

CAS SciFinder Discovery Platform™

사용자 가이드

CAS

A division of the
American Chemical Society



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인터페이스 및 설정



App Switcher: 추가 CAS solutions으로 이동

로그를 클릭하여 홈페이지로 이동

알림

저장한 결과, 검색 기록, 다운로드 등

User Name

업데이트 소식, 세팅, 도움 가이드, 프로필 정보 등

Search Interface CAS SciFinder는 직관적이고 편리한 검색 인터페이스를 제공합니다.

Good Afternoon, SearchSense: 자연어 검색 검색 실행하기

Dehalogenation in heteropent catalyzed by palladium

Ask CAS Newton CAS 데이터 기반 Agentic AI 검색 구조 그리기 툴

Featured Search CAS의 표준화된 컨셉을 활용한 검색

- Advanced Search: Select data fields and search operators to create a focused query.
- Search CAS Lexicon: Build powerful searches using CAS concepts, chemical classes, and taxonomy.
- Patent Markush: Search Patent Markush by structure and view associated references.
- Retrosynthetic Analysis: Make reaction plans, with conditions, yields, catalysts, and experimental procedures.
- Search CAS Sequences: Query BLAST, CDL, and Motif algorithms for nucleotide and protein based sequences.
- Prior Art Discovery: An enhanced prior art search for patent professionals.

고급 검색: 문헌검색, 물질 검색 한정하여 검색

AI를 활용한 특허성 검토

특허 마쿠시 구조 검색

Retrosynthesis 실행

검색 기능 접기/펼치기

SearchSense

별도의 검색 유형 없이 자연어 표현으로도 필요한 정보를 찾을 수 있습니다.

예: Chromium dichloride catalyzed Nozaki-Hiyama-Kishi reactions
 Papers by Albert Einstein
 Boiling point of 79-09-4
 Where can I find the regulation information on sulfur dioxide

Settings

검색 결과 내 필터를 사용자의 편리에 맞게 조정하실 수 있습니다.

User Name 사용자 설정

Mode Preference 연구 중심 검색 모드 특허 중심 검색 모드

필요한 필터 모두 선택 후 한 번에 Apply 기능 적용

필터 상하 이동 가능

사용하지 않는 필터 오른쪽으로 이동하여 숨기기

CAS preferred 이름 대신 Index name 디스플레이

6개 까지 선택 가능

검색결과 별 필터 변경

검색결과에서 보여질 물질의 Key Physical Properties 선택

문헌 상세 페이지 내 물질의 구조 디스플레이

선택하는 판매처 정보 선택



고급 검색

물질명, CAS RN, 특허번호 등 검색어 입력

Drop down으로 검색 필드 선택

화학 구조식 검색

물질 검색

문헌 검색

검색 필드 우선 순위 변경

연산자 변경 AND/OR/NOT

검색 필드 추가

Advanced Search Tips 검색 필드는 50개까지 사용 가능합니다.

논리 연산자(AND, OR, NOT)를 통해 정확한 텍스트 검색어를 정의할 수 있습니다.

연산자는 **OR, AND, NOT** 순서로 처리됩니다.

동어의 등의 논리적 표현을 그룹화하기 위해 괄호를 사용하세요. (예: (flavor or odor) and menthol)

와일드 카드(*, ?)를 사용하면 보다 포괄적이고 정밀한 검색이 가능합니다.

문헌과 물질의 이름 검색에서 사용할 수 있습니다.

*은 알파벳 0개 부터 무제한으로 확장될 수 있으며, ? 는 0개 또는 1개를 대신합니다. (예: immunoglobulin*conjugate*, benzonorbornen?)

큰 따옴표(“”) 안에 있는 용어는 구문으로 검색됩니다.

Substance Search

물질의 명칭, 동의어, CAS Registry Number, 문헌 식별 번호 등 다양한 표기 방법으로 검색할 수 있습니다.

Streptomycin 레코드 검색

CAS Registry number 식별자로 Streptomycin 검색

세가지 검색: Streptomycin, Streptomycin sulfate, and Sulfate

Sulfoximin을 포함한 레코드 검색

특허 내 색인된 모든 물질 검색 (예: WO2019234160)

물성 정보로 검색하여 물질 후보군을 확인할 수 있습니다.

측정/예측 값을 범위로 검색 (예: 끓는점 80-120 °C)

Drug likeness 에 해당하는 조건(Lipinski, LogD, LogP, pKa 등)을 선정하여 빠르게 스크리닝

화학 구조를 그려 다른 검색 필드와 함께 검색할 수 있습니다.

1

Molecular Formula

CAS Registry Number

Chemical Identifier

Document Identifier

Patent Identifier

Experimental Species

Life Science Data

Biological

Chemical Properties

Density

Electrical

Formula

Magnetic

Mechanical

Optical and Scattering

Structure Related

Thermal

Vapor Pressure (Torr)

Reference Search

키워드, 물질명, 문헌 식별자, 특허 번호/분류, Concept 등을 사용해 문헌을 검색할 수 있습니다.

물질명 또는 치환기가 사용된 문헌 검색

특허의 패밀리 기준 검색 및 확인

DOI, PubMed ID 등 고유 식별자 기반 정확 검색

저자, 발명자, 기관명을 기준으로 관련 문헌을 찾을 수 있습니다.

Pharmacology data, ADME, Toxicity, Biomarker 등의 생명과학 정보로 검색할 수 있습니다.

Authors/Inventors

Publication Name

Organization

Title

Abstract/Keywords

Concept

Substances

Life Science Data

Publication Year

Document Identifier

Patent Identifier

Publisher



CAS Draw editor

CAS Draw를 통해 구조식과 반응쿼리를 설정할 수 있습니다.

CAS Draw Drawing Editor 선택
 구조그리기 창 키우기
 Select Search Type
 검색 종류 선택하기
 Substances References Reactions Suppliers Patent Markush All
 구조 업로드/다운로드
 키보드 단축기 확인하기
 예: 헤테로 원자 쉽게 그리기
 Registry Number, SMILES 또는 InChI를 통해 구조 그리기
 Enter a Systematic Name, CAS Registry Number
 Molecular Formula:
 Zoom: 100%
 Cancel OK

올가미 도구 | 선택 도구
 Atom과 Bond 그리기 | 지우개
 주기율표에서 원자 선택하기 | Shortcuts
 구조식에 Variables 선택 | 구조식에 R-Group 생성
 Attachment 설정하기 | Template에 그려진 구조 선택 및 구조 지정하기
 Charge 설정
 반복단위 설정하기 | Carbon 체인 그리기
 링 구조의 여러 위치에 치환체 결합 표시 | 반응 내 역할 선택
 원자 매핑 | Ring fusion 방지 반응 역할 지정
 H atom을 제외한 치환기 차단
 구조식 회전
 구조식 Flip
 끊어지거나 형성될 본드 지정 | 반응물 및 생성물 지정

Hydrogen Deuterium Tritium
 그린 구조식 그대로 E/Z 이중결합 설정
 Unspecified 본드
 3-15-Sided Ring 그리기



ChemDoodle®

CAS Draw editor 외에도 ChemDoodle을 사용하여 원하는 구조식을 그릴 수 있습니다. 특히 ChemDoodle은 태블릿 및 모바일 기기로 검색할 때 유용합니다.

The screenshot shows the ChemDoodle Drawing Editor interface. At the top, there is a title bar with 'ChemDoodle' and 'Drawing Editor 선택' (Drawing Editor selected). A 'Draw 창 확대' (Expand drawing window) button is in the top right. Below the title bar is a 'Select Search Type' section with tabs for 'Substance', 'References', 'Reaction', 'Patent Markush', and 'All'. A '검색 종류 선택하기' (Select search type) label points to this section. Below the tabs is a toolbar with various icons. Labels point to specific icons: '센터' (Center), 'Zoom 인/아웃' (Zoom in/out), '열기 | 저장' (Open | Save), 'CAS Registry Number로 구조 불러오기' (Load structure by CAS Registry Number), '전체 지우기 | 지우개' (Erase all | Eraser), '구조 선택' (Structure selection), '뒤집기' (Flip), '자르기 | 복사 | 붙여넣기' (Cut | Copy | Paste), and '템플릿 불러오기/저장하기' (Load/Save template). The main drawing area contains a chemical structure of a complex organic molecule. At the bottom right of the drawing area is the 'ChemDoodle®' logo. Below the drawing area are 'Cancel' and 'OK' buttons.

A vertical toolbar with various drawing tools and their corresponding labels in Korean:

- Labeling
- Atom 선택하기 (Select atom)
- 본드 그리기 (Draw bond)
- 링 그리기 (Draw ring)
- Charge 그리기 (Draw charge)
- 체인 그리기 (Draw chain)
- 반복 그룹 표시 (Show repeating group)
- 링 구조의 여러 위치에 치환체 결합 표시 (Show substituent attachment at multiple positions on ring structure)
- Atoms/Chains/rRngs 막기 (Lock atoms/chains/rRngs)
- R 그룹 설정 (Set R group)
- 반응식 설정 (Set reaction)
- 반응식 매핑 (Map reaction)
- 본드 break/form 설정 (Set bond break/form)

검색 결과 보기



SearchSense

입력한 검색 쿼리를 해석하여 가장 관련성이 높은 결과를 즉시 제공합니다.

The screenshot shows the CAS SciFinder search results page for the query "biodegradable materials". The page is divided into "References" and "Substances" sections. Annotations include: "검색 쿼리" (Search Query) pointing to the search bar; "결과 탭 전환" (Result Tab Switch) pointing to the navigation tabs; "문헌 결과 더보기" (View More Literature Results) pointing to the "View All References" button; and "물질 결과 더보기" (View More Substance Results) pointing to the "View All Substances" button. The "References" section shows two results with titles like "Environmentally-safe water-based fire retardant biochemical compositions..." and "Biodegradable polymer composition with enhanced room temperature decomposition rate...". The "Substances" section shows a result for "2408284-87-5 Unspecified | EBP 1504".

Search History

완료된 검색은 Search History 페이지에 자동 기록됩니다.

검색화면 하단에서 Recent Search History나, 상단 Menu 아이콘 → History에서 확인할 수 있습니다.
검색 기록 건수는 제한이 없습니다.

The screenshot shows the mobile app menu with the "History" icon highlighted by a red circle and labeled "1". Below it, the text "검색 기록" (Search History) is written.

The screenshot shows the "History" page with a list of "Recent Search History" items. The first item is dated "March 6, 2026" and includes a search for "alzheimer disease biomarker". The second item is for "Suzuki coupling catalysts". Annotations include: "최근 검색 목록" (Recent Search List) pointing to the list; "검색 기록 더보기" (View More Search History) pointing to the "View All Search History" button; and "2" indicating the number of items shown.

The screenshot shows a search results page with various filters and search history items. Annotations include: "결과별 검색결과" (Search Results by Result Type) pointing to the "Result Type" filter; "검색 기간 선택" (Search Date Selection) pointing to the date range filter; "검색 기록 지우기" (Clear Search History) pointing to the trash icon; and "재검색 실행" (Execute Re-search) pointing to the "Re-search" button for a specific result.

검색 결과 보기 - 문헌



Reference Search Results 문헌-물질-반응까지 연결된 정보의 흐름을 따라 탐색합니다.

시각화된 그래프 및 필터로 연도별 트렌드, Concept, 저자, 기관 등의 상세 정보를 빠르고 쉽게 파악할 수 있습니다.

1 쿼리 해석 변경

Query Interpretation

How we're searching your query
recent and biomarkers and alzheimer's disease

We've modified your query.

Search Original Query

AI 기반 검색에서 키워드 검색으로 변경

Try using [Advanced Search](#) to build boolean queries.
Learn more about how our reference search has changed.

2 검색 결과 문헌에 색인된 물질, 반응식, 인용 정보 불러오기

How are these results different? [Learn more.](#)

- Substances
- Reactions
- Citing

Knowledge Graph - 검색된 문헌간의 상관관계를 시각화하는 툴

1 Query Interpretation

CAS Newton **View** All Substances Reactions **References** Suppliers Patent Markush

4,636 Results Sort: Relevance View: Partial Abstract

2 View Related Results

결과 재정렬 결과 표시 방식 변경

Alerts/Save 다운로드 결과 합치기

Analyze Results 결과 분석 시각화

AI 기반 결과 요약

Based on the search results, here's a summary of key findings related to recent and biomarkers and alzheimer's disease:

Recent advancements in Alzheimer's disease (AD) research have led to the development of various biomarkers and diagnostic tools. Biomarkers such as amyloid-beta (Aβ), tau protein, and neurofibrillary tangles play a crucial role in the progression of AD. Recent studies have explored the...

View All

1

Recent findings in Alzheimer disease and nutrition focusing on epigenetics
By Athanopoulos, Dimitrios Karagiannis, George Teotaki, Magda Advances in Nutrition (2016), 7(3), 917-927 | Language: English, Database: C/plus and MEDLINE

A review. **Alzheimer disease** (AD) is a chronic neurodegenerative **disease** with no effective cure so far. The current review focuses on the epigenetic mechanisms of AD and how nutrition can influence the course of this **disease** through regulation of gene expression, according to the latest scientific findings. The search strategy was the use of scientific databases such as PubMed and Scopus in order to find relative research or review articles published in the years 2012-2015. By showing the latest data of...

색인된 물질 확인 색인된 인용문헌 확인 제목 선택하여 문헌 정보 확인

2

Recent advances in small molecular near-infrared fluorescence probes for a targeted diagnosis of the Alzheimer disease
By Liu, Yue, Chuang, Gangping, Wang, Jingping, Huang, Haiyan, Li, Rui Zhang, Wu, Chaojun, Deng, Yuanfei, Hu, Genmin, Guo, Bing Analysis (Cambridge, United Kingdom) (2022), 147(21), 4701-4723 | Language: English, Database: C/plus and MEDLINE

A review. Nowadays, it is still quite challenging to achieve an early diagnosis of the **Alzheimer disease** (AD) in clinics. The burgeoning near-IR fluorescence (NIRF) imaging fulfills the requirements for a precise diagnosis with good sensibility and a high signal-to-background ratio and offers opportunities for the... The pathogenesis of AD is quite complex, there is an ongoing exploration of target AD **biomarkers** (e.g., amyloid β (Aβ) plaques, neurofibrillary (NF) tangles, synaptic dysfunction, and metabolism).

저널 전문 액세스

View More

3

Recent Progress in the Pharmacotherapy of Alzheimer's Disease
By Khoury, Rita Patel, Kadir, Gold, Jake, Hints, Stephanie, Grossberg, George I. Drugs & Aging (2017), 34(11), 611-626 | Language: English, Database: C/plus and MEDLINE

A review. **Alzheimer's disease** is the most common major neurocognitive disorder with substantial

결과 구제화를 위한 필터 선택

Filter Results

Analyze Results

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

Document Type

- Journal (5,539)
- Patent (1)
- Review (2,934)
- Biography (1)
- Clinical Trial (50)

View All

Publication Year

Language

Flags

- Is Open Access (1,503)
- Has DOI (5,280)
- Has Claims (5)
- Has PatentPak (6)
- Has Related Substances (2,187)
- Has Related Reactions (15)

Patent Office

Patent Status

- Alive (5)
- Transitional (4)
- Dead (5)

Classification Code

Available at My Institution

Author/Inventor

Publications over Time

Patent Offices



Preparation of sulfonylhydrazide derivatives as anticancer agents

Assignee: King Saud University

Novel sulfonylhydrazide derivatives, a method of synthesizing said compounds, a pharmaceutical composition comprising said compounds and a suitable carrier, and a method of using the compounds. The sulfonylhydrazide derivative compounds, identified as TXA₂ inhibitors, are useful as anticancer and/or antitumor agents.

인용맵 보기

관련 정보 바로가기

- Claims
- Classifications
- CAS Concepts
- CAS Concepts
- Markush Structures
- Substances
- Reactions
- Pharmacological Data
- Cited Documents

대표 도면, 그래프, 구조식 등

Log Concentration (nM)	% Inhibition
-1	0
0	25
1	55
2	80
3	85

유사 문헌 더보기

Keywords: sulfonylhydrazide, preparation anticancer

문헌 서지 정보

Patent Number	Publication Date	Application Number	Application Date	Assignee
US12234265 B1	2025-02-25	US2024-1967193S	2024-05-22	King Saud University, Saudi Arabia

Source: United States
Database Information: APL 2025/038522
Language: English

유사 문헌 모두보기

유사 문헌 빠르게 넘겨보기

마쿠시구조 상세보기

기술 키워드 상세보기

물질 정보 상세보기

반응식 상세보기

CAS 과학자들에 의해 색인 및 추가된 문헌 내 주제, 포مول레이션, 물질 및 인용문헌

검색 결과 보기 - 물질



Substance Search Results 물질-반응-판매처까지 연결된 정보의 흐름을 따라 탐색합니다.

1 구조식 기반 검색 시 구조 매치 별 필터 가능

결과 구조화를 위한 필터 선택

물질 상세정보
Life Science 정보
반응식 확인
합성법 확인
역합성 플래너
색인된 인용문헌
물질 판매처
CAS BioFinder로 이동 (개별구독)



Substance detail

CAS Registry Number를 클릭하여 구조, 분자식, 물성 및 추가 데이터가 포함된 물질 상세 정보가 표시됩니다.

CAS Registry Number: 6493-05-6

8,397 433 54 View in CAS BioFinder

Download Print

분자식

GHS 경고표지

C₁₃H₁₈N₄O₃

1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-1-(5-oxohexyl)- (RCL ACI)

물질명

Patents Containing Substance in Claims

Method of treating one or more aphthous ulcers in an individual using fibroblasts and fibroblasts organoids
 Patent Number: WO202010870
 Publication Date: 2020-01-08

Composition for the care of hair and/or scalp
 Patent Number: FR1763896
 Publication Date: 2020-01-02

Method of treating localised scleroderma of type of sclerotic atrophic lichen
 Patent Number: RU27852432
 Publication Date: 2020-12-23

[View All Patents](#)

Properties	Value	Condition
Molecular Weight	278.31	-
Melting Point (Experimental)	105 °C	-
Boiling Point (Predicted)	531.314; 55.00 °C	Press: 750.00 Torr
Density (Experimental)	1.3 g/cm ³	-
pKa (Experimental)	0.28	-

주요 물성

Other Names and Identifiers

Canonical SMILES
 O=C1C2=CN=CN2C(=O)N1C(C)CCCC(=O)OCC

INChI
 INChI=1=C13H18N4O3=1-6186-4-5-T-15.1217810-1114-8-15102116315172008H4-7H2.1-3H3

INChI Key
 #HFKZ2ZUJWMEJLHFFA0YSA-N

31 Other Names for this Substance

- 3,7-Dihydro-3,7-dimethyl-1-(5-oxohexyl)-1H-purine-2,6-dione (ACI)
- Theobromine, 1-(5-oxohexyl)- (7O, 8C)
- 1-(5-Oxohexyl)-3,7-dimethylxanthine
- 1-(5-Oxohexyl)theobromine
- 3,7-Dimethyl-1-(5-oxo-hexyl)-3,7-dihydro-purine-2,6-dione
- 3,7-Dimethyl-1-(5-oxohexyl)-1H,3H-purin-2,6-dione
- 3,7-Dimethyl-1-(5-oxohexyl)-1H-purine-2,6(1H,7H)-dione
- 3,7-Dimethyl-1-(5-oxohexyl)purine-2,6-dione
- 3,7-Dimethyl-1-(5-oxohexyl)xanthine

다양한 명칭: 문헌에서 추출되며, 개발코드 뿐 아니라 체계적이고 다양한 상표명으로 구성

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Pharmacological Data
- ADME
- Toxicity
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- GHS Hazard Statements
- Additional Details

실험 물성
 실험 스펙트럼
 약리학적 데이터
 흡수, 분포, 대사, 배설
 독성
 예측 물성
 생물학적 활성 지표
 타겟 지표
 규제 정보
 GHS 위험 문구
 추가 세부 정보

Expand All | Collapse All

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Reaction searches 반응식 검색어로는 물질명, CAS Registry Numbers, CAS Reaction Number, 문서 식별자 (DOI) 또는 구조식이 가능합니다.

- 지정된 반응물의 역할과 Functional Groups, 두개 이상의 검색어 (불 연산자 포함) 및 반응 관련 문구로 검색 가능합니다.
- Scheme으로 그룹화 된 경우에 한해서, 정렬 순서는 검색 관련도, 등록일, 수율, 스텝 수 순서로 정렬할 수 있습니다.
- Scheme 내 반응식들은 수율 순서대로 정렬됩니다.

검색 예시

- *Camphorsulfonic acid* catalyzed conversion of *3,4-Dihydro-2H-pyran* to *224315462* in *water*
- *Preparation of spiro lactone from 13934-61-7*
- 10.1021/acs.orglett.7b03668 and 2170309-48-3

Results Filters

다양한 필터를 활용하여 관련된 반응식을 빠르게 찾으실 수 있습니다.

- Non-Participating Functional Groups: 반응에 참여하지 않는 치환기
- Commercial Availability: Starting Materials 또는 Products가 구매 가능한 물질인 반응식
- Reaction Notes: 특정 환경에서 진행한 반응정보
- Source References: 반응식 출처



Reaction Details

용매, 촉매, 반응물, 조건을 포함한 세부정보, 문헌, 그리고 Supplement에서 추출한 실험 프로토콜을 나타냅니다.

Reaction Overview

Steps: 2 Yield: -

JOURNAL

Short and efficient process for the synthesis of trans-4-aminocyclohexanecarboxylic acid derivatives

By: Patil, Pankaj S.; et al.
View All

Organic Process Research & Development (2009) 13(6), 1141-1144

[View Source](#) [Full Text](#)

Company/Organization
API R & D Centre
Emcure Pharmaceuticals Ltd.
Pune 411057
India

스텝별 반응 조건 정보

Suppliers (10)

Suppliers (140)

Suppliers (3)

Suppliers (97)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Triethylamine	-	Methanol	rt, 25 - 30 °C, 3 - 4 h, 25 - 30 °C

CAS Reaction Number: 31-366-CAS-6730116

상세 절차를 포함한 실험 프로토콜 보기

Experimental Protocols

Synthetic Methods Experimental Procedure

Products [1-Methylethyl trans-4-\[\[\[1,1-dimethylethoxy\]carbonyl\]amino\]cyclohexanecarboxylate](#), Yield: 97%

Reactants [Di-tert-butyl dicarbonate](#)
[1-Methylethyl trans-4-aminocyclohexanecarboxylate](#)

Reagents [Triethylamine](#)

Solvents [Methanol](#)

Procedure

1. Dissolve isopropyl trans-4-aminocyclohexanecarboxylate (5.40 mol) in methanol (80 L) at ambient temperature.
2. Add triethylamine (7 kg, 7.01 mol) dropwise to the reaction mixture at 25-30 °C under stirring.
3. Add BOC anhydride (11.78 kg, 5.40 mol) to the reaction mixture in methanol (20 L) at 25-30 °C under stirring at 25-30 °C.
4. Stir the reaction mass for 3-4 hours.
5. After completion of the reaction (monitored by TLC), remove methanol under vacuum completely.
6. Add 3M water (40 L) to the reaction mixture.
7. Extract the reaction mixture with dichloromethane (2 x 25 L).
8. Dry the combined dichloromethane layer over sodium sulfate.
9. Concentrate the combined dichloromethane layer under reduced pressure at 40-45°C.
10. Purify the sample by column chromatography.

Transformation Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarbonates

Scale milligram

Characterization Data

1-Methylethyl trans-4-[[[1,1-dimethylethoxy]carbonyl]amino]cyclohexanecarboxylate

Proton NMR Spectrum	400 MHz, CDCl ₃ δ = 1.13-1.14 (d, 6H), 1.36 (s, 9H), 1.76-1.82 (m, 4H), 2.12 (m, 1H), 3.16 (m, 1H), 4.82-4.88 (sep, 1H), 6.76 (d, 1H).
Carbon-13 NMR	100 MHz, CDCl ₃ δ = 21.65, 27.27, 27.65, 28.29, 32.58, 42.49, 48.84, 67.25, 78.95, 135.05, 174.84.
Elemental Analysis	For C ₁₅ H ₂₇ NO ₂ : Calcd C, 63.13; H, 9.54; N, 4.91. Found C, 63.01; H, 9.51; N, 4.90.
Mass Spectrum	MS Cl calcd for C ₁₅ H ₂₇ NO ₂ (M + H) 286.39, found (M + H): 286.39. White solid, mp: 86-87 °C.
State	white solid.

CAS Method Number 3-366-CAS-6730116

대체 반응 조건 보기

Alternative Steps (1)

원문에서의 실험방법 확인하기

반응 결과 분석 데이터

주요 반응식 명칭

Transformations
1. Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarbonates



Suppliers Searching

물질명, 화학 구조식 또는 기타 식별자를 통해 판매처 검색을 하여 카탈로그에 직접 연결이 가능합니다.
자연어 검색을 통해 판매처와 추정 가격을 확인할 수 있습니다.

Hydrogen Peroxide
58-08-2

How much is hydrogen peroxide?
Who sells caffeine?

Results for "how much is hydrogen peroxide?"

CAS Newton **NW** All Substances Reactions References Suppliers Patent Markush

7722-84-1
Hydrogen peroxide

Estimated Commercial Pricing
\$6.37 USD/kg

Supplier price is the average of Hydrogen peroxide
[Learn more](#)

Suppliers
Showing 3 of 123 Suppliers [View All Suppliers](#)

	Thermo Fisher Scientific Product List 2025-04-08	7722-84-1 Hydrogen peroxide	Order From Supplier \$ 25 ml, USD 55.90
	Thermo Fisher Scientific Product List 2025-04-08	7722-84-1 Hydrogen peroxide	Order From Supplier \$ 25 ml, USD 48.90
	Aladdin Scientific Product Listing 2026-01-12	7722-84-1 Hydrogen peroxide solution	Order From Supplier \$ 100 ml, USD 85.90

정렬 방식 판매처 우선순위

상세정보로 이동

Sort: Price: High to Low [Sort](#)

- Relevance
- Price: Low to High
- Price: High to Low
- Supplier: A to Z
- Supplier: Z to A
- Ships Within
- Purity

선호 판매처만 보기

Supplier	Substance	Purity	Quantity Information	Availability	Ordering
Thermo Fisher Scientific Product List	7722-84-1 Hydrogen peroxide	>90%	25 ml, USD 55.90	Maintained in stock Ships within 1 week United States	Order From Supplier \$ Order Number:
Thermo Fisher Scientific Product List	7722-84-1 Hydrogen peroxide		25 ml, USD 48.90	Maintained in stock Ships within 1 week United States	Order From Supplier \$ Order Number: 42600258
Aladdin Scientific Product Listing	7722-84-1 Hydrogen peroxide solution		100 ml, USD 85.90	Maintained in stock Ships within 1 week United States	Order From Supplier \$ Order Number: H755825

TCI Research Chemicals (KRW)

Supplier Contact Information

주소: http://www.tci.com/kr/...
Order: 010-8000-2400
Email: order@tci.com/kr
Phone: 82-2066-2400
Fax: 82-2066-2400

연락처 정보

선호 유무 선택

주문 링크

카탈로그 세부정보

Chemical Name: Hydrogen Peroxide (20% in Water)
Order Number: H75582
Quantity Information: 250 ml, 4.5oz (2000.00)
Stock Status: Maintained in stock
Ships Within: 1 Week
Pricing Information (USD 48.90): \$ 206.250

HO—OH



CAS Roles

Roles는 물질에 연결되며 문헌 내 특정 역할과 연관된 문헌을 찾을 수 있습니다.

- Super roles는 광범위한 범주이며, 관련된 모든 특정 역할로 구성됩니다. 예로는 Analytical Study, Preparation, Occurrence 등이 있습니다.
- Specific roles는 상세한 범주이며, 분석연구에서 분석물질 (Analyte)로 사용하거나 천연 추출물 (Natural Product Occurrence)와 같은 내용을 찾아볼 수 있습니다.

Roles in substance results

물질 검색에서의 **Role** 필터는 문헌의 물질과 연결된 역할 종류를 나타냅니다.

Roles in reference results

Role 필터는 검색한 물질이 문헌 내에 색인되어 있는 경우에 나타납니다. 물질명이나 구조 그리기를 통해 검색 후 관련 문헌 리스트를 볼 수 있습니다.

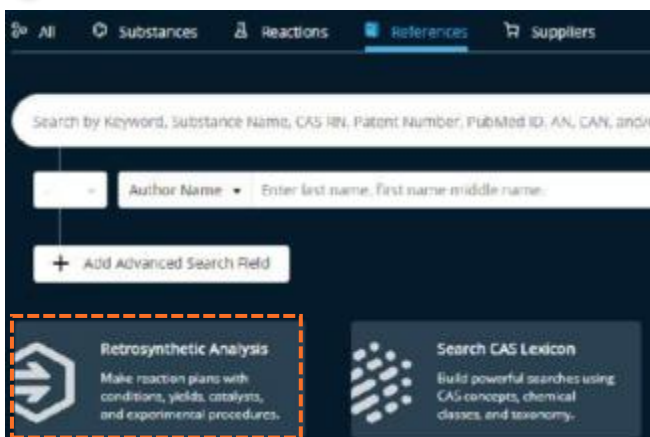
예시: 해양 오염에 관심이 많은데, 폴리프로필렌이 구체적 오염 물질로 기술된 문헌을 어떻게 찾을 수 있을까요?

폴리프로필렌을 검색하면 많은 수의 문헌이 나타납니다. Substance Role 필터에는 폴리프로필렌에 적용되는 모든 역할이 표시됩니다. 그 중 **Pollutant**는 폴리프로필렌을 오염 물질로 표기 및 설명한 1,657개의 문헌이 있음을 나타냅니다.



Launch Plan Generation SciFinder Retrosynthesis Planner를 시작하는 두가지 방법

1 Retrosynthesis 탭을 클릭하여 시작



2 물질 구조의 플라이아웃 창을 열고 생성 시작



Plan Options

플랜 옵션을 선택하여 아래와 같은 사항을 설정할 수 있습니다.

- Protect bonds를 통한 전체 합성 경로 설정
 - 첫번째 Disconnection 설정
 - Starting material의 비용 한도 설정
 - 유의미한 대안으로 플랜 설정
- 예: poly- or heterocyclic molecules

Predicted Reaction Rules 예측의 기반이 되는 검증된 규칙

Common Rule에는 실험실에서 자주 사용되는 반응 유형이 포함되며, 많은 문헌 예제를 포함한 강력한 반응 유형을 볼 수 있습니다.

Uncommon, Rare Rule을 통해서는 잠재적으로 더 새로운 합성법을 도출해낼 수 있습니다.

역합성 플래너 (Retrosynthesis)



Open Plan

Experimental Plan은 몇 초 안에 사용할 수 있으며, Predictive Retrosynthesis Plan (예측 역합성 플랜)은 조금 더 오래 걸릴 수 있습니다.

Retrosynthesis Plan for drawn structure

제외시킨 물질/반응식 확인

다운로드

플랜 정보

Predictive step 온/오프 스위치

플랜 스텝 상세보기

물질 정보 확인하기

파란색 실선은 Experimental step (실험 스텝)을 뜻함. 문헌에 보고된 스텝

녹색 점선은 Predictive step (예측 스텝)을 뜻함

물질 판매처 보기

Alternative Steps 다른 대안을 선택하여 플랜을 재구성 할 수 있습니다.

- 모든 실험 및 예측된 disconnection에 대한 개요를 제공하며, 증거로 사용된 반응식은 반응식 결과세트로 표시됩니다.
- 증거로 사용된 반응식은, ① Plan Scheme 또는 ② Step Overview, ③ Alternative reaction scheme에서 찾아보실 수 있습니다.

View all alternatives (6)

View evidence (3,517)

Exclude this step

D의 disconnection 증거 반응식(Predictive)

Step	Evidence
Maximum Yield: 86%	Catalytic: Palladium
Evidence (1)	Solvents: Ethanol; 12 h, 60 °C
Alternative steps (17)	View All
C → F + G	1.1 Reagents: Pyridine; 0 °C; overnight
Maximum Yield: 66%	
Evidence (7)	
Alternative steps (24)	
D → H	1.1 Reagents: N-Bromosuccinimide
Average Yield: 72%	Solvents: Dimethylformamide; 0 °C
Evidence (3,517)	
Alternative steps (6)	

대안 선택 - 계획 재구성

Reactions from Retrosynthesis Plan Evidence



Patent Markush Search

CAS에서 구축한 Markush 구조 전문 데이터베이스인 MARPAT으로 화합물군을 체계적으로 탐색·검증합니다.

Patent Markush search for drawn structure

Markush Search Results

Markush 구조 그리기

구조 매칭 설정

필터 옵션 설정

특허 상세 보기

Patent Markush 2

Markush 결과 상세 보기

특허 상세 보기

Markush 구조의 위치

PatentPak®

특허 워크플로 솔루션으로, 전체 텍스트 특허를 신속·정확하게 검색하고, 관련 화학물질 파악 시간을 줄일 수 있습니다.

- **PDF:** 특허 전문 PDF; 문서 내 텍스트 검색 가능
- **PDF+:** 주요 물질이 마크업 된 특허 전문 PDF. 문서 내 텍스트 검색 가능
- **PatentPak Viewer:** 주요 물질의 마크업이 연결된 특허 PDF. 아래 참조:

PDF 다운로드 화학 주석이 포함된 PDF 다운로드

CAS PatentPak

특허 내 해당 물질의 위치 표시

특허 물질 위치 링크

연관 정보로의 연결

특허 내 주요 물질이 색인됨



Prior Art Analysis

CAS 인덱싱 기술과 AI를 활용하여 해당 특허의 선행 기술을 자동 분석합니다.

- AI 기반 연관성 예측
- 단일 특허 문헌을 기반으로 분석 시작
- CAS Concepts, 인덱싱한 물질, IPC 코드 및 추가적인 텍스트를 종합적으로 분석
- 특허 및 비특허 문헌을 포함하여 해당 특허보다 이전에 알려진 문서를 관련도 순으로 생성

PatentPak Viewer | Get Prior Art Analysis | Full Text

Patent Family

Patent	Language	Class	Options	Publication Date	Application Number	Application Date
WO2004011464	English	A2	PDF PDF+ Viewer	2004-02-05	WO2003-FR2354	2003-07-25
FR2842805	French	A1	PDF	2004-01-30	FR2002-9519	2002-07-25
CA2493402	Undetermined	A1		2004-02-05	CA2003-2493402	2003-07-25

문헌 상세보기에서 선행기술 조사 실행

References: 10:44 AM

Prior Art Analysis (154)
Novel substituted pyrazolo[1,5-a]1,3,5-triazine derivatives and their analogs, pharmaceutical compositions containing them, their use as drugs, particularly as neurotrophic factor production enhancers, and methods for their preparation

View Results | Complete

Search History에서 View Results 클릭

Prior Art Discovery

출원 전 단계에서도 발명/연구 내용만으로 선행 기술을 찾을 수 있습니다.

기존 특허 없이, 발명/연구 내용을 담은 영문 텍스트(≥ 200자)와 CAS Draw 구조(선택), 우선권일을 입력하면, 다중 AI 알고리즘으로 유사한 문헌을 제시합니다.

Prior Art Discovery
AI-enhanced prior art search for patent professionals.

검색 조건 입력

텍스트 입력

우선일 설정

구조식 작성

What is claimed is:
A method of forming a self-assembled monolayer (SAM) on a first surface of a substrate by exposing the substrate to a first precursor, wherein the substrate has at least one feature comprising the first surface and a second surface and wherein the first precursor comprises a heterocyclic carbene; selectively depositing a linear on the second surface by exposing the substrate to a second precursor; and removing the SAM from the second surface by exposing the substrate to a third precursor, wherein the first surface comprises a metal, and the second surface comprises a dielectric material.

Priority Date: 2009-11-10

Add Structure (Optional)

Search

검색 결과

특허

비특허 문헌

Search Details

Your Inputs

Text

What is claimed is:
What is:
Priority Date:
Structure:

Method of forming a metal liner for interconnect structures
Assigned: Applied Materials, Inc.
US20030020481 A1, Publication Date: 2003-01-09 | Priority Date: Unknown

...A self-assembled monolayer (SAM) is formed on the bottom of the gap, and a barrier layer is formed on the SAM before selectively depositing a metal liner on the barrier layer. The SAM is removed after selectively depositing the metal liner on the...

Metal surface blocking molecules for selective deposition
Assigned: Applied Materials, Inc.
WO2002191527 A1, Publication Date: 2002-10-26 | Priority Date: 2002-06-01

Methods for selectively depositing on metallic surfaces and disclosed. Some embodiments of the disclosure utilize a metal-cermyl containing precursor to form a self-assembled monolayer (SAM) on metallic surfaces.



문헌 상세 페이지에서는 약리·ADME·독성 정보를 제공합니다.

- 해당 문헌에 관련 정보가 수록된 경우에 한해 인덱싱되어 표시되므로, 각 문헌의 데이터 특성에 따라 제공되는 범위가 달라질 수 있습니다.

문헌 결과 필터 중 Life Science Data로 필터하여 해당 콘텐츠를 포함한 문헌으로 결과를 좁힐 수 있습니다.

Pharmacological profiles of a highly potent and long-acting angiotensin II receptor antagonist, fimasartan, in rats and dogs after oral administration

In This Reference: Abstract, Citations, Life Science Data, Cited Documents

Abstract: The pharmacological profile of fimasartan, (S)-N-(5-(4-(2-(2-ethylhexafluoroethyl)-5-methyl-2-oxo-1,2,4-triazol-5-yl)phenyl)-4-oxo-1,2,3,4-tetrahydro-1H-benzopyridin-3-yl)propanoic acid, a new non-peptide angiotensin type 1 (AT1) selective angiotensin II receptor antagonist, has been investigated in a variety of *in vitro* and *in vivo* experimental models. In the present study, fimasartan showed dose-dependent and reversible binding to AT1 subtype receptors in membrane fractions of HEK-293 cells with a K_{d} of 3.03 nM and a B_{max} of 66.7 nM. The inhibitory effect of fimasartan on angiotensin II (Ang II)-induced contractions persisted longer after washout than that of losartan or candesartan. In conscious rats, a single dose of fimasartan (0.3, 1, or 3 mg/kg per os up to 3 days) independently antagonized Ang II-induced protein responses. Both orally administered fimasartan and losartan dose dependently decreased mean arterial pressure in fentanyl-anesthetized rats and dogs, and fimasartan administered orally at 1, 3, or 10 mg/kg reduced blood pressure in conscious spontaneously hypertensive rats. Taken together, these findings indicate that fimasartan has potent and sustained binding affinity at the AT1 receptor subunit and reveal the rat, being responsible for the marked lowering of blood pressure in various conscious rats and dogs models after oral administration.

Keywords: angiotensin II receptor antagonist; fimasartan; blood pressure; hypertension; angiotensin type II receptor blocker; blood pressure; fimasartan; hypertension

Publication Information: Journal

Source	Database Information	Company/Organization	Publisher	Language
Biological & Pharmaceutical Bulletin Volume: 43 Issue: 7 Pages: 1041-1047 Journal Article 2017 DOI: 10.1248/bpb.1315-8087	AS: 2018-24791 CAS: 133-10584 PubMed ID: 28574263 CAS and MEDLINE	CasRx Research Institute Weyang Pharm. Co., Ltd. Ansan, Gyeonggi 415-828 Korea, Republic of	Pharmaceutical Society of Japan	English

- 1 Pharmacological Data
- 2 Toxicity
- 3 ADME

1 약리학 데이터

Ligand	Target	Function	Value	Disease	Organism	Assay
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail
134771-45-4	Type 1 angiotensin II receptor	antagonist	1000	hypertension	Rattus norvegicus	view detail

2 ADME(흡수·분포·대사·배설)

Ligand	Target	Function	Parameter	Value	Disease	Organism	Assay
134771-45-4	-	inhibitor	IC50	2.01 µg/mL	disease of cellular proliferation	Human	view detail
134771-45-4	-	inhibitor	IC50	1.282 µg/mL	disease of cellular proliferation	Human	view detail
134771-45-4	-	inhibitor	IC50	1.073 µg/mL	disease of cellular proliferation	Human	view detail
134771-45-4	-	inhibitor	IC50	1.269 µg/mL	disease of cellular proliferation	Human	view detail
134771-45-4	-	inhibitor	IC50	0.767 µg/mL	disease of cellular proliferation	Human	view detail
134771-45-4	-	inhibitor	IC50	1.148 µg/mL	disease of cellular proliferation	Human	view detail
134771-45-4	-	inhibitor	IC50	1.272 µg/mL	disease of cellular proliferation	Human	view detail
134771-45-4	-	inhibitor	IC50	1.081 µg/mL	disease of cellular proliferation	Human	view detail


3 독성정보

Ligand	Target	Function	Parameter	Value	Disease	Organism	Assay
134771-45-4	Angiotensin II receptor	inhibitor	LD50	88.8 µg	-	-	view detail
134771-45-4	Angiotensin II receptor	inhibitor	LD50	3.2 µM	-	-	view detail



Life Sciences 관련 정보는 문헌뿐 아니라 물질 상세 페이지를 통해서도 확인할 수 있습니다. 특정 물질과 연관된 Pharmacological Data, ADME, Toxicity 정보를 확인하세요.

CAS Registry Number: 137862-53-4



Properties

Property	Value	Condition
Molecular Weight	374.52	-
Boiling Point (Experimental)	216-217 °C	-
Boiling Point (Predicted)	284.91245336 °C	Press: 760 (0) Torr
Density (Experimental)	1.286 g/cm ³	-
pKa (Experimental)	3.8 (Carbonic Acid)	-

Patents Containing Substance in Claims

- Pharmaceutical composition containing ligand neuropeptide and hybrid for enhancing telomerase production
Patent Number: WO2008079791
Publication Date: 2008-07-23
- Oral solid dosage forms of nebulant containing pharmaceutically acceptable excipients
Patent Number: WO2008080811
Publication Date: 2008-07-23
- Composition of fixed dose combination of olmesartan and valsartan for antihypertensive activity against marketed formulation
Patent Number: WO2011101402
Publication Date: 2011-03-10

Experimental Properties / Spectra

- Pharmacological Data **1**
- ADME **2**
- Toxicity **3**

1 약리학 데이터

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
β-AR1/β2	inhibitor	Inhibition (IC50)	9.0	Hypertension, congestive heart failure	Human	View Detail	(1) CAS
β-AR1/β2	inhibitor	IC50	9.4 × 10 ⁻⁶ μM	Hypertension, congestive heart failure	Human	View Detail	(2) CAS
Multiple Inhibitor Type: Substrate (inhibitor-substrate assay)	inhibitor	IC50	2.0 × 10 ⁻⁶ μM	Radio-receptor	Human	View Detail	(3) CAS
Multiple Inhibitor Type: Substrate (inhibitor-substrate assay)	inhibitor	IC50	1.9 × 10 ⁻⁶ μM	Radio-receptor	Human	View Detail	(4) CAS
Multiple Inhibitor Type: Substrate (inhibitor-substrate assay)	inhibitor	IC50	2.7 × 10 ⁻⁶ μM	Radio-receptor	Human	View Detail	(5) CAS

Assay Detail 확인하기

Assay Data

Ligand: 137862-53-4

Target: β-AR1 expression (receptor)

Assay Name: Aβ1-receptor expressing HEK cell based assay

Procedure: Aβ1-receptor expressing HEK cell based assay

Assay Context: Aβ1-receptor expressing HEK cell based assay

Condition: 37°C, 5% CO2, DMEM

Parameter: IC50

Value: 2.00E-06

Measurement Method: Spectrophotometry

Ligand Box: Ligand Box

Measurement System: In vitro, Microassays, with 96-well formatting Aβ1-receptor HEK

Notes: The ligand binds to the Aβ1-receptor and activates the Aβ1-receptor. The Aβ1-receptor is a G-protein coupled receptor (GPCR) and is involved in the regulation of various cellular processes. The Aβ1-receptor is a member of the Aβ1-receptor family and is found in the human brain. The Aβ1-receptor is a member of the Aβ1-receptor family and is found in the human brain.

2 ADME(흡수·분포·대사·배설)

Target	Function	Parameter	Value	Disease	Organism	Assay
Cystostatic NS323	inhibitor	IC50	2.8 × 10 ⁻⁶ μM	Cancer, metastatic disease	Human	View Detail
Cystostatic NS323	Substrate	IC50	9.4	Phenothiazine	Human	View Detail
-	Antagonist	IC50	0.28 U/g	-	Human	View Detail (1) CAS
-	Antagonist	IC50	0.28 U/g	-	Human	View Detail (2) CAS
-	Antagonist	IC50	0.22 U/g	-	Human	View Detail (3) CAS
-	Antagonist	IC50	0.22 U/g	-	Human	View Detail (4) CAS
-	Antagonist	IC50	0.22 U/g	-	Human	View Detail (5) CAS
-	Antagonist	IC50	0.22 U/g	-	Human	View Detail (6) CAS
-	Antagonist	IC50	0.22 U/g	-	Human	View Detail (7) CAS
-	Antagonist	IC50	0.22 U/g	-	Human	View Detail (8) CAS
-	Antagonist	IC50	0.22 U/g	-	Human	View Detail (9) CAS
-	Antagonist	IC50	0.22 U/g	-	Human	View Detail (10) CAS

3 독성정보

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
HU-75142	-	Toxicity	10.2 %	Hepatitis C	-	View Detail	(1) CAS
-	-	TDL0	10 mg/kg	-	Rattus norvegicus	View Detail	(2)
-	-	TDL0	6.4 mg/kg	-	Rattus norvegicus	View Detail	(3)
-	Antagonist	LD50	307.5 mg/kg	Hypertension	Rattus norvegicus	View Detail	(4) CAS
-	-	Cytotoxicity	0 %	neurodegenerative disease	Rat	View Detail	(5) CAS
-	-	Cytotoxicity	0 %	neurodegenerative disease	Rat	View Detail	(6) CAS

(1) Galarraga, R. (Proceedings of the National Academy of Sciences of the United States of America (2010), 107(1), 291-296, doi:10.1073/pnas.0911030107, C.A.P. and MEDLINE
 (2) FCLPH: Fundamental & Clinical Pharmacology (Oxford: Blackwell Science, 2007 - volume/year/page/year) 12, 315, 2003
 (3) APHNER: Annals of Pharmacotherapy (Harcourt Whitney Books Co., POB 42696, Cincinnati, OH 45242) 9, 26-1992 - volume/year/page/year: 37, 102, 2003
 (4) Nak, Yung-yun; Bioorganic & Medicinal Chemistry (2012), 20(8), 2743-2761, C.A.P. and MEDLINE
 (5) Akasaka, K. (United States, US20110330611 A1 2011-10-26, C.A.P.)

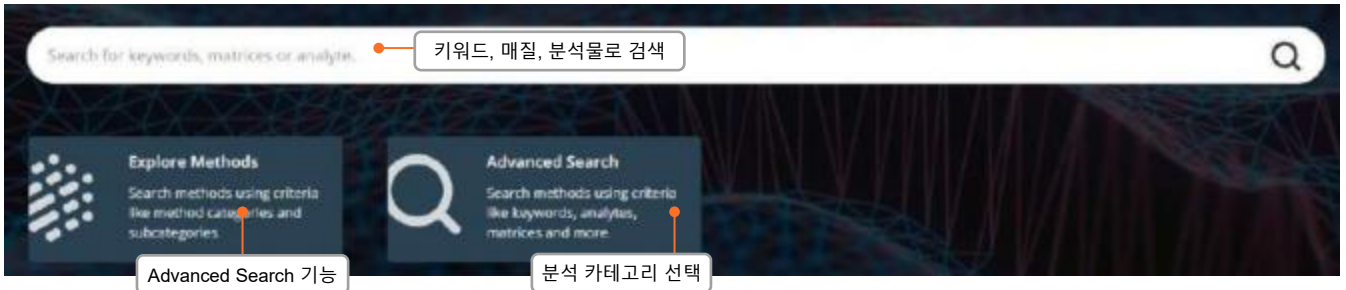




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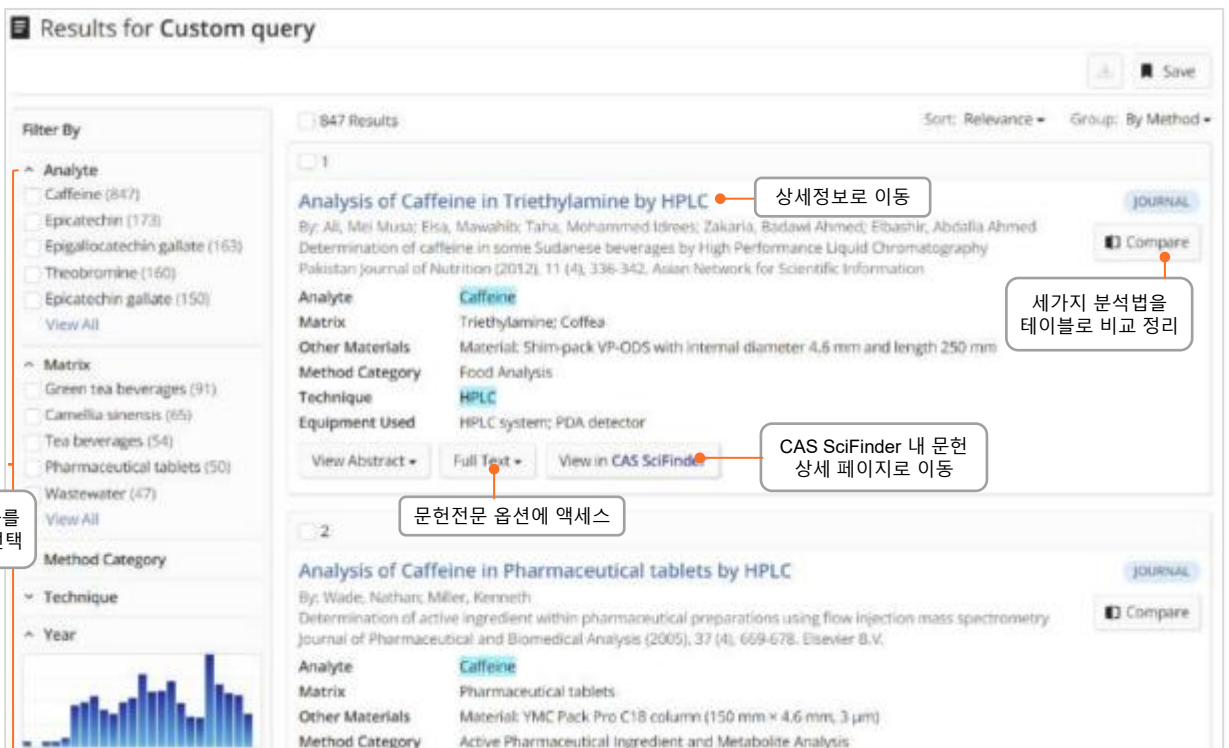
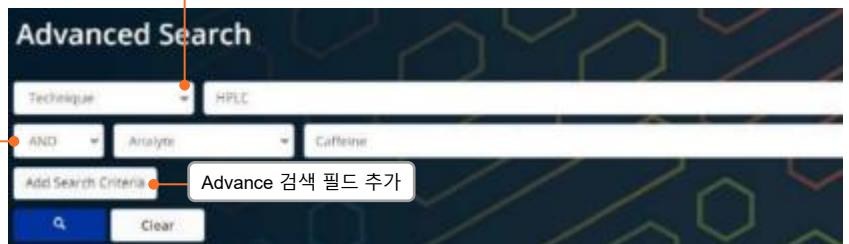
- 실험실에 바로 가져갈 수 있는 단계별 스킴을 제공합니다.
- 집중 영역에는 약리학, HPLC, 식품 분석, 천연 제품 분리 분석 및 수질 분석이 포함됩니다.



Advanced Search

키워드, Analyte, Matrix, Method Category, Technique, CAS Method Number, Publication name 중 선택 후 검색

AND, OR, NOT 중 불연산자 선택





Analytical Methods Details

기기명부터 샘플링, 분석 방법까지 한눈에 검토하실 수 있습니다.

■ Analysis of Dibutyl phthalate in Drinking waters by Solid phase extraction

[PDF, XLS 포맷으로 다운로드](#)
↓
↓
↓

CAS Method Number 분석법 식별번호

1-143-CAS-356206

Method Category 적용 분야

Water / Wastewater / Sludge Analysis

Technique 분석 기법

UV-visible spectroscopy; HPLC; Solid phase extraction

Analyte
Dibutyl phthalate

Matrix
Drinking waters

Material
Nanoparticles Molecularly imprinted polymers Filter (200 nm) Symmetry column (150 ×

Reagent
Ethylene glycol dimethacrylate Methacrylic acid Azobisisobutyronitrile Methanol

Biological Reagent
-

분석에 사용된 Analyte, materials, reagent 등 확인

Equipment Used

High performance liquid chromatograph, LC-2010A, Shimadzu, Kyoto, Japan

Pump, LC-2010A, Shimadzu, Kyoto, Japan

UV detector, Shimadzu, Kyoto, Japan

Conditions

Instrument

column: Symmetry column (150 × 4.6 mm, 5 μm); mobile phase: water/methanol (15:85, v/v); flow rate: 1 mL/min; injection volume: 10 μL

detection wavelength: 224 nm

Source 출처 정보

JOURNAL

Synthesis of surface molecular imprinted polymers based on carboxyl-modified silica nanoparticles with the selective detection of **dibutyl phthalate** from tap water samples

Xu, Wanzhen; Zhang, Xiaoming; Huang, Weihong; Luan, Yu; Yang, Yanfei; Zhu, Maiyong; Yang, Wenming

Applied Surface Science (2017), 426, 1075 - 1083. Elsevier B.V.

CODEN : ASUJSEE | ISSN : 01694332 | DOI : 10.1016/j.apsusc.2017.07.241

View Abstract + Full Text +

Instructions

Preparation of water samples

1. Collect samples of tap water samples for analysis.
2. Filter using a 200 nm filter to remove the insoluble impurities prior to use.

샘플링 방법

Synthesis of carboxyl-modified SiO₂ particles (COOH@SiO₂)

1. Add 12 mL of tetraethylorthosilicate (TEOS) to a mixture of ethanol (200 mL), deionized solution ammonium (12 mL) with mechanical stirring at 30 °C.
2. Continue the reaction for 12 h.
3. Separate the resultant SiO₂ nanoparticles by centrifugation and wash repeatedly with ethyl alcohol and water.
4. Dry in a vacuum oven at 35 °C for 24 h.
5. Add 15 mmol of (3-aminopropyl)triethoxysilane (APTES) to a solution containing *o*s-butenedioic anhydride (15 mmol) and *N,N*-dimethylformamide (DMF, 5 mL).
6. Disperse the resulting product in 100 mL DMF containing 1 g of SiO₂ nanoparticles.
7. Stir the solution for 24 h at 30 °C.
8. Collect the resultant residue by centrifugation and wash frequently with ethyl alcohol and distilled water.
9. Obtain the COOH@SiO₂ particles and dry in a vacuum oven at 30 °C for 12 h.

상세 분석 방법

Synthesis of molecular imprinted polymers @COOH@SiO₂ (MIPs@COOH@SiO₂)

1. Disperse 1 g COOH@SiO₂ particles in 100 mL acetonitrile.
2. Dissolve 1 mmol **dibutyl phthalate** (DBP) and 0.5 mmol methacrylic acid (MAA) into the above system.
3. Shake the mixture at 150 rpm for 1.5 h at 25 °C in a thermostatic shaker for pre-assembly.
4. Add 10 mmol ethylene glycol dimethacrylate (EGDMA) and 20 mg azobisisobutyronitrile (AIBN) and stir the solution at 60 °C for 24 h under violent mechanical condition.
5. Wash the template DBP of the MIPs with methanol/acetic acid (9:1, v/v) several times until no template detection occurs by HPLC at 224 nm.

Solid phase extraction

1. Add 30 mg of MIPs into the tap water sample and keep shaking at 30 °C for 1 h.
2. Centrifuge the solutions and filter.
3. Elute the DBP adsorbed onto MIPs sorbent with 2 mL of methanol/acetic acid (9:1, v/v) for 60 min.
4. Dry the collected eluent under N₂ flow.
5. Reconstitute the residues in 2 mL of distilled water for HPLC analysis.

High performance liquid chromatography-UV spectroscopy (HPLC-UV)

1. Perform the analysis using a Shimadzu LC-2010A HPLC system (Shimadzu, Kyoto, Japan) consisting of two LC-2010A pumps and a UV detector with a changeable wavelength in the range of 190 - 600 nm.
2. Conduct separation on a Waters Symmetry column (150 × 4.6 mm, 5 μm).
3. Use a mixture of water/methanol (HPLC grade, 15:85, v/v) as the mobile phase at a flow rate of 1 mL/min under isocratic conditions.
4. Inject a sample volume of 10 μL.
5. Perform detection at a UV detection wavelength of 224 nm.

검증 데이터

Validation	
Linearity Range	5.0 - 30.0 μmol/L
Limit of Detection	0.05 μmol/L
Accuracy	86.0, 89.0 and 95.3% (recovery) in 0.05, 0.1 and 1.0 mg/L spiked concentrations, respectively

분석에 사용한 기기정보

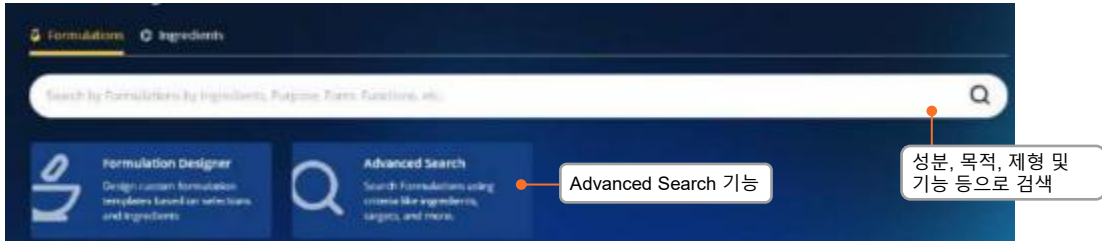


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Formulation 정보를 성분, 공정 및 실험 활동을 포함하여 제제/제형의 세부 사항을 확인할 수 있습니다. CAS Formulus® 를 사용하려면, <https://formulus.cas.org> 에서 로그인 하거나, App switcher를 통해 이동할 수 있습니다.



Search Formulation 제형, 성분, 목적 또는 기능 등의 정보를 입력하여 검색할 수 있습니다.



Formulation Results

산업 분야, 목적, 제형의 상태 및 이동경로 까지 확인하고 필터로 활용 가능합니다.

결과 필터하기

78,209 Results | Sort: Relevance | Group: By Family

Aqueous Hair Color-Altering Composition: Hair Coloring Agent (상세 보기)

Location: Example 1, 2, 3, Table 1, 2, 3-1
 Purpose: Hair dyes
 Target: Hair, Hair dyes
 Physical Form: Solutions

Component 정보

Component	Function	Amount Reported
Group: pulverulent hair bleaching composition	Bleaching agents	1
Ammonium persulfate	Bleaching agents	11.60 wt. %
Carboxylic acids	-	3.9 wt. %
Urea	Keratolytic agents	2.50 wt. %
Sodium stearate	Gelation agents	4.21 wt. %

원문 보기 (선택한 formulation을 add to compare 클릭 후 비교 (3개까지 비교 가능))

Patent
 Thermal control of hair color-altering compositions
 Assignee: L'Oréal
 US11324683
 Language: English
 Patent PDF | View in CAS SciFinder (CAS SciFinder 내 문헌 상세 페이지로 이동)

물질 정보 보기

Additional group components reported

Component	Function	Amount Reported
Group: developer composition	Carriers, mask	1
Tridecem-2 carboxamide MEA	Carriers, mask	0.1-0.3 wt. %
Alcohols, C ₁₀₋₁₈	-	-
Alcohols, C ₁₀₋₁₈ ethoxylated	-	-
Hydrogen peroxide	Oxidizing agents	11.75 wt. %

View Formulation Detail (상세 보기)

10 Similar Formulations - View All (유사한 제형/제제 탐색)



Formulation Details 제형/제제에 관련한 상세한 정보를 빠르게 검토하실 수 있습니다.

- 조성
- 제조 방법
- 유효 선량
- 실험 값

검색 결과 저장
PDF 다운로드
Save

Aqueous Hair Color-Altering Composition: Hair Coloring Agent

Purpose	Target	Delivery Route	Physical Form	Source
Hair dyes	Hair, Hair dyes	-	Solutions	View

Formulation Ingredients Expand All Groups | Collapse All Groups

Component	Function	Amount Reported	Optionality
Group: pulverulent hair bleaching composition	bleaching agents	1	Mandatory
Carboxylic acids	-	3.64 wt. %	Mandatory
Urea	-	2.50 wt. %	Mandatory
Sodium alkylate	-	4.21 wt. %	Mandatory
Potassium persulfate	-	41.60 wt. %	Mandatory
Dioctylmethylsulfoniacetate	-	0.95 wt. %	Mandatory
C.I. Pigment Blue 29	-	0.05 wt. %	Mandatory
Hydrocarbon oils	-	2.00 wt. %	Mandatory
Bases	alkaline agents	11.50 wt. %	Mandatory
Sodium metasilicate (Na ₂ SiO ₃)	-	14.00 wt. %	Mandatory
Sodium silicate	-	5.85 wt. %	Mandatory
Ammonium persulfate	-	11.50 wt. %	Mandatory
Thickening agents	Thickening agents	1.09 wt. %	Mandatory
Surfactants	surfactants	0.80 wt. %	Mandatory
Water	-	0.01 wt. %	Mandatory
Group: developer composition	-	1	Mandatory

More Formulations like this...

Anhydrous Bleaching Compositions Hair Bleaching

Purpose: hair bleaching

Target: hair

Delivery Route: -

Physical Form: anhydrous

Anhydrous Bleaching Compositions Hair Bleaching

Purpose: hair bleaching

Target: hair

Delivery Route: -

Physical Form: anhydrous

Bleaching Compositions Hair Bleaching

Purpose: hair bleaching

Target: human skin

Delivery Route: -

Physical Form: -

Anhydrous Bleaching Compositions Hair Bleaching

Purpose: hair bleaching

Target: human hair

Delivery Route: -

Physical Form: anhydrous

Process

A method for preparing an aqueous hair color-altering composition comprising mixing a pulverulent hair bleaching composition and a developer composition to form an aqueous mixture.

Experimental Activity

Descriptor	Notes	Details
Thermal control assessment	thermal control was measured by conducting a bowl test in which 60 g of the pulverulent hair bleaching composition and 60 g of the 40% developer composition were mixed together in a bowl to prepare hair color-altering compositions, which were allowed to rest in ambient conditions with a temperature probe in mixture within 25 minutes	51.5°C

Source Patent

Thermal control of hair color-altering compositions

Assignee: L'Oréal
 US11324683
 Language: English
 Location: Example 1, 2, 3, Table 1, 2, 3, 1

[Patent PDF](#) [View in CAS SciFinder](#)

제형/제제 기본 정보

각 성분의 기능 및 조성

유사한 제형/제제 바로가기

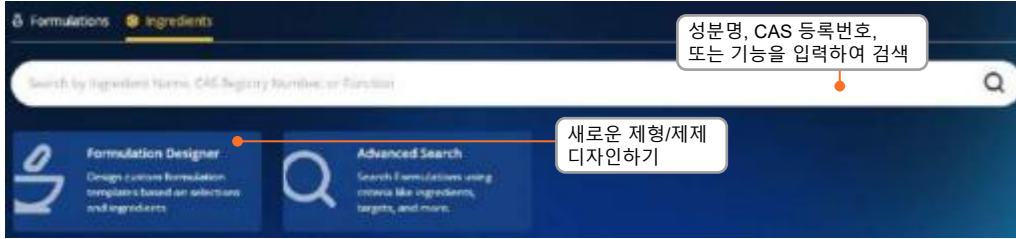
제조 방법

실험 값

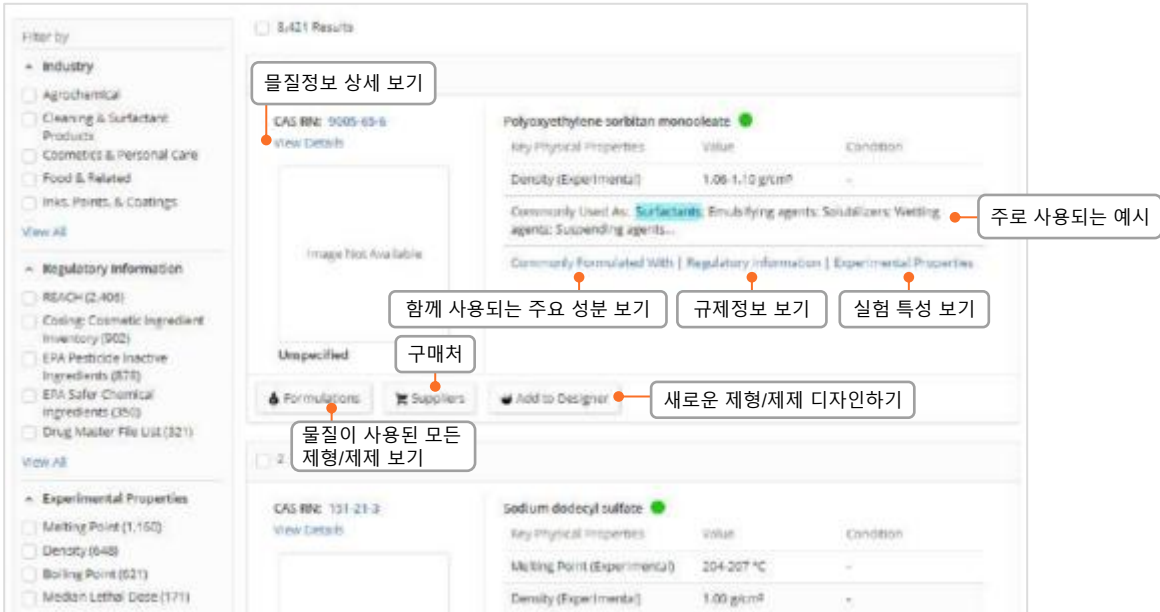
원문 바로가기



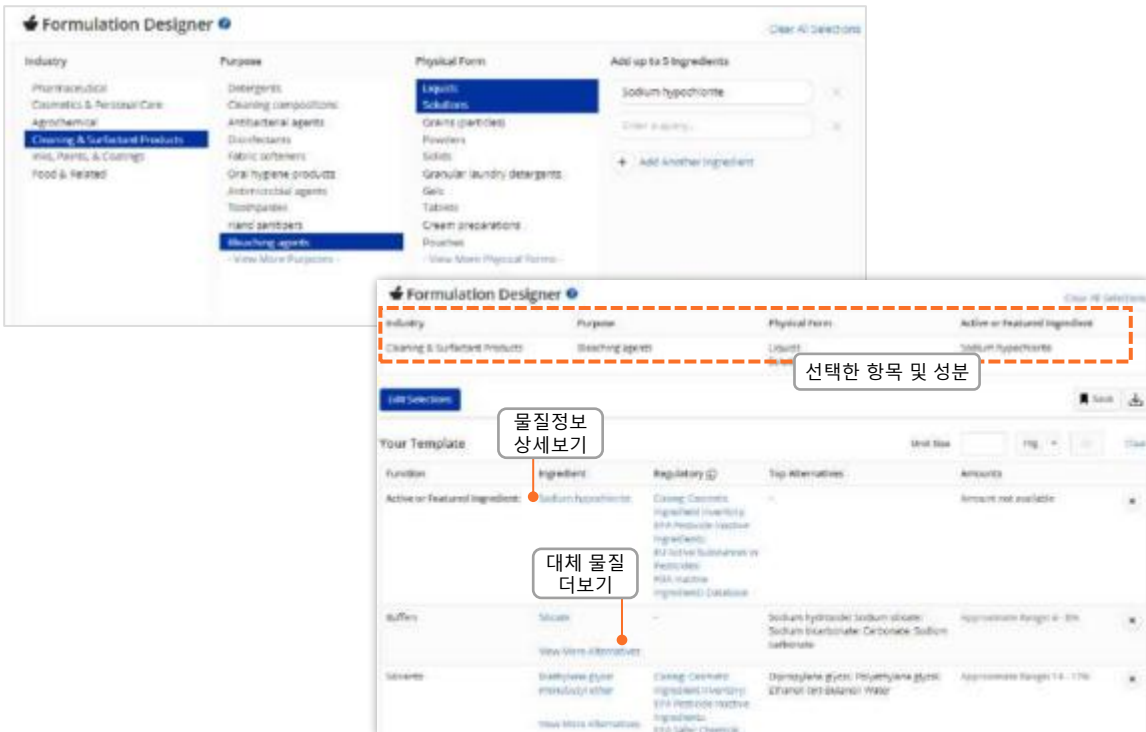
Search ingredients 구성 물질을 검색하여 다양한 formulation을 확인해보세요.



Ingredient Results 성분 물질로부터 새로운 제형/제제의 아이디어를 얻을 수 있습니다.



Formulation Designer 선택 항목과 성분을 기반으로 맞춤형 제형/제제를 디자인합니다.





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- CAS Formulus: <https://formulus.cas.org>

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<https://www.cas.org/resources/events>

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CAS Contacts

CAS Korea Team, korea@acs-i.org

국내 담당자의 도움이 필요하실 때에는 CAS Korea Team으로 문의 주시기 바랍니다.