

CAS SCIFINDER DISCOVERY PLATFORM™

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科学突破之间
数据关联
至关重要**

借助 CAS SciFinder Discovery Platform,
让您的研究想法更快地实现。

CAS

A division of the
American Chemical Society



CAS SciFinder Discovery Platform

加速您的科学发现

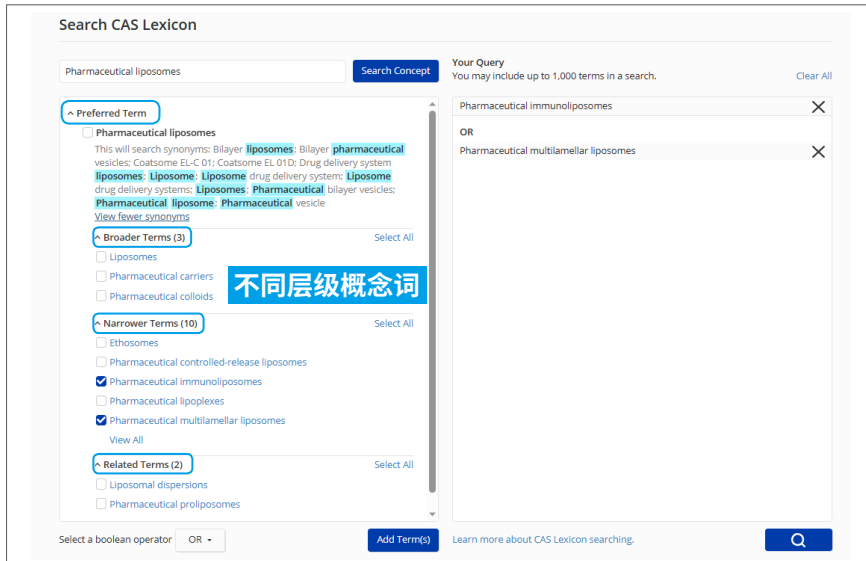
随着科学信息量不断高速增长，在纷繁复杂的信息中快速找到真正所需的科研信息可能极具挑战。CAS SciFinder Discovery Platform 是美国化学文摘社 (CAS) 隆重发布的新一代权威科学研究工具，是业界领先的检索引擎之一。CAS 国际科学家团队追踪全球科技进展，收录汇总、标引、关联全球专利、科技期刊等内容，学科收录涵盖化学及相关领域，如生物、医药、材料、食品、应用化学、化学工程、农学、高分子、物理等跨学科的科技信息；收录文献类型包括期刊、专利、会议论文、学位论文、图书、技术报告、评论、预印本和网络资源等。无论您是找寻并确定新的研究课题、申请基金、撰写论文，还是为新的项目制定实验计划或找寻合作者以推动您所在领域的研究进程，CAS SciFinder Discovery Platform 助力您更快地找到相关见解。

CAS SciFinder Discovery Platform 包括：化学及相关学科智能研究平台 CAS SciFinder、化学分析方法解决方案 CAS Analytical Methods 及制剂（配方）解决方案 CAS Formulus。

- 利用业界领先的相关性搜索引擎更快定位关键信息。
- 全面获取物质信息，自信地开展实验。
- 利用逆合成分析工具 (Retrosynthesis) 快速实现对已知和新物质的逆合成分析，确定最优路线。
- 专利解决方案 CAS PatentPak 在定位和分析大量专利中的化学结构方面，可以为师生节省一半以上的时间。
- 马库什结构 (Markush) 检索有助于快速判定化合物的新颖性和创造性。
- 利用引文地图 (Citation Map)，全面了解相关学科全景。
- 利用构效关系 (SAR)、吸收、分布、代谢、排泄和毒性 (ADMET) 数据，探索药物 - 靶点 - 毒性的相互作用。
- 检索和分析生物序列及其相关文献，助力生命科学研究。
- 运用配方设计功能 (Formulation Designer) 为配方设计提供思路。
- 利用最古老的德国化学文摘 (ChemZent) 的英文版，可追溯化学科学起源、丰富学生的化学历史知识。

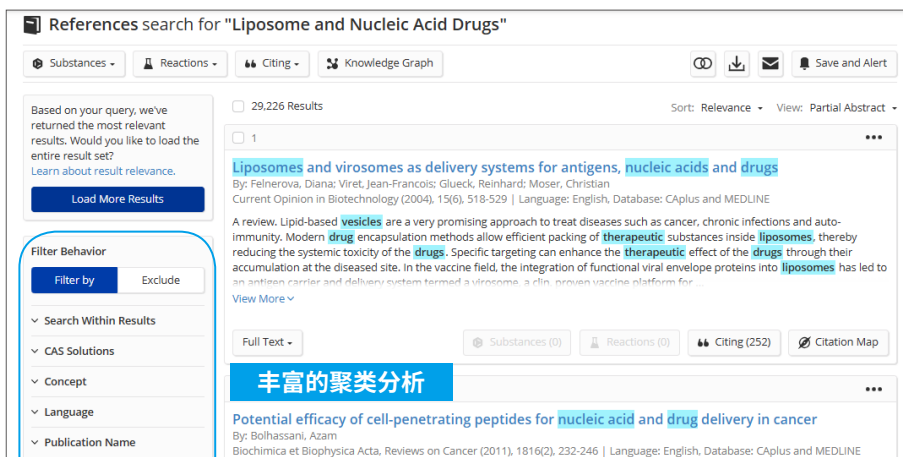
CAS 词库

CAS Lexicon: CAS 信息科学家创建的叙词表，建立数据间的关联，形成独特的 CAS 知识图谱，提高信息检索效率和精准性。



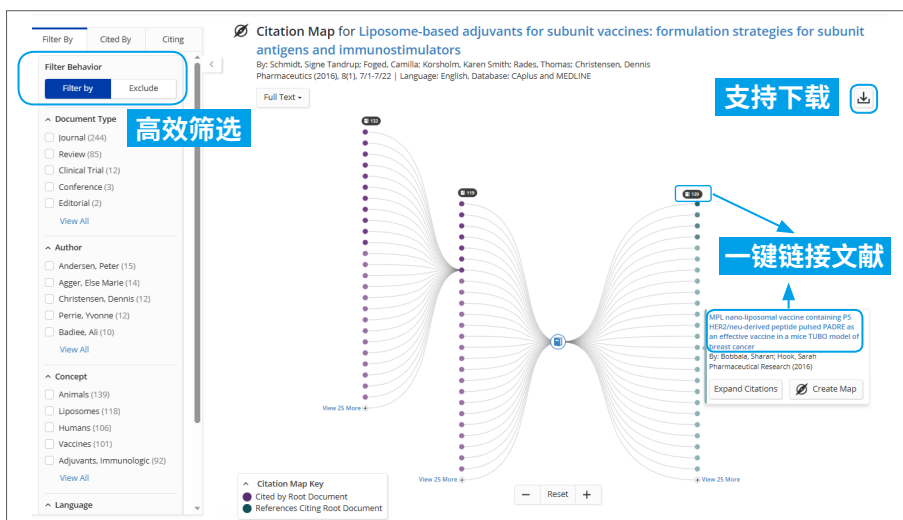
文献检索

References: 结果集按相关性排列，提供多个聚类筛选项，节省文献分析时间。



引文地图

Citation Map: 便捷地追踪前向、后向引用，并提供多个筛选项对引文进行筛选。



物质检索

Substances: 获得物质参与的反应、研究物质的文献、物质详情, 提高理解物质信息的效率。

The screenshot displays the CAS Substances search interface. On the left, there are filters for 'Structure Match' (As Drawn (2), Substructure (6,704), Similarity (242K)), 'Filter Behavior' (Filter by, Exclude), and 'Search Within Results'. The main area shows search results for 'Functional Group: Unsaturated ketone', 'Aromatic Rings: 1', and 'Stereochemistry: 3 Selected'. Three results are shown: 1) 24-Norchola-4,20,22-trien-3-one, 21,23-epoxy-11β-hydroxy- (C₂₃H₃₀O₃), 2) 17-Naphtho[2',3':13,17]-18-norandrost-4-en-3-one, 4',17-dihydro-11-hydroxy-4'-m... (C₂₇H₃₂O₂), and 3) Androst-4-en-3-one, 17-benzoyl-3,11-dihydroxy-, (11β,17β)- (C₂₆H₃₂O₃). Each result includes a chemical structure and buttons for 'References', 'Reactions', and 'Suppliers'.

便捷切换精准、亚结构、相似结构

生物活性数据

Bioactivity Data: 利用 SAR 和 ADMET 数据, 探索药物 - 靶标 - 毒性的相互作用, 评估化合物的安全性。

The screenshot shows the CAS Bioactivity Data interface. It features filters for 'Structure Activity Relationships', 'Absorption, Distribution, Metabolism, and Excretion Data', and 'Toxicity'. Below the filters, there are dropdown menus for 'Ligand', 'Target', 'Function', 'Parameter...', 'Value', 'Disease', and 'Organism'. A table displays search results for ligand 2460476-35-9, target GLP-1R, and function Inhibition. The table includes columns for 'Parameter', 'Value', 'Disease', and 'Organism', with a 'View Detail' link for each entry.

Ligand	Target	Function	Parameter	Value	Disease	Organism	Assay Information
2460476-35-9	GLP-1R	Inhibition	IC50	0.54 nM	Malaria	-	View Detail
2460476-35-9	GLP-1R	Inhibition	IC50	0.75 nM	Malaria	-	View Detail
2460476-35-9	GLP-1R	Inhibition	IC50	21 nM	Malaria	-	View Detail

序列检索

Sequences: 支持多种序列检索选项, 包括 BLAST 检索、输入 CDR 区检索抗体以及用可变符号检索序列。

The screenshot displays the CAS Sequences search interface. It shows 'Sequences search for your query' with a 'References' button. The 'BLAST Search Details' section includes 'Sequence Type: Protein', 'Search Within: Proteins', 'BLAST Algorithm: BLASTp', 'NCBI Included: Yes', 'Alignment Identity: -', 'Query Coverage: 90%', 'E-Value: 10', 'Match with Gaps?: No', 'Gap Costs: Existence 11', 'Extension 1', and 'Word Size: 3'. The 'Bioscope Analysis' section includes 'Visually explore sequence similarity with a new tool.' and a 'Create Bioscope Analysis' button. The 'Query Details' section shows 'Query: GFSGLQGPPG PPGSPGEGP SGASGAFGPR' and '935 Results'. The 'Alignment' section shows a sequence alignment with 'Alignment Identity: 100%' and 'Matches: 30, Mismatches: 0'. The 'Alignment Data' section shows 'BLAST Score: 170' and 'E-Value: 4.01429e-14'. The 'References' section includes a 'References' button and a 'View Less' dropdown.

一致性详情

关联文献

反应检索

Reactions: 获得物质参与的反应信息, 发现物质的最优合成方法, 加速方法的开发。

Structure Match: As Drawn (2,837), Substructure (7.5M)

Filter Behavior: Filter by, Exclude

Search Within Results

Yield

Reaction Scale: Milligram (63), Gram (8), No Scale Provided (219)

Non-Participating Functional Groups

Filtering: Yield: 90-100% X, Reaction Scale: Gram X, Clear All Filters

8 Results, Group: By Scheme, Sort: Yield, View: Collapsed

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

Suppliers (81), Supplier (1)

31-239-CAS-8822125, Steps: 1, Yield: 100%

One-Pot Formation of Functionalized Indole and Benzofuran Derivatives Using a Single Bifunctional Ruthenium Catalyst

By: Nair, Reji N.; et al
Topics in Catalysis (2010), 53(15-18), 1045-1047

Full Text

逆合成路线设计

Retrosynthesis: 快速提供最优的逆合成路线, 支持获取预测路线, 可自主选择替代路线。

CAS SciFinder, Reactions - Enter a query...

Retrosynthesis Plan for draw structure, Powered by ChemPlanner

Overview, Steps, Predicted Results ON, View Excluded Options, Save

Plan Information: Estimated Yield: 42%, Overall Price: \$653.24 (USD per 100 grams), Commercially Available: B, C, D, E, F, G, H

Plan Options: Synthetic Depth: 3, Predicted Rules: Common, Break & Protect Bonds: No, Starting Material Cost Limit: \$1,000.00/mol, Edit Plan Options

Scoring Profiles: Complexity Reduction, Convergence, Evidence, Cost, Yield, Atom Efficiency

已知反应, 预测型反应, 灵活调整参数

合成实验方法详情

Synthetic Methods: 获取可直接用于实验的合成方法, 直观展示每一步详细操作信息, 节省分析、归纳全文的时间。

Experimental Protocols

Synthetic Methods

Products: 1-Butanamminium, N,N,N-tributyl-, (SP-4-3)-bis(cyano-κC)[(3-methyl-1H-imidazol-1-yl)-2(3H)-ylidene]-3,2-naphthalenediylplatinat(1-), (1:1), Yield: 69%

Reactants: Di-μ-chlorobis(3-methyl-1H-imidazol-1-yl)-2(3H)-ylidene)-2,3-naphthalenediyl]diplatinum, Potassium cyanide, Tetrabutylammonium chloride

Reagents: Silver perchlorate

Solvents: Acetonitrile, Methanol, Water

Procedure: 1. Dissolve AgClO₄ (75 mg, 0.36 mmol) and [Pt₂(μ-Cl)₂(mpi)₂] (163 mg, 0.19 mmol) in methanol (30 mL). 2. Stir the reaction mixture for 4 hours in the dark. 3. Filter the mixture through Celite and evaporate the yellow filtrate to dryness. 4. Suspend the resulting yellow solid in methanol (30 mL). 5. Add KCN (47 mg, 0.72 mmol) to the mixture. 6. Stir the suspension for 2 hours and filter the mixture. 7. Evaporate the solution to dryness. 8. Suspend the resulting yellow solid in H₂O (30 mL). 9. Add n-Bu₄NCl (132 mg, 0.41 mmol) to the mixture. 10. Collect the precipitated solid by filtration. 11. Recrystallization from methanol/Et₂O to obtain the product.

Transformation: Transmetalation, Coordination of a Metal to Carbon and Heteroatom, Ligand Substitution

Scale: milligram

Characterization Data

1-Butanamminium, N,N,N-tributyl-, (SP-4-3)-bis(cyano-κC)[(3-methyl-1H-imidazol-1-yl)-2(3H)-ylidene]-3,2-naphthalenediylplatinat(1-), (1:1)

Proton NMR Spectrum: (CD₃CN, 270 MHz): δ 8.49 (t, J = 28.6 Hz, 1H), 7.77-7.69 (m, 2H), 7.62 (d, J = 1.9 Hz, 1H), 7.57 (t, J = 5.0 Hz, 1H), 7.34-7.30 (m, 2H), 7.10 (d, J = 1.9 Hz, 1H), 4.12 (s, 3H), 3.09-3.03 (m, 8H), 1.63-1.51 (m, 8H), 1.34 (sext, J = 7.5 Hz, 8H), 0.95 (t, J = 7.3 Hz, 12H).

Elemental Analysis: C₃₂H₄₇N₅Pt: C, 55.16; H, 6.80; N, 10.05%. Found: C, 55.02; H, 6.80; N, 9.96%.

State: pale-yellow crystals

马库什检索

Markush: 利用马库什结构检索快速判断化合物新颖性和创造性, 为化合物可专利性提供支持, 降低侵权风险。

Patent Markush Match

As Drawn (35)

Substructure (809)

Filter Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (22)

United States (5)

China (4)

European Patent Organization

35 Results Sort: Patent Number: Descending

1

WO2022204827

Application of halcinonide and derivatives thereof for preparing drug treating and/or preventing cerebrovascular disease

By: Chen, Xiping; Zhao, Wenyang; Liu, Jingjing; Li, Xiangxiang
World Intellectual Property Organization, WO2022204827 A1 2022-10-06 | Language: Chinese, Database: CAPLUS
Assignee: Lanzhou University

Patent claim 1

PatentPak Full Text

There are no notes to display for this structure.

CAS 科学家标引的马库什结构

专利浏览工具

CAS PatentPak: CAS 科学家对专利深度标引, 快速、精准定位专利中的重要物质。

CAS PatentPak

PAGE 238 / 543 ZOOM DOWNLOAD PDF PDF+ 下载专利原文

Key Substances in Patent

CAS RN 192704-52-2

Analyst Markup Locations (1)

Page 235

CAS RN 209253-58-7

Analyst Markup Locations (2)

Page 236

Page 238

一键定位

WO 98/25948 PCT/US97/23090

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combined methylene chloride layers were then dried over sodium sulfate to provide 45 g of a solid which was mixture of 11 α -hydroxycanrenone and the product, 7 α -cyano-11 α ,17-dihydroxy-3-oxo-17 α -pregn-4-ene-21-carboxylic acid, γ -lactone.

5 A sample of the product was analyzed by HPLC (column: 25cm x 4.6mm, 5 μ Altima C₁₈LL); solvent gradient: solvent A = water/trifluoroacetic acid = 99.9/0.1, solvent B = acetonitrile/ trifluoroacetic acid = 99.9/0.1, flow rate = 1.00 mL/minute, gradient = 65:30 (v/v) (A:B--initial), 35:65 (v/v) (A:B--after 20 minutes), 10:90 (v/v) (A:B--after 25 minutes); diode array detector) which revealed a λ_{max} of 238 nm.

10 The reaction mixture was analyzed by HPLC-NMR

15 using the following conditions: HPLC--column: Zorbax RX-

追溯早期科学研究

ChemZent®: 最早期的化学文摘——德国化学文摘的英文版, 唯一提供可用英文获取德国化学文摘的解决方案, 将化学研究相关文献回溯至十九世纪初。

28

Ausser dass in der Lymphe mehr Wasser vorhanden ist, als im Blutwasser (hier 922, dort 950 Theile) unterscheiden sich beide Flüssigkeiten noch in dem Verhältnisse der festen Bestandtheile zu den Salzen, welches in der erstern Flüssigkeit wie 88,7 : 11,3, in der letztern wie 91,2 : 8,8 ist. Gerade dieser Umstand ist es wohl, der die viel grössere Klebrigkeit des Serums bedingt, die keineswegs blos von der grössern Concentration der Eiweisslösung abhängig ist. (SIMON'S Beiträge zur phys. u. pathol. Ch. I. p. 449—457.)

Alkalische Reaction der Borsäure und ihrer Salze, nach HERZOG.

Die Färbung des Curcumapapiers durch Borsäure hängt nach den Versuchen des Verf. von der grösseren oder geringeren Intensität der gelben Farbe dieses Papiers ab, und muss man daher besonders bei vergleichenden Versuchen auf ein völlig egal gefärbtes Papier Rücksicht nehmen.

Die in Wasser gelöste reine Säure verändert die Farbe langsamer und ein wenig schwächer, als die in Alkohol gelöste, und geschieht solches wohl schon deshalb, weil der Alkohol rascher verdun-

CHEMZENT® A CAS SOLUTION

高效获取分析实验详情

CAS Analytical Methods: 便捷获取和对比来自权威期刊及专利中的分析方法详情, 提高分析化学研究的效率。

Analysis of Bacteria in Air by Microbial cell culture

分析试剂、材料、介质

CAS Method Number 1-103-CAS-263631	Method Category Air Analysis	Technique Microbial cell culture
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Analyte Bacteria	Matrix Air	Material Circular copper plate electrode (6 and 16 mm diameter)	Reagent Sodium chloride
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实验仪器

Equipment Used: High voltage supply, 205B-15R, Bertan Associate, Inc., Valhalla, NY

操作步骤

Instructions: Development of the automated electrostatic sampler (AES)

- Construct a AES sampler consisting of a half-ball shape steel electrode (radius is 45 mm) with three aerosol inlets (radius is 3.5 mm) on the top and a circular copper plate electrode (6 and 16 mm diameter) suited inside a circular plastic support.
- Build a plastic cylindrical reservoir (14 mm in diameter and 1 mm in height) with one inlet and one outlet made of copper (2 mm in diameter) above the plate electrode.
- During the sampler's operation, connect the AES sampler to a high voltage supply (model 205B-15R from Bertan Associate, Inc., Valhalla, NY) and draw the air from three air inlets where a particle charger (two copper sticks and one voltage supply up to 1.5 V) is also equipped.
- When the electrostatic field is present, collect the airborne particles into the liquid reservoir both by gravitational and electrostatic forces.
- Deliver the liquids containing the air samples in the reservoir to an antibody-based biosensor through the liquid outlets and a peristaltic pump.
- Model the electrostatic field distribution between two electrodes using ANSYS software.
- Operate the AES sampler (central electrode D = 16 mm) with sampling flow rate of 1.2 L/min at the applied sampling voltage of 20 kV.
- Operate the button aerosol sampler at the sampling flow rate of 5 L/min.
- Use a 30 min sampling to limit possible overgrowth of the collected microorganisms on 25 mm filter area.
- Culture the collected air sampling filters directly on Tryptic Soy Agar (TSA) plates at 26 °C for 3 days.
- For the AES sampler, filter the collected air samples in the reservoir first through a mixed cellulose ester (MCE) filter and then culture directly with the filter on TSA plates at 26 °C for 3 days.
- During the sampling, add 400 µL of 0.9% NaCl solution into the liquid reservoir.
- Count the colony forming units (CFUs) manually and calculate the biological collection efficiencies as the total CFU obtained per m³ of air sampled.

数据有效性

Validation: Concentration 250 CFU/m³ (sample data)

制剂 (配方) 检索工具

CAS Formulus: 高效获取制剂或配方的工艺、实验评估、目标成分及其常见配伍成分等信息, 探索合规要求。同时支持个性化设计配方或制剂。

Curcumin Loaded Oil-in-Water Nanoemulsions: Antifungal Agent or Drug Delivery System

制剂原料

Component	Function	Amount Reported
Oil-in-water nanoemulsions	-	49.5 µL
N-[2-(Dimethyloxidoamino)ethyl]pentadecanamide	pharmaceutical surfactant	3 w/w %
Glyceryl monocaprylate	-	2 w/w %
Water	-	95 w/w %
Curcumin	antimicrobial agent	-

工艺信息

Process: N-[2-(dimethyloxidoamino)ethyl]pentadecanamide and glyceryl monocaprylate were thermostatically maintained in baths at 25 °C, with stirring to equilibrate after step-wise addition of water to obtain oil-in-water nanoemulsion. curcumin solution (dissolved in dimethyl sulfoxide) was then encapsulated into the nanoemulsions to obtain curcumin loaded oil-in-water nanoemulsions.

实验评估

Descriptor	Notes	Details
antifungal activity	the effect of curcumin loaded oil-in-water nanoemulsions on reducing the growth of Candida albicans was assessed against Candida albicans, ATCC 10231 yeast strain.	27 %
cytotoxicity	the effect of curcumin loaded oil-in-water nanoemulsions on in-vitro cytotoxicity was assessed in NHDF cells human skin fibroblasts and the result was based on the cell viability.	the cell viability was diminished and as concentration increased, toxicity at higher doses was observed.
particle size	particle size of the nanoemulsion was assessed via dynamic light scattering using a Zetasizer nano ZS.	85 nm ± 3 nm
polydispersity index	particle size of the nanoemulsion was assessed via dynamic light scattering using a Zetasizer nano ZS.	0.17 ± 0.02
skin penetration efficacy	the effect of curcumin loaded oil-in-water nanoemulsions on ex-vivo skin penetration and interactions with stratum corneum was assessed after 5 h of exposure of pig ear skin, upon encapsulation of the composition with Nile red fluorescent probe.	A better promotion of Nile red penetration into the stratum corneum and its accumulation in the skin was observed.

相似制剂

- Terbutaline Sulfate Tablet; Bronchodilators; Purpose: Bronchodilators; Target: Asthma; Bronchitis; Bronchosp.; Delivery Route: Oral drug delivery syst...; Physical Form: Tablets
- Terbutaline Sulfate; Bronchodilators; Purpose: Bronchodilators; Target: Homo sapiens; Delivery Route: Oral drug delivery syst...; Physical Form: tablet
- Terbutaline Sulfate-Tablet; Bronchodilators; Purpose: Bronchodilators; Target: Asthma; Bronchitis; Bronchosp.; Delivery Route: Oral drug delivery syst...; Physical Form: Tablets
- Terbutaline Sulfate; Bronchodilators; Purpose: Bronchodilators; Target: Homo sapiens; Delivery Route: Oral drug delivery syst...; Physical Form: Tablets

Source Journal

Role of architecture of N-oxide surfactants in the design of nanoemulsions for Candida skin infection
Colloids and Surfaces, B: Biointerfaces
Language: English
Location: Article Page 1, 2, 3, 4, 5, 7, 10, Table 1, 2
Full Text | View in CAS SciFinder



美国化学文摘社 (CAS) 链接全球科学知识加速科学突破，以实现改善人们生活的愿景。CAS 助力全球创新者在当今复杂的数据环境中高效定位，在创新之旅的每个阶段做出自信的决策。作为科学知识管理专家，CAS 建立了全球权威的人工标引科学数据合集，提供不可或缺的信息解决方案、定制服务和专业资源。不同行业的科学家、专利专业人士和商业领袖信赖 CAS，从而发现机会、降低风险、解锁共享知识，更快地获得灵感实现创新。CAS 是美国化学会分支机构。

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