学术版

CAS SCIFINDER DISCOVERY PLATFORM™

快速入门指南

CAS

A division of the
American Chemical Society

目录

CAS SciFinder

主界面及文献检索

检索界面

CAS SciFinder拥有简洁的检索界面。

文献结果集界面

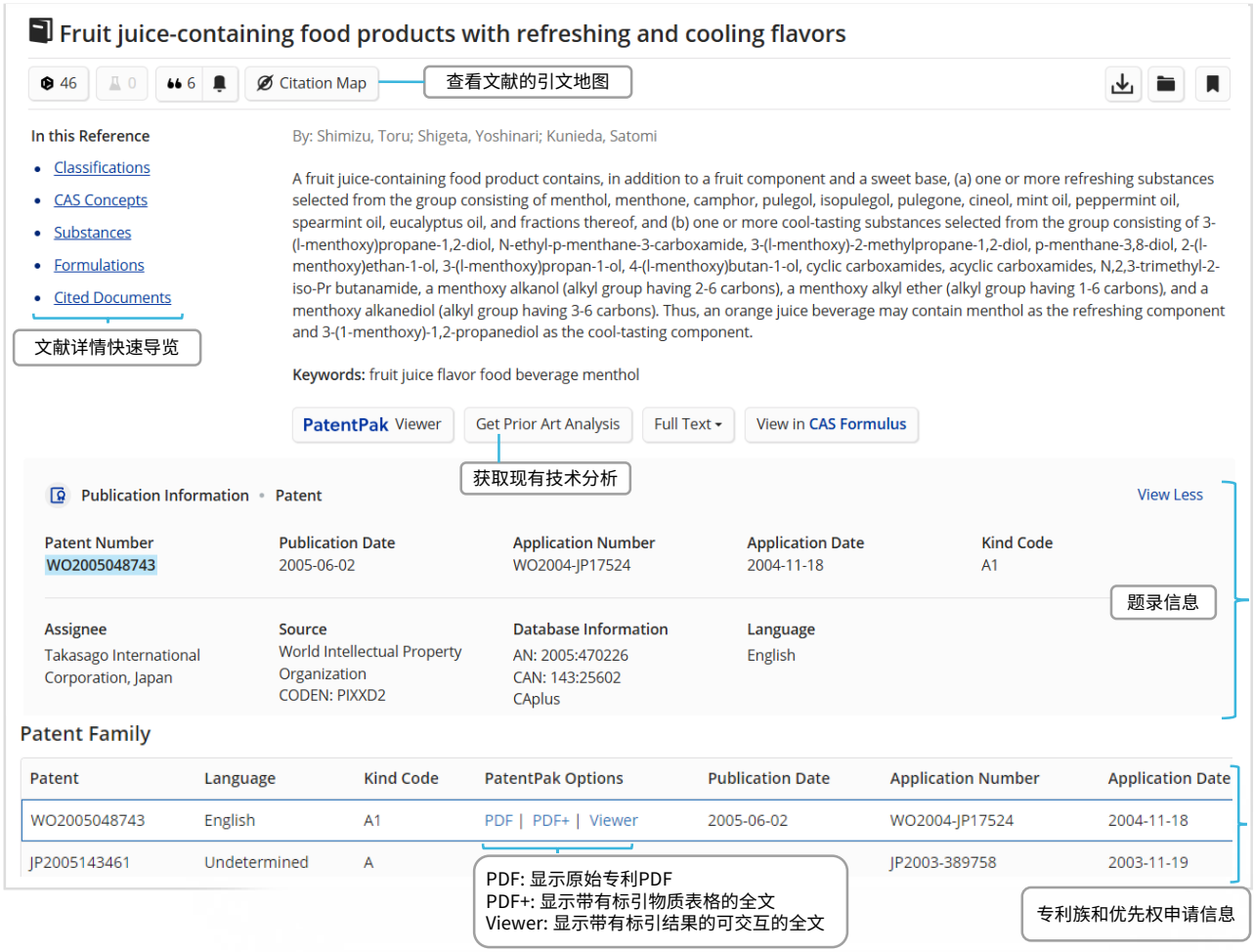
进行文献检索时，您可以在一个易于使用的界面中访问完整的检索结果集：

- 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

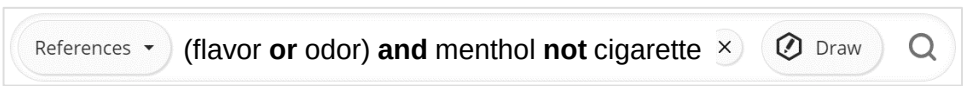
文献详情

获取 CAS SciFinder 中每篇文献的详细信息。



布尔逻辑运算符

如下所示，您可以使用布尔逻辑运算符进行文献检索，可以通过使用括号对逻辑运算符进行优先运算。



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?

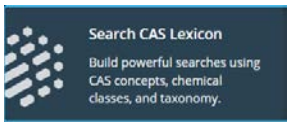
包含双引号的短语将作为精确短语进行检索。
例如：搜索“Programmed cell death protein”只会找到完全匹配“Programmed cell death protein”的结果。

CAS Lexicon

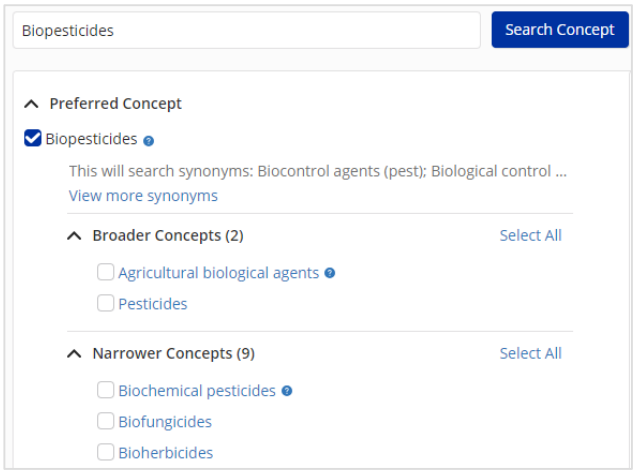
CAS Lexicon概述

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。

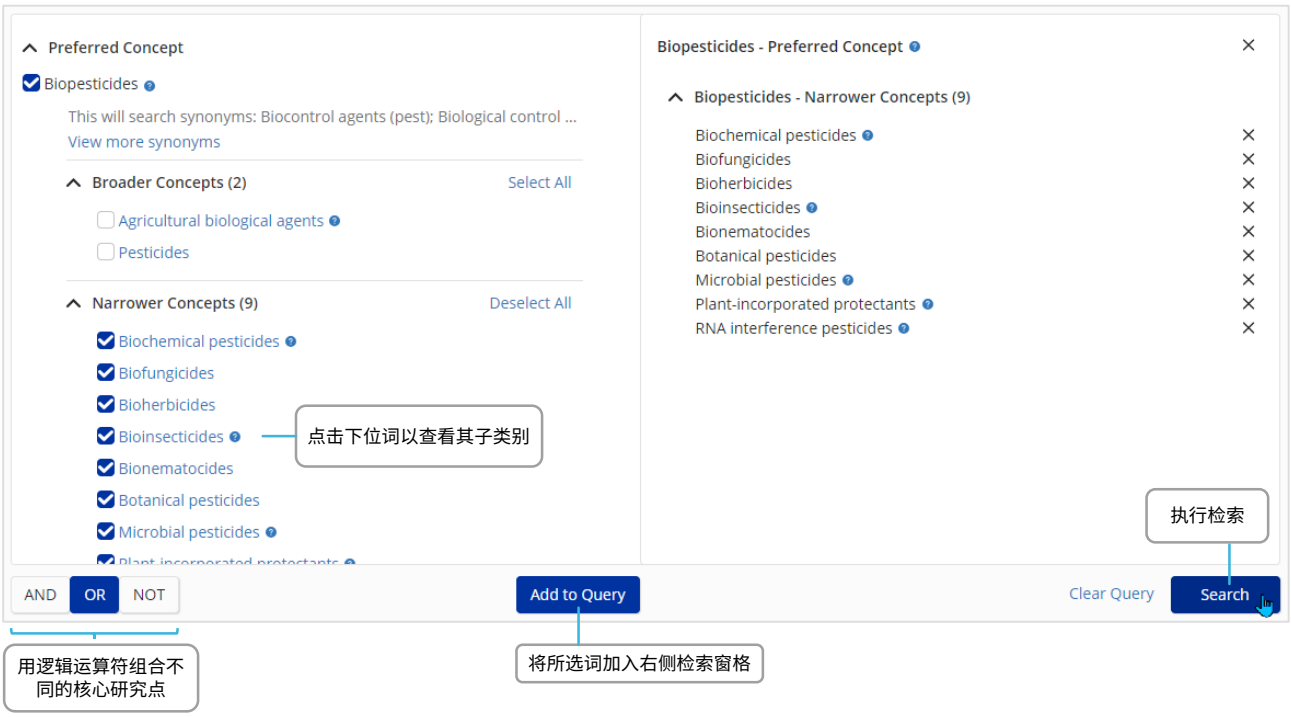
访问和浏览



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。

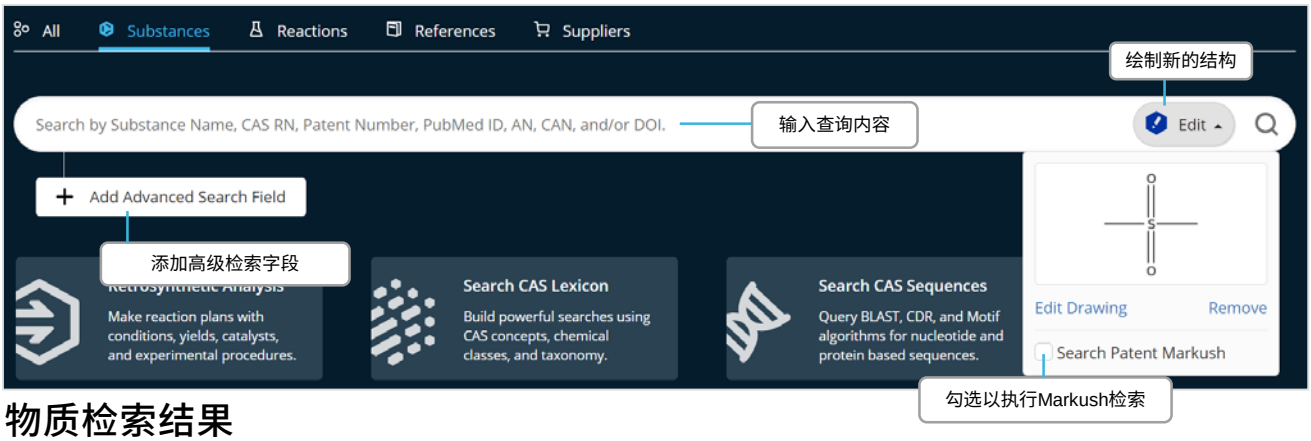


物质名称及结构式检索

物质检索

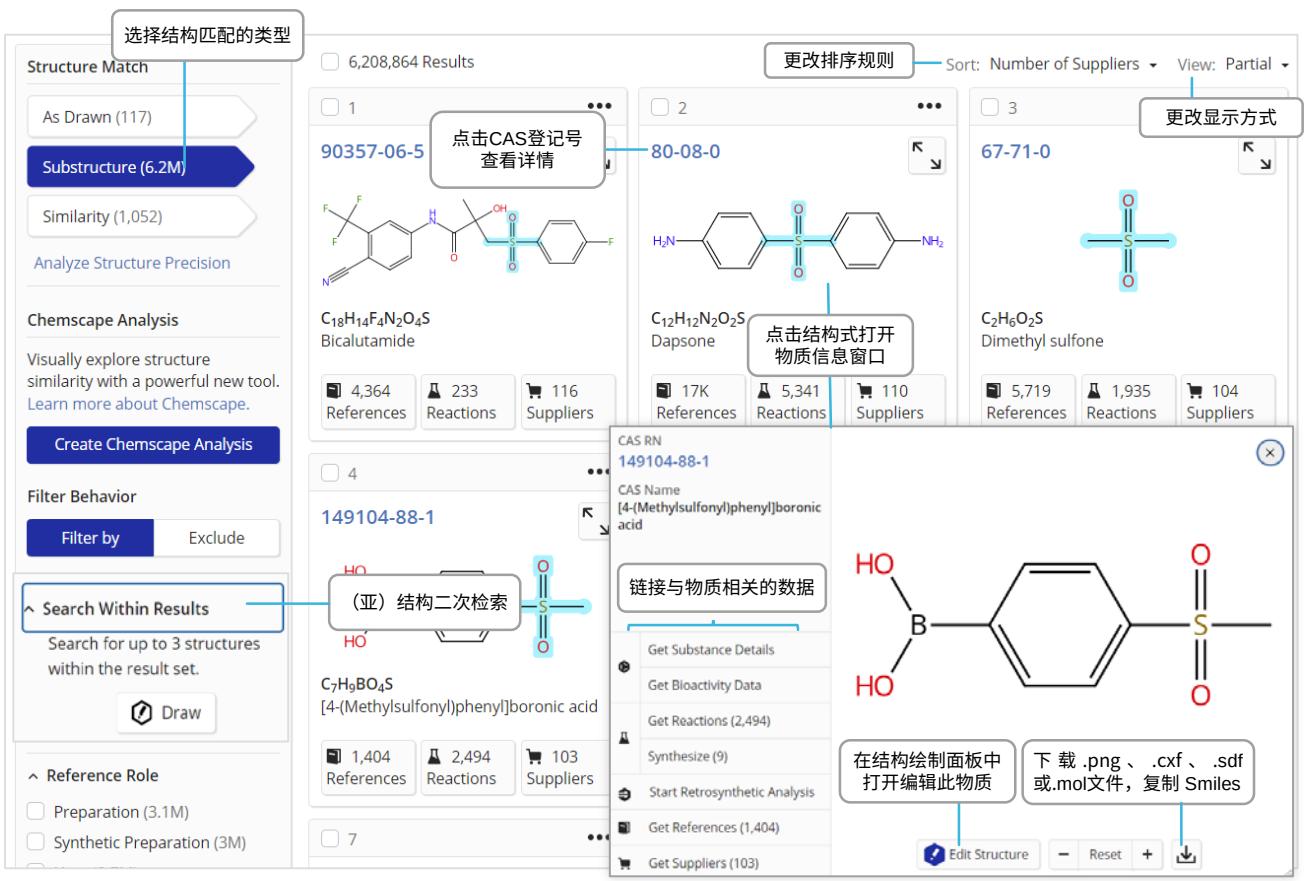
可以通过在检索框中输入一个或多个物质名称或标识符来检索物质。还可以通过绘制或编辑结构式进行检索。以下是物质检索的示例：

Streptomycin
57-92-1
"Streptomycin sulfate"
Sulfoximin*
WO2019234160



物质检索结果

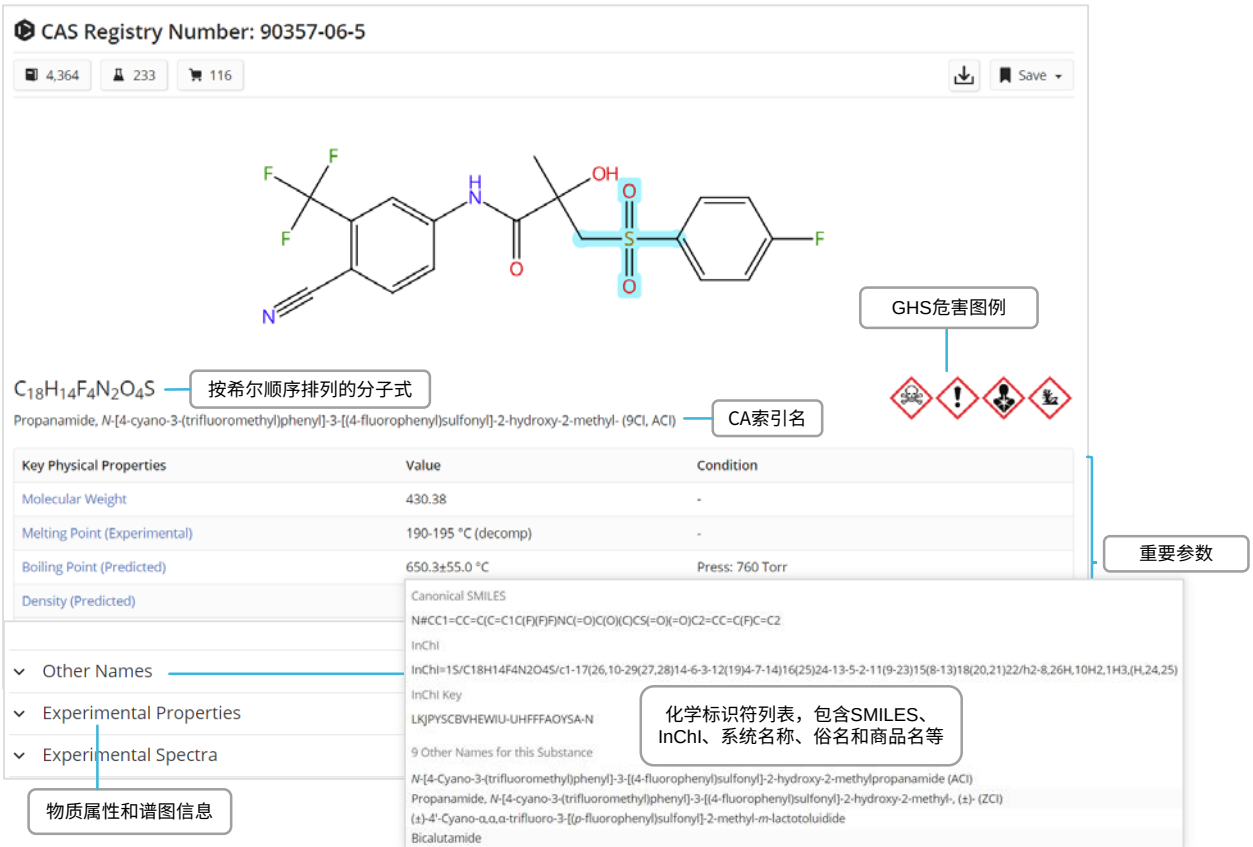
物质检索结果在一个直观的界面中呈现，您将看到与您的检索最相关的结果，包括物质名称、CAS登记号和高分辨率结构式图像。



物质详情和结构绘制面板

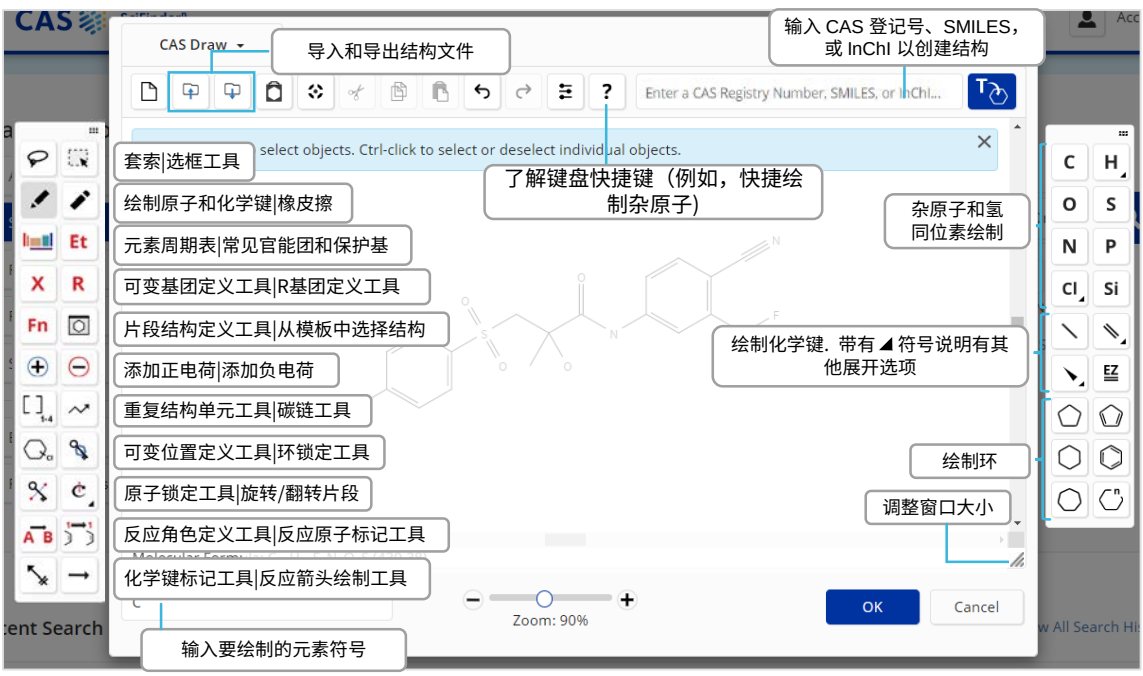
物质详情

点击某个物质检索结果的 CAS 登记号时，会显示该物质的详细信息，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。

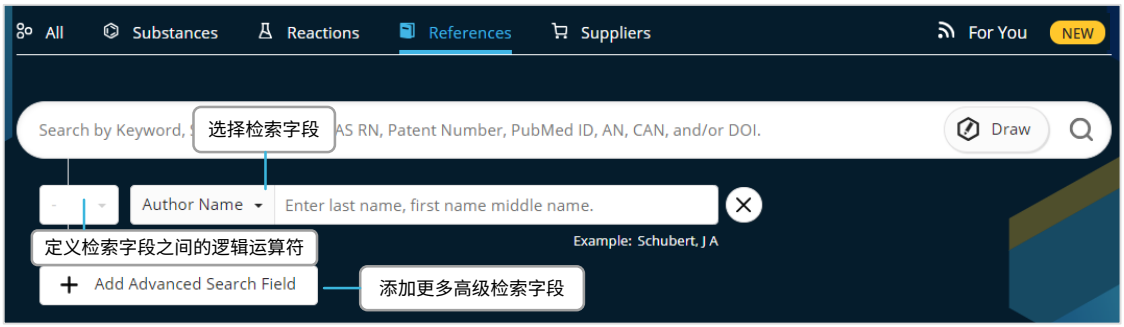


高级检索

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，无需使用逻辑运算符
- 允许使用通配符，例如 pollut*
- 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）

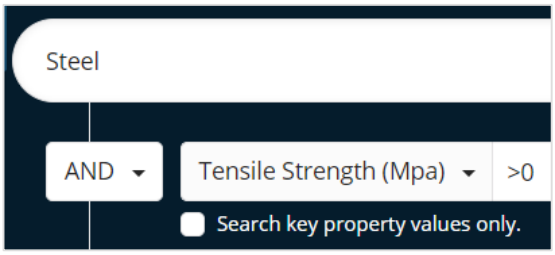


高级检索示例

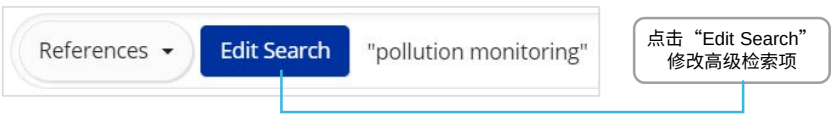
高级文献检索

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
- 生命科学数据
- 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
- 生命科学数据
- 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，您可以聚焦感兴趣的物质及其特定研究角色相关的文献。

- 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）使用。

物质检索结果中的Roles

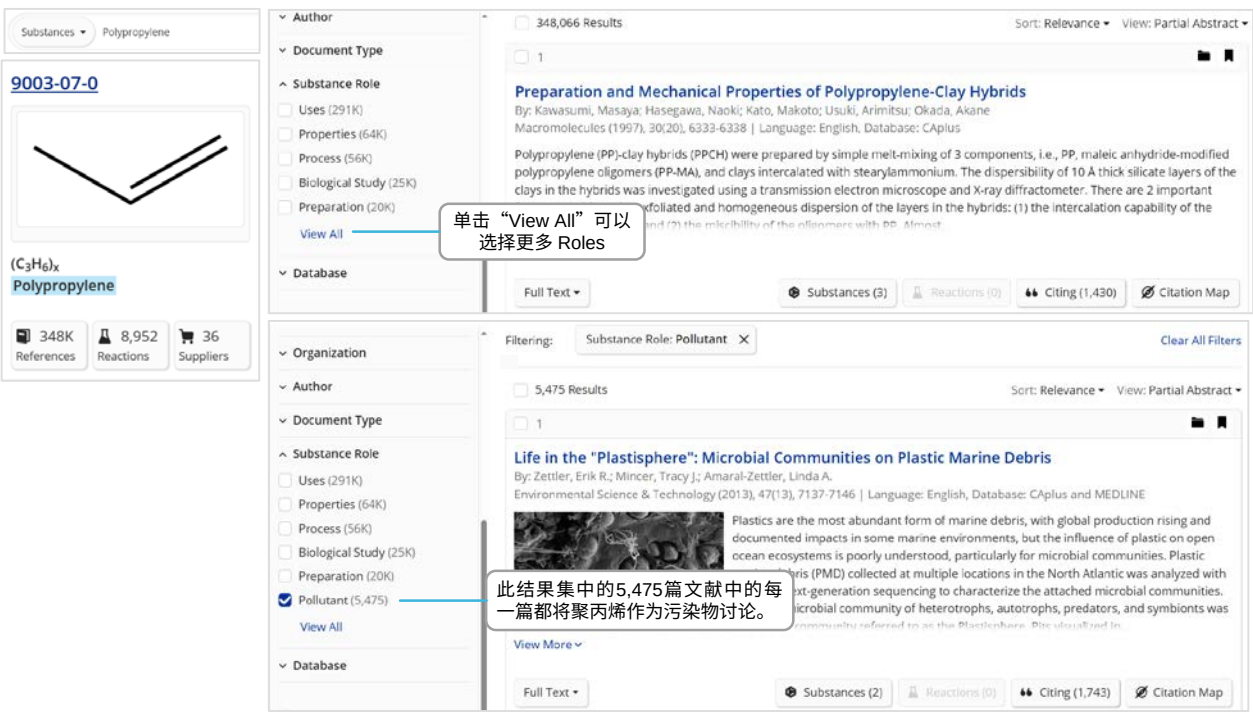
在物质检索结果集中，Roles的筛选项表示对应物质在文献中的Role。

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，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5,475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。



检索CAS序列

检索选项

可以使用三种不同的方式检索序列：

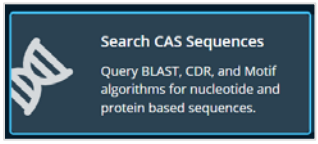
- BLAST：检索相似序列
- CDR：利用 CDR 检索抗体或T细胞受体
- Motif：检索氨基酸或核苷酸位点可变的序列

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。

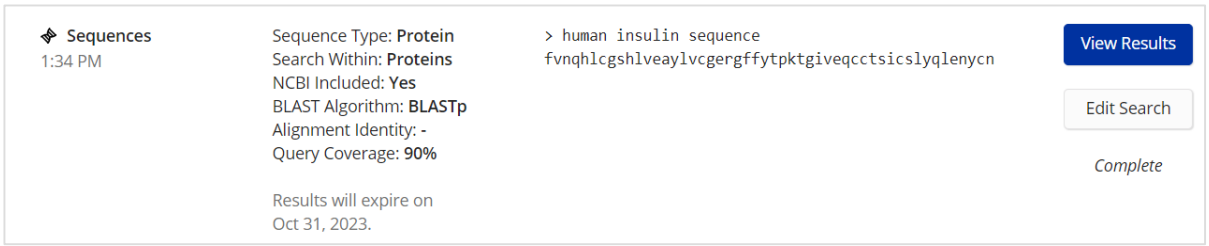


BLAST 结果分析

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。

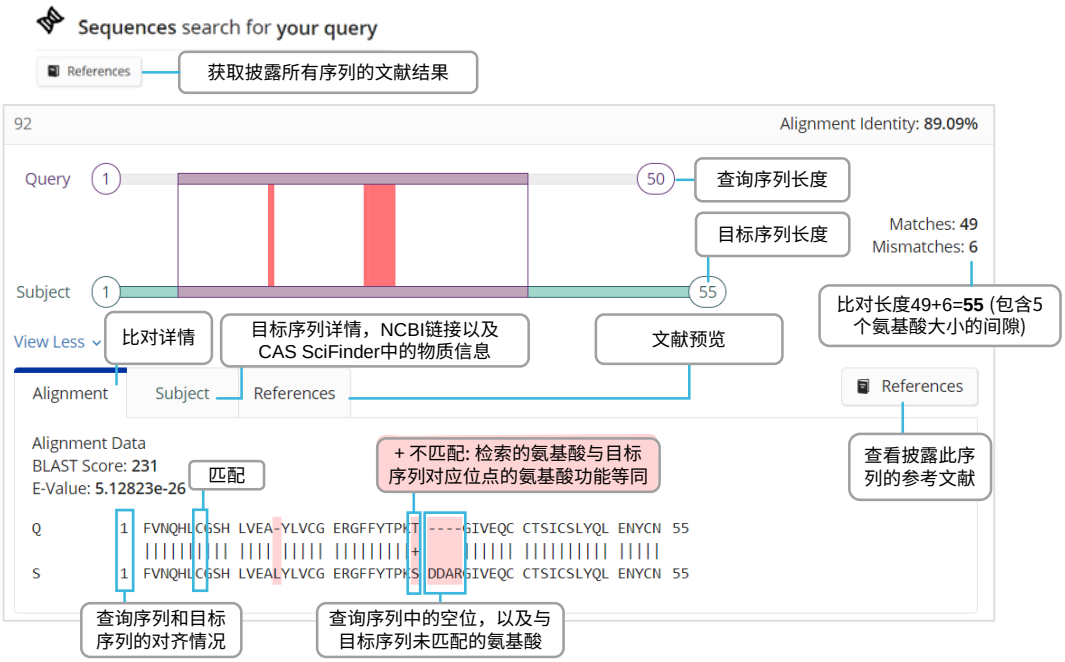
点击 “View Results” 查看序列检索结果。



查看结果

在查看BLAST序列相似性结果时：

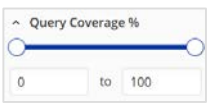
- 比对结果按序列一致性排序。
- 简化的图形概览显示比对质量。
- 不匹配部分以红线标示。
- 详细比对结果可在“Alignment”标签中查看。
- 目标序列详情和相关专利预览可在单独的标签中查看。
- 点击 References 可获取相关文献。
- 支持下载 XLSX 格式的结果文件。



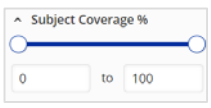
筛选结果

检索结果会随着筛选项调整而动态改变。

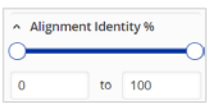
E-值（期望值）



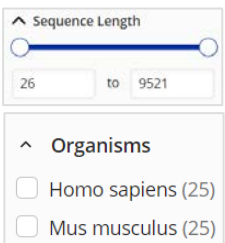
比对上的序列长度 / 查询序列长度



比对上的序列长度 / 目标序列长度



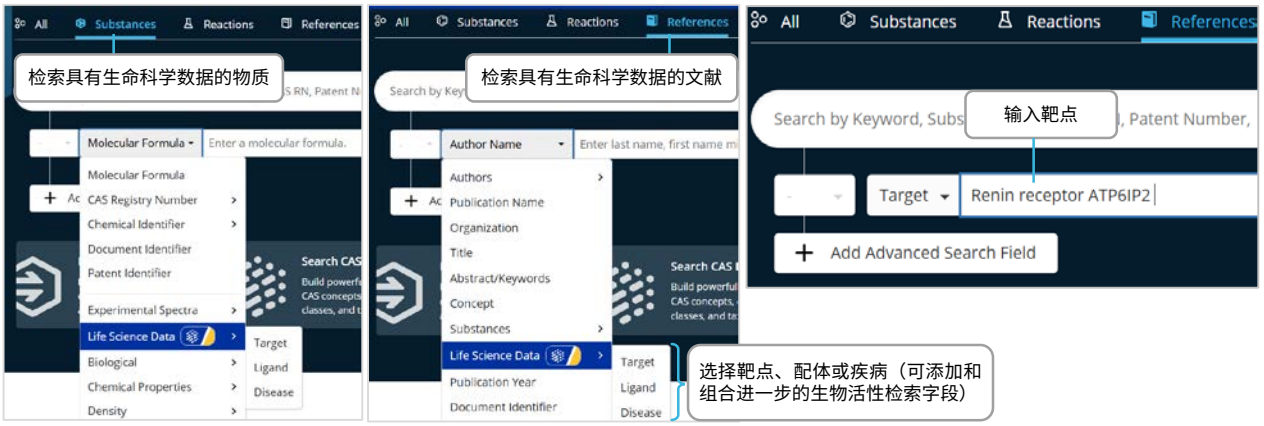
匹配上的氨基酸或碱基对的数量 / 比对上的序列长度



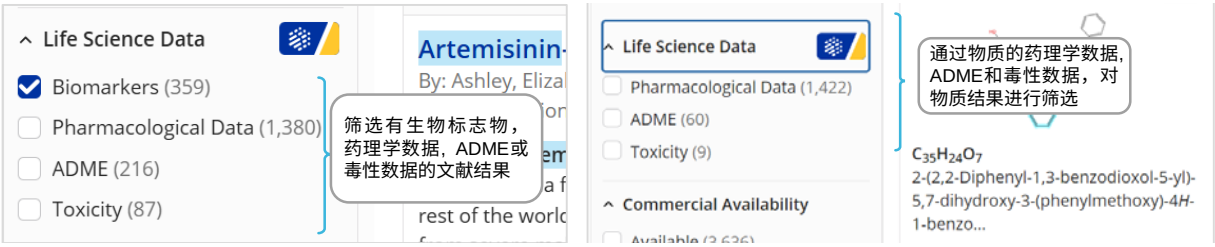
生命科学数据

检索靶点、配体和疾病

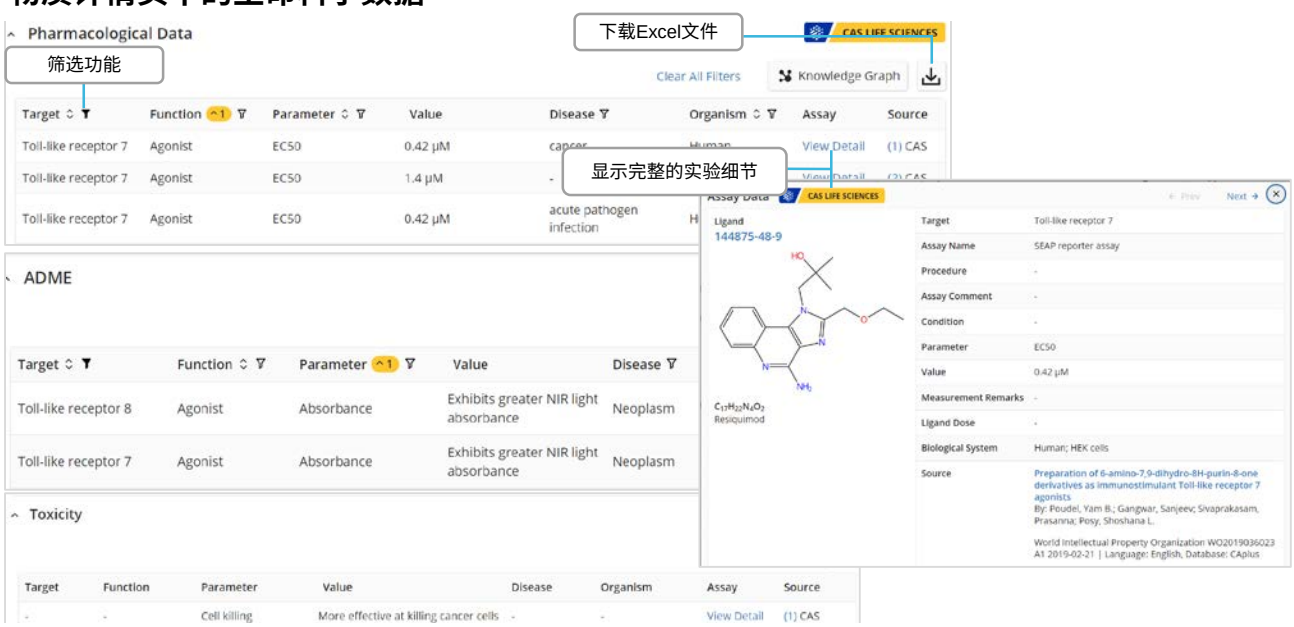
在 CAS Life Sciences 中利用高级检索字段进行物质检索或文献检索，您可以找到与靶点、配体和疾病相对应的生命科学数据。



文献检索和物质检索中的生命科学数据筛选项



物质详情页中的生命科学数据

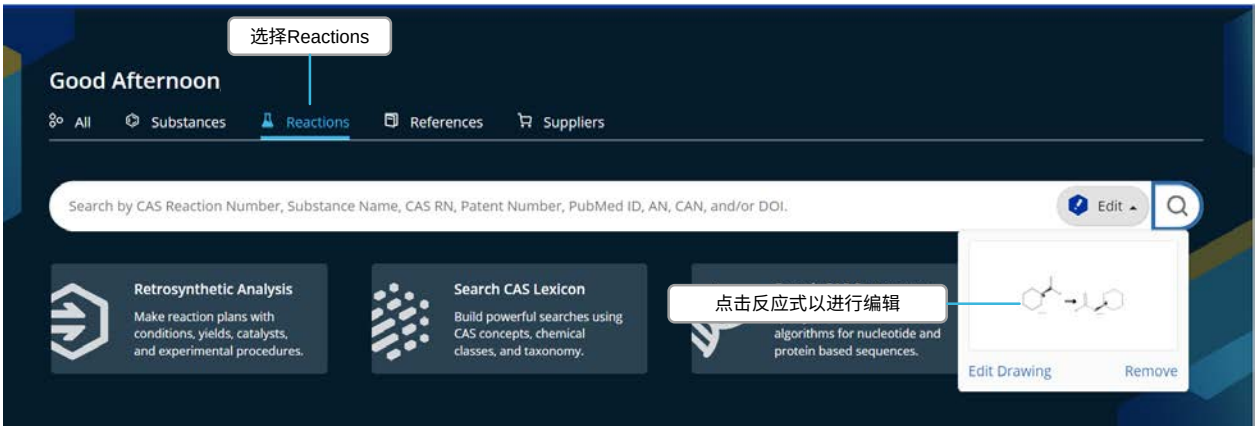


文献详情页中的生命科学数据

反应检索

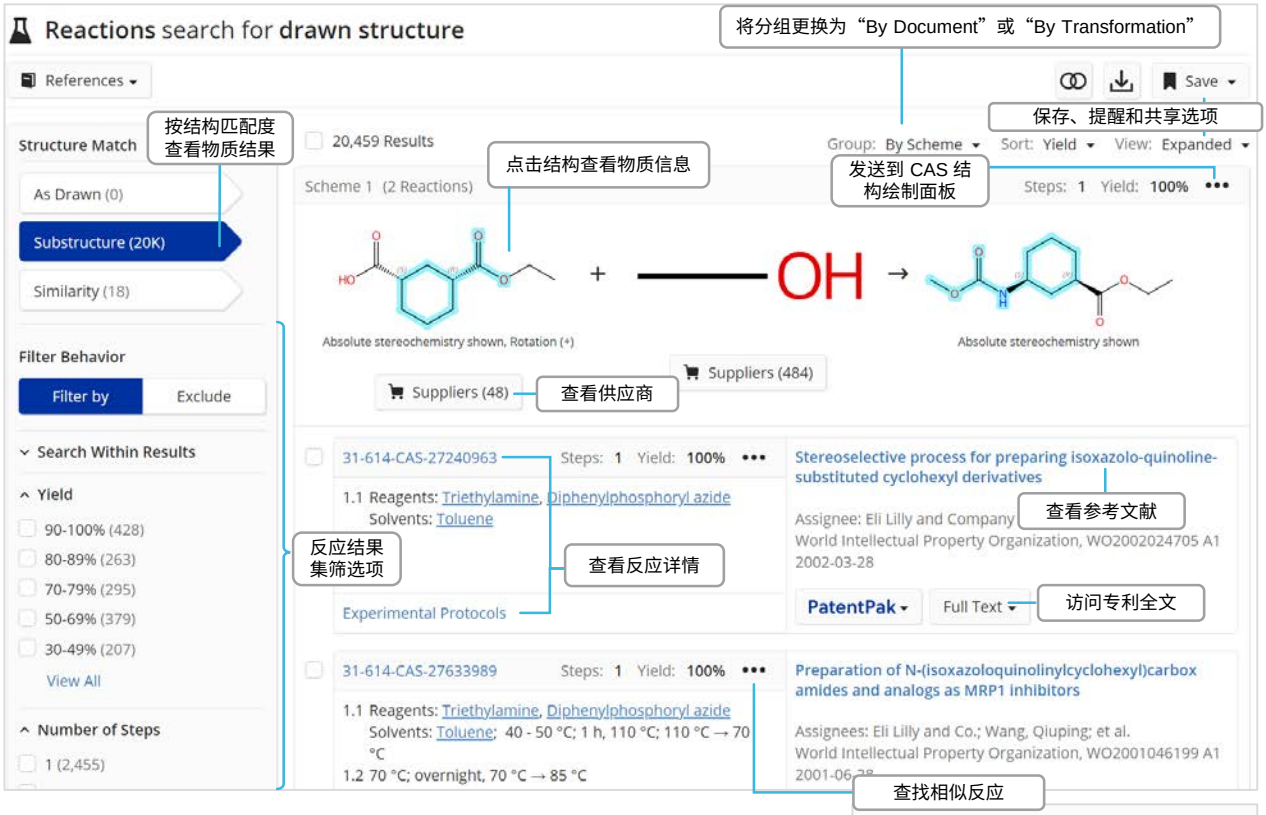
进行反应检索

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的设置进行分组。



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

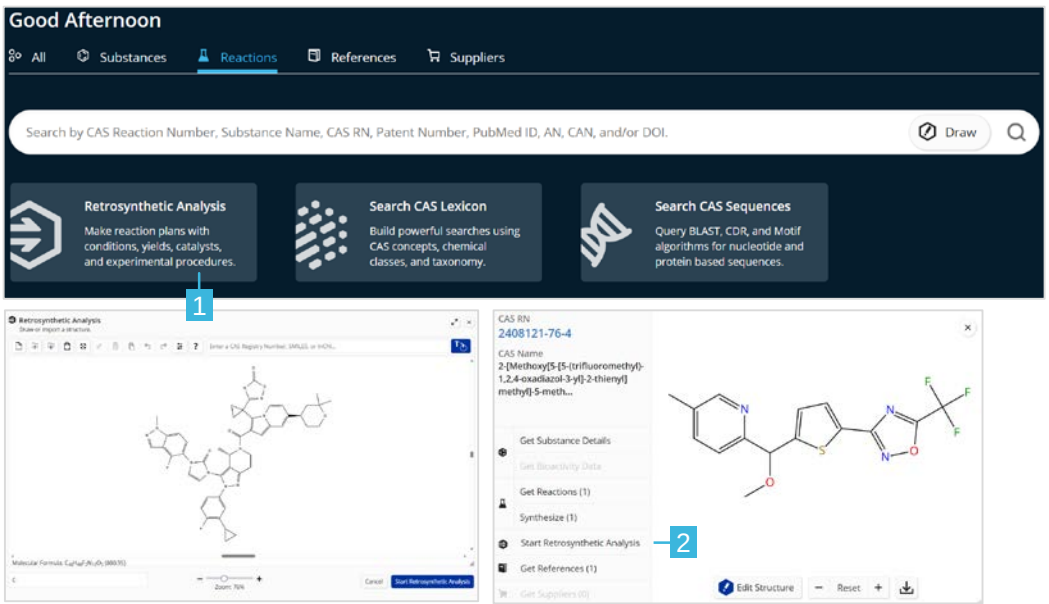
反应详情页为您提供了从文献及其 Supporting Information 中提取的信息，包括溶剂、催化剂、试剂、反应条件和表征数据等。

逆合成反应路线设计工具

开启逆合成设计

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。

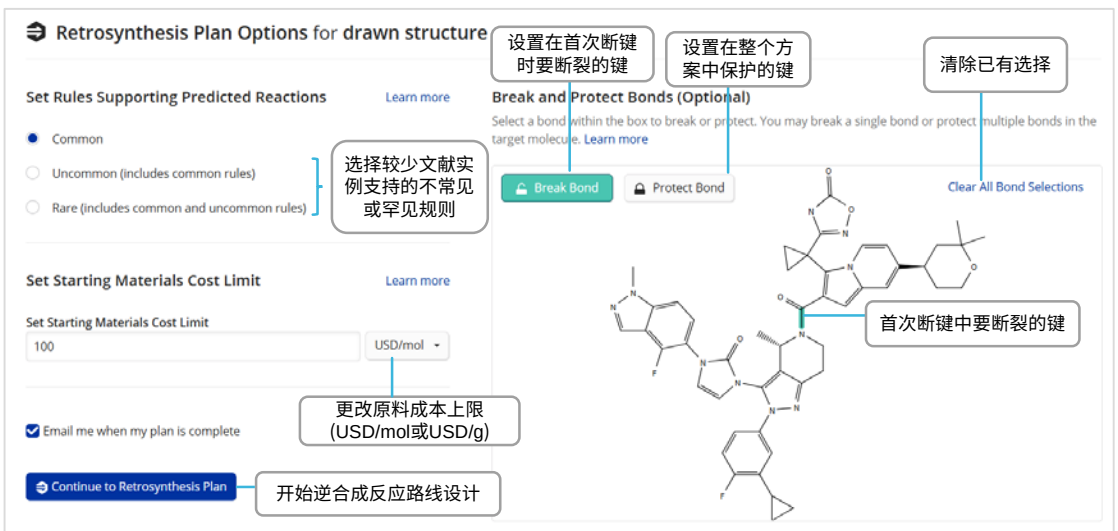


参数设置

您可以编辑方案选项以：

- 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。

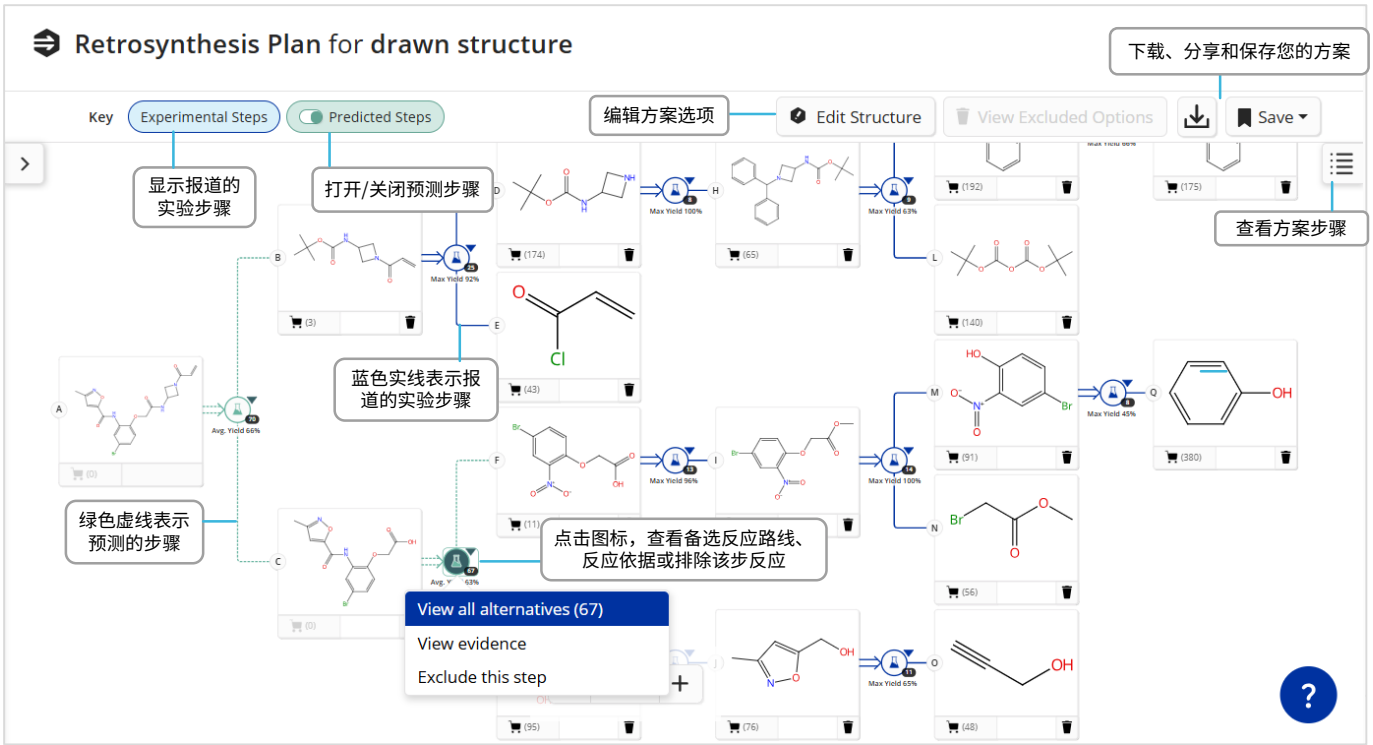
设置好了所需的选项后，点击 “Continue to Retrosynthesis Plan”



逆合成方案和备选路线

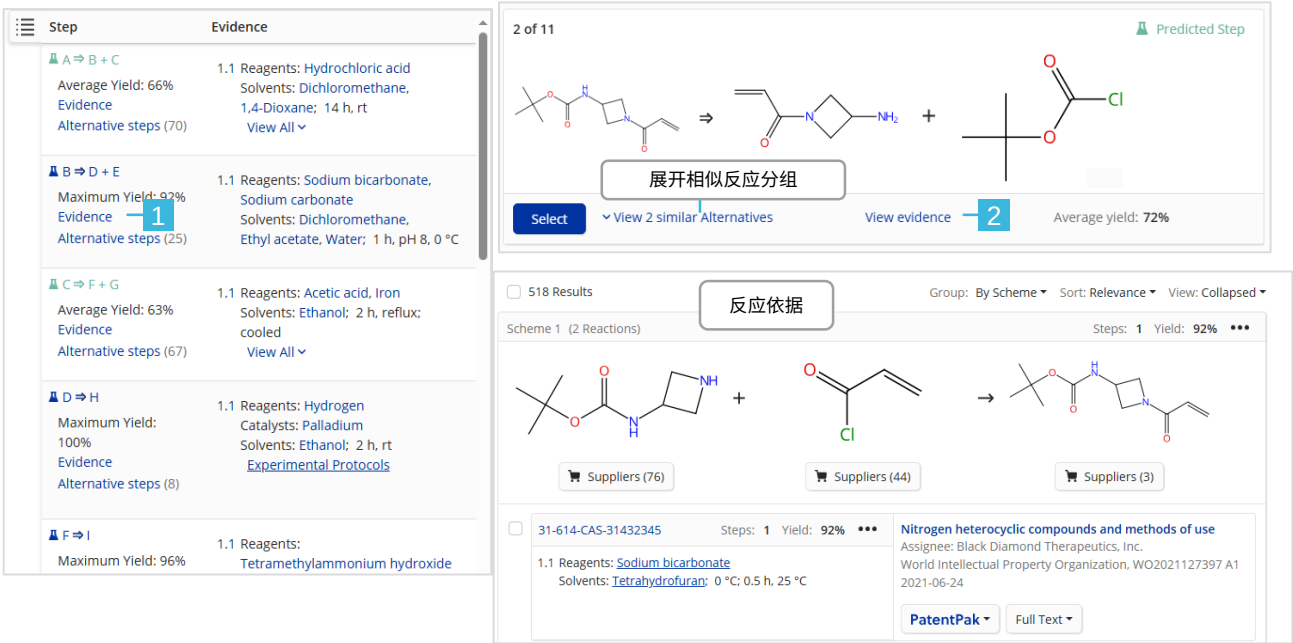
打开方案

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反应依据：(1)步骤概览中的链接，或(2)备选反应路线的反应式。



CAS Markush 检索及 CAS PatentPak

CAS Markush 检索

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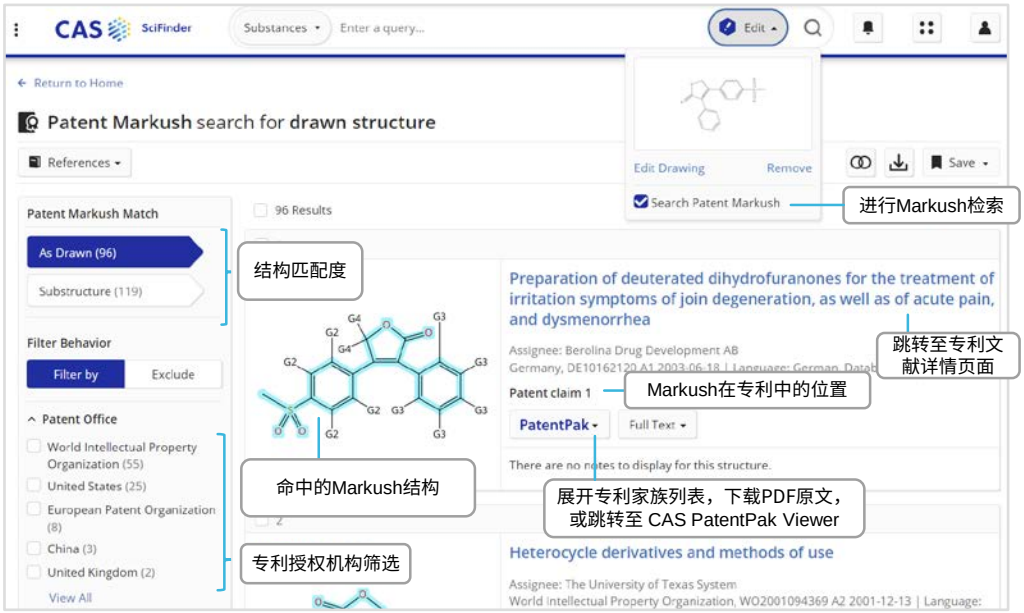

CAS PatentPak

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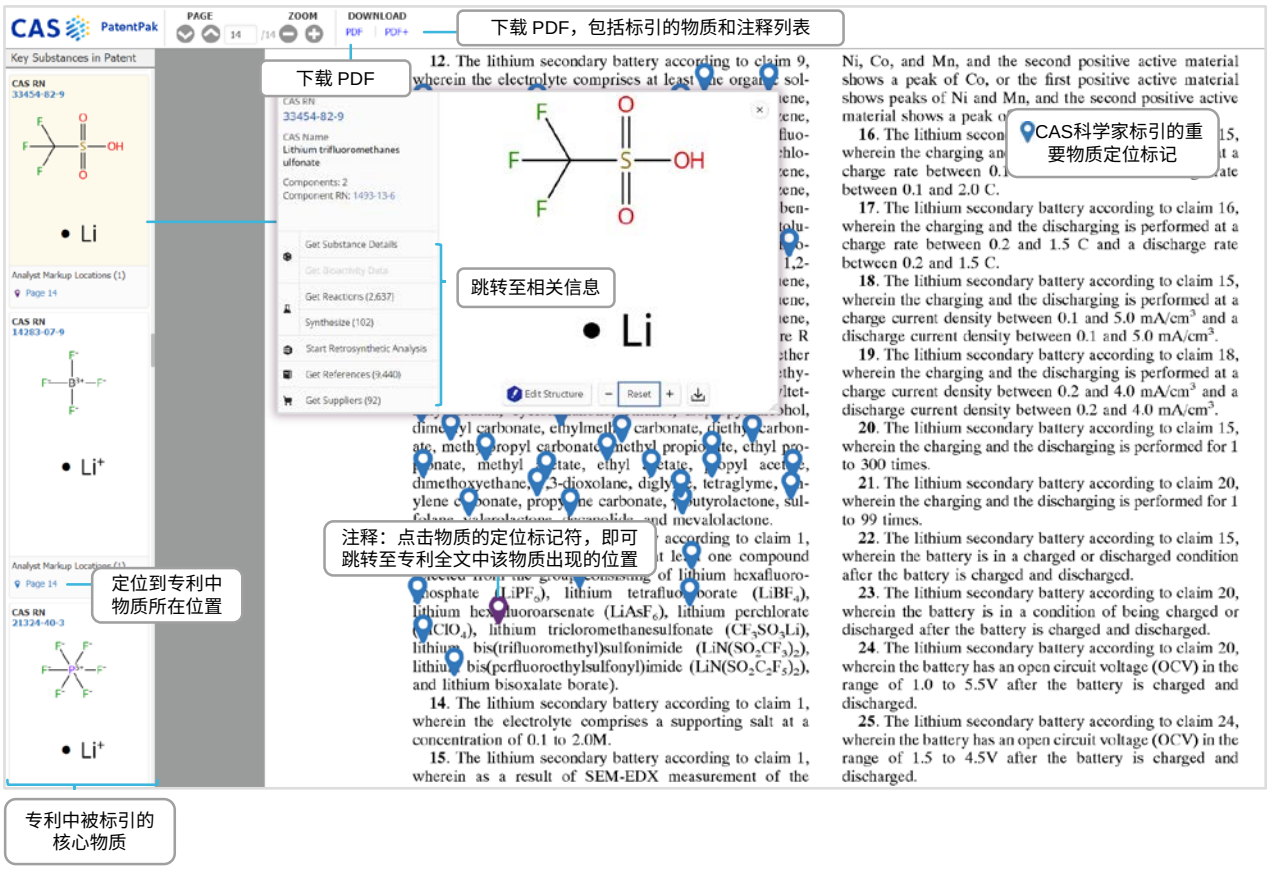
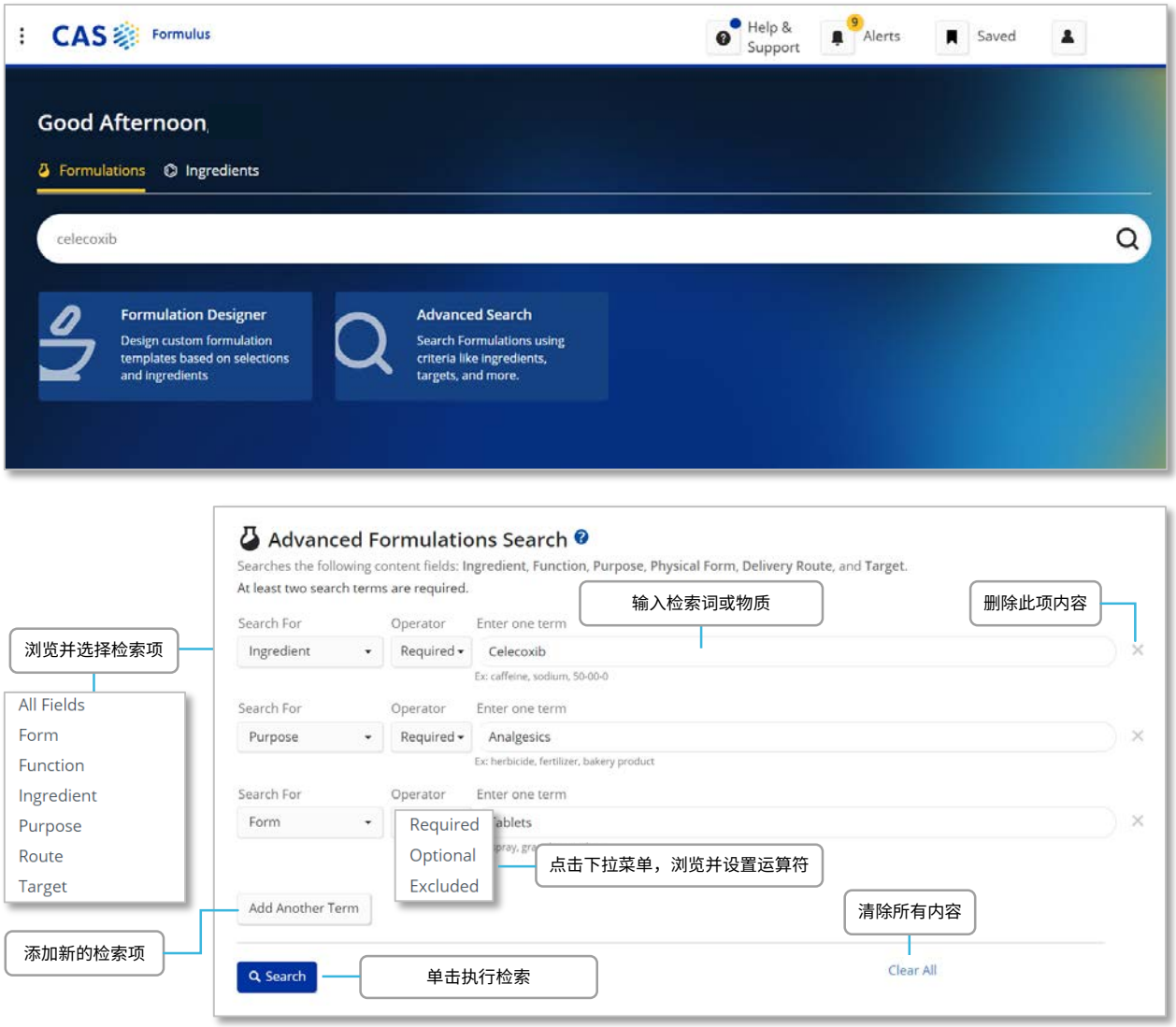
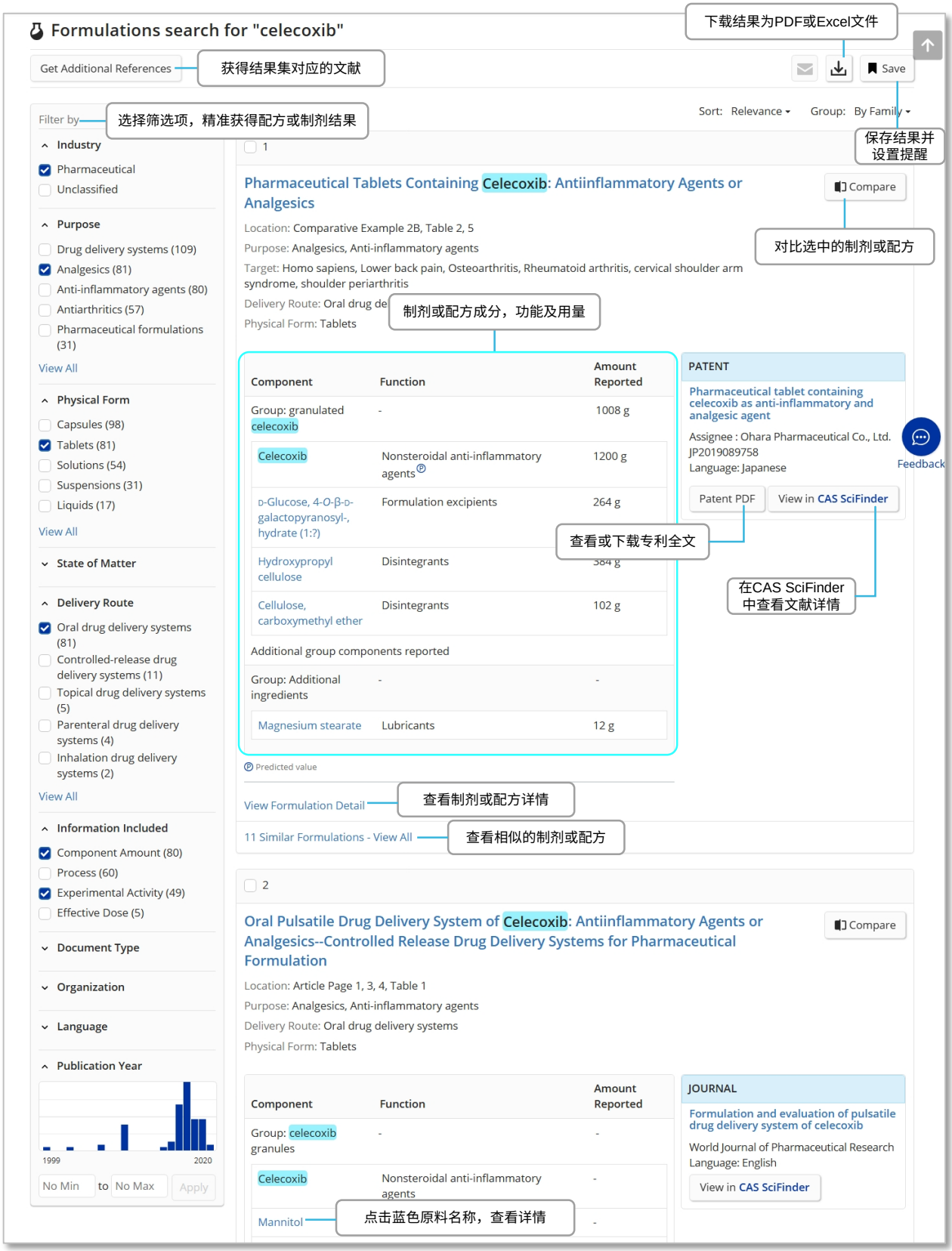


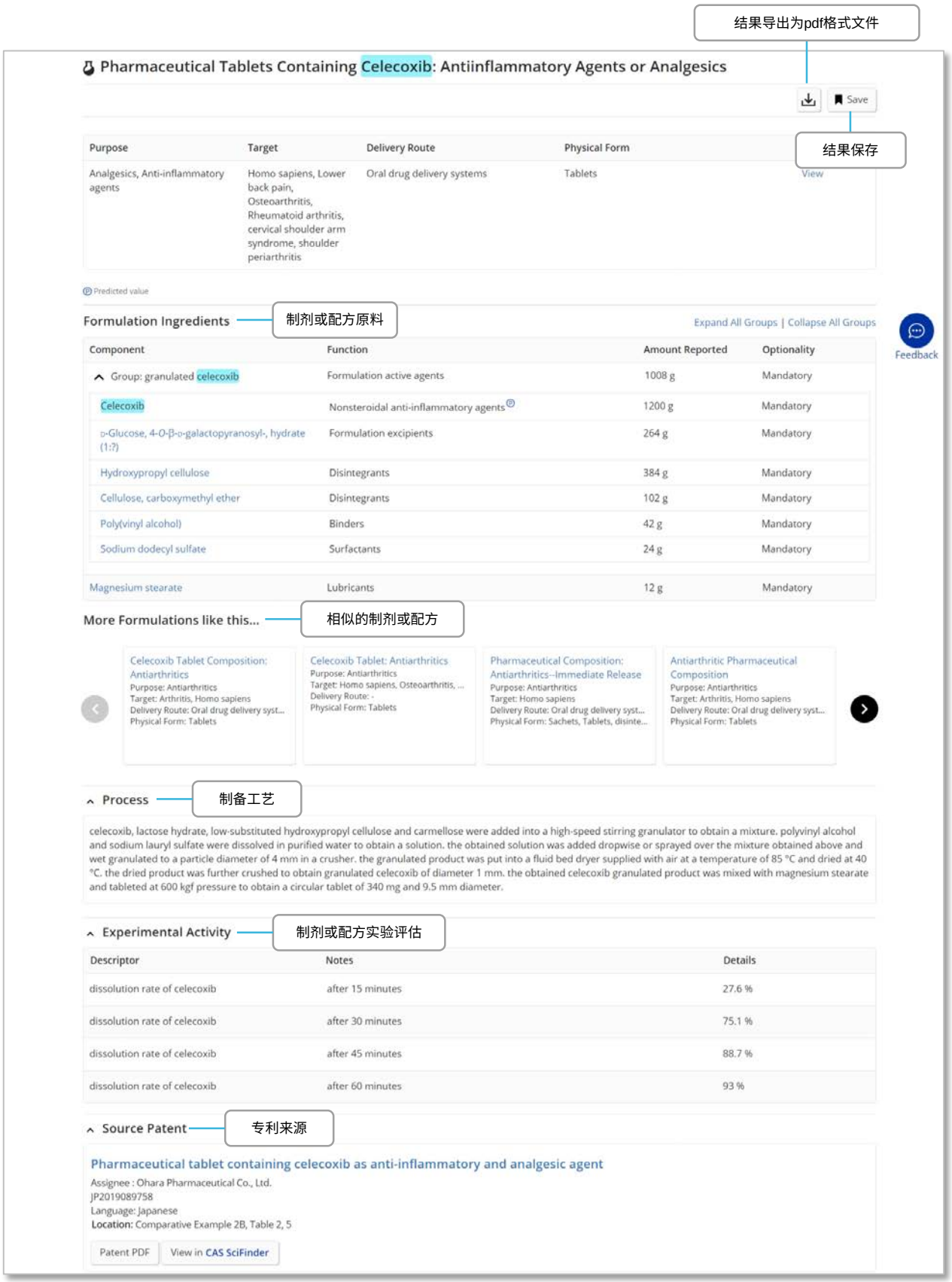
CAS Formulus

检索制剂或配方



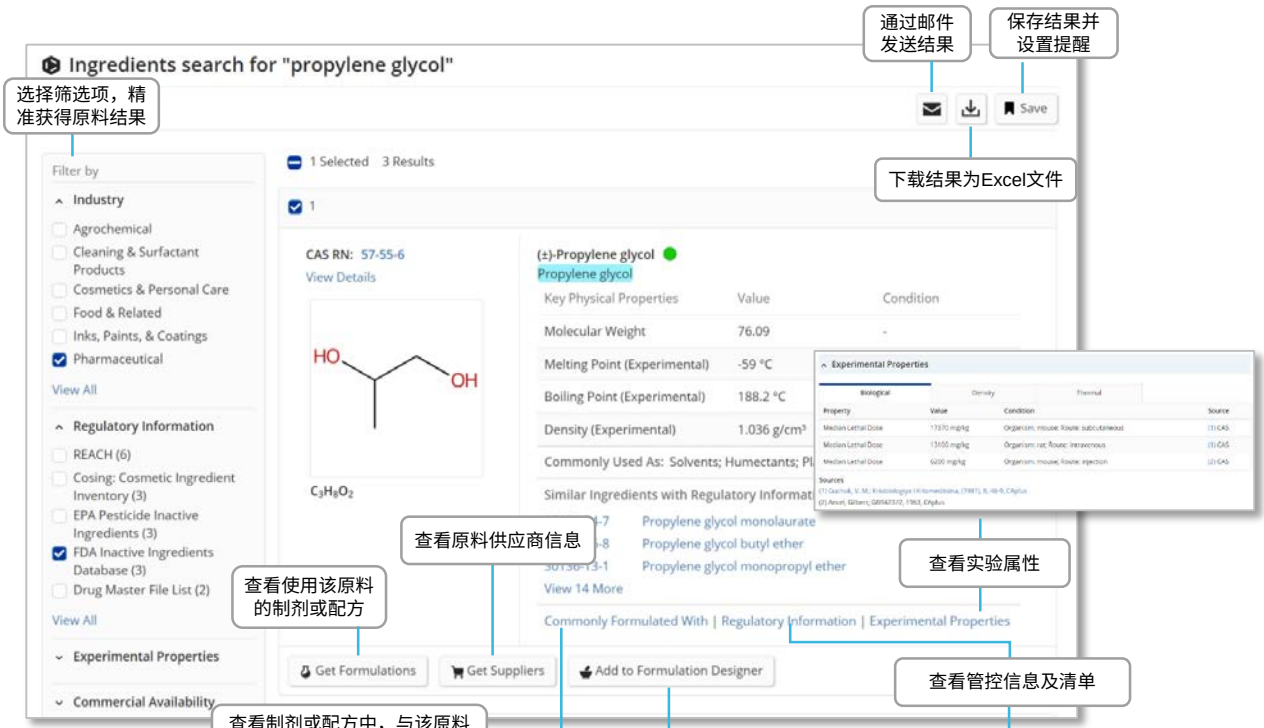

Formulations search for "celecoxib"
下载结果为PDF或Excel文件
Get Additional References
获得结果集对应的文献
Save
Filter by
选择筛选项，精准获得配方或制剂结果
Sort: Relevance
Group: By Family
保存结果并设置提醒
Industry
Pharmaceutical
Unclassified
Purpose
Drug delivery systems (109)
Analgesics (81)
Anti-inflammatory agents (80)
Antiarthritics (57)
Pharmaceutical formulations (31)
View All
Physical Form
Capsules (98)
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 (60)
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
Compare
对比选中的制剂或配方
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 de
Physical Form: Tablets
制剂或配方成分，功能及用量
Component
Function
Amount Reported
Group: granulated celecoxib
-
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
384 g
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
Feedback
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
Compare
Location: Article Page 1, 3, 4, Table 1
Purpose: Analgesics, Anti-inflammatory agents
Delivery Route: Oral drug delivery systems
Physical Form: Tablets
Component
Function
Amount Reported
Group: celecoxib granules
-
-
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

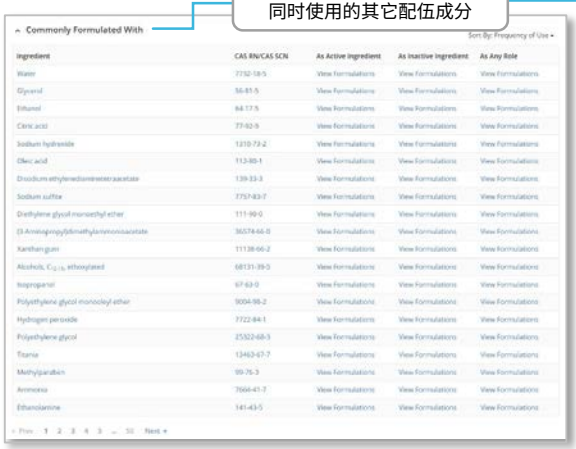
制剂或配方详情

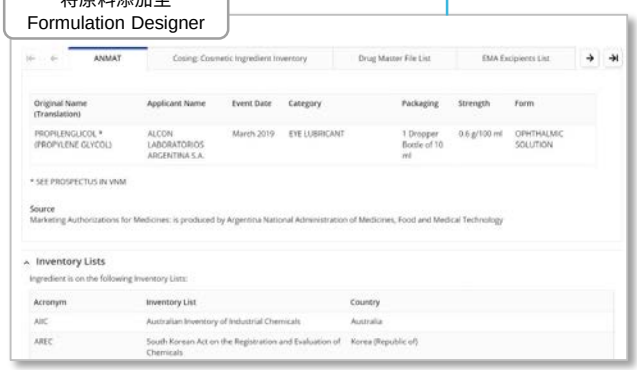

结果导出为pdf格式文件
Pharmaceutical Tablets Containing Celecoxib: Antiinflammatory Agents or Analgesics
Save
结果保存
Purpose
Target
Delivery Route
Physical Form
Analgesics, Anti-inflammatory agents
Homo sapiens, Lower back pain, Osteoarthritis, Rheumatoid arthritis, cervical shoulder arm syndrome, shoulder periarthritis
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

检索配方成分

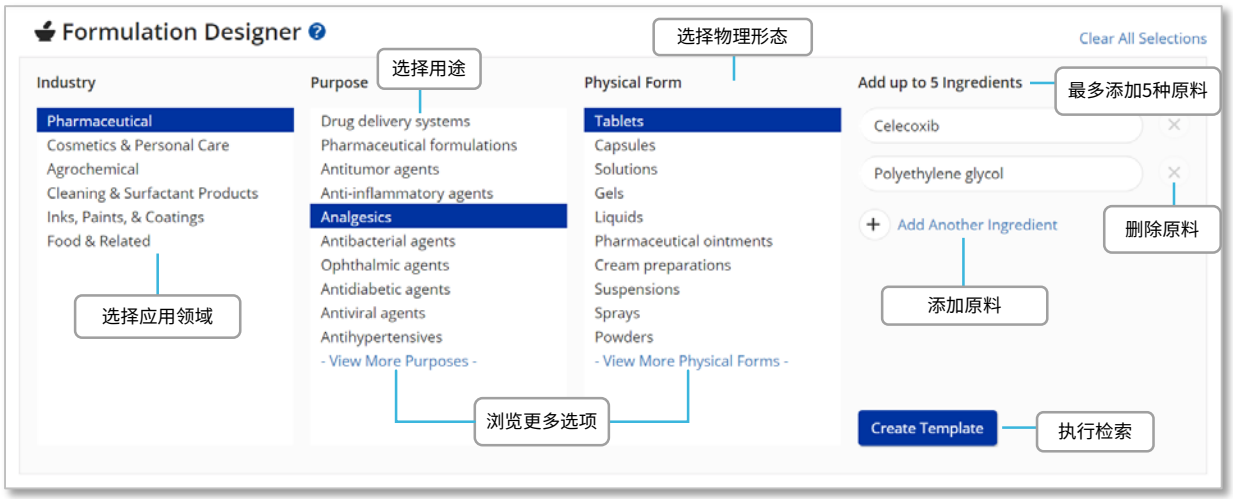

CAS Formulus
Help & Support
9
Alerts
Saved
Good Afternoon
选择Ingredients
Formulations
Ingredients
propylene glycol
可输入原料名称、CAS登记号或功能信息进行检索

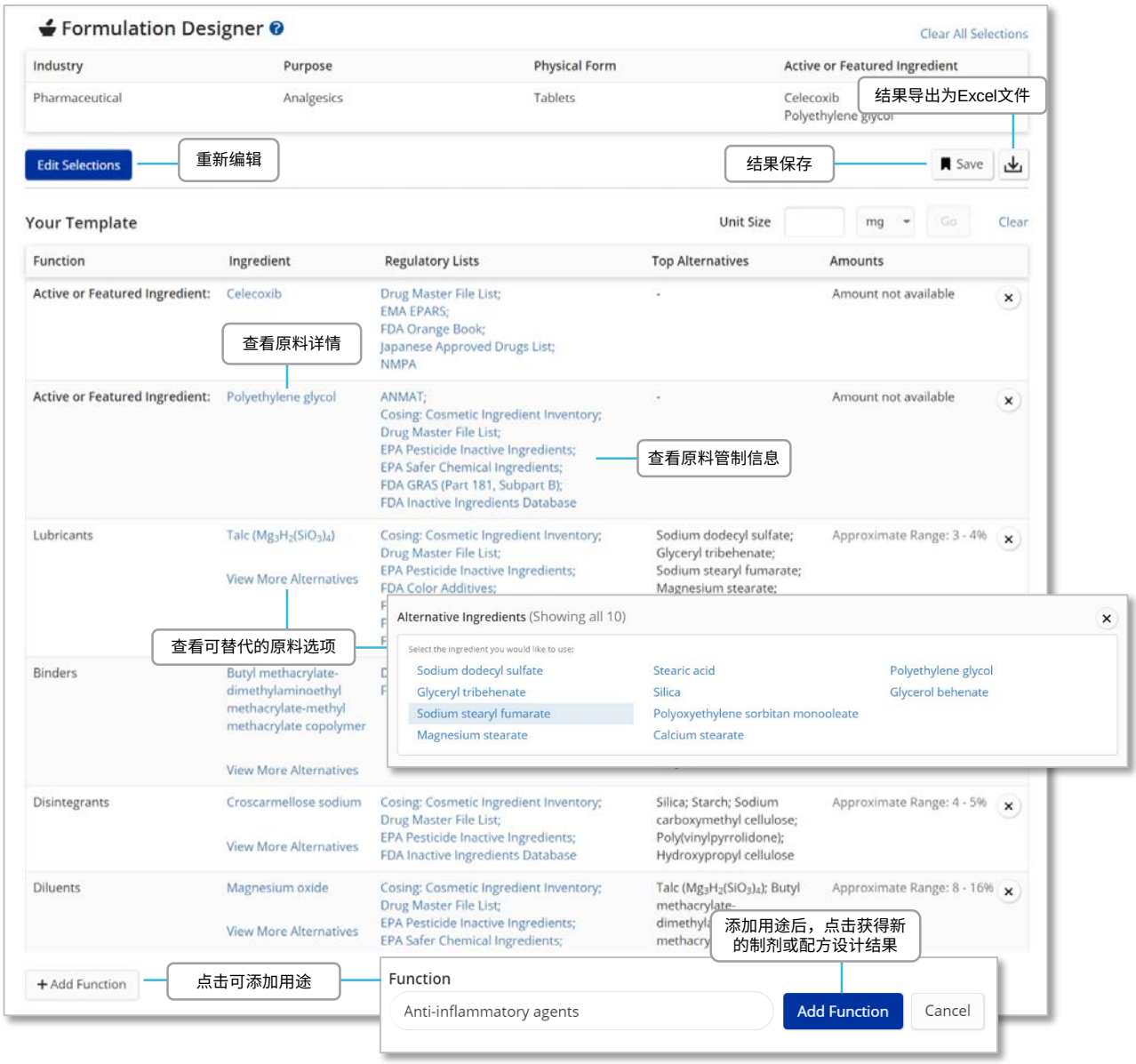

通过邮件发送结果
保存结果并设置提醒
选择筛选项，精准获得原料结果
Ingredients search for "propylene glycol"
Save
下载结果为Excel文件
Filter by
Industry
Agrochemical
Cleaning & Surfactant Products
Cosmetics & Personal Care
Food & Related
Inks, Paints, & Coatings
Pharmaceutical
View All
Regulatory Information
REACH (6)
Cosing: Cosmetic Ingredient Inventory (3)
EPA Pesticide Inactive Ingredients (3)
FDA Inactive Ingredients Database (3)
Drug Master File List (2)
View All
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 ether
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
Inventory Lists





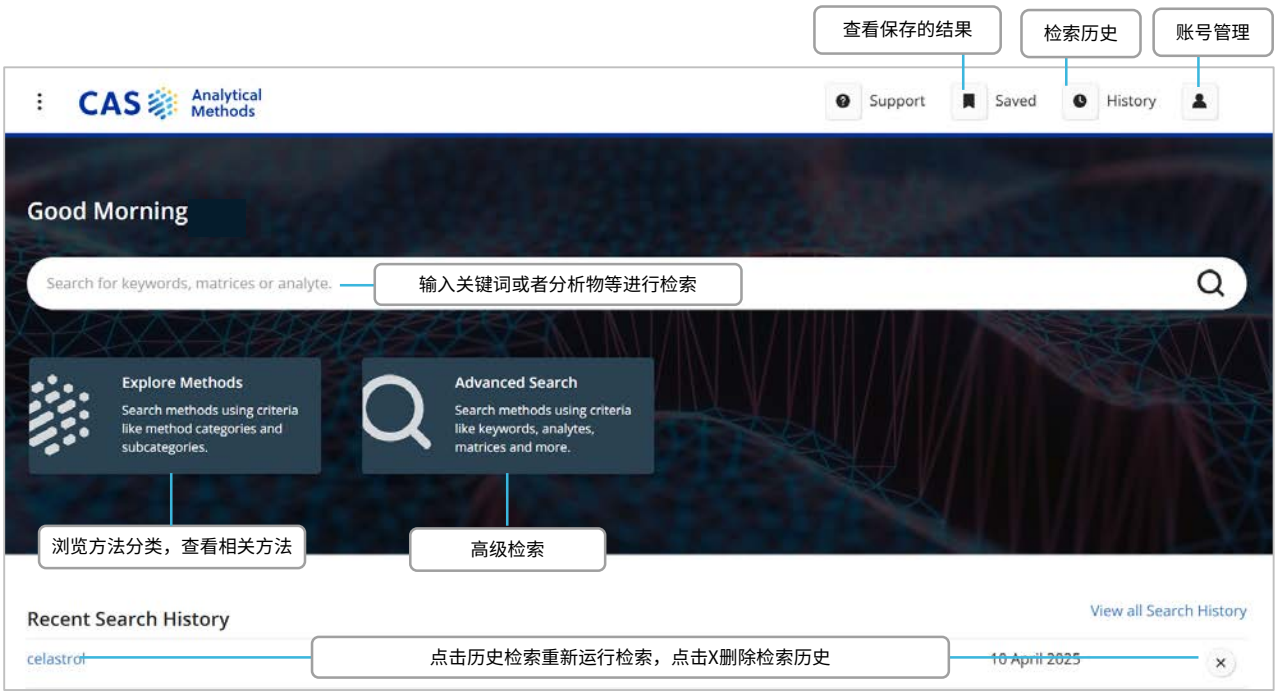
设计制剂或配方


Formulation Designer
选择物理形态
Clear All Selections
Industry
Purpose
选择用途
Physical Form
Add up to 5 Ingredients
最多添加5种原料
Pharmaceutical
Cosmetics & Personal Care
Agrochemical
Cleaning & Surfactant Products
Inks, Paints, & Coatings
Food & Related
Drug delivery systems
Pharmaceutical formulations
Antitumor agents
Anti-inflammatory agents
Analgesics
Antibacterial agents
Ophthalmic agents
Antidiabetic agents
Antiviral agents
Antihypertensives
- View More Purposes -
Tablets
Capsules
Solutions
Gels
Liquids
Pharmaceutical ointments
Cream preparations
Suspensions
Sprays
Powders
- View More Physical Forms -
Celecoxib
Polyethylene glycol
Add Another Ingredient
删除原料
选择应用领域
添加原料
浏览更多选项
Create Template
执行检索


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
重新编辑
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
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
查看原料管制信息
Amount not available
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%
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

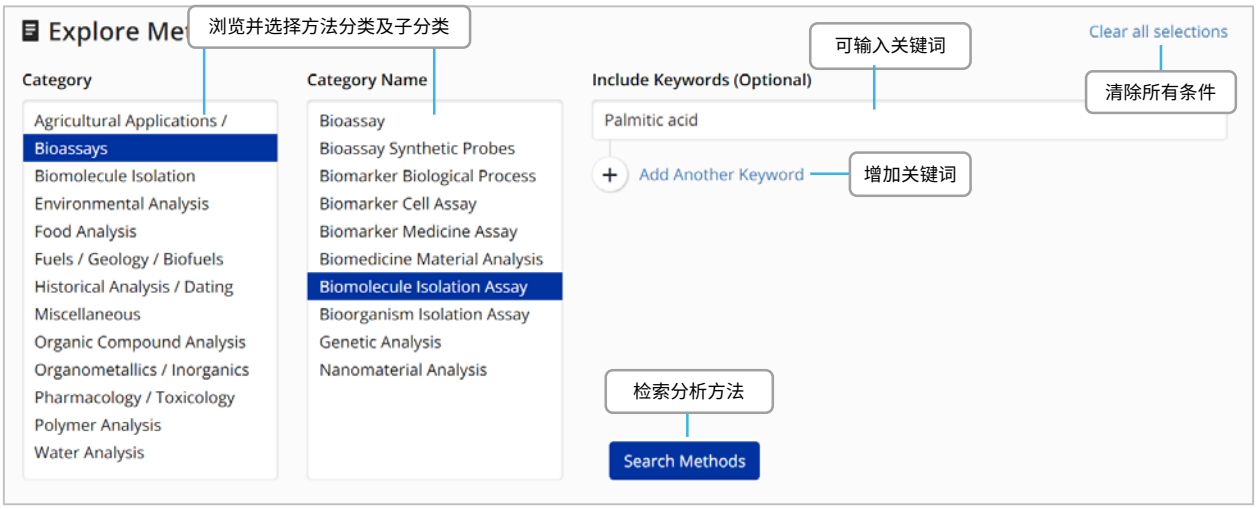
CAS Analytical Methods

分析方法检索

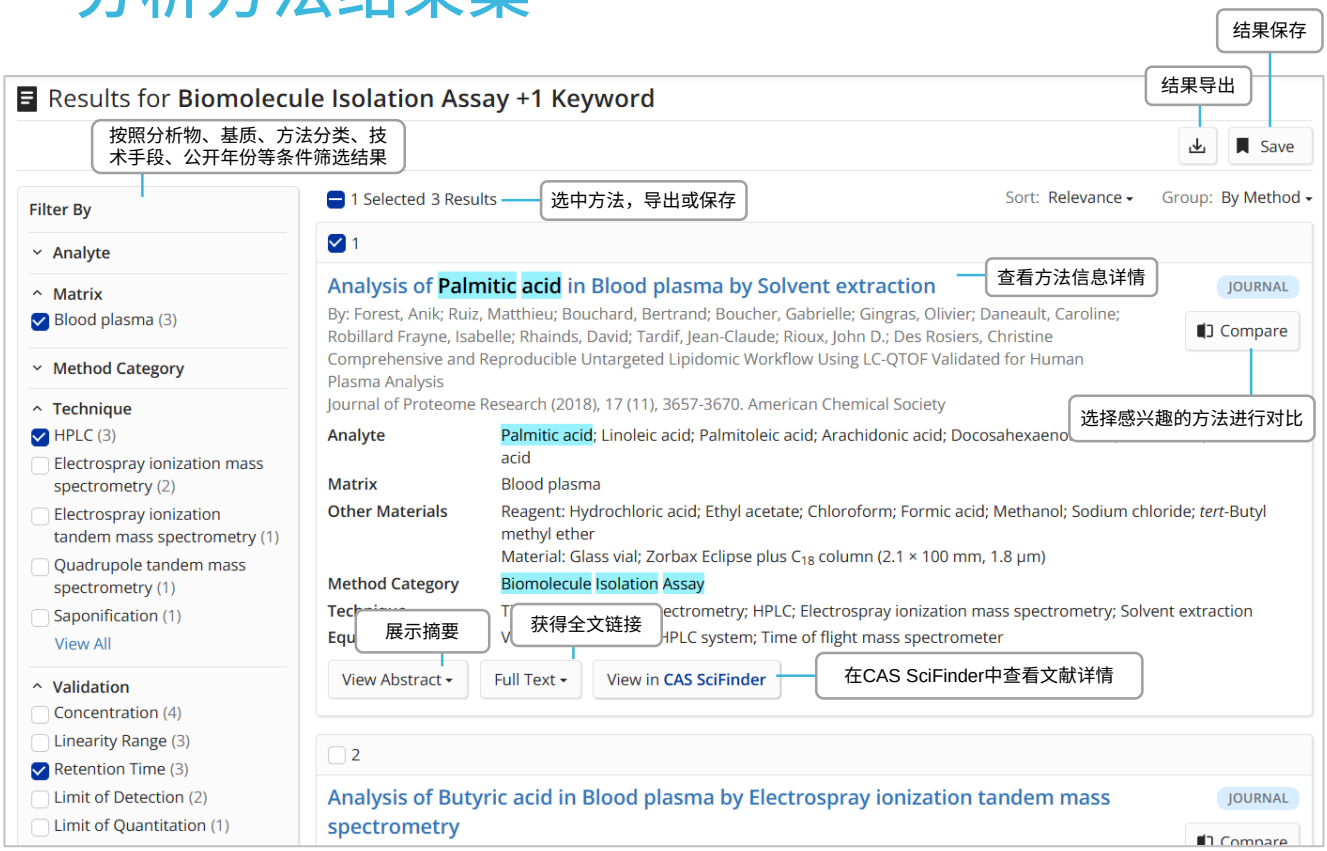


高级检索

分析方法的分类检索



分析方法结果集



分析方法详情及结果对比

Analysis of Myristic acid in Blood plasma by Solvent extraction

结果导出

Save

结果保存

CAS Method Number

1-122-CAS-534418

Method Category

分析物、基质、材料、试剂等分类展示

Technique

Mass spectrometry; HPLC; Solvent extraction

Analyte	Matrix	Material	Reagent	Biological Reagent
cis-Octadecenoic acid (*Z*)-Hexadecenoic acid *cis*-Octadecadienoic acid Palmitic acid Myristic acid	Blood plasma	Atlantic T3 C18 column (2.1 × 150 mm, 3 µm) Ethylenediaminetetraacetic acid-loaded vacuum tubes	Chloroform Methanol	-

所用仪器信息

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

Source

来源文献题录信息

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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展示摘要

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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

Comparing your 3 selected Methods

删除方法

下载方法比较结果为pdf或excel格式

	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

登录，培训，支持

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https://www.cas.org/cas-webinars?attendance=Coming+soon

过往活动和网络研讨会录像：
https://www.cas.org/cas-webinars?attendance=On+demand

培训内容：
https://www.cas.org/training/platform/cas-scifinder-discovery-platform

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网址：https://www.cas.org/contact

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SCIACDENGREF101245240414-A4

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