

# CAS FORMULUS® 検索ガイド

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- CAS Formulus® の概要
- 配合検索の流れ
- 成分検索の流れ
- CAS SciFinder® との連携
- Formulation Designer

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# CAS FORMULUS<sup>®</sup> の概要

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## CAS Formulus の概要

製剤・配合・成分情報を効率的に検索

重点分野：

- 医薬品、農薬、化粧品

一部収録分野：

- コーティング剤、日用品、食品、材料

内容収録：

- 配合の構成成分や機能、形状、各成分の価格情報や規制情報

文献および医薬添付文書から製剤・配合の情報を抽出し、  
項目ごとに整理してデータベース化



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# CAS Formulus の概要

製剤・配合・成分情報を効率的に検索

**成分検索**

Paclitaxel

Key Physical Properties Value

Molecular Weight 853.91

Melting Point (Experimental) 213-216 °C

Commonly Used As: Antitumor agents; Antiproliferative Coating materials...

Commonly Formulated With | Regulatory Information

C47H51NO14

View in CAS SciFinder®

Get Formulations Suppliers Add to Formulation Designer

Commonly Used As

**配合検索**

ized Paclitaxel Nanocrystals: Drug Delivery or Anticancer--Controlled Release

Location: Article page 2, 4, Table 1

Purpose: Antitumor agents; Drug delivery systems

Target: Drugs; cancer cell growth

Physical Form: Nanocrystals

Add to Compare

Component Function reported

Paclitaxel	Antitumor agents	20 mg
Trastuzumab	Antitumor agents®	0.25 mg/mL

Ⓞ Predicted value

成分情報へのリンク

JOURNAL

Herceptin-functionalized pure paclitaxel nanocrystals for enhanced delivery to HER2-positive breast cancer cells

International Journal of Pharmaceutics (Amsterdam, Netherlands)

Language: English

CAS SciFinder との連携

Full Text View in CAS SciFinder®

## 成分検索

- 物質名や機能性のキーワードから検索
- 物性、配合中の用途、配合情報へのリンク
- CAS SciFinder の物質詳細へのリンク

## 配合検索

- 配合成分や用途、ターゲット等から検索
- 成分や機能など配合の詳細、成分情報へのリンク
- CAS SciFinder の出典文献へのリンク



# CAS Formulus の概要

収録範囲

項目	内容
収録源	CAS SciFinder に収録の特許、雑誌論文、DailyMed 由来の医薬品添付文書
収録分野	重点分野: 医薬品、農薬、化粧品 一部収録分野: コーティング剤、日用品、食品、材料化学
レコード構成	製剤配合単位
収録期間	<ul style="list-style-type: none"> <li>・英語の特許: 1996 年～</li> <li>・日本語、中国語、韓国語、ドイツ語、フランス語の特許: 2000 年～</li> <li>・雑誌論文: 2014 年～</li> </ul>
規制情報の収録	FDA Orange Book of Approved Drugs FDA Generally Regarded as Safe (GRAS) PMDA Japanese Approved Drugs List EMA Excipients EU Active Substances in Pesticides List など



# 配合検索の流れ

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## ① アクセス

アクセス URL: <https://formulus.cas.org/>

CAS Formulus

Log in to Formulus

Username or Email Address

Username (ID)、パスワードは CAS SciFinder と共通

Can't log in?

CAS SciFinder

CAS Formulus

CAS SciFinder® からアクセス可能

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## ② 検索の実行

**Formulations を選択**

Search by Formulations by Ingredients, Purpose, Form, Functions, etc.

**Formulation Designer**  
Design custom formulation templates based on selections and ingredients

**Advanced Search**  
Search Formulations using criteria like ingredients, targets, and more.

キーワード検索  
成分情報や配合の目的、剤型、機能など配合に関するキーワードから検索する

**詳細検索**  
演算子\* を利用して成分や機能など複数の情報を組み合わせて検索

**\* 演算子の種類**  
Required : 必須  
Optional : 任意  
Excluded : 除外

**Advanced Formulations Search**

Search For	Operator	Enter one term
Ingredient	Required	Celecoxib <small>Ex: caffeine, sodium, 50-00-0</small>
Function	Required	Anti-inflammatory <small>Ex: binder, surfactant, carrier</small>

Add Another Term



## ③ 検索結果

Formulations search for "+Ingredient:"Celecoxib" +Function:"Anti-inflammatory""

Get Additional References

Compare (1/3) Save

Sort: Relevance Group: By Family

2 Selected 28 Results

Filter by

- Industry
  - Pharmaceutical
- Purpose
- Physical Form
- State of Matter
- Delivery Route
- Information Included
- Document Type
  - Journal (7)
  - Article (7)
  - Patent (28)
  - Claim (1)
  - Example (27)
- Organization
- Language
- Publication Year

1

Pharmaceutical **Celecoxib** Nanoparticles: Antiinflammatory Agents

Location: Example 1, Figure 1G, Sample DL  
Purpose: Anti-inflammatory agents  
Target: Homo sapiens, Pain  
Physical Form: Particles

Component	Function	Amount Reported
Group: Additional ingredients	-	-
Celecoxib	Anti-inflammatory agents	10 % (w/w)
Group: Additional ingredients	-	-
Sorbitol	Formulation excipients	90 % (w/w)

Remove from Compare

PATENT  
Novel formulation of meloxicam  
Assignee: Fundacionuniversidad Norte  
US20120141548  
Language: English  
View in CAS SciFinder

View Formulation Detail → ④ 配合の詳細へ

成分名・機能・用量などの配合情報

出典文献を CAS SciFinder で確認

回答の保存、ダウンロード、共有、比較

回答の並べ替え、グループ化

配合の分野、目的、剤型、収録情報、投与の経路、書誌情報などで絞り込みが可能 (複数選択可)



## ④ 回答の詳細を表示 (1/2)

**タイトル**

**製品情報**

**成分情報**

**類似配合情報**

**その他の情報**  
(配合のプロセス、有効量、実験情報)

**収録源**  
(書誌情報、配合の記載位置、全文へのリンク、CAS SciFinder へのリンク)

**タイトル**

Pharmaceutical **Celecoxib** Nanoparticles: Antiinflammatory Agents

目的、ターゲット、投与の経路等の製品情報

Purpose	Target	Delivery Route	Physical Form
Anti-inflammatory agents	Homo sapiens, Pain	-	Particles

成分の名称、機能、配合量等の成分情報

**Formulation Ingredients**

Component	Function	Amount Reported	Optionality
<b>Celecoxib</b>	Anti-inflammatory agents	10 % (w/w)	Mandatory
Sorbitol	Formulation excipients	90 % (w/w)	Mandatory

**類似配合情報**

More Formulations like this...

- Naproxen Containing Pharmaceutical Nanoparticle: Antiinflammatory Agents  
Purpose: Anti-inflammatory agents  
Target: Homo sapiens, Pain  
Delivery Route: -  
Physical Form: Particles
- Naproxen Containing Pharmaceutical Nanoparticle: Antiinflammatory Agents  
Purpose: Anti-inflammatory agents  
Target: Homo sapiens, Pain  
Delivery Route: -  
Physical Form: Particles
- Naproxen Containing Pharmaceutical Nanoparticle: Antiinflammatory Agents  
Purpose: Anti-inflammatory agents  
Target: Homo sapiens, Pain  
Delivery Route: -  
Physical Form: Particles
- Naproxen Containing Pharmaceutical Nanoparticle: Antiinflammatory Agents  
Purpose: Anti-inflammatory agents  
Target: Homo sapiens, Pain  
Delivery Route: -  
Physical Form: Particles

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## ④ 回答の詳細を表示 (2/2)

**タイトル**

**製品情報**

**成分情報**

**類似配合情報**

**その他の情報**  
(配合のプロセス、有効量、実験情報)

**収録源**  
(書誌情報、配合の記載位置、全文へのリンク、CAS SciFinder へのリンク)

**配合のプロセス、実験情報等の文献由来の情報**

Process

celecoxib and sorbitol in a variety of formulations to obtain the pharmaceutical celecoxib nanoparticles

**Experimental Activity**

Descriptor	Notes	Details
particle size	particle size (D(5.0) μm) of the composition was examined.	16.031 μm
particle size	percentage of less than 2.0 μm sized particle present in the composition was examined.	0.8 %
yield		46 %

**収録源**

**Source Patent**

Novel formulation of meloxicam  
Assignee: Fundacionuniversidad Del Norte  
US20120141548  
Language: English  
Location: Example 1, Figure 1G, Sample DL

出典文献を CAS SciFinder で確認

Patent PDF [View in CAS SciFinder](#)

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## 【参考】アラートの設定

検索した結果を保存する際にアラートを登録すると、設定した頻度で最新情報をメールで配信できる

アラートの結果の確認

Save Results and Set Alerts

Your Saved results can be found on the Saved page in CAS Formulus. You can change Alert frequency, edit, or rerun your search at any time.

Name  
Pigment Red

Alert Frequency  
 No Alerts  Weekly  Monthly

Save Cancel

アラートの配信頻度を設定する

アラートの結果の確認

Return to Home

Formulations search for "+Ingredient:'980-26-7'"

Get Additional References

Filter by

- Industry
- Purpose
- Physical Form
- State of Matter
- Delivery Route
- Information Included
- Document Type

3,215 Results

1

Black/Gray Pigment

Location: Example  
Purpose: pigment

Component	Function	Amount Reported
Group: neutral black ink	Formulation active agents	-
Pigment Red 122	-	1,300-0.780 %

PATENT

Neutral gray or black inks for ink-jet printing

Assignee : Hewlett-Packard Development Company, L.P.  
US20050171240  
Language: English

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## 【参考】製剤・配合情報の比較

Formulations search for "+Ingredient:"Celecoxib" +Function:"Anti-inflammatory"'

Get Additional References

2,697 Results

Sort: Relevance Group: By Family

1

Pharmaceutical Composition Containing Antiinflammatory Agent for Treating and/or Preventing Inflammatory Condition in Milk-Producing Animal: Antiinflammatory Agents

Location: Claim 3, 4, 5, 16, 28, 29, 30, 31, 32, 33, 34, 40, 43, 44, 45, 46, 47, 50, 53, 55, 57, 60

Purpose: Anti-inflammatory agents

Target: Animals, Inflammation

Delivery Route: Infusion drug delivery systems

① 比較したい配合の Add to Compare をクリック

② 最大 3 件の配合情報を表形式で出力する

Compare (2/3)

Add to Compare

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## 【参考】製剤・配合情報の比較（続き）

出力した表は PDF 形式で  
ダウンロード可能

配合情報の各項目を  
表形式で簡単に比較

Comparing your Formulations

	Formulation 1	Formulation 2	Formulation 3
	Pharmaceutical Composition Containing Antiinflammatory Agent for Treating and/or Preventing Inflammatory Condition in Milk-Producing Animal: Antiinflammatory Agents	Antiinflammatory Composition: Antiinflammatory Agents	Pharmaceutical Formulation: Antiinflammatory Agents
Purpose	Anti-inflammatory agents	Anti-inflammatory agents	Anti-inflammatory agents
Target	Animals, Inflammation	Homo sapiens	Homo sapiens, Osteoarthritis, Rheumatoid arthritis
Delivery Route	Infusion drug delivery systems	-	-
Physical Form	-	-	Pharmaceutical injections
Experimental Activity	Not Available	Not Available	Not Available

## 成分検索の流れ

## ① 検索の実行

CAS Formulus

Ingredients を選択

Formulations Ingredients

Sunscreens

Formulation Designer  
Design custom formulation templates based on selections and ingredients

Advanced Search  
Search Formulations using criteria like ingredients, targets, and more.

成分の名称や CAS 登録番号 (CAS RN®)、機能に関するキーワードから検索する

## ② 検索結果

Ingredients search for "sunscreens"

1 Selected 799 Results

Filter by

- Industry
- Regulatory Information
  - REACH (267)
  - Cosing: Cosmetic Ingredient Inventory (137)
  - EPA Pesticide Inactive Ingredients (57)
  - Drug Master File List (29)
  - FDA Inactive Ingredients Database (13)
- View All
- Experimental Properties
- Commercial Availability
  - Available (478)
- Toxicity/Ecological Toxicity
  - Available (93)

③ 成分の詳細へ

回答の保存、ダウンロード、共有

CAS RN: 70356-09-1

Property	Value	Condition
Molecular Weight	310.39	-
Melting Point (Experimental)	83.5 °C	-

Commonly Used As: Sunscreens; UV absorbers; UV stabilizers; Stabilizing agents; Filters...

Commonly Formulated With | Regulatory Information | Experimental Properties

C<sub>20</sub>H<sub>22</sub>O<sub>3</sub>

Get Formulations | Get Suppliers | Add to Formulation Designer

CAS RN: 118-60-5

2-Ethylhexyl salicylate

Property	Value	Condition
Key Physical Properties		

### ③ 成分の詳細を表示

- 基本情報  
(CAS RN、構造図、分子式、基本物性値など)
- 成分の一般的な用途
- この成分とよく配合される他の成分
- 毒性情報
- 規制情報
- 実測物性値
- 化学物質名

Ingredient Detail (1 of 799)

CAS RN: 70356-09-1

Avobenzene

Key Physical Properties	Value
Molecular Weight	310.39
Melting Point (Experimental)	83.5 °C

Commonly Used As: [Sunscreens](#); UV absorbers; UV stabilizers; Stabilizing agents; Filters...

Commonly Formulated With | [Regulatory Information](#) | [Experimental Properties](#)

Get Formulations | Get Suppliers | Add to Formulation Designer

- Commonly Used As
- Commonly Formulated With
- Toxicity
- Ecological Toxicity
- Regulatory Information
- Experimental Properties
- Other Names

## CAS SCIFINDER® との連携

# CAS SciFinder で製剤・配合情報を確認

① CAS SciFinder で文献を検索し、配合情報が収録されている回答に限定する

CAS Formulus に  
配合情報が収録  
されている文献に  
限定できる

配合の目的で限定  
ができる

The screenshot shows the CAS SciFinder interface with search results for 'Sunscreens'. The left sidebar contains filters for 'CAS Solutions' (Formulus 3,541) and 'Formulation Purpose' (Sunscreens 3,541, Cosmetics and Personal care products 2,296, Shampoos 730, Skin conditioners 704, Lipsticks 455). The main content area displays three search results, with the second one, 'Combination sunscreen and insect repellent', highlighted with a blue box and a circled '2'.

# CAS SciFinder で製剤・配合情報を確認

② Formulations のタブで配合情報が確認できる

The screenshot shows the 'Formulations' tab for the selected article. It includes a table of components and their functions. A blue box highlights the 'View CAS Formulus® Detail' link, and another blue box contains the text 'CAS Formulus で配合の詳細が確認できる'.

Component	Function	Amount Reported
Group: Sunscreens	active agent, sunscreen agent	0.5-30 % by weight
N,N-Diethyl-m-toluamide	insect repellents	0.5-95 % by weight
Agrochemical carriers	carrier	-

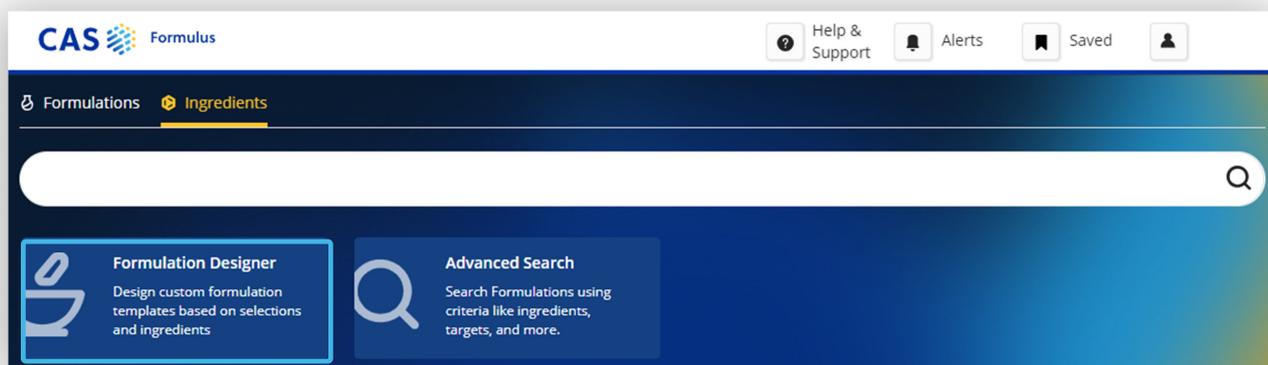
# FORMULATION DESIGNER

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## 配合テンプレートの作成

① ホーム画面の Formulation Designer を選択する



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# 配合テンプレートの作成

② 産業分野、目的、形状、成分を入力する

The screenshot shows the 'Formulation Designer' interface with the following selections:

- Industry:** Cosmetics & Personal Care
- Purpose:** Sunscreens
- Physical Form:** Cosmetic lotions
- Add up to 5 Ingredients:** Avobenzone, 56-81-5

A 'Create Template' button is visible at the bottom right.

# 配合テンプレートの作成

③ 配合テンプレートが作成される

The screenshot shows the 'Your Template' section with the following details:

Function	Ingredient	Regulatory Lists	Top Alternatives	Amounts
Active or Featured Ingredient:	Avobenzone	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients	-	Amount not available
Active or Featured Ingredient:	Glycerol	ANMAT; Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 182, Subpart A); FDA GRAS (Part 182, Subpart B); FDA Inactive Ingredients Database; NMPA	-	Amount not available
Solvents	Benzyl alcohol <a href="#">View More Alternatives</a>	Cosing: Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA Inactive Ingredients Database; FDA Orange Book	Hexylene glycol; 1,3-Butanediol; Propylene carbonate; Isopropyl myristate; 1,5-Pentanediol	Approximately 1%

② で指定した条件

テンプレートの保存、ダウンロード

機能、成分、規制情報、代替成分、配合量をまとめたテンプレートが作成される

JAICI ヘルプデスク

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