CAS SciFinder Discovery Platform™ (Academic)

全面高效获取科技信息

刘子露
ZLiu@acs-i.org
美国化学文摘社(CAS)北京代表处

CAS
A division of the
American Chemical Society

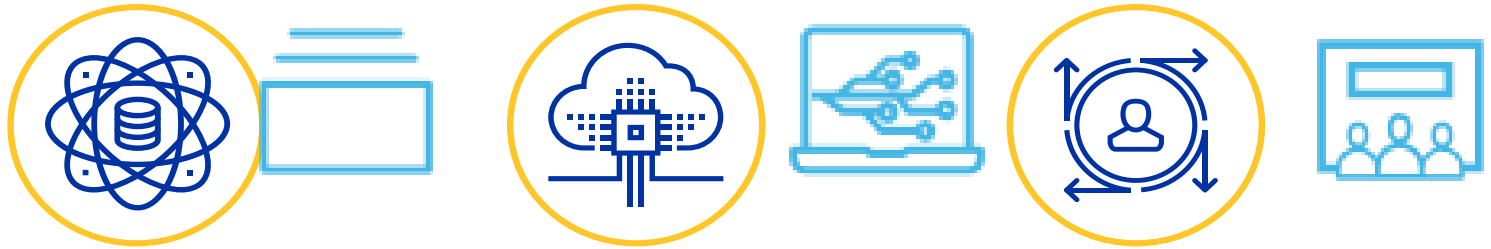
大纲

- 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
A division of the American Chemical Society

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

CAS
A division of the
American Chemical Society

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：**

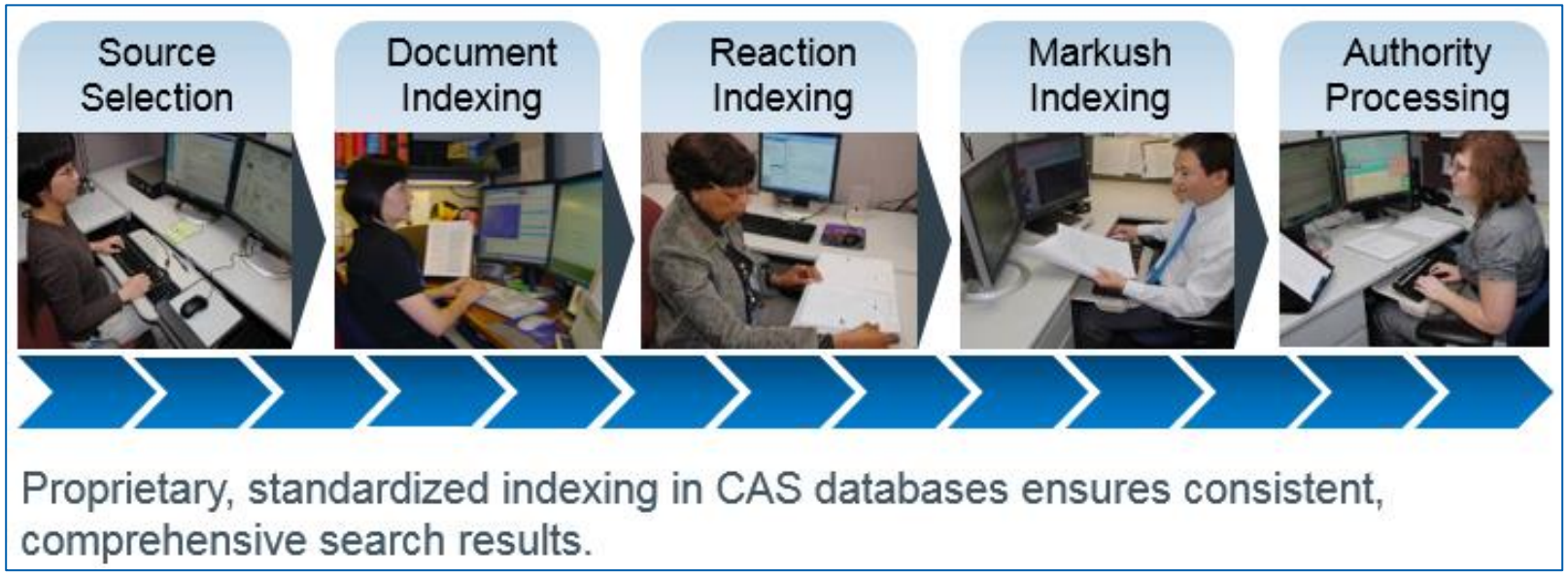
  大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金

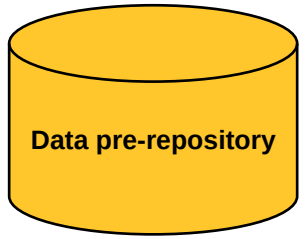
- **物理、无机、分析化学各领域：**

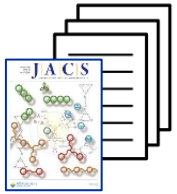
  表面化学、催化剂、相平衡、核现象、电化学

CAS
A division of the American Chemical Society

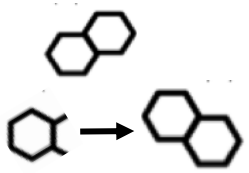
CAS科学家的智力标引

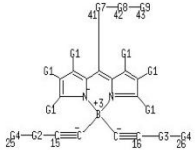






1990
Smith, M.
anthracene





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

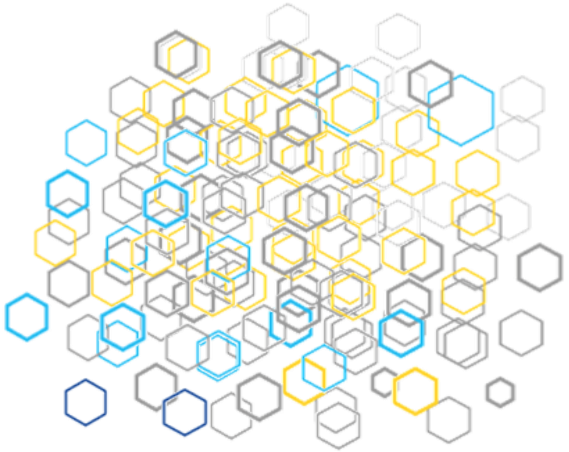
CAS
A division of the American Chemical Society

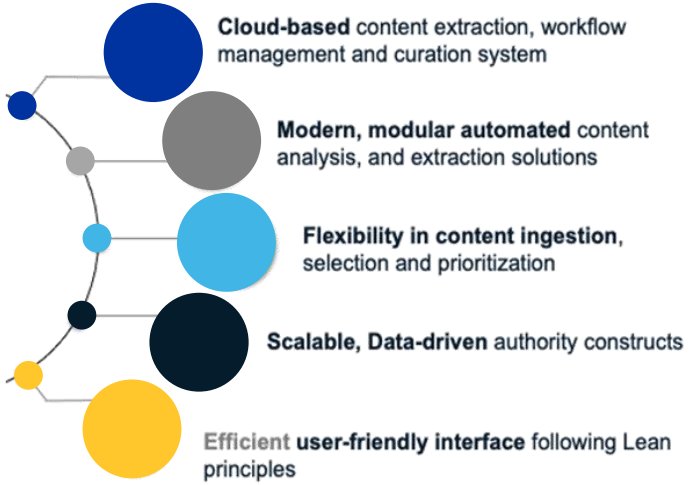
Data frame process at CAS

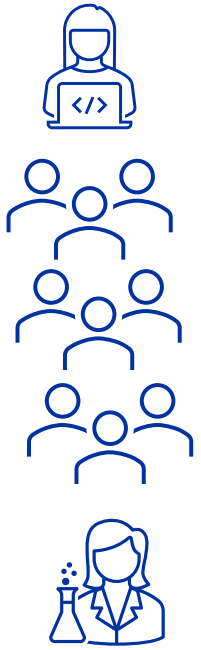
Expert scientists combined with a wide range of ML optimize connections

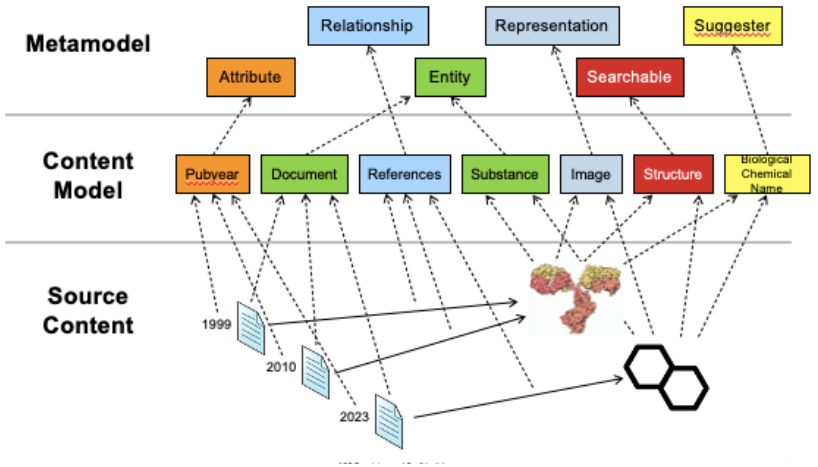
Published content ⟶ **Curated, modeled data**

Continually acquire scientific content	Classify and align to workflows	Human driven, supervised science value collection	Data modeling and data lake creation









CAS
A division of the American Chemical Society

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℠

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

CAS
A division of the American Chemical Society

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。

CAS
A division of the American Chemical Society

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
A division of the American Chemical Society

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

用户需求的演进、内容的增长和广度的扩展推动

新的技术解决方案的出现！

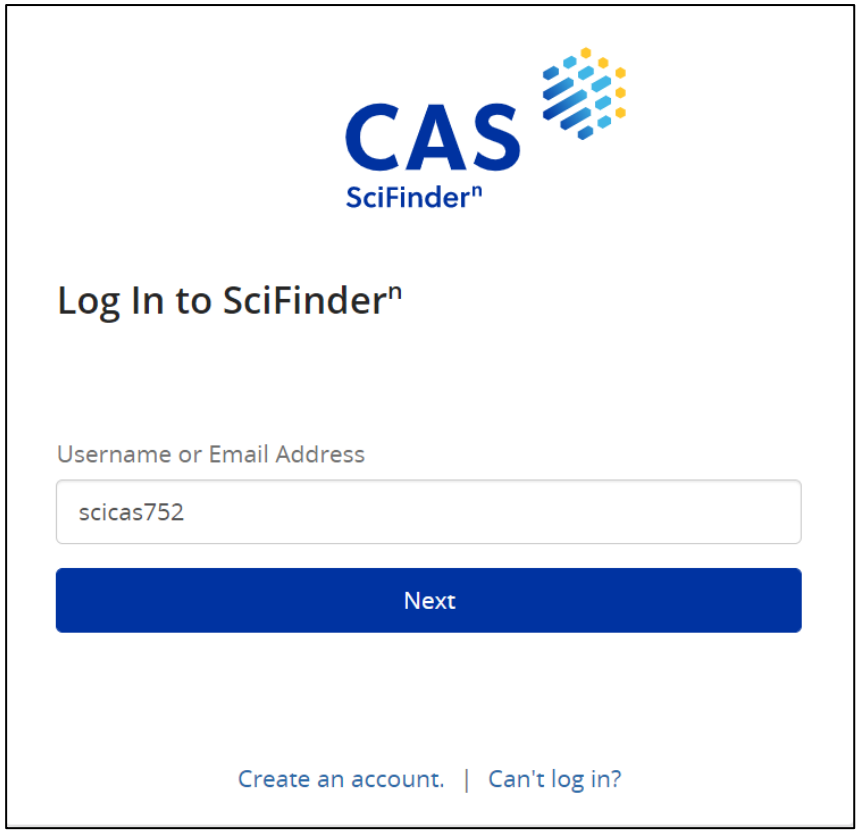
CAS
A division of the American Chemical Society

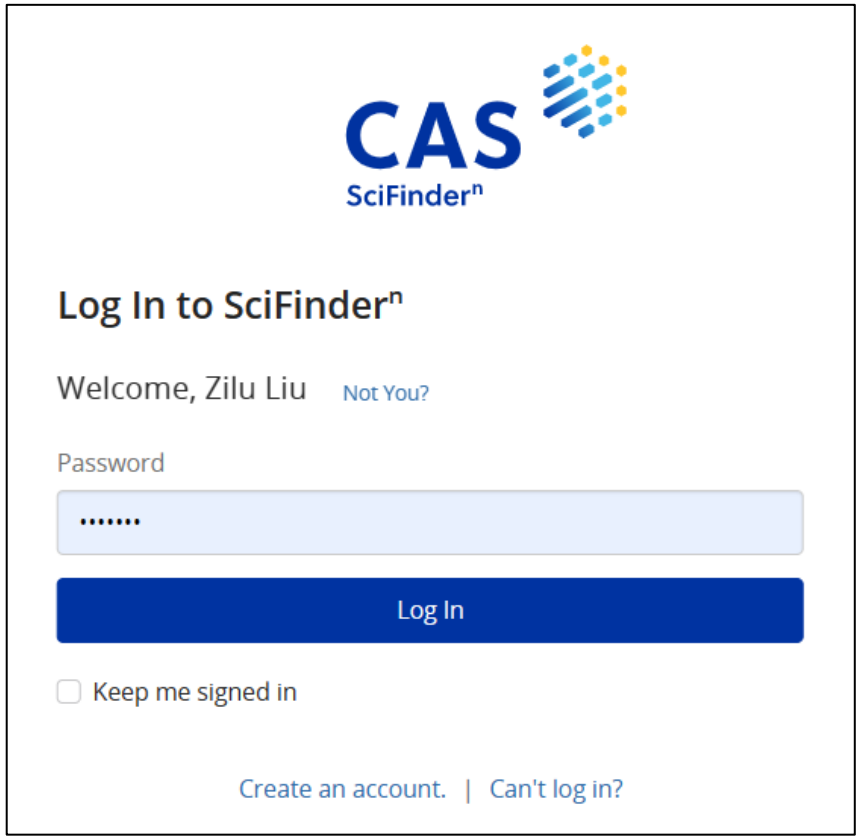
CAS独特的内容合集

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

CAS
A division of the American Chemical Society

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

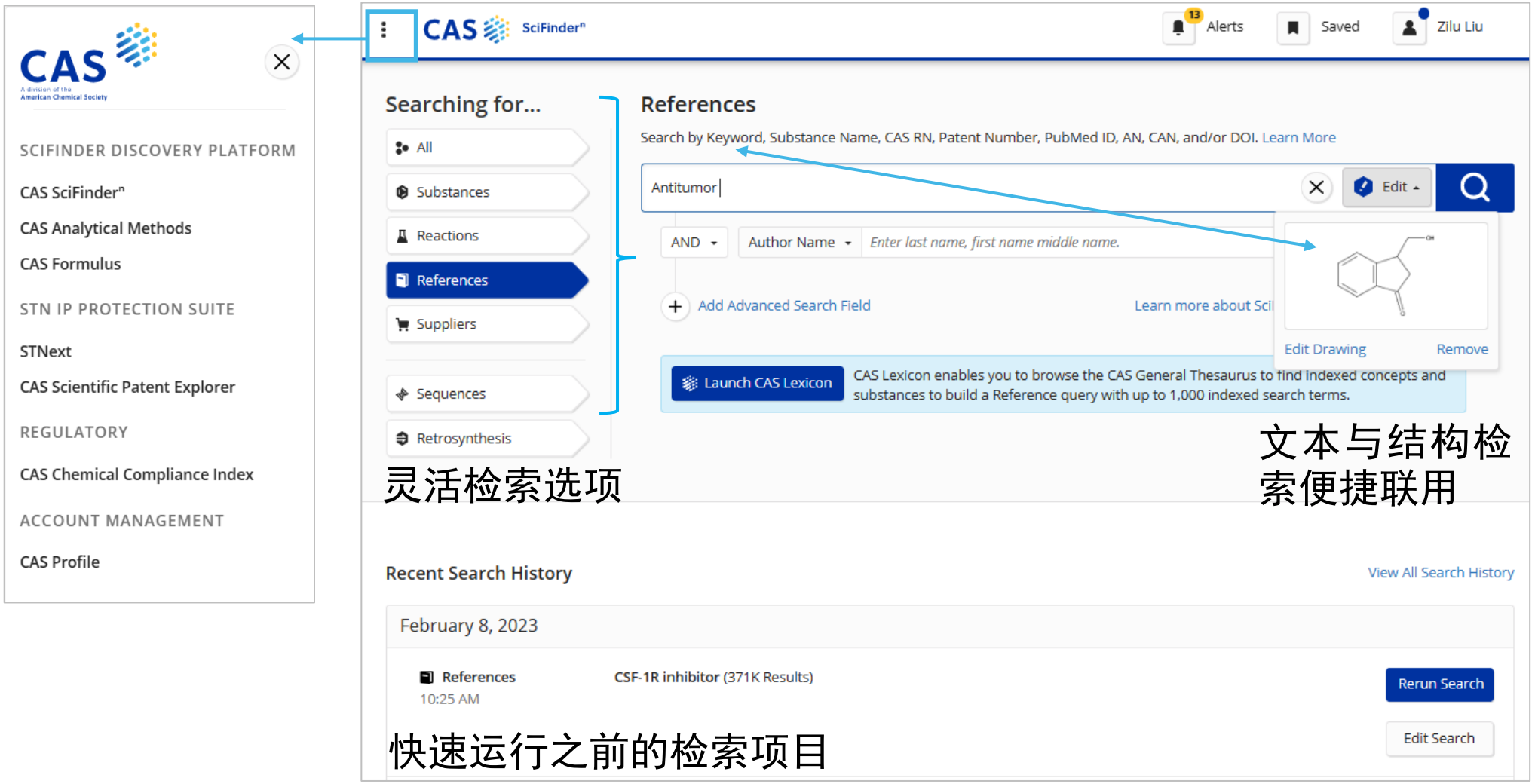




账号与CAS SciFinder相同

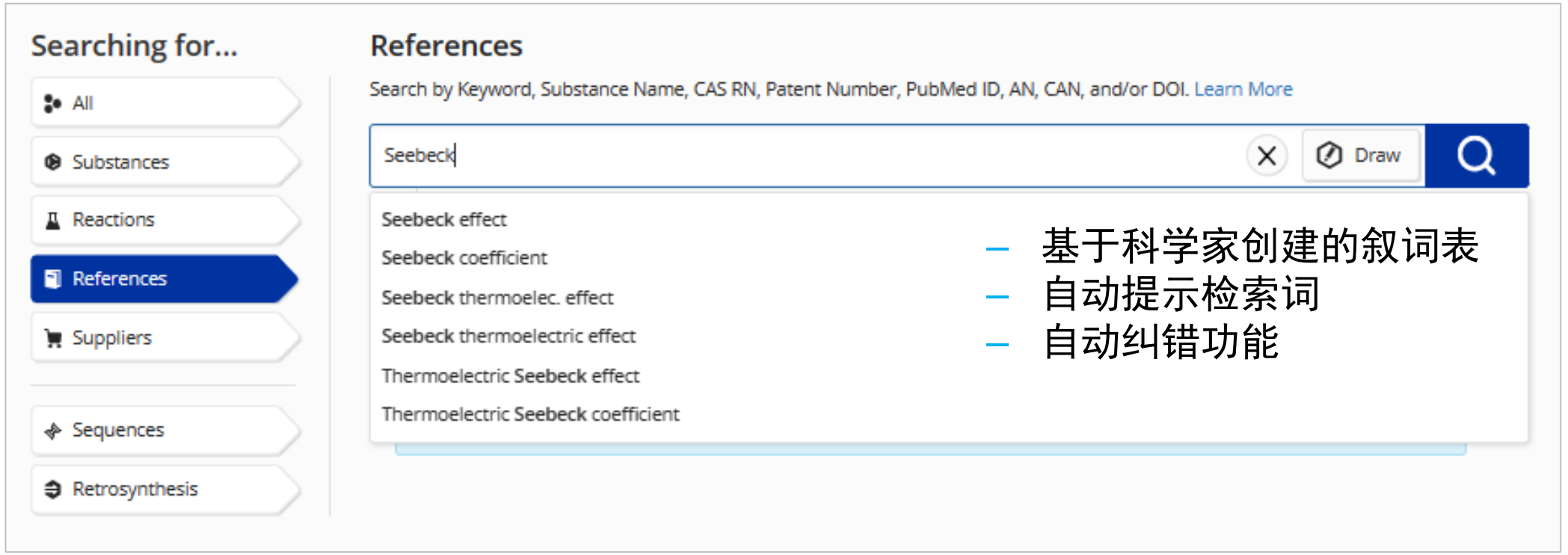
CAS
A division of the American Chemical Society

CAS SciFinder^{n}主界面



CAS
A division of the American Chemical Society

文献检索——主题词

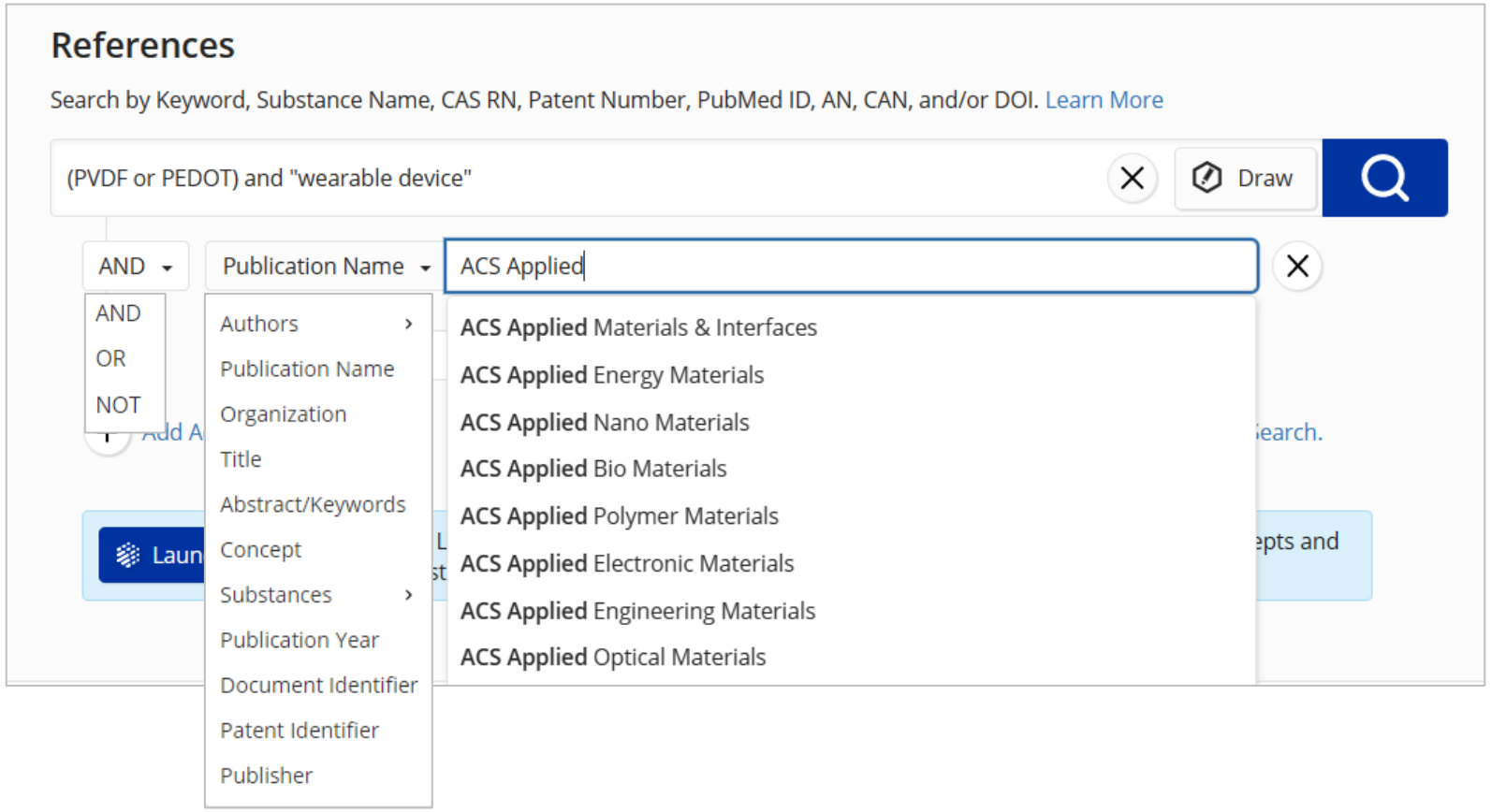


- 基于科学家创建的叙词表
- 自动提示检索词
- 自动纠错功能

- 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）

CAS
A division of the American Chemical Society

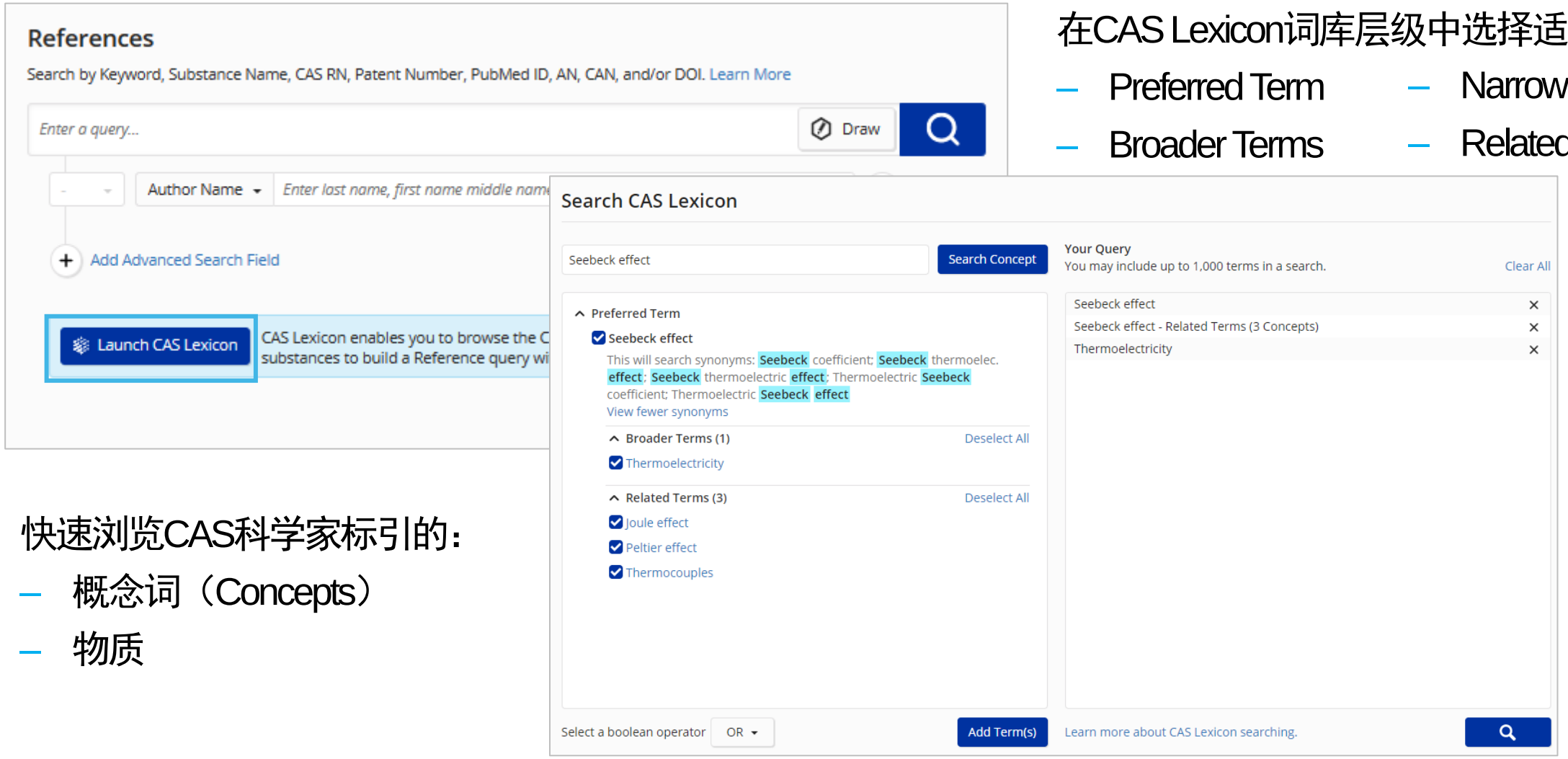
高级检索—高效实现多项自定义组合检索



- 可单独使用，或可联用以下检索方法：
- 关键词、物质名称、CAS RN®、文献号；
- 高级检索：刊物名、Concepts、物质等
- 结构检索

CAS
A division of the American Chemical Society

CAS Lexicon—利用词库选词启发检索



在CAS Lexicon词库层级中选择适合的主题词：

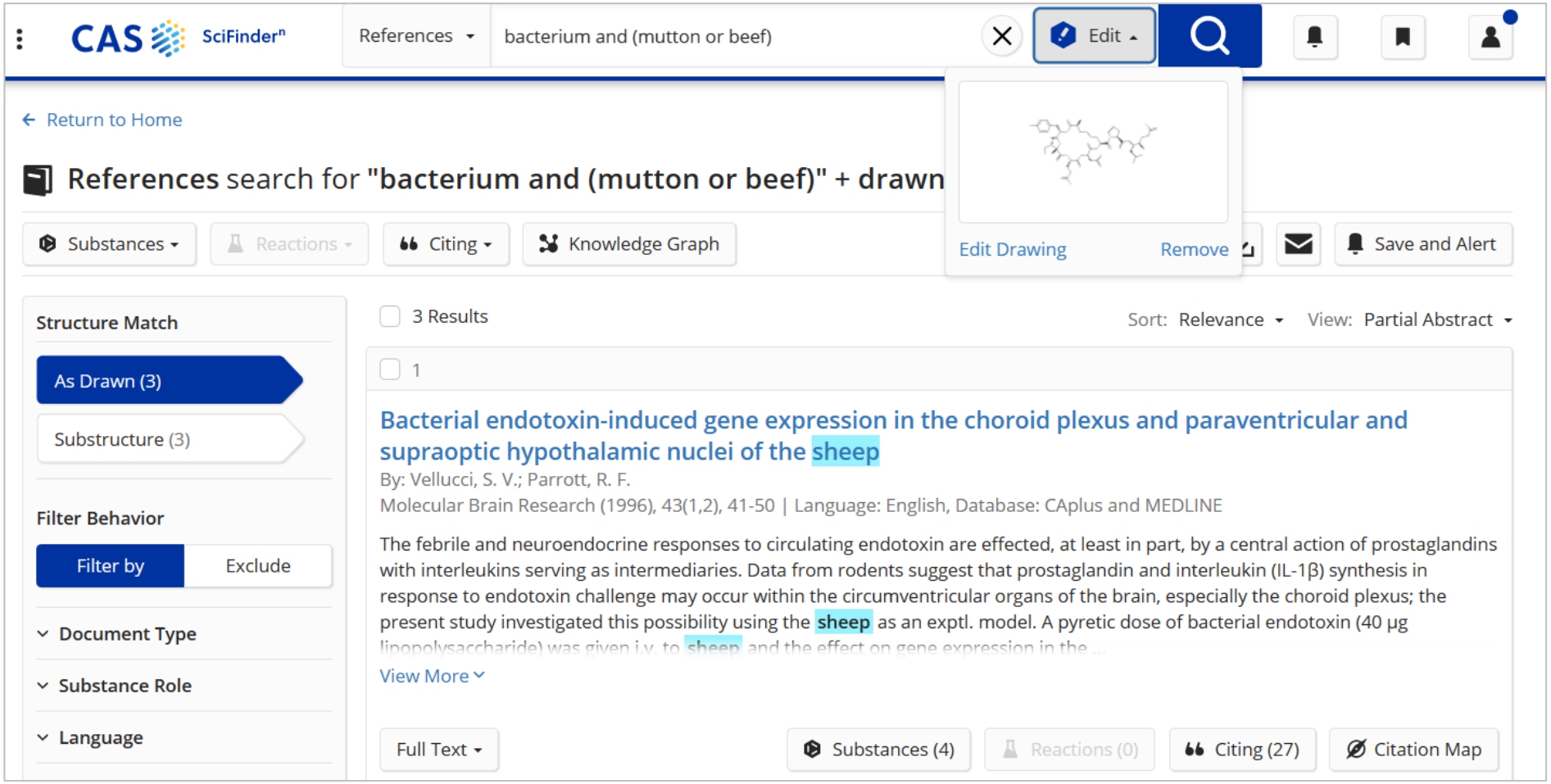
- Preferred Term
- Broader Terms
- Narrower Terms
- Related Terms

快速浏览CAS科学家标引的：

- 概念词（Concepts）
- 物质

CAS
A division of the American Chemical Society

文献检索—主题词+结构联合检索



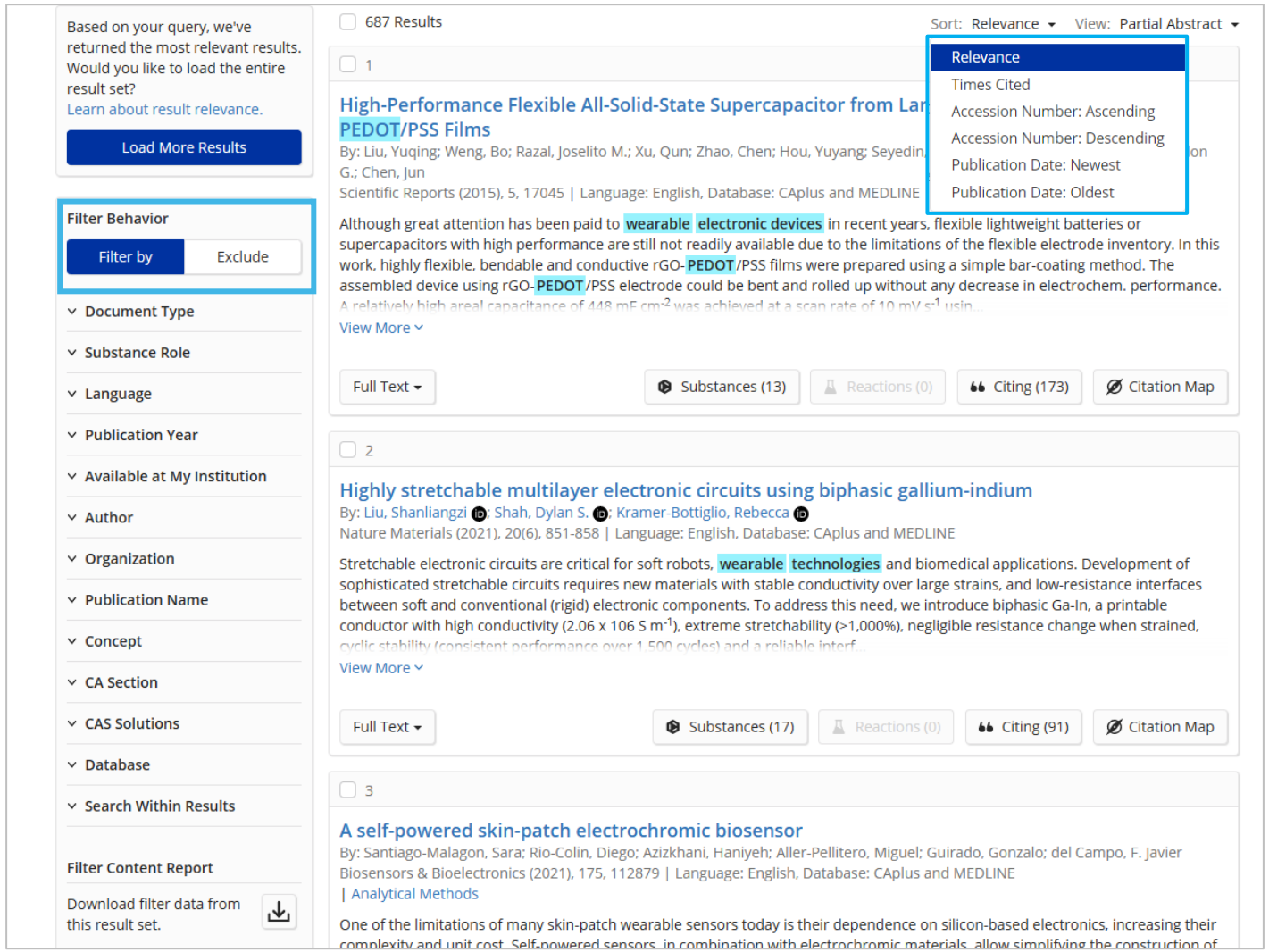
主题词+结构联合检索，大大提高检索的效率

CAS
A division of the American Chemical Society

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

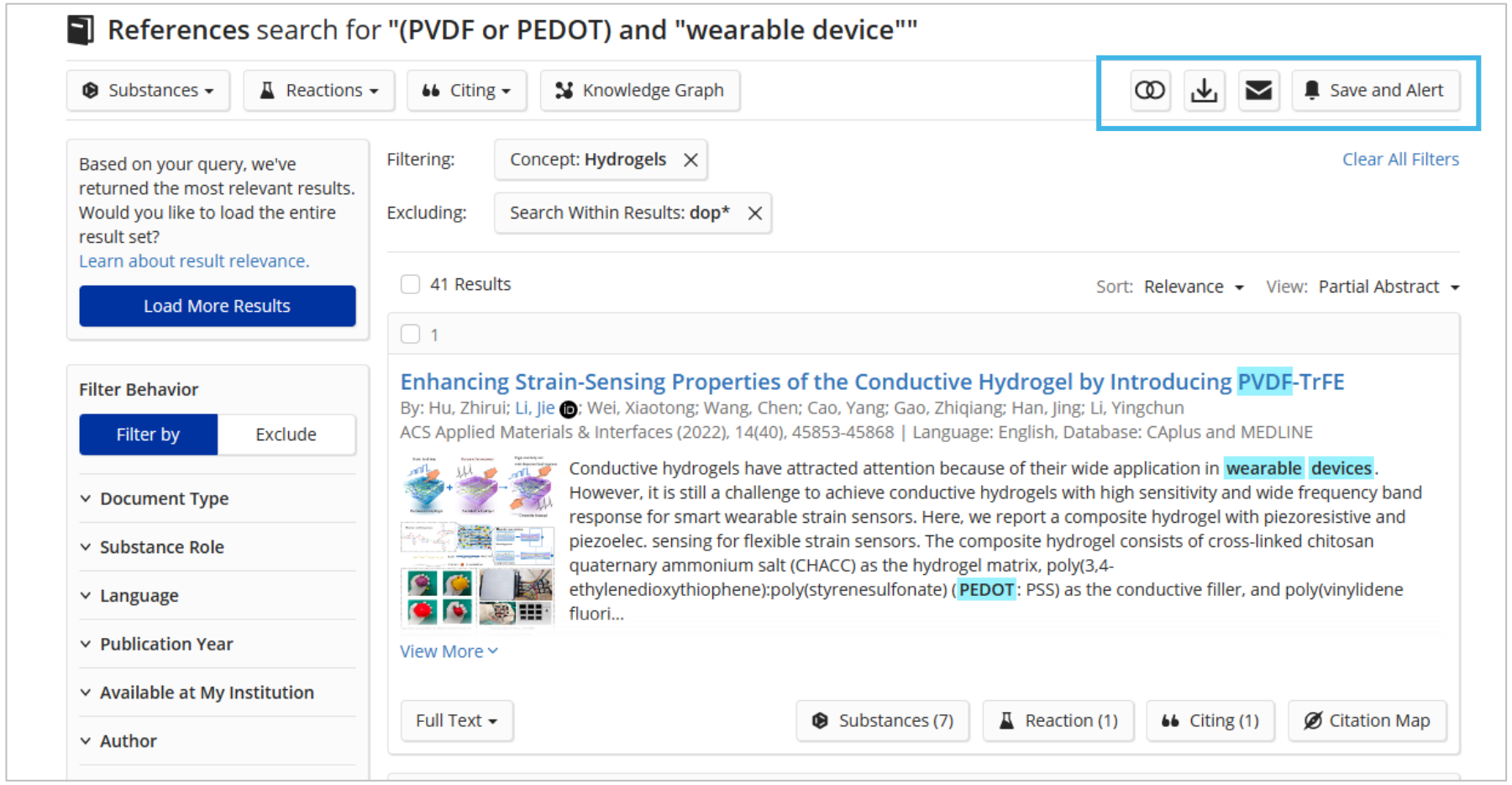
文献类型
文献语言
出版年份
作者
机构名
刊物名
Concept
CA Section
二次检索
……



- 排序：
- 更快锁定目标信息

CAS
A division of the American Chemical Society

文献结果集的处理、下载、保存及定题追踪

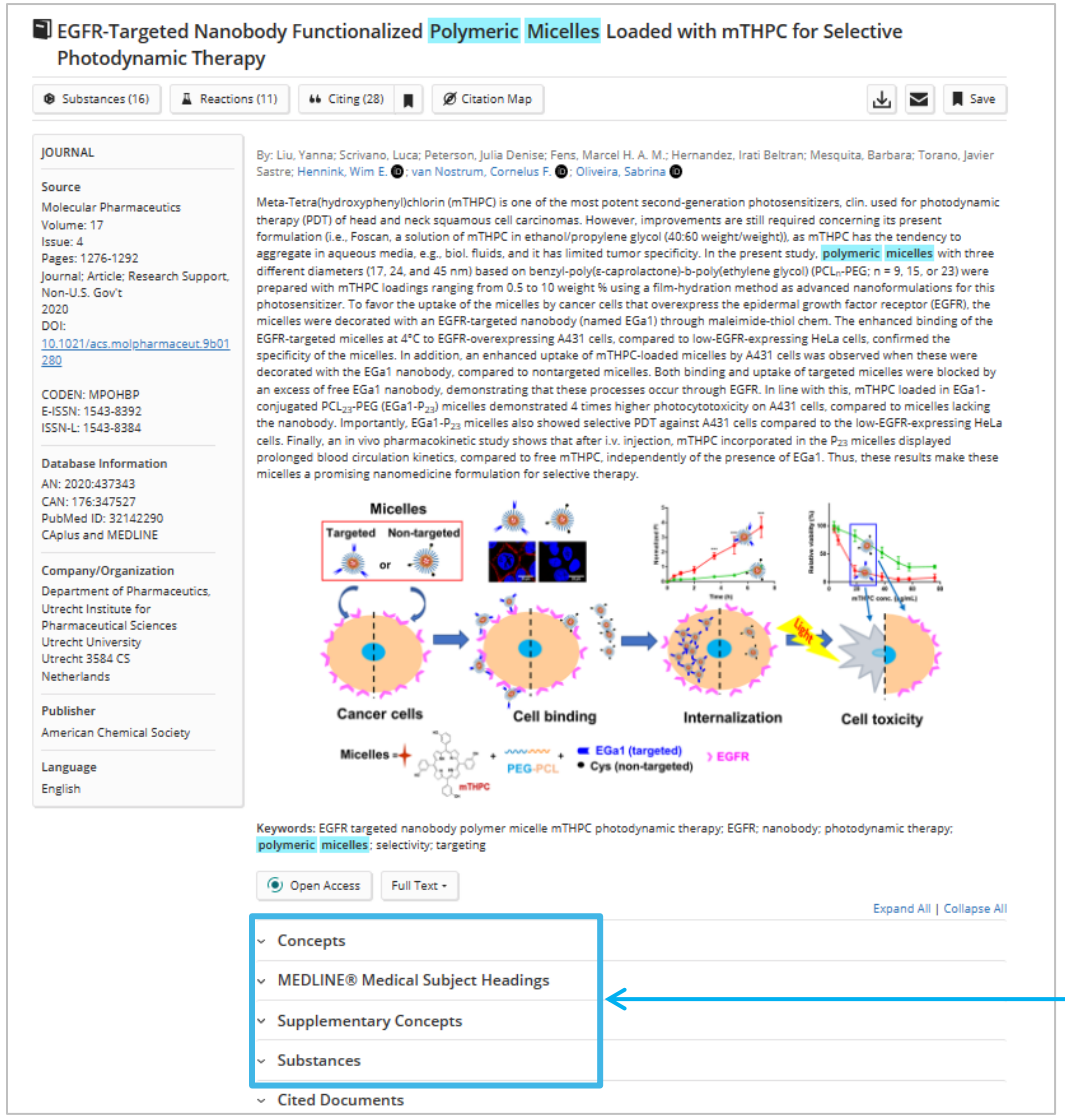


支持结果集的：

- 合并、交集和去重
- 下载保存
- 邮件分享
- 设置提醒

CAS
A division of the American Chemical Society

文献详情



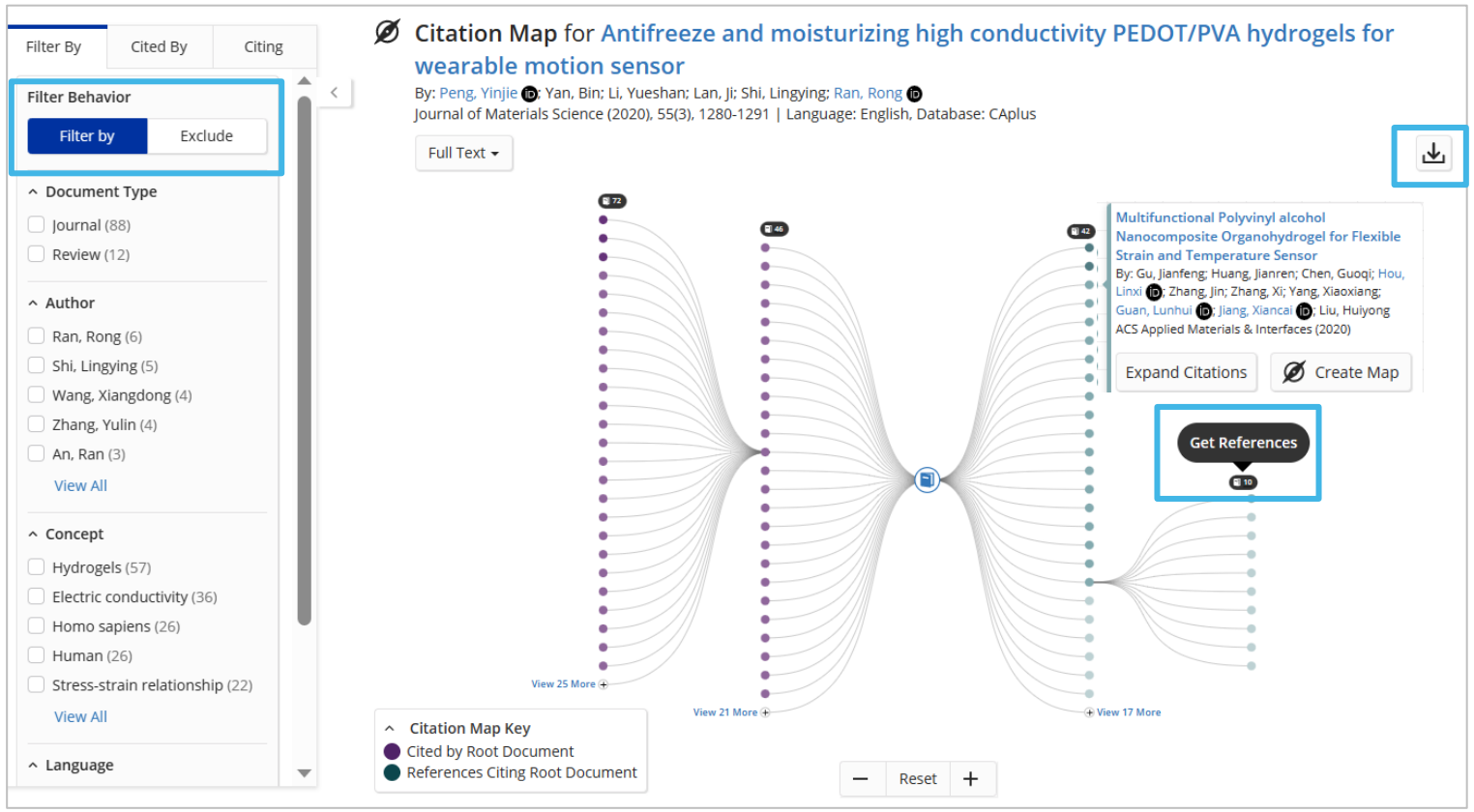
文献详情界面包括：

- 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

CAS
A division of the American Chemical Society

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

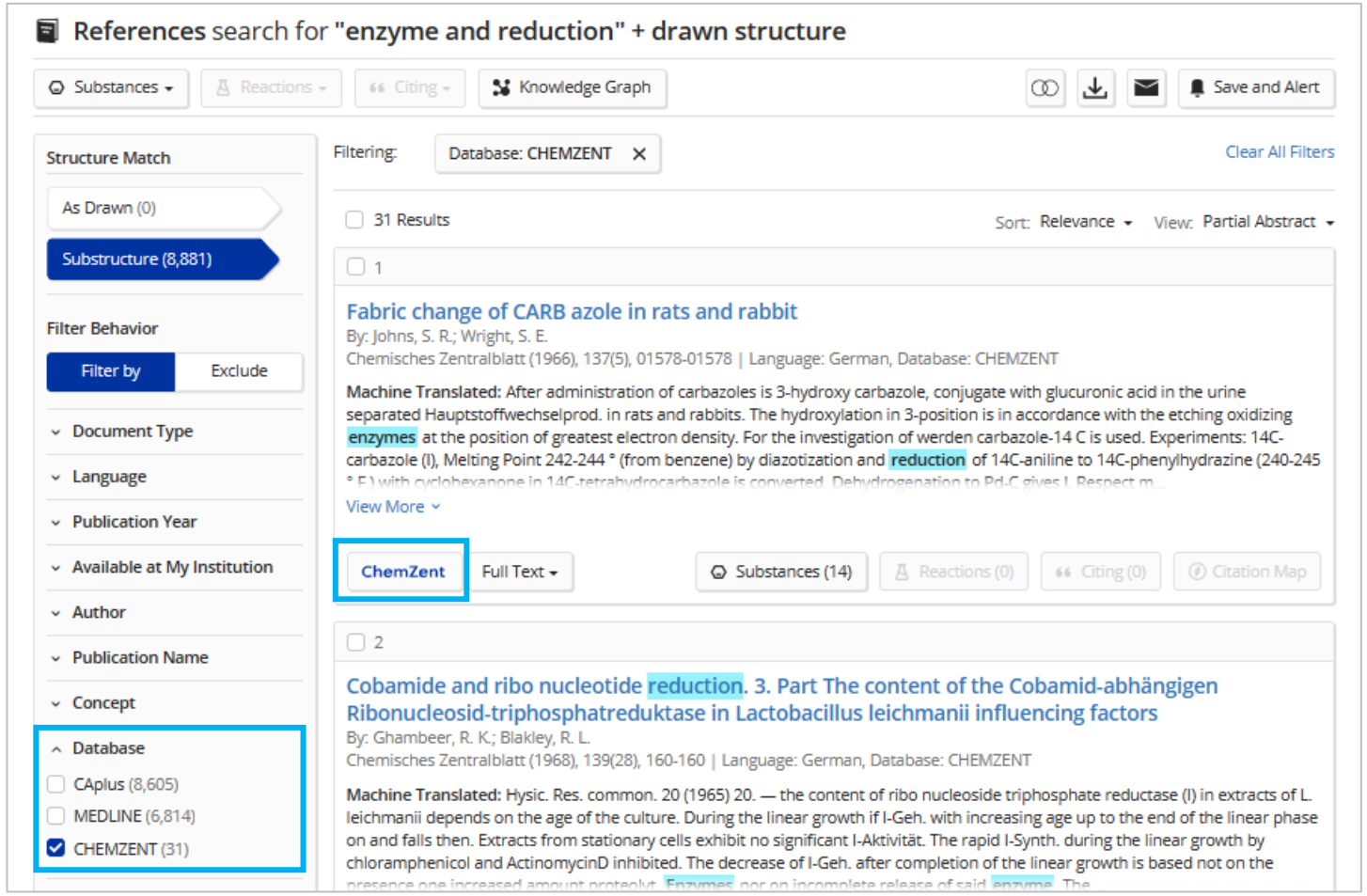
Citations: 参考文献

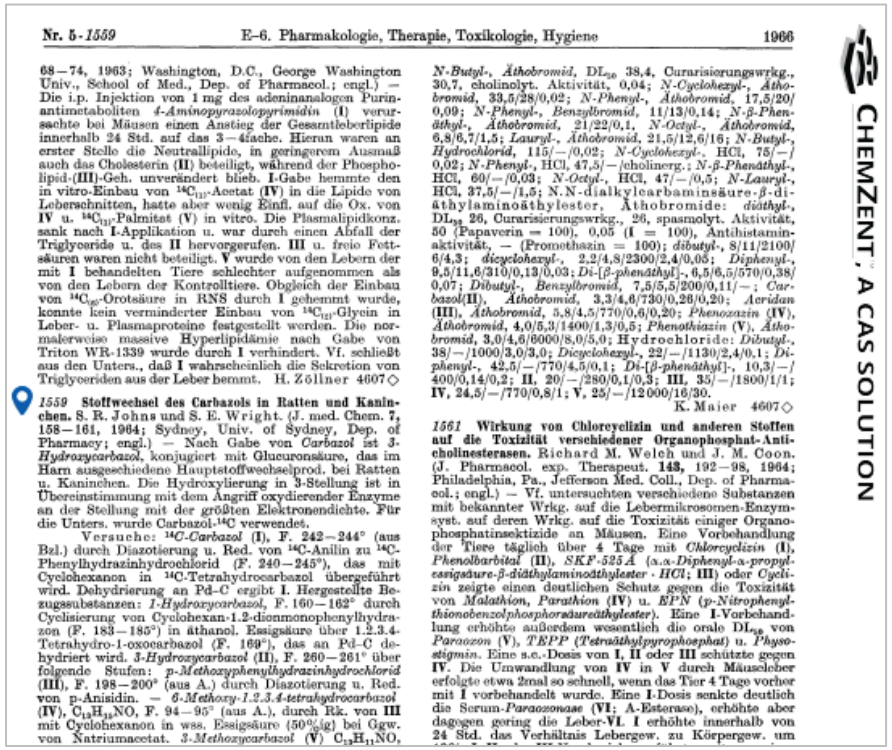
Cited By: 引用当前文献的文献

CAS
A division of the American Chemical Society

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





CAS
A division of the American Chemical Society

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
- 安全、快捷地获得来自全球46个专利授权机构的PDF格式专利文件
  - 无需在多个不同专利局网站上耗费时间
  - 可获得的专利数量是其他科学信息检索工具的7倍
  - 新的专利文件每日上传更新
- 通过CAS PatentPak浏览器，快速定位专利PDF文件中的重要物质页码信息， 迅速找到难以查找的化学信息，可为研究人员节省一半以上的时间
- 在CAS专利族文献中找到您所熟悉语言的专利

CAS
A division of the American Chemical Society

专利文献详情

PATENT

Patent Number
WO2015011254

Publication Date
2015-01-29

Application Number
WO2014-EP66007

Application Date
2014-07-25

Kind Code
A1

Assignee
INSERM (Institut National de la Sante et de la Recherche Medicale), France

Universite de Droit et de la Sante

Institut Pasteur de Lille, France

Universite de Lille 1 Sciences et Technologies, France

ETH Zurich, France

Universidad de la Republica, France

Source
World Intellectual Property Organization
CODEN: PIXXD2

CAN: 162:266207
CAplus

Language
English

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

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

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, polymixins, and lipopeptides.

Keywords: antibacterial toll like recept tic TLR agonist antibacterial combination therapy bacterial infection

获取现有技术文献

PatentPak Viewer | Get Prior Art Analysis | Full Text

专利族信

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

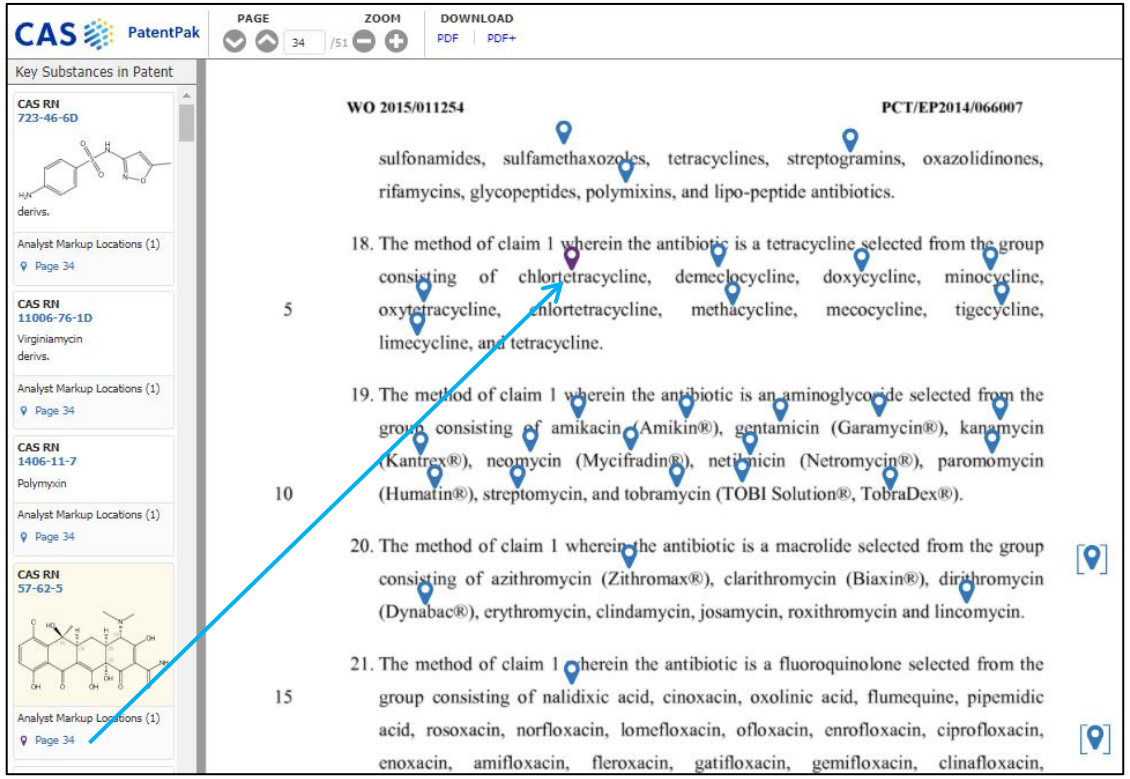
优先权信

Priority Application

Priority Application Number	Application Date
EP2013-306086	2013-07-26
EP2014-749736	2014-07-25
WO2014-EP66007	2014-07-25

Expand All | Collapse Al

IPC Data



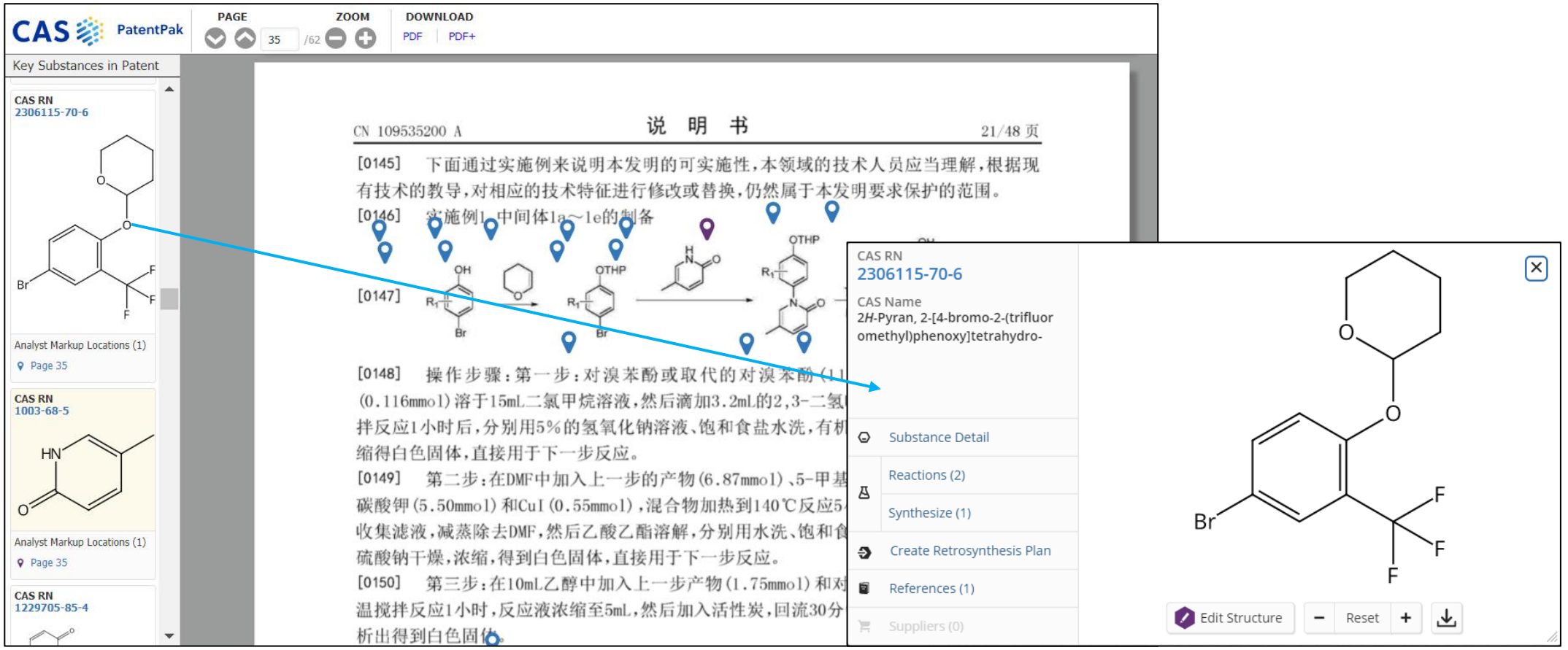
CAS PatentPak：

- 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

CAS
A division of the American Chemical Society

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



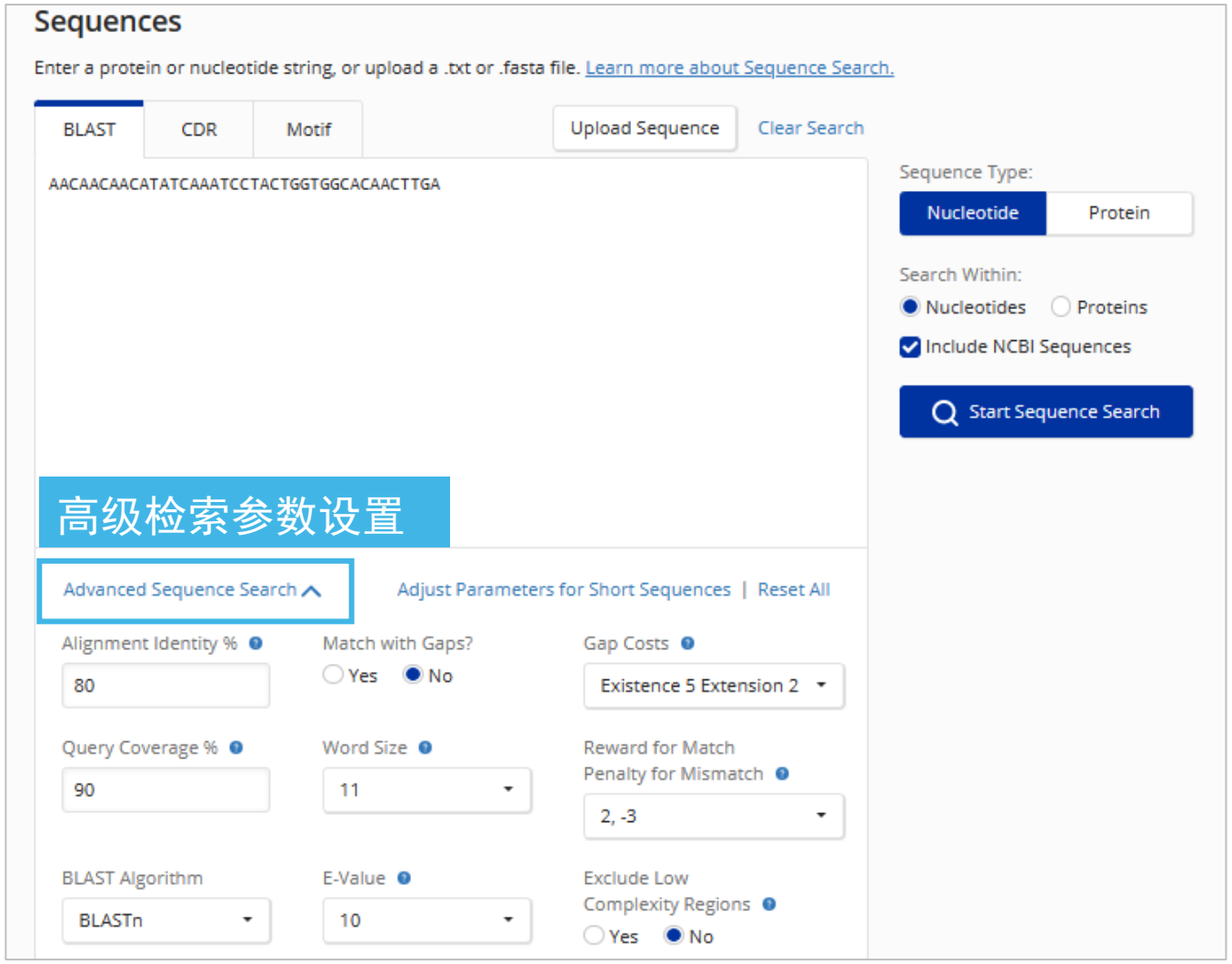
CAS
A division of the American Chemical Society

CAS Sequences™—分子生物学解决方案

- 超过14亿条序列
- 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
A division of the American Chemical Society

CAS Sequences™— Blast检索



BLAST：检索核酸或蛋白

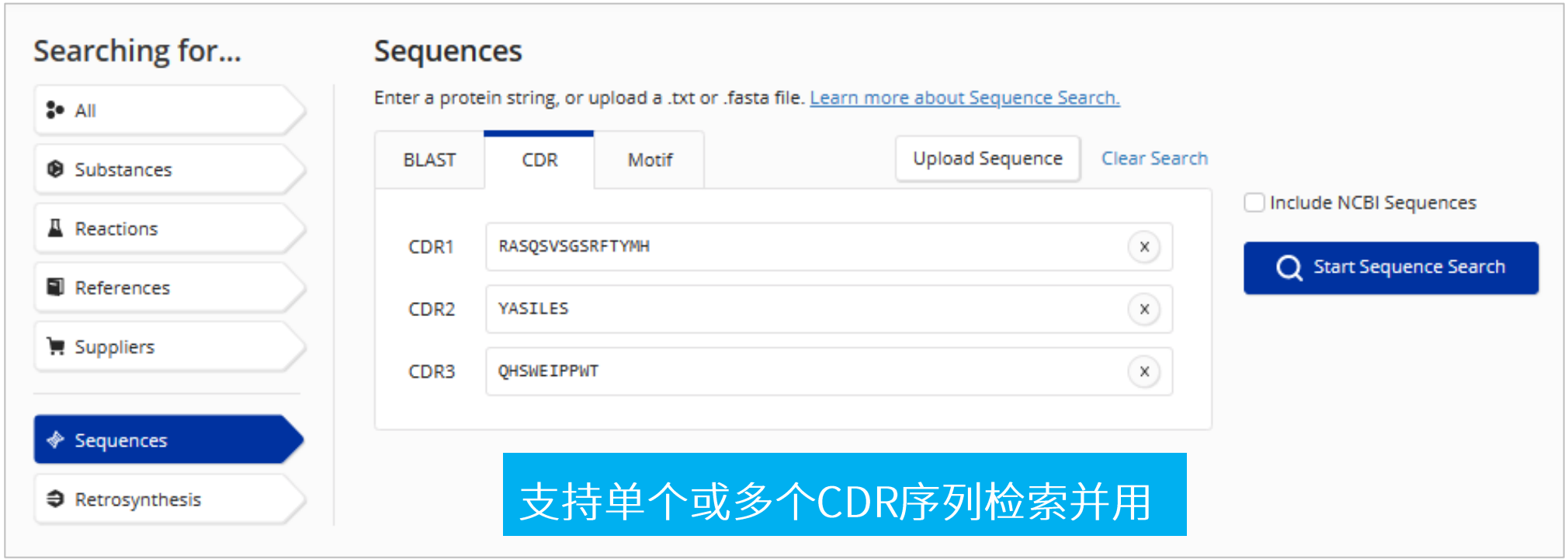
选择是否包含NCBI中的序列

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

CAS
A division of the American Chemical Society

CAS Sequences™—CDR检索

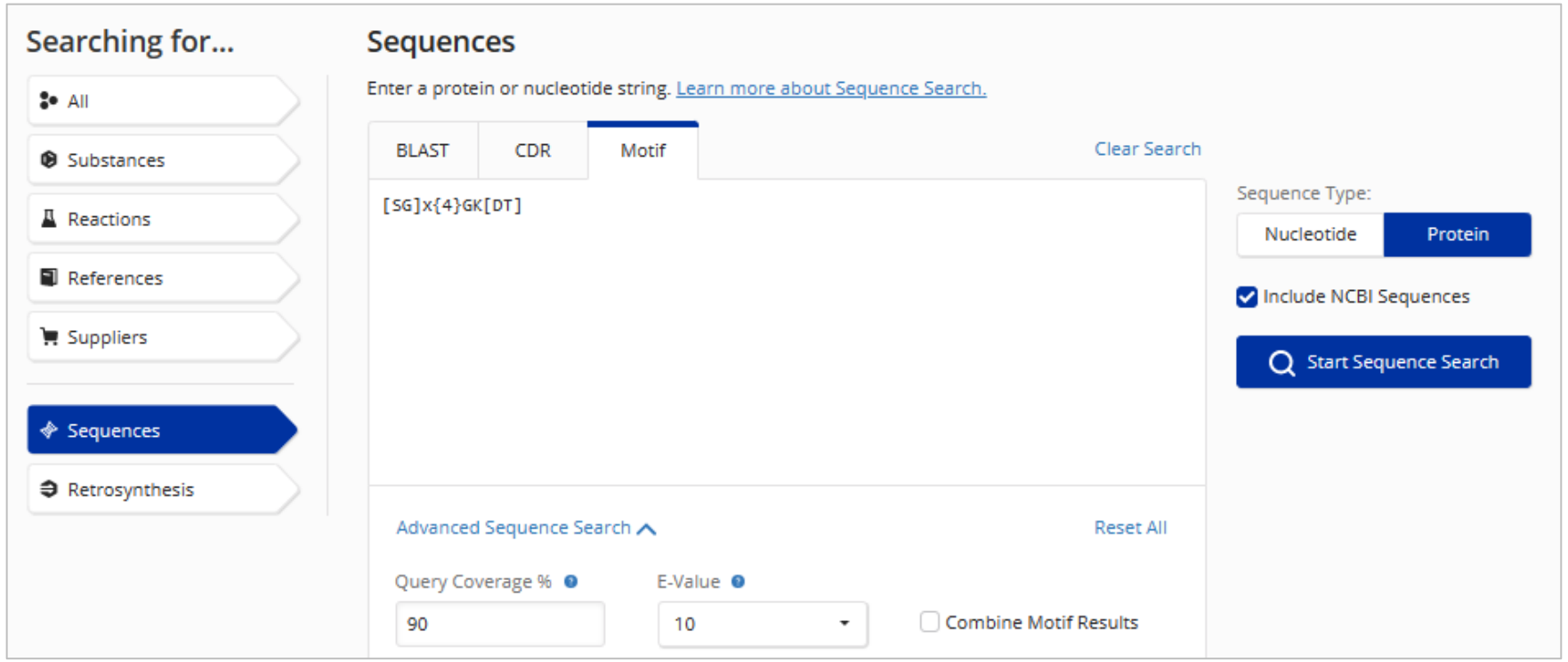
CDR: 抗体或细胞中的互补决定区



CAS
A division of the American Chemical Society

CAS Sequences™—Motif检索

Motif：可用于检索序列中有不确定位点的DNA、RNA或蛋白；推荐检索短序列。



- [ ]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

CAS
A division of the American Chemical Society

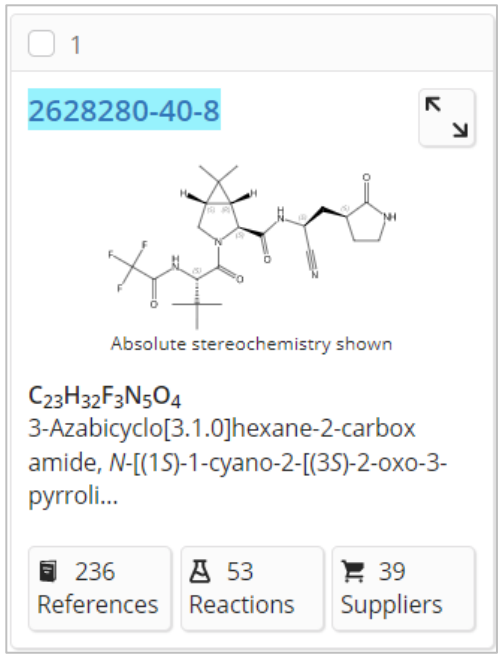
CAS Retrosynthesis Tool—逆合成工具

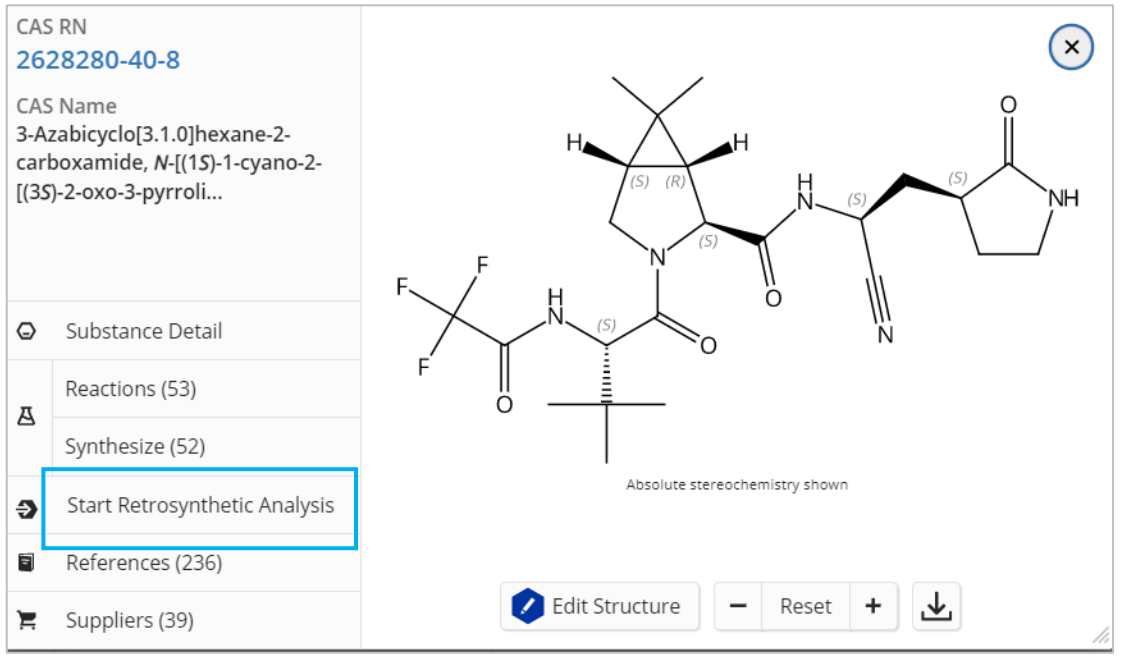
- 依据一个确定的结构进行设计
- 有报道且结构明确的物质，无论是否有反应信息报道
- 未报道且结构明确的物质
- 节省设计、实施合成新方法所花费的时间

CAS
A division of the American Chemical Society

CAS Retrosynthesis Tool—由物质获得

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



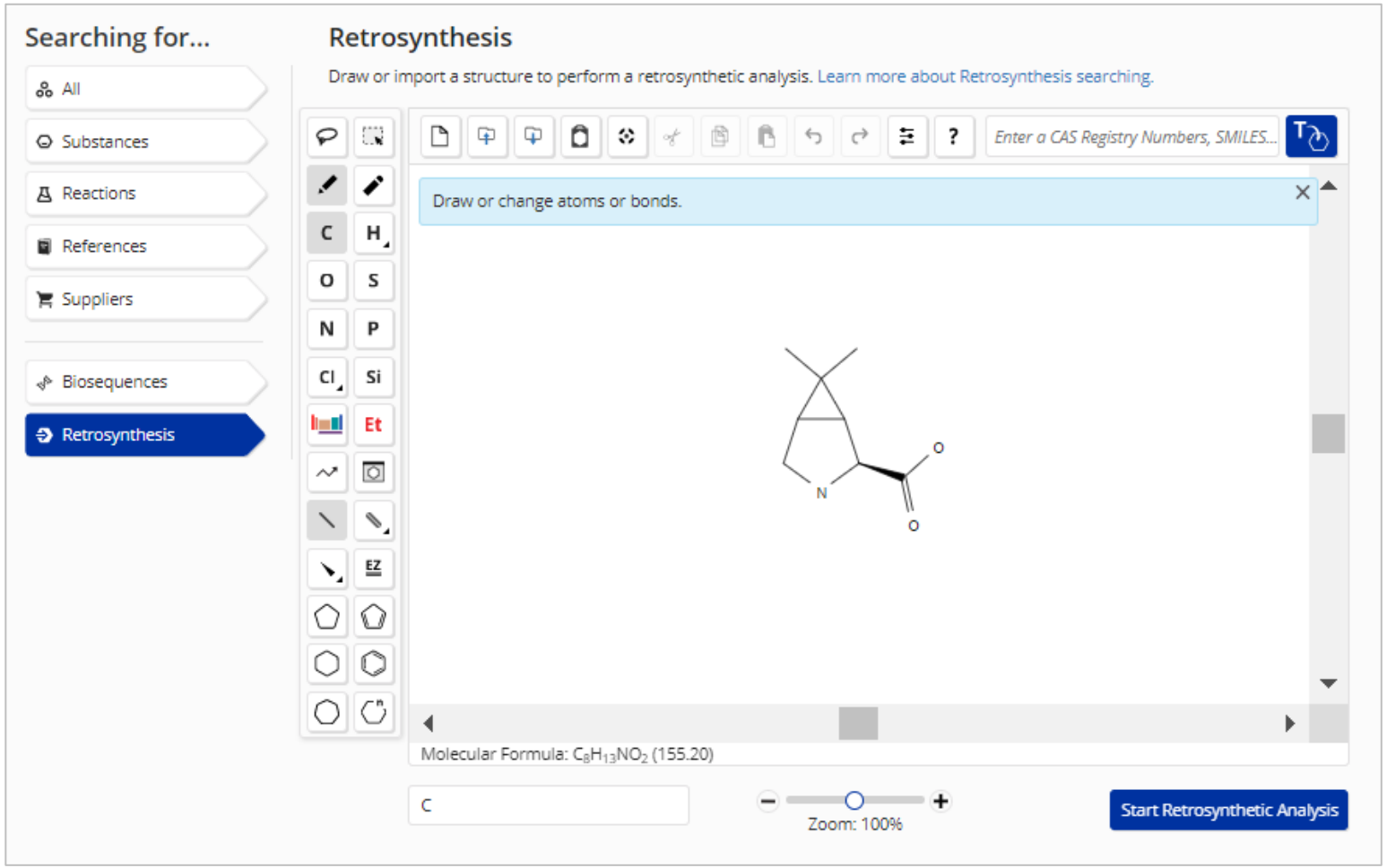


- 逆合成反应路线设计功能
- 启发合成实验设计思路
- 高效获取逆合成反应路线

CAS
A division of the American Chemical Society

CAS Retrosynthesis Tool—直接绘制结构

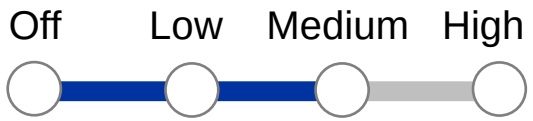
绘制目标化合物：
从Retrosynthesis检索项打开绘图板，绘制目标化合物，获得实验路线



CAS
A division of the American Chemical Society

CAS Retrosynthesis Tool—已知化合物

获得逆合成路线后，可继续通过Scoring灵活调整预测参数



Scoring Profiles：

降低每步原料结构的复杂性

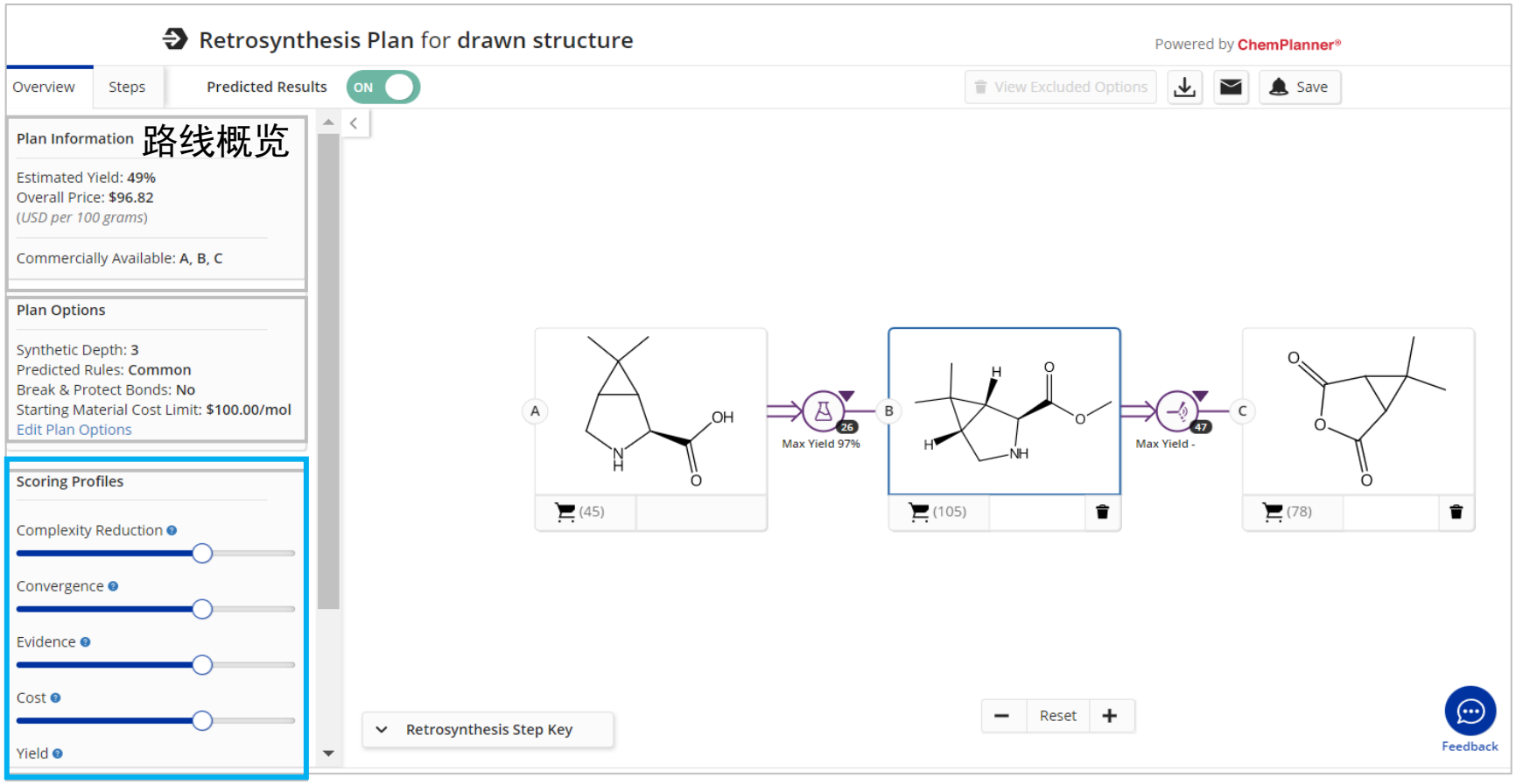
逆合成路线中前体的数量

支持预测路线的文献数量多少

预测路线大概成本

每步的产率

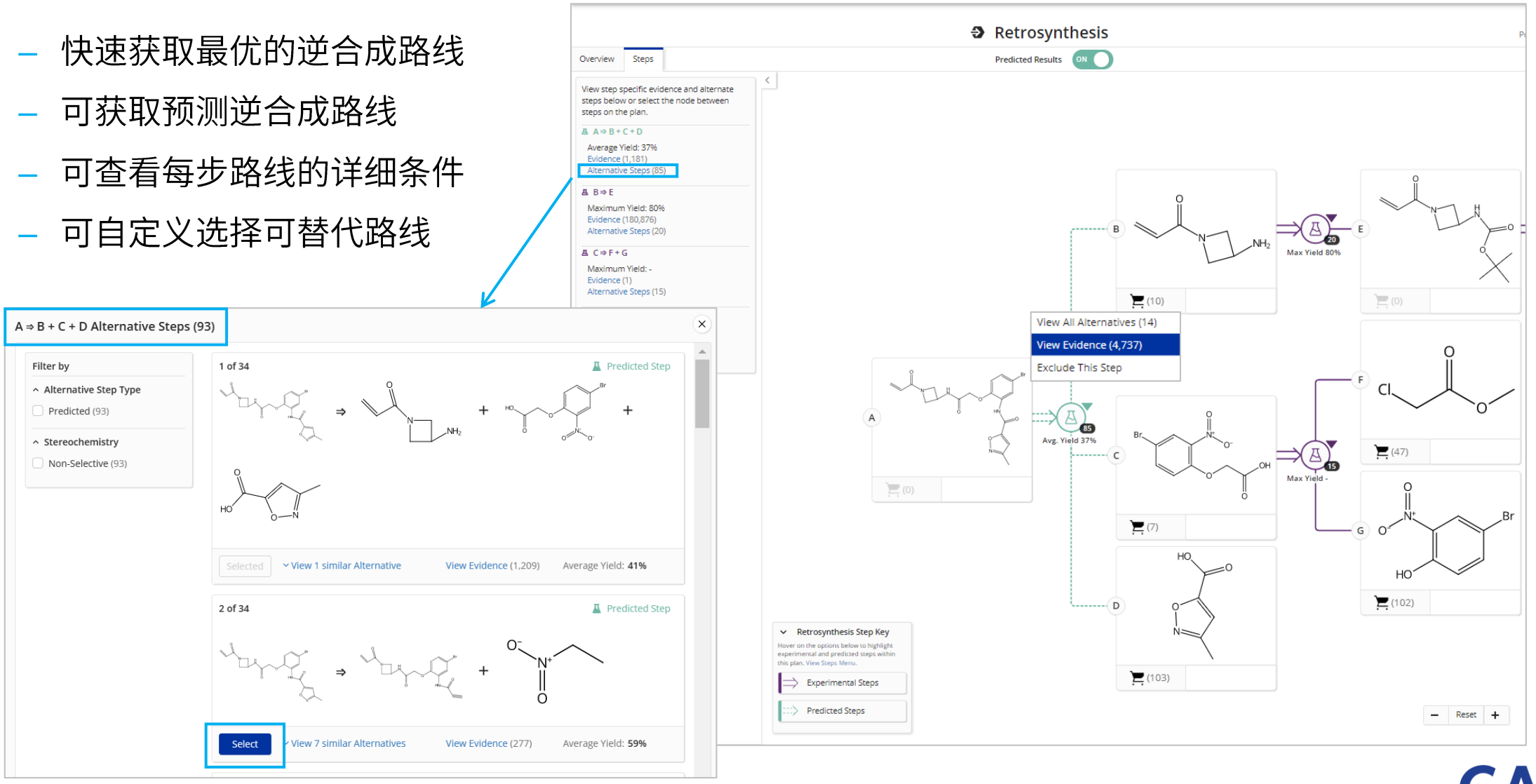
每步的原子转化效率



CAS
A division of the American Chemical Society

CAS Retrosynthesis Tool—已知化合物

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



CAS
A division of the American Chemical Society

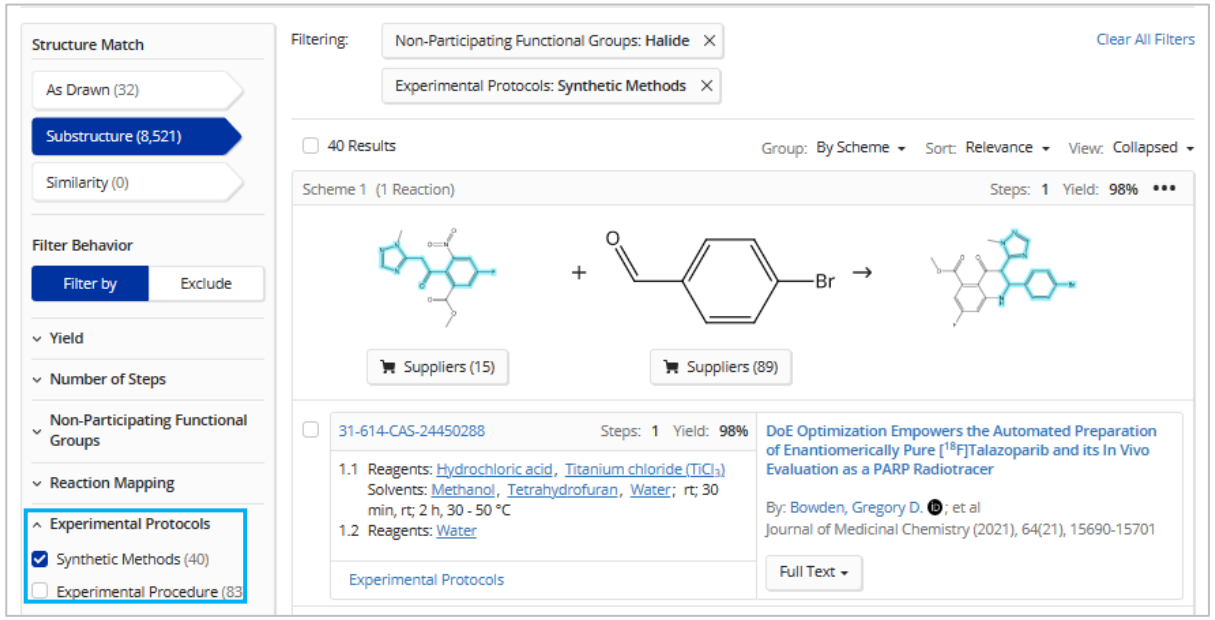
Synthetic Methods™: 合成方法详情解决方案

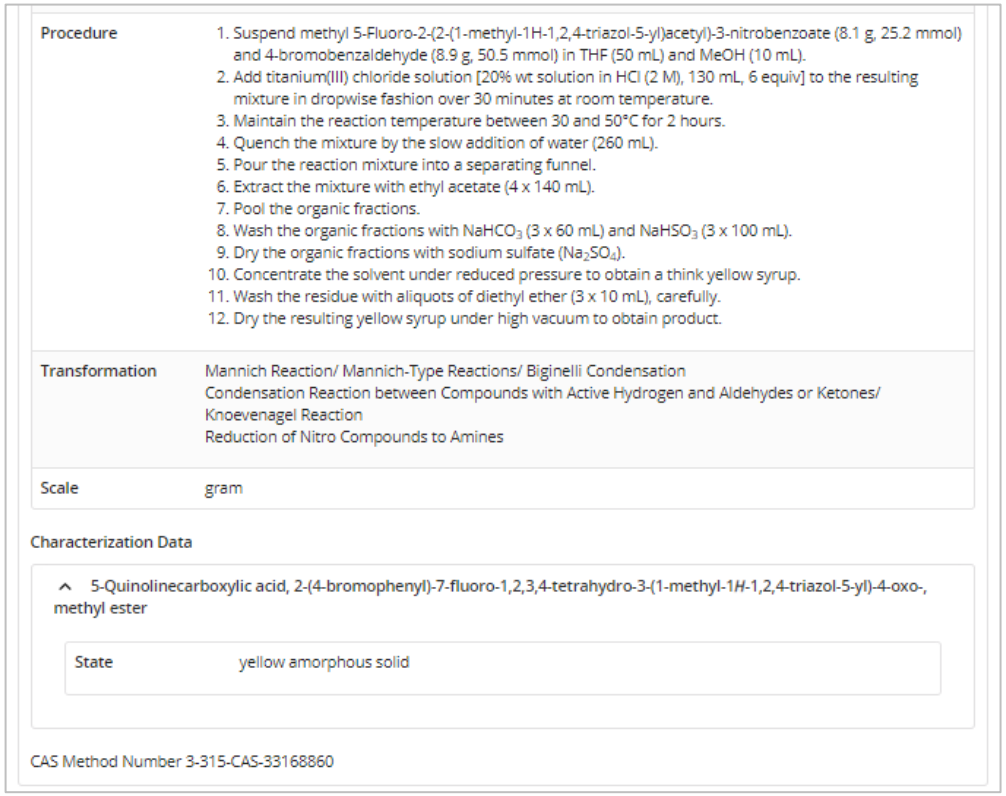
- 迄今为止全球最大的为合成科学家提供的实验方法详情解决方案
- CAS科学家通过分析大量的顶级科技期刊及专利原文，收集、整理、筛选出来的实验方法
- 无需下载阅读全文，即可获得合成实验所需的所有信息
- 极大节省在期刊全文中查找信息的时间

CAS
A division of the American Chemical Society

Synthetic Methods™: 合成方法详情解决方案

- 分类显示详尽信息，方便操作
- 不仅包含原文中描述的实验内容，还包括supporting information中涉及的实验内容





CAS
A division of the American Chemical Society

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
A division of the American Chemical Society

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…

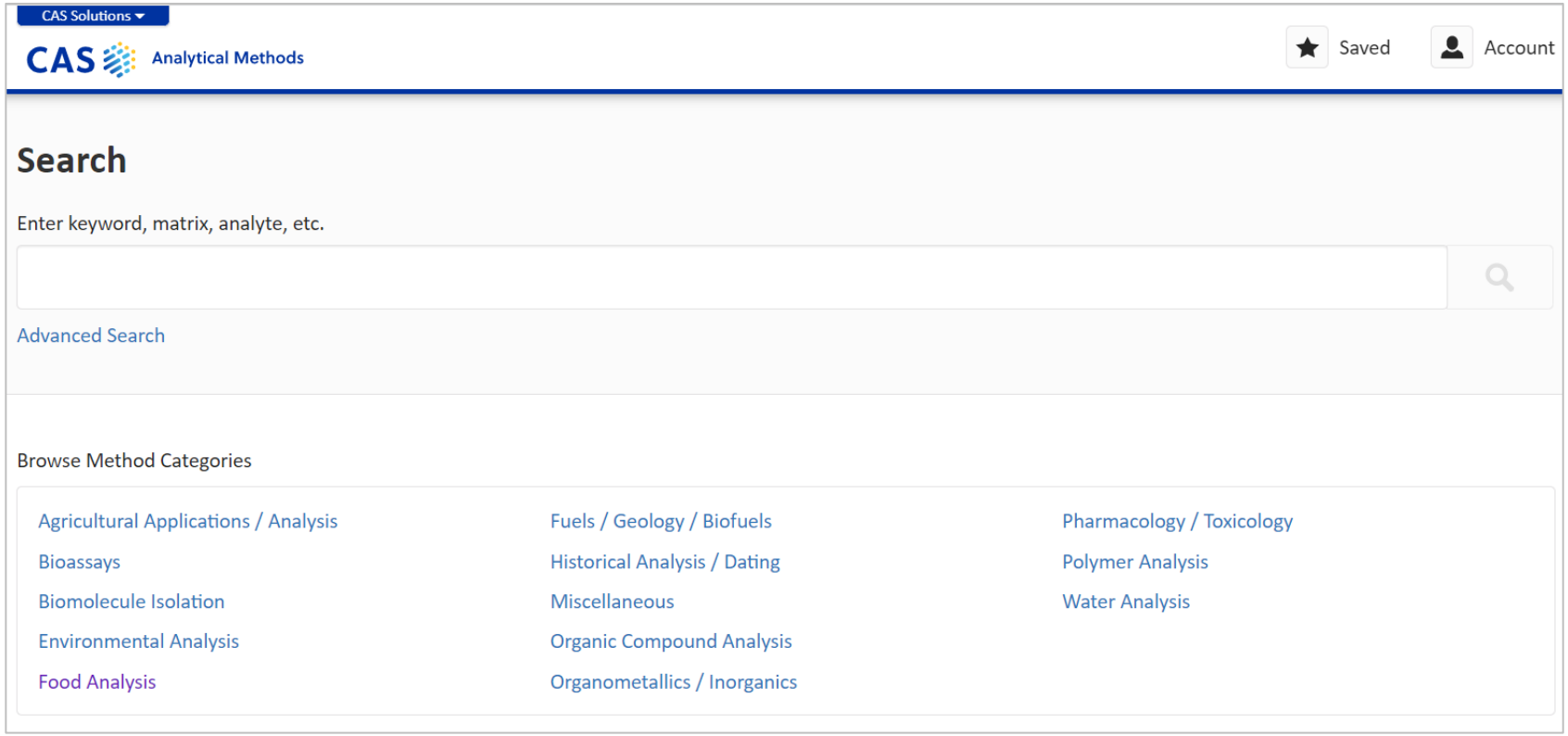
Polymer: 聚合物分析…

CAS
A division of the American Chemical Society

分析实验方法的获取

https://methods.cas.org（与SciFinder-n登录账号相同）

- 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



CAS
A division of the American Chemical Society

分析方法详情

Analysis of Titanium in Kerosene by Inductively coupled plasma mass spectrometry

CAS MN: 1-135-CAS-84928

Method Category: Petroleum Product Analysis

Technique: Inductively coupled plasma mass spectrometry

实验原料

Materials	Role	Image	CAS RN
Cadmium	analyte	View Structure	7440-43-9
Mercury	analyte	View Structure	7439-97-6
Lead	analyte	View Structure	7439-92-1
Silver	analyte	View Structure	7440-22-4
Iron	analyte	View Structure	7439-89-6
Vanadium	analyte	View Structure	7440-62-2
Tin	analyte	View Structure	7440-31-5
Titanium	analyte	View Structure	7440-32-6
Chromium	analyte	View Structure	7440-47-3

Equipment Used

实验仪器

ICP-MS system, Elan 6000, PE-SCIEX1, PerkinElmer, ON, Canada

Microflow nebulizer

Syringe pump, 140C, Applied Biosystems, Foster City, CA, USA

Pump, Smartline Pump 1000, Knauer, Berlin, Germany

Thermostat, Neslab RTE-111, Thermo Fisher Scientific, Waltham, MA

分析条件

Conditions

Instrument

RF power: 1300 W; Ar nebulizer gas: 0.8 L/min and auxiliary O_2 flow: 45 mL/min; integration time per isotope: 20 ms

Flow rate: 20 µL/min

操作步骤

Instructions

Sample Preparation

1. Collect petroleum samples (kerosene, gasoline and full range gas condensate).

Standards Preparation

1. Use conostans monoelemental standards in oil (1000 mg/kg) and multielemental S-21 oil (100 mg/kg) as standards.

ICP-MS analysis

1. Analyze the sample using a PerkinElmer Elan 6000 (PE-SCIEX1, ON, Canada).
2. Introduce the sample using microflow nebulizer consisting of a fused silica capillary of 180 µm i.d. (375 µm o.d.) and heated spray chamber (jacketed to allow the

Source

Sensitivity improvement in ICP MS analysis of fuels and light petroleum matrices using a microflow nebulizer and heated spray chamber sample introduction

Caumette, Guilhem; Lienemann, Charles-Philippe; Merdrignac, Isabelle; Paucot, Hugues; Bouyssiere, Brice; Lobinski, Ryszard

Talanta (2009), 80 (2), 1039 - 1043. Elsevier B.V.

CODEN: TLNTA2 | ISSN: 00399140 | DOI: 10.1016/j.talanta.2009.08.017 | View in SciFinder[n]

文献来源

Full Text

Abstract

Reasons for signal suppression during the anal. of light petroleum matrixes by inductively coupled plasma mass spectrometry (ICP MS) were examined A decrease of the ionization efficiency of the plasma was the principal factor responsible for this loss of sensitivity. Consequently, an interface based on a total consumption micronebulizer and a heated spray chamber was constructed to alleviate this problem. A method based on flow-injection ICP MS using this interface was developed for the direct multielement anal. of undiluted fuels (gasoline, kerosene) and gas condensates offering an increase in sensitivity by at least a factor of 3-4 in comparison with the existing setups.

Validation

数据有效性

Linearity Range	1 - 250 µg/kg
Limit of Detection	0.8 µg/kg (gasoline), Titanium
	0.1 µg/kg (gasoline), Vanadium
	5 µg/kg (gasoline), Chromium
	7 µg/kg (gasoline), Iron
	0.04 µg/kg (gasoline), Silver
	0.3 µg/kg (gasoline), Cadmium
	0.2 µg/kg (gasoline), Tin
	1 µg/kg (gasoline), Mercury
	0.1 µg/kg (gasoline), Lead

CAS
A division of the American Chemical Society

直观的分析方法对比

Compare Methods

Expand All | Collapse All

	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)

CAS
A division of the American Chemical Society

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
A division of the American Chemical Society

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

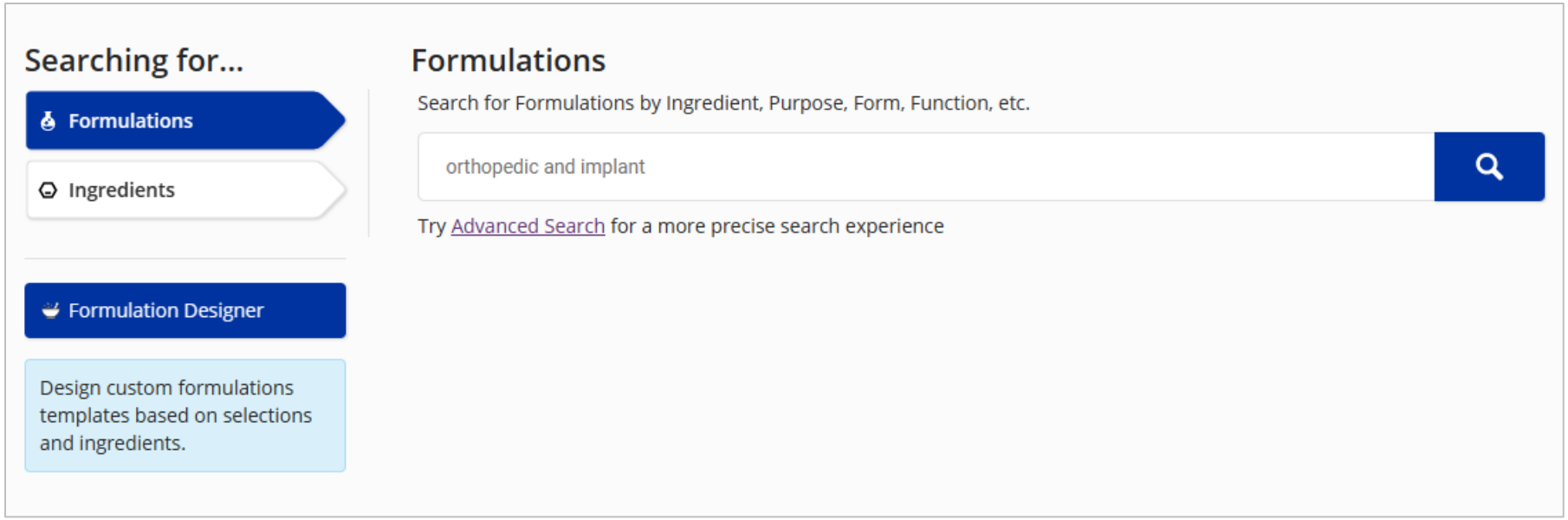
检索配方或制剂

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

配方/制剂检索

原料检索

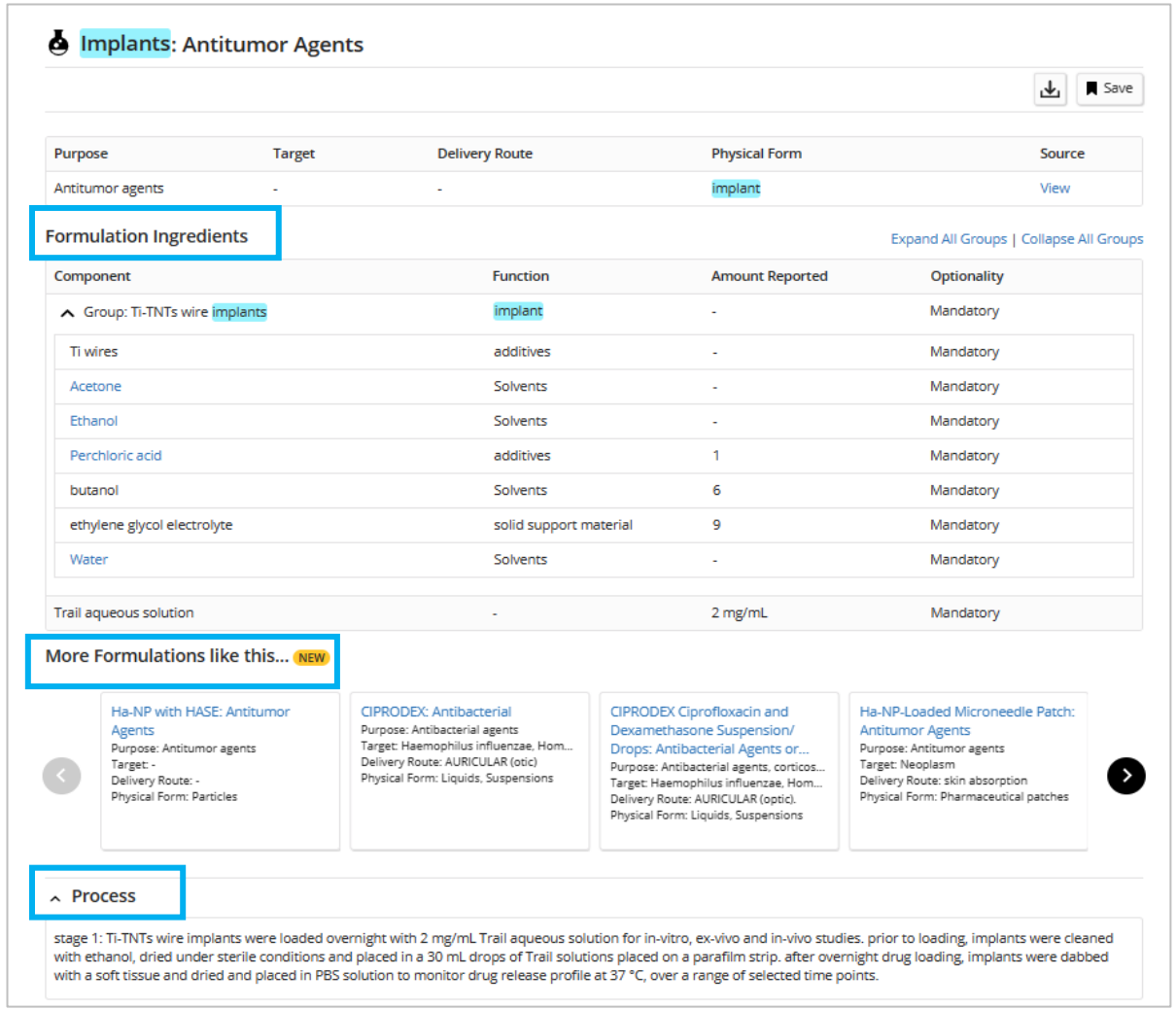
配方/制剂设计

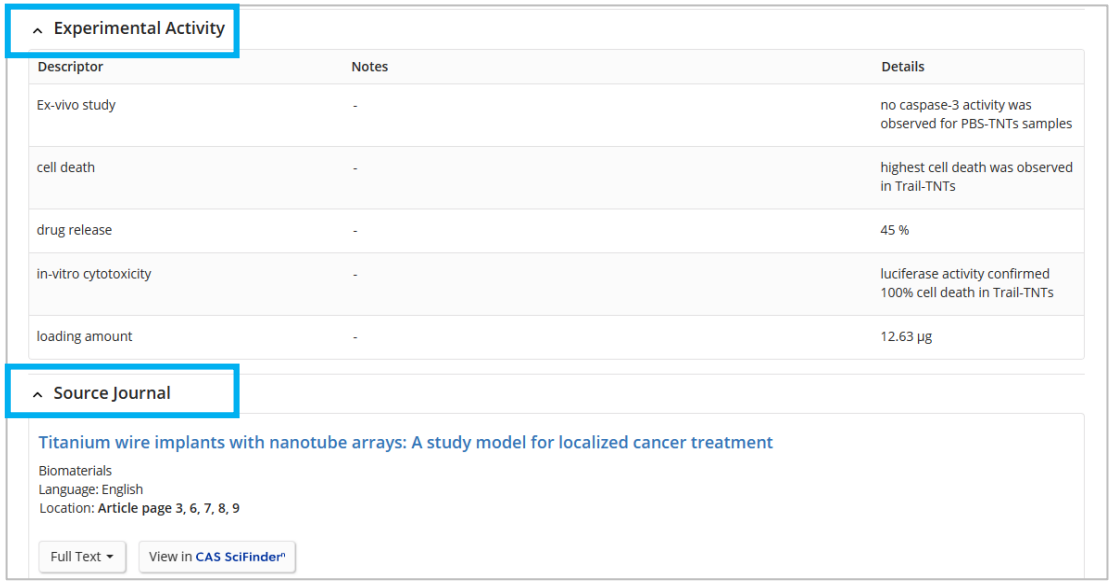


在检索框输入检索式，如制剂或配方的原料、用途、物理形态、功能或文献识别符进行检索

CAS
A division of the American Chemical Society

制剂或配方详情

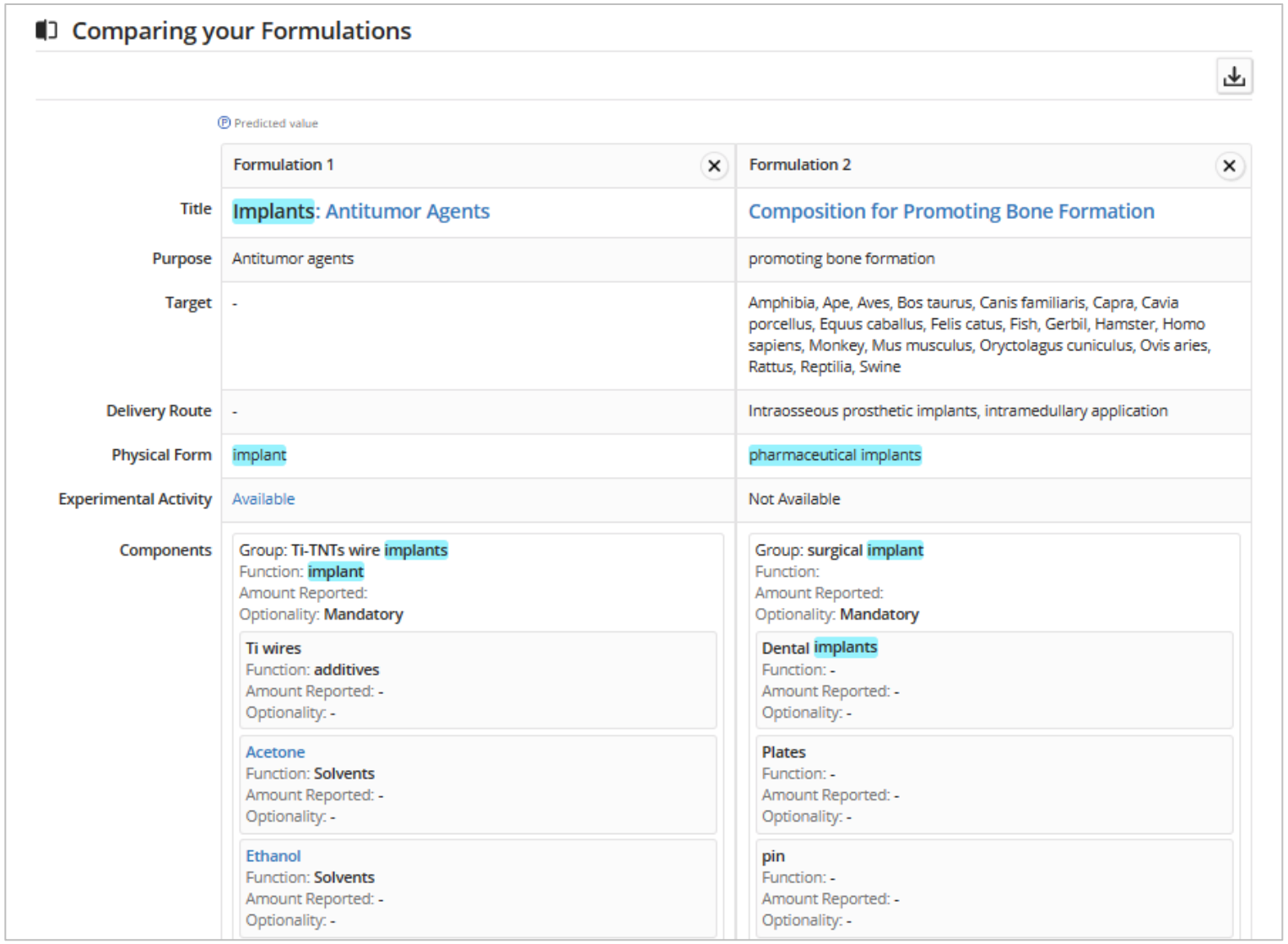




- 制剂或配方原料
- 相似的制剂或配方
- 制备工艺
- 制剂或配方实验评估
- 专利来源

CAS
A division of the American Chemical Society

不同制剂或配方信息的直观对比



Comparing your Formulations

Predicted value

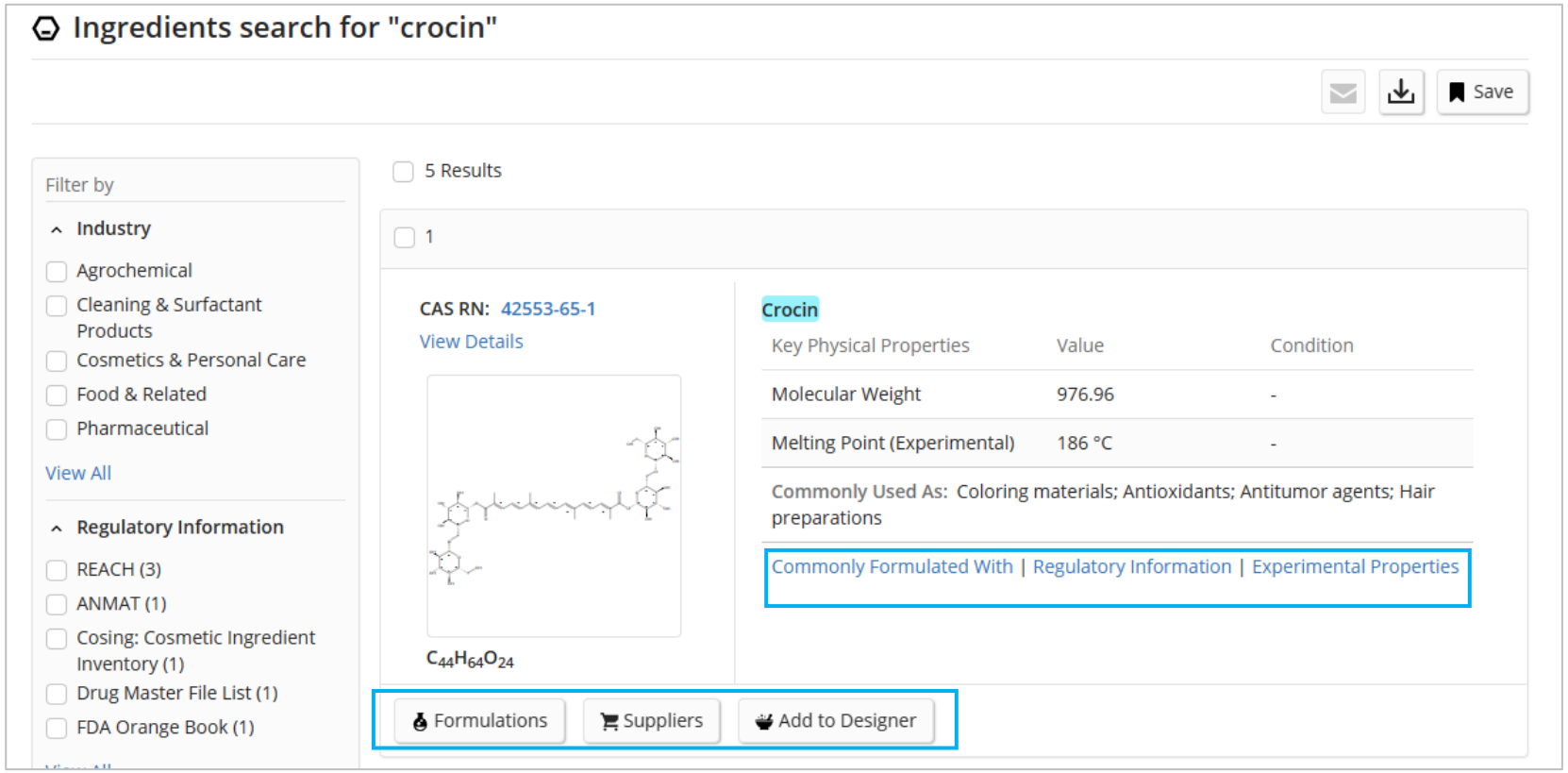
	Formulation 1	Formulation 2
Title	Implants: Antitumor Agents	Composition for Promoting Bone Formation
Purpose	Antitumor agents	promoting bone formation
Target	-	Amphibia, Ape, Aves, Bos taurus, Canis familiaris, Capra, Cavia porcellus, Equus caballus, Felis catus, Fish, Gerbil, Hamster, Homo sapiens, Monkey, Mus musculus, Oryctolagus cuniculus, Ovis aries, Rattus, Reptilia, Swine
Delivery Route	-	Intraosseous prosthetic implants, intramedullary application
Physical Form	implant	pharmaceutical implants
Experimental Activity	Available	Not Available
Components	Group: Ti-TNTs wire implants Function: implant Amount Reported: Optionality: Mandatory **Ti wires** Function: additives Amount Reported: - Optionality: - **Acetone** Function: Solvents Amount Reported: - Optionality: - **Ethanol** Function: Solvents Amount Reported: - Optionality: -	Group: surgical implant Function: Amount Reported: Optionality: Mandatory **Dental implants** Function: - Amount Reported: - Optionality: - **Plates** Function: - Amount Reported: - Optionality: - **pin** Function: - Amount Reported: - Optionality: -

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

CAS
A division of the American Chemical Society

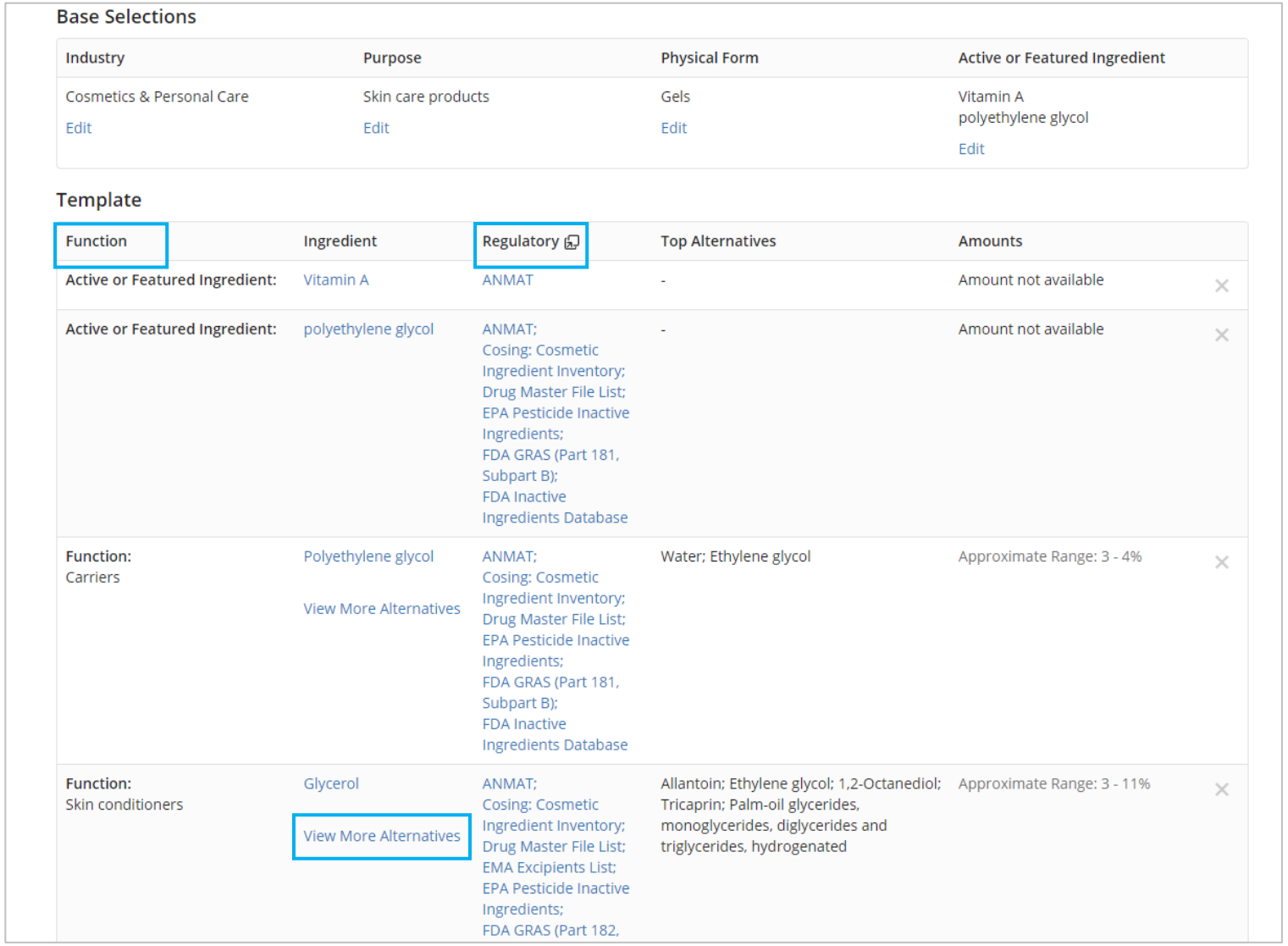
检索原料

- 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



CAS
A division of the American Chemical Society

制剂或配方的设计



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%

- 原料详情
- 原料管制信息
- 可替代的原料选项

CAS
A division of the American Chemical Society

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

CAS
A division of the American Chemical Society

THANK YOU!

CAS
A division of the
American Chemical Society

美国化学文摘社北京代表处
ACS International, Ltd. – Representing CAS
Unit 1010, Tower B, Raycom InfoTech Park
2 Kexueyuan Nanlu, Haidian District, Beijing, China
+86-10-6250 8026/7
cas.org

CAS
A division of the
American Chemical Society