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Agenda

- Introduction of CAS
- What is SciFinderⁿ?
- Content and Coverage in SciFinderⁿ
- A few online Case studies – General interest
 - Substance searching
 - Reference searching and PatentPak
 - Reaction searching and MethodsNow Synthesis
- CAS Retrosynthesis planner
- Markush structure searching
- Questions and Answers

Chemical Abstract Service

- More than 2,500 scientists, engineers are behind creation of SciFinderⁿ.
- They intellectually analyze published articles, patents and “structure” them with standard concepts/ keywords for easy retrieval.



Value added Indexing



(12) 发明专利申请

(10) 申请公布号 CN 102836446 A

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(71) 申请人 华中科技大学 A61P 35/00(2006.01)

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代理人 曹葆青

(51) Int. Cl.

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A61K 49/22(2006.01)

A61K 9/10(2006.01)

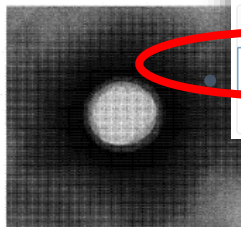
权利要求书 2页 说明书 11页 附图

(54) 发明名称

体内相转变肿瘤靶向纳米泡及其制备方法和用途

(57) 摘要

本发明属于生物医药技术领域,具体为一种体内相转变肿瘤靶向纳米泡及其制备方法和用途。纳米泡以偶联肿瘤靶向因子的聚磷酸酯-聚酯共聚物为包膜材料,可在体内发生液-气相转变的全氟戊烷为泡心填充物质,采用预复乳-中空膜管乳化方法制备。纳米泡进入体内后,液态全氟戊烷在体温下发生液-气相转变,形成含气纳米泡,通过靶向因子与肿瘤细胞的特异性结合,纳米泡富集在肿瘤病灶部位,从而改善肿瘤



Preparation method of in-vivo phase-transition tumor targeting nanobubble and its application

By: Liu, Wei; Xu, Haibo; Chen, Yunchao; Yang, Xiangliang; Cheng, Xin; Li, Huan; Luo, Binhua; Wan, Jiangling; Zhou, Xiaoshun

Abstract: The title nanobubble comprises filling material with perfluoropentane as core, which can have liquid-gas phase transition in vivo, and tumor targeted factor modified biodegradable polyphosphate-polyester copolymer as coating material, and the nanobubble contains polyphosphate-polyester copolymer 1-30%, tumor targeted factor 0.1-10%, liquid perfluoropentane 0.1-5% and pure water. The polyphosphate-polyester copolymer (average mol. weight 2000-60000, polyphosphate:polyester 1:5-5:1) has chem. structure as in patent. The particle size of nanobubble (PDI \leq 0.35) is 30-1000 nm. The polyphosphate is polyethyl alkyl phosphate (C₁-C₁ alkyl) or polypropyl alkyl phosphate (C₁-C₁ alkyl). The polyester is D,L-lactide, poly L-lactide or the like. The tumor targeted factor includes folic acid, lactoferrin or the like. The preparation method consists of dissolving polyphosphate-polyester copolymer in mixture of Et acetate and THF to obtain oil phase 1, using liquid perfluoropentane as oil phase 2, mixing oil phases by high shear(5000-30000 rpm) in ice bath, dripping oil phase into water phase by magnetic stirring in ice bath to obtain O₂/O₁/W, pushing mixture through hollow-membrane tube, pouring mixture into normal saline, stirring at 25°C by magnetic force, removing organic solvent by extraction The hollow-membrane tube is prepared with polyethylene, polypropylene or the like. The MRI contrast agent (0.01-3%) is added into nanobubble. The title nanobubble is used for delivery of anti-cancer drugs, which include paclitaxel, docetaxel or the like.

PATENTPAK PDF Full Text

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
CN102836446	Chinese	A	PDF	2012-12-26	CN2012-10158275	2012-05-21
CN102836446	Chinese	B	PDF	2014-08-27	CN2012-10158275	2012-05-21



Value added Indexing

Abstract

Belonging to the technical field of biomedicine, the invention specifically relates to an in-vivo phase transition tumor targeted nanobubble, its preparation method and application. The nanobubble takes a polyphosphate-polyester copolymer of a coupling tumor targeting factor as a coating material, adopts perfluoropentane able to undergo liquid-gas phase transition in vivo as a bubble core filling material, and is prepared by a pre-multiple emulsion-hollow membrane tube emulsification method. When the nanobubble enters the body, the liquid perfluoropentane undergoes liquid-gas phase transition at body temperature to form a gas-containing nanobubble. By means of the specific combination of a targeting factor and a tumor cell, the nanobubble can cooperate with a tumor cell, thus improving the tumor focus ultrasonic imaging effect. The nanobubble can be used as an MRI contrast agent to improve the tumor focus MRI imaging effect. The nanobubble is loaded with an antitumor drug and used for targeted treatment of tumors, diagnosis-treatment integrated multifunctional imageological nano-contrast agent.

Chinese patent

CN102836446B

China

Download PDF Find Prior Art Similar

Other languages: Chinese

Inventor: 刘卫 徐海波 陈云超 杨祥良 程欣 李欢 罗斌华 万江陵

Preparation method of in-vivo phase-transition tumor targeting nanobubble and its application

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Abstract: The title nanobubble comprises filling material with perfluoropentane as core, which can have liquid-gas phase transition in vivo, and tumor targeted factor modified biodegradable polyphosphate-polyester copolymer as coating material, and the nanobubble contains polyphosphate-polyester copolymer 1-30%, tumor targeted factor 0.1-10%, liquid perfluoropentane 0.1-5% and pure water. The polyphosphate-polyester copolymer (average mol. weight 2000-60000, polyphosphate:polyester 1:5-5:1) has chem. structure as in patent. The particle size of nanobubble (PDI ≤ 0.35) is 30-1000 nm. The polyphosphate is polyethyl alkyl phosphate (C₁-C₁ alkyl) or polypropyl alkyl phosphate (C₁-C₁ alkyl). The polyester is D,L-lactide, poly L-lactide or the like. The tumor targeted factor includes folic acid, lactoferrin or the like. The preparation method consists of dissolving polyphosphate-polyester copolymer in mixture of Et acetate and THF to obtain oil phase 1, using liquid perfluoropentane as oil phase 2, mixing oil phases by high shear(5000-30000 rpm) in ice bath, dripping oil phase into water phase by magnetic stirring in ice bath to obtain O₂/O₁/W, pushing mixture through hollow-membrane tube, pouring mixture into normal saline, stirring at 25°C by magnetic force, removing organic solvent by extraction. The hollow-membrane tube is prepared with polyethylene, polypropylene or the like. The MRI contrast agent (0.01-3%) is added into nanobubble. The title nanobubble is used for delivery of anti-cancer drugs, which include paclitaxel, docetaxel or the like.

PATENTPAK PDF Full Text

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
CN102836446	Chinese	A	PDF	2012-12-26	CN2012-10158275	2012-05-21



Concepts

Antibodies and Immunoglobulins

Role: Biological Use, Unclassified

Antitumor agents

Ceramics

Dissolution

Extraction

Fluoropolymers

Role: Other Use, Unclassified

Imaging agents

Lactoferrins

Role: Reactant

Liver neoplasm

Microstructure

NMR imaging

NMR imaging agents

Particle size

Particle size distribution

Physiological saline solutions

Polycarbonates

Role: Other Use, Unclassified

Polysulfones

Role: Other Use, Unclassified

Stability

Transferrins

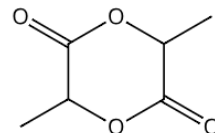
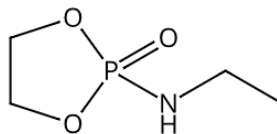
Role: Reactant

Zeta potential

Substances

Substances (33)

1417421-76-1

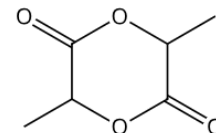
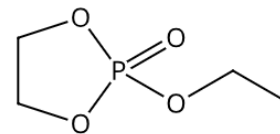


$(C_6H_8O_4 \cdot C_4H_{10}NO_3P)_x$

1,4-Dioxane-2,5-dione, 3,6-dimethyl-, polymer with *N*-ethyl-1,3,2-dioxaphospholane...

Role: Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

326604-67-5



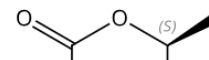
$(C_6H_8O_4 \cdot C_4H_9O_4P)_x$

1,4-Dioxane-2,5-dione, 3,6-dimethyl-, polymer with 2-ethoxy-1,3,2-dioxaphospholane...

Role: Properties, Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

99896-85-2

33135-50-1



Content and coverage

Reference

- >48M references available
- Patents from 63 patent issuing authorities
- 10,000+ Journal Publications
- **PatentPak**

Substances

- >148M substances
- >7.6B Property values
- >1M Markush structures
- Back referencing for substances till 1800

Reactions

- >116M reactions available
- **MethodsNow Synthesis**
- **CAS Retrosynthesis planner**

How to Log in into SciFinder-n

1. Go to <https://www.cas.org/> > Login to > SciFinder-n

The screenshot shows the CAS website interface. At the top right, there is a 'Log In To:' dropdown menu. The dropdown is open, showing a list of products: 'Choose a product', 'Choose a product', 'SciFinderⁿ', 'SciFinder', 'Formulus', 'STNext', 'MethodsNow', and 'NCI Global'. The 'SciFinderⁿ' option is highlighted in blue. The main content area features the CAS logo (A DIVISION OF THE AMERICAN CHEMICAL SOCIETY) and a navigation menu with 'What We Do', 'Products', 'Services', 'Resources', and 'Blog'. A blue banner contains the text: 'CAS has released an open access dataset of chemical compounds with known or potential antiviral activity to support COVID-19 research. Available to download now.' Below this, there are social media icons for Facebook (1.4K), Twitter, LinkedIn, and Email (6.9K). The main heading reads 'Solve Scientific Information Challenges' over a background image of a molecular structure.

Enter your Login credentials



SciFinderⁿ is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.

Log In with your CAS Username

[Learn more](#)

Username

Password

Keep me signed in

Log In

[Forgot Username or Password?](#)

New To SciFinderⁿ? [Register for enterprise or government use](#) OR [request academic access.](#)

By using SciFinderⁿ®, you agree to the [License Agreements and Policies](#)

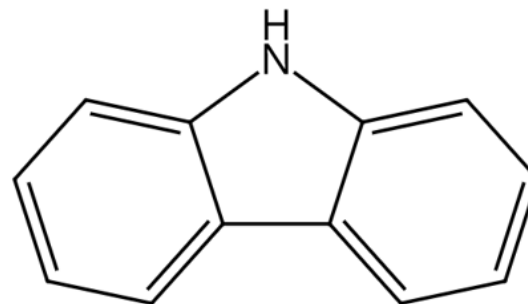
SciFinder-n interface

The screenshot displays the SciFinder-n interface. At the top left is the SciFinder-n logo with the tagline "A CAS SOLUTION". To the right of the logo are three navigation buttons: "Saved" (star icon), "History" (clock icon), and "Account" (person icon). Below the logo is a "Search" section with a vertical list of navigation options: "All", "Substances" (highlighted in purple), "Reactions", "References", and "Suppliers". The main search area contains a text input field with the placeholder "Enter a query...", a "Draw" button with a chemical structure icon, and a search button with a magnifying glass icon. Below the search field, there is a link for "Advanced Search" and a note: "Use Advanced Search for Molecular Formula, Substance Property, or Experimental Spectra".

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- Introduction of CAS
- What is SciFinderⁿ?
- Content and Coverage searchable in SciFinderⁿ
- A few online Case studies – General interest
 - **Substance searching**
 - Reference searching and PatentPak
 - Reaction searching
- CAS Retrosynthesis planner
- Markush structure searching
- Questions and Answers

Substance searching



- Search substance query: **Carbazole**
 1. Search substance by name (Commercial name, IUPAC name or CAS registry number)
 2. Search substance using structure

1. Search substance by name

The screenshot displays the SciFinder-n search page. At the top left is the SciFinder-n logo with the tagline 'A CAS SOLUTION'. On the top right, there are navigation links for 'Saved', 'History', and 'Account'. The main search area is titled 'Search' and features a sidebar with filters: 'All', 'Substances' (highlighted), 'Reactions', 'References', and 'Suppliers'. The search input field contains the text 'carbaz' and is followed by a 'Draw' button and a search icon. A dropdown menu of suggestions is visible below the input field, listing various chemical entities related to 'carbaz'. A purple box highlights the search icon.

Search by Substance Name, CAS RN, Patent Number, etc.

carbaz

- Carbazepine
- Carbazole**
- Carbazotic acid
- Carbazole, 9-vinyl-, homopolymer
- Carbazole, 9-vinyl-, polymer
- Carbazole, 9-vinyl-, polymers
- Carbazamide
- Carbazimidic acid
- Carbazole, 9,9'-(4,4'-biphenylene)di-
- Carbazinc

SciFinder-n provides
autosuggestions for search
query

Search substance by name

The screenshot shows the SciFinder interface. At the top, the search term 'carbazole' is entered. A sidebar on the left lists various filters such as 'Commercial Availability', 'Reaction Role', and 'Reference Role'. The main content area displays 'Substances (1)' with a search result for Carbazole (CAS RN 86-74-8). Below the name, the chemical structure is shown, along with its molecular formula $C_{12}H_9N$. At the bottom of the result, statistics are provided: 17K References, 13K Reactions, and 104 Suppliers.

This panel provides a detailed view of the Carbazole entry. It includes the CAS RN (86-74-8) and the CAS Name (Carbazole). The chemical structure is displayed prominently. A menu on the left offers several actions: 'Substance Detail', 'Reactions (13K)', 'Synthesize (1,217)', 'Create Retrosynthesis Plan', 'References (17K)', and 'Suppliers (104)'. At the bottom, there are controls for 'Edit Structure', 'Reset', and a download icon.

Retrieve all reactions, references, suppliers and create retrosynthesis plan on single click

Substance details

Download, share and export substance details

Substances ▾ carbazole

Substance Detail

References (17K) Reactions (13K) Suppliers (104)

CAS Registry Number
86-74-8

C1=CC=C2C(=C1)C(=CN2)C3=CC=CC=C3

$C_{12}H_9N$
9H-Carbazole

Key Physical Properties	Value	Condition
Molecular Weight	167.21	-
Melting Point (Experimental)	245 °C	-
Boiling Point (Experimental)	355 °C	-
Density (Experimental)	1.10 g/cm ³	Temp: 18 °C
pKa (Predicted)	17.00±0.30	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

- Other Names
- Experimental Properties
- Experimental Spectra
- Predicted Properties
- Predicted Spectra

¹H NMR ¹³C NMR

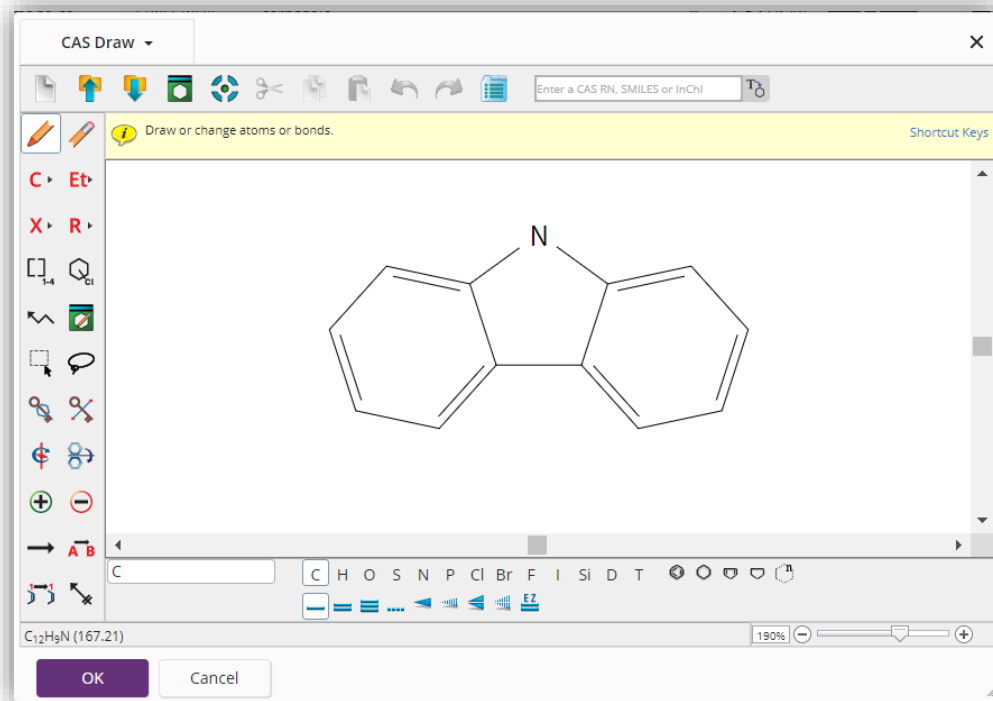
	Source
View Proton NMR Spectrum	(1) ACDNMR

Sources

(1) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V11.01 (© 1994-2020 ACD/Labs)

- Regulatory Information
- Additional Details

2. Search substance using structure



Substance search

SCIFINDERⁿ
A CAS SOLUTION

Substances ▾ Enter a query... Edit ▾ 🔍 ☆ ⌚ 👤

Structure Match

- As Drawn (475)
- Substructure (665K)
- Similarity (47K)

Analyze Structure Precision

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator

Search Within Results

Draw

Draw using current structure

Substances (475) Sort: Relevance ▾ View Partial ▾

References ▾ Reactions ▾ Suppliers ▾

1 86-74-8 C12H9N Carbazole
17K References 13K Reactions 104 Suppliers

2 51555-21-6 (C12H9N)4 Polycarbazole
650 References 50 Reactions 0 Suppliers

3 14541-25-4 C12H9N 9H-Carbazol-9-yl
41 References 1 Reaction 1 Supplier

4 23560-25-0 C12H9N 9H-Carbazole, ion(1-)
30 References 9 Reactions 3 Suppliers

5 53318-00-6 C12H9N 9H-Carbazole, radical ion(1+)
17 References 0 Reactions 0 Suppliers

6 38537-24-5 C12HD9N 9H-Carbazole-1,2,3,4,5,6,7,8-d₆
11 References 7 Reactions 16 Suppliers

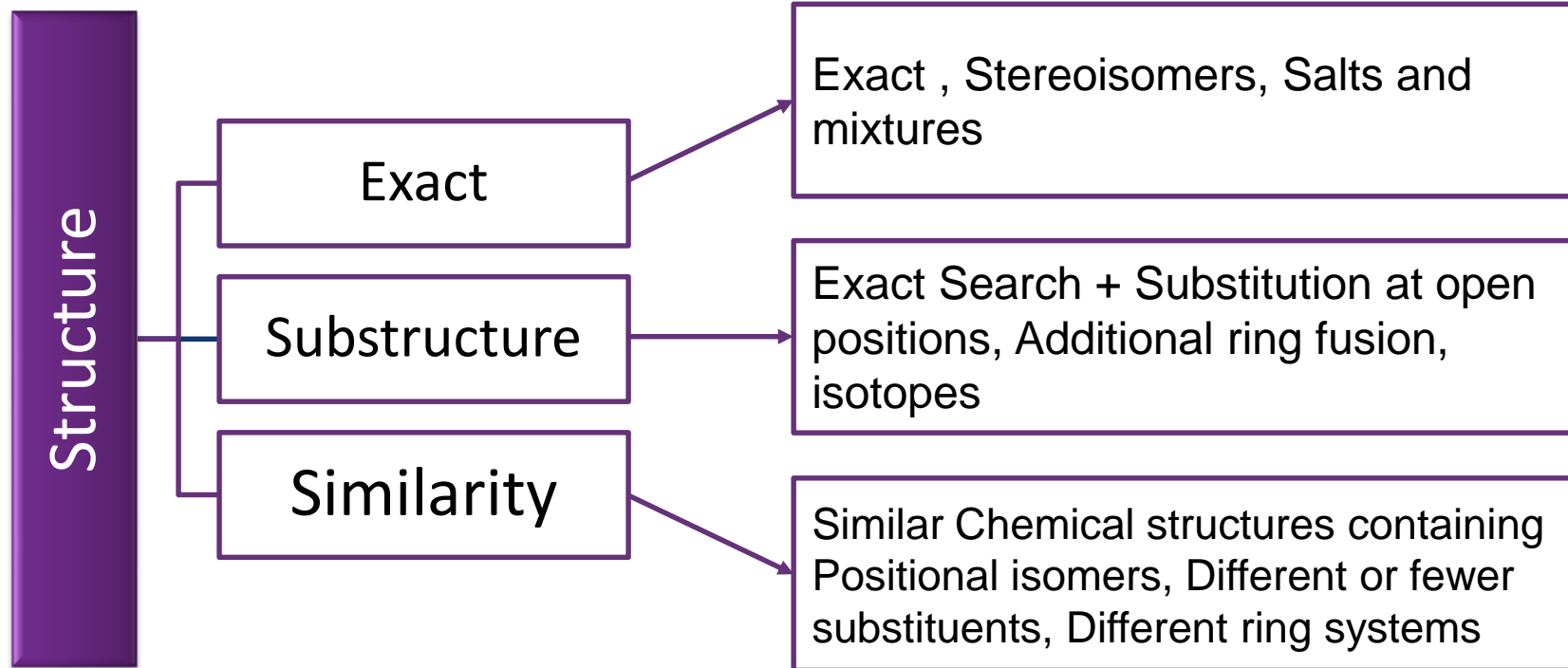
7 97960-58-2

8 42952-94-3

9 34479-78-2

Type of structure searches

Answers retrieved



Agenda

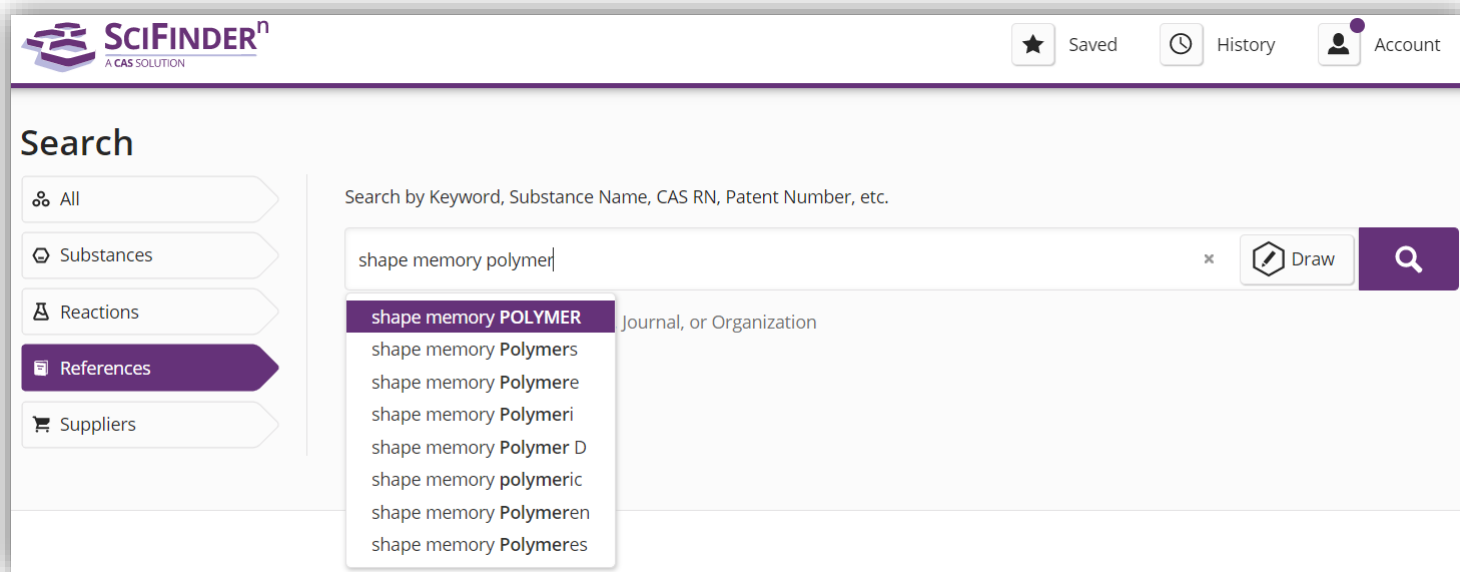
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Case study

Search references for Shape memory polymers

1. Search for ***Shape memory polymer*** as a keyword
2. Retrieve all references and filter all references by document type Patent
3. Explore all other refinement options

Key word search



The screenshot displays the SciFinder search interface. At the top left is the SciFinder logo with the tagline 'A CAS SOLUTION'. To the right are navigation icons for 'Saved', 'History', and 'Account'. The main search area is titled 'Search' and features a sidebar with filters: 'All', 'Substances', 'Reactions', 'References' (highlighted), and 'Suppliers'. The search input field contains the text 'shape memory polymer' and includes a 'Draw' button and a search icon. Below the input field, a dropdown menu lists suggestions: 'shape memory POLYMER Journal, or Organization', 'shape memory Polymers', 'shape memory Polymere', 'shape memory Polymeri', 'shape memory Polymer D', 'shape memory polymeric', 'shape memory Polymeren', and 'shape memory Polymeres'.

References retrieved

A new, proprietary algorithm presents the most relevant answers for your immediate review and evaluation alongside other important criteria

The screenshot displays the SciFinder search results page for the query "shape memory POLYMER". The interface includes a top navigation bar with the SciFinder logo, search filters, and a search bar. The main content area shows a list of references, with the first two results highlighted. The first result is titled "Shape-memory polymers" by Behl, Marc; Lendlein, Andreas, published in Materials Today (Oxford, United Kingdom) in 2007. The second result is also titled "Shape-memory polymers" by Lendlein, Andreas; Kelch, Steffen, published in Angewandte Chemie, International Edition in 2002. The interface includes filters for Document Type, Language, and Publication Year, and a "Load More Results" button. The search results are sorted by Relevance and shown as Partial Abstracts.

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#)

[Load More Results](#)

Filter by

- Document Type
 - Journal (518K)
 - Patent (204K)
 - Review (72K)
 - Biography (1)
 - Book (4,710)
- Language
 - English (550K)
 - Japanese (69K)
 - Chinese (55K)
 - Russian (24K)
 - German (23K)
- Publication Year

[View All](#)

References (763,315) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By

1

Shape-memory polymers
By: Behl, Marc; Lendlein, Andreas
Materials Today (Oxford, United Kingdom) (2007), 10(4), 20-28 | Language: English, Database: CAlplus

A review. **Shape-memory polymers** are an emerging class of active **polymers** that have dual-**shape** capability. They can change their **shape** in a predefined way from **shape A** to **shape B** when exposed to an appropriate stimulus. While **shape B** is given by the initial processing step, **shape A** is determined by applying a process called programming. We review fundamental aspects of the mol. design of suitable **polymer** architectures, tailored programming and recovery processes, and the quantification of the **shape-memory** effect. **Shape-memory** research was initially founded on the thermally induced dual-**shape** of...

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Full Text Substances (0) Reactions (0) Cited By (600) Citation Map

2

Shape-memory polymers
By: Lendlein, Andreas; Kelch, Steffen
Angewandte Chemie, International Edition (2002), 41(12), 2034-2057 | Language: English, Database: CAlplus

A review. Material scientists predict a prominent role in the future for self-repairing and intelligent materials. Throughout the last few years, this concept has found growing interest as a result of the rise of a new class of **polymers**. These so-called **shape-memory polymers** by far surpass well-known metallic **shape-memory** alloys in their **shape-memory** properties. As a consequence of the relatively easy manufacture and programming of **shape-memory polymers**, these materials represent a cheap and efficient alternative to well-established **shape-memory** alloys. In **shape-memory** polymers, the consequenc...

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Full Text Substances (0) Reactions (0) Cited By (1,484) Citation Map

Different filtration options

Filter by

^ **Document Type**

- Journal (518K)
- Patent (204K)
- Review (72K)
- Biography (1)
- Book (4,710)


[View All](#)

^ **Language**

- English (550K)
- Japanese (69K)
- Chinese (55K)
- Russian (24K)
- German (23K)

[View All](#)

^ **Publication Year**



1874 2020

No Min to No Max

[View Larger](#)

^ **Author**

- Zaikov, G. E. (780)
- Wang, Wei (720)
- Anonymous (677)
- Matyjaszewski, Krzysztof (652)
- Zhang, Wei (619)

[View All](#)

^ **Organization**

- Chinese Academy of Sciences (7,295)
- Sichuan University (3,035)
- Zhejiang University (2,678)
- Russian Academy of Sciences (2,614)
- Tokyo Institute of Technology (2,555)

[View All](#)

^ **Publication Name**

^ **Publication Name**

^ **Concept**

- Polymers (352K)
- Polymer morphology (110K)
- Polymer blends (49K)
- Polyesters (40K)
- Glass transition temperature (36K)

[View All](#)

^ **CAS Solutions**

^ **Formulation Purpose**

^ **Database**

^ **Search Within Results**

Refine references using concept titles

Concept [X]

Top Count | Alphanumeric | Search

0 Selected

<input type="checkbox"/> Polymers (352K)	<input type="checkbox"/> Elongation at break (15K)	<input type="checkbox"/> Temperature (9,828)
<input type="checkbox"/> Polymer morphology (110K)	<input type="checkbox"/> Crystallization (15K)	<input type="checkbox"/> Surface structure (9,778)
<input type="checkbox"/> Polymer blends (49K)	<input type="checkbox"/> Polycarbonates (14K)	<input type="checkbox"/> Molecular structure (9,723)
<input type="checkbox"/> Polyesters (40K)	<input type="checkbox"/> Adsorption (14K)	<input type="checkbox"/> Particle size distribution (9,686)
<input type="checkbox"/> Glass transition temperature (36K)	<input type="checkbox"/> Fracture surface morphology, polymeric (14K)	<input type="checkbox"/> Polymer electrolyte fuel cells (9,359)
<input type="checkbox"/> Thermal stability (31K)	<input type="checkbox"/> Polymer morphology, fracture-surface (14K)	<input type="checkbox"/> Peptides (9,324)
<input type="checkbox"/> Acrylic polymers (30K)	<input type="checkbox"/> Crosslinking (14K)	<input type="checkbox"/> Plastic films (9,292)
<input type="checkbox"/> Tensile strength (29K)	<input type="checkbox"/> Melting point (13K)	<input type="checkbox"/> Impact strength (9,260)
<input type="checkbox"/> Simulation and Modeling (29K)	<input type="checkbox"/> Molecular weight (13K)	<input type="checkbox"/> Films (9,102)
<input type="checkbox"/> Nanoparticles (27K)	<input type="checkbox"/> Swelling, physical (13K)	<input type="checkbox"/> Polymer degradation (9,093)
<input type="checkbox"/> Nanocomposites (26K)	<input type="checkbox"/> Plastics (13K)	<input type="checkbox"/> Polymer electrolytes (9,090)
<input type="checkbox"/> Crystallinity (25K)	<input type="checkbox"/> Polymerization (12K)	<input type="checkbox"/> Crystal structure (8,959)
<input type="checkbox"/> Young's modulus (25K)	<input type="checkbox"/> Chemical chains (12K)	<input type="checkbox"/> Fusion enthalpy (8,874)
<input type="checkbox"/> Polyoxyalkylenes (24K)	<input type="checkbox"/> Diffusion (12K)	<input type="checkbox"/> Biocompatible materials (8,874)
<input type="checkbox"/> Microcavity (23K)		

Apply Cancel

Concept [X]

Top Count | Alphanumeric | Search

Concept Name

nano [Search]

Select All on Page

<input type="checkbox"/> Agrochemical nanocapsules (1)	<input type="checkbox"/> Nanocatalysts (157)	<input type="checkbox"/> Nanoflowers (28)
<input type="checkbox"/> Carbon nanofibers (247)	<input type="checkbox"/> Nanochannels (26)	<input type="checkbox"/> Nanoflowers, nanoroses (1)
<input type="checkbox"/> Carbon nanostructured materials (50)	<input type="checkbox"/> Nanoclusters (278)	<input type="checkbox"/> Nanofluidic devices (4)
<input type="checkbox"/> Carbon nanotube fibers (335)	<input type="checkbox"/> Nanocoils (17)	<input type="checkbox"/> Nanofluidics (9)
<input type="checkbox"/> Carbon nanotubes (11K)	<input type="checkbox"/> Nanocolloids (18)	<input type="checkbox"/> Nanofluids (116)
<input type="checkbox"/> Cellulosic nanofibers (33)	<input type="checkbox"/> Nanocomposites (26K)	<input type="checkbox"/> Nanogels (191)
<input type="checkbox"/> Core-shell nanoparticles (565)	<input type="checkbox"/> Nanoconfinement (20)	<input type="checkbox"/> Nanohorns (70)
<input type="checkbox"/> Cosmetic nanoemulsions (21)	<input type="checkbox"/> Nanoconjugates (34)	<input type="checkbox"/> nano-hydroxyapatite-collagen (3)
<input type="checkbox"/> Electric nanogenerators (29)	<input type="checkbox"/> Nanocrystalline materials (156)	<input type="checkbox"/> Nanoimprint lithography (532)
<input type="checkbox"/> Electron beam nanolithography (16)	<input type="checkbox"/> Nanocrystalline metals (134)	<input type="checkbox"/> Nanoliposomes (1)
	<input type="checkbox"/> Nanocrystallites (36)	<input type="checkbox"/> Nano-liquid chromatography

← Prev 1 2 Next →

Apply Cancel

Citation Map

Reference Detail (1 of 763,315)

Substances (0) Reactions (0) Cited By (600) Citation Map

Journal

Source
Materials Today (Oxford, United Kingdom)
Volume: 10
Issue: 4
Pages: 20-28
Journal: General Review
2007
DOI:
10.1016/s1369-7021(07)70047-0

Database Information
AN: 2007:501552
CAN: 149:105215
CAplus

Company/Organization
Center for Biomaterial Development, GKSS Research Center Geesthacht
Institute of Polymer Research
Teltow D-14513
Germany

Publisher
Elsevier Ltd.

Language
English

Shape-memory polymers

By: Behl, Marc; Lendlein, Andreas

Abstract: A review. **Shape-memory polymers** are an emerging class of active polymers that have dual-shape capability. They can change their **shape** in a predefined way from **shape A** to **shape B** by the initial processing step. **shape A** is determined by the initial processing step, **shape A** is determined by applying mol. design of suitable **polymer** architectures, tailored program **memory** effect. **Shape-memory** research was initially founded extended to other stimuli by either indirect thermal actuation or level. Finally, **polymers** are introduced that can be multifunctional biofunctional or biodegradable. Potential applications for such

Full Text ▾

Concepts

Citations

Citation Map

Shape-memory polymers

By: Behl, Marc; Lendlein, Andreas
Materials Today (Oxford, United Kingdom) (2007), 10(4), 20-28 | Language: English, Database: CAplus

Abstract: A review. Shape-memory polymers are an emerging class of active polymers that have dual-shape capability. They can change their shape in a predefined way from shape A to shape B when exposed to an appropriate stimulus. While shape B is given by the initial processing step, shape A is determined by applying a process called programming. We review fundamental aspects of the mol. design of suitable polymer architectures, tailored programming and recovery processes, and the quantification of the shape-memory effect. Shape-memory research was initially founded on the thermally induced dual-shape ef...

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Full Text ▾

Filter by

- Document Type
 - Journal (643)
 - Patent (4)
 - Review (96)
 - Conference (23)
 - Preprint (3)
- Author
 - Leng, Jinsong (36)
 - Liu, Yanju (31)
 - Lendlein, Andreas (30)
 - Li, Guoqiang (14)
 - Huang, W. M. (12)
- View All
- Concept
 - Shape memory materials (325)
 - Shape memory effect (324)
 - Glass transition temperature

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- Designing materials for biology and medicine
Nature (London, United Kingdom) (2004)
Cited By 2,435 [Map](#)
- Shape-memory polymers
Angewandte Chemie, International Edition (2002)
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Science (New York, N.Y.) (2002)
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- Carbon nanotube composites for thermal management
Applied Physics Letters (2002)
Cited By 1,175 [Map](#)
- Light-induced shape-memory polymers
Nature (London, United Kingdom) (2005)
Cited By 1,139 [Map](#)
- Remotely actuated polymer nanocomposites-stress-recovery of carbon-nanotube-filled thermoplastic elastomers
Nature Materials (2004)
Cited By 689 [Map](#)

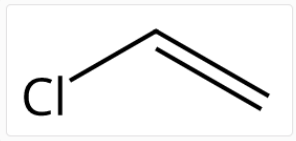
References Citing This Document

- 25th Anniversary Article: Rational Design and Applications of Hydrogels in Regenerative Medicine
Advanced Materials (Weinheim, Germany) (2014)
Citing 586 [Map](#)
- Multifunctional Shape-Memory Polymers
Advanced Materials (Weinheim, Germany) (2010)
Citing 545 [Map](#)
- Shape-memory polymers and their composites: Stimulus methods and applications
Progress in Materials Science (2011)
Citing 522 [Map](#)
- Recent advances in shape memory polymers and composites: a review
Journal of Materials Science (2008)
Citing 472 [Map](#)
- Recent advances in shape memory polymer
Polymer (2011)
Citing 430 [Map](#)
- A review of stimuli-responsive shape memory polymer composites
Polymer (2013)
Citing 379 [Map](#)

Combine text and structure searching

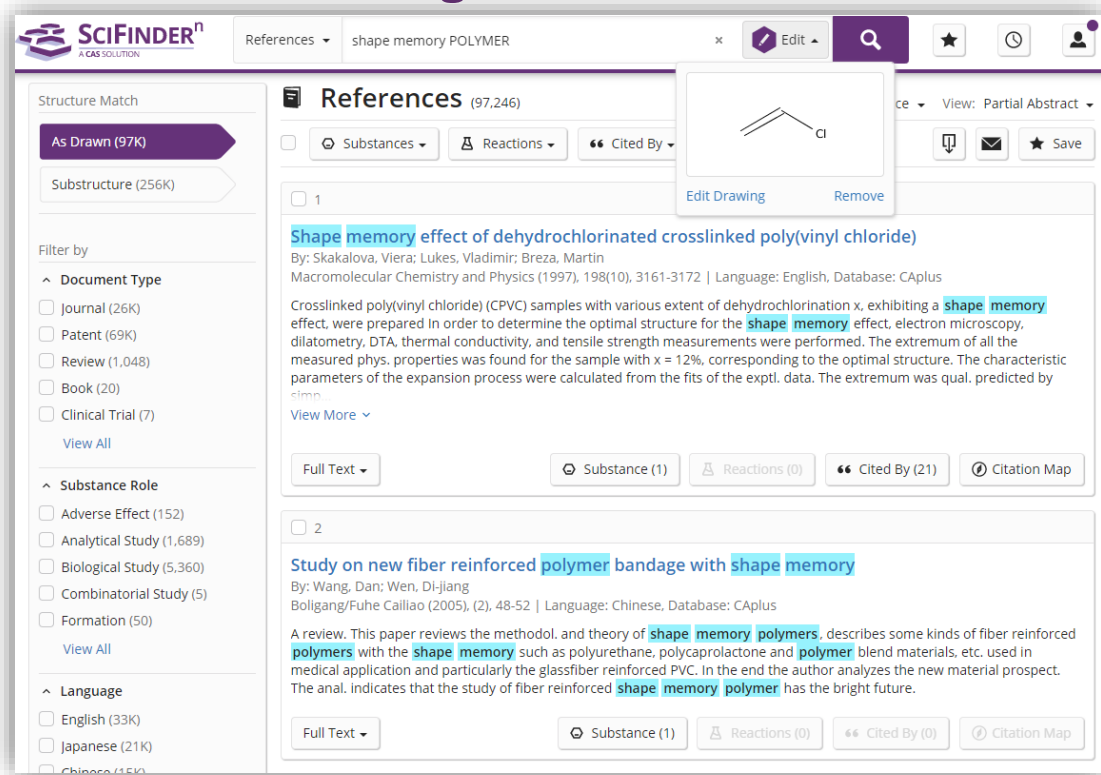
Draw structure within
“Draw” option
available to combine
Keyword and
structure query

9002-86-2



$(C_2H_3Cl)_x$
Polyvinyl chloride

199K References 1,248 Reactions 29 Suppliers



SciFinderⁿ A CAS SOLUTION

References shape memory POLYMER

Structure Match

- AS Drawn (97K)
- Substructure (256K)

Filter by

- Document Type
 - Journal (26K)
 - Patent (69K)
 - Review (1,048)
 - Book (20)
 - Clinical Trial (7)
- Substance Role
 - Adverse Effect (152)
 - Analytical Study (1,689)
 - Biological Study (5,360)
 - Combinatorial Study (5)
 - Formation (50)
- Language
 - English (33K)
 - Japanese (21K)
 - Chinese (15K)

References (97,246)

Substances Reactions Cited By

1

Shape memory effect of dehydrochlorinated crosslinked poly(vinyl chloride)

By: Skakalova, Viera; Lukes, Vladimir; Breza, Martin
Macromolecular Chemistry and Physics (1997), 198(10), 3161-3172 | Language: English, Database: CAplus

Crosslinked poly(vinyl chloride) (CPVC) samples with various extent of dehydrochlorination x , exhibiting a **shape memory effect**, were prepared in order to determine the optimal structure for the **shape memory effect**, electron microscopy, dilatometry, DTA, thermal conductivity, and tensile strength measurements were performed. The extremum of all the measured phys. properties was found for the sample with $x = 12\%$, corresponding to the optimal structure. The characteristic parameters of the expansion process were calculated from the fits of the exptl. data. The extremum was qual. predicted by simn.

View More

Full Text Substance (1) Reactions (0) Cited By (21) Citation Map

2

Study on new fiber reinforced polymer bandage with shape memory

By: Wang, Dan; Wen, Di-jiang
Bolgang/Fuhe Cailliao (2005), (2), 48-52 | Language: Chinese, Database: CAplus

A review. This paper reviews the methodol. and theory of **shape memory polymers**, describes some kinds of fiber reinforced **polymers** with the **shape memory** such as polyurethane, polycaprolactone and **polymer** blend materials, etc. used in medical application and particularly the glassfiber reinforced PVC. In the end the author analyzes the new material prospect. The anal. indicates that the study of fiber reinforced **shape memory polymer** has the bright future.

Full Text Substance (1) Reactions (0) Cited By (0) Citation Map

One of the reference

Reference Detail (1 of 97,269)

← Prev Next →

Substance (1) Reactions (0) Cited By (21) Citation Map Save

Journal

Source
Macromolecular Chemistry and Physics
Volume: 198
Issue: 10
Pages: 3161-3172
Journal
1997
DOI:
10.1002/macp.1997.021981014

Database Information

AN: 1997:697123
CAN: 127:359349
CAplus

Company/Organization

Faculty Chemical Technology
Slovak Technical University
Bratislava 81237
Slovakia

Publisher

Huethig & Wepf

Language

English

Shape memory effect of dehydrochlorinated crosslinked poly(vinyl chloride)

By: Skakalova, Viera; Lukes, Vladimir; Breza, Martin

Abstract: Crosslinked poly(vinyl chloride) (CPVC) samples with various extent of dehydrochlorination x , exhibiting a **shape memory** effect, were prepared in order to determine the optimal structure for the **shape memory** effect, electron microscopy, dilatometry, DTA, thermal conductivity, and tensile strength measurements were performed. The extremum of all the measured phys. properties was found for the sample with $x = 12\%$, corresponding to the optimal structure. The characteristic parameters of the expansion process were calculated from the fits of the exptl. data. The extremum was qual. predicted by simplified quantum chem. models of a double PVC chain using the semiempirical AM1 method. The generalized zip mechanism of CPVC dehydrochlorination might explain the extremum due to mutual chain reorientation with increasing x .

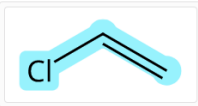
Full Text ▾ [Expand All](#) | [Collapse All](#)

Concepts

Substances

Substance (1)


9002-86-2



$(C_2H_3Cl)_x$
Poly(vinyl chloride)

Role: Physical, Engineering or Chemical Process, Properties, Process

Notes: dehydrochlorinated



SciFinderⁿ
A CAS SOLUTION

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27

PatentPak is a CAS solution to ease the substance search in patents



- Types of issues & challenges faced in day-today while searching patents
- What is PatentPak? And how does it work?
- Coverage and Content of PatentPak
- What if an important Patent is not in English?
- Conclusion

Search patented references published in English language

Explore patent
in PatentPak

Reference Detail (2 of 17,205) ← Prev Next →

Substances (19) Reactions (0) Cited By (5) Citation Map 📄 📧 ★ Save

Patent

Patent Information

Patent Number
WO2004033539

Publication Date
2004-04-22

Application Number
WO2003-US32329

Application Date
2003-10-10

Kind Code
A1

Assignee
University of Connecticut, United States

Source
World Intellectual Property Organization

Database Information
AN: 2004:333773
CAN: 140:322355
CAplus

Language
English

Blends of amorphous and semicrystalline **polymers** having **shape memory** properties

By: Mather, Patrick T.; Liu, Changdeng

Abstract: Blends of amorphous and semicrystalline **polymers** having **shape memory** properties were prepared by blending a crystalline **polymer** such as poly(vinylidene fluoride), polylactide, poly(hydroxybutyrate), poly(ethylene glycol) polyethylene, polyethylene-co-vinyl acetate, poly(vinyl chloride), poly(vinylidene chloride) and copolymers of poly(vinylidene chloride) and poly(vinyl chloride) and an amorphous **polymer** such as poly(vinyl acetate), poly Me acrylate, poly Et acrylate, atactic poly Me methacrylate, isotactic poly Me methacrylate, syndiotactic poly Me methacrylate and other poly alkyl methacrylates. The method for preparing the polymeric materials and applications thereof, for example, as smart medical devices, are also disclosed.

PATENTPAK Viewer Full Text ▾

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2004033539	English	A1	PDF PDF+ Viewer	2004-04-22	WO2003-US32329	2003-10-10
		P			US2002-60418023P	2002-10-11
		P			US2003-60466401P	2003-04-29
		P			US2003-60488323P	2003-07-18
CA2501549	Undetermined	A1		2004-04-22	CA2003-2501549	2003-10-10
CA2501551	Undetermined	A1		2004-04-22	CA2003-2501551	2003-10-10
CA2501617	Undetermined	A1		2004-04-22	CA2003-2501617	2003-10-10
CA2501643	Undetermined	A1		2004-04-22	CA2003-2501643	2003-10-10
WO2004032799	English	A2	PDF	2004-04-22	WO2003-US32308	2003-10-10
WO2004033515	English	A2	PDF PDF+ Viewer	2004-04-22	WO2003-US32059	2003-10-10
WO2004033553	English	A1	PDF PDF+ Viewer	2004-04-22	WO2003-US32138	2003-10-10

PatentPak viewer

5 polymer, for example, PLA, with an amorphous polymer, for example PVAc. The polymer blends are totally miscible at all blend ratios within the experimental ranges and form only one single glass transition temperature for each formulation. Additionally, the degree of crystallinity of the blends decreases monotonically with increasing PVAc and PVAc and PVDF fraction. This, in turn, governs the rubbery modulus important to shape memory.

10 Thus, the present disclosure advantageously provides a shape memory polymeric material that is characterized by a T_g exceeding room temperature whose rubber modulus and elasticity are derived substantially from physical crosslinks comprising a bond of a crystalline polymer selected from the group consisting of poly(vinylidene fluoride), polyglycolides, polylactide and copolymers thereof, poly(hydroxybutyrate), poly(ethylene glycol), polyethylene, polyethylene-co-vinyl acetate, poly(vinyl chloride), poly(vinylidene chloride) and copolymers of poly

15 vinylidene chloride and poly vinyl chloride with an amorphous polymer selected from the group consisting of poly(vinyl acetate), poly methyl acrylate, poly ethyl acrylate, atactic poly methyl methacrylate, isotactic poly methyl methacrylate and syndiotactic poly methyl methacrylate.

The present disclosure also advantageously provides a method of preparing a shape memory polymer material characterized by a T_g exceeding room temperature whose rubber

Situation 1: Patent disclosed substances only by IUPAC name

vacuo and collected in EtOH, azeotroping to dryness to afford the title compound.

Step 2: 5-Amino-2-fluoro-4-methylbenzoic acid

- 10 2-Fluoro-4-methyl-5-nitrobenzoic acid (900 mg, 4.52 mmol) in MeOH (70 ml) was treated with ammonium formate 1(425 mg, 22.60 mmol) and Pd (Carbon) (144 mg, 1.356 mmol). The mixture was degassed thoroughly refilling with nitrogen and heated to 60 °C for 2 hrs. The mixture was filtered through silica gel. The filtrate was passed through SCX-2 resin (30g 0.67 μm) (250 ml) followed by 2M ammonia in MeOH (250 ml). The solvents were evaporated to dryness and the resulting crude residue was recrystallised from MeOH to afford the title compound; LC-MS: Rt 0.53 mins; MS m/z 170 {M+H}⁺; Method 10minLC_v003

Step 3: 5-Amino-2-fluoro-4-methyl-N-(2-(4-methylpiperazin-1-yl)benzyl)benzamide

- 20 A mixture comprising (2-(4-methylpiperazin-1-yl)phenyl)methanamine (413 mg, 2.010 mmol) and 5-amino-2-fluoro-4-methylbenzoic acid (step 2)(340 mg, 2.010 mmol) in DMF (3 ml) was treated with DIPEA (0.351 ml, 2.010 mmol) followed by HATU (764 mg, 2.010 mmol) and stirred at 25 °C for 24 hrs. The mixture was partitioned between water and EtOAc. The organic portion was washed with sat. aq. NaHCO₃, 0.5 M LiCl and brine (each back extracted with EtOAc). The combined organic layers were dried (MgSO₄), filtered and evaporated to dryness to give a pink oil. Purification

If the patent is big, it is difficult to find the substance by just its name.....



Situation 2: Name or structure not given - Only data is available.

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PAGE 40 / 171 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

polymers

Analyst Markup Locations (1)

CAS RN
1526905-74-7

Analyst Markup Locations (2)

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Page 49

CAS RN
1526905-75-8

Analyst Markup Locations (2)

Page 29
Page 49

CAS RN
1526905-78-1

integrally supported into a process cartridge and detachably attached to the main body of the electrophotographic apparatus using a guiding member 10, such as a rail.

EXAMPLES

25

[0101] The present invention will be described in more detail below by examples. Here, the term "part(s)" in examples indicates "part(s) by mass". Synthesis examples of electron-transporting substances according to an embodiment of the present invention will now be described. Synthesis example 1

30 [0102] First, 5.4 parts of naphthalenetetracarboxylic dianhydride (manufactured by Tokyo Chemical Industry Co., Ltd.), 4 parts of 2-methyl-6-ethylaniline (manufactured by Tokyo Chemical Industry Co., Ltd.), and 3 parts of 2-amino-1-butanol were added to 200 parts of dimethylacetamide under a nitrogen atmosphere. The mixture was stirred at room temperature for 1 hour to prepare a solution. After the preparation of the solution, the solution was refluxed for 8 hours. The precipitate was separated by filtration and recrystallized in ethyl acetate to give 1.0 part of compound A1-8.

35 Synthesis example 2

[0103] First, 5.4 parts of naphthalenetetracarboxylic dianhydride and 5 parts of 2-aminobutyric acid (manufactured by Tokyo Chemical Industry Co., Ltd.) were added to 200 parts of dimethylacetamide under a nitrogen atmosphere. The mixture was stirred at room temperature for 1 hour to prepare a solution. After the preparation of the solution, the solution was refluxed for 8 hours. The precipitate was separated by filtration and recrystallized in ethyl acetate to give 4.6 parts of compound A1-42.

40 Synthesis example 3

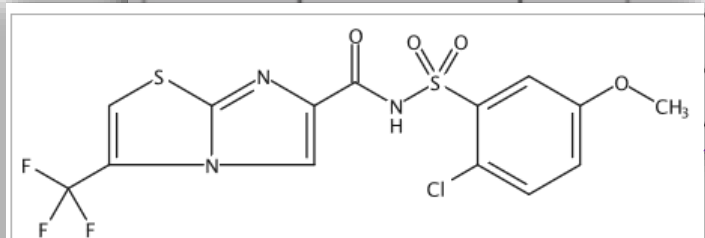
45 [0104] First, 5.4 parts of naphthalenetetracarboxylic dianhydride, 4.5 parts of 2,6-diethylaniline (manufactured by Tokyo Chemical Industry Co., Ltd.) and 4 parts of 4-2-aminobenzenethiol were added to 200 parts of dimethylacetamide under a nitrogen atmosphere. The mixture was stirred at room temperature for 1 hour to prepare a solution. After the preparation of the solution, the solution was refluxed for 8 hours. The precipitate was separated by filtration and recrystallized in ethyl acetate to give 1.3 parts of compound A1-39.

50 Synthesis example 4

55 [0105] To a solvent mixture of 100 parts of toluene and 50 parts of ethanol, 7.4 parts of 3,6-dibromo-9,10-phenanthrene-dione, which was synthesized from 2.8 parts of 4-(hydroxymethyl)phenylboronic acid (manufactured by Sigma-Aldrich Japan K.K.) and phenanthrenequinone (manufactured by Sigma-Aldrich Japan K.K.) under a nitrogen atmosphere by a synthetic method described in Chem. Educator No. 6, pp. 227-234, (2001), was added. After 100 parts of an aqueous solution of 20% sodium carbonate was added dropwise to the mixture, 0.55 parts of tetrakis(triphenylphosphine)palladium

Situation 3: Disclosed/Claimed compounds are in tabular form.

Example	R ¹	n	A	R ^a	R ^b	R ^c	R ^d	R ^e	Remarks
I-1-28	2-CF ₃	1	CH	CH ₃	H	H	Cl	H	
I-1-29	3-CF ₃	1	C-R ¹	Cl	H	H	OMe	H	NMR
I-1-30	3-CF ₃	1	C-R ¹	Cl	H	H	H	Cl	NMR
I-1-31	3-CF ₃	1	C-R ¹	Cl	H	H	Cl	H	NMR
I-1-32	3-CF ₃	1	C-R ¹	Cl	H	H	CH ₃	H	
				Cl	H	H	Et	H	
				CH ₃	H	H	Cl	H	
				F	H	H	OMe	H	



CAS RN 164-8720-97-1
assigned by Chemical
Abstract Service

Situation 4: Disclosed/Claimed compounds have a different common name (which you are not aware)

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Key Substances in Patent

Search in SciFinder | View Detail

Analyst Markup Location
page 80

CAS RN 55-98-1

CC(=O)OCCCCOS(=O)(=O)C

Search in SciFinder | View Detail

Analyst Markup Location
page 80

CAS RN 7689-03-4

CC1=C2C(=C(C=C1)C(=O)O)N3C=CC=CC=C3N2

73. The method of claim 72, wherein the one or more additional chemotherapeutic agents includes aminoglutethimide, amsacrine, anastrozole, asparaginase, Bacillus Calmette-Guérin vaccine (bcg), bicalutamide, bleomycin, bortezomib, busulfan, busulfan, camptothecin, capecitabine, carboplatin, carfilzomib, carmustine, chlorambucil, chloroquine, cisplatin, cladribine, clodronate, colchicine, cyclophosphamide, cyproterone, cytarabine, dacarbazine, dactinomycin, daunorubicin, demethoxyviridin, dexamethasone, dichloroacetate, dienestrol, diethylstilbestrol, docetaxel, doxorubicin, epirubicin, estradiol, estramustine, etoposide, everolimus, exemestane, filgrastim, fludarabine, fludrocortisone, fluorouracil, fluoxymesterone, flutamide, gemcitabine, genistein, goserelin, hydroxyurea, idarubicin, ifosfamide, imatinib, interferon, irinotecan, letrozole, leucovorin, leuprolide, levamisole, lomustine, lonidamine, mechlorethamine, medroxyprogesterone, megestrol, melphalan, mercaptopurine, mesna, metformin

We had searched by "Sulfabutin" and were not aware that it's also called "busulfan"

How to use Boolean operators

Separate keyword search for
hand wash and hand
sanitizer

The screenshot shows the SciFinder interface with the search term "hand wash" entered in the search bar. The search results page displays "References (37,203)". The first result is titled "Hand wash and manual skin wipes." by Brouwer, D H; Boeniger, M F; van Hemmen, J. The abstract discusses techniques for dermal exposure and sampling protocols. The left sidebar shows filter options for Document Type (Journal, Patent, Review, Biography, Book) and Language (Chinese, English, Korean, Japanese, German).

The screenshot shows the SciFinder interface with the search term "hand sanitizer" entered in the search bar. The search results page displays "References (1,726)". The first result is titled "Environmentally hand sanitizer containing alcohol" by Lin, Cisheng. The abstract describes an environmentally friendly sanitizer with specific components. The left sidebar shows filter options for Document Type (Journal, Patent, Review, Clinical Trial, Commentary) and Language (Chinese, English, Korean, Japanese, German).

Use 'OR' Boolean operator to get combined search for both keywords

The screenshot shows the SciFinder interface with a search query 'hand wash OR hand sanitizer' entered in the search bar. The search results page displays 1,027,581 references. The first result is titled 'Hand wash and manual skin wipes.' by Brouwer, D H; Boeniger, M F; van Hemmen, J, published in The Annals of occupational hygiene (2000), 44(7), 501-10. The abstract text indicates that hand wash and skin wipes are major techniques for dermal exposure sampling. The interface includes filters for document type and language, and options to view full text or citation maps.

References (1,027,581) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By

1

Hand wash and manual skin wipes.
By: Brouwer, D H; Boeniger, M F; van Hemmen, J
The Annals of occupational hygiene (2000), 44(7), 501-10 | Language: English, Database: MEDLINE

Hand wash and skin wipes are major techniques that have been used for dermal exposure sampling. Both techniques remove chemicals either deposited on or transferred to the skin contaminant layer by a combination of chemical and mechanical actions. The paper overviews identified methods and techniques, with emphasis on sampling parameters and sampling efficiency. It is concluded that identified sampling protocols, including sampling techniques, deviate at possible key issues, which hampers comparisons of study results. It is recommended to conduct sampling efficiency studies prior to field sampling.

View More

Full Text Substances (0) Reactions (0) Cited By (59) Citation Map

2

Use of 'AND' Boolean operator to get references containing both keywords/ concepts in same reference

The screenshot shows the SciFinder interface with a search query 'hand wash AND Hand sanitizer' entered in the search bar. The search results are displayed under the heading 'References (766)'. The first result is titled 'Wash-free hand sanitizer for antibacterial' by Liang, Wenqi, published in 2018. The second result is titled 'High performing, high impact fragrant materials' by Teixeira, Miguel A.; Unno, Masakatsu; Helweg, Hendrik; Kay, Lay Meng; Shin, Jung Chul, published in 2018. The interface includes a filter sidebar on the left with options for Document Type, Language, and Publication Year. The search bar is highlighted with a red box.

SciFinderⁿ
A CAS SOLUTION

References - hand wash AND Hand sanitizer

Draw

Return to Home

Filter by

- Document Type
 - Journal (312)
 - Patent (453)
 - Review (19)
 - Biography (2)
 - Clinical Trial (38)
 - View All
- Language
 - English (388)
 - Chinese (307)
 - German (23)
 - Japanese (21)
 - Korean (12)
 - View All
- Publication Year

References (766)

Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

1

Wash-free hand sanitizer for antibacterial

By: Liang, Wenqi
China, CN107550818 A 2018-01-09 | Language: Chinese, Database: CAplus

The invention discloses a **wash-free hand sanitizer** for antibacterial, which has the advantages of good effect, safe use, no stimulation, and can also soften cuticle, skin care, nourishing and moisturizing. The **hand sanitizer** comprises the following raw materials in percentage by weight: A.SAP 0.1%-0.5%, glycerol 2%-5%, hypromellose 0.1%-0.5%, hyaluronic acid 0.1%-0.5%, plant extract 0.1%-0.5%, allantoin 0.1%-0.5%, water balance; wherein the plant extract consists of aloe vera extract 4-6 parts, Herba Portulacae extract 0.8-1.3 parts, Alternanthera philoxeroides extract 1.2-1.5 parts, and Corte...

View More

PATENTPAK Full Text Substances (4) Reactions (0) Cited By (0) Citation Map

2

High performing, high impact fragrant materials

By: Teixeira, Miguel A.; Unno, Masakatsu; Helweg, Hendrik; Kay, Lay Meng; Shin, Jung Chul
World Intellectual Property Organization, WO2018071897 A1 2018-04-19 | Language: English, Database: CAplus

Disclosed are fragrance accords each containing (i) at least 7 wt% of one or more Class 1 fragrance ingredients, (ii) 5 to 85 wt% of one or more Class 2 fragrance ingredients, and (iii) 0 to 80 wt% of one or more Class 3 fragrance ingredients. The Classes 1, 2, and 3 fragrance ingredients are defined by exptl. velocity. Also disclosed are delivery systems and consumer products

Use of 'NOT' Boolean operator to exclude one of the keyword from main search

SciFinderⁿ A CAS SOLUTION

Reference: hand wash NOT Hand sanitizer

Return to Home

Filter by

- Document Type
 - Journal (5,420)
 - Patent (1,645)
 - Review (423)
 - Biography (9)
 - Clinical Trial (326)
 - View All
- Language
 - English (5,772)
 - German (569)
 - Chinese (274)
 - Japanese (238)
 - French (96)
 - View All
- Publication Year
 - 1870
 - 2020

References (7,084)

Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

1

Alpha alkylation of aldehyde with a polycyclic olefin

By: Quintaine, Julie; MacMillan, David W. C.
World Intellectual Property Organization, WO2018192923 A1 2018-10-25 | Language: English, Database: CAPlus

alkenediyl; and n is 1 or 2.
[View More](#)

PATENTPAK Full Text Substances (13) Reactions (2) Cited By (0) Citation Map

2

Personal care compositions in the form of dissolvable solid structures

By: Pratt, Michael Sean; Hilvert, Jennifer Elaine; Keune, Pamela Ann; Massa, Alessandra; Kay, Melanie Anne; Hamersky, Mark William
World Intellectual Property Organization, WO2018140676 A2 2018-08-02 | Language: English, Database: CAPlus

Described are effervescent, dissolvable solid structures having fibers formed from a

Use of parenthesis with Boolean operators

This will search references in which keyword/concept of Hand sanitizer and disinfectant is mentioned together but not Hand wash

The screenshot shows the SciFinder search interface. At the top, the search bar contains the query "(hand sanitizer AND disinfectant) NOT hand wash", which is highlighted with a purple box. Below the search bar, the interface displays search results for "References (641)". The results are sorted by "Relevance" and viewed as "Partial Abstract". A filter panel on the left shows "Document Type" filters: Journal (402), Patent (225), Review (31), Conference (8), Dissertation (5), and Preprint (1). The first result is titled "Inactivation and removal of Bacillus cereus by sanitizer and detergent" by Peng, Jui-Sen; Tsai, Wei-Chong; Chou, Cheng-Chun, published in the International Journal of Food Microbiology (2002), 77(1-2), 11-18. The abstract text mentions "sanitizers" and "detergent". At the bottom of the result, there are buttons for "Full Text", "Substances (5)", "Reactions (0)", "Cited By (103)", and "Citation Map".

Use of quotation marks to search exact phrase along with Boolean operator

SCI FINDERⁿ
A CAS SOLUTION

References ▾ "hand sanitizer" NOT "hand wash" × Draw 🔍 ★ 🕒 👤

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)
Load More Results

References (1,690) Sort: Relevance ▾ View: Partial Abstract ▾

Substances ▾ Reactions ▾ Cited By ▾ Save

1

Environmentally hand sanitizer containing alcohol
By: Lin, Cisheng
China, CN107898675 A 2018-04-13 | Language: Chinese, Database: CAPlus

The present invention provides an environmentally **hand sanitizer** comprising the following component in parts by weight such as 6-12 parts of plant ash, 0.1-0.4 parts of surfactant, 0.5-0.8 parts of lemon flavor, 4-8 parts of alc., 3-6 parts of glycerol, 8-18 parts of deionized water, and 0.1-0.2 parts of diallyl trisulfide. The **hand sanitizer** is degradable, and reduces water pollution.

PATENTPAK ▾ Full Text ▾ Substances (2) Reactions (0) Cited By (0) Citation Map

2

Processing method of ice-cold hand sanitizer
By: Zhao, Yingxiang; Guo, Ziming; Zhao, Qingwen; Yang, Jing
China, CN108324584 A 2018-07-27 | Language: Chinese, Database: CAPlus

The invention discloses a processing method of ice-cold **hand sanitizer**, which has the advantages of good cleaning effect, antibacterial disinfection and skin care. The **hand sanitizer** is made from the following raw materials in parts by weight: menthol 0.5-1 parts, ethanol 300-400 parts, glycerin 50-60 parts, water 150-200 parts, and perfume 1-2 parts.

PATENTPAK ▾ Full Text ▾ Substances (3) Reactions (0) Cited By (0) Citation Map

Filter by

Document Type

- Journal (526)
- Patent (1,153)
- Review (41)
- Clinical Trial (56)
- Commentary (9)

[View All](#)

Language

- Chinese (888)
- English (723)
- Korean (27)
- Japanese (15)
- German (13)

[View All](#)

Special characters and wildcard searching

- *Use of Asterisk (*) mark*

Query Disinfect* will match Disinfectant, disinfection, disinfecting, disinfected etc.

SciFinderⁿ
A CAS SOLUTION

References | disinfect*

1
Bactericidal Activity of TiO₂ Photocatalyst in Aqueous Media: Toward a Solar-Assisted Water Disinfection System
By: Wei, Chang; Li, Wen Yuan; Zainal, Zulkarnain; Williams, Nathan E.; Zhu, Kai; Kruzic, Andrew P.; Smith, Russell L.; Rajeshwar, Krishna
Environmental Science and Technology (1994), 28(5), 934-8 | Language: English, Database: CAplus
Irradiation of suspensions of *Escherichia coli* (~10⁵ cells/mL) and TiO₂ (anatase) with UV-visible light of wavelengths longer than 380 nm resulted in the killing of the bacteria within minutes. Oxygen was a prerequisite for the bactericidal properties of the photocatalyst. Bacterial killing was found to adhere to first-order kinetics. The rate constant was proportional to the square root of the concentration of TiO₂ and proportional to the incident light intensity in the range ~180~1660 μE s⁻¹ m⁻². The trends in these simulated laboratory experiments were mimicked by outdoor tests conducted u
View More ▾
Full Text ▾ | Substance (1) | Reactions (0) | Cited By (371) | Citation Map

2
Antimicrobial nanomaterials for water disinfection and microbial control: Potential applications and implications
By: Li, Qilin; Mahendra, Shaily; Lyon, Delina Y.; Brunet, Lena; Liga, Michael V.; Li, Dong; Alvarez, Pedro J., Jr.; Wang, Qifeng
Water Research (2008), 42(18), 4591-4602 | Language: English, Database: CAplus
A review. The challenge to achieve appropriate disinfection without forming harmful disinfection byproducts by conventional chemical disinfectants, as well as the growing demand for decentralized or point-of-use water treatment and recycling systems calls for new technologies for efficient disinfection and microbial control. Several natural and engineered nanomaterials have demonstrated strong antimicrobial properties through diverse mechanisms including photocatalytic production of reactive oxygen species that damage cell components and viruses (e.g., TiO₂, ZnO, and fullerenes), compromising the ha
View More ▾
Full Text ▾ | Substances (0) | Reactions (0) | Cited By (1,233) | Citation Map

3
Antiseptics and disinfectants: activity, action, and resistance
By: McDonnell, Gerald; Russell, A. Denver
Clinical Microbiology Reviews (1999), 12(1), 147-179 | Language: English, Database: CAplus

Substance Role
 Patent (388K)
 Review (43K)
 Biography (111)
 Book (798)
View All

Substance Role
 Adverse Effect (1,124)
 Analytical Study (8,847)
 Biological Study (21K)
 Combinatorial Study (22)
 Formation (691)
View All

Language
 English (422K)
 Chinese (193K)
 Japanese (59K)
 German (49K)
 Undetermined (22K)
View All

Publication Year
1832 to 2020
No Min to No Max Apply
View Larger

Author
McDonnell, Gerald; Russell, A. Denver

Special characters and wildcard searching

- *Use of question mark (?)*

Search query: Colo?r.
it helped retrieving references where color or colour is mentioned.

Agenda

- Introduction of CAS
- What is SciFinderⁿ?
- Content and Coverage searchable in SciFinderⁿ
- A few online Case studies – General interest
 - Substance searching
 - Reference searching and PatentPak
 - **Reaction searching**
- CAS Retrosynthesis planner
- Markush structure searching
- Questions and Answers

Reaction searching

- Search reactions for Pitavastatin

SciFINDERⁿ
A CAS SOLUTION

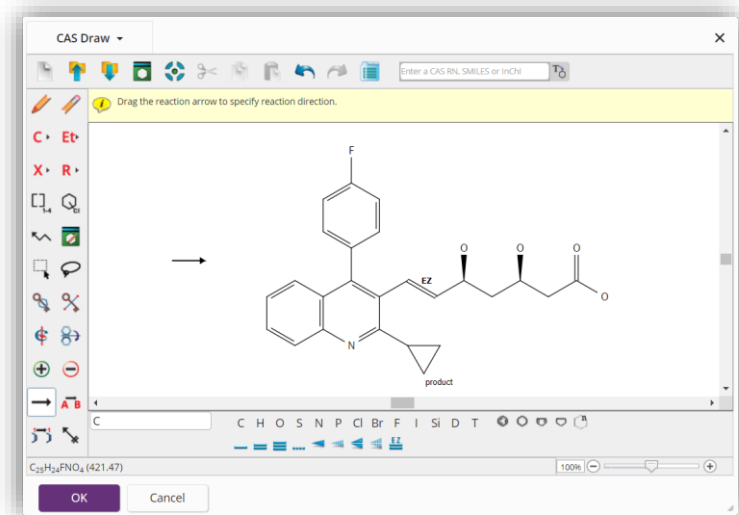
Search

All
Substances
Reactions
References
Suppliers

Search by Keyword, Substance Name, CAS RN, I

Pitavastatin

- Pitavastatin
- Pitavastatin calcium
- Pitavastatin hemicalcium
- Pitavastatin lactone
- Pitavastatin sodium



Synthetic reactions for Pitavastatin

Selecting all required refinement options, available reactions

Structure Match

As Drawn (1,109)

Substructure (2,015)

Filter by

- Yield
 - 90-100% (29)
 - 80-89% (21)
 - 70-79% (9)
 - 50-69% (10)
 - 30-49% (2)
- View All
- Number of Steps
- Non-Participating Functional Groups
 - Acyclic alkene (62)
 - Alkene (62)
 - Halide (62)
 - Imine (62)
 - Phenyl halide (62)
- View All
- Experimental Protocols
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst

Reactions (1,052)

References

Scheme 1 (2 Reactions) Steps: 1 Yield: 100%

Absolute stereochemistry shown, Rotation (+) Double bond geometry shown Suppliers (15)

Absolute stereochemistry shown, Rotation (+) Double bond geometry shown Suppliers (38)

Reaction Summary Steps: 1 Yield: 100% The synthesis of [¹⁸F]pitavastatin as a tracer for hOATP using the Suzuki coupling

1.1 Reagents: Sodium hydroxide Solvents: Methanol, Water; 30 min, rt

By: Yagi, Yusuke; et al Organic & Biomolecular Chemistry (2015), 13(4), 1113-1121

View Reaction Detail Experimental Protocols Full Text

Reaction Summary Steps: 1 Process for the preparation of statins

1.1 Reagents: Sodium hydroxide Solvents: Methanol, Water; 2 h, 20 °C

1.2 Reagents: Hydrochloric acid Solvents: Ethyl acetate, tert-Butyl methyl ether, Water; pH 4.5

PATENTPAK Full Text

View Reaction Detail Experimental Protocols

Collapse Scheme

Scheme 2 (2 Reactions) Steps: 1 Yield: 99%

Stereochemistry

- Absolute Stereo Match (1,016)
- Absolute Stereo Mirror Image (8)
- Relative Stereo Match (28)
- Stereo that Doesn't Match Query (26)
- No Stereo in Answer Structure (31)

SciFinder-n will consider stereostructures. We can select required stereochemistry

Search for exact reaction using various refinement options available

Filter by

^ **Yield**

- 90-100% (29)
- 80-89% (21)
- 70-79% (9)
- 50-69% (10)
- 30-49% (2)

[View All](#)

^ **Number of Steps**

- 1 (151)
- 2 (147)
- 3 (141)
- 4 (120)
- 5 (97)

[View All](#)

^ **Non-Participating Functional Groups**

- Acyclic alkene (62)
- Alkene (62)
- Halide (62)
- Imine (62)
- Phenyl halide (62)

[View All](#)

^ **Experimental Protocols**

- MethodsNow: Synthesis (142)
- Experimental Procedure (257)

^ **Reaction Type**

- Full (874)
- Product Only (178)

^ **Stereochemistry**

- Absolute Stereo Match (1,016)
- Absolute Stereo Mirror Image (8)
- Relative Stereo Match (28)
- Stereo that Doesn't Match Query (26)
- No Stereo in Answer Structure (31)

^ **Reagent**

^ **Catalyst**

^ **Solvent**

- Water (840)
- Tetrahydrofuran (520)
- Methanol (468)
- Dichloromethane (359)
- Toluene (338)

[View All](#)

^ **Commercial Availability**

^ **Reaction Notes**

- Stereoselective (463)
- Prophetic Reaction (27)
- Regioselective (19)
- Microwave Irradiation (15)
- Chemoselective (12)

[View All](#)

^ **Search Within Results**

Source Reference

^ **Document Type**

- Journal (248)
- Patent (804)

^ **Language**

^ **Publication Year**

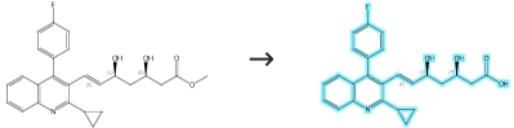
1992 to 2019

to

[View Larger](#)

^ **Publication Name**

Exploring one of the reaction Scheme



Absolute stereochemistry shown,
Rotation (-)
Double bond geometry shown

Suppliers (15)

Absolute stereochemistry shown,
Rotation (+)
Double bond geometry shown

Suppliers (38)

Step 1

Alternative Steps (1)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Sodium hydroxide	-	Methanol Water	2 h, 20 °C
2	Hydrochloric acid	-	Ethyl acetate <i>tert</i> -Butyl methyl ether Water	pH 4.5

MethodsNow Synthesis

- MethodsNow provides detailed description of the synthetic experimental procedures utilized in the lab.
- Finding these methods and protocols in the literature is time consuming.
- MethodsNow[®] is a single source for searching the latest published scientific methods by featuring step-by-step instructions that you can take right to the lab and synthesize the compound.

Experimental details using MethodsNow synthesis

Reaction Detail (Scheme 1, Reaction 1 of 1)

← Prev Next

↓ ↑ ✉ ★

Steps: 3

Step 1 | Step 2 | Step 3

Suppliers (150) | Suppliers (93)

Absolute stereochemistry shown, Rotation (+), Double bond geometry shown

Absolute stereochemistry shown, Rotation (+), Double bond geometry shown

26%

Suppliers (15) | Suppliers (38)

Absolute stereochemistry shown, Rotation (+), Double bond geometry shown

Absolute stereochemistry shown, Rotation (+), Double bond geometry shown

63%

100%

Reference

The synthesis of [¹⁸F]pitavastatin as a tracer for hOATP using the Suzuki coupling

By: Yagci, Yusuke; et al
View All

Organic & Biomolecular Chemistry (2015), 13(4), 1113-1121

Full Text

Stage	Reagents	Catalysts	Solvents	Conditions
1	Potassium carbonate	Dichloro[1,1'-bis(diphenylphosphino)ferrocene]palladium(II) dichloro methane adduct	Dimethyl sulfoxide	4 h, 70 °C

CAS Reaction Number: 31-142-CAS-18176672

^ Experimental Protocols

MethodsNow: Synthesis (142)

Experimental Procedure (257)

Experimental details using MethodsNow synthesis

Experimental Protocols

MethodsNow™

Products	6-Heptenoic acid, 7-[2-cyclopropyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-quinolinyl]-3,5-dihydroxy-, methyl ester, (3R,5S,6E)-, Yield: 26%
Reactants	Bis(pinacolato)diborane 6-Heptenoic acid, 7-(4-bromo-2-cyclopropyl-3-quinolinyl)-3,5-dihydroxy-, methyl ester, (3R,5S,6E)-
Reagents	Potassium carbonate
Catalysts	Dichloro[1,1'-bis(diphenylphosphino)ferrocene]palladium(II) dichloromethane adduct
Solvents	Dimethyl sulfoxide
Procedure	<ol style="list-style-type: none"> 1. Stir a of methyl (3R,5S,6E)-7-(4-bromo-2-cyclopropylquinolin-3-yl)-3,5-dihydroxyhept-6-enoate (1.00 g, 2.40 mmol), bis(pinacolato)-diboron (12) (0.790 g, 3.12 mmol) and K_2CO_3 (1.00 g, 7.20 mmol) in DMSO (40.0 mL) under an argon atmosphere. 2. Add $PdCl_2(dppf)CH_2Cl_2$ (0.19 g, 0.240 mmol) to the above reaction mixture. 3. Stir the resulting mixture for 4 hours at 70 °C. 4. Add silica gel to the reaction and filter the resulting mixture through celite. 5. Extract the filtrate with EtOAc and wash the organic layer with water and brine. 6. Dry the reaction mixture over Na_2SO_4. 7. Concentrate the solvent under reduced pressure to obtain a residue. 8. Subject the residue to azeotropic dehydration with MeCN and purify by HPLC to obtain a brown oil. 9. Powder the resulting oil with a 1 : 1 (v/v) mixture of diisopropyl ether and n-heptane to obtain methyl (3R,5S,6E)-7-[2-cyclopropyl-4-(4,4,5,5-tetramethyl-1,3-dioxabolan-2-yl)quinolin-3-yl]-3,5-dihydroxyhept-6-enoate.
Transformation	Preparation of Borates and Boronic Acids
Scale	gram

Characterization Data

^ 6-Heptenoic acid, 7-[2-cyclopropyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-quinolinyl]-3,5-dihydroxy-, methyl ester, (3R,5S,6E)-

Proton NMR Spectrum	(500 MHz, $CDCl_3$) δ : 7.91 (d, J = 9.2 Hz, 1H), 7.89 (d, J = 9.2 Hz, 1H), 7.56 (t, J = 9.2 Hz, 1H), 7.40 (t, J = 9.2 Hz, 1H), 7.19 (dd, J = 16.0, 1.4 Hz, 1H), 6.03 (dd, J = 16.0, 5.4 Hz, 1H), 4.66 (br, 1H), 4.38 (br, 1H), 3.75 (br, 1H), 3.73 (s, 3H), 3.32 (br, 1H), 2.56 (d, J = 3.4 Hz, 1H), 2.54 (s, 1H), 2.28 (tt, J = 8.0, 4.6 Hz, 1H), 1.87-1.78 (m, 2H), 1.46 (s, 12H), 1.25-1.20 (m, 2H), 0.98 (dd, J = 8.0, 3.1 Hz, 2H)
Carbon-13 NMR	(125 MHz, $CDCl_3$): δ 172.9, 159.6, 146.3, 138.2, 135.6, 129.2, 128.9 (2C), 128.4, 127.2 (2C), 125.4, 84.7 (2C), 72.4, 68.5, 51.9, 42.7, 41.3, 25.3 (2C), 25.2 (2C), 15.4, 9.5, 9.3
Optical Rotatory Power	$[\alpha]^{20}_D$: +22.932 (c 1.00, MeOH)
HRMS	calcd for $C_{26}H_{34}BNO_6$ (M^+): 467.2479, found 467.2481
Mass Spectrum	MS (EI): 467 (M^+ , 6.8), 346 (100), 322 (80), 220 (92), 206 (57)
State	pale yellow solid

Agenda

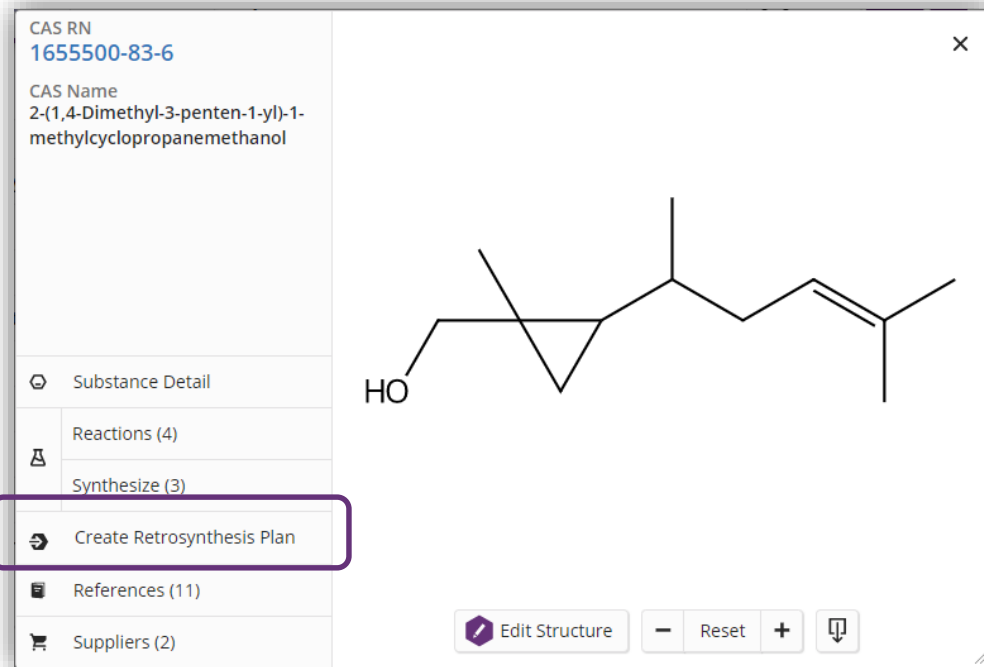
- Introduction of CAS
- What is SciFinderⁿ?
- Content and Coverage searchable in SciFinderⁿ
- A few online Case studies – General interest
 - Substance searching
 - Reference searching and PatentPak
 - Reaction searching
- **CAS Retrosynthesis planner**
- Markush structure searching
- Questions and Answers

CAS Retrosynthesis Planner

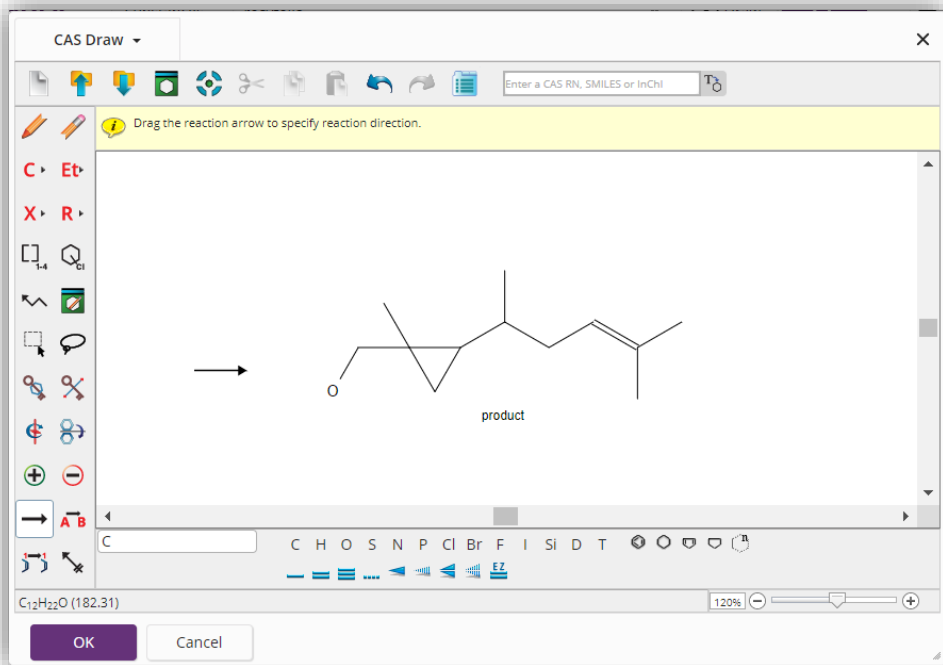
- For new or known molecules, SciFinderⁿ will perform a full retrosynthetic analysis utilizing the renowned CAS collection of reactions, presenting results in a highly intuitive and interactive synthesis plan.
- It will help,
 - Synthesizing new molecular innovations
 - Process development and scale up
 - Evaluating new synthetic options
 - Identifying opportunities for new breakthroughs in methods development

Creating retrosynthetic plan for required compound

- Built retrosynthetic plan for *Rosyfolia*



Creating retrosynthetic plan for required compound



The screenshot shows the retrosynthesis plan creation interface. It features a search bar at the top right, an "Edit" button, and a search icon. The main area displays a chemical structure with a retrosynthetic arrow pointing to it. Below the structure are two buttons: "Edit Drawing" and "Remove". A purple box highlights the "Create Retrosynthesis Plan" button, which is located below the "Edit Drawing" and "Remove" buttons. Below the highlighted button is the text "Set Plan Options".

Retrosynthesis plan

Retrosynthesis [Edit Plan Options](#) Powered by ChemPlanner®

Overview Steps

Step Key

- ⇒ B Experimental
- ⇒ A Predicted

Plan Information

Estimated Yield: 11%
Overall Price: \$15,054.94
(USD per 100 grams)

Commercially Available:
A, B, C, D, E, F, G, H

Suppliers (2) Max. Yield: 72% Suppliers (4) Max. Yield: 98% Suppliers (8) Max. Yield: 66% Suppliers (5) Suppliers (68) Max. Yield: 93% Suppliers (53)

Reset

Feedback

Searching alternative step

Retrosynthesis [Edit Plan Options](#) Powered by ChemPlanner®

Overview Steps 📄 ✉ ★ Save

A ⇒ B
Maximum Yield: 72%
Evidence (3)
Alternative Steps (67)

B ⇒ C
Maximum Yield: 98%
Evidence (34,348)
Alternative Steps (109)

C ⇒ D + E
Maximum Yield: 66%
Evidence (3)
Alternative Steps (68)

E ⇒ F
Maximum Yield: 93%
Evidence (10)
Alternative Steps (26)

F ⇒ G
Maximum Yield: -
Evidence (1)
Alternative Steps (2)

G ⇒ H
Maximum Yield: -
Evidence (1)
Alternative Steps (94)

Suppliers (2) Max. Yield: 72% Suppliers (4) Max. Yield: 98% Suppliers (8) Max. Yield: 66% Suppliers (5) Suppliers (68) Max. Yield: 93% Suppliers (53)

Reset Feedback

Alternative steps (Experimental and Predictive)

Check for the type of alternative step, evidence reactions and average yield

Alternative Steps (109)

Filter by

- Alternative Step Type
 - Experimental (1)
 - Predicted (108)

1 of 109

CC(C)C(C)C(O)C=C >> CC(C)C(C)C=O

Selected Experimental Step Evidence (34,348) Maximum Yield: 98%

2 of 109

CC(C)C(C)C(O)C=C >> CC(C)C=C + CC(C)CO

Select Predicted Step Evidence (848) Average Yield: 71%

3 of 109

CC(C)C(C)C(O)C=C >> CC(C)C=C + CC(C)CO

Select Predicted Step Evidence (6,235) Average Yield: 58%

Incorporating predictive step

Retrosynthesis [Edit Plan Options](#) Powered by ChemPlanner®

Overview Steps

Step Key

- ⇒Ⓐ Experimental
- ⇒Ⓐ Predicted

Plan Information

Estimated Yield: 24%
Overall Price: \$82.20
(USD per 100 grams)

Commercially Available:
A, B, C, D, E, F, G

Reaction Plan Summary:

Step	Starting Material	Reagents/Conditions	Max. Yield	Suppliers
A	<chem>CC(C)C(C)C(C)C</chem>		72%	2
B	<chem>CC(C)C(C)C(C)C</chem>		71% (Avg)	4
C	<chem>CC(C)C=C</chem>		95%	8
D	<chem>CC(C)C(O)C=C</chem>		-	57
E	<chem>CC(C)C=C</chem>		-	43
F	<chem>CC(C)C=O</chem>		-	71
G	<chem>CC(C)C#C</chem>		-	19

Reset +

Feedback

Evident reactions

Retrieves all published reactions discussing same type of chemical transformation

The screenshot displays the SciFinder interface for searching reactions. The top navigation bar includes the SciFinder logo, a search bar with the text 'Reactions', and various utility icons. The main content area is titled 'Reactions (848)' and features a 'View Expanded' dropdown. A filter sidebar on the left allows users to refine results by yield, number of steps, non-participating functional groups, experimental protocols, reaction type, stereochemistry, reagent, catalyst, and solvent. The main area shows two reaction schemes. Scheme 1 (1 Reaction) depicts the dimerization of an unsaturated diol to form a saturated diol. Below the reaction is a 'Suppliers (84)' button. Scheme 2 (1 Reaction) shows a reaction involving a nickel complex and an olefin, with a 'Suppliers (20)' button. A 'Reaction Summary' box for Scheme 2 provides details: '1.1 Catalysts: Nickel(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]hydro(tributylphosphine)-, 1,1,1-tri...', 'Solvents: Toluene; 6 h, 40 °C', and a reference: 'By: Kuroda, Junichi; et al Japan, JP2013035759 A 2013-02-21'. Buttons for 'PATENTPAK' and 'Full Text' are also visible.

Edit Plan Options

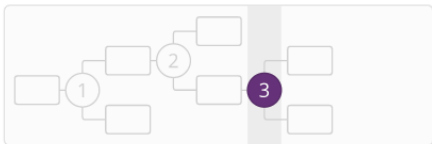
Plan Options

Powered by ChemPlanner®

Select Synthetic Depth

Synthetic depth restricts the number of steps generated in the plan. [Learn More.](#)

- 1
- 2
- 3
- 4



Set Rules Supporting Predicted Reactions

Common rules are supported by many literature examples. Uncommon and Rare rules are supported by fewer examples, but may expose novel approaches. [Learn More.](#)

- Common
- Uncommon (includes Common Rules)
- Rare (includes Common and Uncommon Rules)

➔ Create Retrosynthesis Plan

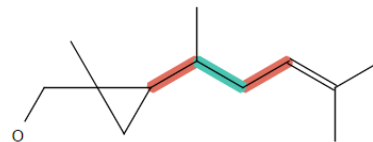
Break and Protect Bonds

You may select one bond to break in the first step of the plan. Any bonds you protect will not break, though their order may change. [Learn More.](#)

Break Bond

Protect Bond

[Clear All Bond Selections](#)



Break Bond

Protect Bond

Export, Share and Save retrosynthesis plan

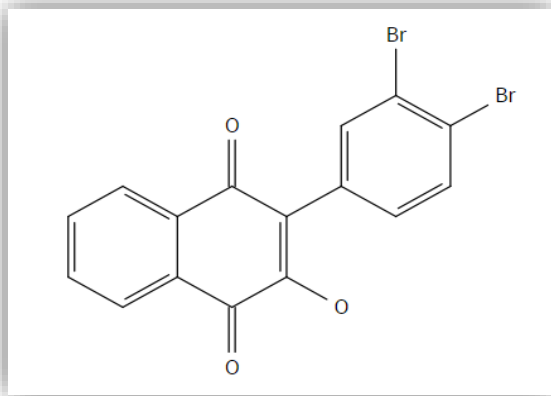
The screenshot displays the ChemPlanner Retrosynthesis interface. At the top, it says "Retrosynthesis" with an "Edit Plan Options" link. A "Powered by ChemPlanner®" badge is in the top right, containing icons for download, email, and a "Save" button. The main workspace shows a retrosynthetic plan with two steps: Step A (Experimental) and Step B (Predicted). Step A shows a bicyclic amine precursor with 2 suppliers and a maximum yield of 72%. Step B shows a linear amine precursor with 4 suppliers and an average yield. A "Save Plan" dialog box is open in the foreground, with fields for "Name", "Tags (optional)" (with checkboxes for Synthesis, process, and substances), and "New Tag (optional)". Buttons for "Save" and "Cancel" are at the bottom of the dialog. On the right side of the interface, there are additional options for "Yield:", "Suppliers (19)", and a "Feedback" button.

Agenda

- Introduction of CAS
- What is SciFinderⁿ?
- Content and Coverage searchable in SciFinderⁿ
- A few online Case studies – General interest
 - Substance searching
 - Reference searching and PatentPak
 - Reaction searching
- CAS Retrosynthesis planner
- **Markush structure searching**
- Questions and Answers

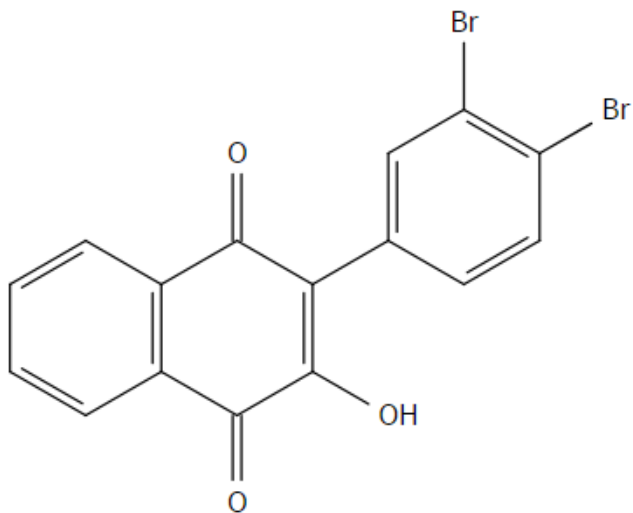
Difficult to find some substances?

- Whether the substance I prepared is novel?
- Is the below substance claimed generically in any patent?



Find it with Markush search

Is this substance indexed?



Structure Match

As Drawn (0)

Substructure (0)

So is this substance is a novel substance?

Indexing substances in patent

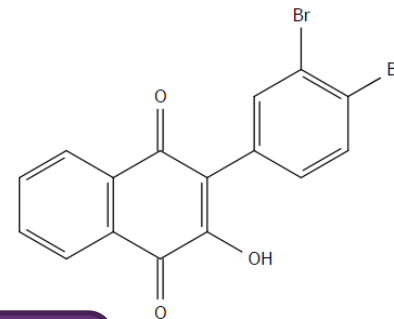
There are generally two types of substance indexing when it come to indexing in patent.

1. **Specific substances:** Represented with an exact structure and name. these substances also get CAS Registry number.
2. **Generic substances:** Represented with general or generic structure. So a single generic structure can represent hundreds of substances at once.

Similar compounds available

The screenshot shows the SciFinder search results page. The search bar at the top contains the text "Enter a query...". The left sidebar has a "Structure Match" section with "Similarity (14K)" selected. The main content area displays a grid of search results for "Substances (29)". The first result is highlighted in blue and is for the compound 860365-57-7. The grid shows chemical structures, molecular formulas, and names for several related compounds.

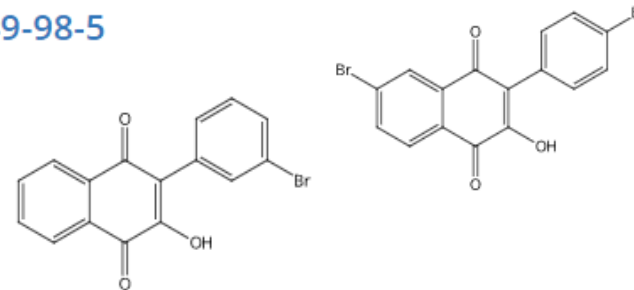
Substance ID	Chemical Formula	Name	References	Reactions	Suppliers
860365-57-7	$C_{16}H_8Br_2O_3$	1,4-Naphthalenedione, 6-bromo-3-(4-bromophenyl)-2-hydroxy-	1	0	0
860249-98-5	$C_{16}H_8BrO_3$	1,4-Naphthalenedione, 2-(3-bromophenyl)-3-hydroxy-	1	0	0
195452-14-3	$C_{16}H_8BrO_3$	2-(4-Bromophenyl)-3-hydroxy-1,4-naphthalenedione	8	5	4
860249-68-9	$C_{17}H_{11}BrO_3$	1,4-Naphthalenedione, 2-(4-bromo-2-methylphenyl)-3-hydroxy-	1	0	0
244245-02-1	$C_{16}H_8BrO_4$	1,4-Naphthalenedione, 2-(3-bromo-4-hydroxyphenyl)-3-hydroxy-	1	1	1
54808-28-5	$C_{16}H_8BrO_3$	1,4-Naphthalenedione, 6-bromo-3-hydroxy-2-phenyl-, radical ion(1-)	1	0	0
54808-27-4					
54808-14-9					
54808-13-8					



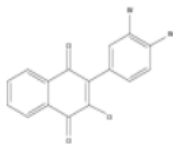
Searched query:
Similar substances:

860365-57-7

860249-98-5



Edit ▾

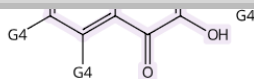


Edit Drawing

Remove

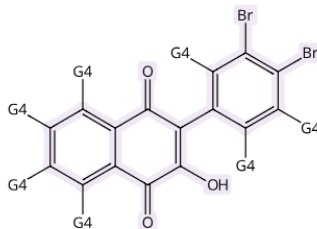
Search Patent Markush

*Know exact
location of
substance using
PatentPak*



WO2011113060

[View Reference Detail](#)



Patent claim 2

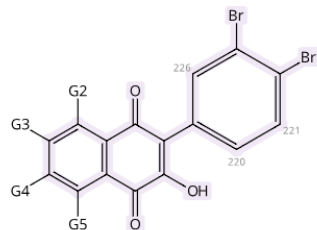
PATENTPAK ▾

Full Text ▾

There are no notes to display for this structure.

JP2006096687

[View Reference Detail](#)



Patent claim 2

PATENTPAK ▾

Full Text ▾

220,221,226: opt. substd. by (up to 3) G7

Patent

Patent Information

Patent Number

JP2006096687

Publication Date

2006-04-13

Application Number

JP2004-282855

Application Date

2004-09-28

Kind Code

A

Assignee

Riron Soyaku Kenkyusho K. K.,
Japan

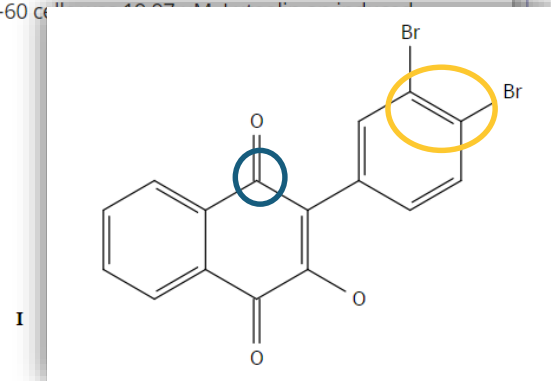
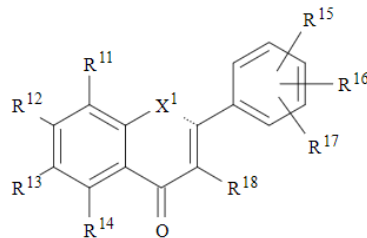
Source

Japan

Glyoxalase I inhibitors containing compounds characterized by specific pharmacophores and screening of compounds showing glyoxalase I inhibiting or apoptosis inducing activity

By: Tanuma, Seiichi; Yoshimori, Atsushi

Abstract: Glyoxalase I (I) inhibitors, which induce apoptosis because of accumulation of methylglyoxal, contain ≥ 1 selected from compounds characterized by specific pharmacophores (a figure is given) and their glycosides. The compounds may be flavones or their analogs I [$R^{11} = \text{H, C}_{1-6}$ alkoxy; $R^{12} = \text{H, OH, C}_{1-6}$ alkoxy, aryl, aryl, aryloxy, halo, etc.; $R^{13} = \text{H, OH, C}_{1-6}$ alkoxy, halo; $R^{14} = \text{H, OH}$; $R^{15}\text{-}R^{17} = \text{H, OH, C}_{1-6}$ alkoxy, aryl, halo, etc.; $R^{18} = \text{H, OH, etc.}$; dotted line = direct bond or none; when dotted line is direct bond, then $X^1 = \text{O, S, CO, SO, SO}_2$, NR^{19} ($R^{19} = \text{H, C}_{1-6}$ alkyl); when dotted line is none, then $X^1 = \text{H, OH, C}_{1-6}$ alkoxy, amino, C_{1-6} alkylcarbonyl, etc.; $X^2 = \text{O, S, CO, SO, SO}_2$, NR^{19}], etc. Method for screening compounds which inhibit I or induce apoptosis, useful as antitumor agents, involves (1) a step to analyze pharmacophores of test compounds, (2) a step to examine whether or not the pharmacophores agree the above specific pharmacophores, and (3) a step to measure I-inhibiting activity. Thus, IC_{50} of luteolin on I derived from HL-60 cells is $10.07 \mu\text{M}$. Method for screening compounds which induce apoptosis of HL-60 cells with ED_{50} $28.3 \mu\text{M}$.



PATENTPAK PDF

Full Text ▾



Search history

Rerun the
resent search.

SciFINDERⁿ
A CAS SOLUTION

★ Saved ⌚ History 👤 Account

Search

🔍 All 🔍 Substances ⚗️ Reactions 📄 References 🏪 Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query... 📐 Draw 🔍

Use [Advanced Search](#) for Author, Journal, or Organization

Recent Search History

June 25, 2019

2:25 PM	References: CAN 169:230865 (13.5M)	Edit	Rerun Search
2:22 PM	References: biodegradation of Paracetamol (185K)	Edit	Rerun Search
1:44 PM	References: formulation of amlodipine and Telmisartan (1,576)	Edit	Rerun Search
1:42 PM	References: formulation of paracetamol and Amlodipine (1,567)	Edit	Rerun Search

Search history

Handpick a type of search from search history

Assign a range of dates or select a particular month to search the history and rerun the search to get all previously viewed data.

References | Enter a query... | Draw | Search | Star | Clock | User

Filter by

Search Type

- All (109)
- Reactions (52)
- References (170)
- Retrosynthesis (5)
- Substances (192)
- Suppliers (8)

Date

Start Date | End Date

mm/dd/yyyy | to | mm/dd/yyyy

June, 2019

SU	MO	TU	WE	TH	FR	SA
26	27	28	29	30	31	1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	1	2	3	4	5	6

Search History (536)

June 25, 2019

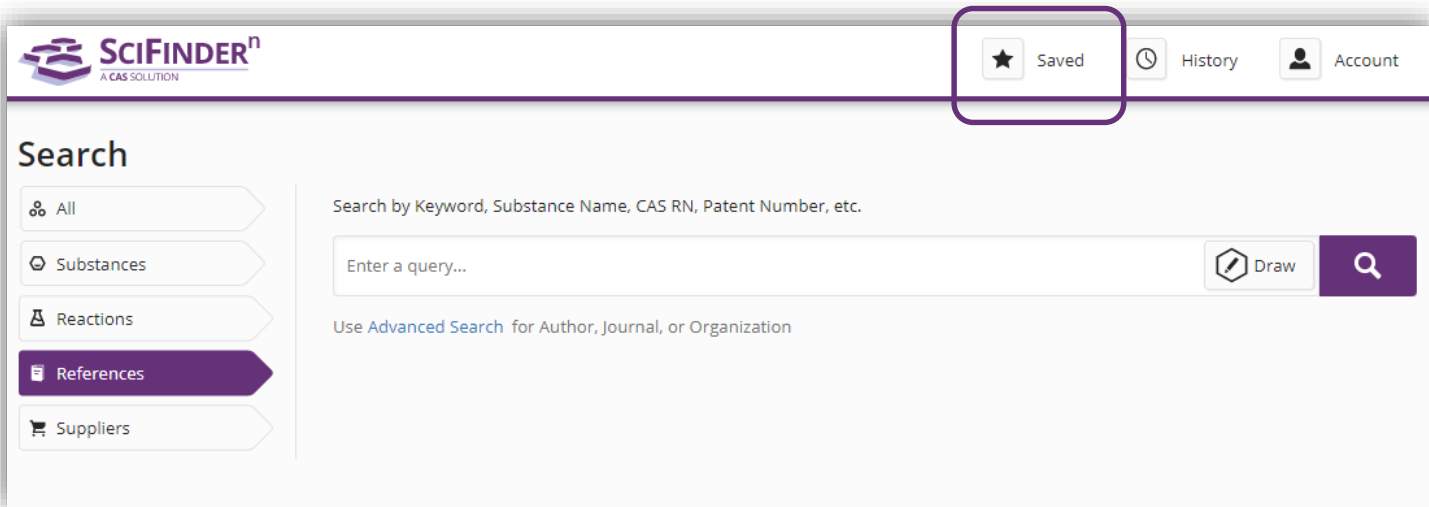
- 2:25 PM
References: CAN 169:230865 (13.5M) | Edit | Rerun Search
- 2:22 PM
References: biodegradation of Paracetamol (185K) | Edit | Rerun Search
- 1:44 PM
References: formulation of amlodipine and Telmisartan (1,576) | Edit | Rerun Search
- 1:42 PM
References: formulation of paracetamol and Amlodipine (1,567) | Edit | Rerun Search
- 12:34 PM
References: Diels-Alder reaction | As Drawn (82), Substructure (108) | Edit | Rerun Search
- 12:00 PM
References: Diels-Alder reaction | As Drawn (82), Substructure (108) | Edit | Rerun Search
- 11:59 AM
References: high pressure reaction | As Drawn (115), Substructure (143) | Edit | Rerun Search

For example

The screenshot shows the SciFinder search history page. On the left, there is a 'Filter by' section with 'Search Type' (All (38), Reactions (22), References (34), Substances (33), Suppliers (4)) and 'Date' (Start Date: 04/01/2019, End Date: 04/30/2019, and a calendar for April 2019). The main area is titled 'Search History (56)' and lists search results by date. Each entry includes a time stamp, a reference title, and 'Edit' and 'Rerun Search' buttons. A purple box highlights the 'Rerun Search' button for the entry on April 26, 2019, at 12:25 PM, which is titled 'Reactions: As Drawn (146). Substructure (6,689)'. A large purple arrow points from this button towards the right-hand screenshot.

The screenshot shows the SciFinder 'Reactions' interface. The top navigation bar includes 'Reactions' and a search bar. The main content area is titled 'Reactions (147)' and shows a list of reaction schemes. 'Scheme 1 (15 Reactions) View All' is selected, displaying a chemical reaction scheme with a yield of 98.99%. Below the scheme are filters for 'Yield' (90-100% (9), 80-89% (5), 70-79% (2), 50-69% (1), No Yield Available (130)), 'Number of Steps' (1 (69), 2 (23), 3 (9), 4 (1)), 'Experimental Protocols', 'Reaction Type', 'Reagent', 'Catalyst', 'Availability', 'Reaction Notes', and 'Search Within Results'. A purple box highlights the 'Catalyst' filter, and a large purple arrow points from this box towards the left-hand screenshot.

Access all saved answer sets



The screenshot shows the SciFinder web interface. At the top left is the SciFinder logo with the text "A CAS SOLUTION". In the top right corner, there are three navigation buttons: "Saved" (with a star icon), "History" (with a clock icon), and "Account" (with a person icon). The "Saved" button is highlighted with a purple rectangular box. Below the navigation bar is a "Search" section. On the left, there is a vertical menu with five options: "All", "Substances", "Reactions", "References" (which is highlighted in purple), and "Suppliers". The main search area contains the text "Search by Keyword, Substance Name, CAS RN, Patent Number, etc." above a search input field with the placeholder "Enter a query...". To the right of the input field are two buttons: "Draw" (with a chemical structure icon) and a search button (with a magnifying glass icon). Below the search input, there is a link that says "Use [Advanced Search](#) for Author, Journal, or Organization".

Overview

The screenshot displays the SciFinder web interface. At the top left is the SciFinder logo with the tagline 'A CAS SOLUTION'. To its right is a search bar with a 'References' dropdown and the text 'Enter a query...'. Further right are icons for 'Draw', search, star, refresh, and user profile.

On the left side, there is a 'Filter by' section with a 'Result Type' dropdown. Under 'Result Type', there are four checkboxes: 'Reactions (1)', 'References (27)', 'Retrosynthesis (1)', and 'Substances (3)'. Below this is a 'Combine Saved Results' section with a 'Combine' button. At the bottom of the left sidebar is a 'Migrate Alerts & Saved Results' section with a 'Migrate' button.

The main content area is titled '★ Saved (32)'. It contains a list of three saved items, each with a checkbox, a title, a timestamp, a category, a sub-name, and a 'Rerun Search' button. The items are:

- diuron / June 20, 2019, 5:21 PM / Substances / diuron
- amlodipine structure / June 20, 2019, 5:21 PM / Substances / amlodipine
- paracetamol / June 20, 2019, 5:20 PM / Substances / paracetamol

Each item also has an 'Alerts' dropdown and an 'Add Tags' button below it.

Search according to result type

Select any result type and rerun the search

The screenshot displays the SciFinder interface with the following elements:

- Header:** SciFinderⁿ A CAS SOLUTION, References, Enter a query..., Draw, Search, Star, Refresh, User.
- Filter by:**
 - Result Type
 - Reactions (1)
 - References (27)
 - Retrosynthesis (1)
 - Substances (3)
- Combine Saved Results:** Combine
- Migrate Alerts & Saved Results:** Migrate
- Results:**
 - ★ Saved (28)**
 - glimepiride** (June 14, 2019, 10:13 AM)
 - Retrosynthesis (with chemical structure image)
 - Open Plan button
 - synthesis if amlodipine** (April 30, 2019, 12:02 PM)
 - References: synthesis of Amlodipine + Filters
 - Rerun Search button
 - sads** (April 12, 2019, 12:39 PM)
 - References: drug
 - Rerun Search button

Migrate from SciFinder

The screenshot shows the SciFinder interface with the following elements:

- Header:** SciFINDERⁿ A CAS SOLUTION, References, Enter a query..., Draw, Search, Star, Clock, User.
- Filter by:** Result Type
 - Reactions (1)
 - References (27)
 - Retrosynthesis (1)
 - Substances (3)
- Combine Saved Results:** Combine
- Migrate Alerts & Saved Results:** Migrate
- Saved (32):**
 - diuron** (June 20, 2019, 5:21 PM) - Substances - Rerun Search
 - amlodipine structure** (June 20, 2019, 5:21 PM) - Substances - Rerun Search
 - paracetamol** (June 20, 2019, 5:20 PM) - Substances - Rerun Search

Migrate all saved references, substances or Keep me posted alerts from SciFinder if any

Combine option

SciFinderⁿ
A CAS SOLUTION

References ▾ Enter a query...

Draw 🔍 ★ ⌚ 👤

Filter by

Result Type

- Reactions (1)
- References (27)
- Retrosynthesis (1)
- Substances (3)

Combine Saved Results

Combine

Migrate Alerts & Saved Results

Migrate

★ Saved (32)

diuron ✎
June 20, 2019, 5:21 PM
Substances diuron

Alerts ▾ Add Tags ▾

amlodipine structure ✎
June 20, 2019, 5:21 PM
Substances amlodipine

Alerts ▾ Add Tags ▾

paracetamol ✎
June 20, 2019, 5:20 PM
Substances paracetamol

Rerun Search

Combine Saved Results

1 — 2 — 3

Select a result type:

Substances No eligible results to combine.

Reactions No eligible results to combine.

References **Select**

[Learn More](#)

Saved reference sets
can be combined,
intersected or
excluded to get
expected set of
references

Select sets of references to run desired combine option

Combine Saved Reference Results ×

✓ 2 3

Select a combine option: ← Prev

- Add Select
- Intersect Select
- Subtract Select

[Learn More](#)

Combine Saved Reference Results: Add ×

✓ ✓ 3

Select up to 5 saved result items: ← Prev

<input type="checkbox"/>	anti cancer drugs german bayer (50)	February 27, 2019, 8:12 AM
<input checked="" type="checkbox"/>	Nanotechnology in shape recovery polymer (85)	February 7, 2019, 11:11 AM
<input checked="" type="checkbox"/>	Nanotechnology in shape memory polymer (793)	February 7, 2019, 11:10 AM
<input type="checkbox"/>	USV (4,542)	December 21, 2018, 2:42 PM
<input type="checkbox"/>	quenching of azide using sodium sulphide (Kws) (4)	December 14, 2018, 10:14 AM
<input type="checkbox"/>	quenching of azides using sodium sulphite (Sub id) (8)	December 14, 2018, 10:12 AM
<input type="checkbox"/>	Amberlite ARP 69 (230)	December 10, 2018, 11:19 AM
<input type="checkbox"/>	Dextramethorpahn (5,511)	December 10, 2018, 11:19 AM
<input type="checkbox"/>	polixtirez (12)	December 10, 2018, 11:18 AM

View Results Cancel Learn More

Stay updated

Assign alerts with
required frequency to
stay updated

The screenshot displays the SciFinder 'Saved' search results page. On the left, there is a 'Filter by' sidebar with a 'Result Type' section containing checkboxes for Reactions (3), References (28), Retrosynthesis (1), and Substances (4). Below this are buttons for 'Combine Saved Results' and 'Migrate Alerts & Saved Results'. The main content area shows a search result for 'synthesis of amlodipine' with a date of 'June 25, 2019, 4:19 PM'. It includes a chemical structure of amlodipine and a 'Rerun Search' button. An 'Alerts' dropdown menu is open, showing options for 'No Alerts', 'Weekly', and 'Monthly'. The 'Frequency' dropdown is also visible, showing the same three options. The search result is categorized as 'Reactions' with '+ Filters As Drawn' and 'From Selected Substance Results + Filters'.

Add tags

Add a pre-saved tag or assign a new tag to saved answer

The screenshot displays the SciFinder interface for a saved search. On the left, a 'Filter by' sidebar includes sections for 'Result Type' (Reactions (3), References (28), Retrosynthesis (1), Substances (4)) and 'Tags' (Synthesis (1)). Below this are buttons for 'Combine Saved Results' and 'Migrate Alerts & Saved Results'. The main area shows a 'Saved (36)' section with a search result for 'synthesis of amlodipine' dated June 25, 2019, 4:19 PM. A chemical reaction scheme for amlodipine synthesis is shown. A 'Rerun Search' button is present. An 'Add Tags' dialog box is open, showing a list of tags with 'Synthesis' selected. Below the list is an 'Add Tag' input field and 'Save' and 'Cancel' buttons.

Protect yourself from all infectious diseases by using these precautions.



Stay home when you are sick



Avoid contact with people who are sick



Get adequate sleep and eat well-balanced meals



Wash hands often with soap and water – 20 seconds or longer



Dry hands with a clean towel or air dry your hands



Avoid touching your eyes, nose, or mouth with unwashed hands or after touching surfaces



Cover your mouth with a tissue or sleeve when coughing or sneezing



Clean and disinfect "high touch" surfaces often



Call before visiting your doctor

Thank You!

For any additional information, please contact us at
info@acs-i.org