

CAS SCIINDER DISCOVERY PLATFORM™

灵感与 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的研究工具，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。

The screenshot shows the 'Search CAS Lexicon' interface. In the search bar, 'Pharmaceutical liposomes' is entered. Below the search bar, there are several expandable sections: 'Preferred Concept' (selected), 'Broader Concepts (3)', 'Narrower Concepts (11)', and 'Related Concepts (2)'. Under 'Preferred Concept', 'Pharmaceutical liposomes' is checked. Under 'Narrower Concepts', 'Pharmaceutical immunoliposomes' and 'Pharmaceutical multilamellar liposomes' are checked. On the right side, a detailed view of the 'Pharmaceutical liposomes - Preferred Concept' is shown, listing 'Pharmaceutical liposomes - Narrower Concept (1)' and 'Pharmaceutical multilamellar liposomes'. At the bottom, there are buttons for 'AND', 'OR', 'NOT', 'Add to Query', 'Clear Query', and 'Search'.

文献检索

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

The screenshot shows the 'References search for "Liposome and Nucleic Acid Drugs"' interface. The search results are sorted by relevance, with 34,061 results found. The first result is 'Liposomes and virosomes as delivery systems for antigens, nucleic acids and drugs' by Felnerova, Diana; Viret, Jean-Francois; Glueck, Reinhard; Moser, Christian. The second result is 'Potential efficacy of cell-penetrating peptides for nucleic acid and drug delivery in cancer' by Bolhassani, Azam. The interface includes a sidebar for 'Filter Behavior' (Filter by, Exclude) and various search filters for Substances, Reactions, Citing, and Knowledge Graph.

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。

The screenshot shows the 'Citation Map for Recent advances in using liposomes for delivery of nucleic acid-based therapeutics' interface. It features a central citation map with nodes representing documents and lines representing citations. A callout box highlights the '一键链接文献' (One-click link to literature) feature. The left sidebar provides '高效筛选' (Efficient filtering) options for Document Type (Journal, Review, Biography, Clinical Trial, Editorial, Historical), Author, Concept (Liposomes, Humans, Animals, Pharmaceutical liposomes, Homo sapiens), and Language. The bottom left shows a 'Citation Map Key' with icons for 'Cited by Root Document' and 'References Cited Root Document'.

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。

Structure Match Filtering: Aromatic Rings: 1 Functional Group: Unsaturated ketone Clear All Filters

As Drawn (2) Substructure (6,732) Similarity (246K)

便捷切换精准、亚结构、相似结构

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

Create Chemscape Analysis Filter Behavior

Filter by Exclude

Search Within Results

572 Results 1 2 3

Sort: Relevance View: Partial

193818-88-1
C₂₃H₃₀O₃
24-Norchole-4,20,22-trien-3-one, 21,23-epoxy-11 β -hydroxy-

6650-43-7
C₂₆H₃₂O₃
Androst-4-en-3-one, 17-benzoyl-3,11-dihydro-, (11 β ,17 β)-

Absolute stereochemistry shown

Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown

2 References 2 Reactions 0 Suppliers 1 Reference 1 Reaction 0 Suppliers 2 References 0 Reactions 0 Suppliers

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。

Structure Activity Relationships CAS LIFE SCIENCES

Absorption, Distribution, Metabolism, and Excretion Data CAS LIFE SCIENCES

Toxicity CAS LIFE SCIENCES

Ligand Target Function Parameter Value Disease Organism Assay Information

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。

Sequences search for your query

References

BLAST Search Details

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 Word Size: 3

Bioscape Analysis

Visually explore sequence similarity with a new tool. Learn more about Bioscape.

Create Bioscape Analysis

100,000 Results Sort: Alignment Identity View: Collapsed

1 Alignment Identity: 100% Matches: 30 Mismatches: 0

Query 1 Subject 1 30

Subject 1 1,394

View Less

Alignment Subject References

Alignment Data BLAST Score: 17 E-Value: 4.02082e-14

Q 1 GFSGLQGPPG PPGSPGEGQP SGASGPAGPR 30 S 1079 GFSGLQGPPG PPGSPGEGQP SGASGPAGPR 1108

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。

The screenshot shows a search results page for a reaction. On the left, there are filters for 'Structure Match' (As Drawn (120)), 'Substructure (3.7M)', 'Similarity (0)', 'Filter Behavior' (selected 'Filter by'), and 'Search Within Results' (Reaction Scale: Gram (7)). The main area displays 'Scheme 1 (1 Reaction)' with a reaction scheme: 2-pyridone reacts to form 2-pyridineamine. Below the scheme are two buttons: 'Suppliers (106)' and 'Suppliers (49)'. A detailed reaction card for entry 31-541-CAS-19736284 is shown, listing reagents (Ethyl chloroformate, Hydrogen), catalyst (Platinum), and conditions (Etano, 2 h, 40 bar, rt). It also includes a link to 'Reduction of Amides to Amines under Mild Conditions via Catalytic Hydrogenation of Amide Acetals and Imidates' from Advanced Synthesis & Catalysis (2019), 361(1), 185-191, and a 'Full Text' button.

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。

The screenshot shows a retrosynthesis plan for a drawn structure. At the top, it says 'Retrosynthesis Plan for drawn structure' and 'Powered by ChemPlanner®'. Below are tabs for 'Experimental Steps' (selected), 'Predicted Steps', and 'Edit Plan Options'. The main area shows a complex network of retrosynthetic steps for a target molecule. A blue box highlights a '已知反应' (Known Reaction) step, which is a standard retrosynthetic step. Another blue box highlights a '预测型反应' (Predictive Reaction) step, which is a novel or suggested retrosynthetic route. Various reaction schemes are shown with yields (e.g., Max Yield 100%, Avg. Yield 60%) and reagents (e.g., H, Pd/C, NaBH4).

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。

The screenshot shows a detailed view of a synthetic method. At the top, it says 'Experimental Protocols' and 'Synthetic Methods'. The 'Products' section lists '1-Butanaminium, N,N,N-tributyl-, (SP-4-3)-bis(cyano-κO)[(3-methyl-1H-imidazol-1-yl-2(3H)-ylidene)-3,2-naphthalenediy]platinum(1-) (1:1)' with a yield of 69%. The 'Reactants' section lists 'Dl- μ -chlorobis[(3-methyl-1H-imidazol-1-yl-2(3H)-ylidene)-2,3-naphthalenediy]diplatinum', 'Potassium cyanide', and 'Tetrabutylammonium chloride'. The 'Reagents' section lists 'Silver perchlorate'. The 'Solvents' section lists 'Acetonitrile', 'Methanol', and 'Water'. The 'Procedure' section provides a numbered list of 11 steps. To the right, there is a 'Transformation' section with 'Transmetalation', 'Coordination of a Metal to Carbon and Heteroatom', and 'Ligand Substitution'. The 'Scale' is listed as 'milligram'. The 'Characterization Data' section includes a 'Proton NMR Spectrum' (CD3CN, 270 MHz) with peaks at 8.49, 7.77-7.69, 7.62, 7.57, 5.0 Hz, 1H, 7.34-7.30, 7.10, 4.12, 3.09-3.03, 1.63-1.51, 1.34, and 0.95 ppm, and an 'Elemental Analysis' table. The 'State' is described as '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 (825)

Filter Behavior Filter by Exclude

Patent Office

World Intellectual Property Organization (22)
United States (5)
China (4)

35 Results

WO9710827 Use of antimineralcorticoid compounds against drug withdrawal syndrome

Assignees: Roussel-UCLAF; Petit, Francis; Philibert, Daniel; Goeders, Nick
World Intellectual Property Organization, WO9710827 A1 1997-03-27 |
Language: French, Database: Cplus

Patent claim 4

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 DOWNLOAD PDF PDF+

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

WO 98/25948 PCT/US97/23090

236

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

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.

The reaction mixture was analyzed by HPLC-NMR using the following conditions: HPLC--column: Zorbax RX-

一键定位

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

Equipment Used	Instructions	操作步骤
High voltage supply, 205B-15R, Bertan Associate, Inc., Valhalla, NY	Development of the automated electrostatic sampler (AES)	1. 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 in diameter) suited inside a circular plastic support. 2. 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. 3. 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. 4. When the electrostatic field is present, collect the airborne particles into the liquid reservoir both by gravitational and electrostatic forces. 5. Deliver the liquids containing the air samples in the reservoir to an antibody-based biosensor through the liquid outlets and a peristaltic pump. 6. Model the electrostatic field distribution between two electrodes using ANSYS software. 7. 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. 8. Operate the button aerosol sampler at the sampling flow rate of 5 L/min. 9. Use a 30 min sampling to limit possible overgrowth of the collected microorganisms on 25 mm filter area. 10. Culture the collected air sampling filters directly on Tryptic Soy Agar (TSA) plates at 26 °C for 3 days. 11. 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. 12. During the sampling, add 400 µL of 0.9% NaCl solution into the liquid reservoir. 13. Count the colony forming units (CFUs) manually and calculate the biological collection efficiencies as the total CFU obtained per m ³ of air sampled.
Validation	数据有效性	Concentration 250 CFU/m ³ (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。

制剂原料				
Purpose	Target	Delivery Route	Physical Form	Source
Drug delivery systems, Fungicides	Candida albicans, Homo sapiens, Oral candidiasis, Vulvovaginal candidiasis, Wound infection, curcumin, fungal skin infections, skin candidiasis	Topical drug delivery systems	Emulsions	View

相似制剂		
Component	Function	Amount Reported
Group: oil-in-water nanoemulsions	-	49.5 µL
N-[2-(Dimethylhydroxidoamino)ethyl]pentadecanamide	pharmaceutical surfactant	3 w/w %
Glycerol monocaprylate	-	2 w/w %
Water	-	95 w/w %
Curcumin	antimicrobial agent	-

[More Formulations like this... NEW](#)

Turbulaine Sulfate Tablet: Bronchodilators	Turbulaine Sulfate: Bronchodilators	Turbulaine Sulfate-Tablet: Bronchodilators	Turbulaine Sulfate: Oral drug delivery system
Purpose: Bronchodilators	Purpose: Bronchodilators	Purpose: Bronchodilators	Purpose: Bronchodilators
Target: Asthma, Bronchitis, Bronchosp...	Target: Homo sapiens	Target: Homo sapiens	Target: Homo sapiens
Delivery Route: Oral drug delivery syst...			
Physical Form: Tablets	Physical Form: tablet	Physical Form: tablets	Physical Form: Tablets

工艺信息

N-[2-(Dimethylhydroxidoamino)ethyl]pentadecanamide and glycerol 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.

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, 6, 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。

欢迎联系我们 cas.org



010.62508026/7 | china@acs-i.org

© 2025 American Chemical Society. All rights reserved.

