CAS SCIFINDER
DISCOVERY PLATFORM™

快速入门指南

学术版

CAS
A division of the
American Chemical Society

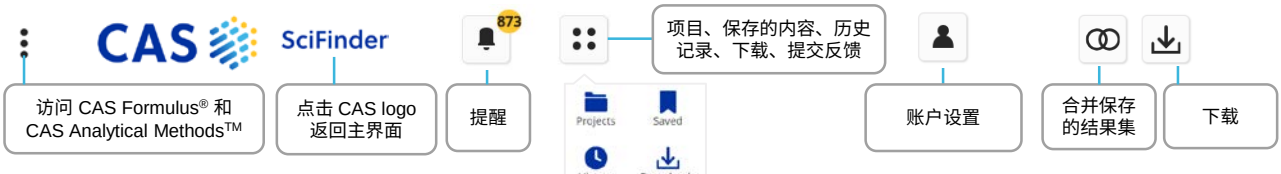
目录

CAS SciFinder

页面及文献检索

主界面

以下选项可在 CAS SciFinder 的主界面上找到。



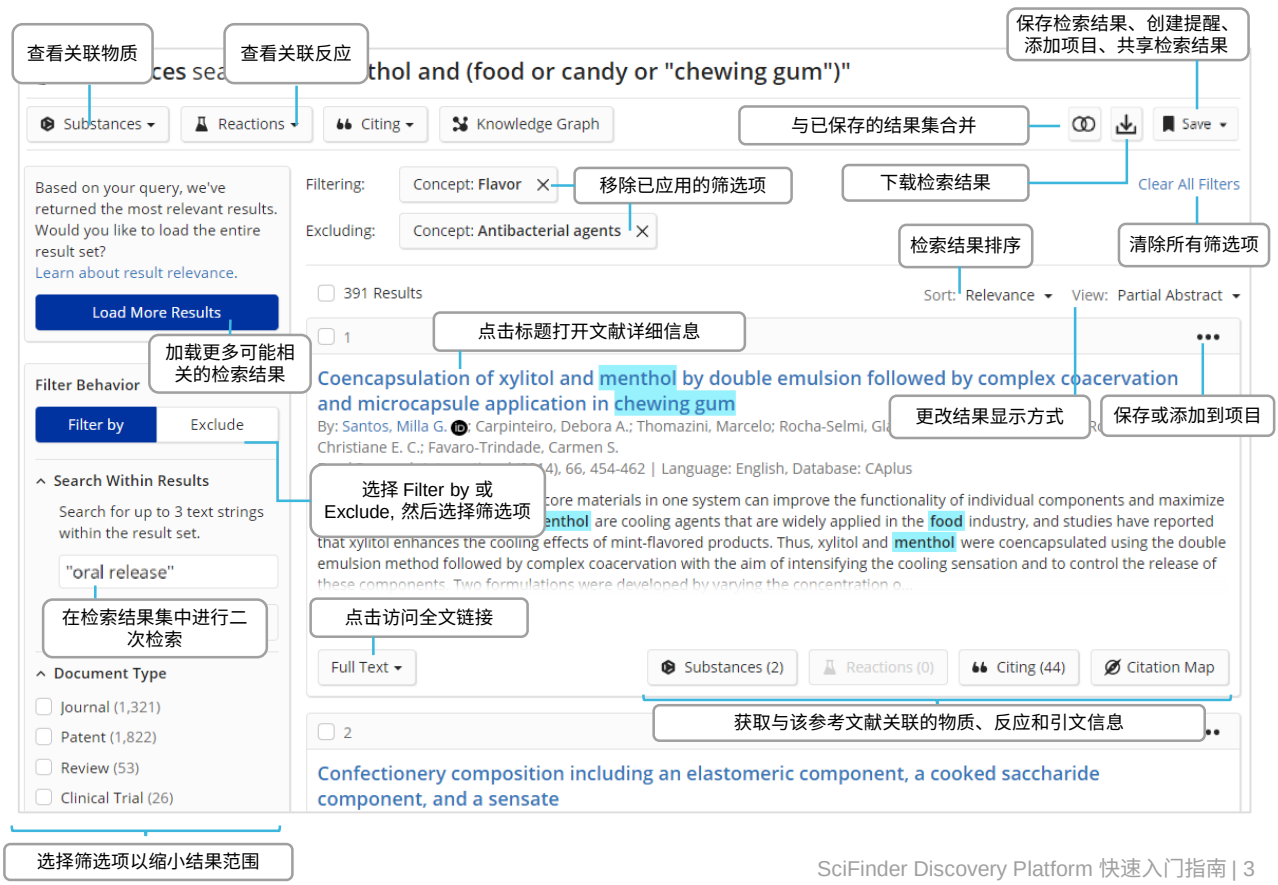
检索界面

CAS SciFinder拥有简洁的检索界面。

检索界面

进行文献检索时，您可以在一个易于使用的界面中访问完整的检索结果集：

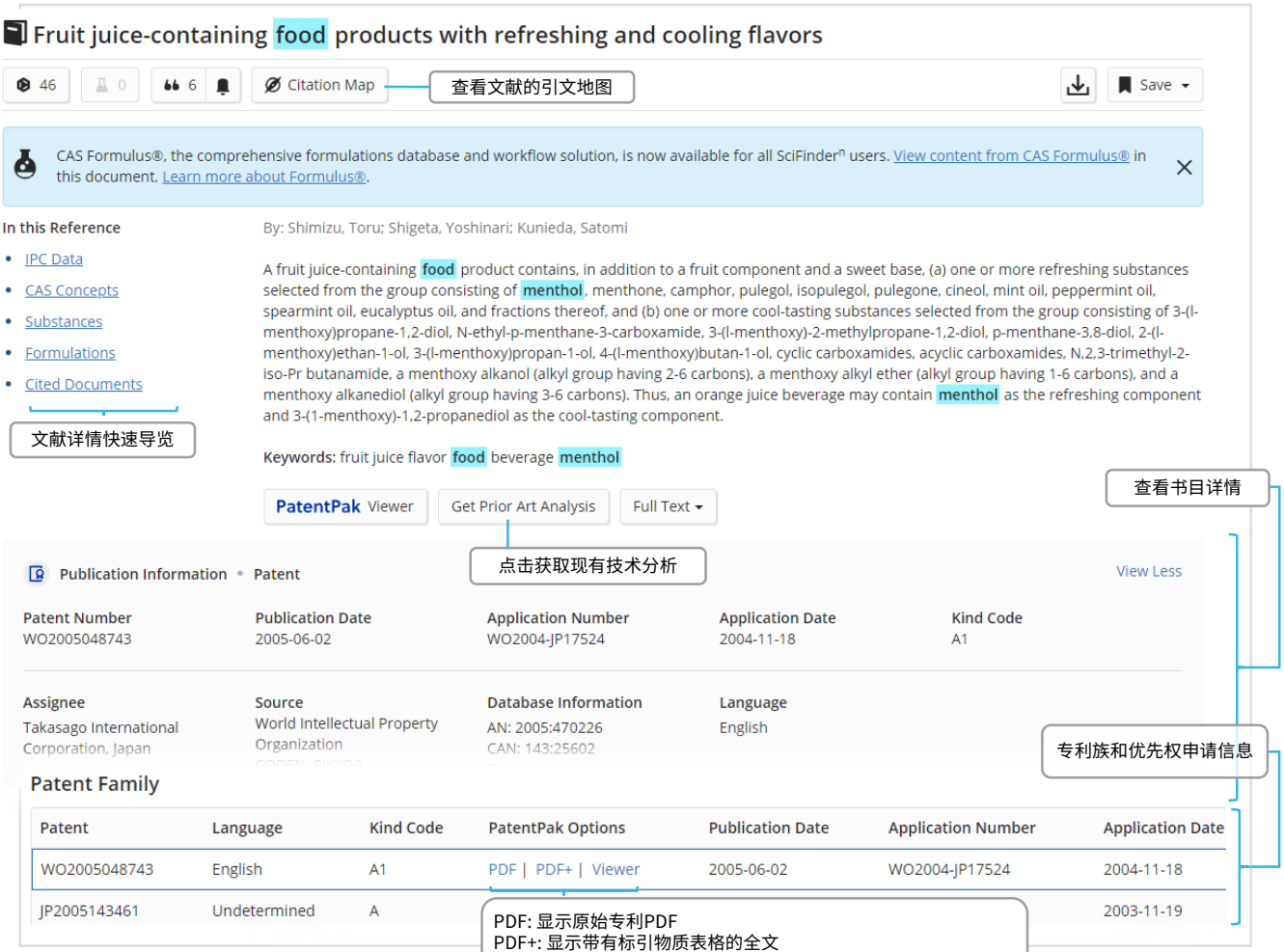
- 文献检索结果按照上一次设置偏好排序。
- 可以使用筛选项进一步缩小检索结果范围。
- 可以保存检索结果，发送链接，设置提醒，或将检索结果添加到项目列表。



文献详情和检索操作符

文献详情

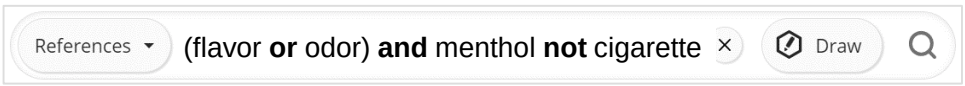
获取 CAS SciFinder 中每篇文献的详细信息。



布尔逻辑运算符

您可以使用布尔逻辑运算符进行文献检索。

使用括号表明对此逻辑运算符进行优先运算，例如使用“OR”连接相关术语，如下所示:



AND 要求文献结果中同时出现两个术语。

OR 要求文献结果中至少出现其中一个术语或两个术语都出现。

NOT 从检索结果中排除包含NOT后面的词语的文献结果。

使用通配符可在文献检索、物质检索以及二次筛选检索中获得更全面的结果。

通配符可用于词中或者词尾。

*	可替换0到多个字符	例如: polymorph* | immunoglobulin*conjugate*
?	可替换0个或者1个字符	例如: benzonorbornen?

包含双引号的短语将作为精确短语进行检索。

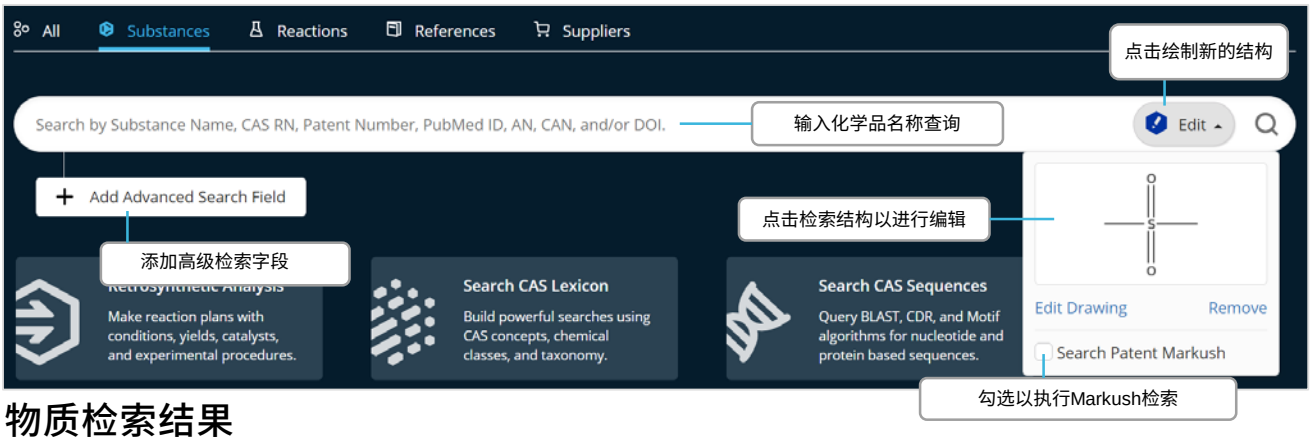
例如：搜索“Programmed cell death protein”只会找到完全匹配“Programmed cell death protein”的结果。

物质名称及结构式检索

物质检索

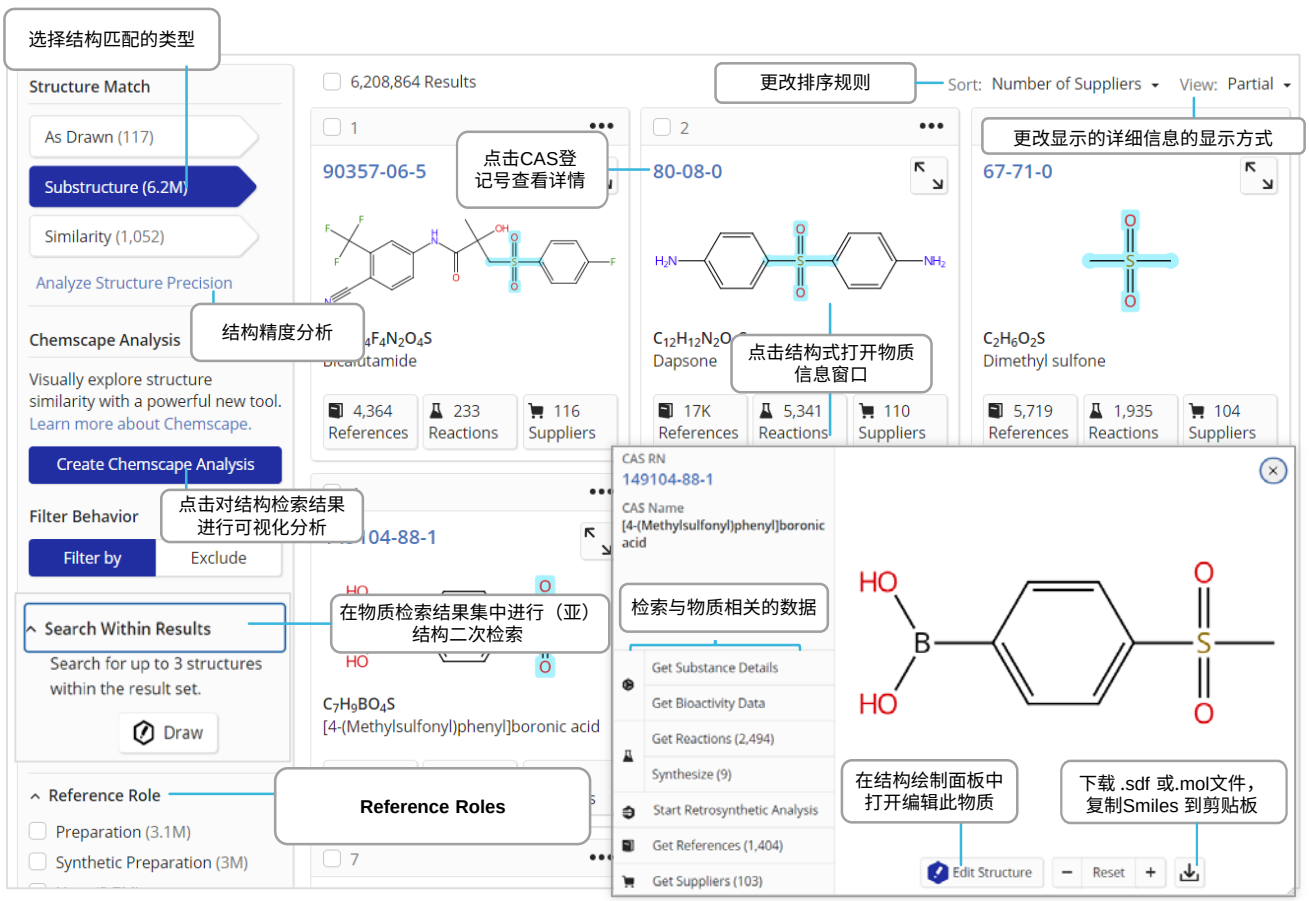
可以通过在检索框中输入一个或多个物质名称或标识符来检索物质。还可以通过绘制或编辑结构式进行检索。以下是通过物质名称进行检索的示例选项。

Streptomycin	检索 Streptomycin 记录
57-92-1	检索使用CAS Registry Number作为标识符的物质记录
Streptomycin sulfate	检索三项记录: Streptomycin, Streptomycin sulfate 和 Sulfate
"Streptomycin sulfate" Streptomycin	检索两项记录: Streptomycin sulfate 和 Streptomycin
Sulfoximin*	检索所有以 Sulfoximin 开头的名称
WO2019234160	检索该专利的所有标引物质



物质检索结果

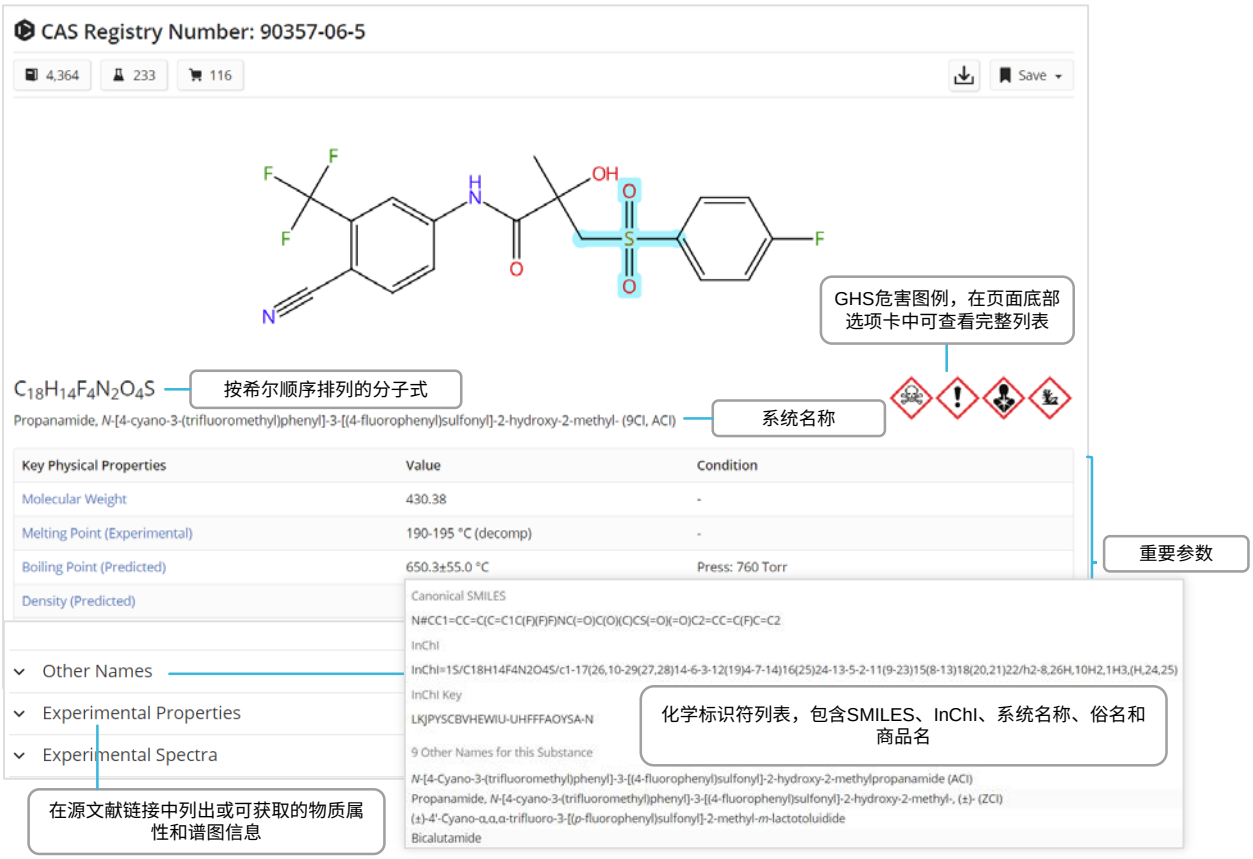
物质检索结果在一个直观的界面中呈现，您将看到与您的检索最相关的结果，包括其关键属性信息和高分辨率结构式图像。



物质详情和结构绘制面板

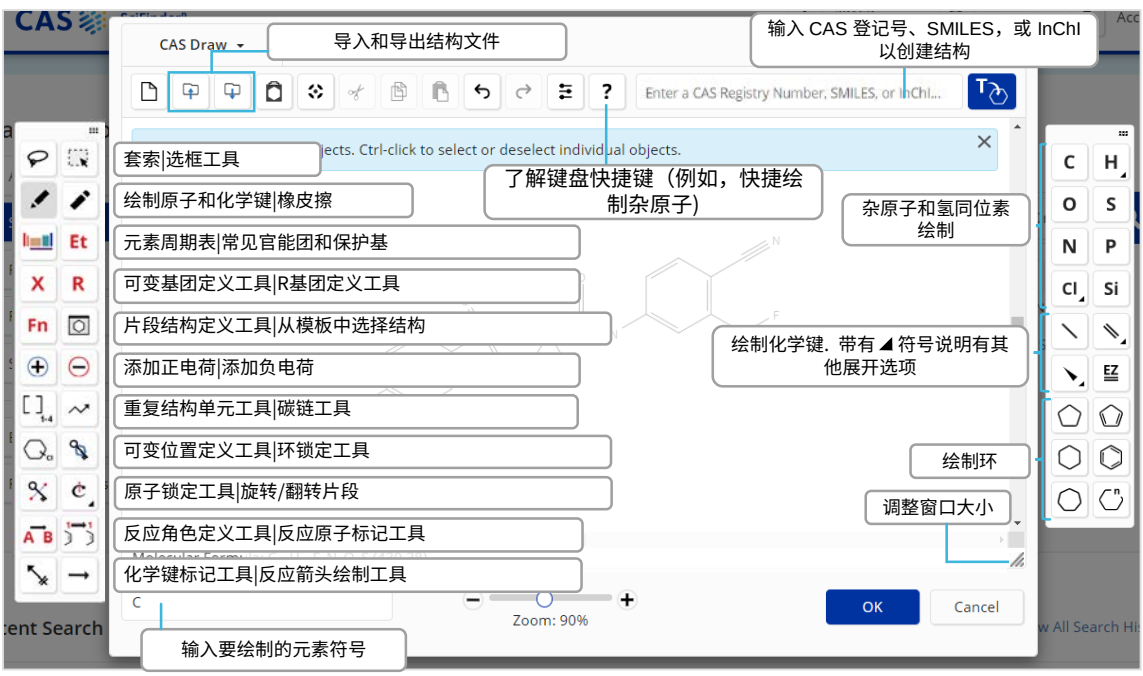
物质详情

当点击某个物质检索结果的 CAS 登记号时，会显示该物质详细信息，包括结构式、分子式、物质性质及其他信息。



CAS 结构绘制面板

您可以使用 CAS 结构绘制面板绘制结构式和反应式进行查询。

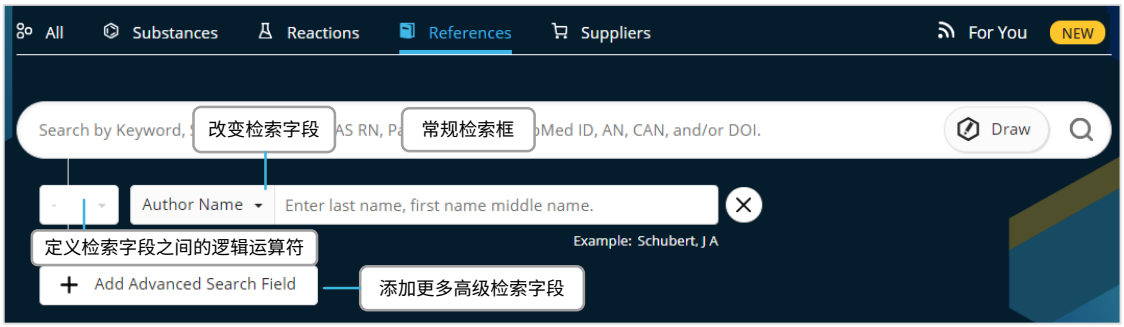


高级检索

执行高级检索

您可以使用 CAS SciFinder 主搜索界面上的高级检索字段进行特定的文献检索和物质检索。

- 逻辑运算符的处理顺序为：**OR**, **AND**, **NOT**
- 仅使用单个高级检索字段时，不能使用逻辑运算符
- 允许使用通配符，例如 peek*
- 最多使用50个高级检索字段（如果主检索字段也被使用，则为49个）

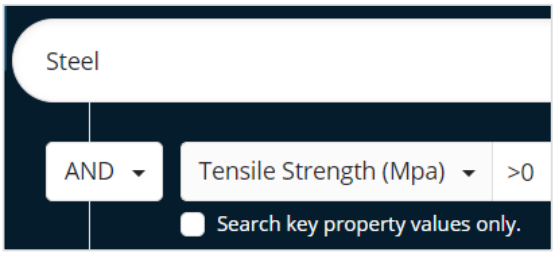


高级检索示例

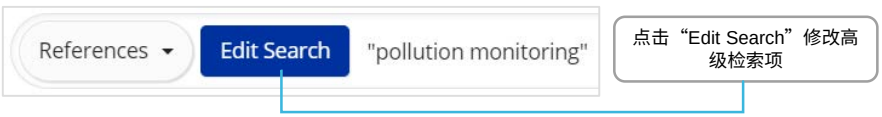
高级文献检索

检索说明：
检索“pollution monitoring”以及（polyethylene or polypropylene）

高级物质检索



检索说明：
检索钢材拉伸强度性能信息



可用的高级检索字段

您可以在高级检索项中利用多个检索字段和类别，包括:

文献检索

- 作者
- 期刊名称
- 发表机构
- 标题
- 摘要/关键字
- 核心研究点
- 物质
- 生物活性数据
- 出版年份
- 文档标识符
- 专利标识符
- 出版商

物质检索

- 分子式
- CAS 登记号
- 化学标识符
- 文献标识符
- 专利标识符
- 实验谱图
- 生物活性数据
- 生物学数据
- 化学性质
- 密度
- 电学
- Lipinski
- 磁
- 机械属性
- 光学与散射
- 结构相关数据
- 热学

CAS Roles

CAS Roles 概述

Roles 与物质相关联，使您可以聚焦将感兴趣的物质与其在文献中的具体Role相关联的文献。

- Super roles 是广泛的类别，包括所有相关的具体的Role。例如分析研究（Analytical Study）。
- Specific roles 更为精确，比如分析研究中物质作为分析物（Analyte）的使用。

物质检索结果中的Roles

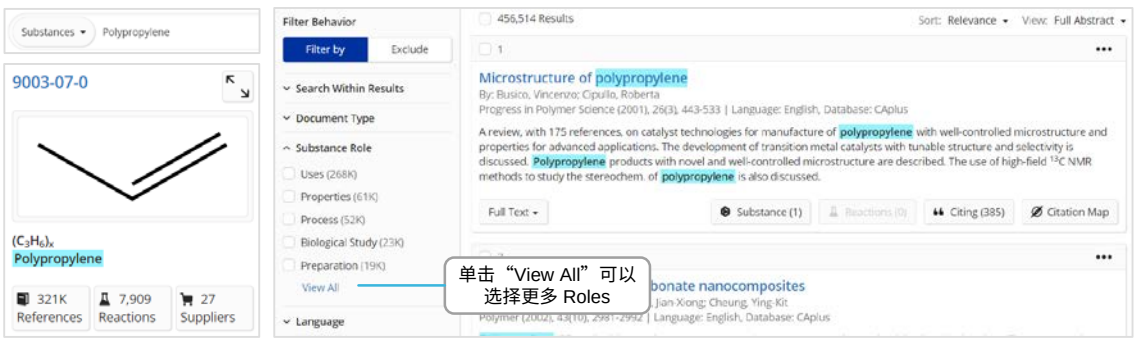
在物质检索结果集中，Roles的筛选项表示对应物质在文献中的Role。

文献检索结果中的 Roles

每当您的检索信息命中物质的标引信息部分，也就是说，通过检索物质名称，或进行基于物质检索之后的关联检索时，Roles将作为文献检索结果中的筛选项出现。

示例：我对（海洋）污染这一课题很感兴趣。我怎样才能找到专门将聚丙烯描述为污染物（pollutant）的文献？

检索聚丙烯会得到许多文献结果。其中 Substance role 窗口显示了此检索结果集中的聚丙烯的所有适用 Roles。其中 Pollutant 这一项Role表明有3,661篇文献将聚丙烯描述为污染物(pollutant)。通过二次检索功能，或通过核心研究点筛选，可将检索结果限定于海洋污染。

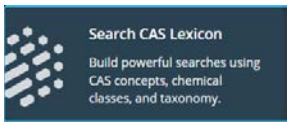


CAS Lexicon

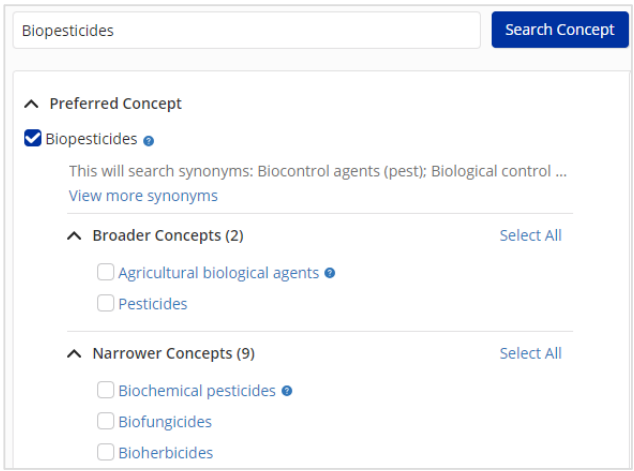
CAS Lexicon概述

可以通过 CAS Lexicon，在CAS总的词库层级中浏览CAS科学家标引的概念词或核心研究点，以及重要的物质，并建立用于文献检索的检索式。

访问和浏览



首先点击主界面上的“CAS Lexicon”，输入检索词，然后浏览多层级词库列表。



可以通过选择核心研究点并将其添加到右侧的检索窗口，来构建高度精准的 CAS Lexicon 检索。只有选定的CAS核心研究点会被检索。

检索CAS序列

检索选项

可以使用三种不同的方式检索序列：

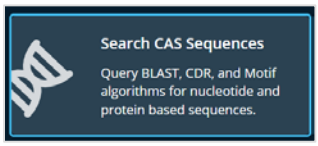
- BLAST：检索相似序列
- CDR：利用 CDR 检索抗体或T细胞受体
- Motif：检索氨基酸或核苷酸位点可变的序列

BLAST 相似性检索

BLAST 可用于检索相似的核苷酸或氨基酸序列。序列比对结果以直观的图形布局显示，并提供便捷的精确筛选功能，可根据比对一致性和覆盖率百分比进行筛选。可以直接查看命中序列的关联文献。

要执行BLAST搜索，请按照以下步骤操作：

- 在CAS SciFinder主界面中打开CAS Sequences模块。
- 从文件中加载序列，或粘贴序列到检索窗格中。
- 充分利用支持的格式，例如：包含由单字母代码表示的残基的序列（例如，在FASTA格式中）。
- 注意，序列输入可支持批量检索。
- 根据需要调整BLAST参数，然后启动序列检索。

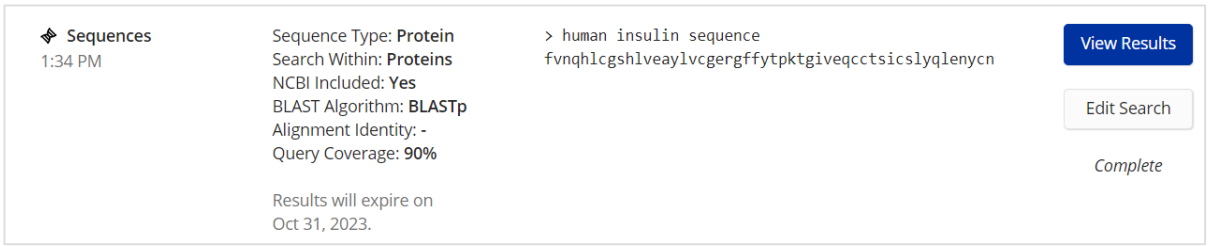


BLAST 结果分析

访问结果

序列检索结果在最近检索历史（Recent Search History）和检索历史（Search History）中呈现。

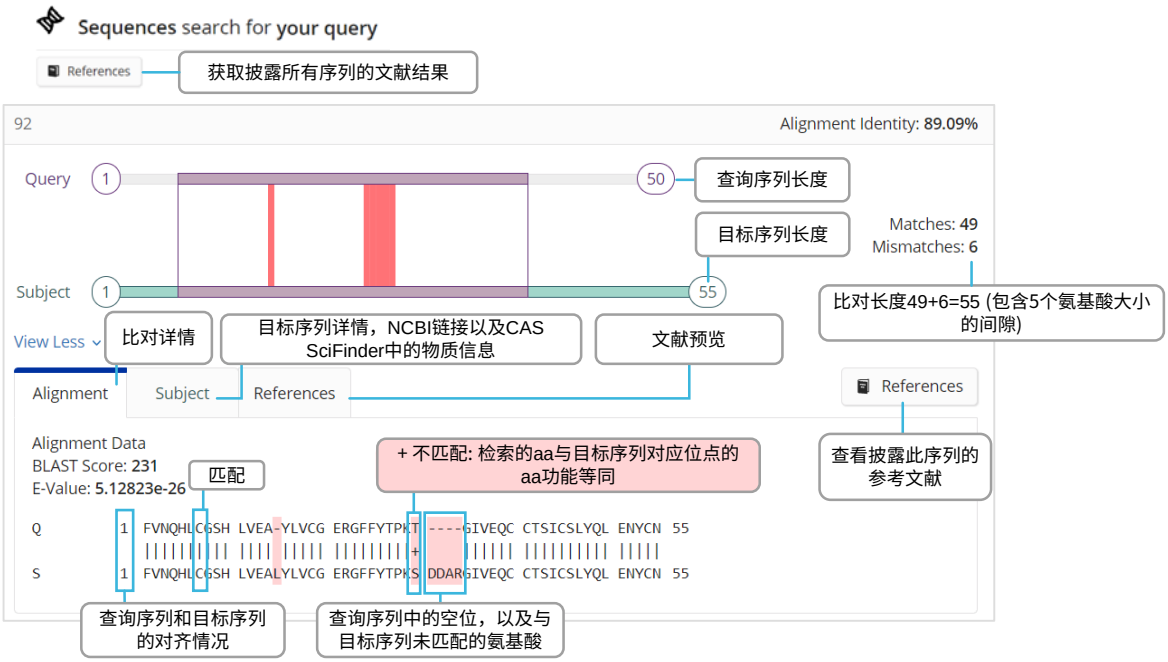
点击 “View Results” 查看序列检索结果。



查看结果

在查看BLAST序列相似性结果时：

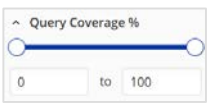
- 比对结果按序列一致性排序。
- 简化的图形概览显示比对质量。
- 不匹配部分以红线标示。
- 详细比对结果可在“Alignment”标签中查看。
- 目标序列详情和相关专利预览可在单独的标签中查看。
- 点击 References 可获取相关文献。
- 支持下载 XLSX 格式的结果文件。



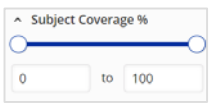
筛选结果

检索结果会随着筛选项调整而动态改变。

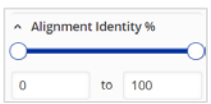
E-值（期望值）



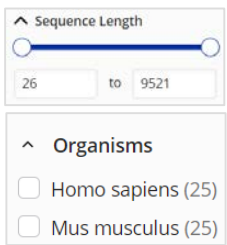
比对上的序列长度 / 查询序列长度



比对上的序列长度 / 目标序列长度



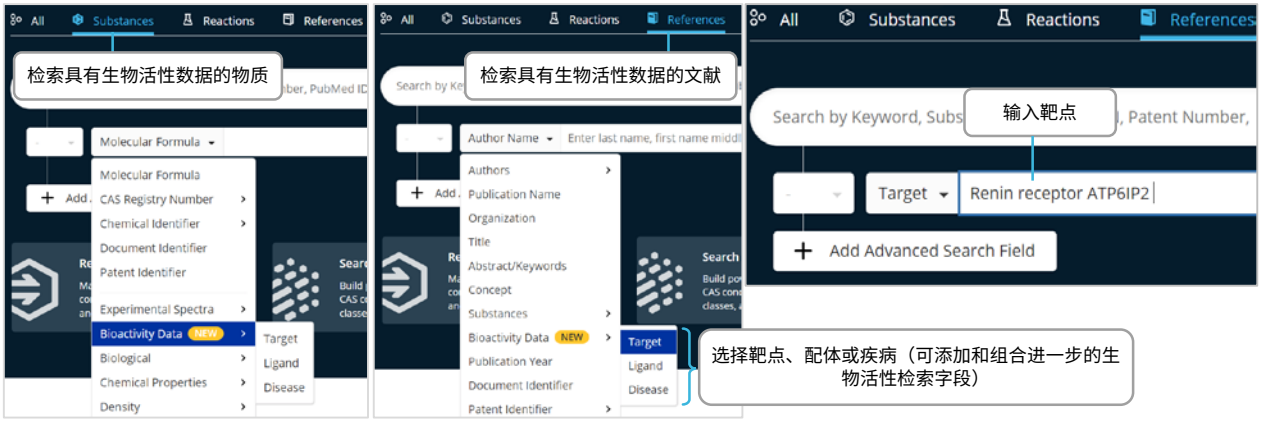
匹配上的氨基酸或碱基对的数量 / 比对上的序列长度



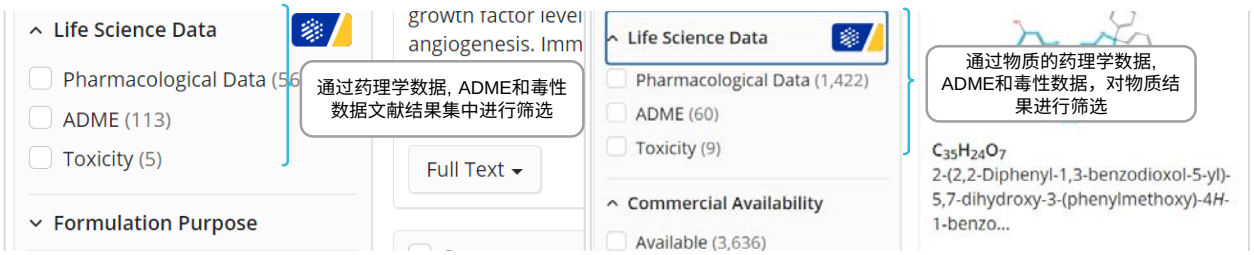
生物活性数据

检索靶点、配体和疾病

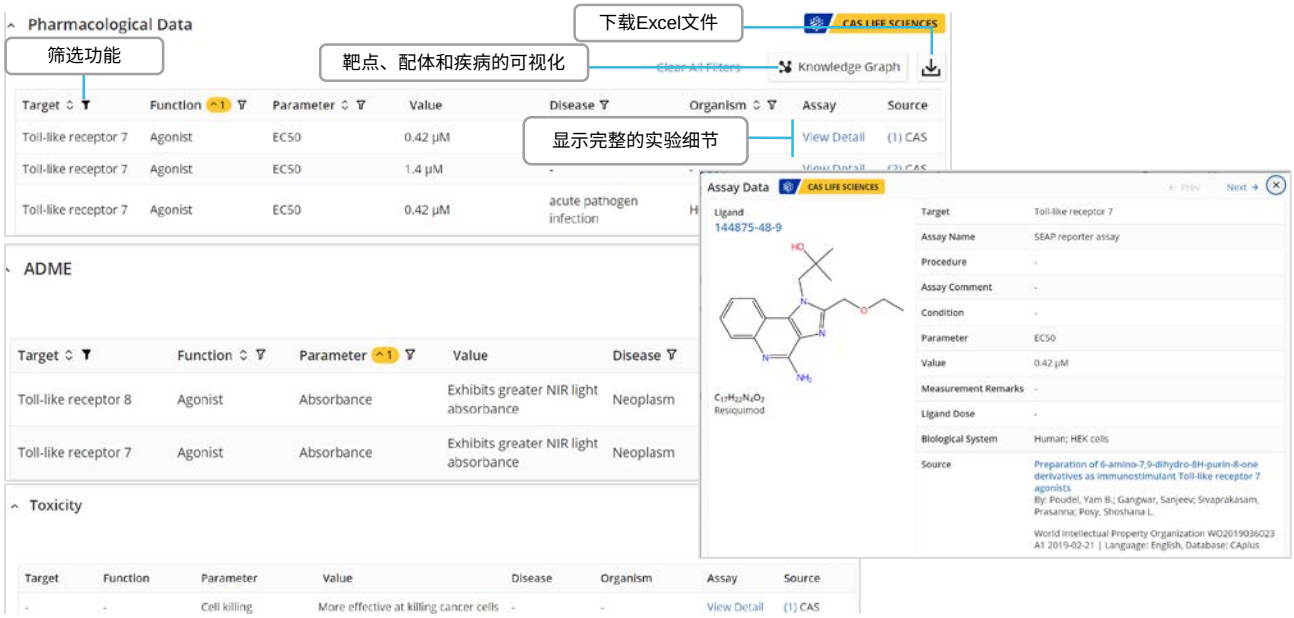
通过物质检索和文献检索的高级检索字段，您可以找到与靶点、配体和疾病相对应的生物活性数据。这将在 CAS Life Sciences 中检索物质和/或文献。



文献检索和物质检索中的生物活性数据筛选项



物质详情页中的生物活性数据

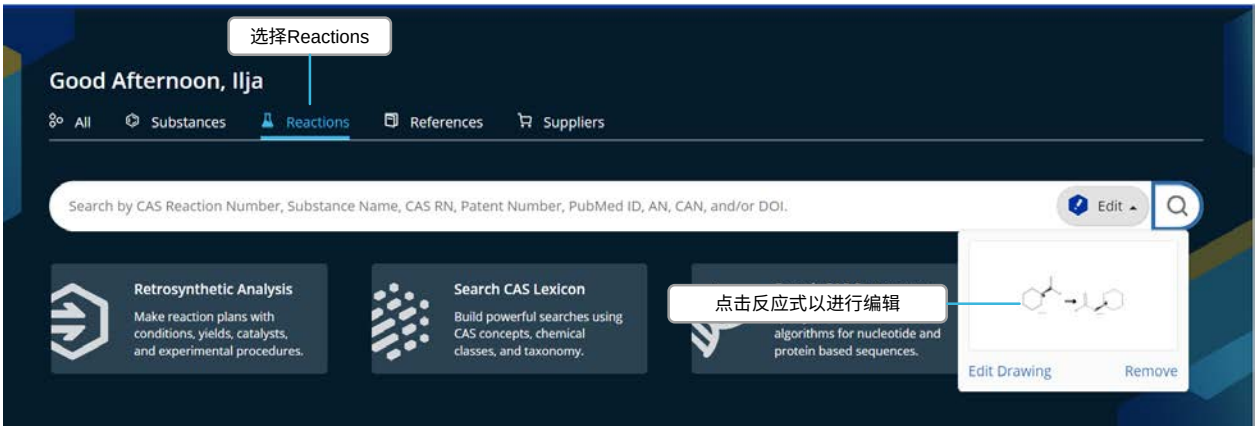


文献详情页中的生物活性数据

反应检索

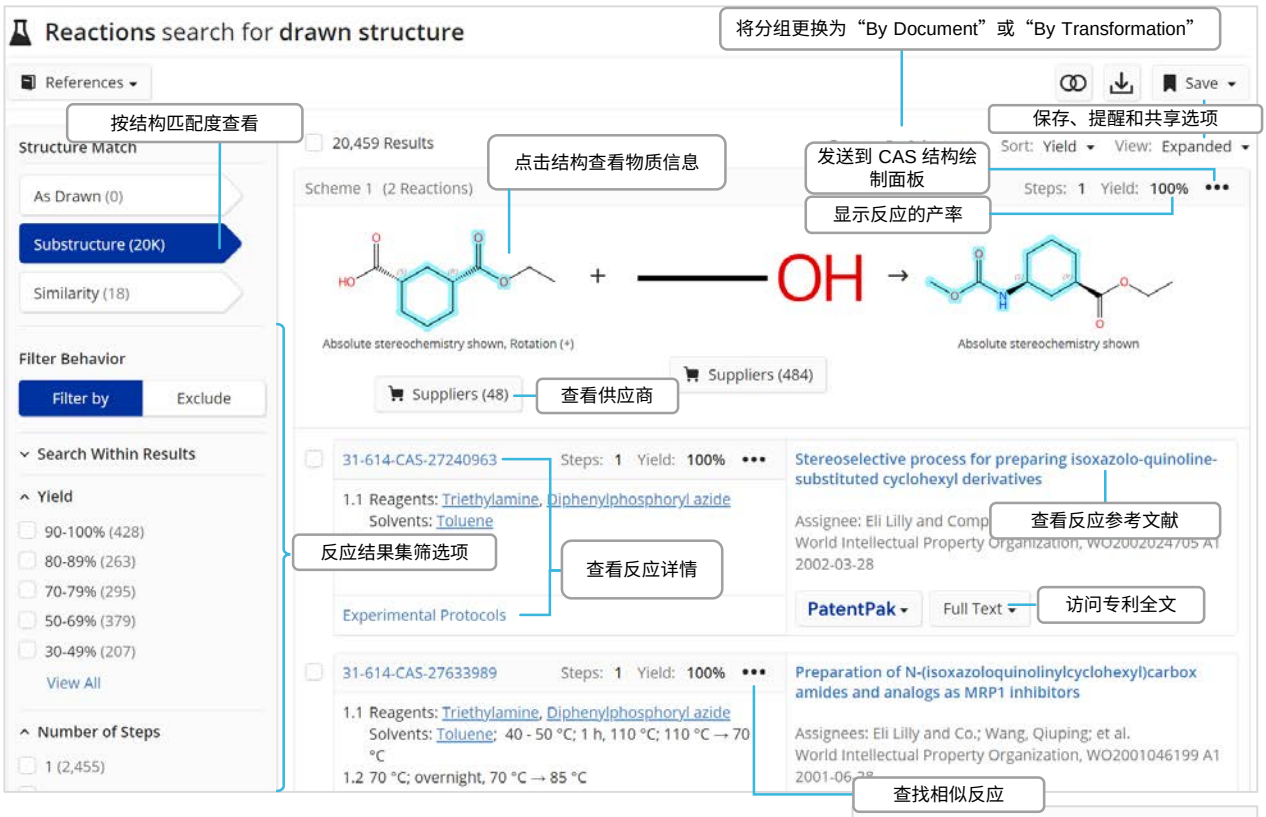
进行反应检索

可以使用CAS反应登记号、物质名称、CAS 登记号、文献标识符、化学结构或基于文本来进行反应检索。



反应检索结果

默认情况下，反应检索结果按照上一次设置进行分组。



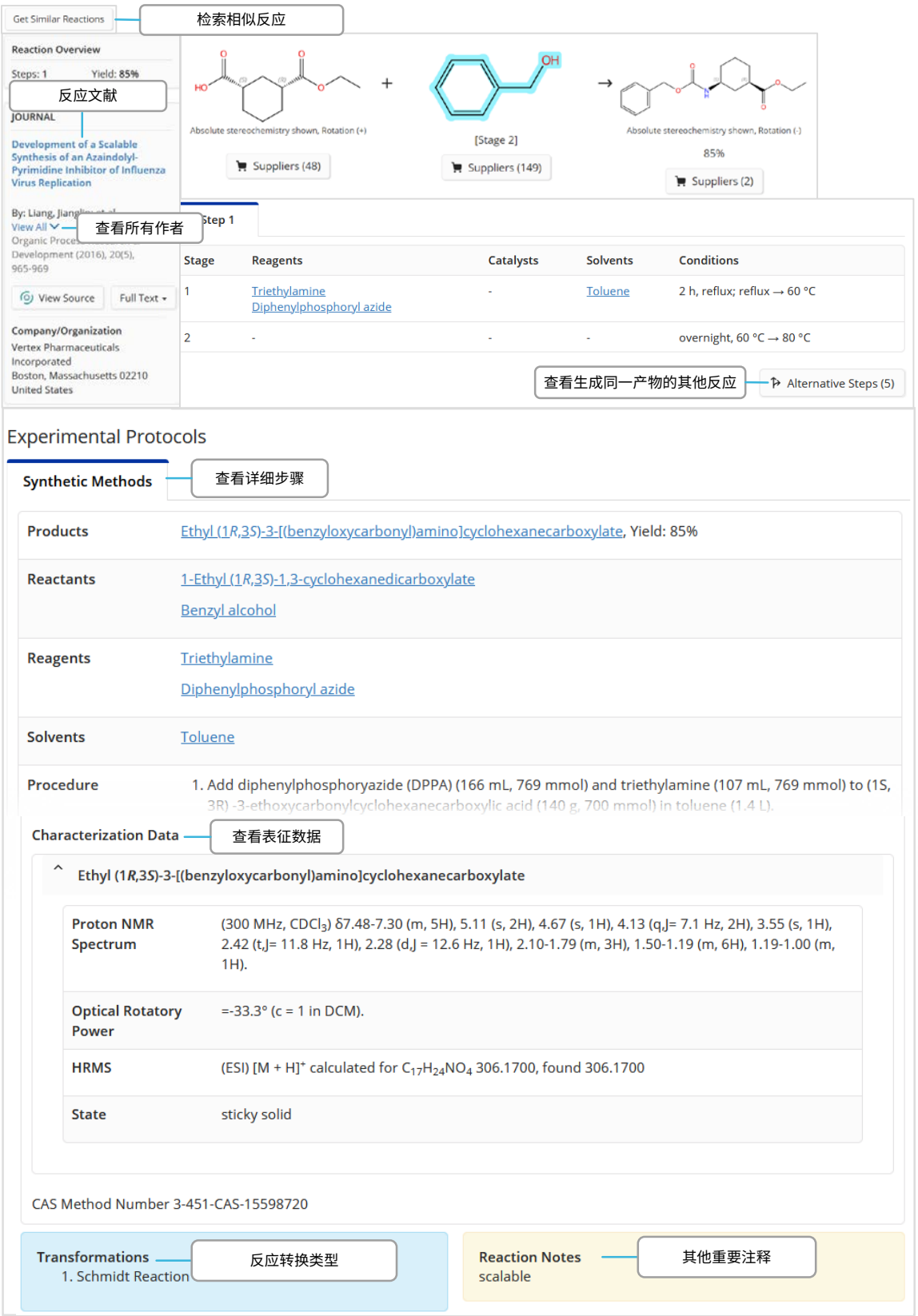
对于单步反应，你可以根据相邻原子与特定反应中心的相似性来获取相似反应。

- **Broad**：获取反应中心一致的反应；
- **Medium**：获取反应中心一致，相邻原子一致的反应；
- **Narrow**：获取反应中心一致，相邻原子、拓展原子和键一致的反应。

反应详情

查看反应详情

反应详情页为您提供了从文献及其 Supporting Information 中提取的信息，包括溶剂、催化剂、试剂、反应条件和表征数据等。

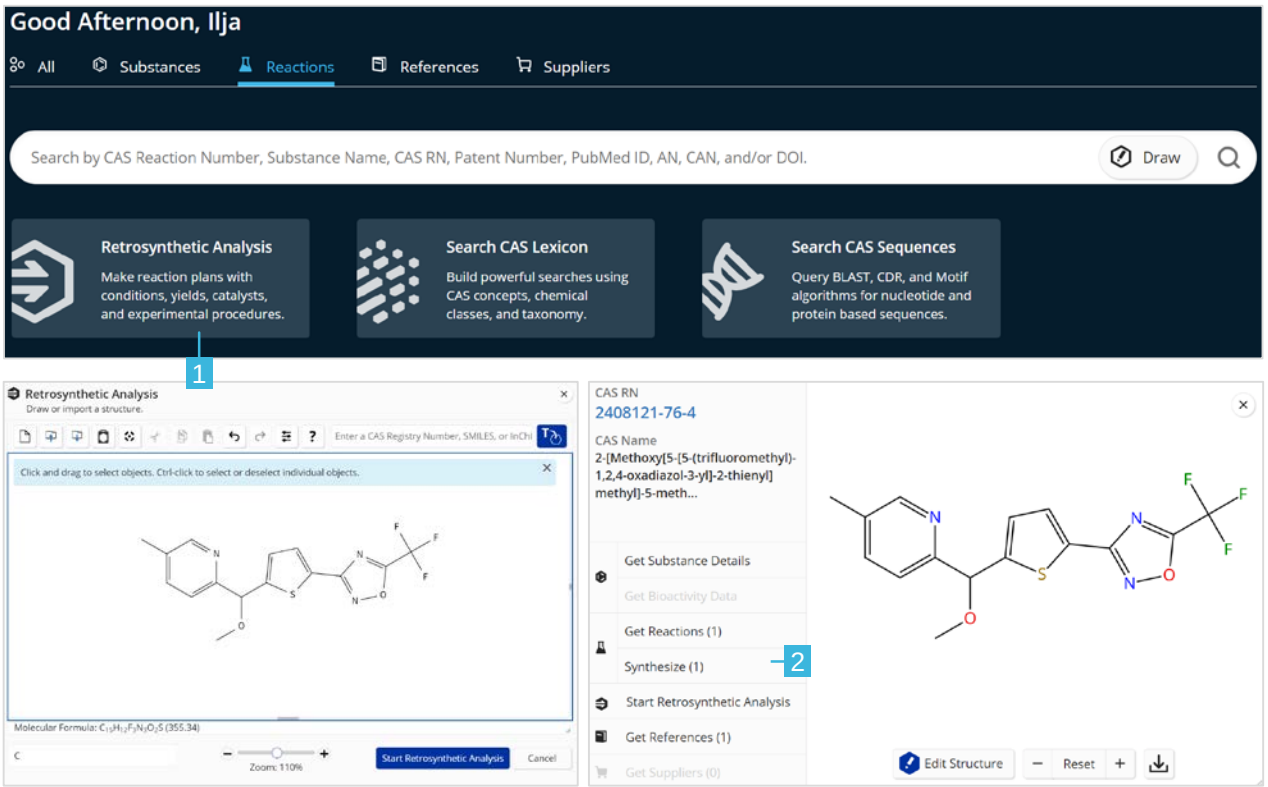


逆合成反应路线设计工具

启动工具

在CAS SciFinder中启动“Retrosynthetic Analysis”主要有两种方式：

1. 点击主界面上的“Retrosynthetic Analysis”选项，在绘制窗口中绘制或导入一个结构。绘制的物质可以是一个新颖结构（无文献报道过合成方法）。
2. 在现有物质的弹出窗口上点击 “Start Retrosynthetic Analysis” 选项。



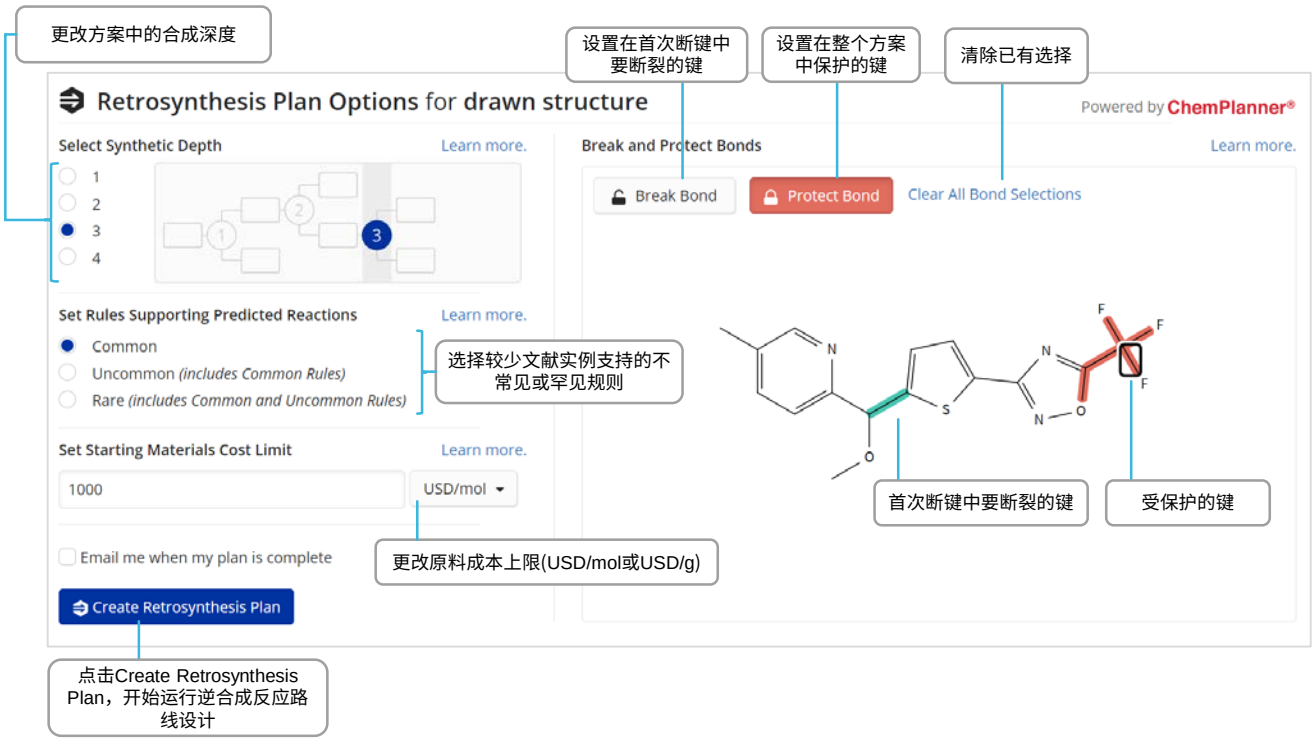
逆合成反应路线设计工具

选择方案选项

您可以编辑方案选项以：

- 修改合成深度。
- 在整个合成路线保护指定的化学键。
- 定义在首次断键中要断裂的键。
- 更改起始原料的成本限制。
- 选择较少文献实例支持的不常见或罕见规则。

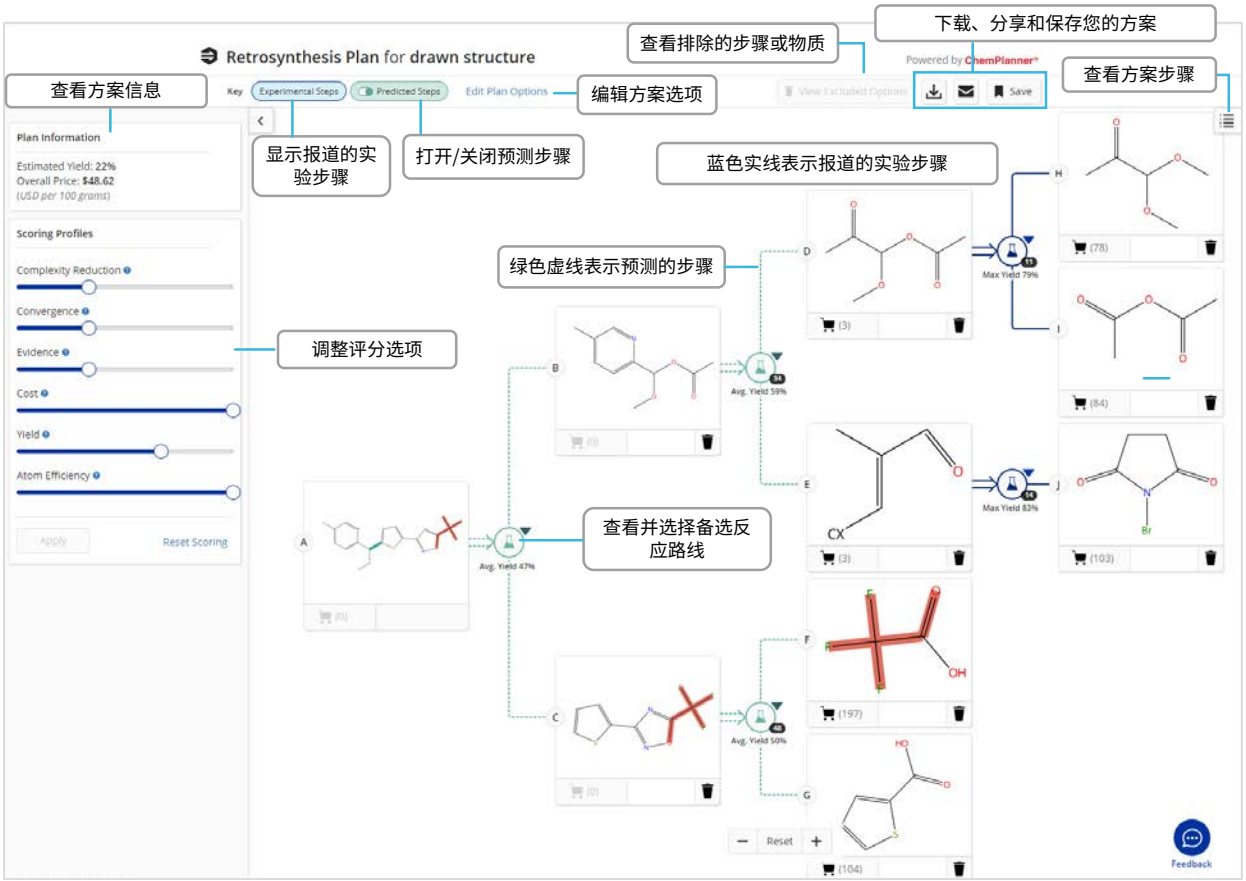
设置好了所需的选项后，点击 “Create Retrosynthesis Plan”



逆合成方案和备选路线

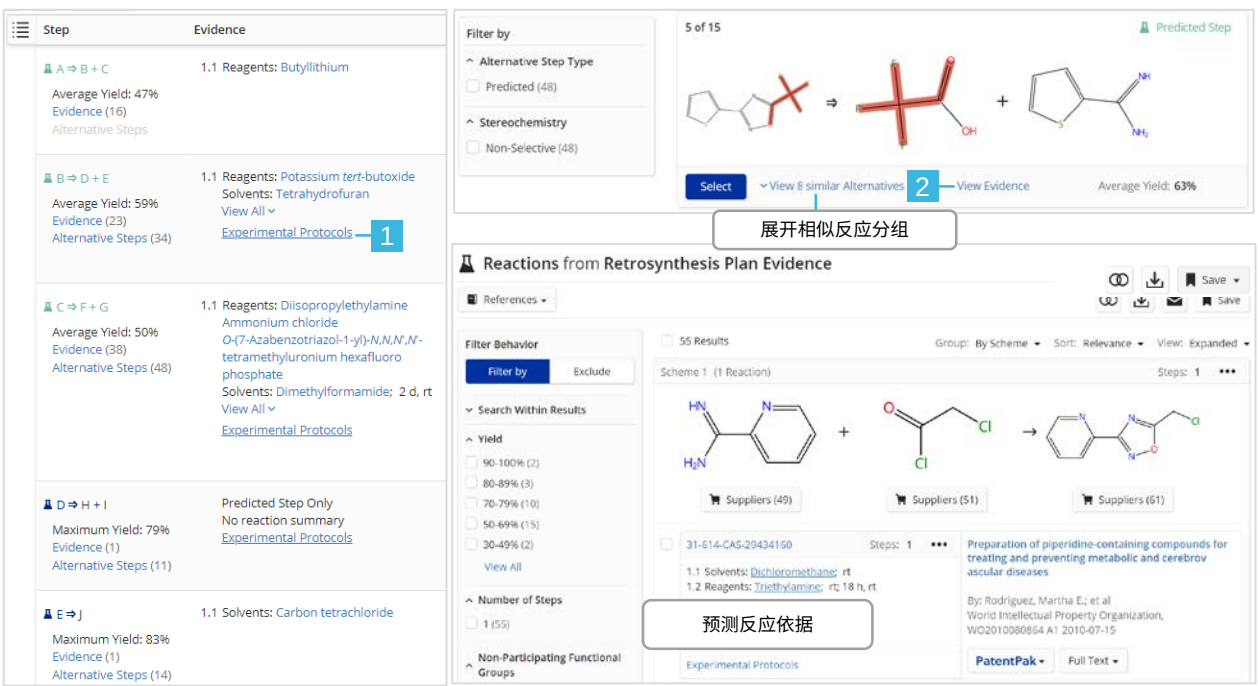
打开方案

有报道的实验方案通常会在几秒钟内生成。预测的逆合成方案的计算可能需要更长的时间。



备选路线

您可以概览所有实验报道的和预测的反应，并将其与反应依据一起作为反应结果集显示。您可以通过以下方式访问这些反应依据：(1)步骤概览中的链接，或(2)备选反应路路线的反应式。



逆合成评分选项

评分选项

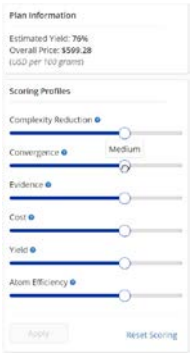
对于包含预测步骤的方案，您可以增加或减少预测步骤和替代反应路线中每个选项中的分数权重，以决定在逆合成方案/替代反应路线中所显示的内容。

- 每个评分项可以设置为“Off （最左），Low, Medium，或者High（最右）。
- 如下图所示，每个评分项的默认设置为 “Medium” 。

评分简介

For plans with predicted steps, you may increase or reduce the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

Each scoring profile may be set to **Off** (extreme left), **Low, Medium**, or **High** (extreme right); the default setting for each profile is "Medium," as shown below. Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor step selection or alternative ranking.



Complexity Reduction

Reduces the complexity of a step's reactants compared to its product.

In retrosynthesis plans, you typically want high complexity reduction.

Convergence

Determines how "branched" the plan is; **you typically want the plan to be as branched as possible (high convergence)**, rather than linear.

For a given step, the more precursors there are, and the closer their relative sizes are, the more it's considered convergent.

Increasing Convergence displays steps/alternatives with more reactants.

Evidence

Ranks plan steps/alternatives based on the number of evidence examples supporting the particular reaction type.

More evidence examples for a step **means that the reaction type has more applications and is more versatile in terms of conditions and substrates**, and hence predictions made based on it are probably more reliable.

Increasing Evidence displays steps/alternatives with more supporting examples.

Cost

Weighs the expenses of the reactions by ranking starting materials based on the lowest price found amongst catalogs.

Yield

Applies to the yield of each step in the plan, which contributes to the yield of the target molecule.

Increasing the Yield displays a higher yield target molecule and steps/alternatives.

Atom Efficiency

Reduces reactant parts not included in a plan step's product.

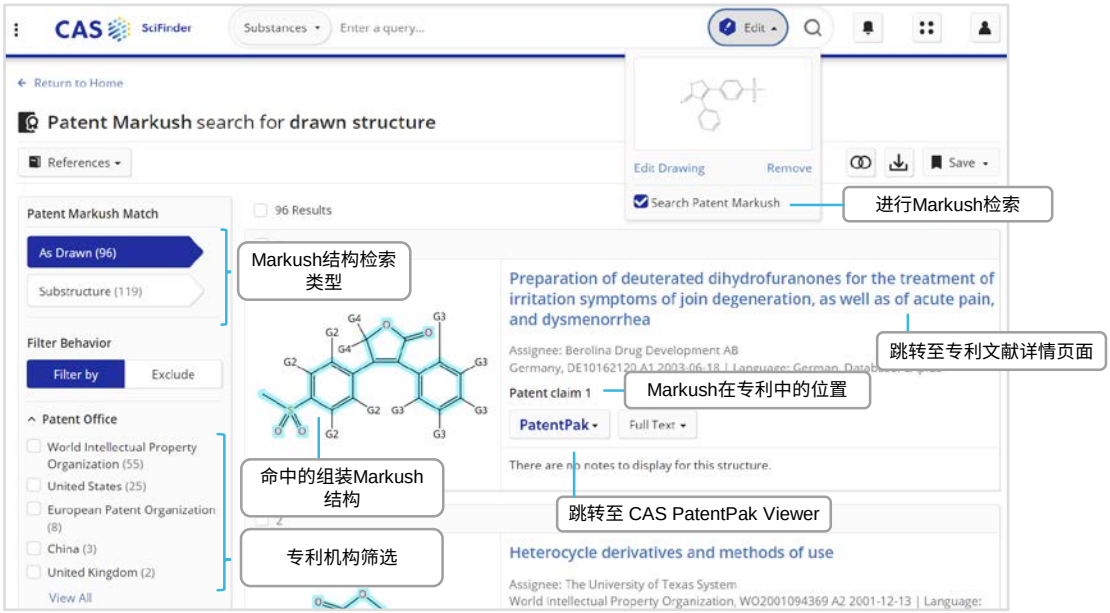
Increasing Atom Efficiency displays steps/alternatives with the least amount of reactant atoms that do not map to the product.

Clicking the **Apply** button redraws the retrosynthesis plan with the revised scoring profiles; clicking **Reset Scoring** restores the "Medium" default.

CAS Markush 检索及 CAS PatentPak

CAS Markush 检索

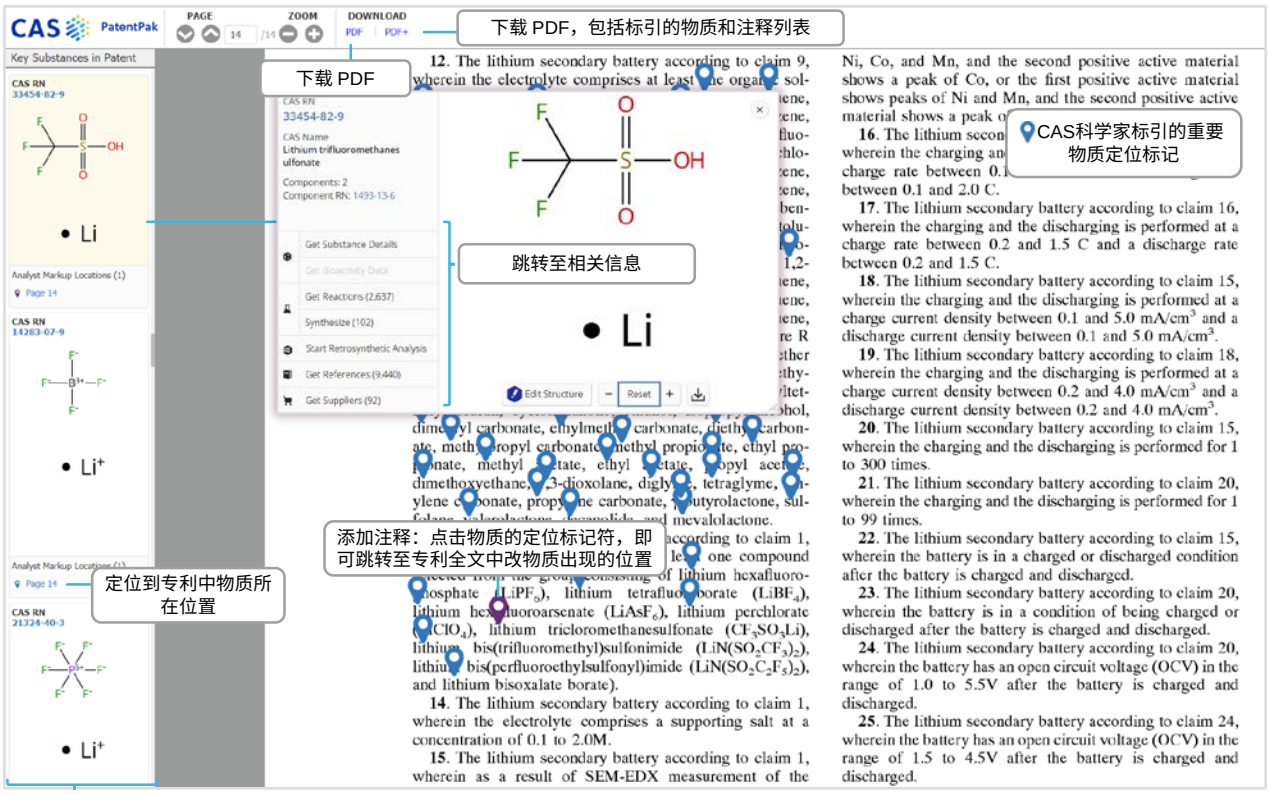
在物质检索模式下，可以使用“Search Patent Markush”选项执行Markush结构检索。



CAS PatentPak

在 CAS PatentPak 中有三种查看专利PDF的方式：

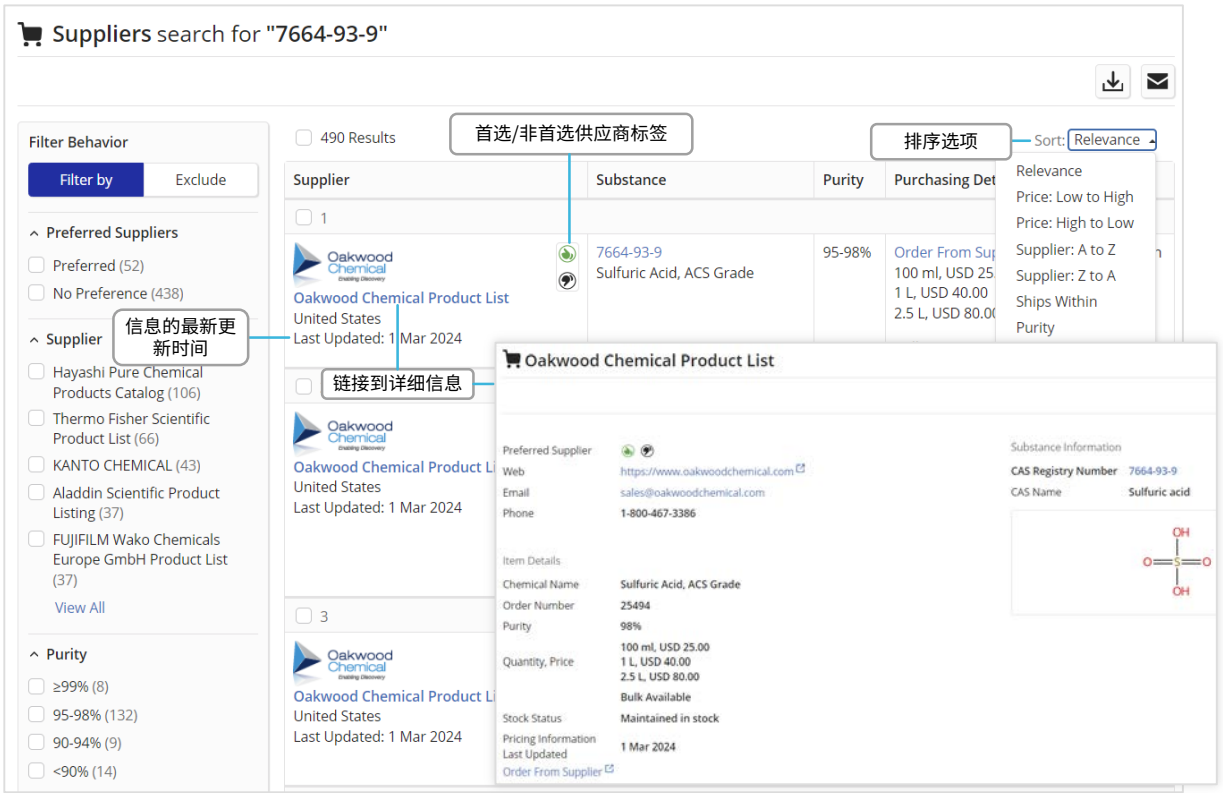
- **PDF**：仅提供支持文本搜索的专利PDF文件
- **PDF+**：附有标引关键物质专利全文PDF文件
- **Viewer**：附有标引关键物质定位符（见下）的专利PDF



供应商检索及 ChemDoodle

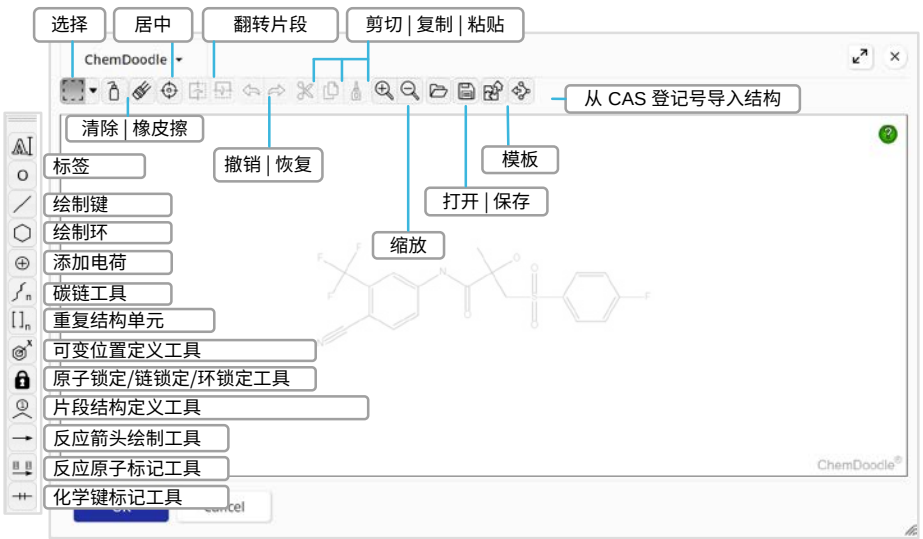
供应商检索

供应商检索允许您根据化学结构、名称或其他标识符查找化学品供应商信息。



ChemDoodle

ChemDoodle 是除了标准的CAS结构绘制面板之外，另一个可选的结构编辑器。 ChemDoodle非常适用于平板电脑等移动设备。

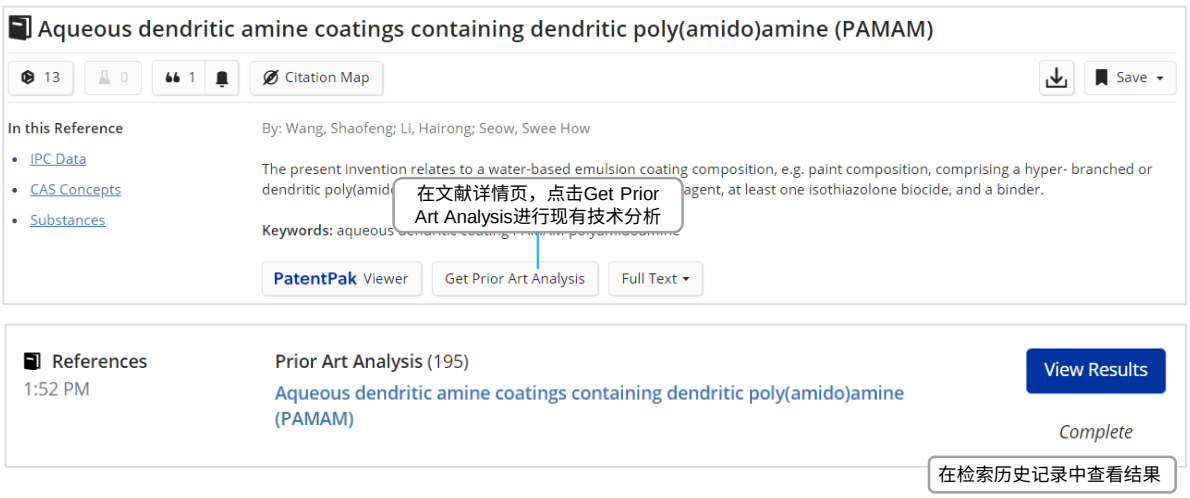


现有技术分析

回顾现有技术

在专利文献详情页中，提供了 “Get Prior Art Analysis”的选项。其结果也会呈现在检索历史中。其工作原理如下：

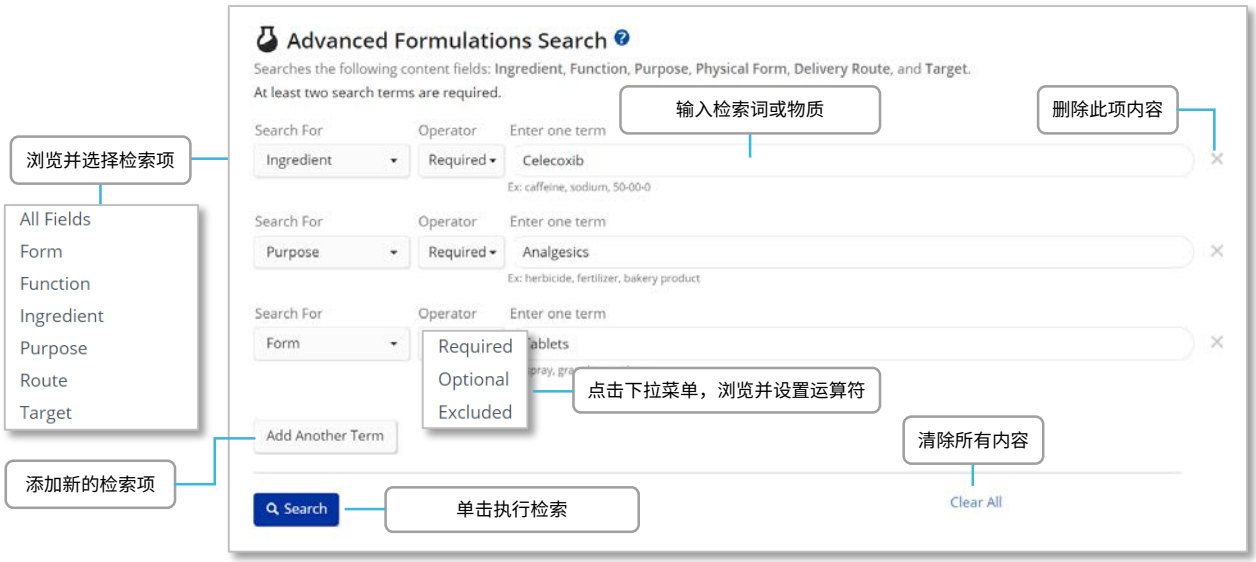
- 提供基于人工智能的相关性预测。
- 以单一专利文件作为分析起点。
- 包括对 CAS 核心研究点、标引的物质、IPC专利分类号和专利题目、摘要等内容的分析。
- 生成一份按照相关性排序的已知文献列表，涵盖专利文献和非专利文献。

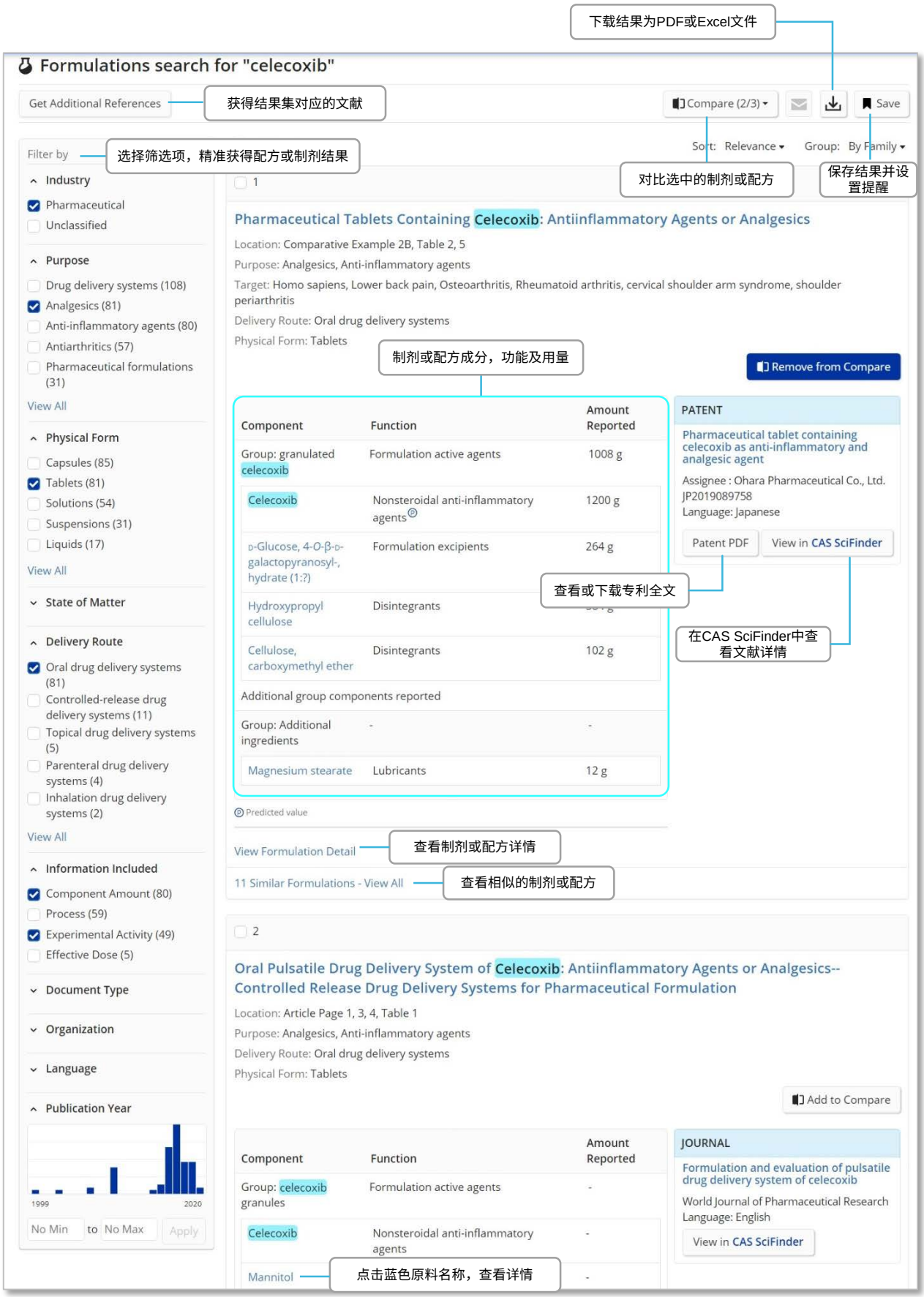


CAS Formulus

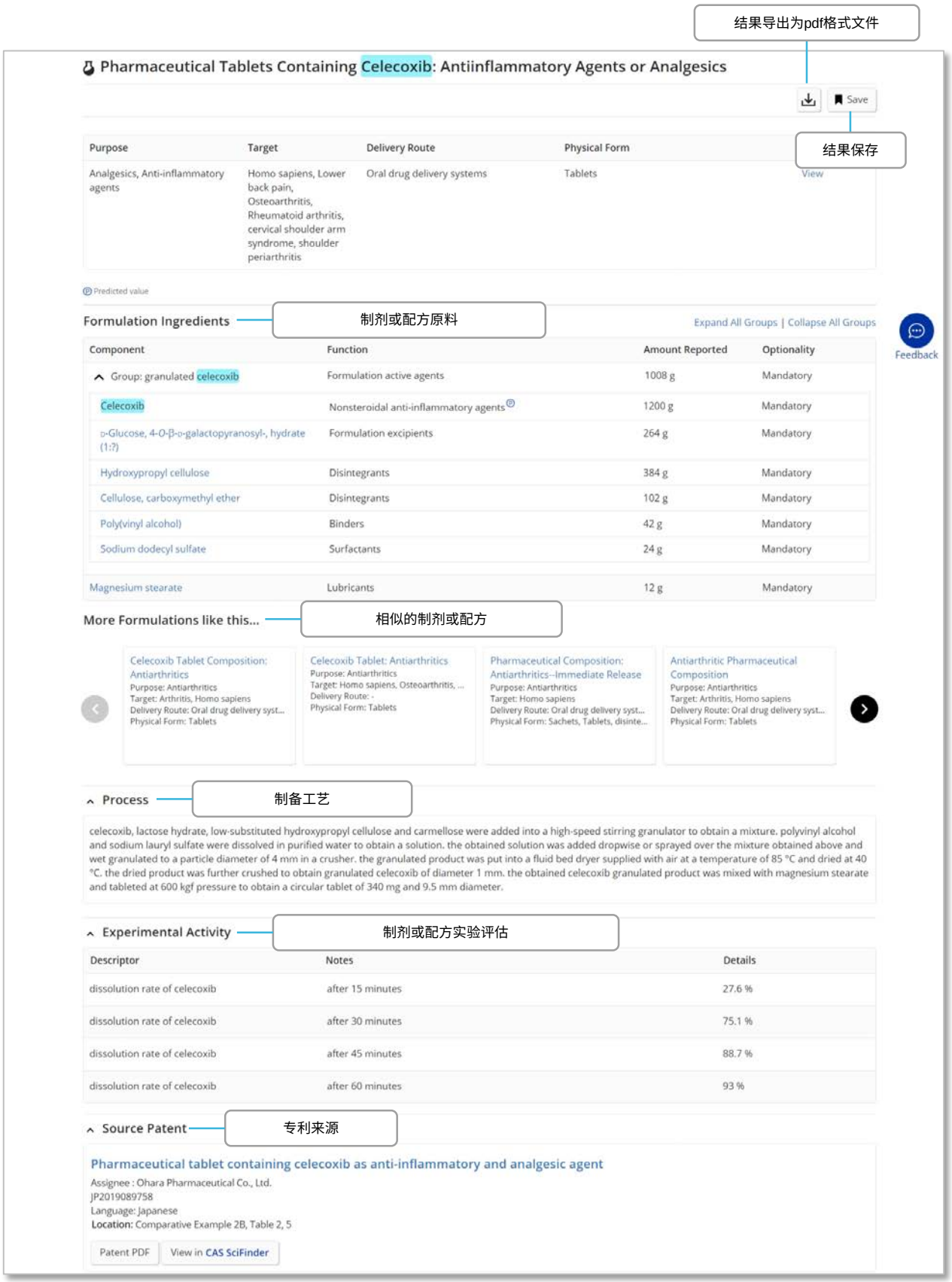
检索制剂或配方


CAS Formulus
Help & Support
9
Alerts
Saved
Good Afternoon, Liu
Formulations
Ingredients
celecoxib
输入制剂或配方的原料、用途、物理形态、功能或文献识别符（包括专利号、DOI号等），单击放大镜执行检索
Formulation Designer
Design custom formulation templates based on selections and ingredients
Advanced Search
Search Formulations using criteria like ingredients, targets, and more.


Advanced Formulations Search
Searches the following content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target.
At least two search terms are required.
输入检索词或物质
删除此项内容
浏览并选择检索项
Search For
Operator
Enter one term
Ingredient
Required
Celecoxib
Ex: caffeine, sodium, 50-00-0
Purpose
Analgesics
Ex: herbicide, fertilizer, bakery product
Form
Tablets
All Fields
Form
Function
Ingredient
Purpose
Route
Target
Required
Optional
Excluded
点击下拉菜单，浏览并设置运算符
Add Another Term
添加新的检索项
清除所有内容
Search
单击执行检索
Clear All

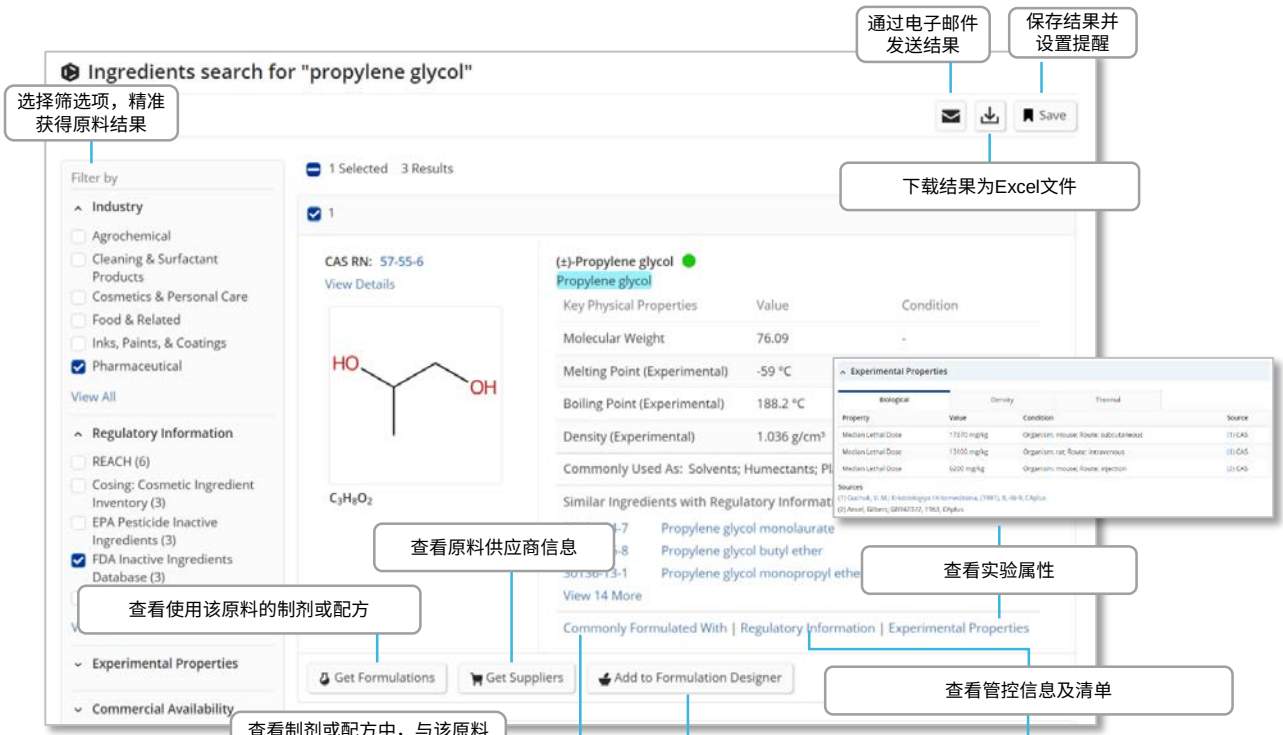

下载结果为PDF或Excel文件
Formulations search for "celecoxib"
Get Additional References
获得结果集对应的文献
Compare (2/3)
Save
Filter by
选择筛选项，精准获得配方或制剂结果
Sort: Relevance
Group: By Family
对比选中的制剂或配方
保存结果并设置提醒
Industry
Pharmaceutical
Unclassified
Purpose
Drug delivery systems (108)
Analgesics (81)
Anti-inflammatory agents (80)
Antiarthritics (57)
Pharmaceutical formulations (31)
View All
Physical Form
Capsules (85)
Tablets (81)
Solutions (54)
Suspensions (31)
Liquids (17)
View All
State of Matter
Delivery Route
Oral drug delivery systems (81)
Controlled-release drug delivery systems (11)
Topical drug delivery systems (5)
Parenteral drug delivery systems (4)
Inhalation drug delivery systems (2)
View All
Information Included
Component Amount (80)
Process (59)
Experimental Activity (49)
Effective Dose (5)
Document Type
Organization
Language
Publication Year
1999
2020
No Min
to
No Max
Apply
1
Pharmaceutical Tablets Containing Celecoxib: Antiinflammatory Agents or Analgesics
Location: Comparative Example 2B, Table 2, 5
Purpose: Analgesics, Anti-inflammatory agents
Target: Homo sapiens, Lower back pain, Osteoarthritis, Rheumatoid arthritis, cervical shoulder arm syndrome, shoulder periarthritis
Delivery Route: Oral drug delivery systems
Physical Form: Tablets
制剂或配方成分，功能及用量
Remove from Compare
Component
Function
Amount Reported
Group: granulated celecoxib
Formulation active agents
1008 g
Celecoxib
Nonsteroidal anti-inflammatory agents
1200 g
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?)
Formulation excipients
264 g
Hydroxypropyl cellulose
Disintegrants
Cellulose, carboxymethyl ether
Disintegrants
102 g
Additional group components reported
Group: Additional ingredients
-
-
Magnesium stearate
Lubricants
12 g
Predicted value
PATENT
Pharmaceutical tablet containing celecoxib as anti-inflammatory and analgesic agent
Assignee : Ohara Pharmaceutical Co., Ltd.
JP2019089758
Language: Japanese
Patent PDF
View in CAS SciFinder
查看或下载专利全文
在CAS SciFinder中查看文献详情
View Formulation Detail
查看制剂或配方详情
11 Similar Formulations - View All
查看相似的制剂或配方
2
Oral Pulsatile Drug Delivery System of Celecoxib: Antiinflammatory Agents or Analgesics--Controlled Release Drug Delivery Systems for Pharmaceutical Formulation
Location: Article Page 1, 3, 4, Table 1
Purpose: Analgesics, Anti-inflammatory agents
Delivery Route: Oral drug delivery systems
Physical Form: Tablets
Add to Compare
Component
Function
Amount Reported
Group: celecoxib granules
Formulation active agents
-
Celecoxib
Nonsteroidal anti-inflammatory agents
-
Mannitol
-
点击蓝色原料名称，查看详情
JOURNAL
Formulation and evaluation of pulsatile drug delivery system of celecoxib
World Journal of Pharmaceutical Research
Language: English
View in CAS SciFinder

制剂或配方详情

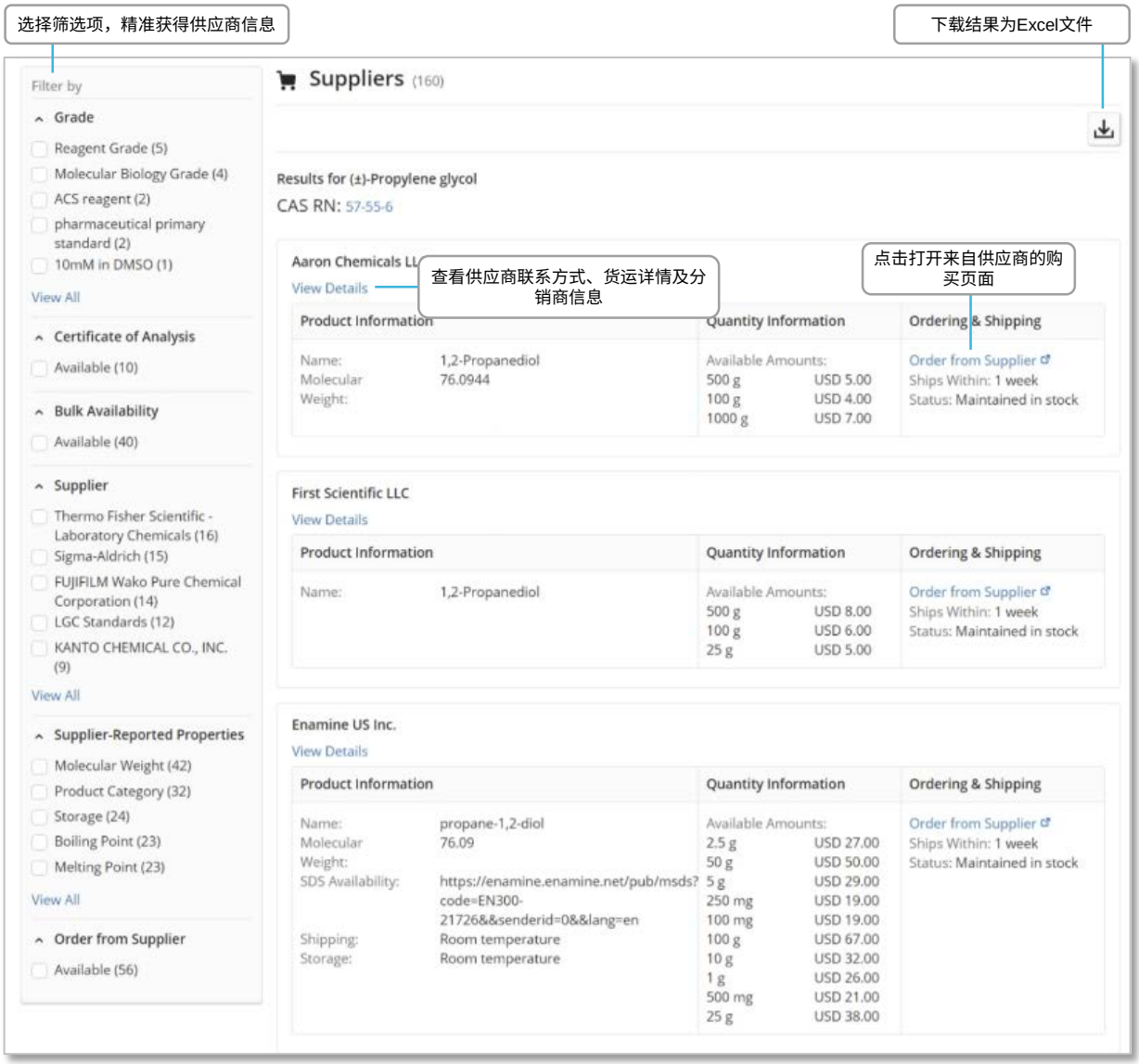

结果导出为pdf格式文件
Pharmaceutical Tablets Containing Celecoxib: Antiinflammatory Agents or Analgesics
Save
结果保存
Purpose
Target
Delivery Route
Physical Form
Analgesics, Anti-inflammatory agents
Homo sapiens, Lower back pain, Osteoarthritis, Rheumatoid arthritis, cervical shoulder arm syndrome, shoulder periarthritis
Oral drug delivery systems
Tablets
View
Predicted value
Formulation Ingredients
制剂或配方原料
Expand All Groups | Collapse All Groups
Feedback
Component
Function
Amount Reported
Optionality
Group: granulated celecoxib
Formulation active agents
1008 g
Mandatory
Celecoxib
Nonsteroidal anti-inflammatory agents
1200 g
Mandatory
D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:?)
Formulation excipients
264 g
Mandatory
Hydroxypropyl cellulose
Disintegrants
384 g
Mandatory
Cellulose, carboxymethyl ether
Disintegrants
102 g
Mandatory
Poly(vinyl alcohol)
Binders
42 g
Mandatory
Sodium dodecyl sulfate
Surfactants
24 g
Mandatory
Magnesium stearate
Lubricants
12 g
Mandatory
More Formulations like this...
相似的制剂或配方
Celecoxib Tablet Composition: Antiarthritics
Purpose: Antiarthritics
Target: Arthritis, Homo sapiens
Delivery Route: Oral drug delivery syst...
Physical Form: Tablets
Celecoxib Tablet: Antiarthritics
Purpose: Antiarthritics
Target: Homo sapiens, Osteoarthritis, ...
Delivery Route: -
Physical Form: Tablets
Pharmaceutical Composition: Antiarthritics--Immediate Release
Purpose: Antiarthritics
Target: Homo sapiens
Delivery Route: Oral drug delivery syst...
Physical Form: Sachets, Tablets, disinte...
Antiarthritic Pharmaceutical Composition
Purpose: Antiarthritics
Target: Arthritis, Homo sapiens
Delivery Route: Oral drug delivery syst...
Physical Form: Tablets
Process
制备工艺
celecoxib, lactose hydrate, low-substituted hydroxypropyl cellulose and carmellose were added into a high-speed stirring granulator to obtain a mixture. polyvinyl alcohol and sodium lauryl sulfate were dissolved in purified water to obtain a solution. the obtained solution was added dropwise or sprayed over the mixture obtained above and wet granulated to a particle diameter of 4 mm in a crusher. the granulated product was put into a fluid bed dryer supplied with air at a temperature of 85 °C and dried at 40 °C. the dried product was further crushed to obtain granulated celecoxib of diameter 1 mm. the obtained celecoxib granulated product was mixed with magnesium stearate and tableted at 600 kgf pressure to obtain a circular tablet of 340 mg and 9.5 mm diameter.
Experimental Activity
制剂或配方实验评估
Descriptor
Notes
Details
dissolution rate of celecoxib
after 15 minutes
27.6 %
dissolution rate of celecoxib
after 30 minutes
75.1 %
dissolution rate of celecoxib
after 45 minutes
88.7 %
dissolution rate of celecoxib
after 60 minutes
93 %
Source Patent
专利来源
Pharmaceutical tablet containing celecoxib as anti-inflammatory and analgesic agent
Assignee : Ohara Pharmaceutical Co., Ltd.
JP2019089758
Language: Japanese
Location: Comparative Example 2B, Table 2, 5
Patent PDF
View in CAS SciFinder

检索原料

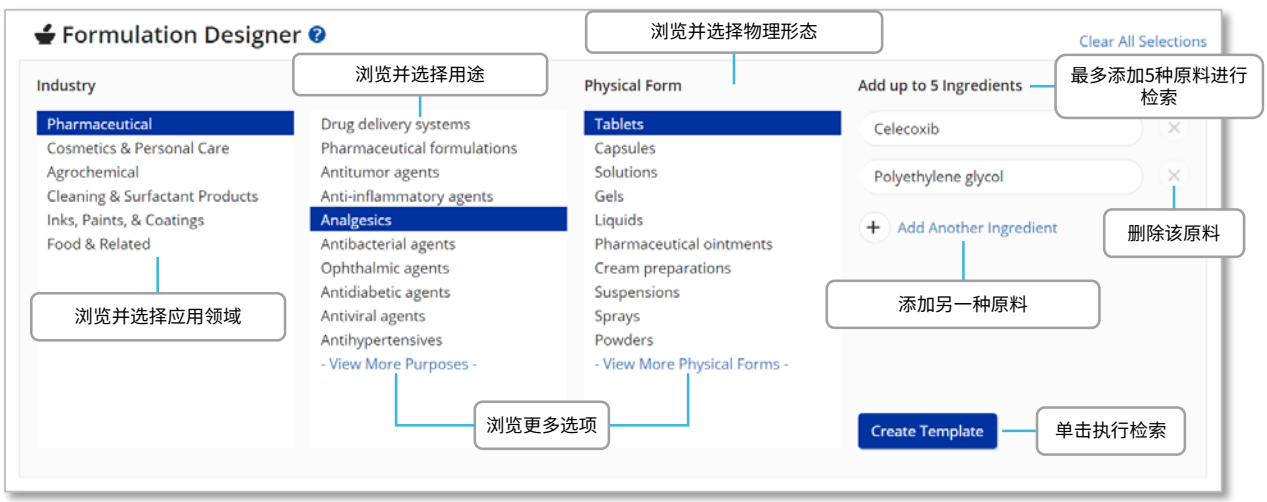

CAS Formulus
Help & Support
9
Alerts
Saved
Good Afternoon, Liu
选择Ingredients
Formulations
Ingredients
propylene glycol
输入原料名称、CAS登记号或功能信息，单击放大镜执行检索

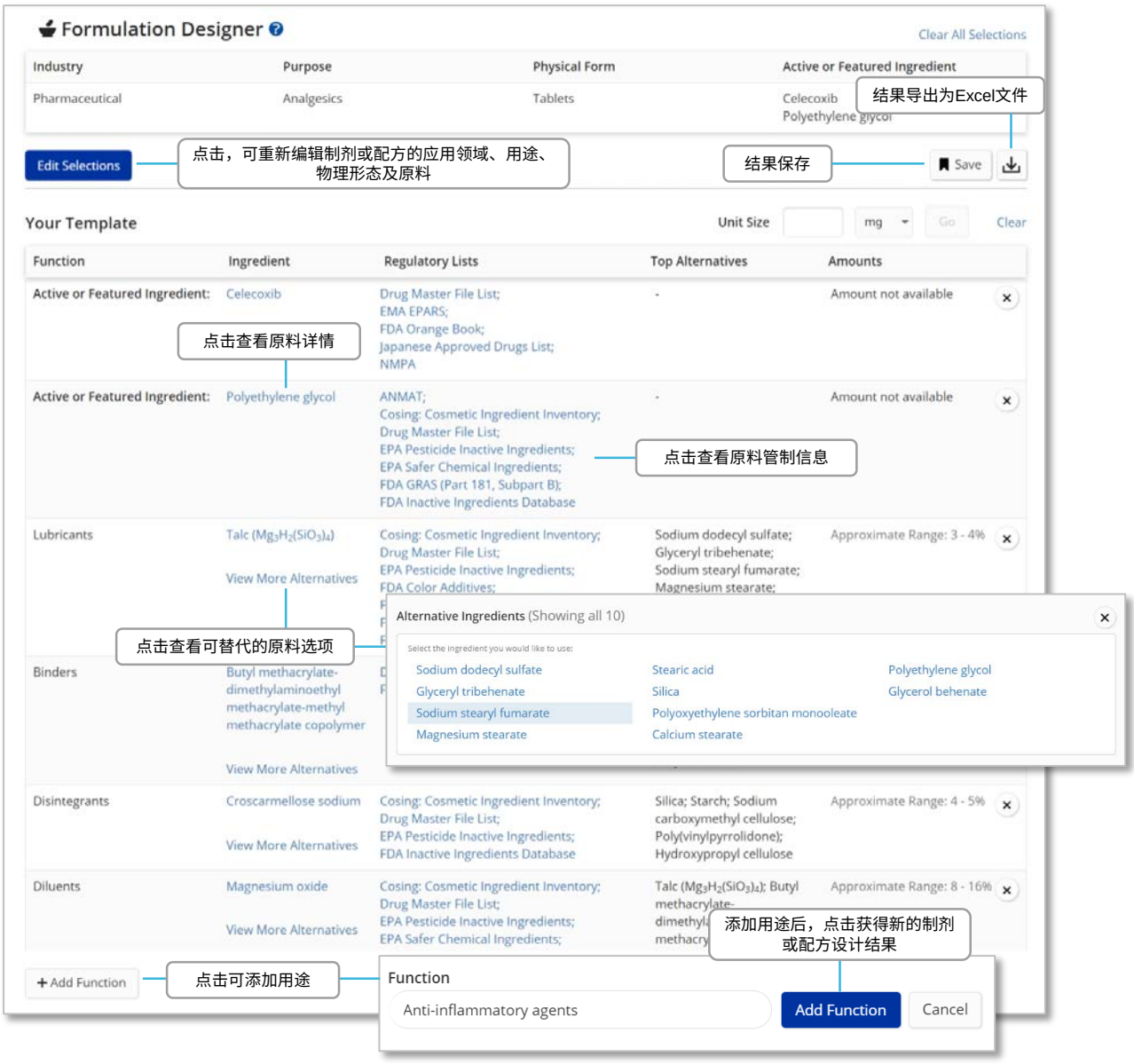

通过电子邮件发送结果
保存结果并设置提醒
Ingredients search for "propylene glycol"
选择筛选项，精准获得原料结果
Save
下载结果为Excel文件
Filter by
Industry
Agrochemical
Cleaning & Surfactant Products
Cosmetics & Personal Care
Food & Related
Inks, Paints, & Coatings
Pharmaceutical
View All
Regulatory Information
REACH (6)
Cosing: Cosmetic Ingredient Inventory (3)
EPA Pesticide Inactive Ingredients (3)
FDA Inactive Ingredients Database (3)
Experimental Properties
Commercial Availability
1 Selected 3 Results
CAS RN: 57-55-6
View Details
(±)-Propylene glycol
Propylene glycol
Key Physical Properties
Value
Condition
Molecular Weight
76.09
Melting Point (Experimental)
-59 °C
Boiling Point (Experimental)
188.2 °C
Density (Experimental)
1.036 g/cm³
Commonly Used As: Solvents; Humectants; Pl
Similar Ingredients with Regulatory Informat
Propylene glycol monolaurate
Propylene glycol butyl ether
Propylene glycol monopropyl ethe
View 14 More
Commonly Formulated With | Regulatory Information | Experimental Properties
Get Formulations
Get Suppliers
Add to Formulation Designer
查看原料供应商信息
查看使用该原料的制剂或配方
查看实验属性
查看管控信息及清单
查看制剂或配方中，与该原料同时使用的其它配伍成分
将原料添加至 Formulation Designer
Commonly Formulated With
ANMAT
Cosing: Cosmetic Ingredient Inventory
Drug Master File List
EMA Excipients List
Original Name (Translation)
Applicant Name
Event Date
Category
Packaging
Strength
Form
PROPILENGLICOL * (PROPYLENE GLYCOL)
ALCON LABORATORIOS ARGENTINA S.A.
March 2019
EYE LUBRICANT
1 Dropper Bottle of 10 ml
0.6 g/100 ml
OPHTHALMIC SOLUTION
* SEE PROSPECTUS IN VNM
Source
Marketing Authorizations for Medicines: is produced by Argentina National Administration of Medicines, Food and Medical Technology
Inventory Lists
Ingredient is on the following Inventory Lists:
Acronym
Inventory List
Country
AIIC
Australian Inventory of Industrial Chemicals
Australia
AIEC
South Korean Act on the Registration and Evaluation of Chemicals
Korea (Republic of)

查看原料供应商信息



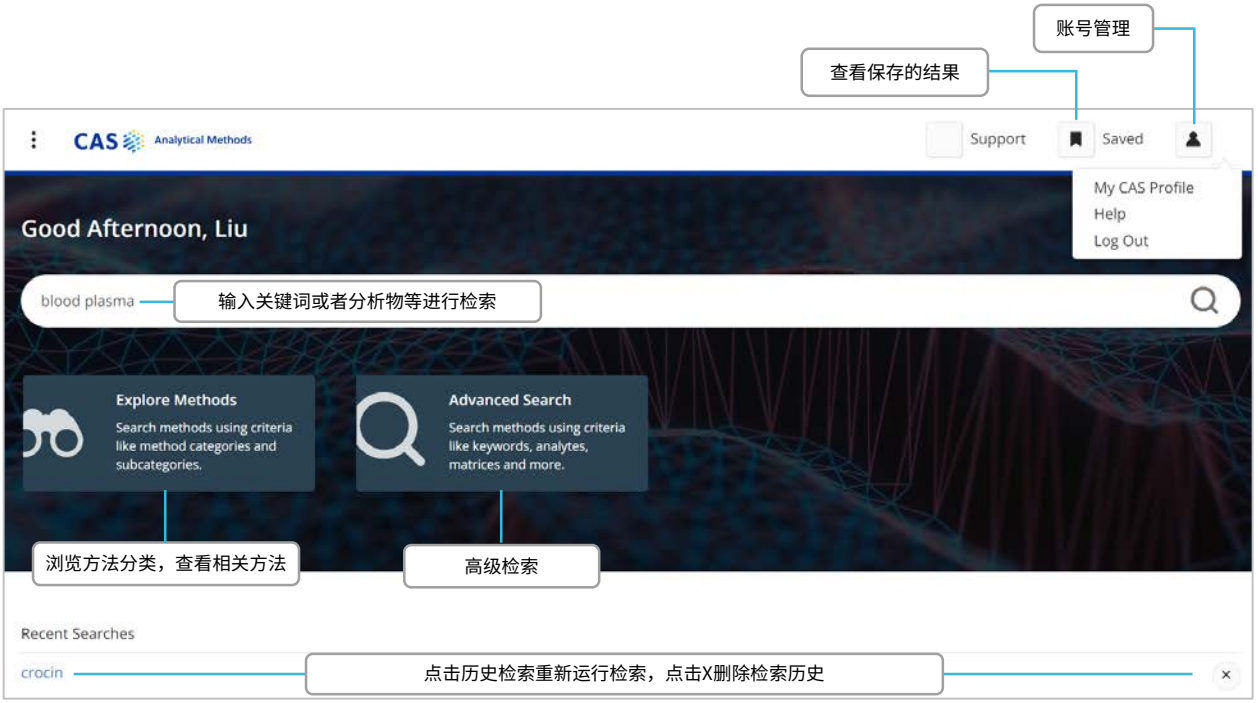
设计制剂或配方




Formulation Designer
Clear All Selections
Industry
Purpose
Physical Form
Active or Featured Ingredient
Pharmaceutical
Analgesics
Tablets
Celecoxib
Polyethylene glycol
结果导出为Excel文件
Edit Selections
点击，可重新编辑制剂或配方的应用领域、用途、物理形态及原料
结果保存
Save
Your Template
Unit Size
mg
Go
Clear
Function
Ingredient
Regulatory Lists
Top Alternatives
Amounts
Active or Featured Ingredient:
Celecoxib
Drug Master File List;
EMA EPARS;
FDA Orange Book;
Japanese Approved Drugs List;
NMPA
Amount not available
点击查看原料详情
Active or Featured Ingredient:
Polyethylene glycol
ANMAT;
Cosing: Cosmetic Ingredient Inventory;
Drug Master File List;
EPA Pesticide Inactive Ingredients;
EPA Safer Chemical Ingredients;
FDA GRAS (Part 181, Subpart B);
FDA Inactive Ingredients Database
Amount not available
点击查看原料管制信息
Lubricants
Talc ($Mg_3H_2(SiO_3)_4$)
View More Alternatives
Cosing: Cosmetic Ingredient Inventory;
Drug Master File List;
EPA Pesticide Inactive Ingredients;
FDA Color Additives;
Sodium dodecyl sulfate;
Glyceryl tribehenate;
Sodium stearyl fumarate;
Magnesium stearate;
Approximate Range: 3 - 4%
点击查看可替代的原料选项
Alternative Ingredients (Showing all 10)
Select the ingredient you would like to use:
Sodium dodecyl sulfate
Glyceryl tribehenate
Sodium stearyl fumarate
Magnesium stearate
Stearic acid
Silica
Polyoxyethylene sorbitan monooleate
Calcium stearate
Polyethylene glycol
Glycerol behenate
Binders
Butyl methacrylate-dimethylaminoethyl methacrylate-methyl methacrylate copolymer
View More Alternatives
Disintegrants
Croscarmellose sodium
View More Alternatives
Cosing: Cosmetic Ingredient Inventory;
Drug Master File List;
EPA Pesticide Inactive Ingredients;
FDA Inactive Ingredients Database
Silica; Starch; Sodium carboxymethyl cellulose; Poly(vinylpyrrolidone); Hydroxypropyl cellulose
Approximate Range: 4 - 5%
Diluents
Magnesium oxide
View More Alternatives
Cosing: Cosmetic Ingredient Inventory;
Drug Master File List;
EPA Pesticide Inactive Ingredients;
EPA Safer Chemical Ingredients;
Talc ($Mg_3H_2(SiO_3)_4$); Butyl methacrylate-dimethyl
Approximate Range: 8 - 16%
添加用途后，点击获得新的制剂或配方设计结果
+ Add Function
点击可添加用途
Function
Anti-inflammatory agents
Add Function
Cancel

CAS Analytical Methods

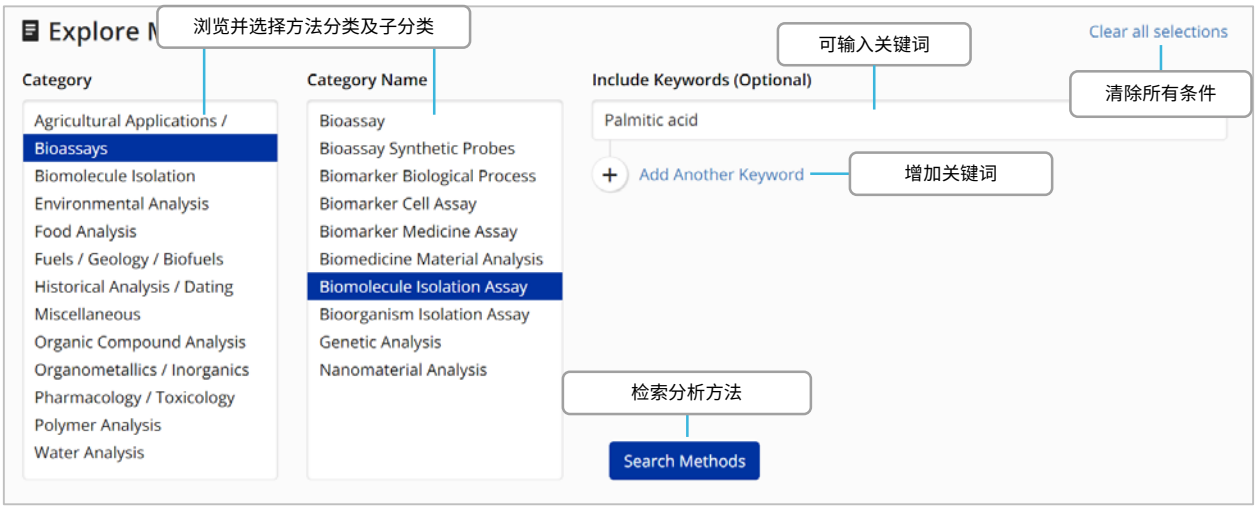
分析方法检索


账号管理
查看保存的结果
CAS Analytical Methods
Support
Saved
My CAS Profile
Help
Log Out
Good Afternoon, Liu
blood plasma
输入关键词或者分析物等进行检索
Explore Methods
Search methods using criteria like method categories and subcategories.
Advanced Search
Search methods using criteria like keywords, analytes, matrices and more.
浏览方法分类，查看相关方法
高级检索
Recent Searches
crocin
点击历史检索重新运行检索，点击X删除检索历史

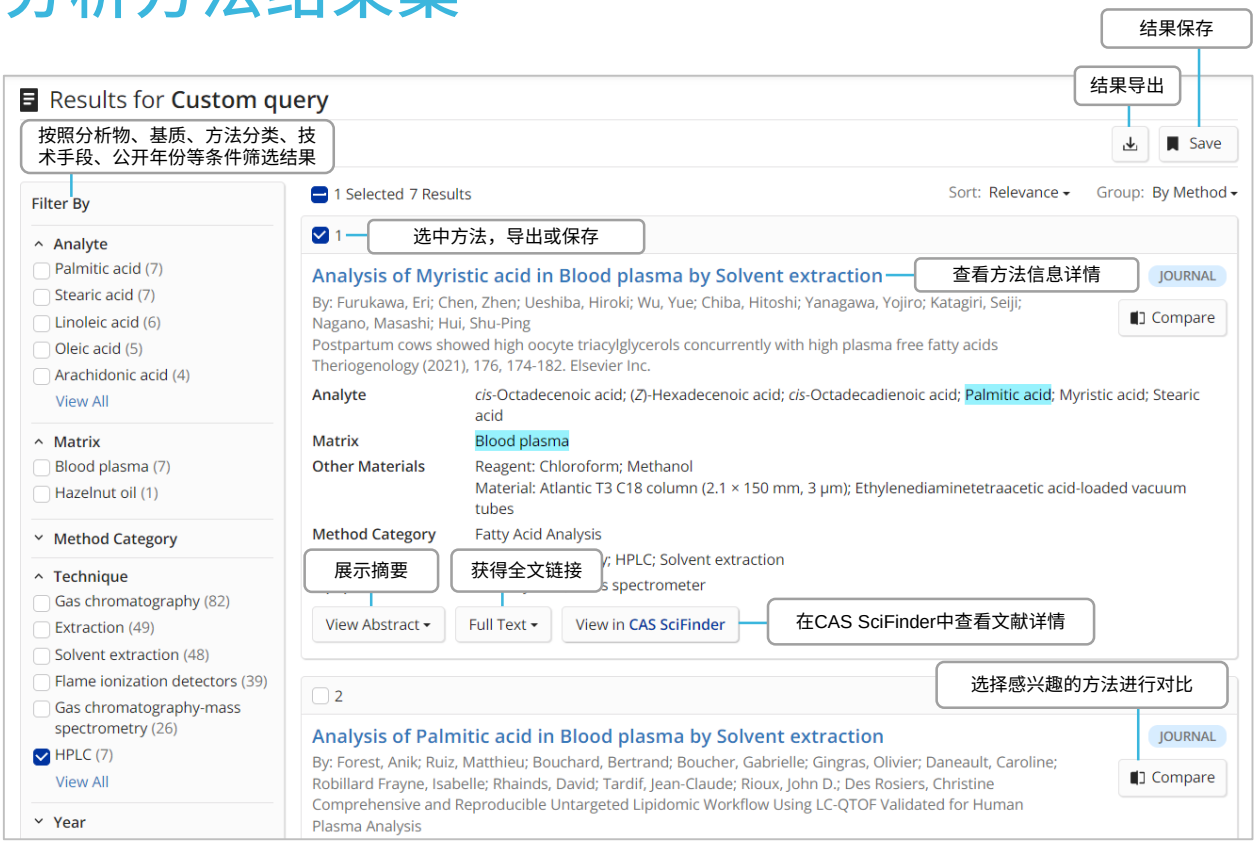
高级检索


AND
OR
NOT
逻辑运算符： and，or，not
增加检索条件
Advanced Search
Analyte
palmitic acid
AND
Matrix
blood plasma
Add Search Criteria
Clear
检索条件包括：关键词，分析物，基质，方法分类，技术手段，CAS方法号，出版物名称
删除检索条件
Keyword
Analyte
Matrix
Method Category
Technique
CAS Method Number
Publication Name

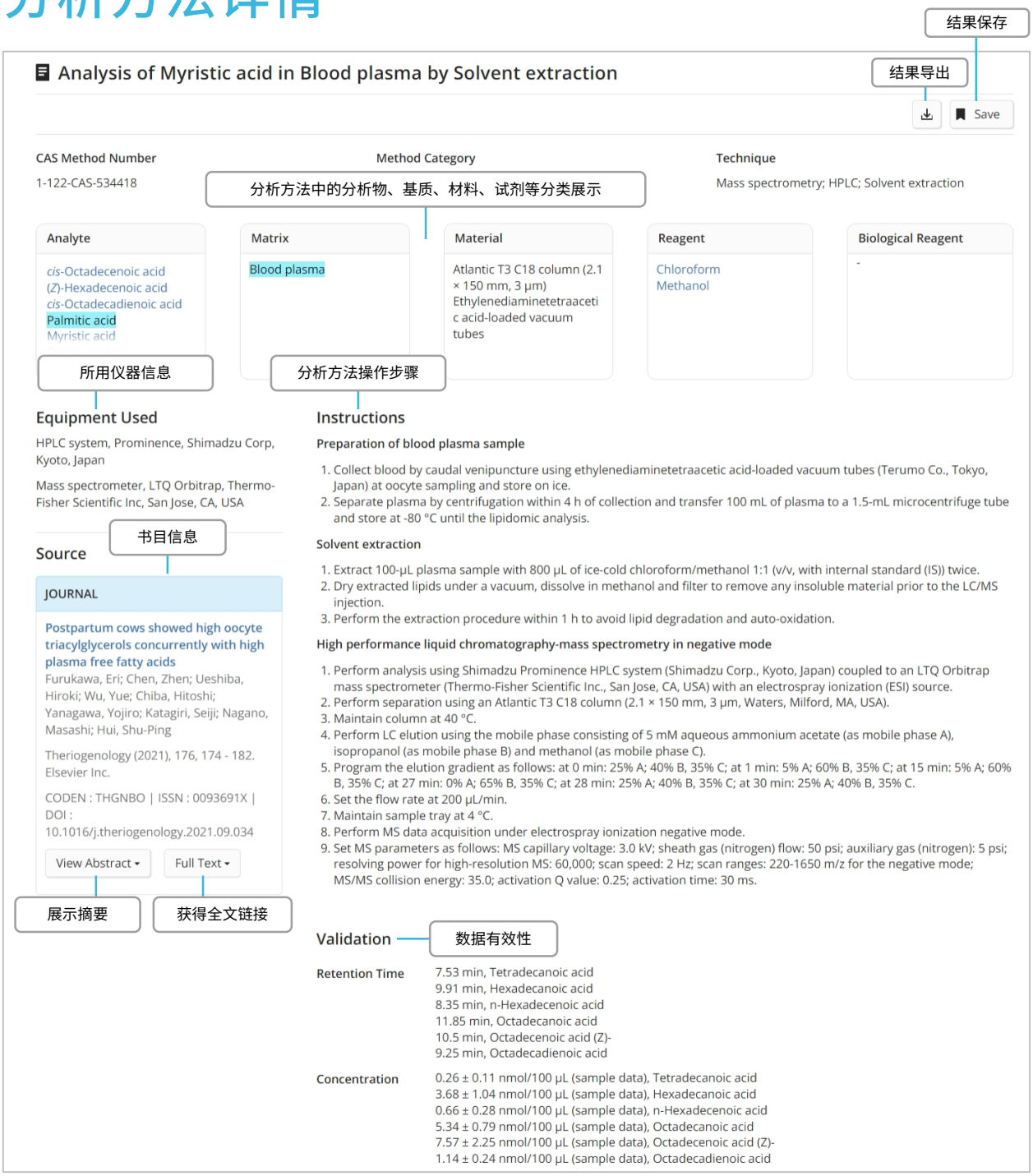
分析方法的分类检索



分析方法结果集



分析方法详情


结果保存
Analysis of Myristic acid in Blood plasma by Solvent extraction
结果导出
Save
CAS Method Number
1-122-CAS-534418
Method Category
分析方法中的分析物、基质、材料、试剂等分类展示
Technique
Mass spectrometry; HPLC; Solvent extraction
Analyte
cis-Octadecenoic acid
(Z)-Hexadecenoic acid
cis-Octadecadienoic acid
Palmitic acid
Myristic acid
Matrix
Blood plasma
Material
Atlantic T3 C18 column (2.1 × 150 mm, 3 µm)
Ethylenediaminetetraacetic acid-loaded vacuum tubes
Reagent
Chloroform
Methanol
Biological Reagent
-
所用仪器信息
分析方法操作步骤
Equipment Used
HPLC system, Prominence, Shimadzu Corp, Kyoto, Japan
Mass spectrometer, LTQ Orbitrap, Thermo-Fisher Scientific Inc, San Jose, CA, USA
书目信息
Source
JOURNAL
Postpartum cows showed high oocyte triacylglycerols concurrently with high plasma free fatty acids
Furukawa, Eri; Chen, Zhen; Ueshiba, Hiroki; Wu, Yue; Chiba, Hitoshi; Yanagawa, Yojiro; Katagiri, Seiji; Nagano, Masashi; Hui, Shu-Ping
Theriogenology (2021), 176, 174 - 182. Elsevier Inc.
CODEN : THGNBO | ISSN : 0093691X | DOI : 10.1016/j.theriogenology.2021.09.034
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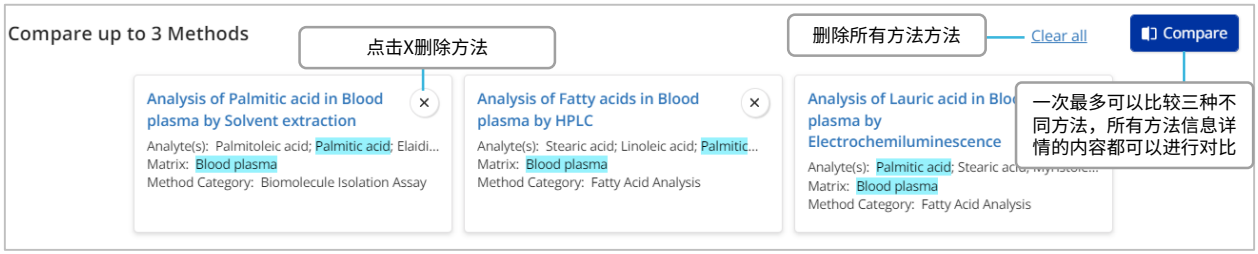
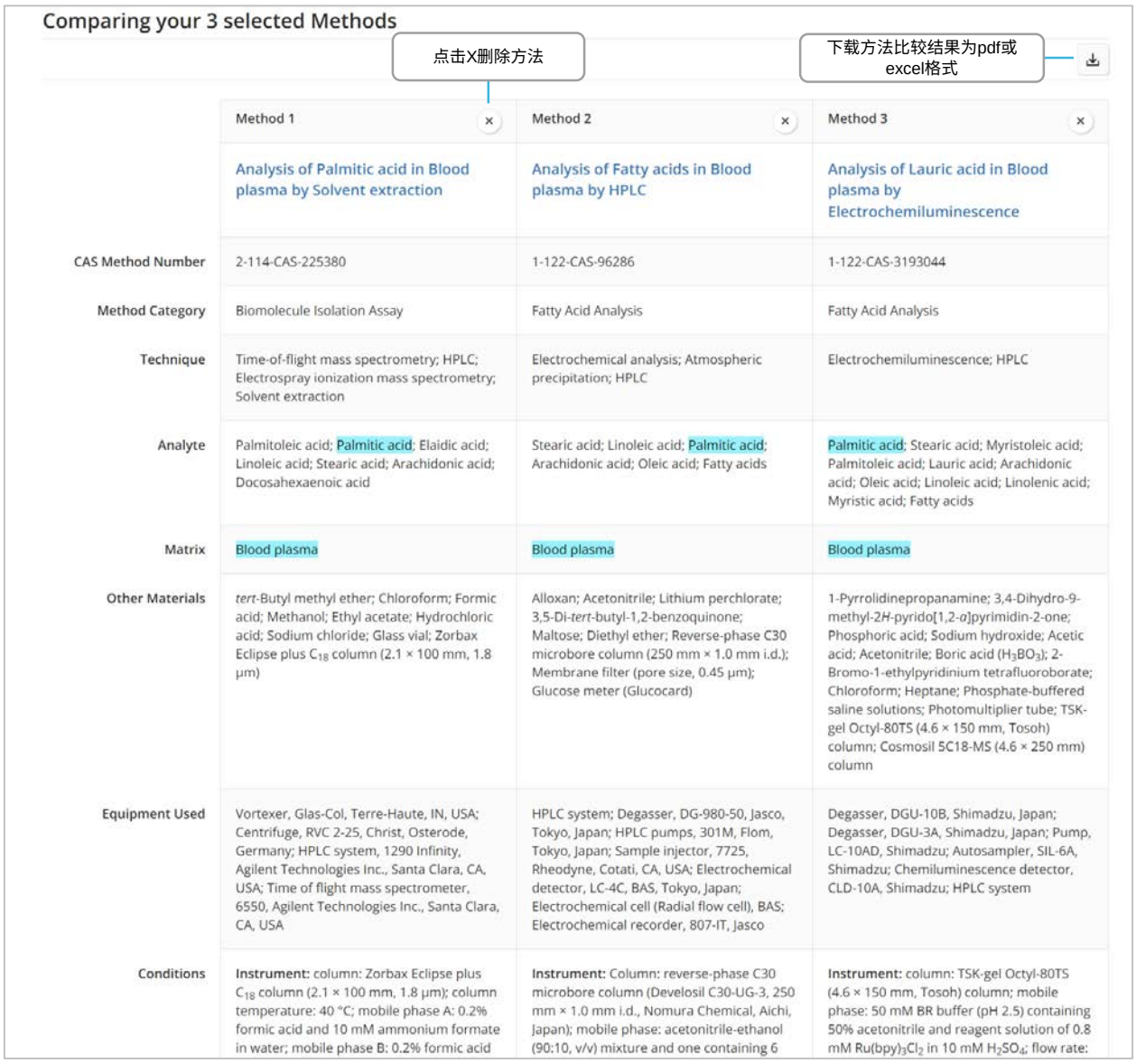
Instructions
Preparation of blood plasma sample
1. Collect blood by caudal venipuncture using ethylenediaminetetraacetic acid-loaded vacuum tubes (Terumo Co., Tokyo, Japan) at oocyte sampling and store on ice.
2. Separate plasma by centrifugation within 4 h of collection and transfer 100 mL of plasma to a 1.5-mL microcentrifuge tube and store at -80 °C until the lipidomic analysis.
Solvent extraction
1. Extract 100-µL plasma sample with 800 µL of ice-cold chloroform/methanol 1:1 (v/v, with internal standard (IS)) twice.
2. Dry extracted lipids under a vacuum, dissolve in methanol and filter to remove any insoluble material prior to the LC/MS injection.
3. Perform the extraction procedure within 1 h to avoid lipid degradation and auto-oxidation.
High performance liquid chromatography-mass spectrometry in negative mode
1. Perform analysis using Shimadzu Prominence HPLC system (Shimadzu Corp., Kyoto, Japan) coupled to an LTQ Orbitrap mass spectrometer (Thermo-Fisher Scientific Inc., San Jose, CA, USA) with an electrospray ionization (ESI) source.
2. Perform separation using an Atlantic T3 C18 column (2.1 × 150 mm, 3 µm, Waters, Milford, MA, USA).
3. Maintain column at 40 °C.
4. Perform LC elution using the mobile phase consisting of 5 mM aqueous ammonium acetate (as mobile phase A), isopropanol (as mobile phase B) and methanol (as mobile phase C).
5. Program the elution gradient as follows: at 0 min: 25% A; 40% B, 35% C; at 1 min: 5% A; 60% B, 35% C; at 15 min: 5% A; 60% B, 35% C; at 27 min: 0% A; 65% B, 35% C; at 28 min: 25% A; 40% B, 35% C; at 30 min: 25% A; 40% B, 35% C.
6. Set the flow rate at 200 µL/min.
7. Maintain sample tray at 4 °C.
8. Perform MS data acquisition under electrospray ionization negative mode.
9. Set MS parameters as follows: MS capillary voltage: 3.0 kV; sheath gas (nitrogen) flow: 50 psi; auxiliary gas (nitrogen): 5 psi; resolving power for high-resolution MS: 60,000; scan speed: 2 Hz; scan ranges: 220-1650 m/z for the negative mode; MS/MS collision energy: 35.0; activation Q value: 0.25; activation time: 30 ms.
Validation
数据有效性
Retention Time
7.53 min, Tetradecanoic acid
9.91 min, Hexadecanoic acid
8.35 min, n-Hexadecenoic acid
11.85 min, Octadecanoic acid
10.5 min, Octadecenoic acid (Z)-
9.25 min, Octadecadienoic acid
Concentration
0.26 ± 0.11 nmol/100 µL (sample data), Tetradecanoic acid
3.68 ± 1.04 nmol/100 µL (sample data), Hexadecanoic acid
0.66 ± 0.28 nmol/100 µL (sample data), n-Hexadecenoic acid
5.34 ± 0.79 nmol/100 µL (sample data), Octadecanoic acid
7.57 ± 2.25 nmol/100 µL (sample data), Octadecenoic acid (Z)-
1.14 ± 0.24 nmol/100 µL (sample data), Octadecadienoic acid

分析方法详情对比





	Method 1	Method 2	Method 3
	Analysis of Palmitic acid in Blood plasma by Solvent extraction	Analysis of Fatty acids in Blood plasma by HPLC	Analysis of Lauric acid in Blood plasma by Electrochemiluminescence
CAS Method Number	2-114-CAS-225380	1-122-CAS-96286	1-122-CAS-3193044
Method Category	Biomolecule Isolation Assay	Fatty Acid Analysis	Fatty Acid Analysis
Technique	Time-of-flight mass spectrometry; HPLC; Electrospray ionization mass spectrometry; Solvent extraction	Electrochemical analysis; Atmospheric precipitation; HPLC	Electrochemiluminescence; HPLC
Analyte	Palmitoleic acid; Palmitic acid; Elaidic acid; Linoleic acid; Stearic acid; Arachidonic acid; Docosahexaenoic acid	Stearic acid; Linoleic acid; Palmitic acid; Arachidonic acid; Oleic acid; Fatty acids	Palmitic acid; Stearic acid; Myristoleic acid; Palmitoleic acid; Lauric acid; Arachidonic acid; Oleic acid; Linoleic acid; Linolenic acid; Myristic acid; Fatty acids
Matrix	Blood plasma	Blood plasma	Blood plasma
Other Materials	*tert*-Butyl methyl ether; Chloroform; Formic acid; Methanol; Ethyl acetate; Hydrochloric acid; Sodium chloride; Glass vial; Zorbax Eclipse plus C_{18} column (2.1 × 100 mm, 1.8 µm)	Alloxan; Acetonitrile; Lithium perchlorate; 3,5-Di-*tert*-butyl-1,2-benzoquinone; Maltose; Diethyl ether; Reverse-phase C30 microbore column (250 mm × 1.0 mm i.d.); Membrane filter (pore size, 0.45 µm); Glucose meter (Glucocard)	1-Pyrrolidinepropanamine; 3,4-Dihydro-9-methyl-2*H*-pyrido[1,2-*a*]pyrimidin-2-one; Phosphoric acid; Sodium hydroxide; Acetic acid; Acetonitrile; Boric acid (H_3BO_3); 2-Bromo-1-ethylpyridinium tetrafluoroborate; Chloroform; Heptane; Phosphate-buffered saline solutions; Photomultiplier tube; TSK-gel Octyl-80TS (4.6 × 150 mm, Tosoh) column; Cosmosil 5C18-MS (4.6 × 250 mm) column
Equipment Used	Vortexer, Glas-Col, Terre-Haute, IN, USA; Centrifuge, RVC 2-25, Christ, Osterode, Germany; HPLC system, 1290 Infinity, Agilent Technologies Inc., Santa Clara, CA, USA; Time of flight mass spectrometer, 6550, Agilent Technologies Inc., Santa Clara, CA, USA	HPLC system; Degasser, DG-980-50, Jasco, Tokyo, Japan; HPLC pumps, 301M, Flom, Tokyo, Japan; Sample injector, 7725, Rheodyne, Cotati, CA, USA; Electrochemical detector, LC-4C, BAS, Tokyo, Japan; Electrochemical cell (Radial flow cell), BAS; Electrochemical recorder, 807-IT, Jasco	Degasser, DGU-10B, Shimadzu, Japan; Degasser, DGU-3A, Shimadzu, Japan; Pump, LC-10AD, Shimadzu; Autosampler, SIL-6A, Shimadzu; Chemiluminescence detector, CLD-10A, Shimadzu; HPLC system
Conditions	**Instrument:** column: Zorbax Eclipse plus C_{18} column (2.1 × 100 mm, 1.8 µm); column temperature: 40 °C; mobile phase A: 0.2% formic acid and 10 mM ammonium formate in water; mobile phase B: 0.2% formic acid	**Instrument:** Column: reverse-phase C30 microbore column (Develosil C30-UG-3, 250 mm × 1.0 mm i.d., Nomura Chemical, Aichi, Japan); mobile phase: acetonitrile-ethanol (90:10, v/v) mixture and one containing 6	**Instrument:** column: TSK-gel Octyl-80TS (4.6 × 150 mm, Tosoh) column; mobile phase: 50 mM BR buffer (pH 2.5) containing 50% acetonitrile and reagent solution of 0.8 mM $Ru(bpy)_3Cl_2$ in 10 mM H_2SO_4; flow rate:

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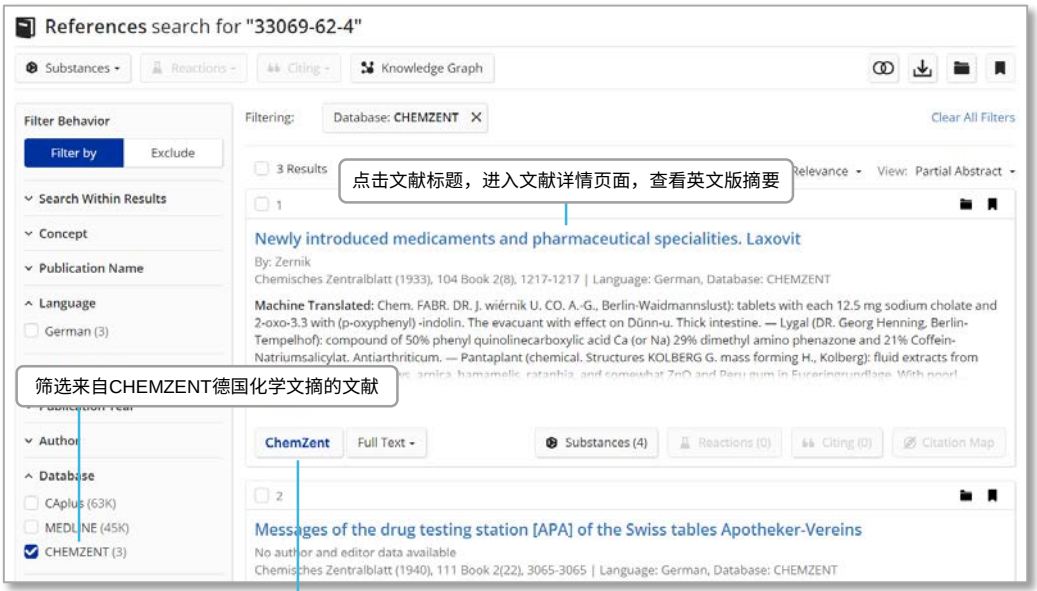

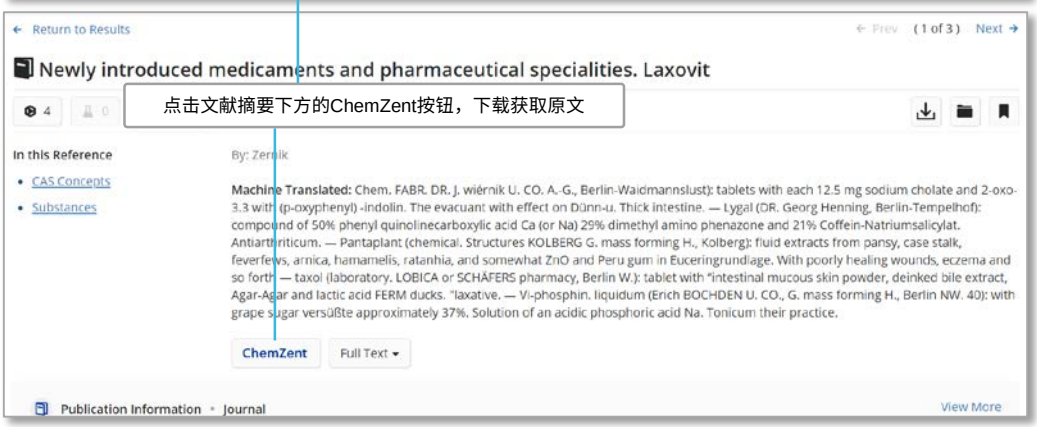

登录，反馈，培训，支持

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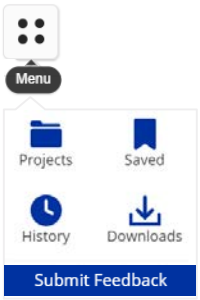

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