Agenda

• Introduction of CAS
• What is SciFinder\textsuperscript{n}?
• Content and Coverage in SciFinder\textsuperscript{n}
• 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 SciFinder™.
• They intellectually analyze published articles, patents and “structure” them with standard concepts/keywords for easy retrieval.
(12) 发明专利申请

(10) 申请公布号 CN102836446 A
(43) 申请公布日 2012.12.26

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(22) 申请日 2012.05.21
(71) 申请人 华中科技大学
地址 430074 湖北省武汉市洪山区珞瑜路 1037 号
(72) 发明人 刘卫 海 刘剑平 杨晓光 陈捷 李欢 万双华 范小轶
(74) 专利代理机构 华中科技大学专利中心
地址 430074 湖北省武汉市洪山区珞瑜路 1037 号
(51) Int.Cl.
A61K 60/18 (2006.01)
A61K 60/22 (2006.01)
A61K 60/30 (2006.01)

(54) 发明名称
体内转移变肿瘤细胞纳米泡及其制备方法和用途

(57) 摘要
本发明属于生物医学工程技术领域，具体为一种体内转移变肿瘤细胞纳米泡及其制备方法和用途。纳米泡作为肿瘤靶向因子的聚乙二醇-聚
乙烯亚胺为包膜材料，以可体内发生液-气
相转变的全氟改性泡沫填料药物，采用预复
合、中空胶囊化方法制备。纳米泡进入体内后，
就整体浸没在液体内发生液-气相转变，形成
含气纳米泡，通过肿瘤因子与肿瘤细胞的特异性
结合，纳米填料集在肿瘤血管部位，从而改变肿瘤

(19) 申请公布日 2012.12.26

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

By: Liu, Wei; Xu, Haihao; Chen, Yunchao; Yang, Xiangfang; Cheng, Xin; Li, Huan; Luo, Binhua; Wan, Jialing; 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 2000-6000, polyphosphate:polyester 1.5:5:1) has chem. structure as in patent. The particle size of nanobubble (PDI ≤ 0.35) is 30-100 nm. The polyphosphate is polyyl alkyl phosphate (C1-C1 alkyl or polyyl alkyl phosphoryl (C1-C1 alkyl). The polyelester is D,L-lactide, polyl-lactide or the like. The tumor targeted factor includes folate 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 all phases by high shear(5000-30000 rpm) in ice bath, dripping oil phase into water phase by magnetic stirring in ice bath to obtain O3/C2/W, pushing mixture through hollow-membrane tube, pouring mixture into normal saline, stirring at 25℃ 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.
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, adsorbs perfluoropentane to undergo liquid-gas phase transition in vivo as a bubble core filling material, and is prepared by a special 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 connect to the tumor tissue, and thus improving the tumor focus ultrasonic imaging effect. The nanobubble can be loaded with an antitumor drug and used for targeted treatment of tumors, as well as diagnosis-treatment integrated multifunctional image-logical nano-contrast imaging agents.

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

By Xu, Wei; Xu, Haibo; Chen, Yunchao; Yang, Xiangliang; Cheng, Xin; Li, Huan; Luo, Binhuo; Wan, Jiangliang; 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 polymer 1:5-9:1) has chem. structure as in paten. The particle size of nanobubble (D<sub>0.35</sub>) is 30-100nm. The polyphosphate is polyethylene alkyl phosphate (C<sub>1-3</sub>-alkyl) or polypropyl alkyl phosphate (C<sub>1-3</sub>-alkyl). The polyester is D,L-lactate, poly L-lactate 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 O<sub>2</sub>O/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.
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
Enter your Login credentials

SciFinder® 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.

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SciFinder-n interface
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• 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

SciFinder-n provides autosuggestions for search query
Search substance by name

Retrieve all reactions, references, suppliers and create retrosynthesis plan on single click
Download, share and export substance details
2. Search substance using structure
Substance search
Type of structure searches

Structure

Exact

Exact, Stereoisomers, Salts and mixtures

Substructure

Exact Search + Substitution at open positions, Additional ring fusion, isotopes

Similarity

Similar Chemical structures containing Positional isomers, Different or fewer substituents, Different ring systems

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

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
- 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

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Refine references using concept titles
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 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 eff...

View More

References Citing This Document

25th Anniversary Article: Rational Design and Applications of Hydrogels in Regenerative Medicine
Advanced Materials (Weinheim, Germany) (2014)
CiteC 586
Multifunctional Shape-Memory Polymers
Advanced Materials (Weinheim, Germany) (2013)
CiteC 549
Shape-memory polymers and their composites: Stimulus methods and applications
Progress in Materials Science (2011)
CiteC 522
Recent advances in shape-memory polymers and composites: a review
CiteC 472
Recent advances in shape-memory polymer
Polymer (2011)
CiteC 459
A review of stimul-responsive shape memory polymer composites
Polymer (2013)
CiteC 379
Combine text and structure searching

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

9002-86-2

(C₂H₃Cl)₂
Polyvinyl chloride

99K
References 1,248
Reactions 29
Suppliers

SciFinder
A CAS Solution

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One of the reference
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
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.

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 blend of a crystalline polymer selected from the group consisting of poly(vinylidene fluoride), polyesters, polylactides, polylactide and copolymers thereof, poly(hydroxybutyrate), poly(ethylene glycol), polyethylene, polyethylene-co-vinyl acetate, poly(vinyl chloride), poly(vinylidene chloride) and copolymers of polyvinylidene 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 ml) (250 ml) followed by 2M ammonia in MeOH (250 ml). The solvent was evaporated to dryness and the resulting crude residue recrystallised from MeOH to afford the title compound;

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

15 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 DPEA (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.

20 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.

Example 1

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 A1-6.

Example 2

First, 5.4 parts of naphthalenetetracarboxylic dianhydride and 5 parts of 2-aminobutyl 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.

Example 3

First, 5.4 parts of naphthalenetetracarboxylic dianhydride, 4.5 parts of 2,6-dimethylamine (manufactured by Tokyo Chemical Industry Co., Ltd.) and 4 parts of 4-3-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.

Example 4

To a solvent mixture of 100 parts of toluene and 50 parts of ethanol, 7.4 parts of 3,6-dibromo-9,10-phenanthroline, 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. 8, pp. 227-234, (2001), was added. After 160 parts of an aqueous solution of 20% sodium carbonate was added dropwise to the mixture, 0.55 parts of tetrais(triphenylphosphine)palladium
Situation 3: Disclosed/Claimed compounds are in tabular form.

<table>
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<tr>
<th>Example</th>
<th>R¹</th>
<th>n</th>
<th>A</th>
<th>R²</th>
<th>R³</th>
<th>R⁴</th>
<th>R⁵</th>
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<td>CH</td>
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<td>H</td>
<td>H</td>
<td>Cl</td>
<td>H</td>
</tr>
<tr>
<td>I-1-29</td>
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<td>1</td>
<td>C-R¹</td>
<td>Cl</td>
<td>H</td>
<td>H</td>
<td>OMe</td>
<td>H</td>
</tr>
<tr>
<td>I-1-30</td>
<td>3-CF₃</td>
<td>1</td>
<td>C-R¹</td>
<td>Cl</td>
<td>H</td>
<td>H</td>
<td>Cl</td>
<td>NMR</td>
</tr>
<tr>
<td>I-1-31</td>
<td>3-CF₃</td>
<td>1</td>
<td>C-R¹</td>
<td>Cl</td>
<td>H</td>
<td>H</td>
<td>Cl</td>
<td>NMR</td>
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<td>Cl</td>
<td>H</td>
<td>H</td>
<td>CH₃</td>
<td>H</td>
</tr>
</tbody>
</table>

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)

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
Use ‘OR’ Boolean operator to get combined search for both keywords
Use of ‘AND’ Boolean operator to get references containing both keywords/ concepts in same reference
Use of ‘NOT’ Boolean operator to exclude one of the keyword from main search
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.
Use of quotation marks to search exact phrase along with Boolean operator

![Image of SciFinder search results]

- **References**
  - "hand sanitizer" NOT "hand wash"

**Environmenally hand sanitizer containing alcohol**
By: Lin, Gisheng
China, CN107898675 A 2018-04-13 | Language: Chinese, Database: Capius

The present invention provides an environmentally **hand sanitizer** comprising the following components 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 alk., 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.

**Processing method of ice-cold hand sanitizer**
By: Zhao, Weigang; Guo, Ziming; Zhao, Qiyuwen; Yang, Jing
China, CN108325884 A 2018-07-27 | Language: Chinese, Database: Capius

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.
Special characters and wildcard searching

- **Use of Asterisk (*) mark**

Query Disinfect* will match Disinfectant, disinfection, disinfecting, disinfected etc.
Special characters and wildcard searching

- Use of question mark (?)

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

• Search reactions for Pitavastatin
Synthetic reactions for Pitavastatin

Selecting all required refinement options, available reactions.

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)
  - 60-69% (10)
  - 50-59% (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
- Publication Name
Exploring one of the reaction Scheme

Step 1

<table>
<thead>
<tr>
<th>Stage</th>
<th>Reagents</th>
<th>Catalysts</th>
<th>Solvents</th>
<th>Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sodium hydroxide</td>
<td>-</td>
<td>Methanol, Water</td>
<td>2 h, 20 °C</td>
</tr>
<tr>
<td>2</td>
<td>Hydrochloric acid</td>
<td>-</td>
<td>Ethyl acetate, tert-Butyl methyl ether, Water</td>
<td>pH 4.5</td>
</tr>
</tbody>
</table>
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
Experimental details using MethodsNow synthesis

| Products | 6-Heptenonic acid, 7-(2-cyclopropyl-4(4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-quinoliny1)3,5-dihydroxy-, methyl ester, (3R,5S,6E). Yield: 26% |
| Reactants | Bispinacolato diborane |
|           | 6-Heptenonic acid, 7-(4-bromo-2-cyclopropyl-3-quinoliny1)-3,5-dihydroxy-, methyl ester, (3R,5S,6E). |
| Regents   | Potassium carbonate |
| Catalysts | Dichloro(1,1-bis(diphenylphosphino)ferrocenyl) palladium(II) dichloromethane adduct |
| Solvents  | Dimethyl sulfoxide |

**Procedure**

1. Stir a 0.5 g (12.1 mmol) of methyl (3R,5S,6E)-7-(4-bromo-2-cyclopropyl-3-quinoliny1)-3,5-dihydroxyhept-6-enoate (1.00 g, 7.20 mmol) in DMF (c. 0.0 mL) under an argon atmosphere.
2. Add 3.0 mL of 0.19 M 1H2O and 3.0 mL of MeCN and stir for 4 hours at 70°C.
3. Add silica gel to the reaction mixture and filter the resulting mixture through celite.
4. Extract the filtrate with EtOAc and wash the organic layer with water and brine.
5. Dry the reaction mixture over Na2SO4.
6. Concentrate the solvent under reduced pressure to obtain a residue.
7. Subject the residue to azeotropic dehydration with MeCN and purify by preparative HPLC to obtain a brown oil.
8. Powder the resulting oil with a 1:1 (v/v) mixture of dichloromethane and n-hexane to obtain methyl (3R,5S,6E)-7-(2-cyclopropyl-4(4,5,5-tetramethyl-1,3-dioxaborolan-2-yl)-3-quinoliny1)-3,5-dihydroxyhept-6-enoate.

**Transformation** Preparation of Borates and Boronic Acids

**Scale** gram
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• Markush structure searching
• Questions and Answers
CAS Retrosynthesis Planner

• For new or known molecules, SciFinder\textsuperscript{n} 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
Retrosynthesis plan

The diagram shows a retrosynthesis plan with steps labeled A to F. Each step has a corresponding yield and supplier information.

- **Step A**: Estimated Yield: 11%, Overall Price: $15,054.94 (USD per 100 grams), Suppliers (2)
- **Step B**: Max. Yield: 72%, Suppliers (4)
- **Step C**: Max. Yield: 98%, Suppliers (8)
- **Step D**: Suppliers (5)
- **Step E**: HD, Max. Yield: 93%, Suppliers (68)
- **Step F**: Suppliers (53)

Other information:
- Commonly Available: A, B, C, D, E, F, G, H

Powered by ChemPlanner®
Searching alternative step
Alternative steps (Experimental and Predictive)

Check for the type of alternative step, evidence reactions and average yield.
Incorporating predictive step
Evident reactions

Retrieves all published reactions discussing same type of chemical transformation
Export, Share and Save retrosynthesis plan
Agenda

• Introduction of CAS
• What is SciFinder\textsuperscript{n}?
• Content and Coverage searchable in SciFinder\textsuperscript{n}
• 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?

So is this substance a novel substance?
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

Searched query:
Similar substances:

860365-57-7
860249-98-5
Know exact location of substance using PatentPak
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} = H, C_{1-6} alkoxy; R^{12} = H, OH, C_{1-6} alkoxy, aryl, aryl, arylxoy, halo, etc.; R^{13} = H, OH, C_{1-6} alkoxy, halo; R^{14} = H, OH; R^{15-17} = H, OH, C_{1-6} alkoxy, aryl, halo, etc.; R^{18} = H, OH, etc.; dotted line = direct bond or none; when dotted line is direct bond, then X^{1} = O, S, CO, SO, SO_{2}, NR^{19}, NR^{19} (R^{19} = H, C_{1-6} alkyl); when dotted line is none, then X^{1} = H, OH, C_{1-6} alkoxy, amino, C_{1-6} alkylcarbonyl, etc.; X^{2} = 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 (20 μM) is an in vitro agent which induces apoptosis of HL-60 cells with ED_{50} 28.3 μM.
Search history

Rerun the resent 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.
For example
Access all saved answer sets
Search according to result type

Select any result type and rerun the search
Migrate all saved references, substances or Keep me posted alerts from SciFinder if any
Saved reference sets can be combined, intersected or excluded to get expected set of references.
Select sets of references to run desired combine option

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- Intersect
- Subtract

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- Nanotechnology in shape recovery polymer (85)
- Nanotechnology in shape memory polymer (793)
- USV (4,542)
- quenching of azide using sodium sulphide (Kw) (4)
- quenching of azides using sodium sulphite (Sub id) (8)
- Amberlite ARP 69 (230)
- Dextramethorphan (5,511)
- poloxatrem (12)

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Protect yourself from all infectious diseases by using these precautions.

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- 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