

CALIS第二十届培训周

CAS SciFinderⁿ增值内容和功能加速创新突破

余敏（中国市场经理）
2022年5月



ACS
International



A division of the
American Chemical Society

大纲

- 美国化学文摘社(CAS)科学家增值的内容
- CAS SciFinderⁿ增值内容和功能加速创新突破
 - 全面的数据覆盖、独特的增值功能与内容
 - 多学科、跨学科中的应用示例



CAS 致力于提高创新效率

CAS的数据和服务是基于对以往知识经验的回顾，对当代前沿研究的洞察，以及对未来发展趋势的前瞻



HINDSIGHT

连接前人的科学发现，创建更美好的未来

INSIGHT

揭示未被发现的数据关联，激发创新火花、加速科学突破

FORESIGHT

预见加速增长的趋势和新机遇

CAS具有最全面的学科连接内容合集



CAS 内容合集来源于化学、超越化学

五大类80小类

— 生物化学：

— 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学

— 有机化学各领域：

— 氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇

— 大分子化学各领域：

— 纤维素、木质素、造纸；涂料、墨水

— 染料、有机颜料；合成橡胶；纺织品、纤维

— 应用化学各领域：

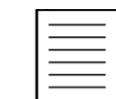
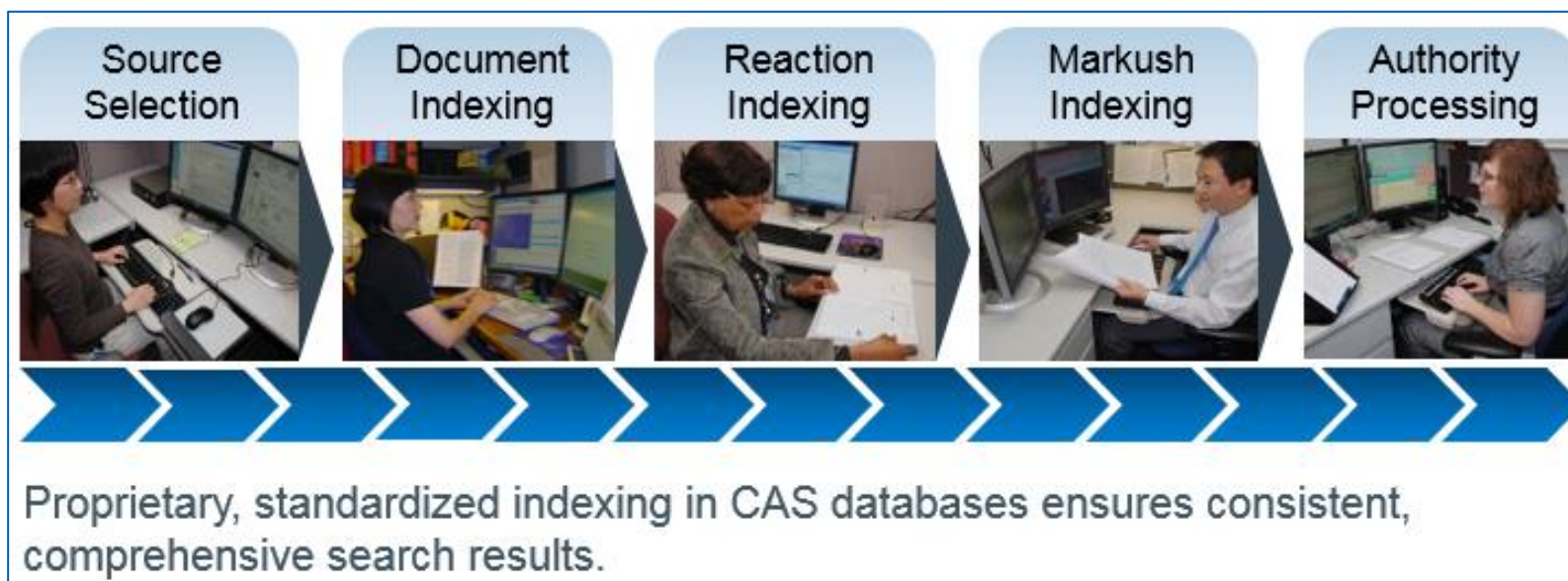
— 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金

— 物理、无机、分析化学各领域：

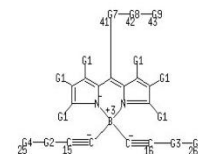
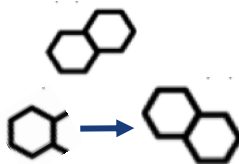
— 表面化学、催化剂、相平衡、核现象、电化学

来源：<https://www.cas.org/support/documentation/references/ca-sections>

CAS科学家的智力标引



1990
Smith, M.
anthracene



Androst-4-en-3-one,
17-hydroxy-17-
methyl-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

独特的CAS内容合集

支持多学科应用的可靠基石



来源:

<https://www.cas.org/cas-data>

<https://www.cas.org/about/cas-content>

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CAS是值得信赖的伙伴

提升各行业创新效率

制药



49

of the top 50

学术



100

of the top 100

生物技术



20

of the top 25

化工



46

of the top 50

专利局



10

of the top 10 global
patent offices

1. Pharm Exec's Top 50 Companies 2020. 2. ShanghaiRanking's Global Ranking of Academic Subjects 2020. 3. Genetic Engineering & Biotechnology News Top 25 Biotech Companies of 2019. 4. C&EN's Global Top 50 for 2020. 5. WIPO IP Facts and Figures 2019.

大纲

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 - 多学科、跨学科中的应用示例

独特的增值功能与内容

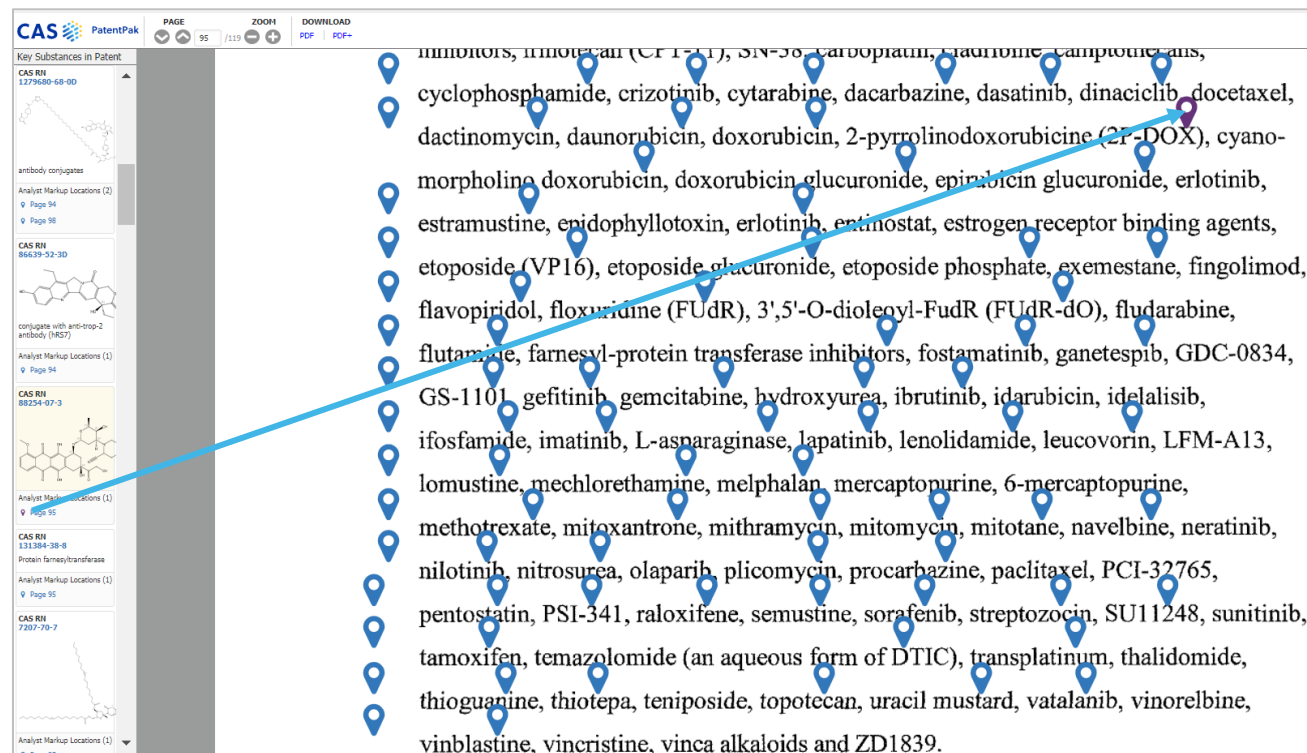
启发科研思路 & 提升获取信息的效率

- 独特的专利流程解决方案— CAS PatentPak
- 独特的合成方法详情解决方案— Synthetic Methods
- 独特的逆合成工具— CAS Retrosynthesis Tool
- 独特的分子生物学解决方案— Biosequences Search

独特的专利解决方案—CAS PatentPak

提升查找和阅读专利的效率

- CAS收录的64家专利局中 46 家主要专利局, 1800多万件专利全文, 专利数量持续增加
- 多种语言撰写的专利, 包括但不限于英语、德语、中文、日语、法语、韩语、俄语、西班牙语、保加利亚语等
- CAS科学家增值标引了物质在专利中的位置信息, 同时提供其结构、CAS登记号等信息
- 可直接下载带有CAS增值的物质位置标记信息、结构式等在内的专利全文(PDF文件)
- 下载熟悉语言撰写的同族专利



CAS PatentPak interface showing a list of substances with their CAS RN numbers and analyst markup locations. The interface includes a search bar, a list of substances, and a detailed view of a specific substance. The detailed view shows the substance name, CAS RN, and analyst markup locations. A blue line highlights a specific entry, and a list of substances is shown on the right side of the interface.

Key Substances in Patent

- CAS RN 1279680-68-00
- analyst Markup Locations (2)
- Page 94
- Page 98

antibody conjugates

- CAS RN 88639-92-3D
- analyst Markup Locations (1)
- Page 94

conjugate with anti-trp-2 antibody (HS7)

- CAS RN 88254-07-3
- analyst Markup Locations (1)
- Page 95

CAS RN 131384-38-8

Protein farnesyltransferase

- analyst Markup Locations (1)
- Page 95

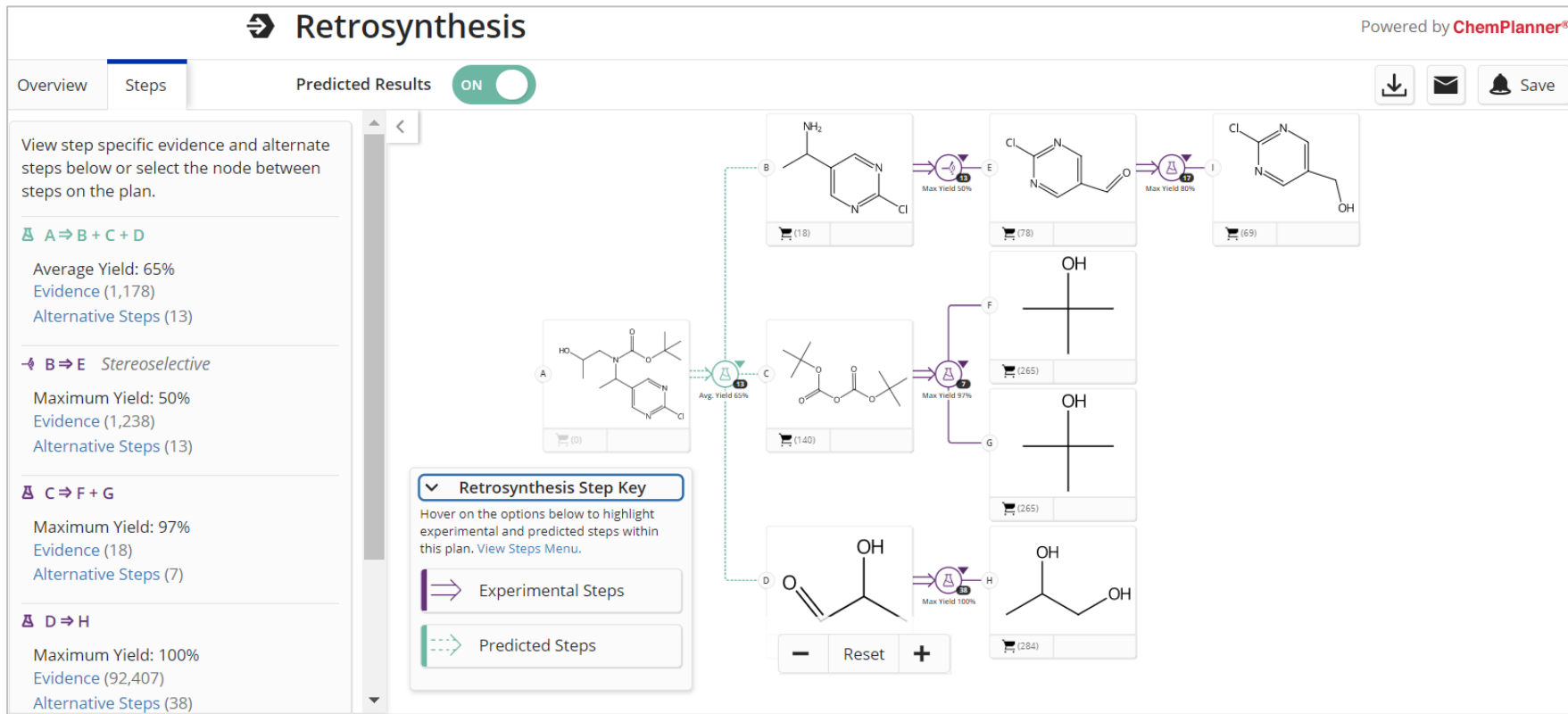
CAS RN 7207-70-7

- analyst Markup Locations (1)

inhibitors, imotican (CF-151), SN-38, carboplatin, irinotecan, camptothecins, cyclophosphamide, crizotinib, cytarabine, dacarbazine, dasatinib, dinaciclib, docetaxel, dactinomycin, daunorubicin, doxorubicin, 2-pyrrolinodoxorubicine (2P-DOX), cyanomorpholine doxorubicin, doxorubicin glucuronide, epirubicin glucuronide, erlotinib, estramustine, epidophyllotoxin, erlotinib, entinostat, estrogen receptor binding agents, etoposide (VP16), etoposide glucuronide, etoposide phosphate, exemestane, fingolimod, flavopiridol, floxuridine (FUDR), 3',5'-O-dioleoyl-FudR (FUDR-dO), fludarabine, flutamide, farnesyl-protein transferase inhibitors, fostamatinib, ganetespib, GDC-0834, GS-1101, gefitinib, gemcitabine, hydroxyurea, ibrutinib, idarubicin, idelalisib, ifosfamide, imatinib, L-asparaginase, lapatinib, lenolidamide, leucovorin, LFM-A13, lomustine, mechlorethamine, melphalan, mercaptopurine, 6-mercaptopurine, methotrexate, mitoxantrone, mithramycin, mitomycin, mitotane, navelbine, neratinib, nilotinib, nitrosourea, olaparib, plicomycin, procarbazine, paclitaxel, PCI-32765, pentostatin, PSI-341, raloxifene, semustine, sorafenib, streptozocin, SU11248, sunitinib, tamoxifen, temazolomide (an aqueous form of DTIC), transplatinium, thalidomide, thioguanine, thiotepa, teniposide, topotecan, uracil mustard, vatalanib, vinorelbine, vinblastine, vincristine, vinca alkaloids and ZD1839.

独特的逆合成工具—CAS Retrosynthesis Tool

节省设计、实施合成新方法所花费的时间



- 支持全新分子及已公开报道分子的逆合成路线设计
- 同时提供预测合成路线和文献报道的路线

独特的合成方法详细信息— Synthetic Methods

无需下载、阅读全文, 即可获得合成实验所需的所有信息

Reaction Detail (Document 1, Reaction 1 of 5)

← Prev Next →
Download Save

Steps: 1
Yield: 90%

Suppliers (106) Suppliers (62) [Stage 4] Suppliers (140) Suppliers (2)

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	-	Methanol	2 h, rt; rt → 0 °C
2	Sodium borohydride	-	-	0 °C; 1 h, 0 °C → rt; rt → 0 °C
3	Ammonium chloride	-	Water	-
4	Triethylamine	-	Tetrahydrofuran	16 h, rt
5	Hydrochloric acid	-	Water	-

CAS Reaction Number: 31-313-CAS-16424766

Experimental Protocols

Synthetic Methods

Products	1,1-Dimethylethyl N-[(1S)-2-hydroxy-1-methylethyl]-N-(phenylmethyl)carbamate, Yield: 90%
Reactants	Benzaldehyde L-Alaninol Di-tert-butyl dicarbonate
Reagents	Sodium borohydride Ammonium chloride Triethylamine Hydrochloric acid

JOURNAL

Substrate-Controlled Diastereoselectivity Reversal in NHC-Catalyzed Cross-Benzoin Reactions Using N-Boc-N-Bn-Protected α -Amino Aldehydes

By: Haghsheenas, Pouyan; et al
View All

Journal of Organic Chemistry (2016), 81(24), 12075-12083

Full Text

Company/Organization
Department of Chemistry
University of Saskatchewan
Saskatoon, Saskatchewan S7N 5C9
Canada

Solvents

Methanol
Water
Tetrahydrofuran

Procedure

1. Add freshly distilled benzaldehyde (1 equivalent) to a solution of the α -amino alcohol (1 equivalent) in dry MeOH (0.25M) at room temperature.
2. Stir the resulting solution for 2 hours.
3. Cool the resulting solution to 0 °C using an ice bath.
4. Add NaBH₄ (5 equivalents) slowly to the mixture in three portions.
5. Warm the resulting suspension to room temperature.
6. Stir the resulting suspension for 1 hour.
7. Cool the suspension once again to 0 °C.
8. Quench the suspension with the addition of saturated NH₄Cl (aqueous).
9. Extract the reaction mixture with EtOAc (×3).
10. Dry the combined organic layers over MgSO₄.
11. Reduce the crude mixture in vacuo.
12. Add triethylamine (1 equivalent) to a solution of N-Bn-amino alcohol (1 equivalent) in THF (0.3M) at room temperature.
13. Add di-tert-butyl dicarbonate (Boc₂O) (1.1 equivalents) to the solution.
14. Stir the solution at ambient temperature for 16 hours.
15. Quench the reaction mixture by addition of HCl (1M).
16. Extract reaction mixture with Et₂O (×3).
17. Wash the combined organic layers with brine.
18. Dry the combined organic over MgSO₄.
19. Purify the crude product by column chromatography.

Transformation

Reductive Alkylation of Ammonia or Amines
Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarbonates

Characterization Data

1,1-Dimethylethyl N-[(1S)-2-hydroxy-1-methylethyl]-N-(phenylmethyl)carbamate

Proton NMR Spectrum	(500 MHz, CDCl ₃) δ 7.35-7.26 (m, 4H), 7.26-7.22 (m, 1H), 4.39 (br s, 2H), 4.05-3.90 (m, 1H), 3.73-2.85 (m, 1H), 2.93 (br s, 1H), 1.43 (s, 9H), 1.14 (br d, J = 4.9 Hz, 3H).
R _f	0.21 (25% EtOAc in hexane).
State	clear colorless oil.

CAS Method Number 3-313-CAS-16424766

— 科学家提炼的实验详细信息

— 可读性高

独特的分子生物学信息— Biosequences

自信地进行查新、可专利性和自由实施检索

Searching for...

- All
- Substances
- Reactions
- References
- Suppliers
- Biosequences**
- Retrosynthesis

Biosequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about Biosequence Search.](#)

BLAST CDR Motif Upload Sequence Clear Search

Enter a query or upload a file...

Sequence Type: **Nucleotide** Protein

Search Within: Nucleotides Proteins

Include NCBI Sequences

Limit Total Sequence Results to: 1000

Start Biosequence Search

Advanced Biosequence Search [^] Adjust Parameters for Short Sequences | Reset All

Alignment Identity % <input type="text" value="80"/>	Match with Gaps? <input type="radio"/> Yes <input checked="" type="radio"/> No	Gap Costs <input type="text" value="Existence 5 Extension 2"/>
Query Coverage % <input type="text" value="90"/>	Word Size <input type="text" value="11"/>	Reward for Match Penalty for Mismatch <input type="text" value="2, -3"/>
BLAST Algorithm <input type="text" value="BLASTn"/>	E-Value <input type="text" value="10"/>	Exclude Low Complexity Regions <input type="radio"/> Yes <input checked="" type="radio"/> No

— 64家专利局出版的专利及数千种期刊中披露的核酸、蛋白、T-细胞等生物大分子

— 超过10亿条序列

— 涵盖NCBI中的序列并可直接链接至NCBI查看序列详情

— CAS科学家增值的修饰信息

独特的分子生物学信息— Biosequences

掌握序列研究全景信息

Filter by

^ E-Value
0 to 10^6

^ Query Coverage %
0 to 100

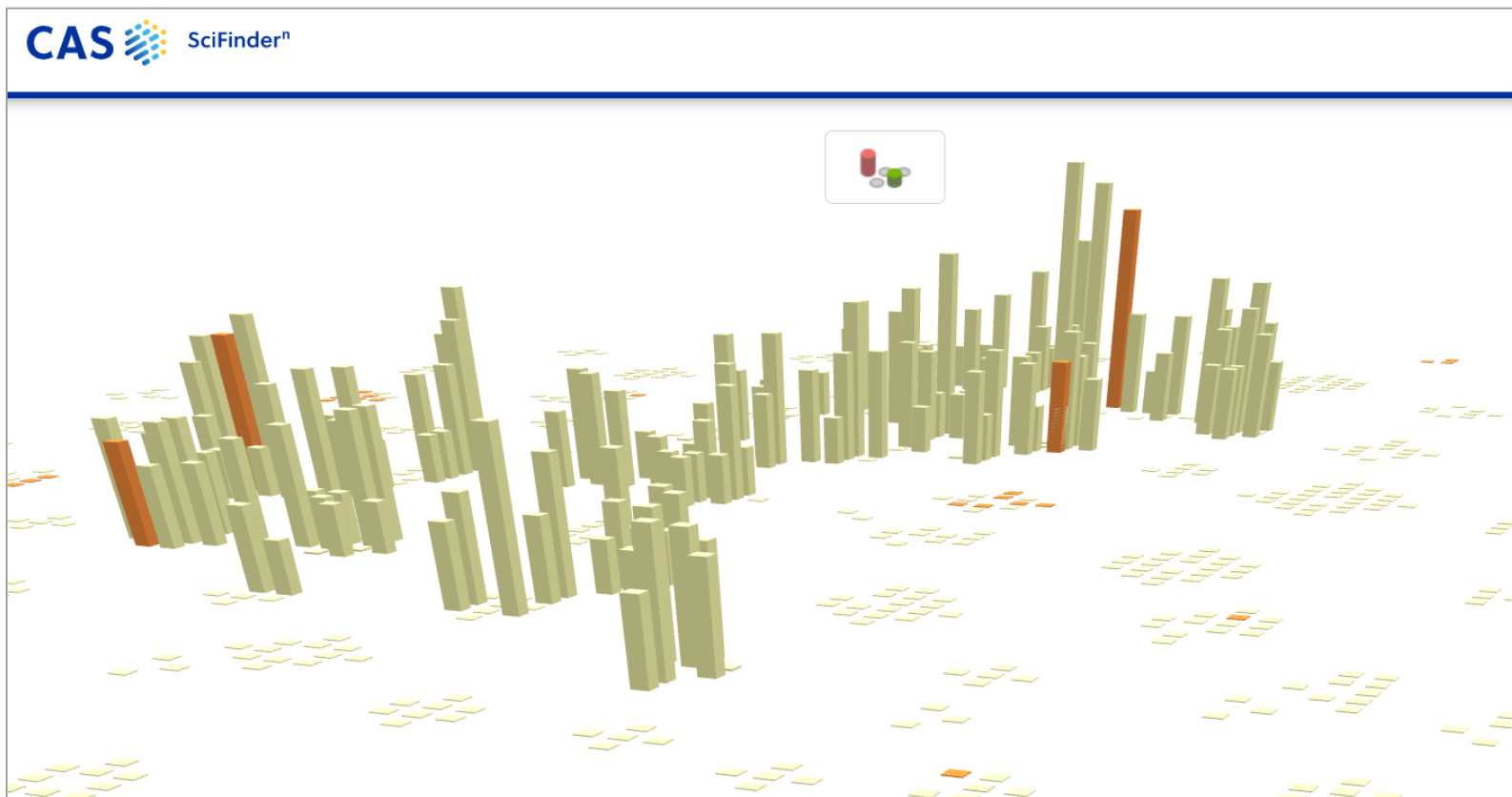
^ Subject Coverage %
0 to 100

^ Alignment Identity %
0 to 100

^ Organisms

- Crocodylus porosus (1)
- Salvia miltiorrhiza (1)

序列来源物种



可视化分析目标序列与查询序列的相似性、目标专利布局、专利法律状态等

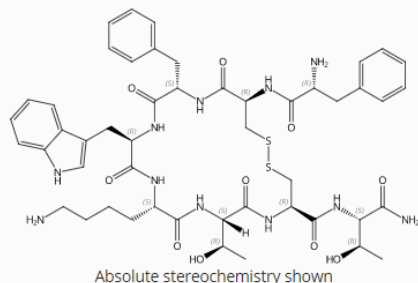
CAS科学家标引的增值序列信息

激发创新火花, 开拓创新思路

Substance Detail (3 of 151)

References (35) Reactions (11) Suppliers (2)

CAS Registry Number
99685-66-2



$C_{49}H_{65}N_{11}O_{10}S_2$

L-Threoninamide, D-phenylalanyl-L-cysteinyl-L-phenylalanyl-D-tryptophyl-L-lysyl-L-threonyl-L-cysteinyl-, cyclic (2-7)-disulfide (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	1032.24	-
Boiling Point (Predicted)	1472.2±65.0 °C	Press: 760 Torr
Density (Predicted)	1.40±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr

Protein/Peptide Sequence

Sequence Length: 8
modified

Related Sequences (714)

点击Related Sequences可以获得不同修饰的和来自不同文献的相关序列

Other Names and Identifiers

Sequence Details

Sequence: linear

1 FCFWKICT - - - -

Sequence Modifications

具体修饰位点信息

Type	Location	Description
terminal mod.	threonine-8	C-terminal amide
bridge	cysteine-2 to cysteine-7	disulfide bridge

Patent Annotations

Source: Not Given
Reference: US6268342, SEQID 21; claimed

Source: Not Given
Reference: WO2007081792, SEQID 101; claimed

大纲

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在降低知识产权风险方面的应用

CAS PatentPak

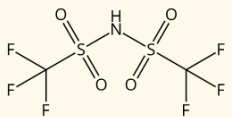
PAGE 25 / 41 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

CAS RN 1443663-24-8
Lithium tin phosphorotetrathioate sulfide (Li₁₀Sn(PS₄)₂S₄)

Analyst Markup Locations (1)
Page 25

CAS RN 90076-65-6



• Li

Analyst Markup Locations (1)
Page 25

Ionic conductivity may be characterized via ionic resistance/conductivity. The SI unit of ionic resistance is the ohm-meter ($\Omega \cdot m$) and that of ionic conductivity is Siemens per meter (S/m), wherein S is ohm^{-1} .

Inventive Example 1 (Ex 1):

5 Solid composite electrolyte composed of sulfide-based solid ionic conducting inorganic particle (LSPS, NANOMYTE® SSE-10; NEI Corporation) and a polymer electrolyte (LiTFSI and Solef®21216) were produced as the following:

10 LiTFSI and PVDF A were dissolved in ACN (acetonitrile) in order to obtain a solution where 3.6 wt% of polymer and 20 wt% of LiTFSI with respect to the polymer is added. 5.9 g of solid electrolyte in powder was added to 7 g of the polymer solution and mixed with a rotor stator. The obtained slurry was cast on an Al support and dried at ambient temperature followed by vacuum drying at 80°C overnight.

Filter by Exclude

Document Type

- Journal (1,044)
- Patent (3,435)
- Review (16)
- Conference (3)
- Preprint (13)

Substance Role

Language

- Japanese (1,096)
- English (827)
- Chinese (748)
- Korean (510)
- French (163)

Solid composite electrolyte

By: Finsy, Vincent; Merlo, Luca
World Intellectual Property Organization

The present invention relates to a solid ionic conducting inorganic particle; and consisting of (co)polymers having recu fluorosilane, acrylate, caprolactone an conducting inorganic particle is from 4 70.0 to 96.0 wt%, based on the total w manufacturing a solid composite elect inorganic particle, (iii) at least one lithi composite electrolyte and to use of the improving ionic conductivity and mech

PATENTPAK Full Text

PatentPak	Language	Kind Code	PatentPak Options
WO2022012007	English	A1	PDF PDF+ Viewer
EP3940846	English	A1	PDF PDF+ Viewer

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在降低知识产权风险方面的应用

利用机器学习，深度分析目标专利相关的现有技术。无需检索人员花费时间阅读专利全文后设计检索策略，自动进行智能化检索并提供全面的现有技术分析

Keywords: lithium ion **battery** **recycling** electrode

PatentPak PDF

Get Prior Art Analysis

Full Text ▾

Patent Family

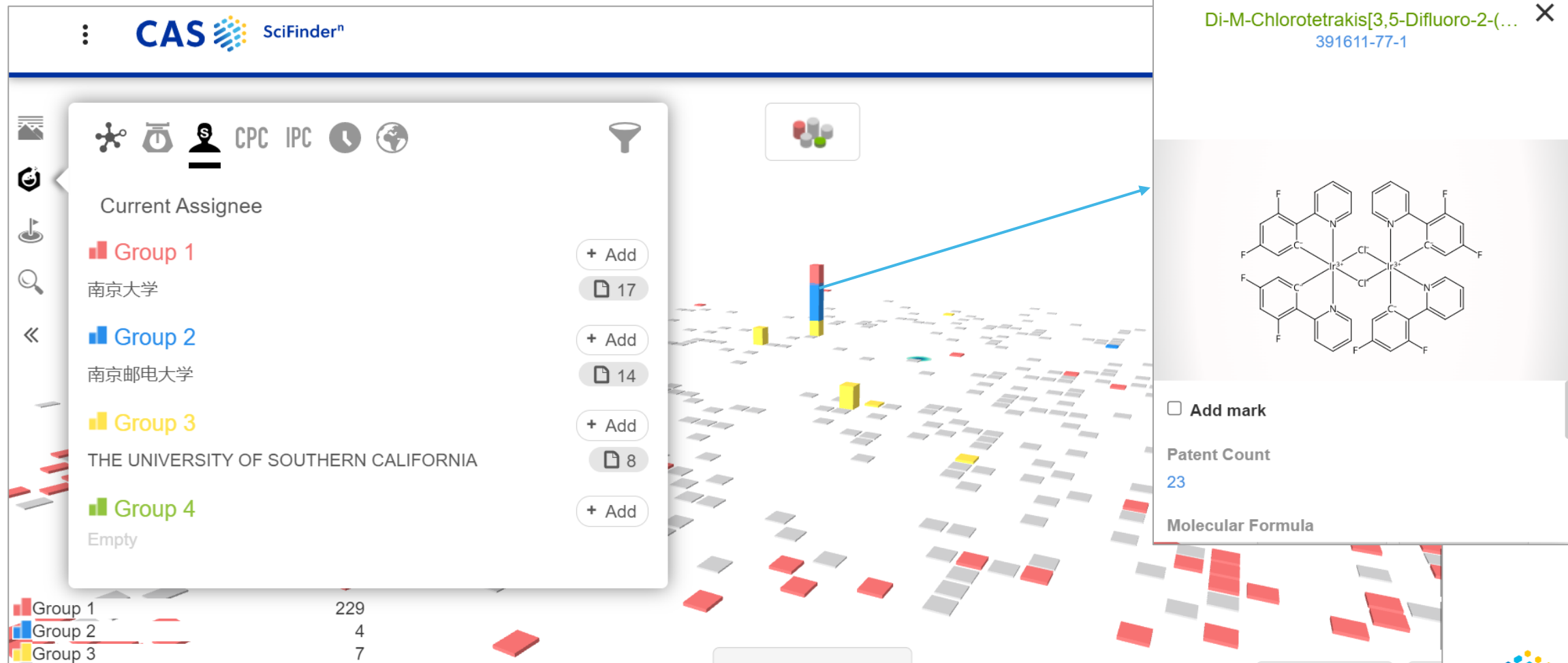
Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
JP2021044180	Japanese	A	PDF PDF+ View			
JP2021044181	Japanese	A	PDF PDF+ View			
JP2021044182	Japanese	A	PDF PDF+ View			
WO2021049668	Japanese	A1	PDF PDF+ View			

IPC Data

Patent	Class	Patent Family Classification Codes
JP2021044180	IPC1	H01M 0010/54; H01M 0010/052; H01M 0010/058; H01M 0050/409
JP2021044181	IPC1	H01M 0004/139; H01M 0010/54
JP2021044182	IPC1	H01M 0010/54
WO2021049668	IPC1	H01M 0004/139; H01M 0010/052; H01M 0010/058; H01M 0010/54; H01M 0050/409

在降低知识产权风险方面的应用

可视化分析有助于了解物质专利全景、发现研究空白及规避专利风险



在食品领域的应用

The screenshot displays the CAS SciFinder search results page. The search query is "food processing" and "food". The interface is divided into several sections:

- References (6,296):** Shows a list of search results. The first result is "Cyclodextrins as food additives and food processing" by Cravotto, Giancarlo; Binello, Arianna; and Bazzani, Roberto. The second result is "Agro-industrial potential of exotic fruits" by Ayala-Zavala, J. F.; Vega-Vega, V.; Rosas-Cordero, J. E.; and Gonzalez-Aguilar, G. A.
- Filter Behavior:** Includes a "Filter by" button and a "Document Type" section with various filters like Journal (1,665), Patent (4,549), Review (600), etc.
- Concept:** A modal window showing a list of concepts related to the search. The "Top Count" tab is selected. The list includes: Food additives (5,705), Food processing (5,478), Syrups (sweetening agents) (909), Confectionery (841), Food gels (821), Flavoring materials (745), Marmalade (647), Flavor (588), Proteins (565), Milk (552), Carbohydrates (437), Food (434), Dietary supplements (235), Fermentation (235), Green tea leaves (228), Food-processing wastes (222), Fish (221), Drying process (220), Emulsifying agents (220), Gelatins (212), Glycine max (212), Soybean (212), Enzymes (209), Carica papaya (206), Papaya (206), Condiments (165), Daucus carota (165), Polysaccharides (165), Amino acids (164), Wheat flour (163), Apple (158), Malus domestica (158), Mineral elements (156), Lipids (155), Fruit and vegetable juices (154), Food viscosity (153), and Solanum lycopersicum (153).

食品添加剂

食品加工

糖浆

糖果

凝胶

风味剂

果酱

风味

蛋白质

牛奶

碳水化合物

膳食补充剂

发酵

绿茶

食品加工废弃物

物

鱼

干燥过程

乳化剂

明胶

大豆

胡萝卜等



在无机材料领域的应用

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All

Substances

Reactions

References

Suppliers

Biosequences

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

"ceramic-metal composites" and wear-resistance

AND

Author Name

Enter last name, first name middle name.

+ Add Advanced Search Field

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文献检索支持布尔逻辑运算符(and, or, not)和
“ ”表示双引号中的内容不作同义词, 相关词拓展



Edit



R₁

设置R1为Ti, Zr

Edit Drawing

Remove



Feedback

在无机材料领域的应用

无机材料研究文献中涉及的具体物质

Structure Match

As Drawn (118)

Substructure (168)

Filter Behavior

Filter by Exclude

Document Type

Substance Role

- Uses (92)
- Process (56)
- Properties (37)
- Preparation (14)
- Formation, Non-preparative (4)

View All

物质特定研究分布

References (118)

Substances

由文献获得物质

Get Substances from References

All Results Selected Results

ogical properties of plasma s

By: Zhang, Fanyong; Li, Chao; Yan, Shu; He, Jining; Liu, Baoxi; Yin, Fuxing
Applied Surface Science (2019), 464, 88-98 | Language: English, Database

In the present work, TiCN-Mo composite coatings were fabricated by using aggregates and metal Mo powders under N₂ condition. Results showed that TiCN matrix to generate nearly alternate ceramic-metal composite coatings. Mo strips and ceramic matrix due to the formation of rim structure. The coatings. The hardness distribution uniformity of composite coatings also composite coatings showed higher friction coefficient than coatings with wear resistance with lower wear rate. Under present sliding wear conditions by thick iron and titanium oxide layer and wear debris contained large amount accompanied with oxidative wear.

Full Text

Substances (5)

Substances (128)

Sort: Relevance View: Partial

References Reactions Suppliers

Filtering: Search Within Results: Drawn Structure

1 7440-32-6 Ti Titanium

Component	Ratio
Ti	1
N	0-1
C	0-1

455K References 3,283 Reactions 890 Suppliers

2 12347-09-0 C.N.Ti Titanium carbide nitride (Ti(C,N))

Component	Percent
Ni	30-50
Al	20-70
Ti	5-20

3,627 References 0 Reactions 0 Suppliers

3 7440-67-7 Zr Zirconium

157K References 1,412 Reactions 442 Suppliers

4 1374584-70-9

5 12045-63-5 B≡Ti≡B

6 14940-68-2 Zr(IV)

在高效低毒农药、生物农药领域的应用

从主题检索开始，了解相关领域研究全景

CAS SciFinder®

References low toxicity and high efficiency and pesticide

References (775) Sort: Relevance View: Partial Abstract

Substances Reactions Citing

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. Use the CAS Solutions: Formulus filter to view available content. [Learn more about Formulus.](#)

Filter Behavior Filter by Exclude

Document Type

- Journal (420)
- Patent (355)
- Review (57)
- Conference (1)
- Report (1)

Language

Publication Year

1

Low toxicity and high efficiency insecticide

By: Tang, Zhijun
China, CN107467085 A 2017-12-15 | Language: Chinese, Database: CAplus

The invention relates to an efficient insecticide, which is retained in the atm. after ejection, but does not affect the man, and is suitable for extensive use. The **pesticide** composition consists of the following components in parts by weight: octadecanol polyethenoxy ether 20-30 parts, hibitane 0.05-0.1 parts, glycerin 3-10 parts, water 40-60 parts, omethoate 2-3 parts, tri-Ph phosphate 1-1.5 parts, imidacloprid 3-4 parts, methamidophos 0.7-0.8 parts, bergamot oil 4-5 parts, salicylic acid 0.4-0.5 parts, Et acetate 2.2-2.3 parts, stearic acid 11-12 parts.

PatentPak Full Text Substances (10) Reactions (0) Citing (0) Citation Map

2

High-efficiency low-toxicity pesticidal seed coating

By: Jia, Hongshan
China, CN1164326 A 1997-11-12 | Language: Chinese, Database: CAplus

The seed coating is composed of chem. **pesticide** 10-50, brassinolide as plant growth regulator 0.001-0.003, microelement fertilizer 2-10, film-forming agent 2-8, sorbitol as plasticizer 1-2, emulsifier 3-10, nekal as wetting agent 0.2-0.8, penetrant JFC 1-5, di-Me silicone oil as defoamer 0.1-0.3, glycol as antifreezing agent 4-8, isopropanol as quick-dryer 5-25, warning color 0.3-0.9, antiseptic

CAS SciFinder®

References biopesticide

References (8,492) Sort: Relevance View: Partial Abstract

Substances Reactions Citing

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Filter Behavior Filter by Exclude

Document Type

- Journal (4,659)
- Patent (3,506)
- Review (921)
- Biography (1)
- Book (15)

View All

Language

Publication Year

1958 to 2022

No Min to No Max Apply

View Larger

Author

Organization

Publication Name

Concept

1

Biopesticides: a review of their action, applications and efficacy

By: Copping, Leonard G.; Menn, Julius J.
Pest Management Science (2000), 56(8), 651-676 | Language: English, Database: CAplus

A review with 106 references of the wide range of different materials and organisms that can be classified as **biopesticides**. Details are given of those currently of com. importance, and future developments in this area are discussed. It is considered that, while in the immediate future **biopesticides** may continue to be limited mainly to niche and specialty markets, there is great potential for long-term development and growth, both in their own right and in providing leads in other areas of pest management science.

Full Text Substances (0) Reactions (0) Citing (244) Citation Map

2

Biopesticides: State of the Art and Future Opportunities

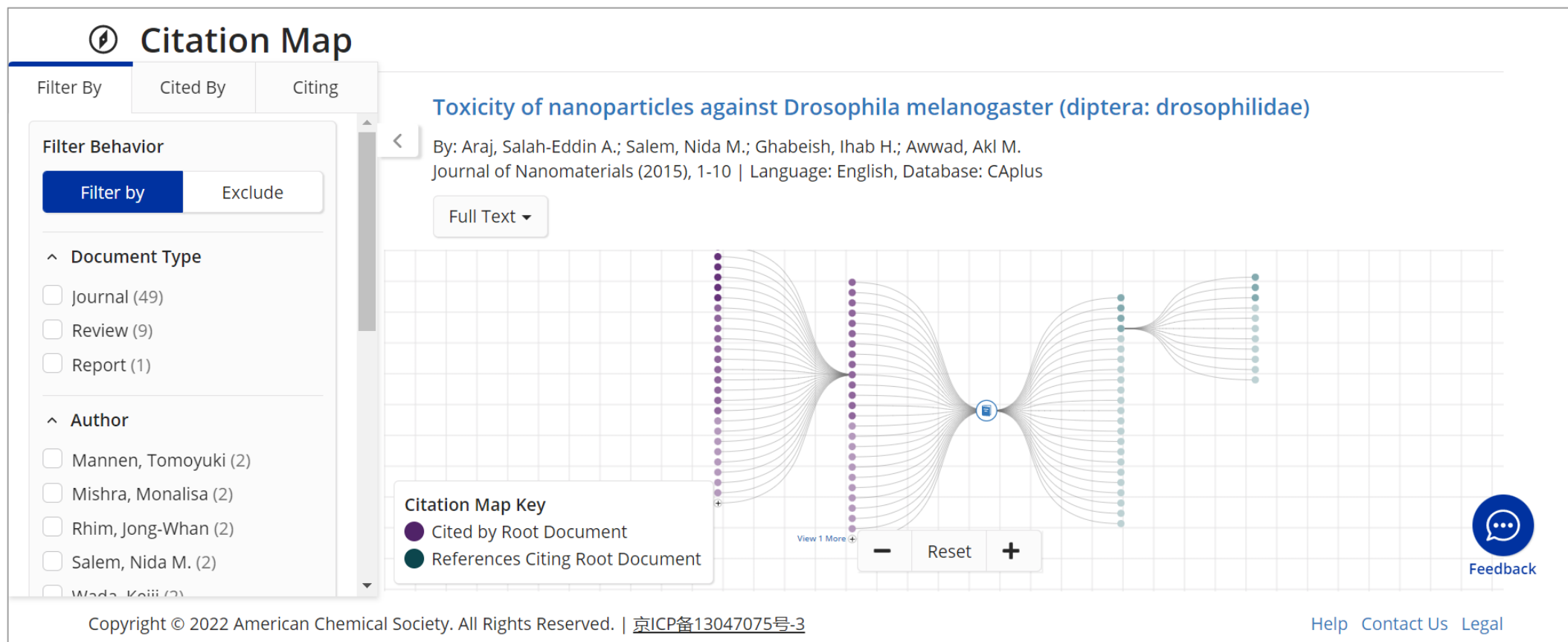
By: Selber, James N.; Coats, Joel; Duke, Stephen O.; Gross, Aaron D.
Journal of Agricultural and Food Chemistry (2014), 62(48), 11613-11619 | Language: English, Database: CAplus and MEDLINE

Protecting produce with biopesticides

A review. The use of **biopesticides** and related alternative management products is increasing. New tools, including semiochems. and plant-incorporated protectants (PIPs), as well as botanical and microbially derived chems., are playing an increasing role in pest management, along with plant and animal genetics, biol. control, cultural methods, and newer synthetics. The goal of this Perspective is to highlight promising new **biopesticide** research and development (R&D), based upon recently published work and that presented in the American Chem. Society (ACS) symposium "**Biopesticides**: State of ...

在高效低毒农药、生物农药领域的应用

多维度获取研究的脉络, 并启发拓展新的研发方向



在高效低毒农药、生物农药领域的应用

CAS科学家人工标引的信息, 助力精准、快速筛选农用物质及化学或生物农药

The screenshot shows the CAS SciFinder interface. The search results are filtered by 'Reference Role: Agricultural Use'. The left sidebar contains navigation options like 'Structure Match' (As Drawn, Substructure, Similarity) and 'Filter Behavior'. The main area displays a grid of substance cards, each with a chemical structure, name, and CAS number. The 'Reference Role' filter is highlighted in blue.

Substances (787)

Filtering: Reference Role: Agricultural Use

Reference Role	Count
Biological Study	1,045
Uses	918
Agricultural Use	787
Biological Study, Unclassified	456
Preparation	158

Substance ID	Chemical Name	References	Reactions	Suppliers
10605-21-7	Carbendazim	15K	291	92
55476-51-2	Carbamic acid, 1H-benzimidazol-2-yl- ¹⁴ C-, methyl ester	4	2	1
70191-39-8	Sulfur	46	0	1
39394-36-0				
106049-27-8				
117936-87-5				
81412-43-3				

The screenshot shows the CAS SciFinder interface with a more detailed filter panel on the left. The search results are filtered by 'Reference Role: Agricultural Use' and 'Substance Class: Nucleic Acid Sequence' and 'Protein/Peptide Sequence'. The 'Substance Class' filter is highlighted in blue.

Substances (27,999)

Filtering: Reference Role: Agricultural Use, Substance Class: 2 Selected

Filter Behavior

- Commercial Availability
- Reaction Role
- Reference Role
 - Properties (51K)
 - Biological Study (50K)
 - Biological Study, Unclassified (44K)
 - Uses (30K)
 - Agricultural Use (27K)**
- Stereochemistry
- Number of Components
- Substance Class**
 - Manual Registration (28K)
 - Nucleic Acid Sequence (22K)**
 - Organic/Inorganic Small Molecule (20K)
 - Protein/Peptide Sequence (5,196)**
 - Mixture (3,360)
- Isotopes

Substance ID	Chemical Name	References	Reactions	Suppliers
64667-10-3	Iturin	415	0	2
138860-28-3	Toxin 2 (Dendroaspis angusticeps)	21	0	0
83785-07-3	Iturin A 2	42	1	1
83777-02-0	Iturin A 6			
1392-60-5	Unspecified Mycosubtilin			
24730-31-2	Surfactin C ₁			

在高效低毒农药、生物农药领域的应用

无需查找全文，即可获取农药配方信息

Reference Detail (1 of 36)

Substances (6) Reactions (0) Citing (0) Citation Map

PATENT

Patent Number: CN109452314

Publication Date: 2019-03-12

Application Number: CN2018-11332267

Application Date: 2018-11-09

Kind Code: A

Assignee: Tianmen Yuanmiao Agricultural Industrialization Development Co., Ltd., China

Source: China, CODEN: CNXXEV

Database Information: AN: 2019:448877, CAN: 170:423518, CAplus

Language: Chinese

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. [View content from CAS Formulus®](#) in this document. [Learn more about Formulus®](#).

Pesticide special for vegetables comprising *Houttuynia cordata* and having **low toxicity** and **low residue**

By: Zhu, Yuanbo

The title **pesticide** is prepared from (by weight) 8-15 parts of veratrine, 4-10 parts of *Houttuynia cordata*, 10-15 parts of allethrin, 5-10 parts of celangulin, 2-5 parts of 64% oxadixyl, 5-8 parts of stearic acid, 3-8 parts of diafenthiuron and 120-200 parts of water. The **pesticide** has the advantages of **high efficiency**, **low toxicity**, **low residue**, simple use, **low cost**, crop safety, good control effect and no drug resistance generation.

Keywords: Chinese medicine vegetable **pesticide** *Houttuynia*

[PatentPak Viewer](#) [Get Prior Art Analysis](#) [Full Text](#)

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
CN109452314	Chinese	A	PDF PDF+ Viewer	2019-03-12	CN2018-11332267	2018-11-09

[Expand All](#) | [Collapse All](#)

IPC Data

Patent	Class	Patent Family Classification Codes
CN109452314	IPC1	A01N 0065/08; A01N 0053/10; A01N 0043/12; A01N 0047/14; A01N 0043/80; A01N 0037/06; A01N 0047/30; A01N 0043/90; A01P 0007/04

Concepts

Substances

Formulations

Pesticide Formulations: Pesticides--Low Residue, Good Control Effect, Etc.

[View CAS Formulus® Detail](#)

Location: Claim 1

Purpose: Pesticides

Target: pests

Component	Function	Amount Reported
Veratrine	pesticide	8-15 pbw
Houttuynia cordata	-	4-10 pbw
Allethrin	insecticide, chemical pesticide	10-15 pbw
2H-3,9a-Methano-1-benzoxepin-4,5,6,7,9,10-hexol, 5a-[[acetyloxy)methyl]octahydro-2,2,9-trimethyl-, 4,6,7,10-tetraacetate 5-benzoate, (3R,4R,5S,5aS,6R,7S,9S,9aS,10R)-	insecticide, pesticide	5-10 pbw

Additional Components Reported in Full Text

通过物质表征数据来获取结构信息

CAS科学家标引的性质数据, 确保用户可灵活选用多种表征数据查询物质信息

Searching for...

- All
- Substances**
- Reactions
- References
- Suppliers
- Biosequences
- Retrosynthesis

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query... Draw 🔍

- **Carbon-13 NMR** 137.6, 136.16, 135.41, 130.28, 129.31, 127.7, 77 to 79 ✕
Allowance of ± 2 ppm. *Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187*

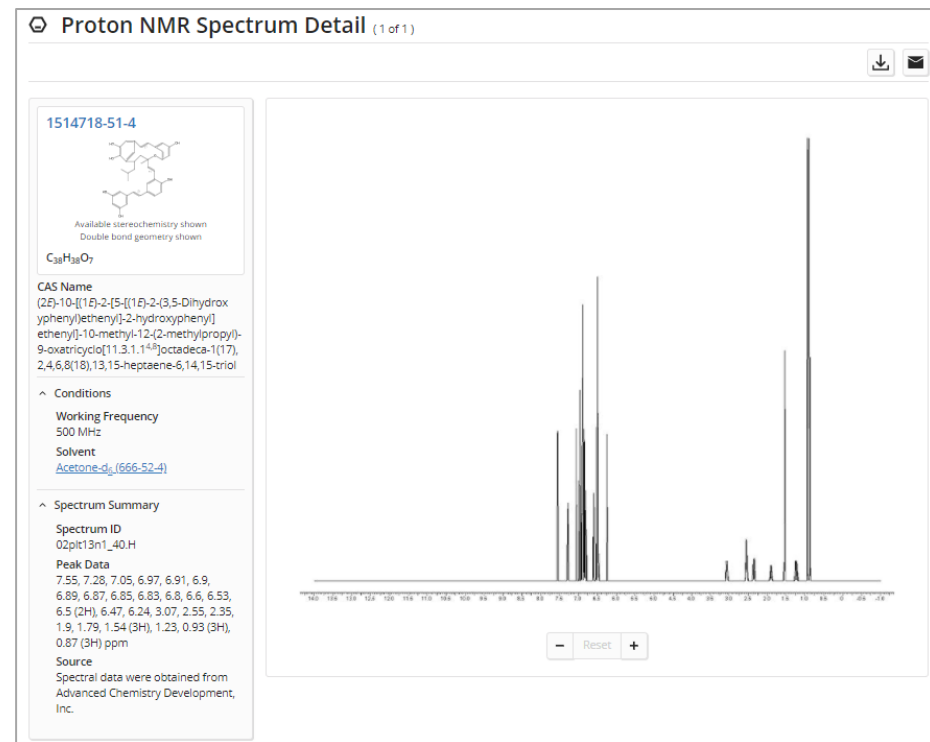
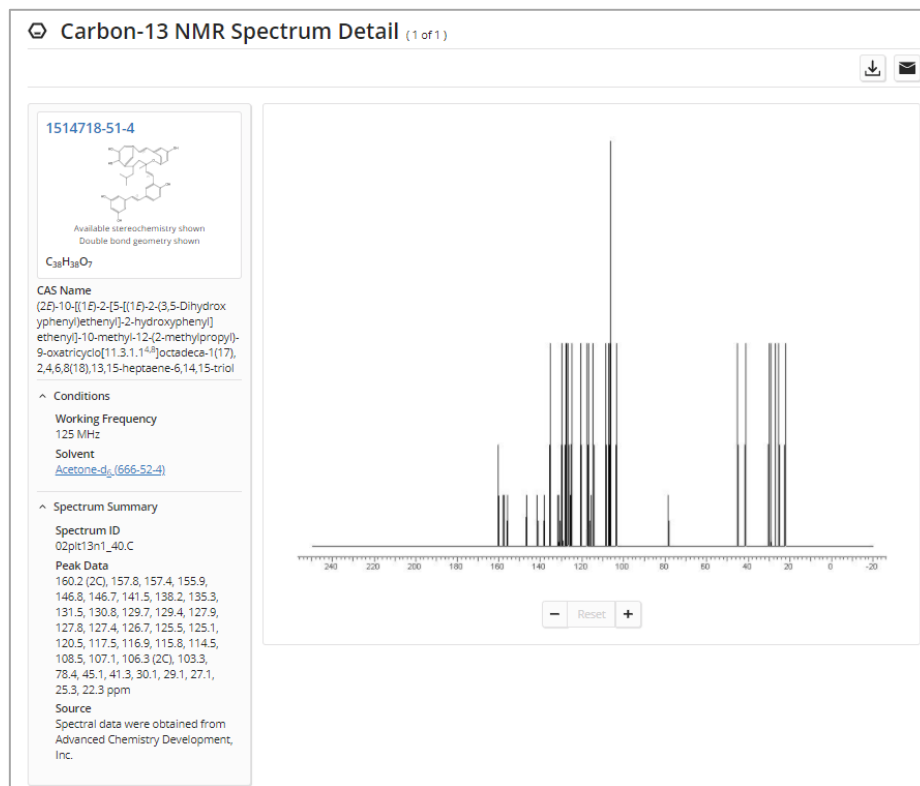
AND **Molecular Weight** 500 to 1000 ✕
Predicted values only. *Examples: 46.07 | 125 to 350 | >300*

+ [Add Advanced Search Field](#) Learn more about SciFinder[®] Advanced Search.

通过物质表征数据来获取结构信息

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- Experimental Property
 - Optical Rotatory Power (110)
 - Melting Point (37)
 - Median Lethal Dose (2)
- Experimental Spectrum
 - Carbon-13 NMR (249)
 - Proton NMR (105)
 - Mass (14)
 - IR Absorption (3)
 - Nitrogen-15 NMR (1)
- Regulatory Data by Country
- Regulatory Data by List
- Bioactivity Indicator
- Target Indicator
- Search Within Results
 - Search for up to 3 structures within the result set.
 -
 -



在天然产物研究领域的应用

The screenshot displays the CAS SciFinder web interface. At the top, the search bar contains the text "medicinal plants". The left sidebar shows a navigation menu with "Analytical Methods (4,293)" highlighted. The main content area is divided into two sections: a list of search results and a detailed view of a selected reference.

Search Results:

- 2. **Microtitre plate-based antibacterial activity of Ginkgo biloba extracts, and its application in the in vitro growth of bacteria**
By: Sarker, Satyajit D.; Nahar, Lutfun; Kumarasamy, S. *Journal of Analytical Methods* (Oxford, United Kingdom) (2007), 42(4), 31-35. | [Analytical Methods](#)
The resazurin assay utilizing microtitre-plate, described here, is a simple, accurate, and rapid method for the determination of the min. inhibitory concentration of antimicrobial fractions or purified compounds against bacteria. It is rapid, robust and reliable, and could be used successfully for the determination of the min. inhibitory concentration of antimicrobial fractions or purified compounds against bacteria.
- 3. **Effect of extraction solvent/technique on the antioxidant activity of selected medicinal plant extracts**
By: Sultana, Bushra; Anwar, Farooq; Ashraf, Muhammad

Reference Detail (3 of 4,293):

JOURNAL

Source
Molecules
Volume: 14
Issue: 6
Pages: 2167-2180
Journal: Article
2009
DOI: [10.3390/molecules14062167](https://doi.org/10.3390/molecules14062167)

Database Information
AN: 2009:785568
CAN: 152:329885
PubMed ID: 19553890
CAlplus and MEDLINE

Company/Organization
Department of Chemistry and Biochemistry
University of Agriculture
Faisalabad 38040
Pakistan

Publisher
Molecular Diversity Preservation

Effect of extraction solvent/technique on the antioxidant activity of selected medicinal plant extracts
By: Sultana, Bushra; Anwar, Farooq; Ashraf, Muhammad

The effects of four extracting solvents [absolute ethanol, absolute methanol, aqueous ethanol (ethanol: water, 80:20 volume/volume) and aqueous methanol (methanol: water, 80:20 volume/volume)] and two extraction techniques (shaking and reflux) on the antioxidant activity of extracts of barks of *Azadirachta indica*, *Acacia nilotica*, *Eugenia jambolana*, *Terminalia arjuna*, leaves and roots of *Moringa oleifera*, fruit of *Ficus religiosa*, and leaves of *Aloe barbadensis* were investigated. The tested plant materials contained appreciable amounts of total phenolic contents (0.31-16.5 g GAE/100g DW), total flavonoid (2.63-8.66 g CE/100g DW); reducing power at 10 mg/mL extract concentration (1.36-2.91), DPPH scavenging capacity (37.2-86.6%), and percent inhibition of linoleic acid (66.0-90.6%). Generally higher extract yields, phenolic contents and plant material antioxidant activity were obtained using aqueous organic solvents, as compared to the resp. absolute organic solvents. Although higher extract yields were obtained by the refluxing extraction technique, in general higher amounts of total phenolic contents and better antioxidant activity were found in the extracts prepared using a shaker.

Keywords: *Azadirachta* *Acacia* *Eugenia* *Terminalia* *Moringa* *Ficus* *Aloe* extraction solvent; antioxidant activity

Concepts: MEDLINE® Medical Subject Headings, Substances, Analytical Methods

Title	CAS Method Number
Analysis of Flavonoids in <i>Azadirachta indica</i> by Solvent extraction	1-131-CAS-3185996



在天然产物研究领域的应用

CAS科学家标引的数据, 无需查找全文即可获得萃取天然产物所需的所有实验信息

CAS Solutions ▾

CAS Analytical Methods

Method Detail (1 of 1)

Analysis of Flavonoids in *Azadirachta indica* by Solvent ext

CAS MN: 1-131-CAS-3185996

Method Category: Natural Product Isolation Analysis
Technique: Spectrophotometry; Solvent extraction

Materials	Role
Flavonoids	
Fruits	
<i>Syzgium cumini</i>	

Equipment Used

Orbital shaker, Gallenkamp, UK
Rotary evaporator, EYELA, SB-651, Rikakikai Co. Ltd., Tokyo, Japan
Spectrophotometer

Conditions

Instrument
Detection wavelength- 510 nm

Instructions

Plant material

1. Collect the barks of *Azadirachta indica* (Neem), *Acacia nilotica* (Desi kiker), *Eugenia jambolana* (Jaman), *Terminalia arjuna* (Arjun), leaves and roots of *Moringa oleifera* (Sohanjana), fruit of *Ficus religiosa* (Peepal) and leaves of *Aloe barbadensis* (Aloe vera) and use for analysis.

Sample extraction (Extraction using absolute methanol by refluxing)

1. Extract the air-dried ground (80 mesh) plant material (20 g for each sample) with absolute methanol (200 mL) for 6 hours at room temperature under reflux on a water bath.
2. Separate the extracts from the residues by filtering through Whatman No. 1 filter paper.
3. Extract the residues twice with the same fresh solvent and combine the extracts.
4. Concentrate the combined extracts and evaporate the solvent under reduced pressure at 45 °C, using a rotary evaporator (EYELA, SB-651, Rikakikai Co. Ltd. Tokyo, Japan).
5. Weigh the dried crude concentrated extracts to calculate the yield and store in a refrigerator (- 4 °C) until use.

Determination of total flavonoid contents (TFC)

1. Dilute the extracts of each plant material (1 mL containing 0.1 mg/mL) with water (4 mL) in a 10 mL volumetric flask.
2. Add 5% NaNO₂ solution (0.3 mL) to each volumetric flask.
3. Add 10% AlCl₃ (0.3 mL) after 5 min.
4. Add 1.0 M NaOH (2 mL) after 6 min.

Validation

Concentration	Value
	5.90 ± 0.16 CE g/100 g of DW (<i>Moringa oleifera</i> leaves)
	1.02 ± 0.03 CE g/100 g of DW (<i>Moringa oleifera</i> root)
	1.99 ± 0.06 CE g/100 g of DW (<i>Eugenia jambolana</i> bark)
	3.92 ± 0.12 CE g/100 g of DW (<i>Acacia nilotica</i> bark)
	2.16 ± 0.08 CE g/100 g of DW (<i>Azadirachta indica</i> bark)
	1.78 ± 0.06 CE g/100 g of DW (<i>Terminalia arjuna</i> bark)
	1.97 ± 0.05 CE g/100 g of DW (<i>Ficus religiosa</i> Fmit)
	2.90 ± 0.07 CE g/100 g of DW (<i>Aloe barbadensis</i> leaves)

↑

CAS SciFinderⁿ增值内容和功能加速创新突破

- CAS科学家人工标引, 能够揭示隐藏在数据间的隐秘关联
- CAS内容合集来源于化学并超越于化学, 支持多学科、跨学科科研创新
- 全面的内容确保不遗漏任何重要的信息
- 强大的功能确保降低文献检索和分析的时间, 将更多宝贵的时间应用于创新工作中, 提升科研创新效率

谢谢关注！



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