPECIALIZED
TECHNOLOGY

UNMATCHED
HUMAN EXPERTISE

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CAS数据覆盖学科

五大类80小类

- **生物化学：**

  农化产品管控信息、生化遗传学、发酵、免疫化学、药理学

- **有机化学各领域：**

  氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇

- **大分子化学各领域：**

  纤维素、木质素、造纸；涂料、墨水

  染料、有机颜料； 合成橡胶； 纺织品、纤维

- **应用化学各领域 ：**

  大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金

- **物理、无机、分析化学各领域：**

  表面化学、催化剂、相平衡、核现象、电化学

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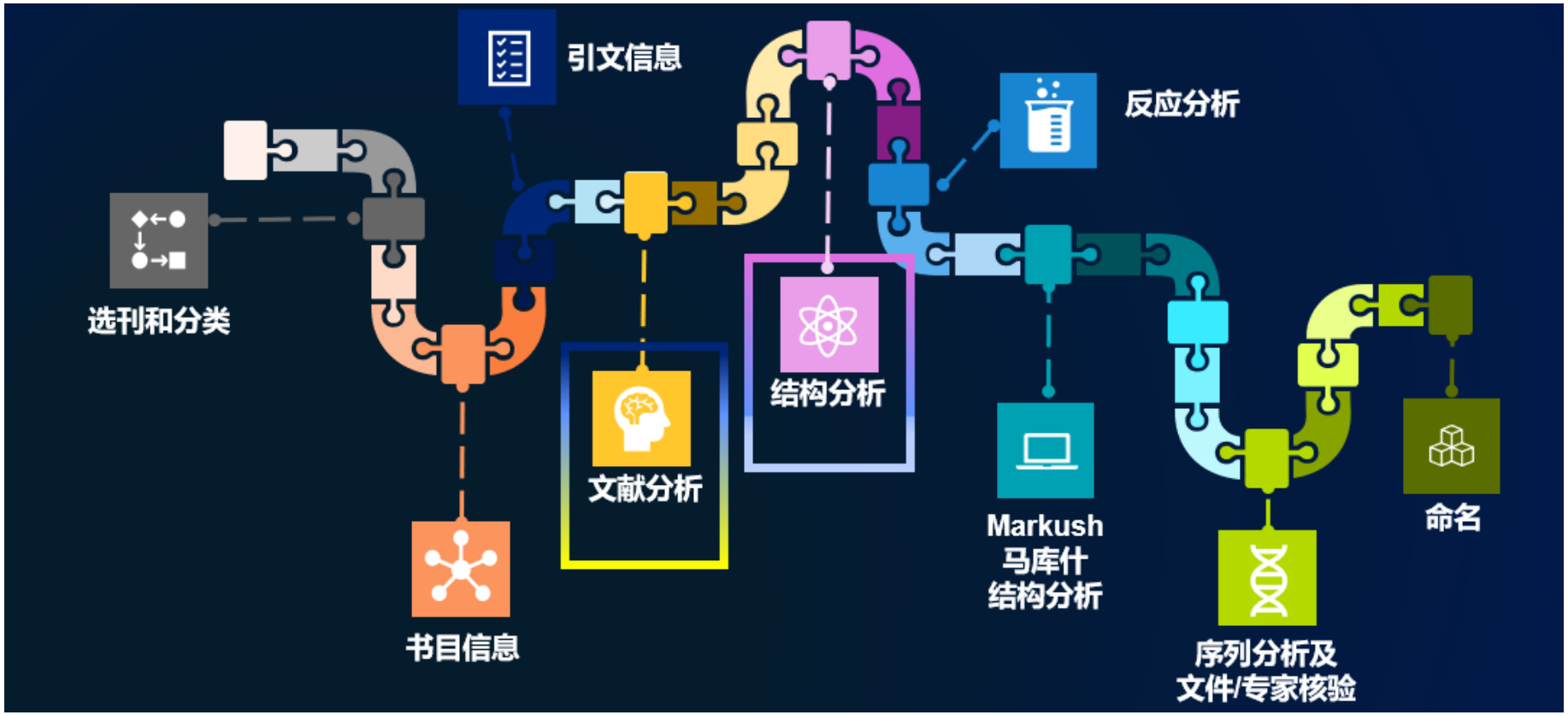
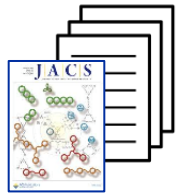
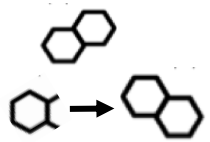
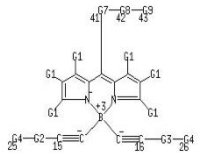
CAS科学家的智力标引





1990
Smith, M.
anthracene





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

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

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经过CAS科学家的揭示，相关信息更易被挖掘

- 人工标引——精准揭示关键技术信息
- 科学家组成的编辑团队深刻理解客户的实际需求
- 审阅、筛选、摘要、标引以覆盖并揭示全球所有已公开的化学及相关信息
- CAS登记号——物质的黄金标准
- CAS Roles (CAS物质角色)——生物研究、性能用途、分析检测、合成制备
- CAS Index Terms (CAS技术词语标准)——揭示技术词语相互间的关联
- CA Sections (CAS学科分类，80个类别)——精准定位具体研究领域

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℠

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CAS SciFinder Discovery Platform 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}——加速科学发现的业界领先的科学工具

- 基于用户习惯、需求、检索策略和革新技术，采用新方法将CAS内容传递给研究人员
- 先进的平台不仅需要实现信息的获取，还要帮助用户发现最佳起点
- CAS的化学信息历史积累、系统知识和人工智力能够加速您的工作

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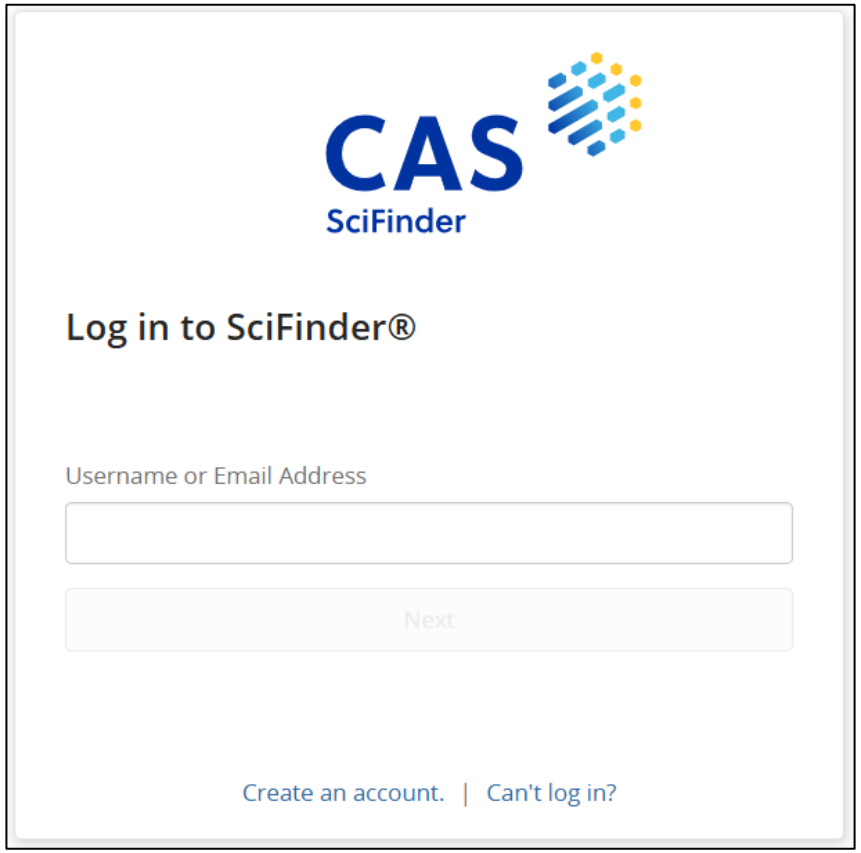
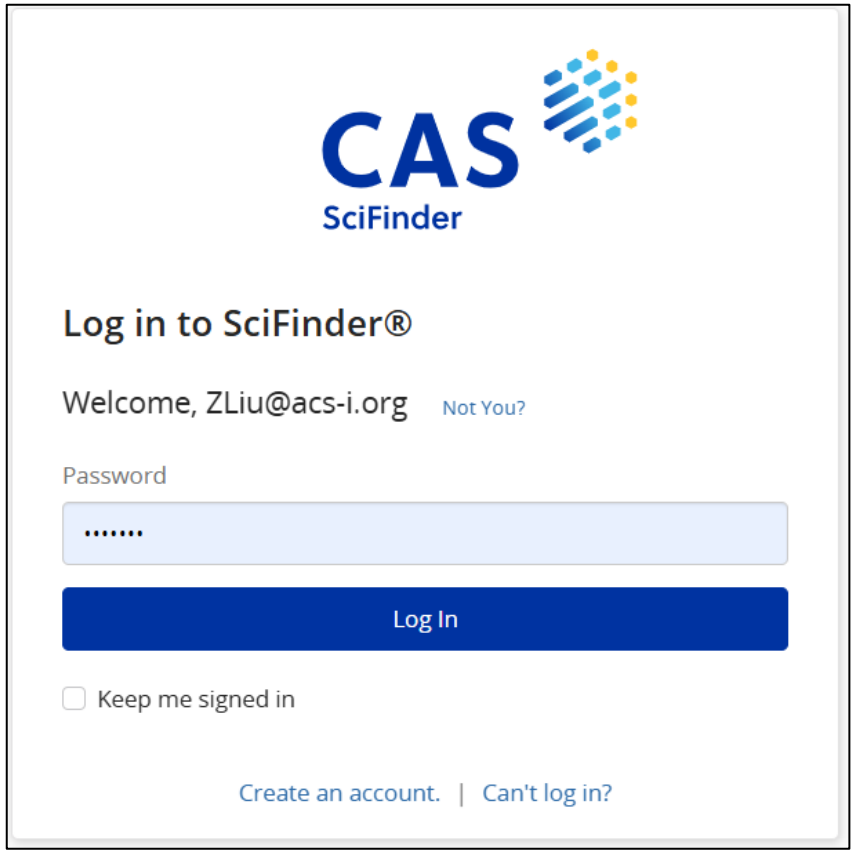
CAS SciFinder^{n}登录网址: https://SciFinder-n.cas.org





账号与CAS SciFinder相同

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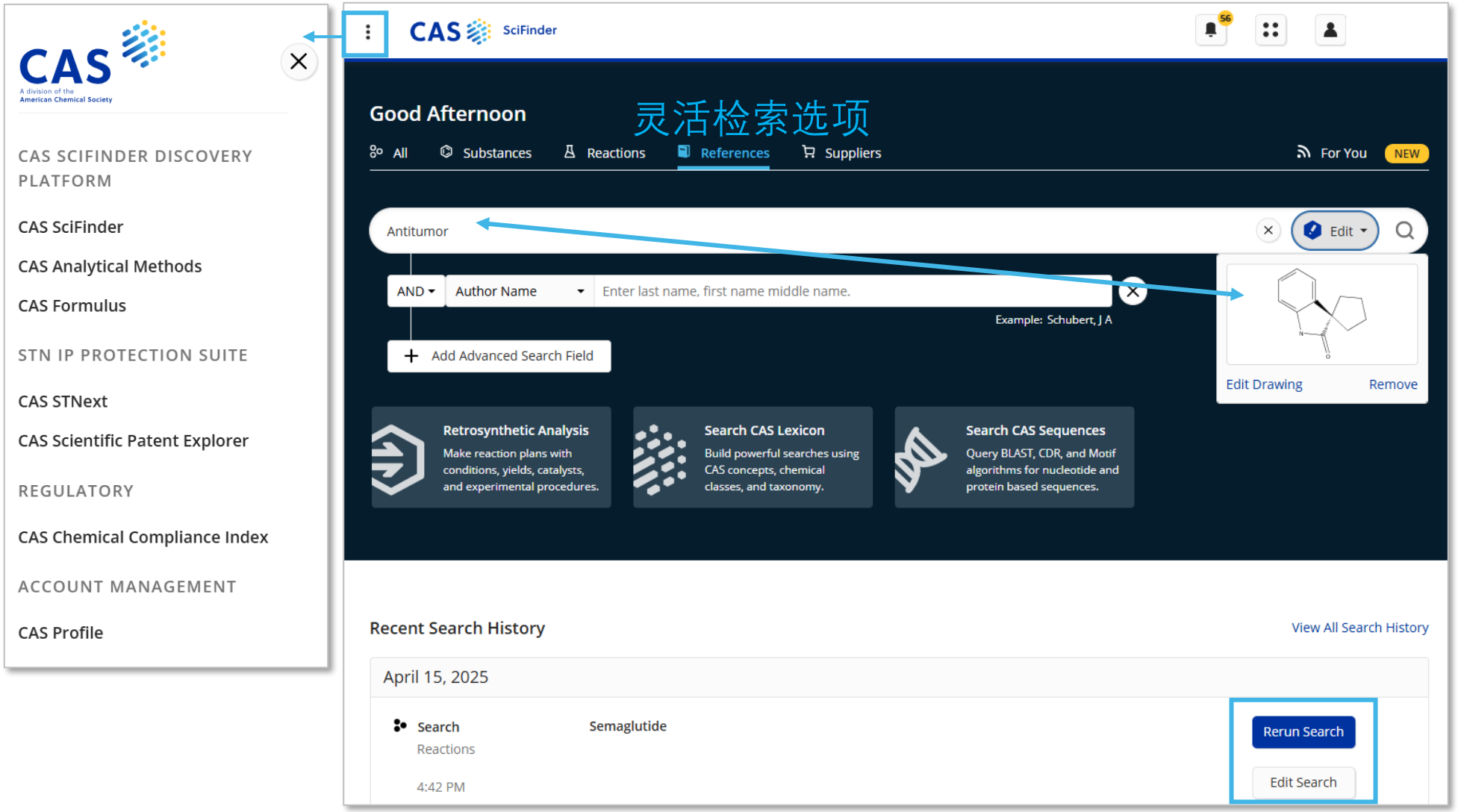
CAS SciFinder^{n}主界面



文本与结构检索便捷联用

快速运行之前的检索项目

文献检索：主题词

- 支持布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not;
- ( ) 优先运算;
- “ ”不允许词形变化，但可出现单数或复数;
- 支持通配符*或？（*代表0或多个字符；？代表0或1个字符）

- 基于科学家创建的叙词表
- 自动提示检索词

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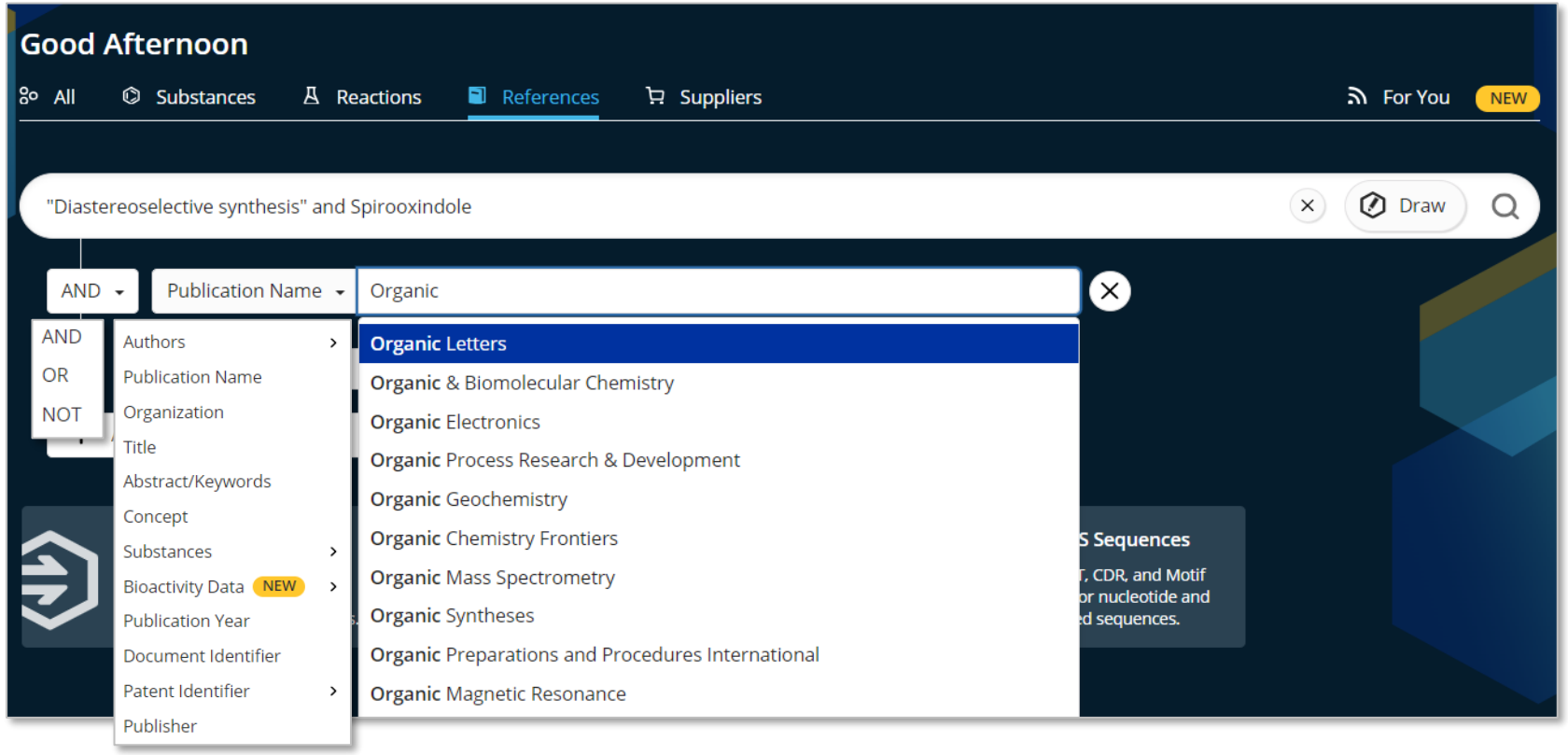
高级检索：高效实现多项自定义组合检索

可单独使用，或联用以下检索方法：

- 关键词、物质名称、CAS Registry Number®、文献号；
- 高级检索：刊物名、Concepts、物质等
- 结构检索



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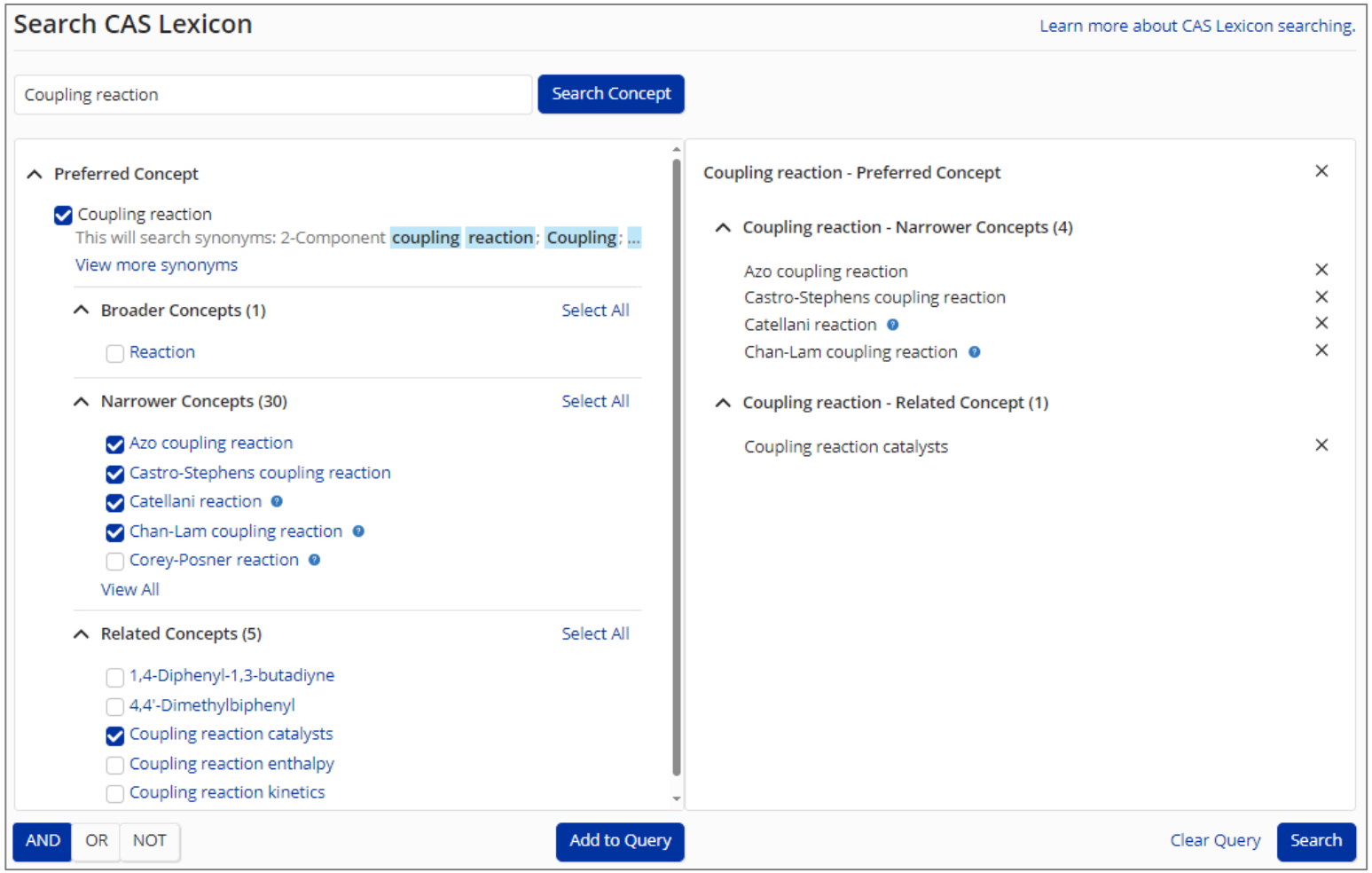
CAS Lexicon：利用词库选词启发检索



快速浏览CAS科学家标引的：

- 概念词（Concepts）
- 物质

在CAS Lexicon词库层级中选择适合的主题词：

- Preferred Concept
- Broader Concepts
- Narrower Concepts
- Related Concepts

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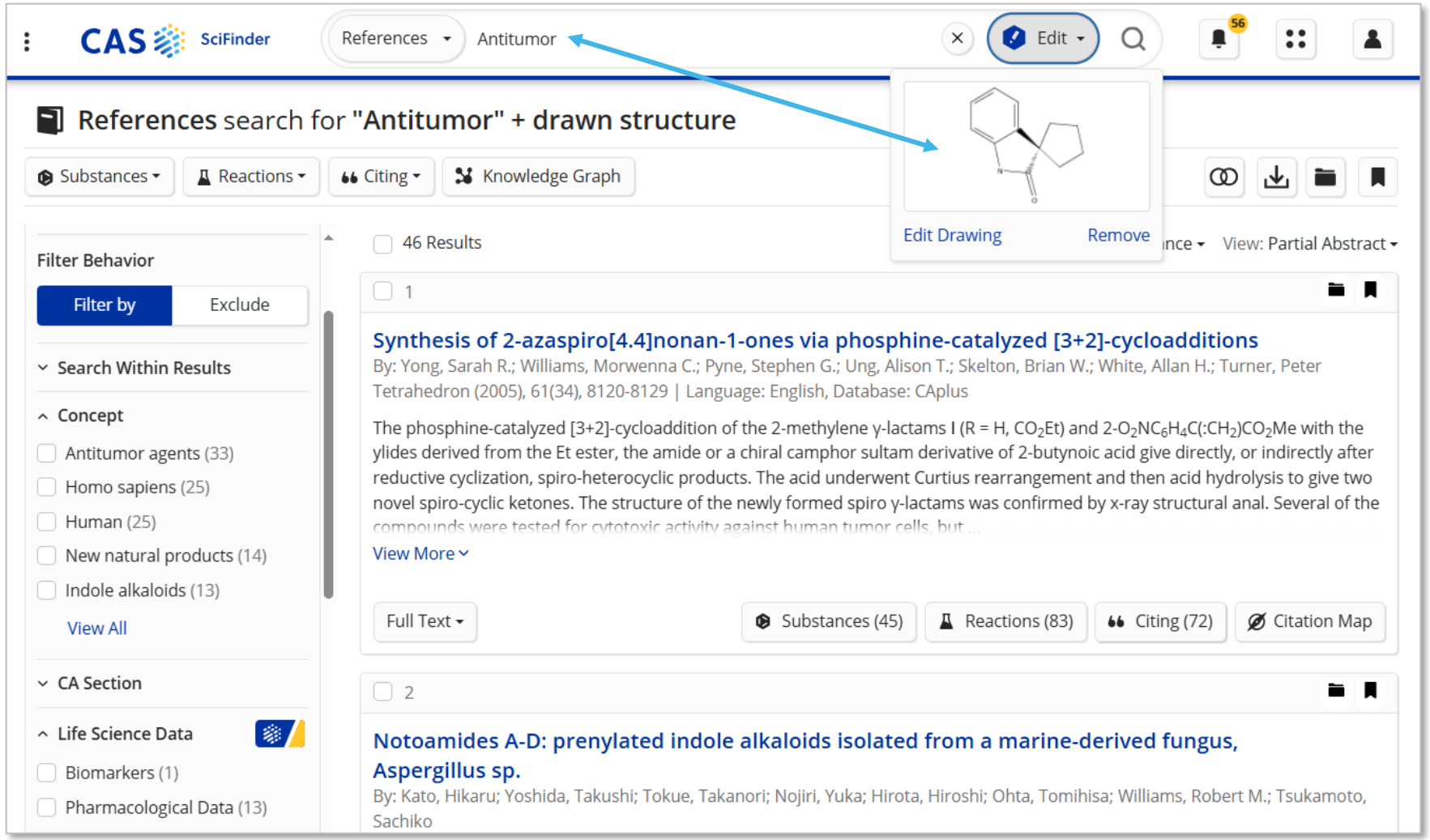
文献检索： 主题词+结构联合检索



主题词+结构联合检索，大大提高检索的效率

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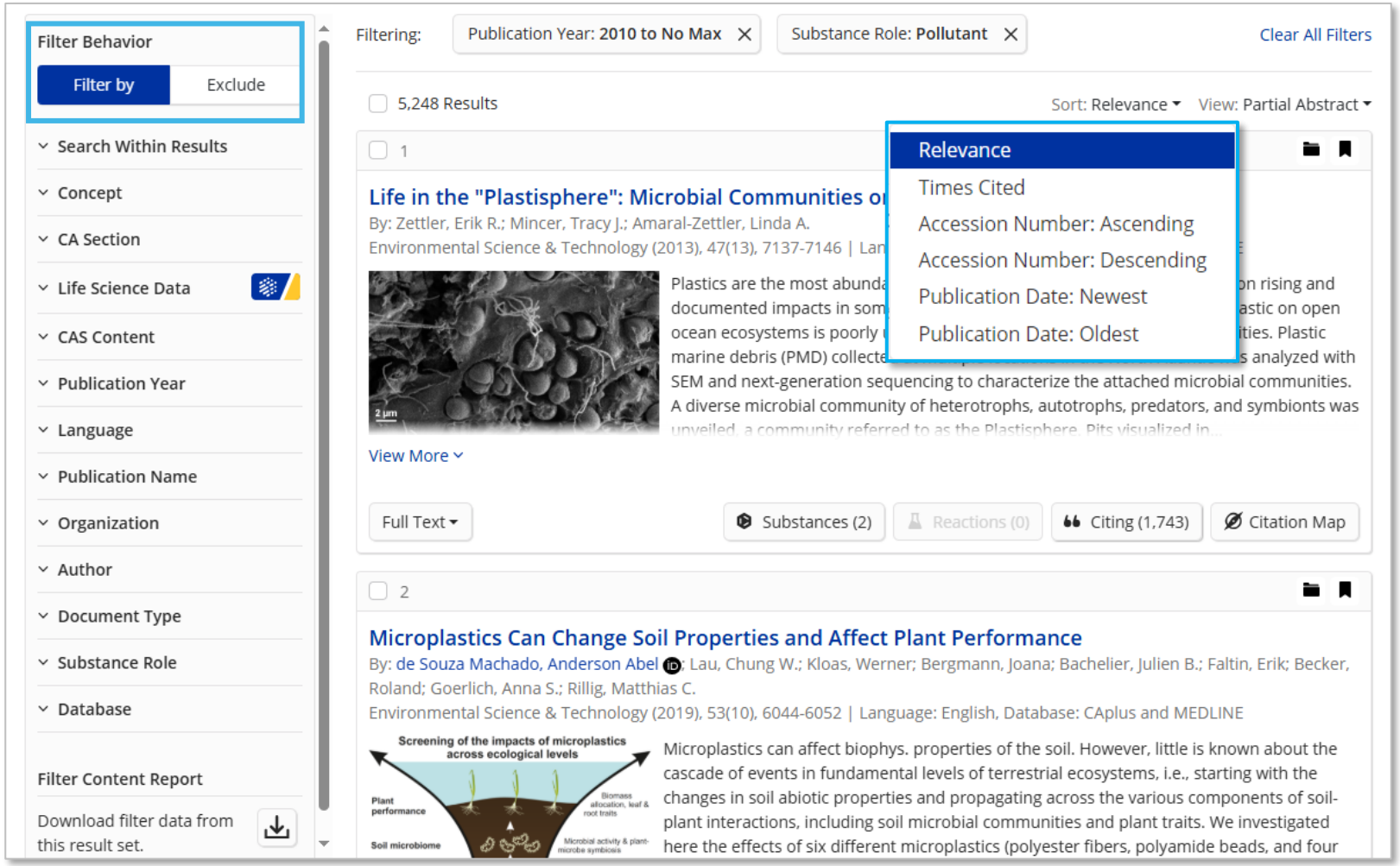
直观的结果页面，丰富的聚类分析



- 聚类筛选项一目了然
- 高效定位所需信息
- 无需逐步二次检索和限定

文献类型
文献语言
出版年份
作者
机构名
刊物名
Concept
CA Section
二次检索
……

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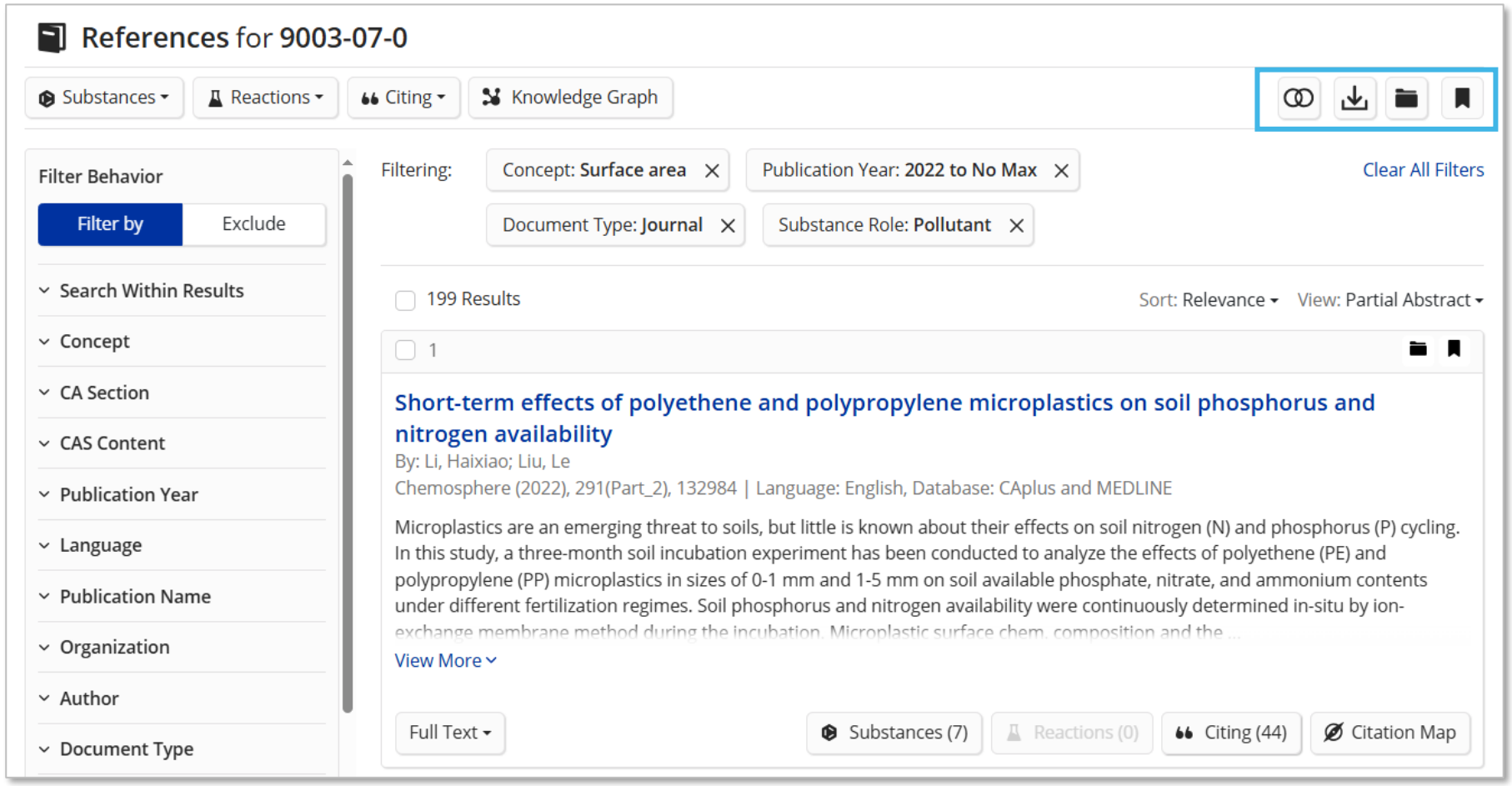
文献结果集的处理、下载、保存及定题追踪



支持结果集的:

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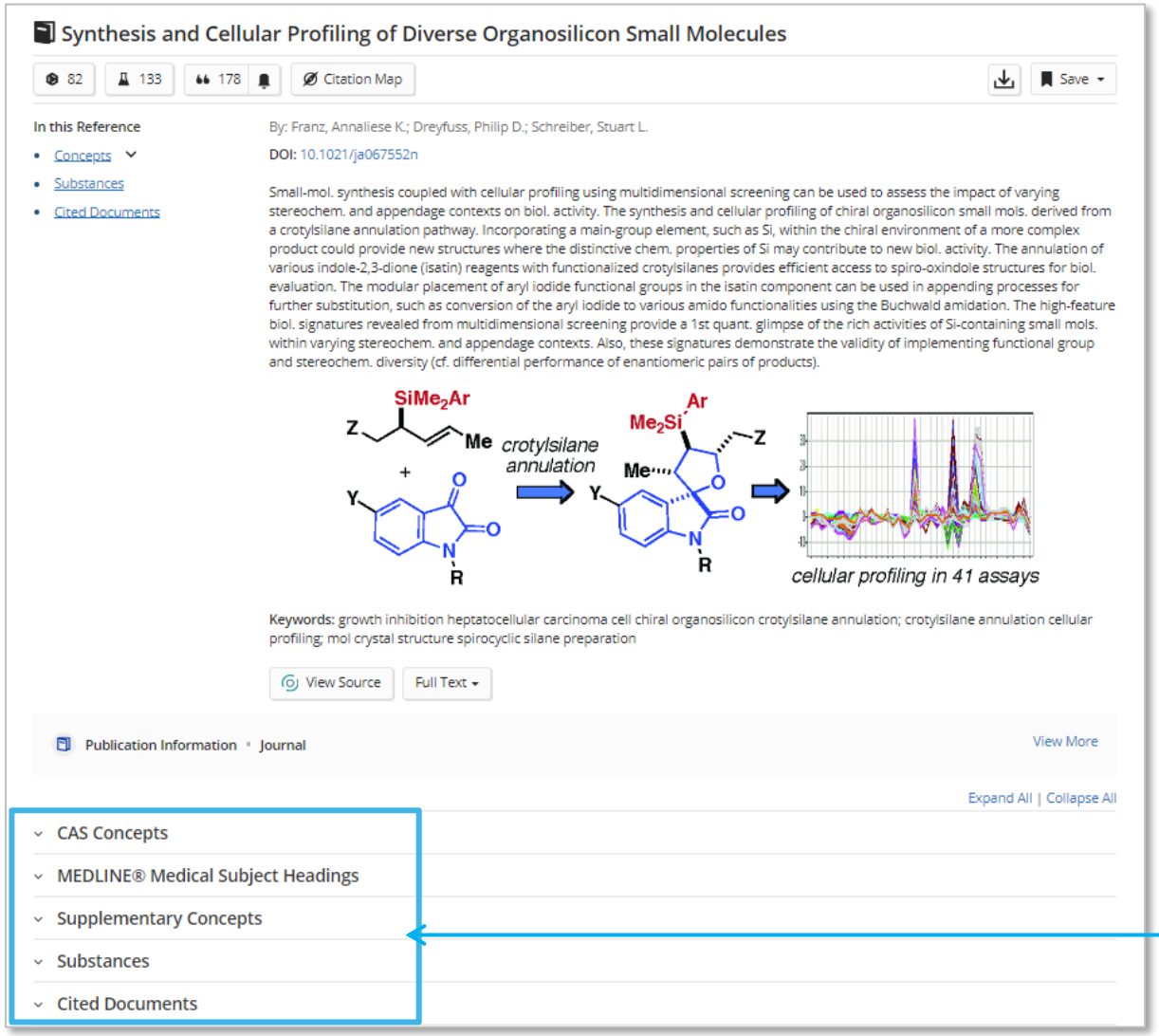
文献详情



文献详情界面包括:

- 标题
- 摘要
- 原文关键词
- 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

CAS科学家增值标引的信息

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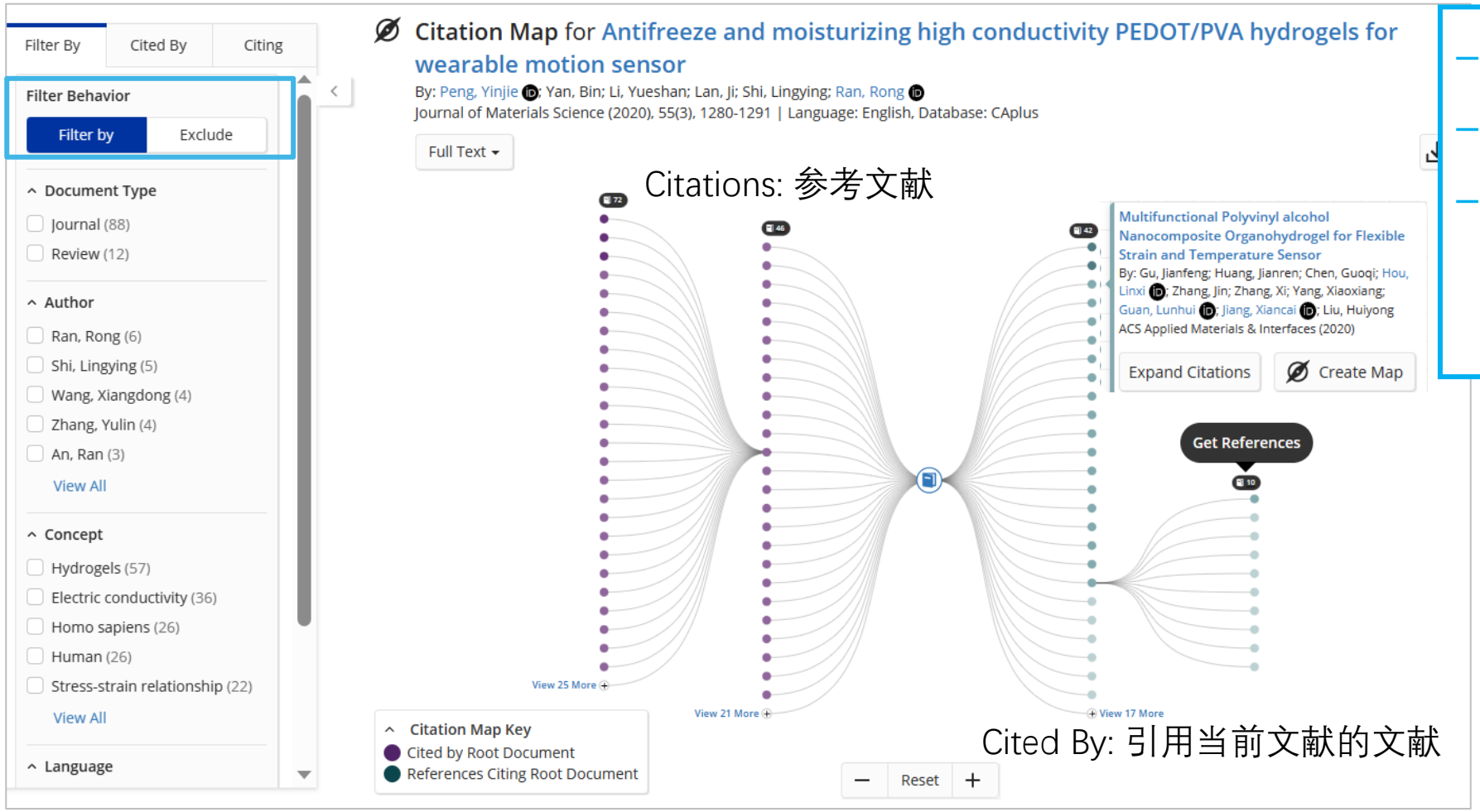
引文地图：便捷地获取关联文献



- 通过聚类选项筛选引文
- 可下载引文地图
- 显示引文和被引文献的数量，点击可链接至对应的文献结果页面

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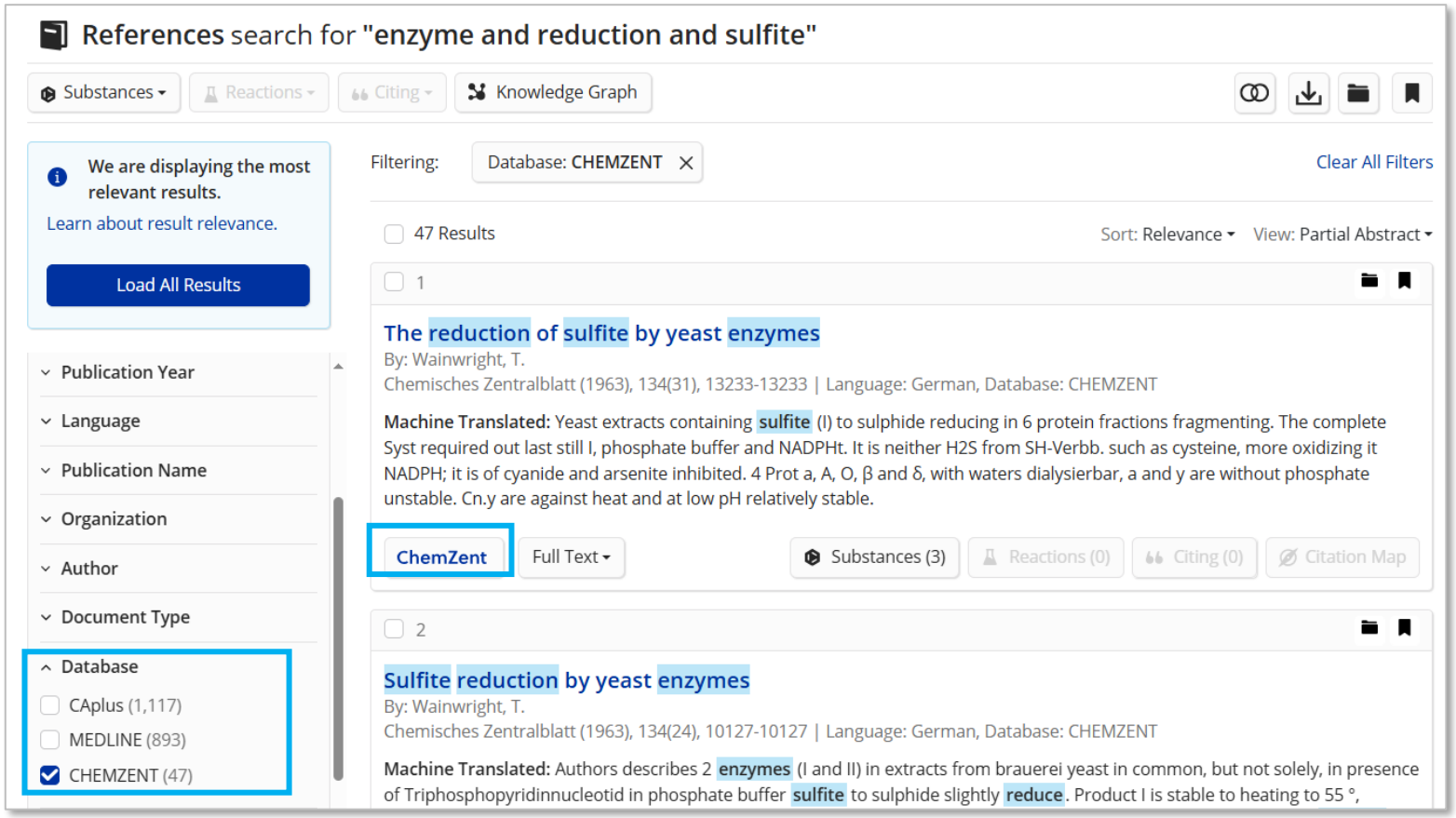
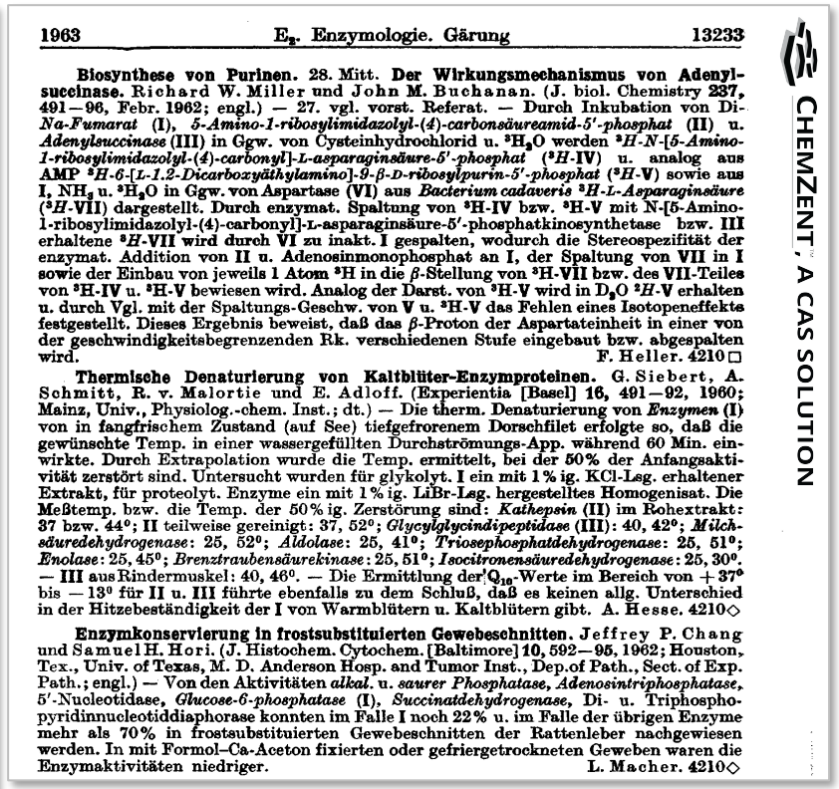
ChemZent®：追溯学科早期的研究

- 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




1963 E$_a$. Enzymologie. Gärung 13233

Biosynthese von Purinen. 28. Mitt. **Der Wirkungsmechanismus von Adenylsuccinase.** Richard W. Miller und John M. Buchanan. (J. biol. Chemistry **237**, 491—96, Febr. 1962; engl.) — 27. vgl. vorst. Referat. — Durch Inkubation von Di-*Na-Fumarat* (I), *5-Amino-1-ribosylimidazolyl-(4)-carbonsäureamid-5'-phosphat* (II) u. *Adenylsuccinase* (III) in Ggw. von Cysteinhydrochlorid u. ^3H_2O werden *^3H-N-[5-Amino-1-ribosylimidazolyl-(4)-carbonyl]-L-asparaginsäure-5'-phosphat* (^3H-IV) u. analog aus AMP *^3H-6-[L-1.2-Dicarboxyäthylamino]-9-β-D-ribosylpurin-5'-phosphat* (^3H-V) sowie aus I, NH_3 u. ^3H_2O in Ggw. von Aspartase (VI) aus *Bacterium cadaveris* *^3H-L-Asparaginsäure* (^3H-VII) dargestellt. Durch enzymat. Spaltung von ^{3}H-IV bzw. ^{3}H-V mit N-[5-Amino-1-ribosylimidazolyl-(4)-carbonyl]-L-asparaginsäure-5'-phosphathinosynthetase bzw. III erhaltene *^3H-VII* wird durch VI zu inakt. I gespalten, wodurch die Stereospezifität der enzymat. Addition von II u. Adenosinmonophosphat an I, der Spaltung von VII in I sowie der Einbau von jeweils 1 Atom ^{3}H in die β-Stellung von ^{3}H-VII bzw. des VII-Teiles von ^{3}H-IV u. ^{3}H-V bewiesen wird. Analog der Darst. von ^{3}H-V wird in D_2O *^2H-V* erhalten u. durch Vgl. mit der Spaltungs-Geschw. von V u. ^{3}H-V das Fehlen eines Isotopeneffekts festgestellt. Dieses Ergebnis beweist, daß das β-Proton der Aspartateinheit in einer von der geschwindigkeitsbegrenzenden Rk. verschiedenen Stufe eingebaut bzw. abgespalten wird. F. Heller. 4210□

Thermische Denaturierung von Kaltblüter-Enzymproteinen. G. Siebert, A. Schmitt, R. v. Malortie und E. Adloff. (Experientia [Basel] **16**, 491—92, 1960; Mainz, Univ., Physiolog.-chem. Inst.; dt.) — Die therm. Denaturierung von *Enzymen* (I) von in fangfrischem Zustand (auf See) tiefgefrorenem Dorschfilet erfolgte so, daß die gewünschte Temp. in einer wassergefüllten Durchströmungs-App. während 60 Min. einwirkte. Durch Extrapolation wurde die Temp. ermittelt, bei der 50% der Anfangsaktivität zerstört sind. Untersucht wurden für glykolyt. I ein mit 1% ig. KCl-Lsg. erhaltener Extrakt, für proteolyt. Enzyme ein mit 1% ig. LiBr-Lsg. hergestelltes Homogenisat. Die Meßtemp. bzw. die Temp. der 50% ig. Zerstörung sind: *Kathepsin* (II) im Rohextrakt: 37 bzw. 44°; II teilweise gereinigt: 37, 52°; *Glycylglycindipeptidase* (III): 40, 42°; *Milchsäuredehydrogenase*: 25, 52°; *Aldolase*: 25, 41°; *Triosephosphatdehydrogenase*: 25, 51°; *Enolase*: 25, 45°; *Brenztraubensäurekinase*: 25, 51°; *Isocitronensäuredehydrogenase*: 25, 30°. — III aus Rindermuskel: 40, 46°. — Die Ermittlung der $^1Q_{10}$-Werte im Bereich von +37° bis −13° für II u. III führte ebenfalls zu dem Schluß, daß es keinen allg. Unterschied in der Hitzebeständigkeit der I von Warmblütern u. Kaltblütern gibt. A. Hesse. 4210◇

Enzymkonservierung in frostsubstituierten Gewebeschnitten. Jeffrey P. Chang und Samuel H. Hori. (J. Histochem. Cytochem. [Baltimore] **10**, 592—95, 1962; Houston, Tex., Univ. of Texas, M. D. Anderson Hosp. and Tumor Inst., Dep. of Path., Sect. of Exp. Path.; engl.) — Von den Aktivitäten *alkal.* u. *saurer Phosphatase*, *Adenosintriphosphatase*, 5'-Nucleotidase, *Glucose-6-phosphatase* (I), *Succinatdehydrogenase*, Di- u. Triphosphopyridinnucleotiddiaphorase konnten im Falle I noch 22% u. im Falle der übrigen Enzyme mehr als 70% in frostsubstituierten Gewebeschnitten der Rattenleber nachgewiesen werden. In mit Formol-Ca-Aceton fixierten oder gefriergetrockneten Geweben waren die Enzymaktivitäten niedriger. L. Macher. 4210◇

CHEMZENT, A CAS SOLUTION

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CAS PatentPak®：专利流程解决方案

- 唯一提供在专利中快速定位物质相关化学信息的工具
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  - 无需在多个不同专利局网站上耗费时间
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- 在CAS专利族文献中找到您所熟悉语言的专利

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专利文献详情

Methods using toll-like receptor (TLR) agonists in combination with antibiotics for the treatment of bacterial infections

208 | 0 | 3 | Citation Map | Save

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In this Reference
- IPC Data
- CAS Concepts
- Substances
- Formulations
- Cited Documents

By: Hardt, Wolf-Dietrich; Kaiser, Patrick; Sirard, Jean-Claude; Carnoy, Christophe; Fougeron, Delphine; Chabalgoity, Jose Alejandro; Munoz, Natalia

The invention relates to methods and pharmaceutical compositions for the treatment of bacterial infections. In particular, the invention relates to a toll-like receptor (TLR) agonist (e.g. flagellin polypeptide, biomols., peptides, antibodies, nucleic acids) for use in a method for the treatment of a bacterial infection in a subject in need thereof wherein the TLR agonist is administered to the subject in combination with at least one antibiotic. In another aspect of the invention the antibiotic is selected from the group consisting of aminoglycosides, beta-lactams, quinolones or fluoroquinolones, macrolides, sulfonamides, sulfamethoxazoles, tetracyclines, streptogramins, oxazolidinones, rifamycins, glycopeptides, polymyxins, and lipopeptides

Keywords: antibacterial toll like r… c TLR agonist antibacterial combination therapy bacterial infection

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专利族信息

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2015011254	English	A1	PDF | PDF+ | Viewer	2015-01-29	WO2014-EP66007	2014-07-25
EP3024476	English	A1		2016-06-01	EP2014-749736	2014-07-25
EP3632458	English	A1	PDF	2020-04-08	EP2019-207885	2014-07-25
US20160151453	English	A1	PDF	2016-06-02	US2016-14906747	2016-01-21
US9919029	English	B2		2018-03-20	US2016-14906747	2016-01-21

Priority Application

Priority Application Number	Application Date
EP2013-306086	2013-07-26
EP2014-749736	2014-07-25

Publication Information • Patent

Patent Number	Publication Date	Application Number	Application Date	Kind Code
WO2015011254	2015-01-29	WO2014-EP66007	2014-07-25	A1

Assignee
INSERM (Institut National de la Sante et de la Recherche Medicale), France
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Institut Pasteur de Lille, France
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ETH Zurich, France
Universidad de la Republica, France

Source
World Intellectual Property Organization
CODEN: PIXXD2

Database Information
AN: 2015:167126
CAN: 162:266207
CAplus

Language
English

优先权信息

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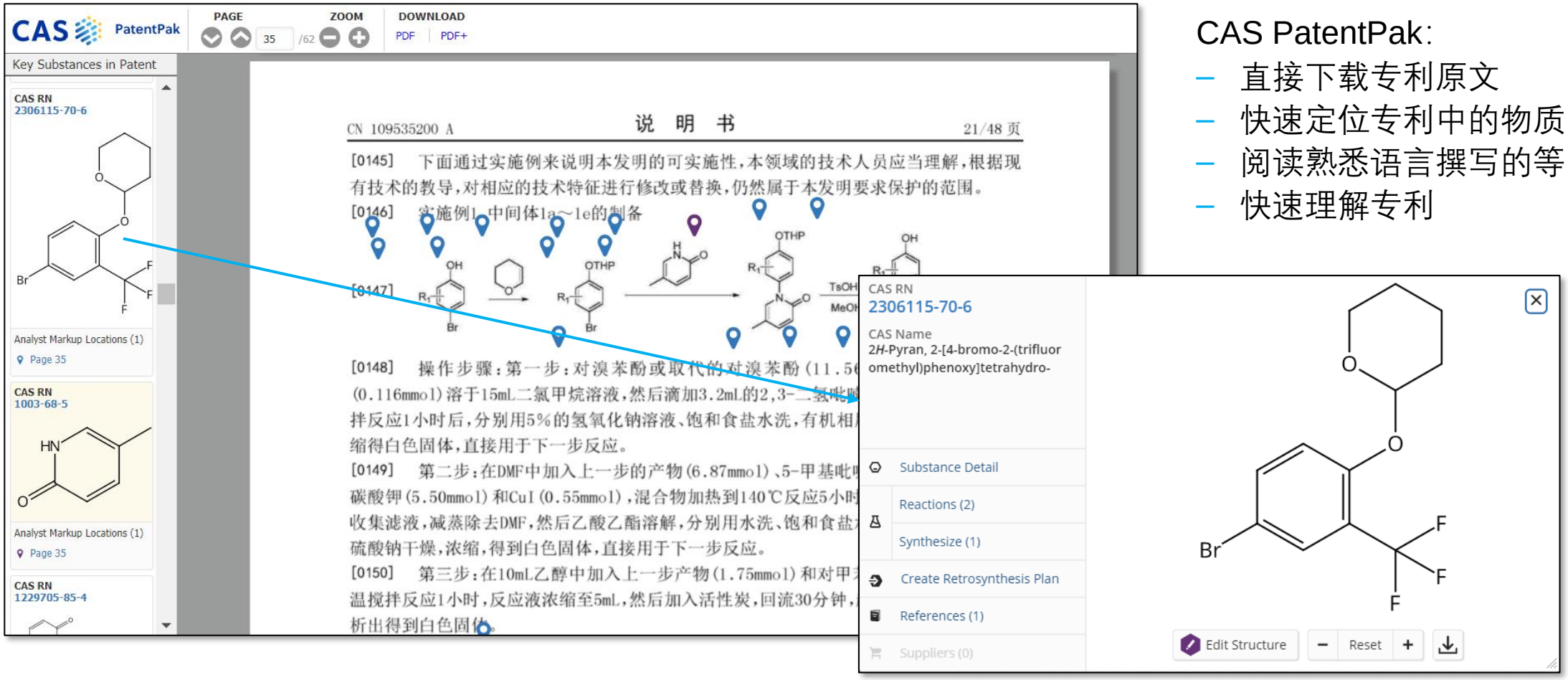
CAS PatentPak：专利流程解决方案

在CAS PatentPak浏览器中单击结构，打开物质菜单检索具体信息



CAS PatentPak:

- 直接下载专利原文
- 快速定位专利中的物质
- 阅读熟悉语言撰写的等同专利
- 快速理解专利

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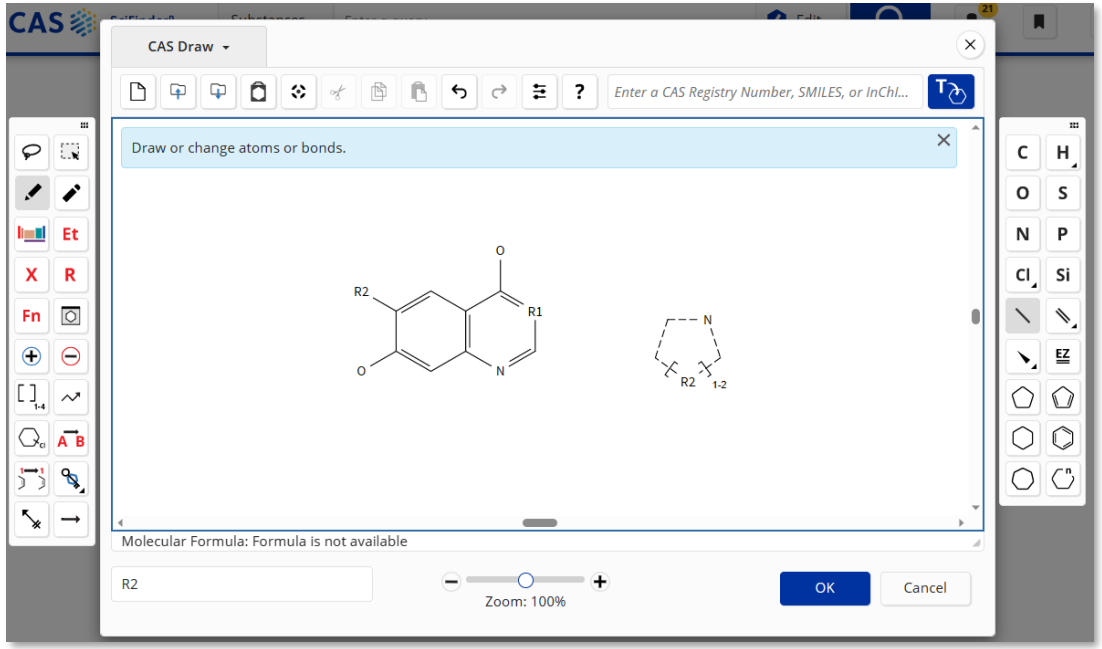
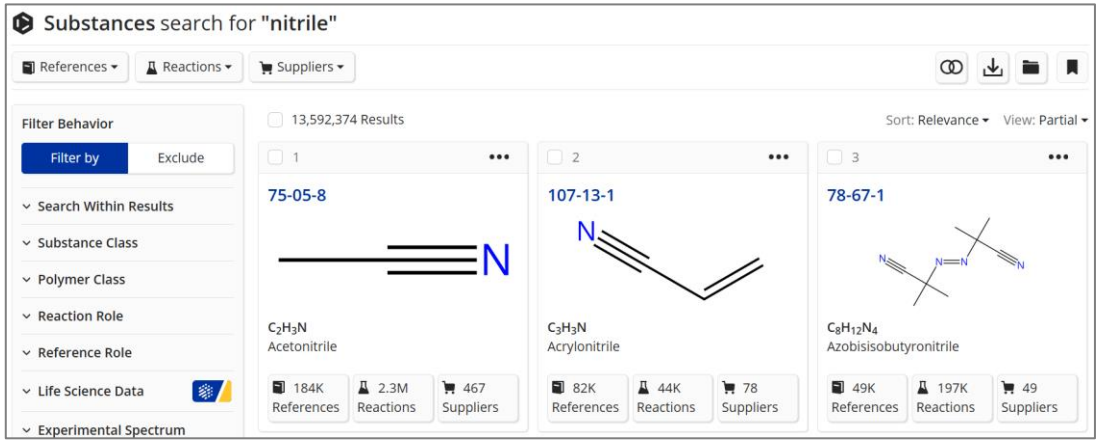
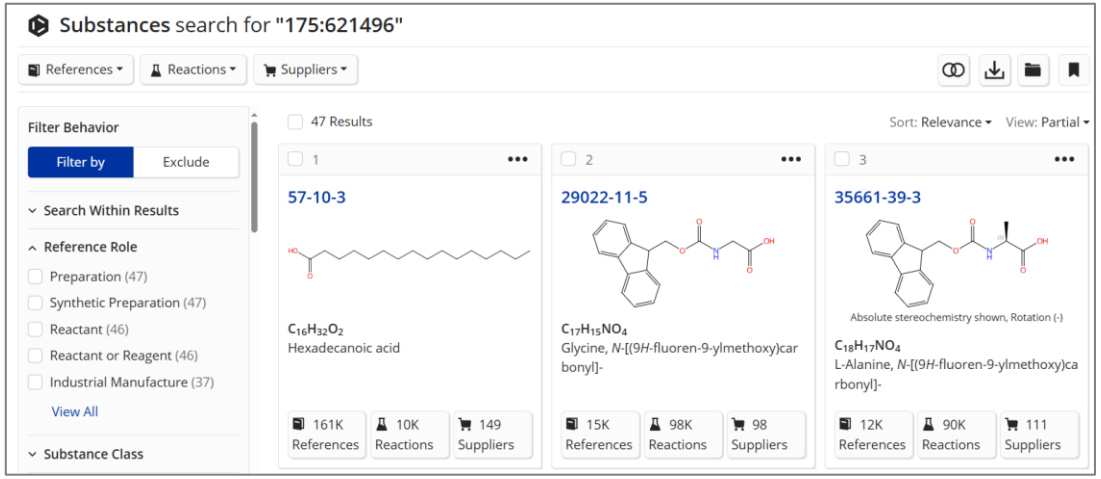
CAS Substances：物质检索

物质检索方法

- 物质或文献标识符
- 结构式
- 高级检索：分子式、属性值、谱图数值检索
- 官能团和物质类别







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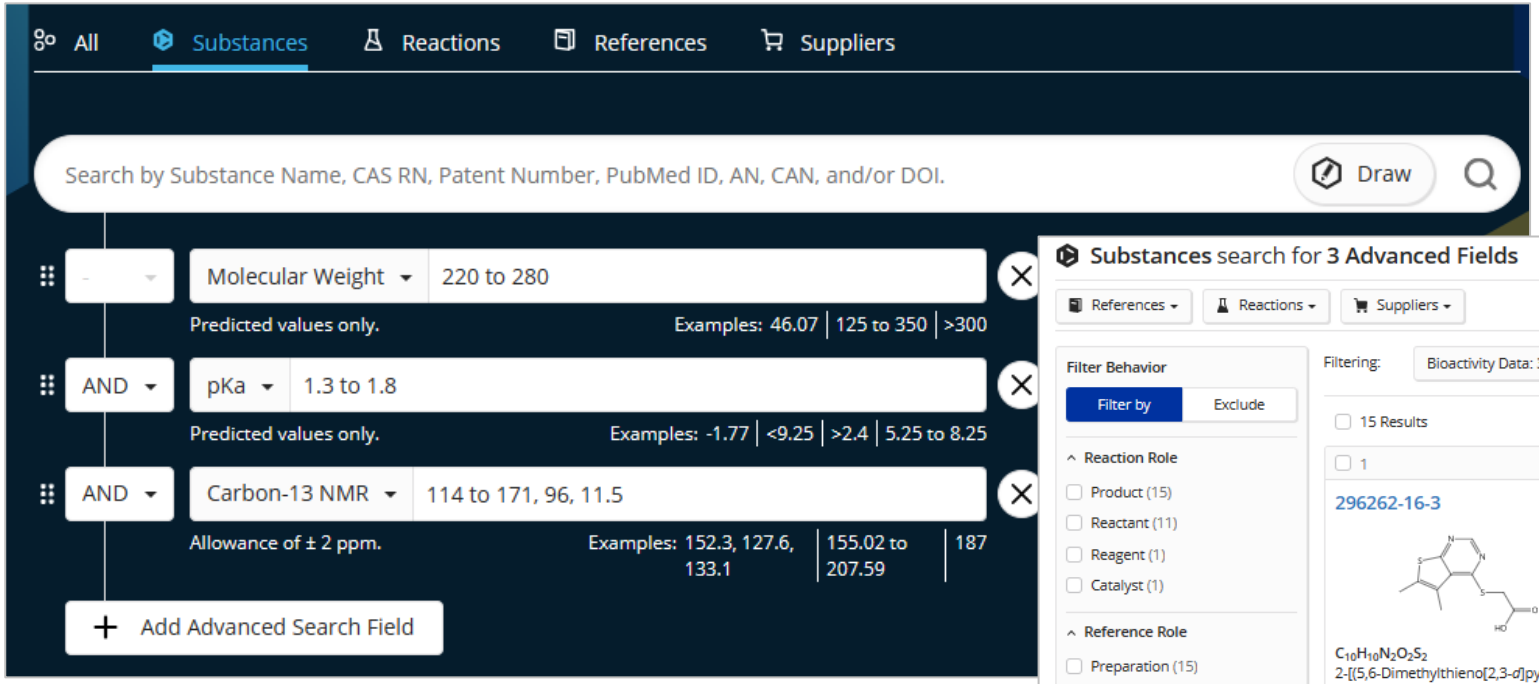
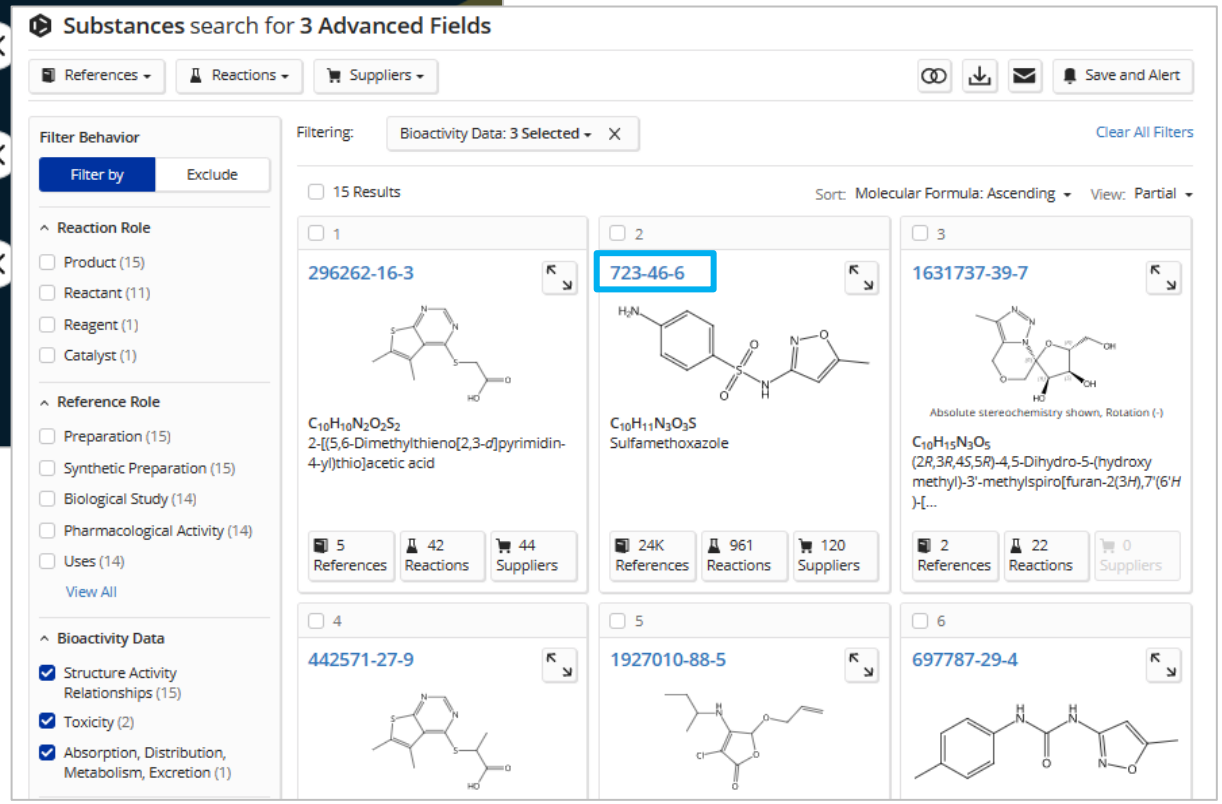
属性值、谱图数值联用检索物质





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

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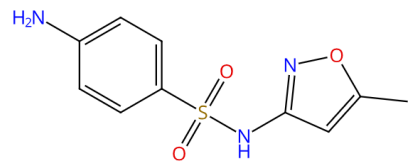
物质详情

CAS Registry Number: 723-46-6

30K | 1,050 | 110 | View in CAS BioFinder



$C_{10}H_{11}N_3O_3S$

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

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point (Predicted)	482.145±55.00 °C	Press: 760.00 Torr
Density (Experimental)	1.08 g/cm³	-
pKa (Predicted)	5.811±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

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
- Regulatory Information
- GHS Hazard Statements
- Additional Details

Structure Activity Relationships — CAS LIFE SCIENCES

Clear All Filters | Knowledge Graph

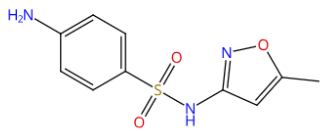
Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Cytochrome P450 2C9	Inhibitor	Activity	-17.1 %	-	HOMO SAPIENS	View Detail	(1) CAS
Cytochrome P450 3A4	Inhibitor	Activity	40 %	-	HOMO SAPIENS	View Detail	(2) CAS
Cytochrome P450 2A6	Inhibitor	Activity	45 %	-	HOMO SAPIENS	View Detail	(2) CAS
Cytochrome P450 2C9	Inhibitor	Activity	95 %	-	HOMO SAPIENS	View Detail	(3) CAS
Cytochrome P450 2C9	Inhibitor	Activity	69 %	-	HOMO SAPIENS	View Detail	(3) CAS
Cytochrome P450 3A4	Inactivator	Enzymatic activity (CYP)	Percentage of P450 enzyme inactivation < threshold at 10 %	-	HOMO SAPIENS	View Detail	(4) CAS

Assay Data — CAS LIFE SCIENCES

← Prev (6 of 27) Next →

Ligand

723-46-6



$C_{10}H_{11}N_3O_3S$

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

Target	Cytochrome P450 3A4
Assay Name	-
Procedure	Percent inactivation of Cytochrome P450 3A4 in human liver microsomes upon incubation for 30 min in 0.1 M sodium phosphate buffer in presence of 250 mM G6P, 20 units/ml G6PDH and 25 mM beta-NADP+ at 100 uM compound concentration using 2.5 uM midazolam as substrate
Assay Comment	-
Condition	-
Parameter	Enzymatic activity (CYP)
Value	Percentage of P450 enzyme inactivation < threshold at 10 %
Measurement Remarks	Percentage of P450 enzyme inactivation < threshold at 10 %
Ligand Dose	-
Biological System	HOMO SAPIENS; liver microsomes; HUMAN
Source	Combination of GSH trapping and time-dependent inhibition assays as a predictive method of drugs generating highly reactive metabolites By: Nakayama, Shintaro; Takakusa, Hideo; Watanabe,

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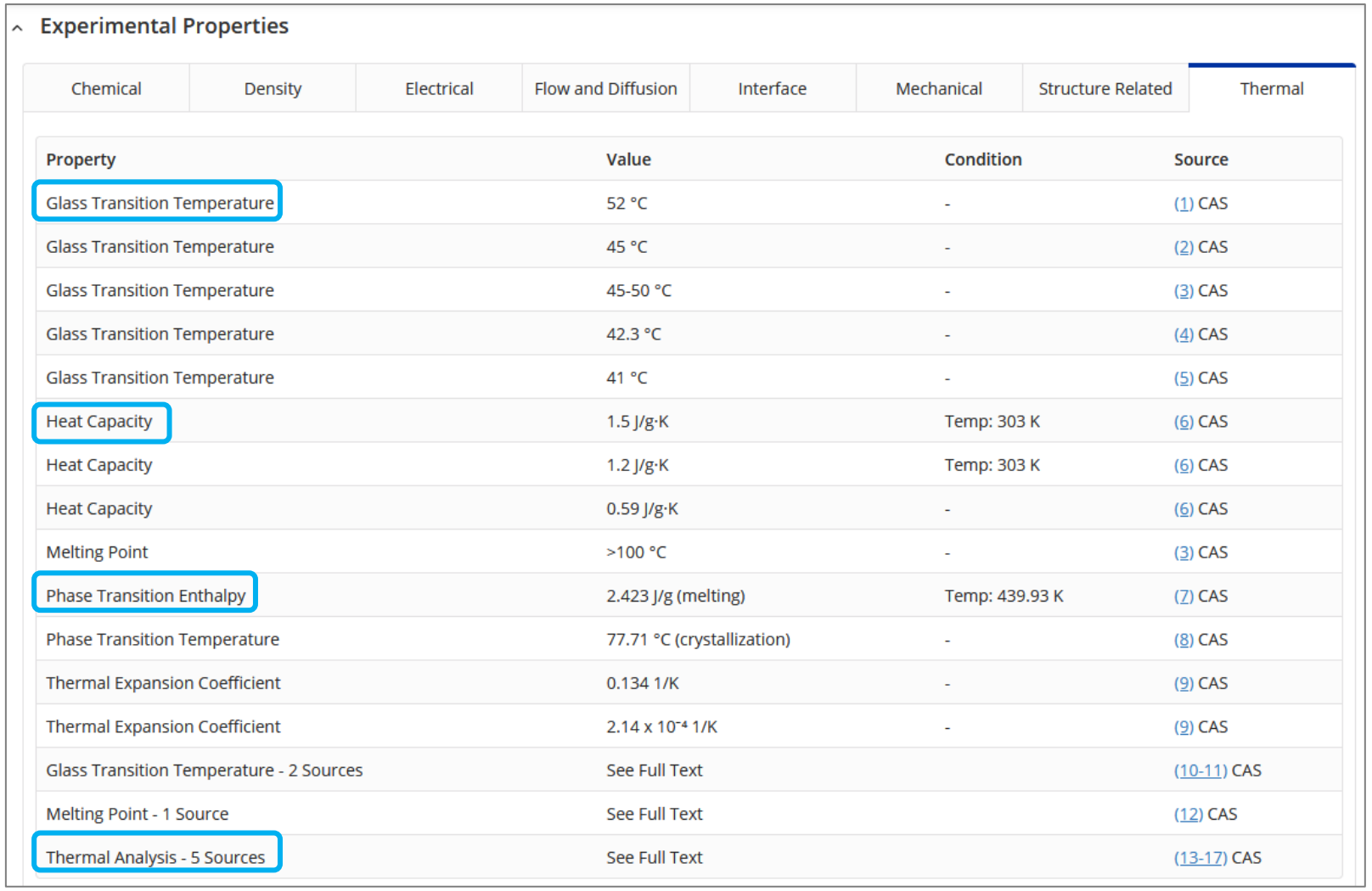
物质详情新增多种属性数据：助力材料、化学化工科研



Experimental Properties

Chemical | Density | Electrical | Flow and Diffusion | Interface | Mechanical | Structure Related | Thermal

Property	Value	Condition	Source
Glass Transition Temperature	52 °C	-	(1) CAS
Glass Transition Temperature	45 °C	-	(2) CAS
Glass Transition Temperature	45-50 °C	-	(3) CAS
Glass Transition Temperature	42.3 °C	-	(4) CAS
Glass Transition Temperature	41 °C	-	(5) CAS
Heat Capacity	1.5 J/g·K	Temp: 303 K	(6) CAS
Heat Capacity	1.2 J/g·K	Temp: 303 K	(6) CAS
Heat Capacity	0.59 J/g·K	-	(6) CAS
Melting Point	>100 °C	-	(3) CAS
Phase Transition Enthalpy	2.423 J/g (melting)	Temp: 439.93 K	(7) CAS
Phase Transition Temperature	77.71 °C (crystallization)	-	(8) CAS
Thermal Expansion Coefficient	0.134 1/K	-	(9) CAS
Thermal Expansion Coefficient	2.14 x 10^{-4} 1/K	-	(9) CAS
Glass Transition Temperature - 2 Sources	See Full Text		(10-11) CAS
Melting Point - 1 Source	See Full Text		(12) CAS
Thermal Analysis - 5 Sources	See Full Text		(13-17) CAS

新增实验属性：

玻璃化转变温度、热分析动力学参数、相点、焓、自由能、热容、流体属性、溶解度、解离常数、偶极距数据等

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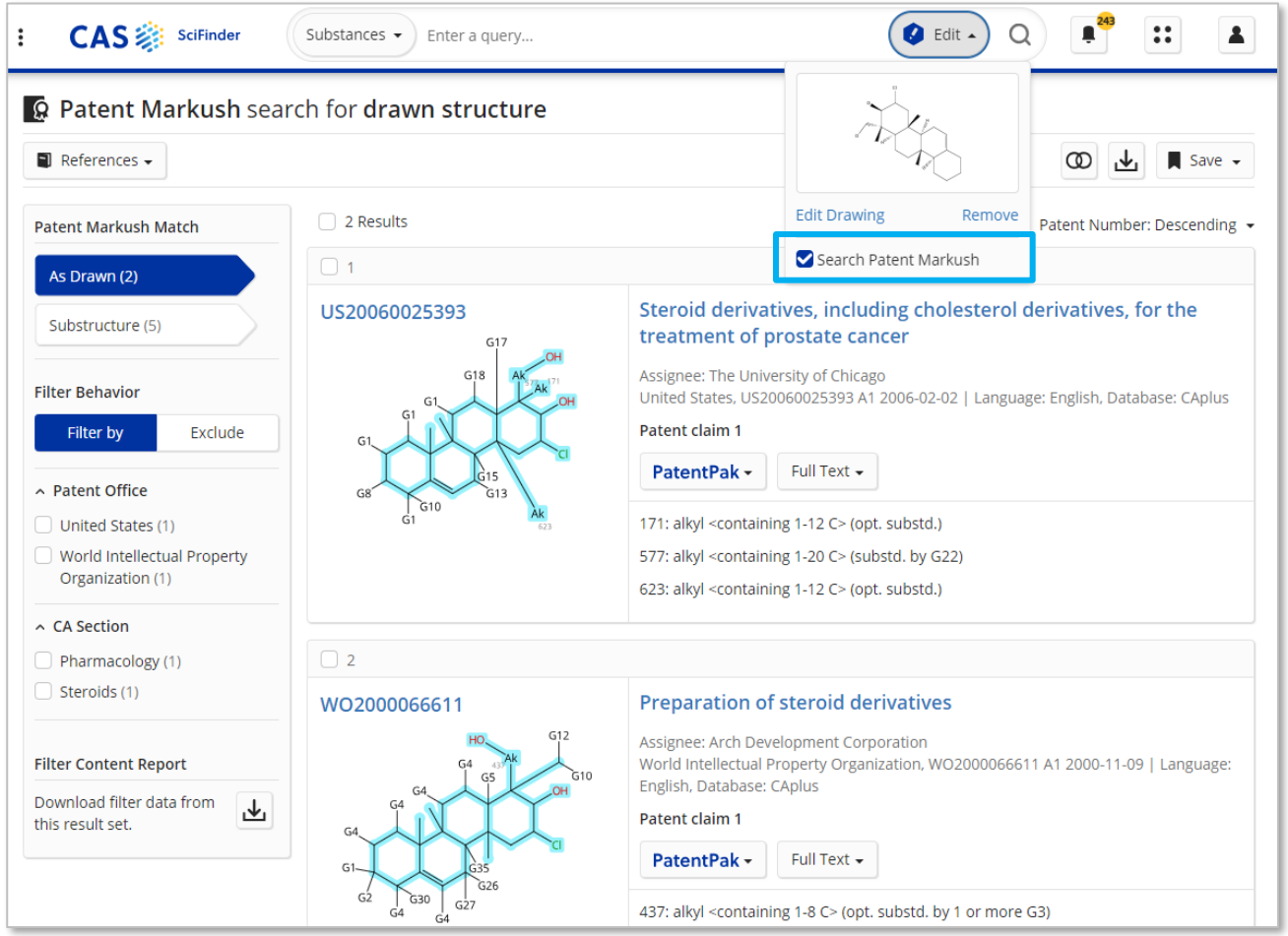
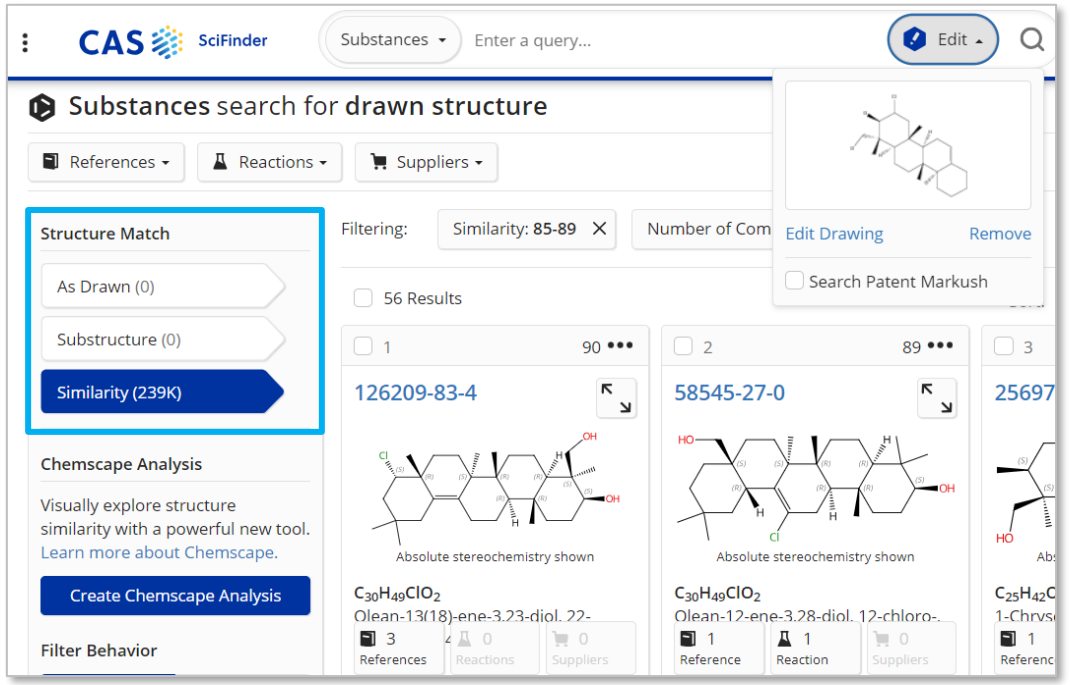
CAS Markush检索



- Markush结构检索、确切结构检索、文献检索相结合
- 评估结构新颖性及专利风险
- 拓展检索范围，获得更多灵感



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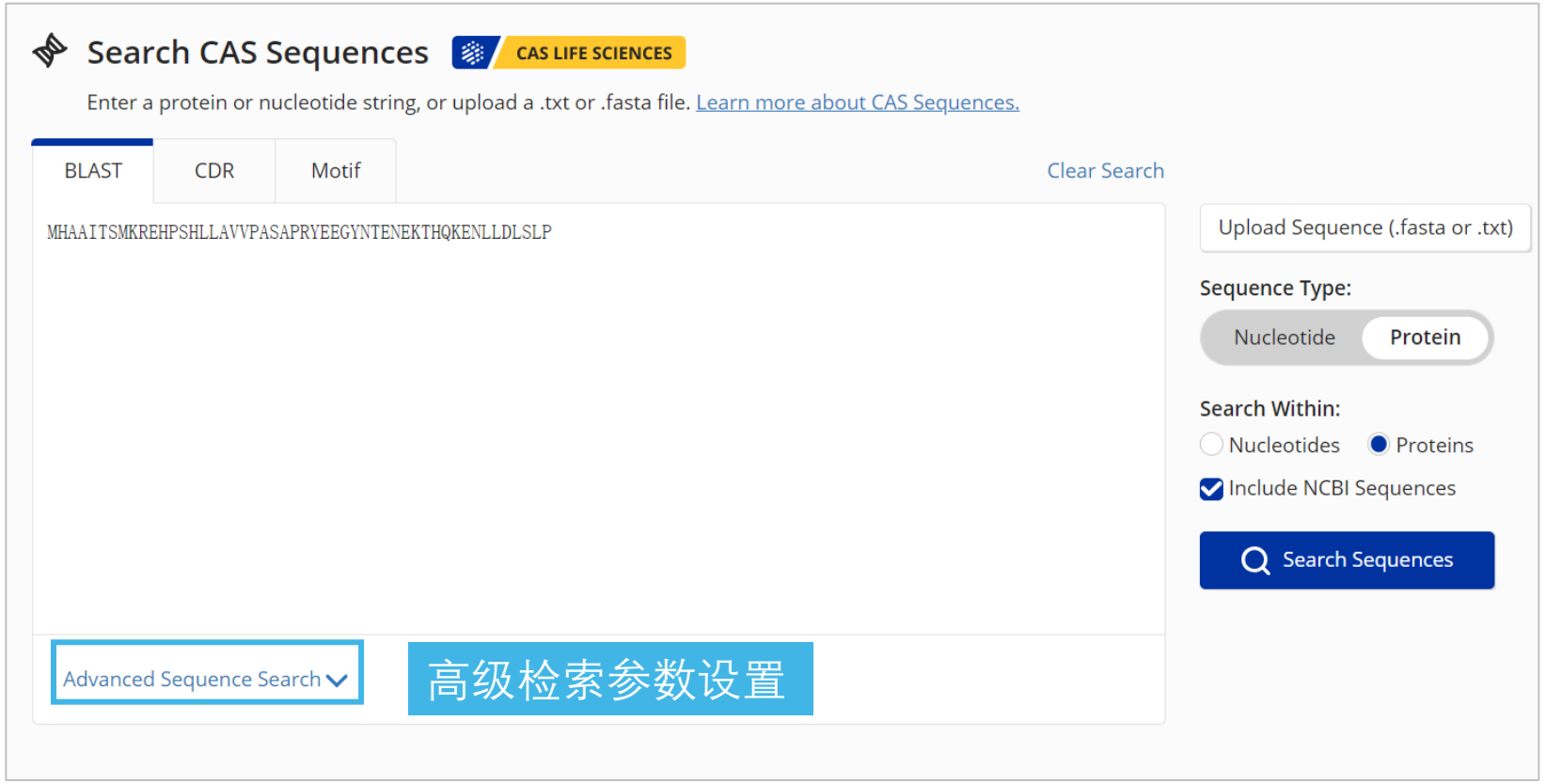
CAS Sequences: 分子生物学解决方案

- 超过13亿条序列
- 涵盖专利、非专利文献披露的序列
- 专有的CAS人工标引的化学修饰序列
- NCBI中的序列
- 可实现新颖性、创造性检索
- 简洁直观的检索界面 & 便捷的筛选、可视化分析、相关信息获取和下载功能
- 三种检索方式：BLAST、CDR、Motif

CAS Sequences: Blast检索

BLAST：检索DNA、RNA、蛋白质、肽



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

选择是否包含NCBI中的序列

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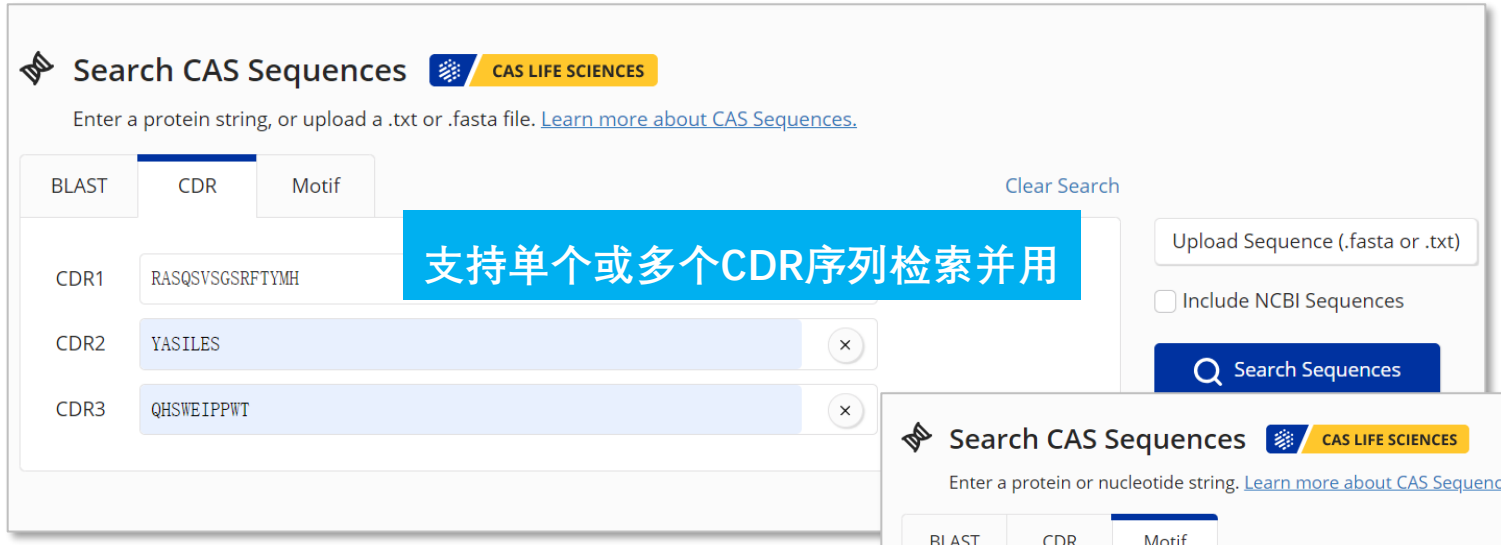
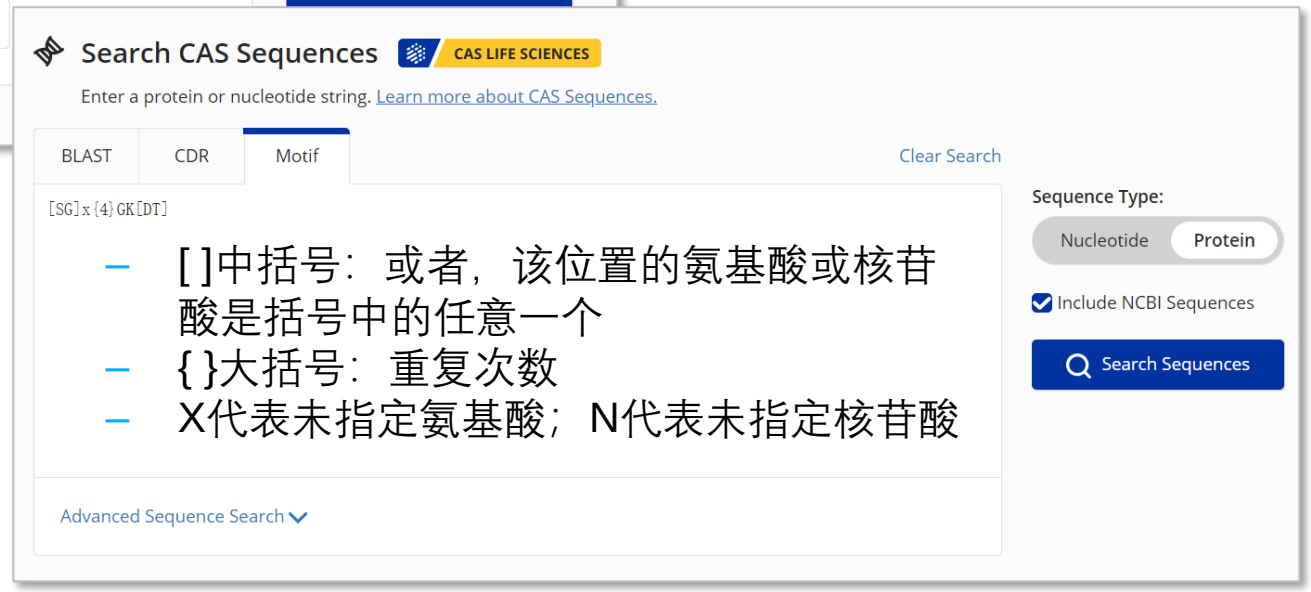
CAS Sequences: CDR和Motif检索

CDR: 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

Motif：检索未指定的氨基酸和核苷酸，且更适合检索短序列。



- [ ]中括号：或者，该位置的氨基酸或核苷酸是括号中的任意一个
- { }大括号：重复次数
- X代表未指定氨基酸；N代表未指定核苷酸

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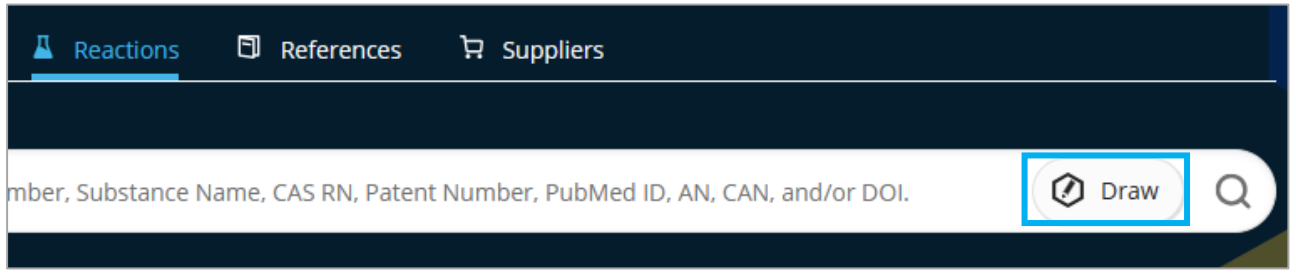
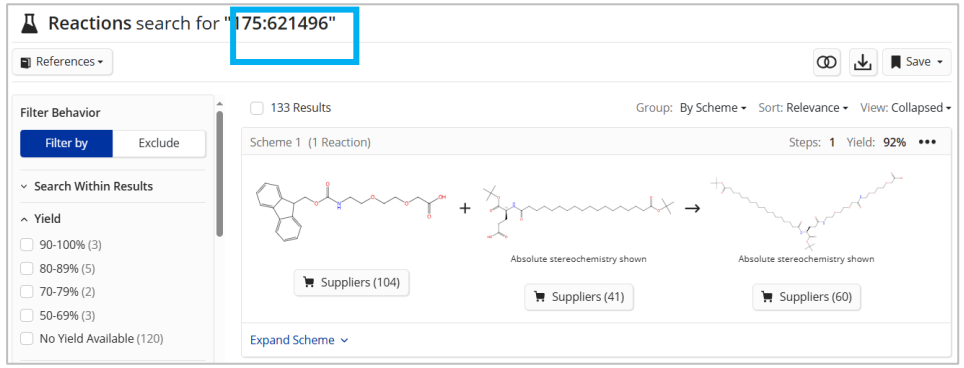
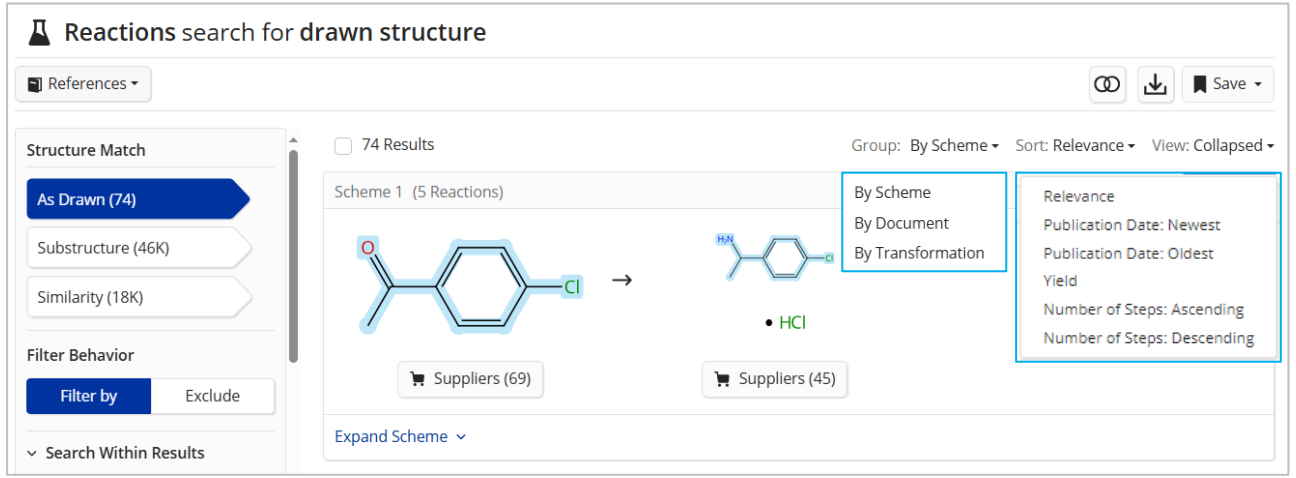
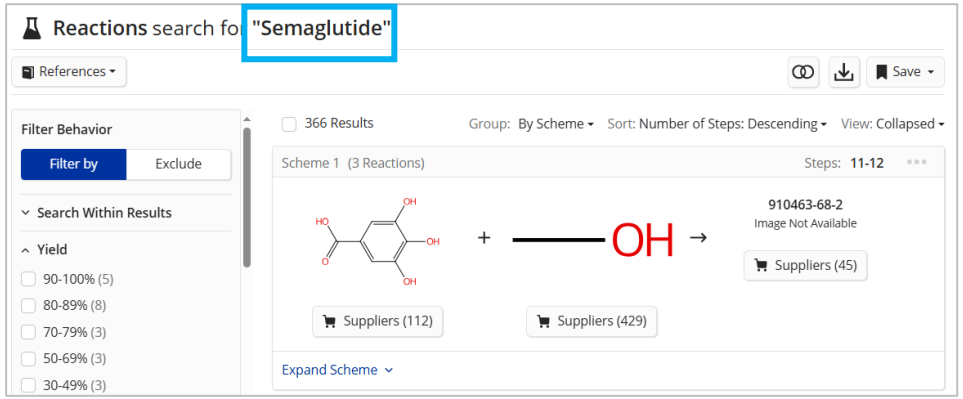
CAS Reactions: 反应检索

- 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
  - 自然语言









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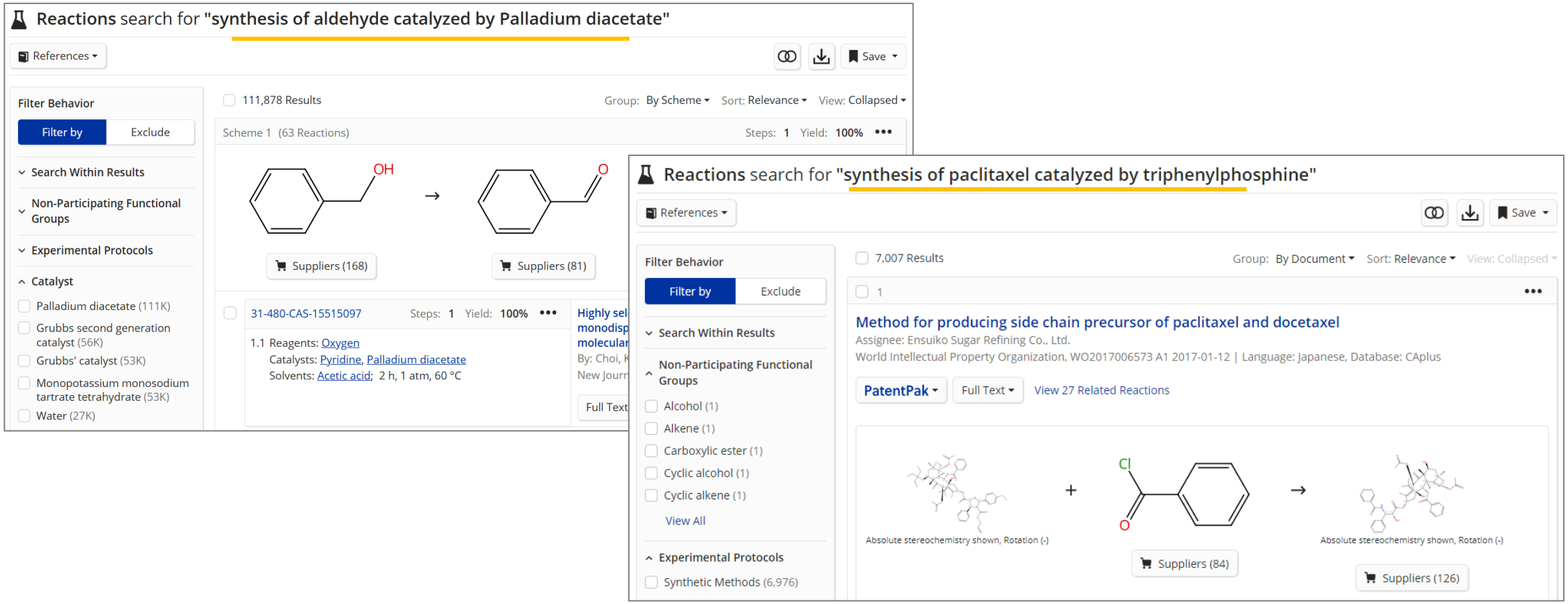
利用自然语言检索反应，降低检索难度

AI识别检索意向，智能识别反应的底物、产物、溶剂、试剂、催化剂、物质类别等信息



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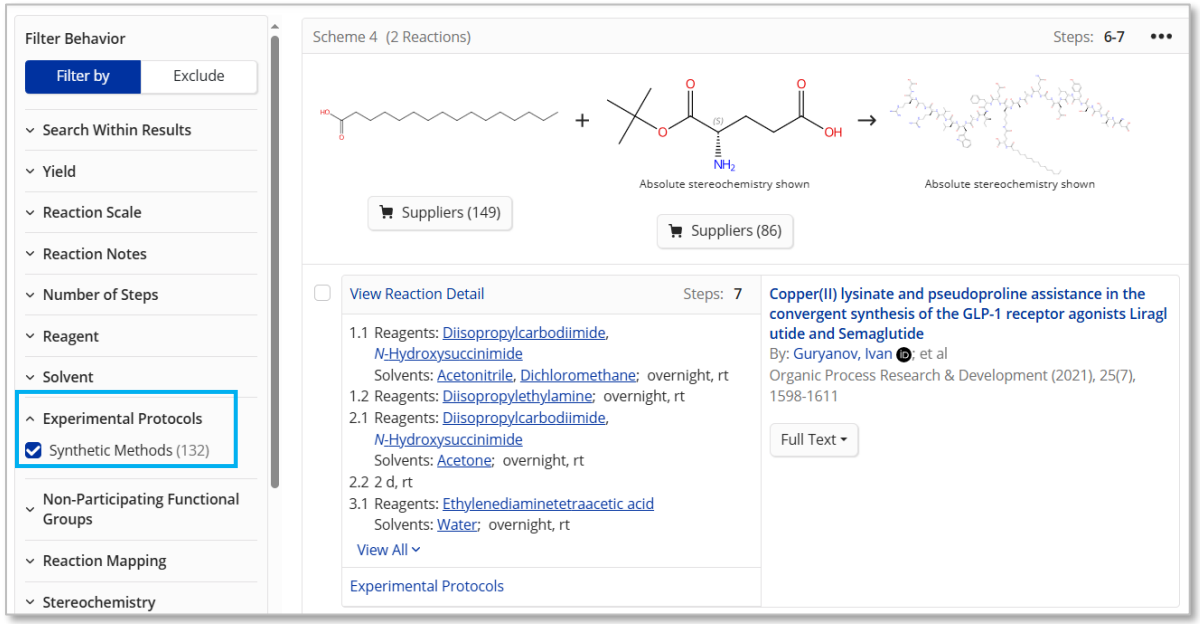
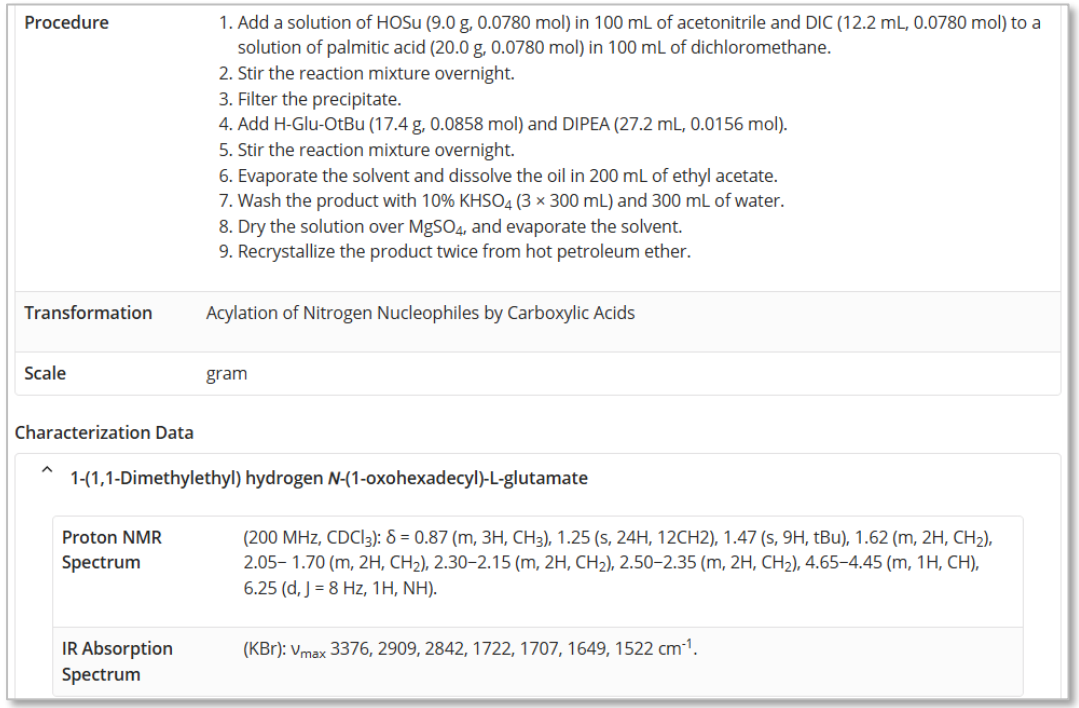
Synthetic Methods: 合成方法详情解决方案

- 迄今为止全球最大的为合成科学家提供的实验方法详情解决方案
- CAS科学家通过分析大量的顶级科技期刊及专利原文，收集、整理、筛选出来的实验方法
- 无需下载阅读全文，即可获得合成实验所需的所有信息
- 极大节省在期刊全文中查找信息的时间





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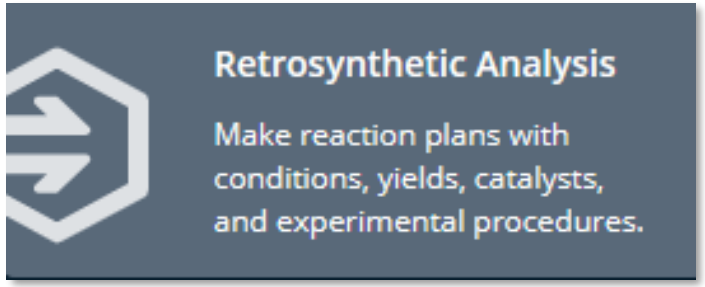
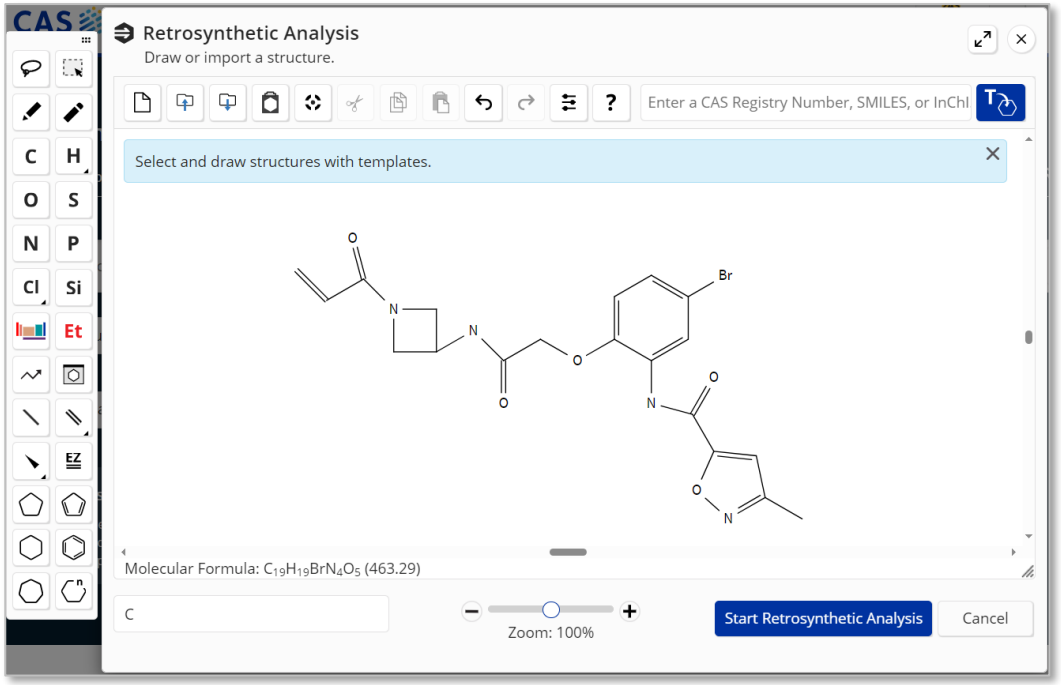
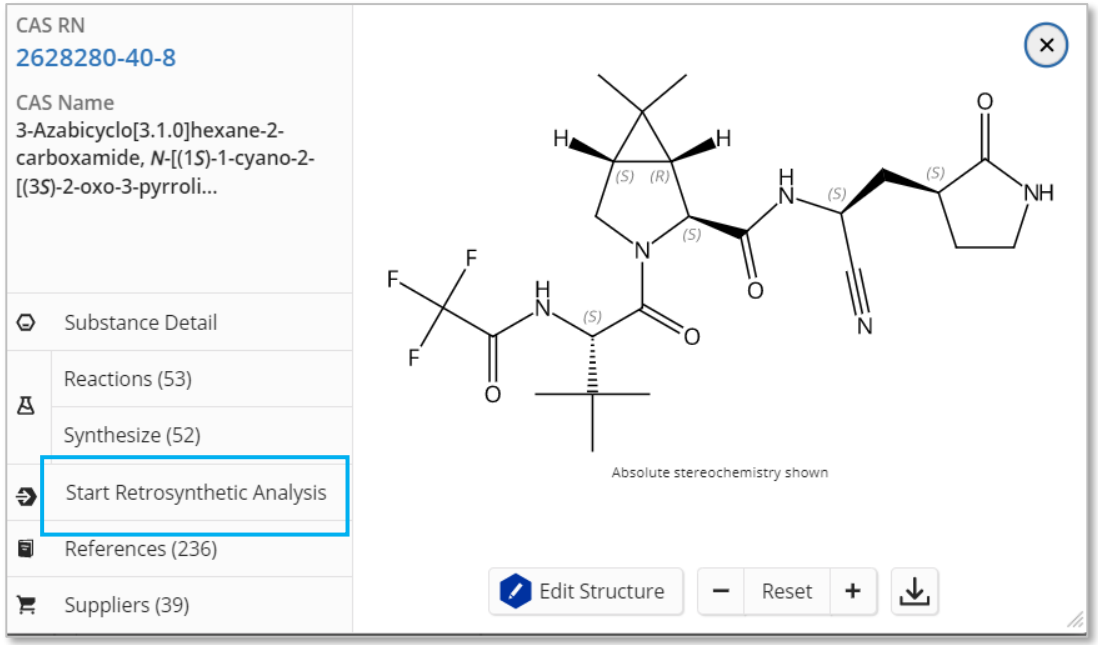
CAS Retrosynthesis Tool: 逆合成工具

- 依据一个确定的结构进行设计
- 有报道且结构明确的物质，无论是否有反应信息报道
- 未报道且结构明确的物质
- 节省设计、实施合成新方法所花费的时间







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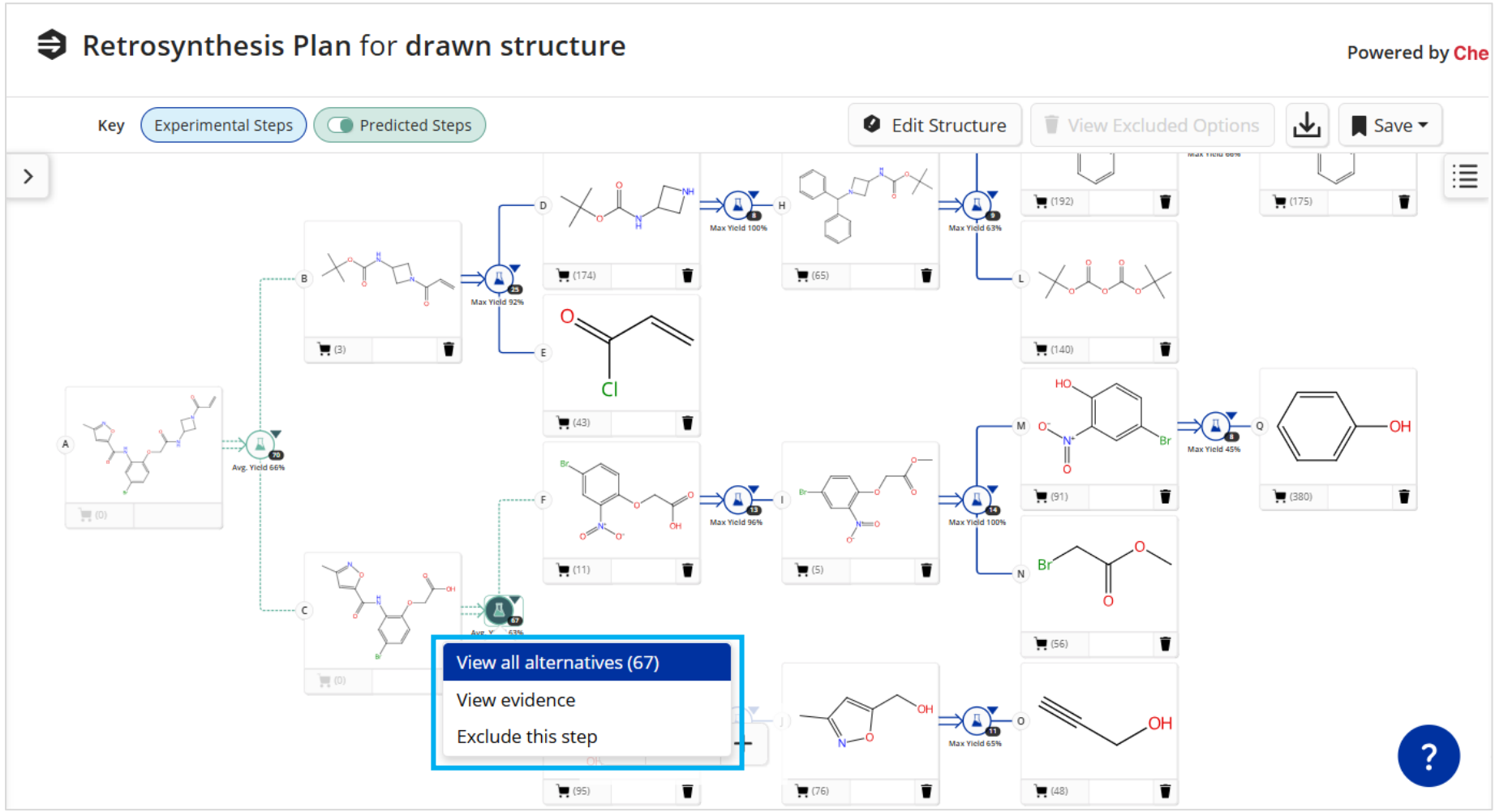
CAS Retrosynthesis Tool: 逆合成工具

获得逆合成路线后，可以查看每一步反应的依据和备选路线



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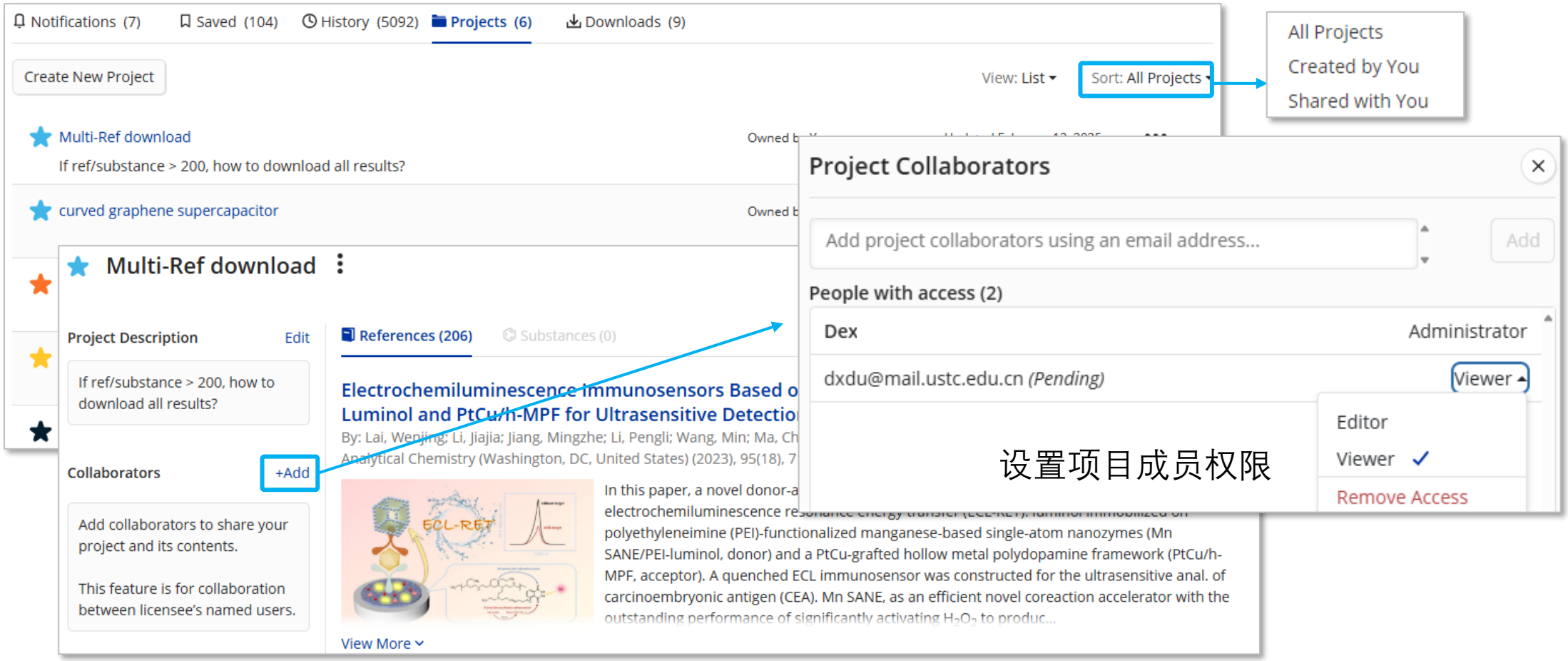
Project项目管理：支持多人协作

可管理文献、物质，并分享项目给其他用户



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大纲

- CAS（美国化学文摘社）及CAS SciFinder Discovery Platform简介
- 新一代科研创新信息工具CAS SciFinder^{n}
- 分析方法解决方案CAS Analytical Methods
- 配方/制剂解决方案CAS Formulus

CAS Analytical Methods: 分析实验方法解决方案

分析方法的类别：13大类45小类；某些子类属多个大类

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

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

Pharmacology / Toxicology: 成瘾药物检测，有毒物检测…

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

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

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

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

Agricultural Applications / Analysis: 除草剂分析…

Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析…

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

Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析…

Water: 阴阳离子分析、环境分析、废水分析、微量元素分析…

Polymer: 聚合物分析…

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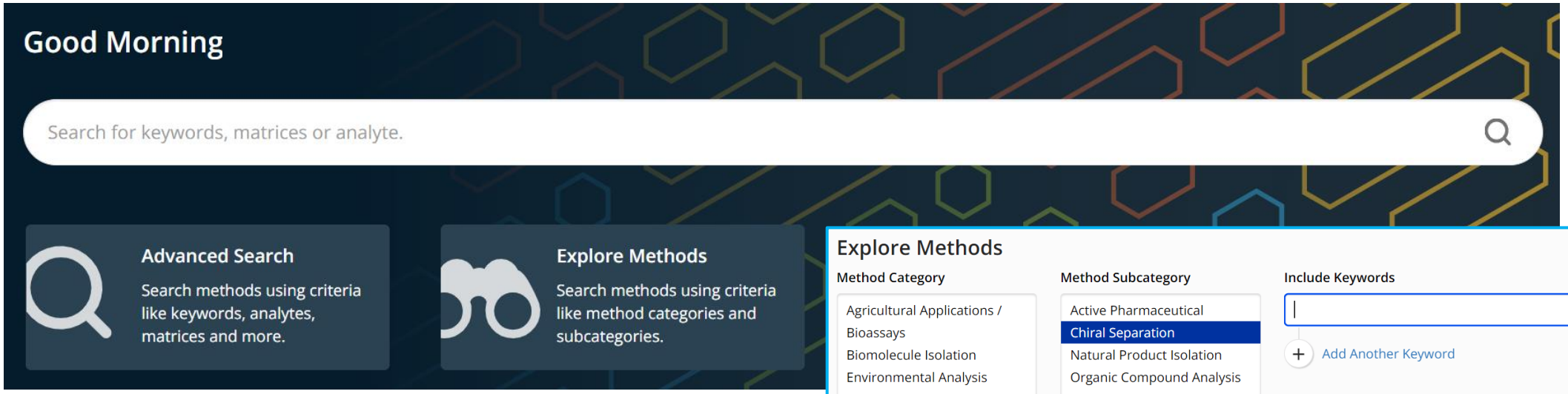
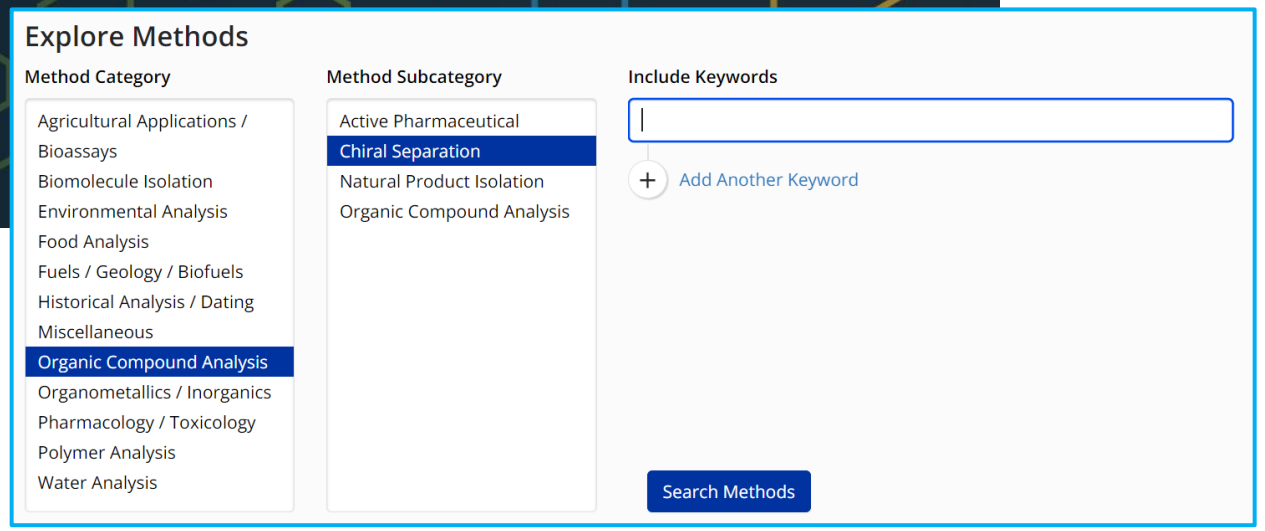
分析实验方法的获取

https://methods.cas.org（与CAS SciFinder^{n}登录账号相同）





- 主题检索或分类浏览；
- 筛选分析物、介质、方法类别、分析技术等

方法分类共13大类，45小类：包括农业应用、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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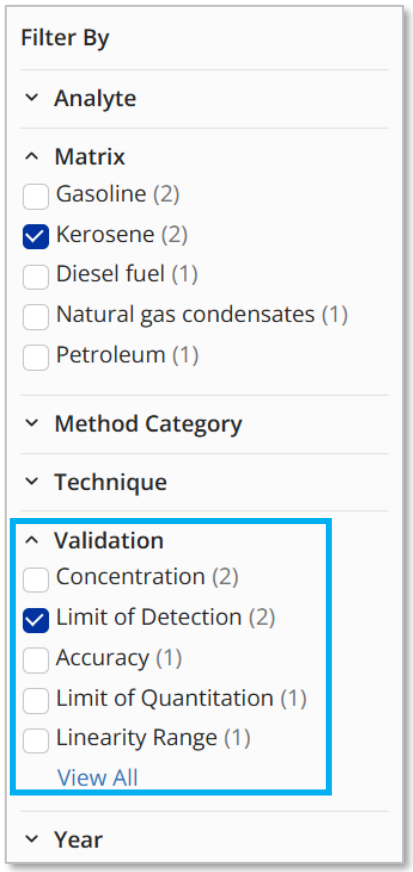
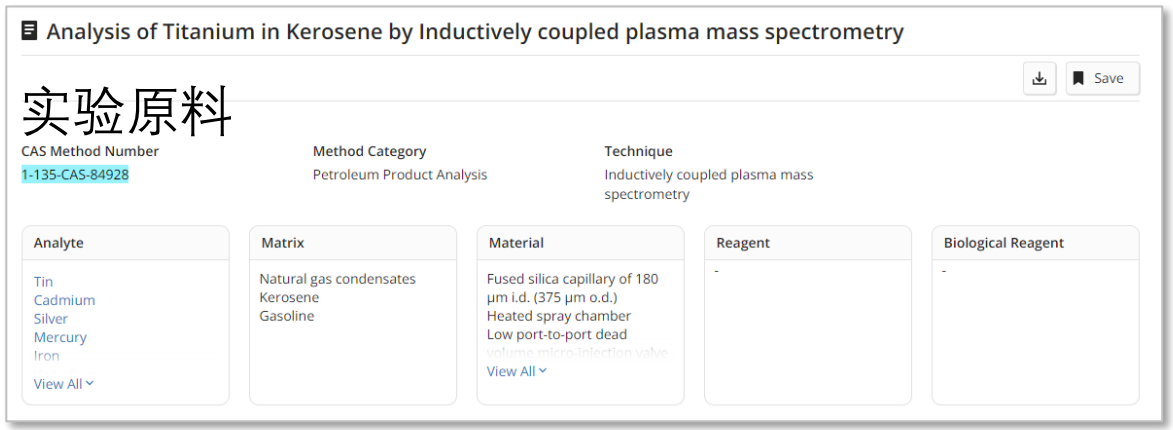
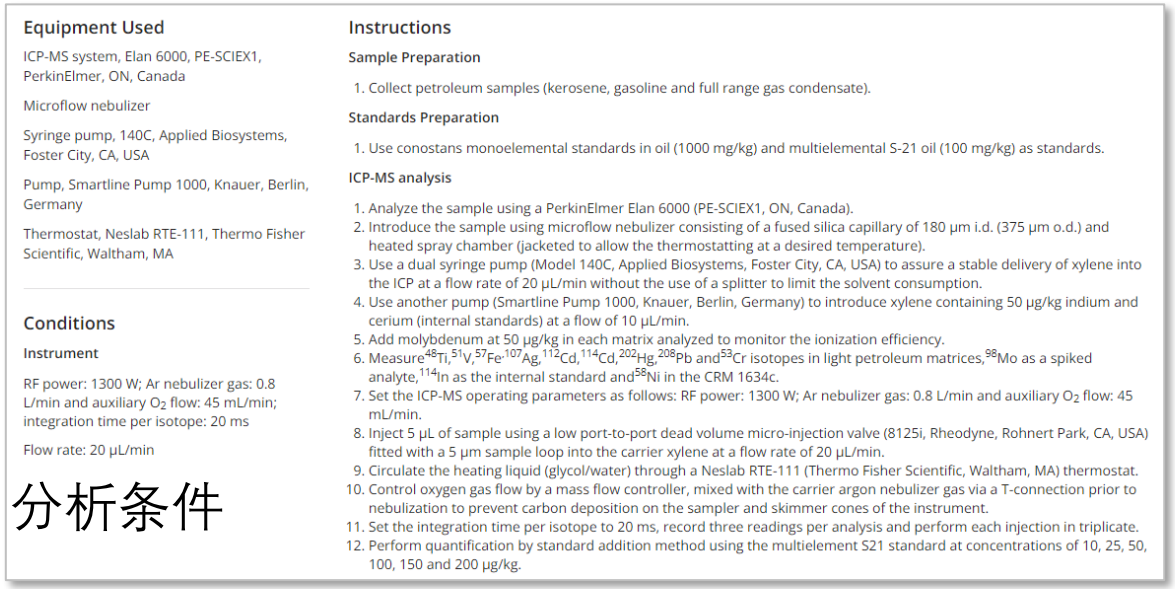
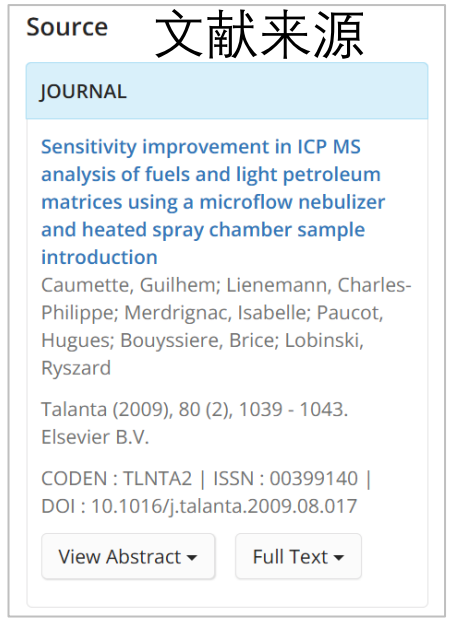
分析方法详情





实验仪器　　操作步骤





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直观的分析方法对比

Compare Methods

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	1	2
Title	Analysis of Chromium in Barium sulfate by Electrothermal atomic absorption spectroscopy	Analysis of Chromium in Barium sulfate by Electrothermal atomic absorption spectroscopy
CAS Method Number	1-142-CAS-3223998	1-142-CAS-3186641
Method Category	Trace Element Analysis; Active Pharmaceutical Ingredient and Metabolite Analysis	Trace Element Analysis; Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Electrothermal atomic absorption spectroscopy	Acid digestion; Electrothermal atomic absorption spectroscopy
Analyte	Chromium	Chromium
Matrix	Barium sulfate	Barium sulfate
Other Materials	Nitric acid; Pyrolytic coated graphite tubes	Nitric acid
Equipment Used	Atomic absorption spectrometer, AAS ZEEnit 60, Analytik Jena, Jena, Germany; Solid sampling system, SSA-5, Analytik Jena, Jena, Germany; Microbalance, M2P, Sartorius, View All	Atomic absorption spectrometer, AAS ZEEnit 60, Analytik Jena, Jena, Germany; Microbalance, M2P, Sartorius, Gottingen, Germany; Sub-boiling system, duoPUR 2.01 E, View All
Conditions	**Instrument:** hollow cathode lamp power: 4 mA; wavelength: 357.9 nm; spectral bandpass: 0.8 nm; integration time: 12 s; atomization temperature: 2400 °C; pyrolysis temperature: View All	**Instrument:** hollow cathode lamp power: 4 mA; wavelength: 357.9 nm; spectral bandpass: 0.8 nm
Source	Chromium determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background View All	Chromium determination in pharmaceutical grade barium sulfate by solid sampling electrothermal atomic absorption spectrometry with Zeeman-effect background View All
Preparation	**Collection and preparation of samples** 1. Obtain the powdered pharmaceutical grade $BaSO_4$ samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h. 2. Spike the samples by addition of chromium reference solutions of 0.48 µg/g. **Preparation of standard solutions** 1. Prepare the reference solutions daily by serial dilutions of stock chromium (Cr) solutions (1 g/L Cr in 2% HNO_3). View Less	**Preparation of nitric acid solution** 1. Doubly distill the concentrated nitric acid in a Milestone sub-boiling system (model duoPUR 2.01 E, Bergamo, Italy) and use this for sample digestion/extraction. **Collection and preparation of samples** 1. Obtain the powdered pharmaceutical grade $BaSO_4$ samples from pharmaceutical industries and dry them in a conventional oven at 105 °C × 2 h. **Preparation of standard solutions** 1. Prepare the reference solutions daily by serial dilutions of stock chromium (Cr) solutions (1 g/L Cr in 2% HNO_3). View Less
Method	**Direct solid sampling (DSS) - electrothermal-atomic absorption spectrometric (ETAAS) analysis** 1. Carry out the chromium determinations using a model View All	**Acid digestion procedure using nitric acid** 1. Perform sample acid digestion (extraction) in closed quartz vessels using a high pressure model Multiwave View All
Linearity Range	100 - 1800 pg	
Limit of Detection	2.4 pg	
Recovery	98% - 103% in 0.48 µg/g spiked concentration	
Concentration	0.45 ± 0.04 µg/g (sample data)	0.32 ± 0.04 µg/g (sample data)

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大纲

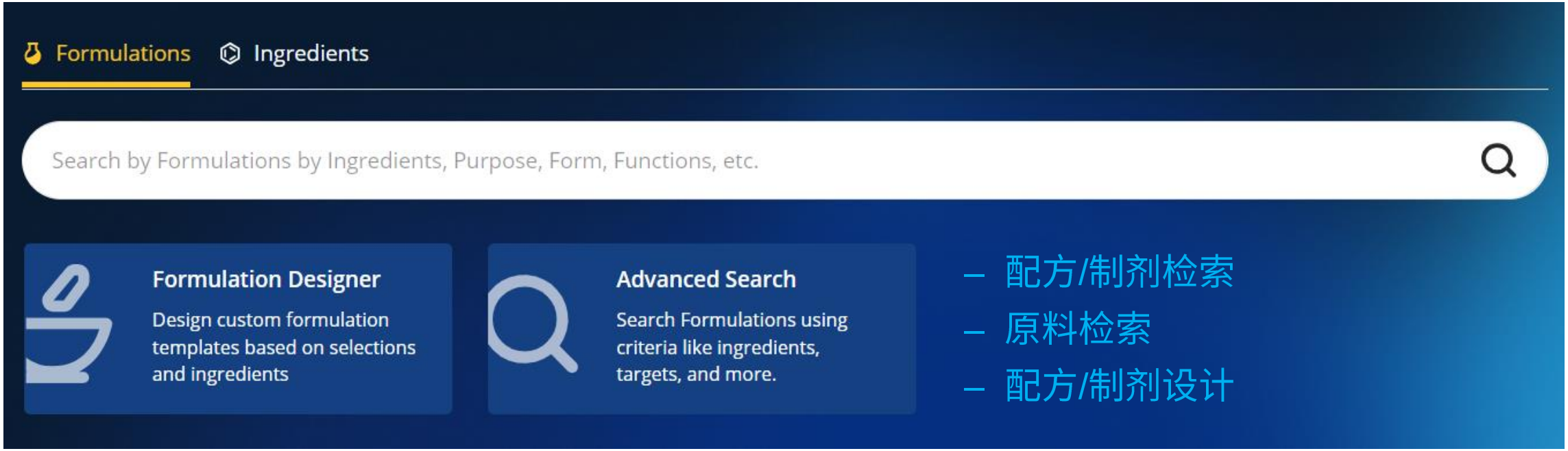
- CAS（美国化学文摘社）及CAS SciFinder Discovery Platform简介
- 新一代科研创新信息工具CAS SciFinder^{n}
- 分析方法解决方案CAS Analytical Methods
- 配方/制剂解决方案CAS Formulus

CAS Formulus: 助力开发安全、有效的产品

- 一个集成配方（制剂）数据与工作流程的解决方案
- 由CAS科学家从期刊、专利、产品说明书中标引的配方信息
- 涵盖制药、化妆品、食品、农化、化妆品、油墨、涂料等众多领域
- 可检索配方及其工艺、成分、目标成分的常见配伍成分、设计配方，探索合规要求等
- 支持自主设计配方/制剂

检索配方或制剂

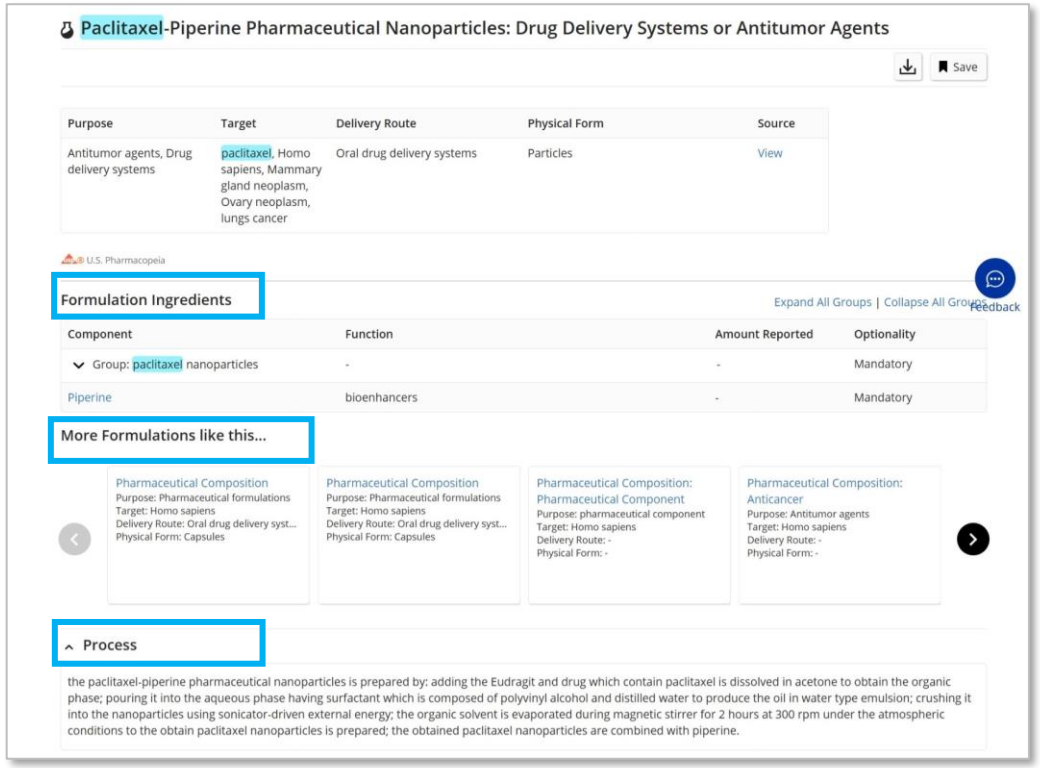
https://formulus.cas.org（与CAS SciFinder^{n}登录账号相同）

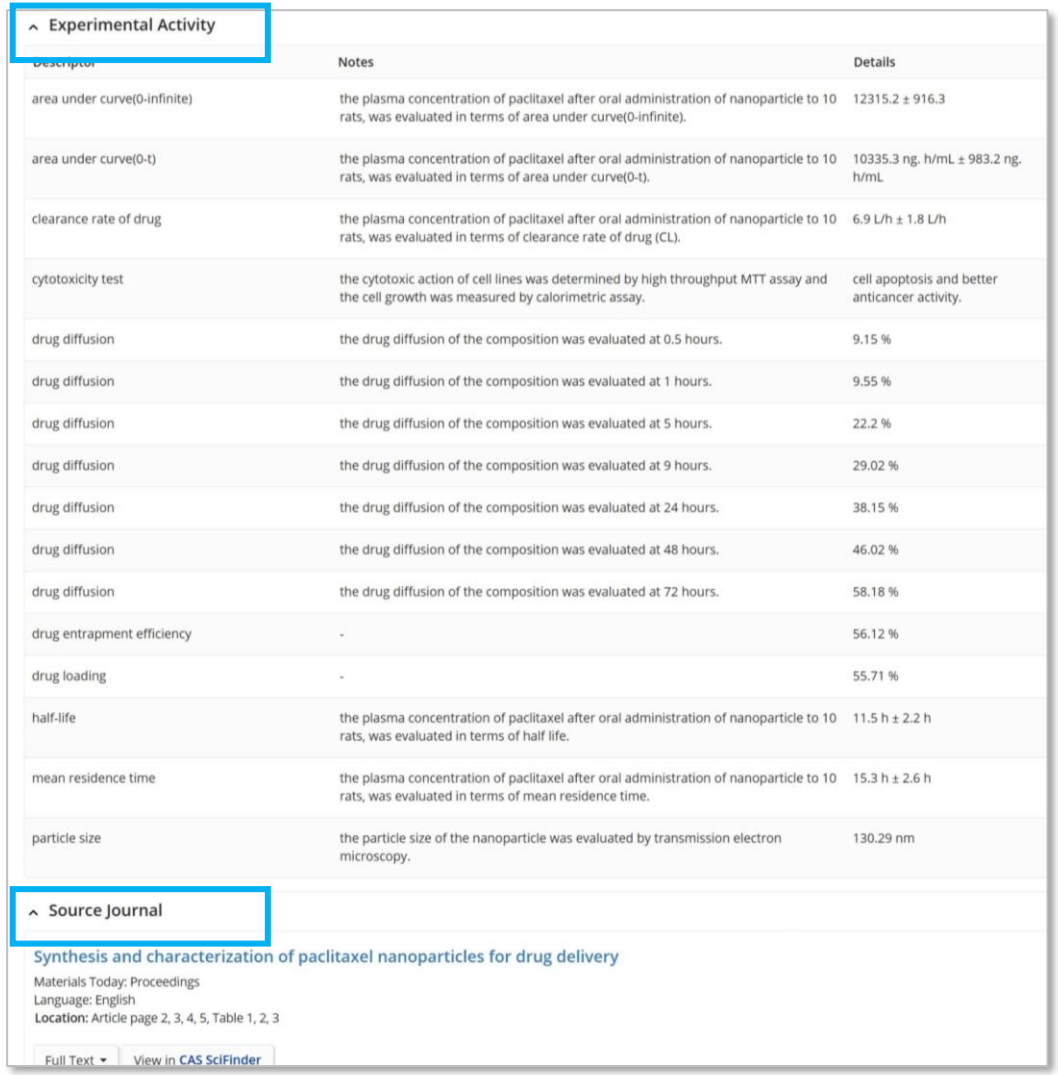


在检索框输入检索式，如制剂或配方的原料、用途、物理形态、功能或文献识别符进行检索

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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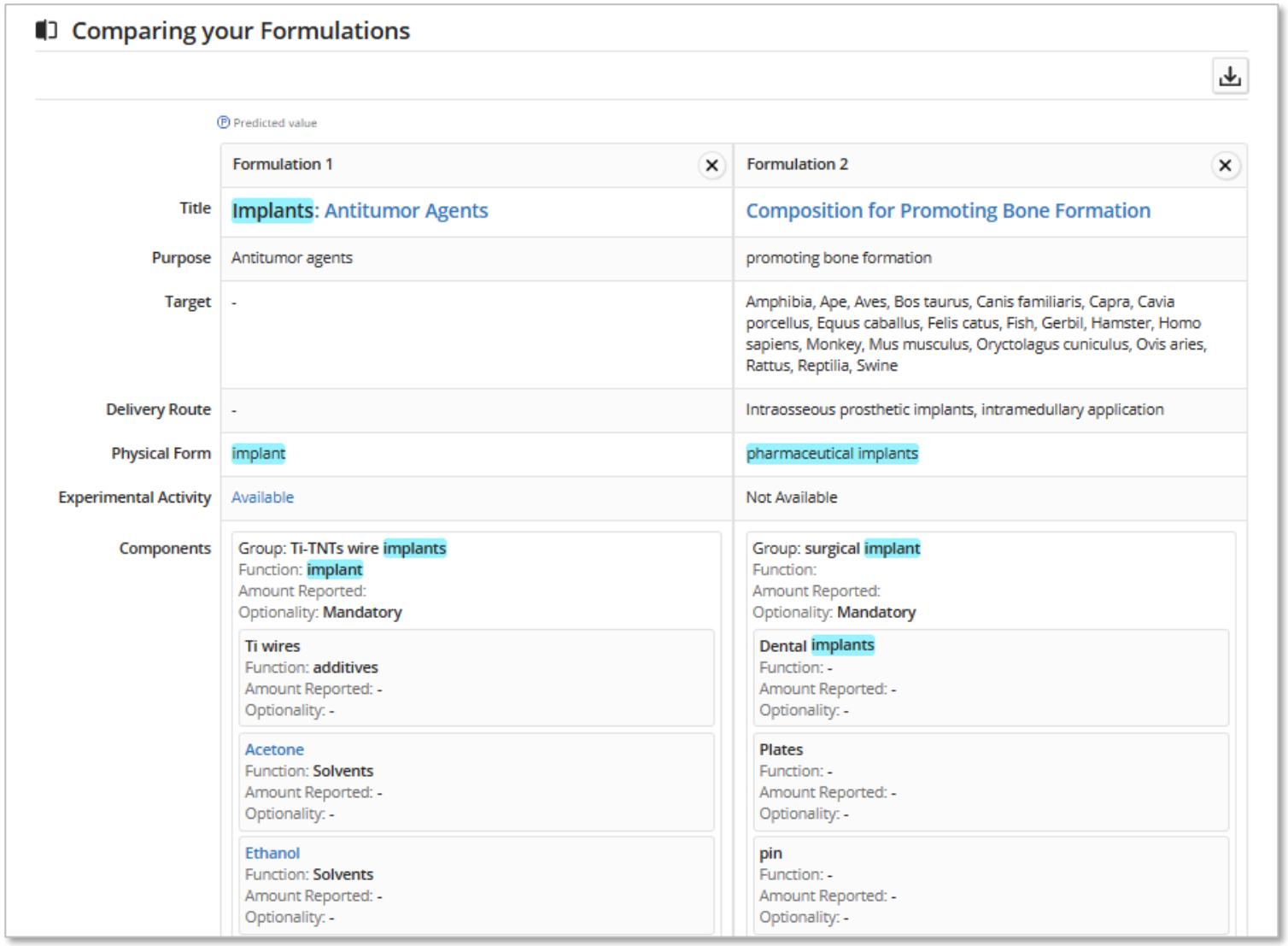
不同制剂或配方信息的直观对比



- 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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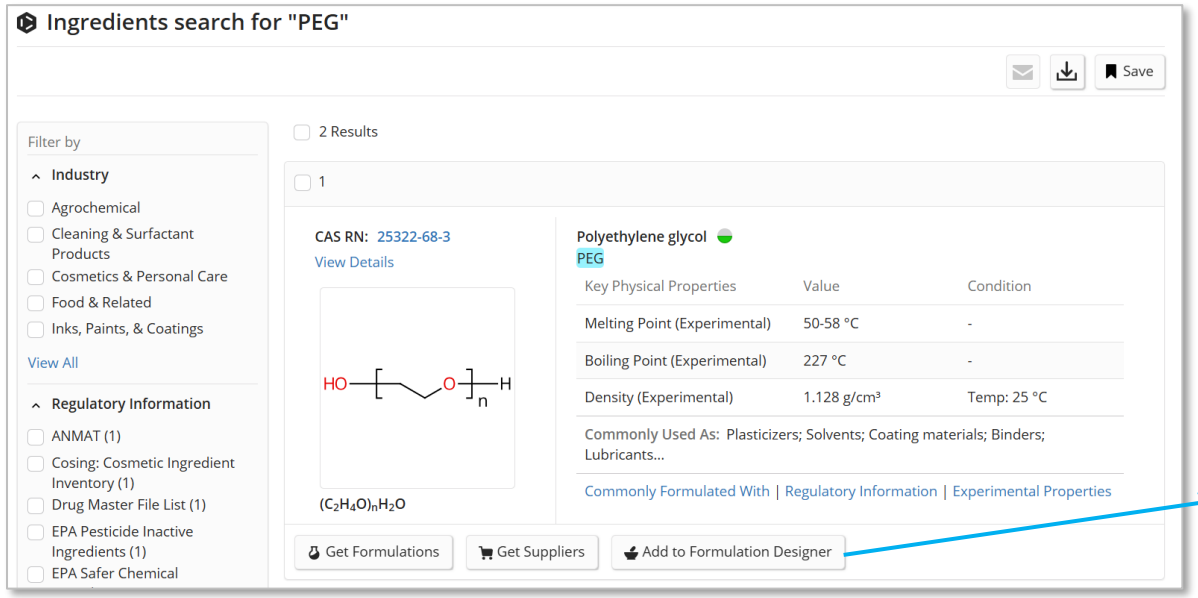
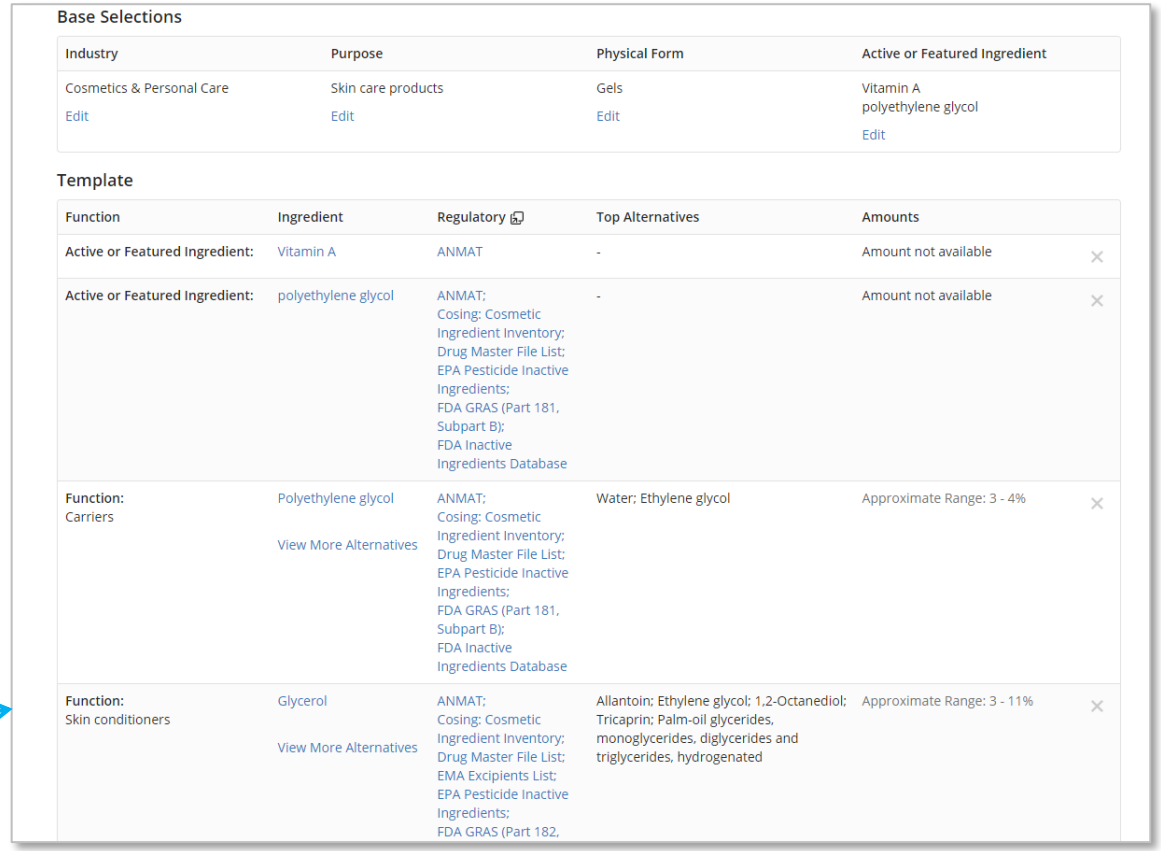
原料检索及配方设计

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





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

- 原料详情
- 原料管制信息
- 可替代的原料选项

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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

THANK YOU!

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