

CAS SciFinder®

CAS SCIFINDER 入門 - 大学向け -

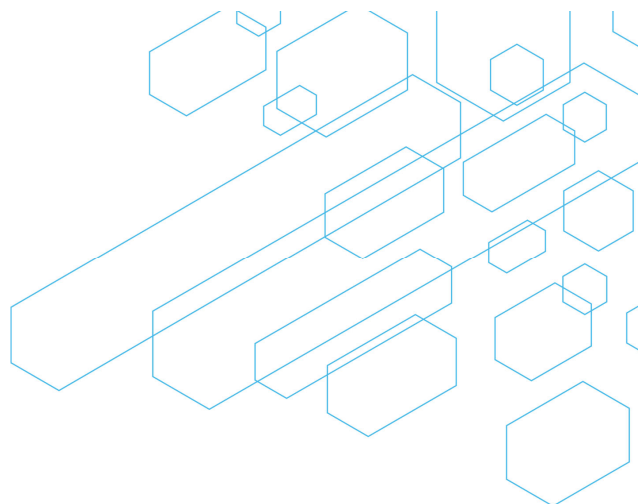
化学情報協会 情報事業部
2025/5/20

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目次

- CAS SciFinder の概要
- References（文献）検索
- Substances（物質）検索
- Reactions（反応）検索
- 便利な機能
- Q&A



CAS SCIFINDER の概要

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研究における情報の必要性

膨大な情報の中から欲しい情報を見つけ出す

研究をする上で重要なこと

- 新規性
網羅的な先行技術の検索
- 信頼性
正確なデータ収集と適切な実験設計
- 効率
適切な方法で迅速に結果を出す



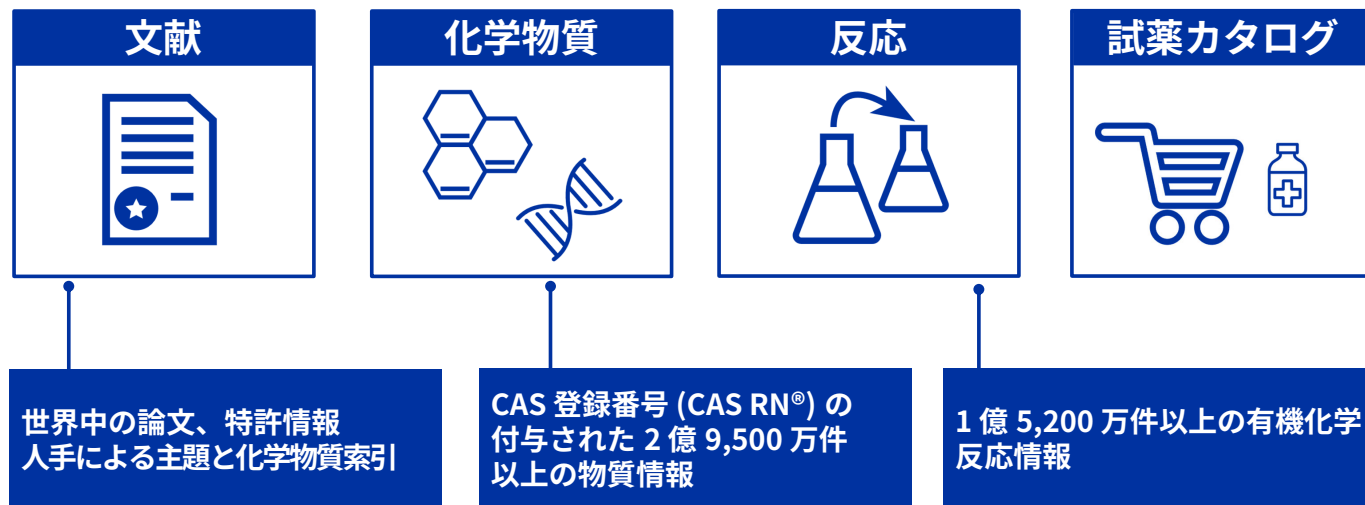
4

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CAS SciFinder とは

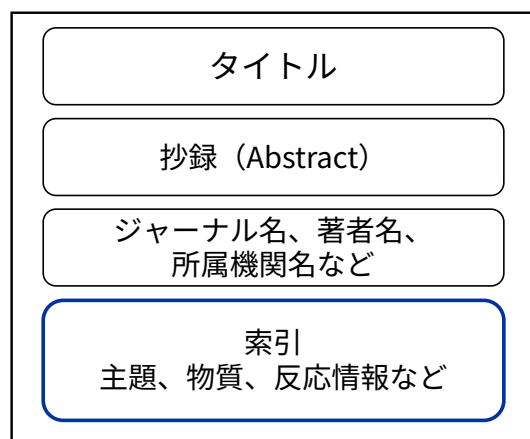
CAS の作成する研究者向けの情報検索ツール



CAS SciFinder の文献情報

原報 (一次資料) の要点をまとめた資料 (二次資料)

CAS SciFinder の文献情報



二次資料のメリット

- 文献の内容を迅速に把握できる
 - 原報を読むべき文献かどうかを判断しやすい
- 要点に基づいた検索が可能
 - ノイズが少なく、必要な情報を見つけやすい

世界 50 以上の言語の文献の二次情報を英語で作成し収録

CAS のアナリストが、著者や発明者が強調している点、文献の主題に関わる概念や化学物質などを索引

CAS SciFinder の物質情報

物質情報は CAS RN® で管理され、収録数は世界最大の2.9億以上

物質情報の収録源

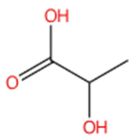
CAS References
CAS Patents

カタログ

その他

CAS RN® の付与・管理

50-21-5



C₃H₆O₃
Lactic acid

- CAS RN®
- 物質名称
- 化学構造式
- 物性値、スペクトル情報など

CAS SciFinder の反応情報

合成的に意義のある反応を収録

原文献



文献情報



合成的に意義がある？

Yes

反応情報



試薬
触媒
溶媒



CAS SciFinder のカタログ情報

市販化学物質製品のカタログ情報を検索可能

Suppliers for 58-08-2

Filter Behavior: **Filter by** Exclude

Filtering: Country/Region: Japan X

27 Results

Sort: Price: Low to High

FUJIFILM Wako Pure Chemical Corporation Product List

Substance	Purity	Quantity Information	Availability	Ordering
58-08-2	95-98%	Product Information	Japan	Order Number: 035-06795
Caffeine		500 g JPY 6250		

Kishida Chemical Product List

Substance	Purity	Quantity Information	Availability	Ordering
58-08-2	95-98%	Product Information	Japan	Order Number: 000-13332
Caffeine		25 g JPY 1800 500 g JPY 6600		

TCI Research Chemicals

Substance	Purity	Quantity Information	Availability	Ordering
58-08-2	95-98%	Product Information	Maintained in stock	Order Number: C2042
Caffeine		25 g JPY 1900 500 g JPY 6900	Ships within 1 week	

FUJIFILM Wako Pure Chemical Corporation Product List

Supplier Contact Information

Web: <https://labchem.wako.fujifilm.com/gp/index.html>

Address: FUJIFILM Wako Pure Chemical Corporation
1-2, Shookomachi 3-Chome
Chuo-Ku, Osaka, 540-8605
Japan

Phone: +81-6-6203-2741

Fax: +81-6-6203-2029

Product Information

Chemical Name: Caffeine

Order Number: 035-06795

Purity: 95.5% (HPLC)

Quantity Information: 500 g JPY 6250

Pricing Information last update: 17 Jun 2024

Distributor Details

Distributor Name: FUJIFILM Wako Chemicals U.S.A. Corporation

Address: 1600 Bellwood Road
Richmond, VA, 23237-1326
United States

Distributor Name: FUJIFILM Wako Chemicals Europe GmbH

Address: Fuggerstrasse 12
Neuss, 51446
Germany

日本の業者や代理店に限定

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CAS SciFinder の特長

索引を基に相互の情報を紐づけた的確で効率的な検索が可能



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CAS 製品の導入実績

CAS のデータベースはその分野の専門家によって作成され、品質管理が行われており、世界の化学・製薬企業、大学、政府機関、特許庁によって利用されている



TOP 25
LIFE SCIENCES
COMPANIES¹



TOP 25
CHEMICAL
COMPANIES²



TOP 25
UNIVERSITIES³



TOP 10
GLOBAL PATENT
OFFICES⁴

1. <https://www.pharmexec.com/view/2024-pharm-exec-top-50-companies>
2. <https://www.chemanalyst.com/ChemAnalyst/ChemicalManufacturers>
3. <https://www.shanghairanking.com/rankings/gras/2024/RS0103>
4. <https://www.wipo.int/edocs/pubdocs/en/wipo-pub-941-2023-en-world-intellectual-property-indicators-2023.pdf>

CAS SciFinder のご利用について

ライセンス（利用規約）を守る

- 必ず自分の **Username (Login ID)** で利用する
- 入手した情報の共有は最小単位の同一研究グループ内でのみ
- データのダウンロードは、1人あたり累計 **5,000** 件を超えないようにする
- 短時間の大量ダウンロードはしないようにする

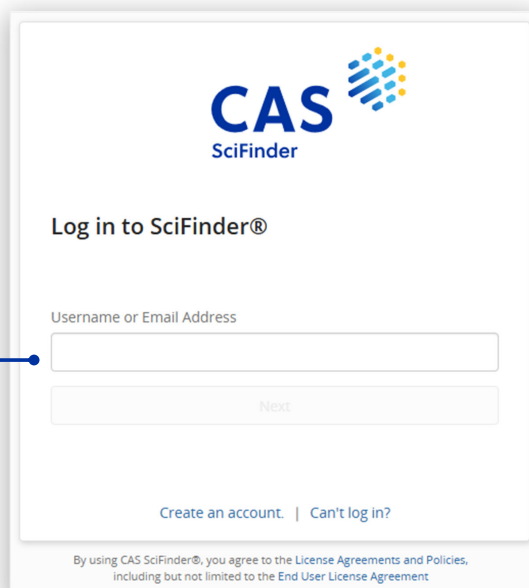
CAS SciFinderへのアクセス

利用にはユーザー登録が必要

• Login URL

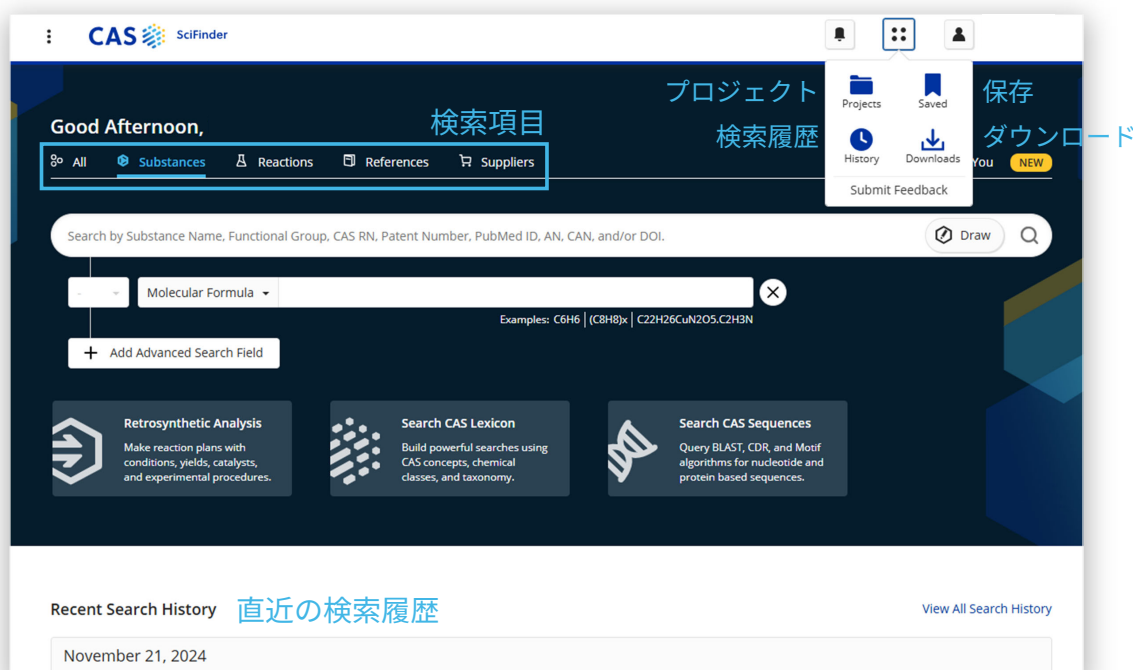
<https://scifinder-n.cas.org/>

自身の Username
パスワードでログイン



The image shows the login page for CAS SciFinder. At the top is the CAS SciFinder logo. Below it is the text "Log in to SciFinder®". There is a text input field labeled "Username or Email Address" and a "Next" button. At the bottom, there are links for "Create an account." and "Can't log in?". A small disclaimer at the very bottom states: "By using CAS SciFinder®, you agree to the License Agreements and Policies, including but not limited to the End User License Agreement."

検索初期画面



The image shows the search homepage of CAS SciFinder. The header includes the CAS SciFinder logo and navigation links for "プロジェクト" (Project) and "検索履歴" (Search History). The main content area features a "Good Afternoon," greeting and a "検索項目" (Search Item) section with tabs for "All", "Substances", "Reactions", "References", and "Suppliers". Below this is a search bar with the text "Search by Substance Name, Functional Group, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." and a "Draw" button. There is also a "Molecular Formula" input field with examples: C6H6, (C8H8)x, C2H26CuN2O5.C2H3N. Below the search bar are three search options: "Retrosynthetic Analysis", "Search CAS Lexicon", and "Search CAS Sequences". At the bottom, there is a "Recent Search History" section with the text "直近の検索履歴" and a "View All Search History" link. The date "November 21, 2024" is displayed.

REFERENCES (文献) 検索

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検索例 ①

新型コロナウイルス感染症の後遺症として多く診断されている症状を調査する

検索の流れ

- キーワード検索：long covid (新型コロナウイルス感染症の後遺症)
- 絞り込み：Search Within Results 「Diagnosis (診断)」
- 解析：Concept

下記のうち、文献報告数が最も多い症状は？

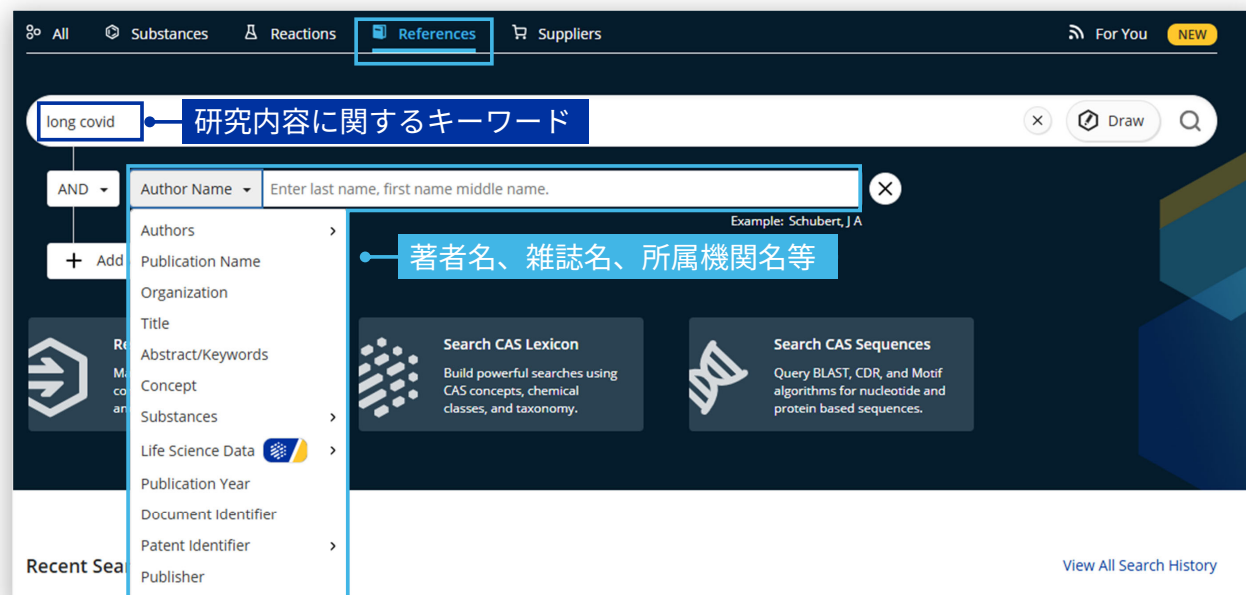
- 嗅覚障害 (Anosmia)
- 疲労 (Fatigue, biological)
- 呼吸困難 (Dyspnea)
- 頭痛 (Headache)

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文献検索画面

検索項目で References を選択し、キーワード (long covid) を入力する

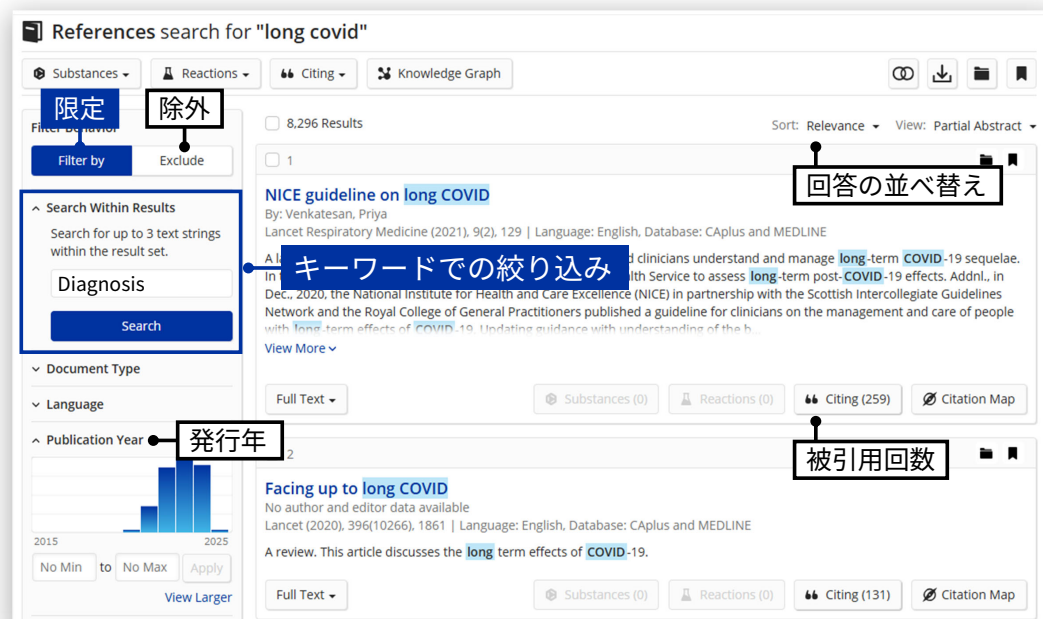


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文献検索の回答一覧画面

Filter by Search Within Results に Diagnosis と入力し、回答を絞り込む



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検索結果の解析

Concept (主題となるキーワード) を解析し、報告数の多い症状を確認する

References search

Substances

Reaction

Filter Behavior

Filter by

Exclude

Search Within Results

Document Type

Language

Publication Year

Available at My Institution

Author

Organization

Publication Name

Concept

COVID-19 (1,066)

Humans (860)

Post-Acute COVID-19 Syndrome (622)

SARS-CoV-2 (561)

Homo sapiens (51)

View All

Concept

Top Count

Alphanumeric

Search

4 Selected

☐ Middle Aged (238)

☐ Long COVID (219)

☐ Aged (184)

☐ Coronavirus infection (122)

☒ Fatigue, biological (119) 疲労

☐ COVID-19 Testing (106)

☐ Pandemics (105)

☐ Child (102)

☐ Depression (102)

☐ Quality of Life (97)

☐ Viral infection (97)

☒ Dyspnea (96) 呼吸困難

☐ Adolescent (93)

☐ Retrospective Studies (92)

☐ Anxiety (90)

☐ Epidemic (85)

☒ Headache (84) 頭痛

☐ Inflammation (80)

☐ Gender (54)

☐ Risk assessment (54)

☐ Prevalence (51)

☒ Anosmia (49) 嗅覚障害

☐ Body mass index (49)

☐ Angina pectoris (48)

☐ Cardiovascular disease (46)

☐ Aging, animal (45)

☐ Immunoglobulin G (45)

☐ Infection (45)

☐ United States (45)

☐ Chronic fatigue syndrome (43)

☐ Surveys and Questionnaires (43)

☐ Disease progression (42)

☐ Hospitalization (42)

☐ Asthma (38)

☐ Blood plasma (30)

☐ Brain (30)

☐ Breathing disorders (30)

☐ Diagnostic biomarkers (30)

☐ Prognosis (30)

☐ Blood serum (29)

☐ COVID-19 Drug Treatment (29)

☐ Longitudinal Studies (29)

☐ Pain (29)

☐ Aged, 80 and over (28)

☐ Chronic obstructive pulmonary disease (28)

☐ Fibromyalgia (28)

☐ Machine learning (28)

☐ Myocarditis (28)

☐ Heart failure (27)

☐ Leukocyte (27)

☐ Health personnel (26)

Cancel

Apply

下記の症状の中で、文献で多く報告されているのは？

- 嗅覚障害 (Anosmia)
- 疲労 (Fatigue, biological)
- 呼吸困難 (Dyspnea)
- 頭痛 (Headache)

文献情報の確認

文献のタイトルをクリックすると詳細ページが開く

検索一覧画面

LONG COVID-A hypothesis for understanding the biological basis and pharmacological treatment strategy

By: Jarrott, Bevyn ● Head, Richard ● Pringle, Kirsty G ● Lumbers, Eugenie R ● Martin, Jennifer H ●

Pharmacology Research & Perspectives (2022), 10(1), e000... | Language: English, Database: CAPUS and MEDLINE

A review. Infection of humans with SARS-CoV-2 virus causes a disease known colloquially as "COVID-19" with symptoms ranging from asymptomatic to severe pneumonia. Initial pathol. is due to the virus binding to the ACE-2 protein on endothelial cells lining blood vessels and entering these cells in order to replicate. Viral replication causes oxidative stress due to elevated levels of reactive oxygen species. Many (~60%) of the infected people appear to have eliminated the virus from their body after 28 days and resume normal activity. However, a significant proportion (~40%) experience a variety of symptoms (loss of smell and/or taste, fatigue, cough, aching pain, "brain fog"). Longitudinal clin. studies in a group of subjects who were infected with SARS-CoV-2 have been compared to a non-infected matched group of subjects. A cohort of infected subjects can be identified by a battery of cytokine markers to have persistent, low level grade of inflammation and often self-report two or more troubling symptoms. There is no drug that will relieve their symptoms effectively. It is hypothesized that drugs that activate the intracellular transcription factor, nuclear factor erythroid-derived 2-like 2 (NRF2) may increase the expression of enzymes to synthesize the intracellular antioxidant, glutathione that will quench free radicals causing oxidative stress. The hormone melatonin has been identified as an activator of NRF2 and a relatively safe chem. for most people to ingest chronically. Thus, it is an option for consideration of re-purposing studies in "LONG COVID" subjects experiencing insomnia, depression, fatigue, and "brain fog" but not tachycardia. Appropriately designed clin. trials are required to evaluate melatonin.

View More

Full Text

Substances (4)

Reaction

LONG COVID-A hypothesis for understanding the biological basis and pharmacological treatment strategy

By: Jarrott, Bevyn ● Head, Richard ● Pringle, Kirsty G ● Lumbers, Eugenie R ● Martin, Jennifer H ●

DOI: 10.1002/prp2.911

A review. Infection of humans with SARS-CoV-2 virus causes a disease known colloquially as "COVID-19" with symptoms ranging from asymptomatic to severe pneumonia. Initial pathol. is due to the virus binding to the ACE-2 protein on endothelial cells lining blood vessels and entering these cells in order to replicate. Viral replication causes oxidative stress due to elevated levels of reactive oxygen species. Many (~60%) of the infected people appear to have eliminated the virus from their body after 28 days and resume normal activity. However, a significant proportion (~40%) experience a variety of symptoms (loss of smell and/or taste, fatigue, cough, aching pain, "brain fog"). Longitudinal clin. studies in a group of subjects who were infected with SARS-CoV-2 have been compared to a non-infected matched group of subjects. A cohort of infected subjects can be identified by a battery of cytokine markers to have persistent, low level grade of inflammation and often self-report two or more troubling symptoms. There is no drug that will relieve their symptoms effectively. It is hypothesized that drugs that activate the intracellular transcription factor, nuclear factor erythroid-derived 2-like 2 (NRF2) may increase the expression of enzymes to synthesize the intracellular antioxidant, glutathione that will quench free radicals causing oxidative stress. The hormone melatonin has been identified as an activator of NRF2 and a relatively safe chem. for most people to ingest chronically. Thus, it is an option for consideration of re-purposing studies in "LONG COVID" subjects experiencing insomnia, depression, fatigue, and "brain fog" but not tachycardia. Appropriately designed clin. trials are required to evaluate melatonin.

Keywords: review long covid infection symptom pharmacol pathophysiol; COVID-19; NRF2; SARS-CoV-2; endothelium; melatonin; oxidative stress; tissue hypoxia; LONG COVID

Open Access

Full Text

文献情報の詳細画面

LONG COVID-A hypothesis for understanding the biological basis and pharmacological treatment strategy

By: Jamari, Bryan; Head, Richard; Pringle, Kirsty; Lumbers, Eugenie; Martin, Jennifer

DOI: 10.1002/prs2.911

抄録
(内容の要約)

約40%の人々が、嗅覚や味覚の喪失、疲労、咳、痛みなどの症状を経験

Keywords: review, long covid, infection symptom, pharmacological pathophysiology, COVID-19, NFR2, SARS-CoV-2, endothelium, melatonin, oxidative stress, tissue hypoxia, LONG COVID

Open Access Full Text

Publication Information - Journal

Source: Pharmacology Research & Perspectives
Database Information: AN: 2022-355399
Company/Organization: Flinders Institute of Neuroscience & Mental Health
Publisher: John Wiley & Sons Ltd.
Language: English

CAS Concepts

主題となるキーワード

Agusia
Anosmia
Antioxidants

Homo sapiens
Human
Insomnia

主題となるキーワード

Long COVID
新型コロナウイルス感染症の後遺症

Diagnosis
診断

Drug repurposing
疲労

Breathing disorders
Long COVID
Nuclear factor erythroid 2 related factor 2 (NFE2L2)
Oxidative stress, biological
Pneumonia
Reactive oxygen species
Severe acute respiratory syndrome coronavirus 2
Tachycardia
Virus replication

MEDLINE® Medical Subject Headings

Substances

重要な化学物質

ACE2
新型コロナウイルスが細胞内に侵入する際の受容体

メラトニン
後遺症の治療薬として検討されている



原報の入手方法 – 雑誌論文の場合 –

原報（フルテキスト）は Full Text リンクから入手可能

4

Stevia rebaudiana Bert. leaf extracts as a multifun

By: Gawel-Beben, Katarzyna; Bujak, Tomasz; Nizioł-Lukaszewska, Zofia; Rybczynska, Kamila

Molecules (2015), 20(4), 5468-5486 | Language: English, Database: C

Analytical Methods

View More

Full Text

Substances (8)

JAICI library
DOI
View all Sources

- In house resource リンク
リンクリゾルバへのリンク
(設定があれば表示される)
- DOI
出版元のページリンク
- View all Sources
原文献へのすべてのリンク



SUBSTANCES（物質）検索

23

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検索例 ②

カフェインの化学構造、CAS RN® および融点を確認する

検索の流れ

- 物質名検索：Caffeine
- 詳細情報の確認

24

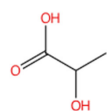
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CAS 登録番号 (CAS RN®) とは

CAS RN® は化学物質の識別番号

50-21-5



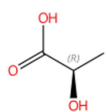
C₃H₆O₃
Lactic acid

一つの物質に一つの
CAS RN® が付与される

乳酸 (Lactic acid) の CAS RN® は 50-21-5

同じ「乳酸」でも
別物質として登録
されるものもある

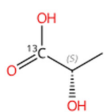
10326-41-7



Absolute stereochemistry shown
C₃H₆O₃
D-Lactic acid

立体異性体

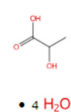
727379-97-7



Absolute stereochemistry shown
C₃H₆O₃
(2S)-2-Hydroxypropanoic-1-¹³C acid

標識化合物

221292-82-6



C₃H₆O₃·4H₂O

塩・水和物

物質検索画面

検索項目で Substances を選択し、物質名 (caffeine) を入力する

The screenshot shows the CAS search interface. The 'Substances' tab is selected. The search bar contains 'caffeine'. A dropdown menu is open, showing various search criteria: Molecular Formula, CAS Registry Number, Chemical Identifier, Document Identifier, Patent Identifier, Experimental Spectra, Life Science Data, Biological, Chemical Properties, Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, and Thermal. The 'Chemical Identifier' option is highlighted. The main search area displays 'caffeine' and a '化学構造' (Chemical Structure) button. Below the search bar, there are sections for 'Search CAS Lexicon' and 'Search CAS Sequences'. The bottom of the screen shows a 'Recent Searches' section with a search for 'caffeine' dated November 3, 2025.

物質検索の回答一覧画面

物質名で検索した場合、検索対象は「名称」と「Notes」

Substances search for "caffeine"

References Reactions Suppliers

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

Product (1)
Reactant (1)
Reagent (1)
Catalyst (1)

Reference Role

Biological Study (22)

26 Results

Sort: Relevance View: Partial

1 58-08-2

CN1C=NC2=C1C(=O)N(C(=O)N2C)C

$C_8H_{10}N_4O_2$
Caffeine

物質名でヒット

72K References 1,788 Reactions 137 Suppliers

2 52622-68-1

Image Not Available

Notes: A pharmaceutical probably contg. **caffeine** Unspecified Coffetyl

Notes* でヒット

3 References 0 Reactions 0 Suppliers

3 155215-75-1

Image Not Available

Notes: A proprietary drug contg. **caffeine** (Saudi Arabia) Unspecified Prontopyrin

1 Reference 0 Reactions 0 Suppliers

* Notes: 索引者による補足情報

物質情報の確認

CAS RN® をクリックすると詳細ページが開く

検索一覧画面

1 58-08-2

CN1C=NC2=C1C(=O)N(C(=O)N2C)C

$C_8H_{10}N_4O_2$
Caffeine

72K References 1,788 Reactions 137 Suppliers

CAS Registry Number: 58-08-2

View in CAS BioFinder

物質情報の詳細

CN1C=NC2=C1C(=O)N(C(=O)N2C)C

$C_8H_{10}N_4O_2$
1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- (9CI, ACI)

Key Physical Properties

Key Physical Properties	Value	Condition
Molecular Weight	194.19	-
Melting Point (Experimental)	178 °C (sublim)	-
Boiling Point (Predicted)	416.789±37.00 °C	Press: 760.00 Torr
Density (Experimental)	1.23 g/cm³	Temp: 18 °C
pKa (Predicted)	0.523±0.70	Most Basic Temp: 25 °C

Experimental Properties | Spectra

物質情報の詳細画面

CAS Registry Number: 58-08-2 CAS RN®

72K 1,788 137 View in CAS Biofinder

化学構造式

分子式
C₈H₁₀N₄O₂
1,3,7-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- (9CI, ACI)

有害性の区分を表すピクトグラム

Key Physical Properties	Value	Condition
Molecular Weight	194.19	-
Melting Point (Experimental)	178 °C (sublim)	-
Boiling Point (Predicted)	416.789±37.00 °C	Press: 760.00 Torr
Density (Experimental)	1.23 g/cm³	Temp: 18 °C
pKa (Predicted)	0.523±0.70	Most Basic Temp: 25 °C

融点→

基本物性値

Experimental Properties | Spectra

Expand All | Collapse All

Other Names and Identifiers

Canonical SMILES
O=C1C=CN2C(=O)N(C(=O)N1C)C2

InChI
InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)/1(13)/2(3)(14)11(6)/h4H,1-3H3

InChI Key
RYYVLZUUVJGH-UHFFFAOYSA-N

41 Other Names for this Substance

Caffeine (9CI)
3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione (ACI)

化学物質名

Experimental Properties

Biological	Chemical	Density	Interface	Lipinski	Optical and Scattering	Structure Related	Thermal
Property	Value					Condition	Source
Melting Point	232-235 °C					-	(25) IC
Melting Point	230 °C					-	(26) CAS
Melting Point	223-224 °C					Solvent: Tetrahydrofuran	(27) IC
Melting Point	178 °C (sublim)					-	(13) NIOSH

Sources
(25) Jansen in de Wal, Helmut; Zeitschrift fuer Chemie, (1989), 29(7), 253-4, Caplus
(26) Schmidt, E.; Archiv der Pharmazie (Weinheim, Germany), (1908), 245, 389-98, Caplus
(27) Yamauchi, Kiyoshi; Journal of Organic Chemistry, (1975), 40(3), 385-6, Caplus

Experimental Spectra
Pharmacological Data
ADME
Toxicity
Predicted Properties
Predicted Spectra
Bioactivity Indicators
Target Indicators
Regulatory Information
GHS Hazard Statements
Additional Details

実測スペクトル
薬理学的データ
ADME
毒性
予測物性値
予測スペクトル

CAS LIFE SCIENCES

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検索例 ③

下記の化合物の名称を確認する

Substances Reactions References Suppliers For You NEW

CAS Draw

Enter a CAS Registry Number, SMILES, or InChI.

Molecular Formula: C₁₅H₁₉O₃ (246.31)

OK Cancel

Zoom: 160%

Draw

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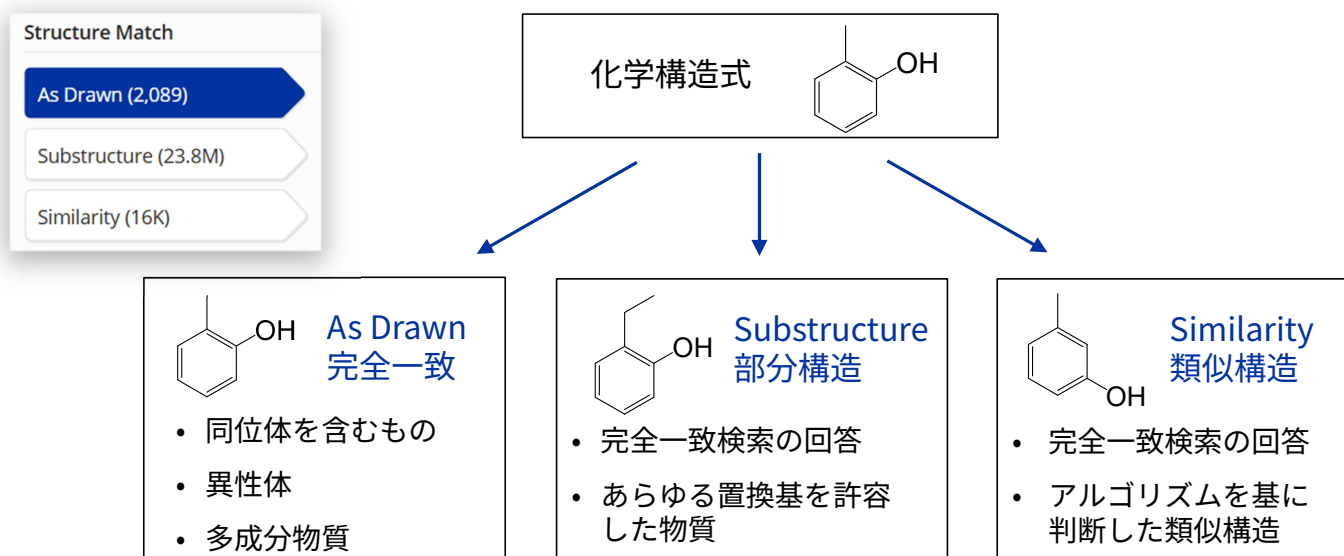


物質検索の回答一覧画面

作図した通りの物質は As Drawn (完全一致検索) で確認する

構造検索のタイプ

化学構造検索を行うと、3つの検索タイプでの構造検索が同時に実行される



REACTIONS (反応) 検索

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検索例 ④

ロキソプロフェンの合成方法を調査する

Substances search 検索例 ③ の物質検索結果

References Reactions Suppliers

Structure Match

As Drawn (245)

Substructure (600)

Similarity (52K)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

245 Results

1

68767-14-6

CC(C)C(=O)Oc1ccc(cc1)Cc2ccccc2C(=O)O

C₁₅H₁₈O₃
Loxoprofen

1,653 References 957 Reactions 85 Suppliers

Reactions for 68767-14-6 反応検索の結果

References

Filter Behavior

Filter by Exclude

Filtering: Substance Role: Product X

Search Within Results

Substance Role

☒ Product (753)

☐ Reactant (204)

Yield

☐ 90-100% (19)

☐ 80-89% (9)

☐ 70-79% (7)

☐ 50-69% (4)

☐ No Yield Available (714)

Number of Steps

Group: By Score

Suppliers (85)

31-244-CAS-7446954 Steps: 1 Yield: 100% Preparation of Assignee: Nippon Japan, JP2001

1.1 Reagents: Hydrogen Catalysts: Palladium Solvents: Ethyl acetate

Experimental Protocols

PatentPal

ロキソプロフェンの役割を生成物に指定

ロキソプロフェンの反応情報が得られる

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反応検索の回答一覧画面

反応情報はスキームごとに表示される

Reactions for 68767-14-6

References

限定 除外

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

☒ Product (753)

☐ Reactant (204)

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Filtering: Substance Role: Product X

Clear All Filters

753 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction) Steps: 1 Yield: 100% ...

反応物

生成物 (ロキソプロフェン)

反応ステップ数 / 収率

市販の有無

Suppliers (85)

31-244-CAS-7446954 Steps: 1 Yield: 100% ...

1.1 Reagents: Hydrogen Catalysts: Palladium Solvents: Ethyl acetate

試薬 触媒 溶媒

Preparation of substituted styrene derivatives

Assignee: Nippon Petrochemicals Co., Ltd. Japan, JP2001081066 A 2001-03-27

PatentPak Full Text

出典文献

Collapse Scheme

35

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反応検索の回答一覧画面 (絞り込み)

反応情報はスキームごとに表示される

Reactions for 68767-14-6

References

限定 除外

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

☒ Product (689)

☐ Reactant (176)

Yield

Number of Steps

Commercial Availability

☐ Products (753)

☒ All Starting Materials (689)

Filtering: Substance Role: Product X Commercial Availability: All Starting Materials X

Clear All Filters

689 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (6 Reactions) Steps: 1 Yield: 85-97% ...

反応物

Suppliers (6)

Suppliers (85)

市販されている

31-352-CAS-14376595 Steps: 1 Yield: 97% ...

1.1 Reagents: Acetic acid, Hydrogen bromide 8 h, reflux

出発物質が市販されているもの

Process for preparation of loxoprofen sodium

Assignee: Zhejiang Apelo Medical Technology Co., Ltd. China, CN101412670 A 2009-04-22

PatentPak Full Text

36

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反応情報の確認

詳細は View Reaction Detail で確認する

Scheme 3 (1 Reaction)

Suppliers (73) Suppliers (56)

☐ View Reaction Detail

Steps: 2

Photo-induced 1,2-aryl migration of 2-chloro-1-aryloxypropane under batch and flow conditions: Rapid, scalable and sustainable approach to 2-arylpropionic acids

By: Li, Qiao; et al

View All

Chinese Chemical Letters (2024), 35(2), 108576

Full Text

Collapse Scheme ^

Multi-Step Reaction for Scheme 3, Reaction 1

Suppliers (73) Suppliers (56) Supplier (1) Suppliers (85)

Reaction Overview

Steps: 2 Yield: -

JOURNAL

Photo-induced 1,2-aryl migration of 2-chloro-1-aryloxypropane under batch and flow conditions: Rapid, scalable and sustainable approach to 2-arylpropionic acids

By: Li, Qiao; et al

View All

Chinese Chemical Letters (2024), 35(2), 108576

View Source Full Text

Company/Organization

College of Chemical Engineering

Zhejiang University of Technology

Hangzhou 310014

China

Step 1 Step 2

Stage	Reagents	Catalysts	Solvents	Conditions
1	Aluminum chloride	-	Dichloromethane	-10 °C, 6 h, 0 °C
2	Water	-	-	cooled

CAS Reaction Number: 31-614-CAS-38851701

Alternative Steps (0)

Experimental Protocols

Synthetic Methods

Products

2-[4-(2-Chloro-1-oxopropyl)phenyl]methylcyclopentanone, Yield: 80%

Reactants

2-Benzylcyclopentanone

2-Chloropropionyl chloride

Reagents

Aluminum chloride

Water

反応情報の詳細画面

詳細画面では反応の全ステップのスキームを確認できる

Multi-Step Reaction for Scheme 3, Reaction 1

全ステップのスキーム

Suppliers (73) Suppliers (56) Supplier (1) Suppliers (85)

Reaction Overview

Steps: 2 Yield: -

JOURNAL

Photo-induced 1,2-aryl migration of 2-chloro-1-aryloxypropane under batch and flow conditions: Rapid, scalable and sustainable approach to 2-arylpropionic acids

By: Li, Qiao; et al

View All

Chinese Chemical Letters (2024), 35(2), 108576

View Source Full Text

Company/Organization

College of Chemical Engineering

Zhejiang University of Technology

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Step 1 Step 2

Stage	Reagents	Catalysts	Solvents	Conditions
1	Aluminum chloride	-	Dichloromethane	-10 °C, 6 h, 0 °C
2	Water	-	-	cooled

CAS Reaction Number: 31-614-CAS-38851701

Alternative Steps (0)

Experimental Protocols

Synthetic Methods

Products

2-[4-(2-Chloro-1-oxopropyl)phenyl]methylcyclopentanone, Yield: 80%

Reactants

2-Benzylcyclopentanone

2-Chloropropionyl chloride

Reagents

Aluminum chloride

Water

Solvents

Dichloromethane

Procedure

1. Add aluminum chloride (8.64 g, 64.8 mmol, 1.08 equiv.) to a solution of substituted benzene (50mmol, 1.0equiv.) in anhydrous dichloromethane (30 mL) at -10°C.
2. Add a solution of 2-chloropropionyl chloride (8.61 g, 67.8 mmol, 1.13 equiv.) in anhydrous dichloromethane (10 mL) dropwise.
3. After complete the addition, stir the reaction mixture at 0°C for 6 h.
4. Pour the reaction mixture onto crushed ice and separate the organic layer.
5. Wash the combined organic layers with 1 M HCl (50mL) followed saturated aqueous NaHCO₃ (50mL).
6. Dry the combined organic layers over anhydrous Na₂SO₄, filter and concentrate under reduced pressure.
7. Purify the residue by silica chromatography (petroleum ether: ethyl acetate = 10: 1).

Transformation

Friedel-Crafts Acylation

Characterization Data

2-[4-(2-Chloro-1-oxopropyl)phenyl]methylcyclopentanone

Proton NMR Spectrum

(400 MHz, CDCl₃) δ 7.90 (d, J = 8.2 Hz, 2H), 7.26 (t, J = 7.4 Hz, 2H), 5.22 (q, J = 6.6 Hz, 1H), 3.15 (dd, J = 13.9, 4.2 Hz, 1H), 2.57 (dd, J = 13.8, 9.3 Hz, 1H), 2.37-2.26 (m, 2H), 2.11-2.01 (m, 2H), 1.97-1.89 (m, 1H), 1.83-1.70 (m, 1H), 1.68 (d, J = 6.7 Hz, 3H), 1.54-1.45 (m, 1H)

Carbon-13 NMR

(100 MHz, CDCl₃) δ 219.5, 193.2, 146.7, 132.2, 129.3, 129.2, 52.8, 50.6, 38.0, 35.6, 29.1, 20.5, 20.0

IR Absorption Spectrum

(cm⁻¹): 2965, 1738, 1689, 1607, 1253, 1154, 955

HRMS

calcd. For C₁₇H₁₇ClO₂Na ([M+Na]⁺) 287.0809, found 287.0808

State

light yellow oil

原報に記載の実験項情報

(参考) Reaction Search

検索初期画面から検索を始める場合

CAS RN® から構造を呼び出し可能

反応ロール (役割) が自動的に付与される

product

Draw

(参考) CAS Retrosynthesis (逆合成解析機能) とは

目的物質を効率的に合成する経路を自動で立案する機能

Experimental Steps Predicted Steps

予測反応を含めた解析で新規化合物の解析にも対応

立体を考慮

反応部位や反応に関与しない結合といった解析条件の設定

多段階のルートを解析

技術資料・動画はこちら



便利な機能

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回答の保存 (Save)

検索式等の保存やアラート登録が可能



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プロジェクト機能

選択した文献、物質をプロジェクト単位で管理可能

The screenshot displays the 'References search for "covid 19"' results page. Two records are selected, indicated by checkboxes and callouts: 'Dexamethasone in the management of covid-19' and 'COVID 19 and its mental health'. Arrows point from these records to the 'Add to Project' dialog box. The dialog box has two sections: 'New Project' and 'Existing Projects'. The 'New Project' section includes fields for 'Project Name', 'Project Color' (set to Light Blue), and 'Project Description (Optional)'. The 'Existing Projects' section shows a list of projects, with 'Lithium Ion Battery - recycling' selected. Callouts in Japanese explain the options: '新規プロジェクトとして登録' (Register as new project) and '既存プロジェクトとして登録' (Register as existing project).

プロジェクト共有機能

作成したプロジェクトを他のユーザーに共有可能

The screenshot shows the 'Project Collaborators' dialog box and the 'Project' page. The 'Project Collaborators' dialog box has a field to 'Add project collaborators using an email address...' and a list of 'People with access (2)'. The list includes 'JAICI (You)' as the 'Administrator' and 'support@jaici.or.jp (Pending)' as a 'Viewer'. A callout points to the 'Remove Access' button, with the text '共有先のユーザーの役割を指定' (Specify the role of the user to share with). The 'Project' page shows two projects: 'Lithium Ion Battery - recycling' and 'Laundry detergents'. A callout points to the 'Share Project' button in the project's menu, with the text 'プロジェクトの編集・共有等' (Edit, share, etc. of the project). Another callout points to the 'Projects' button in the top navigation bar, with the text 'プロジェクトの保存先' (Where to save the project).

回答の共有

検索結果は他のユーザーと共有可能

References search for "covid 19"

Substances Reactions Citing Knowledge Graph

Filter Behavior: Filter by Exclude

Search Within Results: Search for up to 3 text strings within the result set. Enter a query... Search

Searching for... vaccine

Document Type: Journal (64K)

Filtering: Search Within Results: vaccine

2,401 Results

Assessment of booster vaccination of COVID 19 and its impact on health thereof using artificial intelligence, it can be termed into two categories data collected from social medias to find the general opinion of people about booster vaccination and checking authenticity of news about booster dose using Natural Language processing algorithms (NLP) algorithms. NLP are further used to categorize the emotions, public opinions of the people from keywords, images and videos collected from social media websites, blogs, articles and other vlogs. The trustworthy of...

View More

PatentPak Full Text

Substances (0) Reactions (0) Citing (0) Citation Map

リンクをメールで共有
CAS SciFinder から直接送信

URL をコピー
URL をクリップボードにコピー

Save and Alert
Share Results
Copy Search to Clipboard

回答のダウンロード

検索結果は様々な形式でダウンロード可能

- 一人当たりの保存件数 5,000 件を超えないようにする
- 短時間での大量ダウンロードをしない
- 情報共有は最小単位の同一研究グループ内のみ

Substances search for drawn structure

References Reactions Suppliers

Structure Match: As Drawn (79), Substructure (23K), Similarity (118K), Analyze Structure Precision

79 Results

Sort: Relevance View: Partial

1 486-66-8

2 291759-05-2

3 220930-96-1

Download button

Download Substance Results

File Type: Excel (.xlsx), PDF, Rich Text (.rtf), SDFFile (.sdf)

Select Quantity: All Results, Selected Results, Range (ex. 2 to 20)

File Name: Substance_20241001_1319

Include: Task History, Substance Identifiers, Experimental Spectra, Predicted Spectra, Regulatory Information, Experimental Properties, Predicted Properties, Bioactivity Indicators, Target Indicators, GHS Hazard Codes

Download Cancel Learn more about downloads.

まとめ

CAS SciFinder は、科学関連の研究情報を効率的に検索できる

- 世界中の科学関連の研究情報を検索
物質科学領域の研究情報を的確かつ網羅的に調べることができる
- 高品質なデータ
信頼できる情報源から専門家が情報を抽出することで、再現性の高い検索を実現
- 多様な検索機能
キーワードや化学構造を使った柔軟に検索できる
- 関連情報へのスムーズなアクセス
物質の情報から合成法や条件、試薬カタログ情報など欲しい情報がすぐに確認できる

JAICI ヘルプデスク

0120-003-462 (平日 9:00-17:00)

support@jaici.or.jp



ユーザーマニュアル

<https://www.jaici.or.jp/cas-scifinder-discovery-platform/documents/>