

# CAS: SciFindern Discovery Platform 使用說明

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# CAS, Chemical Abstracts Service

- Coverage : CApius, produced by CAS, contains more than 44 million chemistry and chemistry related research records categorized in 80 sections, with references in:

All areas of biochemistry	All areas of organic chemistry	All areas of macromolecular chemistry	All areas of applied chemistry	All areas of physical, inorganic, analytical chemistry
Agrochemical regulators	Amino acids	Cellulose, lignin, paper	Air pollution	Surface chemistry
Biochemical genetics	Biomolecules	Coatings, inks	Ceramics	Catalysts
Fermentation	Carbohydrates	Dyes, organic pigments	Essential oils, cosmetics	Phase equilibrium
Immunochemistry	Organometallic compounds	Synthetic elastomers	Fossil fuels	Nuclear phenomena
Pharmacology	Steroids	Textiles, fibers	Ferrous metals, alloys	Electrochemistry

# Curating the highest quality chemistry content



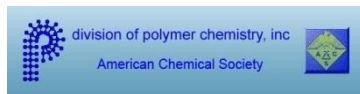
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JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

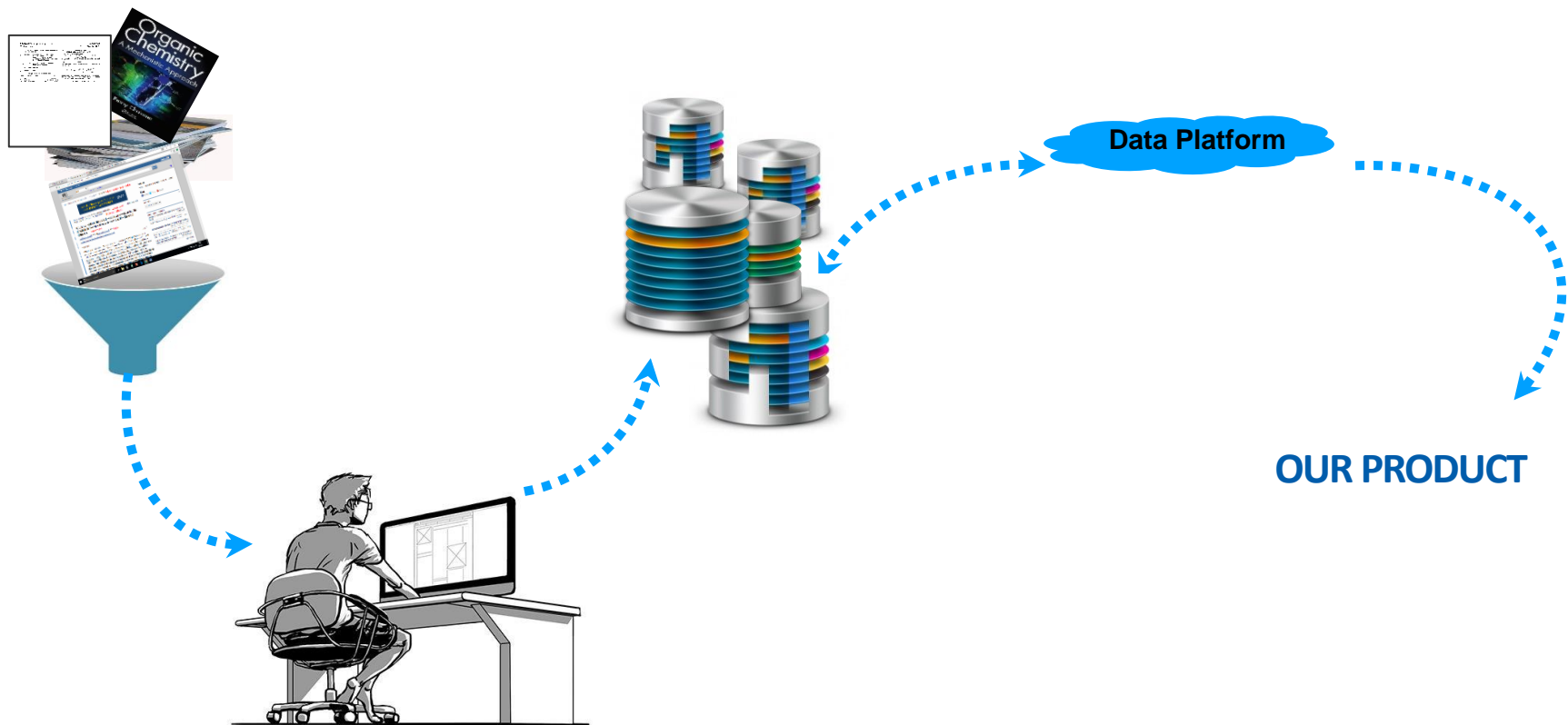


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- Analytics
- Opportunity exploration
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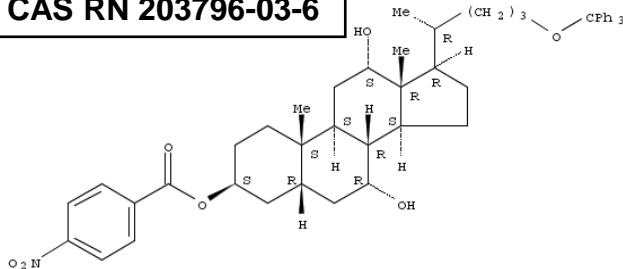
**SciFinder<sup>n</sup>**  
A CAS SOLUTION

# CAS scientists find the chemistry, and save you time!

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste.

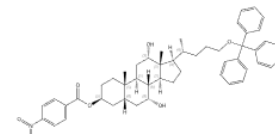
Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding NaHCO<sub>3</sub> solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO<sub>2</sub> chromatography (Et<sub>2</sub>O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529, 1489, 1448, 1345 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m, 9 H) 5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 164.21, 150.56, 144.70, 136.79, 130.77, 64.22, 47.79, 46.79, 42.18, 28.74, 27.71, 26.85, 26.33 (thioglycerol+Na<sup>+</sup> matrix).

CAS RN 203796-03-6



Absolute stereochemistry.

203796-03-6



Absolute stereochemistry shown

C<sub>50</sub>H<sub>99</sub>NO<sub>7</sub>  
Cholane-3,7,12-triol, 24-(triphenylmethoxy)-, 3-(4-nitrobenzoate), (3β, 5β, 7α, 12α)-

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



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## CAS Acquisition Process

- Onsite Acquisitions Team – unique to CAS
- Proprietary processing technology
- Information painstakingly assembled so critical connections are made

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)	
(19) World Intellectual Property Organization International Bureau	
(43) International Publication Date 4 October 2012 (04.10.2012)	(10) International Publication Number <b>WO 2012/135049 A1</b>
	
WIPO   PCT	
(51) International Patent Classification: A01N 43/04 (2006.01) A61K 31/70 (2006.01)	(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.
(21) International Application Number: PCT/US2012/030408	
(22) International Filing Date: 23 March 2012 (23.03.2012)	
(25) Filing Language: English	
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(30) Priority Data: 61/467,661 25 March 2011 (25.03.2011) US	(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).
(71) Applicant (for all designated States except US): UNIVERSITY OF GEORGIA RESEARCH FOUNDATION, INC. [US/US]; Boyd Graduate Studies Research Center, Athens, GA 30602-7411 (US).	Published: — with international search report (Art. 21(3)) — before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments (Rule 48.2(h))
(72) Inventors: and (75) Inventors/Applicants (for US only): BOONS, Geert-Jan [NL/US]; 1321 Lake Wellbrook Drive, Athens, GA 30606 (US). WANG, Zhen [CN/US]; 846 Massachusetts Avenue, Apt. 2F, Arlington, MA 02476 (US).	
(74) Agent: SANDBERG, Victoria, A.; Muetting Raasch & Gebhardt, P.A., P.O. Box 581336, Minneapolis, MN 55458-1336 (US).	





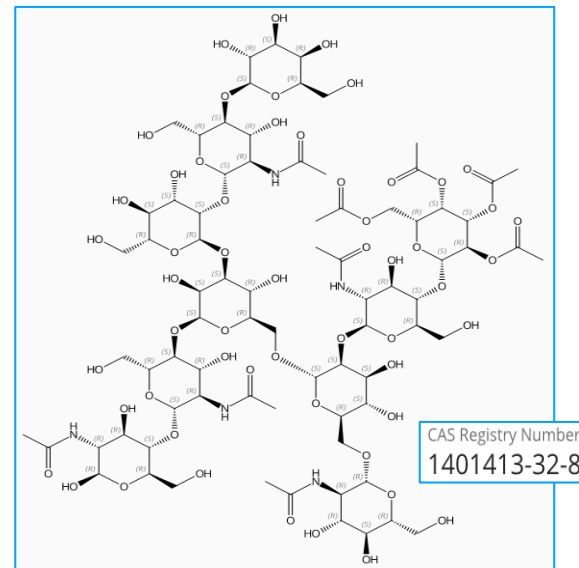
# CONTENT TEAM

## CAS Content Team

- At any given time ~1500 advanced degreed scientists and technologists covering 80 disciplines and 50 languages are working on CAS products and services
- Average experience: 20+ years
- ~\$150,000,000 invested annually in content creation alone

## Rigorous Hiring & Training Process

- Hiring processes includes actual testing of scientific knowledge – our own entrance exam...and hiring rate of ~5% of qualified applicants (lower than both Harvard and Oxford)
- Apprenticeship lasts 1-3 years
- Quality audits of content and workflow



# Scifinder<sup>n</sup> Discovery platform

## \*SciFinderN

### Top 5 key searching function

- Reference searching
- Reaction searching
- Substance searching
- Sequence searching
- Retrosynthesis

## \*CAS Formulation

- Formulation searching

## \*CAS Analytical Methods

- Analytical methods searching

The screenshot displays the CAS SciFinder<sup>n</sup> Discovery platform interface. At the top, the header includes the CAS SciFinder<sup>n</sup> logo, navigation links for 'Saved and Alerts', 'History', and 'Account', and a banner for Retrosynthesis plans. The main search area is titled 'Searching for...' and features a sidebar with search categories: All, Substances (selected), Reactions, References, Suppliers, Biosequences, and Retrosynthesis. The 'Substances' section includes a search bar with the placeholder 'Enter a query...', a 'Draw' button, and a dropdown menu for 'Molecular Formula'. Below the search bar, there is a link to 'Add Advanced Search Field' and a link to 'Learn more about SciFinder<sup>n</sup> Advanced Search'. The 'Recent Search History' section at the bottom shows a search from 'March 2, 2022'. A 'Feedback' button is located in the bottom right corner.

CAS SciFinder<sup>n</sup>

Retrosynthesis plans now have a new rule-set trained on our full collection of single-step reactions, offering greater coverage of synthetic methods and added novelty. [Learn more about Retrosynthesis searching in CAS SciFinder<sup>n</sup>.](#)

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

Molecular Formula

Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N

[Add Advanced Search Field](#)

[Learn more about SciFinder<sup>n</sup> Advanced Search.](#)

Recent Search History

March 2, 2022

View All Search History

Feedback

# Reference:

- An easy-to-read display lets user quickly browse reference
- Filters are available to further narrow results...by year, source type, and organization

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References cancer and Extended-release injection

Return to Home

Filter by

Document Type

- ☐ Journal (151K)
- ☐ Patent (23K)
- ☐ Review (17K)
- ☐ Biography (37)
- ☐ Book (3)

[View All](#)

Language

- ☐ English (150K)
- ☐ Chinese (12K)
- ☐ Japanese (4,136)
- ☐ German (2,835)
- ☐ Undetermined (2,413)

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Publication Year

1831 to 2021

No Min to No Max [Apply](#)

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Available at My Institution

Author

Organization

Publication Name

Concept

CAS Solutions

Formulation Purpose

Database

## References (178,486)

Sort: Relevance View: Partial Abstract

☐ Substances ☐ Reactions ☐ Cited By

☐ 1

### Paclitaxel tumor biodistribution and efficacy after intratumoral injection of a biodegradable extended release implant

By: Shikanov, Ariella; Shikanov, Sergey; Vaisman, Boris; Golenser, Jacob; Domb, Abraham J.  
International Journal of Pharmaceutics (2008), 358(1-2), 114-120 | Language: English, Database: CAPIUS and MEDLINE

Purpose: The aim of this study was to investigate the effectiveness of paclitaxel controlled release from intratumorally injected polymer. Methods: The effectiveness of paclitaxel-polymer formulation injected intratumorally was tested in mouse bladder tumor model. To determine paclitaxel biodistribution in tumor at predetermined time periods the tumor was excised, frozen and sectioned, and the paclitaxel concentrations were determined in the tumor tissue and in plasma by HPLC. Histopathol. evaluation of the necrosis and inflammation was performed on tumor sections. Results: In the paclitaxel/...

[View More](#)

Full Text ☐ Substances (2) ☐ Reactions (0) ☐ Cited By (30) ☐ Citation Map

☐ 2

### Leuprolide acetate given by a subcutaneous extended-release injection: less of a pain?

By: Cox, Michael C.; Scripture, Charity D.; Figg, William D.  
Expert Review of Anticancer Therapy (2005), 5(4), 605-611 | Language: English, Database: CAPIUS and MEDLINE

A review. Androgen deprivation therapy is a mainstay for the treatment of advanced prostate cancer. Hormonal therapy commonly consists of injection of gonadotropin hormone-releasing hormone agonists. Based on the need for improved convenience of administration, a novel formulation of leuprolide acetate (Eligard; Atrix Laboratories Inc. & Sanofi Aventis) which incorporates a mixture of selected polymers and solvents to achieve sustained drug delivery after s.c. injection, was developed. The US Food and Drug Administration has approved 1-, 3-, 4- and 6-mo formulations of leuprolide acetate.

[View More](#)

Full Text ☐ Substances (3) ☐ Reactions (0) ☐ Cited By (17) ☐ Citation Map

☐ 3

### Use of extended release neuregulin for prevention and treatment of cardiac ventricular hypertrophy and other disorders

By: Zhou, Mingdong  
World Intellectual Property Organization, WO2007076701 A1 2007-07-12 | Language: English, Database: CAPIUS

The present invention provides extended release compositions comprising neuregulin 1, 2, 3 or 4 for preventing, treating or delaying various diseases or disorders. Diseases may include cardiovascular disease, cancer, neural growth, muscle disease,

# Reference Detail Page:

## Reference Detail

(3 of 178,486)

Substances (6) Reactions (0)

### Patent

#### Patent Information

Patent Number  
WO2007076701

Publication Date  
2007-07-12

Application Number  
WO2006-CN3694

Application Date  
2006-12-29

Kind Code  
A1

#### Assignee

Zensun (Shanghai) Science & Technology Limited, China

#### Source

World Intellectual Property Organization

#### Database Information

AN: 2007:762994  
CAN: 147:134439  
CAplus

#### Language

English

### Use of ventricles

By: Zhou, M

The present invention provides various drugs for the treatment of muscular dystrophy, schizophrenia, failure and reduction of the differential cytoskeleton.

### Keywords

PATENT

### Patent

Patent

WO2007

AU20063

CA26349

CA28413

US20070

EP19815

CN10139

### Concepts

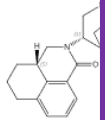
- Alzheimer disease
- Animal gene
- Modifier: NRG1, NRG2, NRG3 and
- Role: Biological Study, Unclassified Activity; Therapeutic Use
- Anti-Alzheimer agents
- Antidiabetic agents
- Antitumor agents**
- Cardiac hypertrophy
- Cardiomyocyte
- Modifier: growth and differentiation
- Cardioprotective agents
- Cardiovascular disease
- Cell differentiation
- Modifier: cardiomyocyte
- Cell proliferation
- Modifier: cardiomyocyte
- Controlled-release drug delivery
- Diabetes mellitus

### Microspheres

Modifier: extended release neuregulin accomplished via

### Substances (4)

135729-61-2

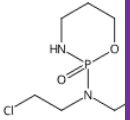


Absolute stereochemistry shown

$C_{19}H_{24}N_2O$   
Palonosetron

Role: Pharmacological Activity, Use, Biological Study, Uses

50-18-0



$C_7H_{15}Cl_2N_2O_2P$   
Cyclophosphamide

Role: Adverse Effect, Including Pharmacological Activity, Therapeutic Use, Biological Study, Uses

### Formulations

#### Collagen Formulation: Anticancer Agents

[View Formulus® Detail](#)

**Location:** Article Page 3, 6  
**Purpose:** Antitumor agents  
**Target:** cancer

Component	Function	Amount Reported
Group: cyclic dinucleotides stock solution	-	-
cyclic dinucleotides	-	6.67 µg
endotoxin-free water	solvent	-
Phosphate-buffered saline solutions	buffer	-
collagen stock solution	carrier	3.5-5 mg/mL

#### Stingel Formulation: Anticancer Agents

[View Formulus® Detail](#)

**Location:** Article Page 3, 6

# PatentPak:

Why waste time slogging through dense patent material with direct access to and understanding of the chemistry within the document

Patent chemistry is fully annotated with structures, nomenclature and more!

The screenshot displays the PatentPak interface, a tool for accessing patent chemistry. The top navigation bar includes 'PAGE' (28 / 37), 'ZOOM' controls, and 'DOWNLOAD' options (PDF, PDF+). The main content area is titled 'CLAIMS' and lists six claims. The left sidebar, titled 'Key Substances in Patent', lists three substances with their CAS RNs and chemical structures. The first substance is CAS RN 2752-65-0. The second substance, CAS RN 81624-55-7, is highlighted with a purple box and has a detailed information panel open, showing its name: 1,2-Ethanediamine, N,N,N',N'-tetrakis[(6-methyl-1H-benzimidazol-2-yl)methyl]-. The third substance is CAS RN 81624-55-7. The main claims list includes: 1. A pharmaceutical composition, comprising: at least one NPM inhibitor; at least one anti-cancer agent; and a pharmaceutically acceptable carrier. 2. The pharmaceutical composition of claim 1, wherein the NPM inhibitor is an siRNA that inhibits NPM expression. 3. The pharmaceutical composition of claim 1, wherein the NPM inhibitor is gambogic acid. 4. The pharmaceutical composition of claim 1, wherein the NPM inhibitor is NSC 348884. 5. The pharmaceutical composition of claim 1, wherein the anti-cancer agent is a target cancer therapy. 6. The pharmaceutical composition of claim 5, wherein the target cancer therapy is sorefenib. The interface also shows 'Analyst Markup Locations (1)' and a 'Page 28' indicator.

Important chemistry locations are identified by CAS expert scientists

# Get to actionable results more quickly with a streamlined new interface

Streamlined search navigation saves you clicks

Immediately run past searches

The screenshot shows the SciFinder search interface. At the top, there's a navigation bar with 'Saved', 'History', and 'Account' links. Below this is a 'Search' section with a sidebar on the left containing 'All', 'Substances', 'Reactions', 'References' (highlighted), and 'Suppliers'. The main search area has a text input field containing 'treatment of cancer', which is circled in purple. Above the input field is the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.'. To the right of the input field is a purple search button with a magnifying glass icon. Below the input field is a link for 'Advanced search'. In the 'Recent Searches' section, there are three entries. The first entry is dated 'March 28, 2017' at '11:55 AM' and shows 'References: high temperature low density plasma (424K)'. The second entry is dated 'March 28, 2017' at '10:14 AM' and shows 'References: Advanced Search (6)' and 'Organization: Memorial Sloan-Kettering Cancer Ctr.'. The third entry is dated 'March 27, 2017' at '5:33 PM' and shows 'Reactions:' followed by a chemical structure of a pyrimidine derivative. To the right of the chemical structure is the text 'As Drawn (9), Substructure (39)'. A purple circle highlights a chemical structure drawing tool in the top right corner, with 'Edit Drawing' and 'Remove' buttons below it. A purple arrow points from this circle to the 'treatment of cancer' search input field. Another purple arrow points from the same circle to the 'References: high temperature low density plasma (424K)' entry in the 'Recent Searches' section.

More conveniently search structures and text

# Reaction: Information presented to facilitate rapid understanding

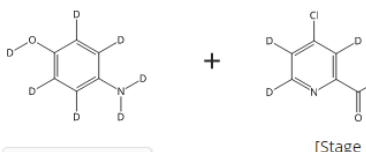
Powerful filtering capabilities allow rapid focus

The screenshot displays the SciFinder Reactions interface. On the left, a sidebar titled 'Structure Match' offers filtering options: 'As Drawn (5)' and 'Substructure (18)'. Below this, a 'Filter by' section includes 'Substance Role' (Product (13) selected, Reactant (5)), 'Yield' (various percentage ranges), 'Number of Steps' (1 (13) selected), 'Experimental Protocols' (MethodsNow Available (2), Procedure Available (6)), 'Reaction Type', 'Reagent', 'Catalyst', 'Solvent', 'Commercial Availability', 'Reaction Notes', 'Source Reference', 'Publication Year', 'Document Type', and 'Language'. The main panel, titled 'Reactions (13)', shows 'Scheme 1 (2 Reactions) View'. It features a chemical reaction scheme with two reactants and a product, along with 'Suppliers (3)' and 'Suppliers (6)' buttons. Below the scheme, a 'Reaction Summary' table lists reagents (Sodium acetate, Acetic acid, manganese(3+) salt (3:1)), catalysts, solvents (Acetic acid), and conditions. To the right of the table, text describes the reaction as 'Carbon-carbon bond-forming reactions promoted by trivalent manganese' by Melikyan, Gagik G. (1997), with a yield of 92%. A 'Full Text' button is also present. The interface includes a 'View - Select -' dropdown and a 'Save' button in the top right corner.

Intuitive information layouts fosters quick comprehension



# Go right to the lab with step-by-step synthetic procedures extracted and summarized from the literature



[Stage 2]

Suppliers (7)

**Step 1**

Stage	Reagents	CAS
1	Potassium <i>tert</i> -butoxide	-
2	Potassium carbonate	-
CAS Reaction Number		31

**Experimental Protocols**

**MethodsNow™** Experimental Procedure

**Products** 2-Pyridine-3,5,6-*d*<sub>3</sub>-carboxamide, 4-(4-aminophenoxy-2,3,5,6-*d*<sub>4</sub>)-*N*-(methyl-*d*<sub>3</sub>)-, Yield: 87%

**Reactants** 4-(Amino-*d*<sub>2</sub>)phen-2,3,5,6-*d*<sub>4</sub>-ol-*d*  
2-Pyridine-3,5,6-*d*<sub>3</sub>-carboxamide, 4-chloro-*N*-(methyl-*d*<sub>3</sub>)-

**Reagents** Potassium *tert*-butoxide  
Potassium carbonate

**Solvents** Dimethylformamide

**Procedure**

1. Add potassium *tert*-butoxide (222 mg, 1.98 mmol) to a solution of d7-4-aminophenol (222 mg, 1.91 mmol; 97 atom % D (CDN Isotopes)) in DMF (2.0 mL).
2. Stir the reaction for 1 h.
3. Add a solution of 4-chloro-3,5,6-*d*<sub>3</sub>-*N*-(methyl-*d*<sub>3</sub>)picolinamide (305 mg, 1.73 mmol) in DMF (0.6 mL) via cannula to the mixture follow with a 0.6 mL DMF rinse.
4. Add K<sub>2</sub>CO<sub>3</sub> (129 mg, 0.935 mmol) to the mixture and heat the mixture to 80°C for 12 h.
5. Cool the reaction to room temperature.
6. Dilute the mixture with EtOAc and pour into a separatory funnel containing EtOAc and brine.
7. Wash the organic layer twice with brine.
8. Wash the combined aqueous solutions once with EtOAc.
9. Dry the combined organic solutions over Na<sub>2</sub>SO<sub>4</sub>.
10. Filter the mixture.
11. Concentrate the filtrate in vacuo.
12. Purify the residue on an ISCO instrument (0% to 90% EtOAc in hexanes) to afford 4-(4-aminophenoxy-*d*<sub>4</sub>)-3,5,6-*d*<sub>3</sub>-*N*-(methyl-*d*<sub>3</sub>)picolinamide.

**Transformation** Aromatic Substitution by Oxygen Nucleophiles

**Scale** milligram

**Characterization Data**

2-Pyridine-3,5,6-*d*<sub>3</sub>-carboxamide, 4-(4-aminophenoxy-2,3,5,6-*d*<sub>4</sub>)-*N*-(methyl-*d*<sub>3</sub>)-

**Mass Spectrum** MS (M + H): 254.0

Key chemical components of the reaction are identified with links to additional information

Go directly to the lab with step-by-step instructions

Additional useful information is included



**SciFinder<sup>n</sup>**  
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# Retrosynthesis

Powered by ChemPla

Overview

Steps

Scoring



Overview

Steps

Scoring

⚡ A ⇒ B + C Stereoselective

Maximum Yield: -

Evidence (3)

Alternatives

ON

Overview

Steps

Scoring

Scoring Profiles

Complexity Reduction ⓘ

Convergence ⓘ

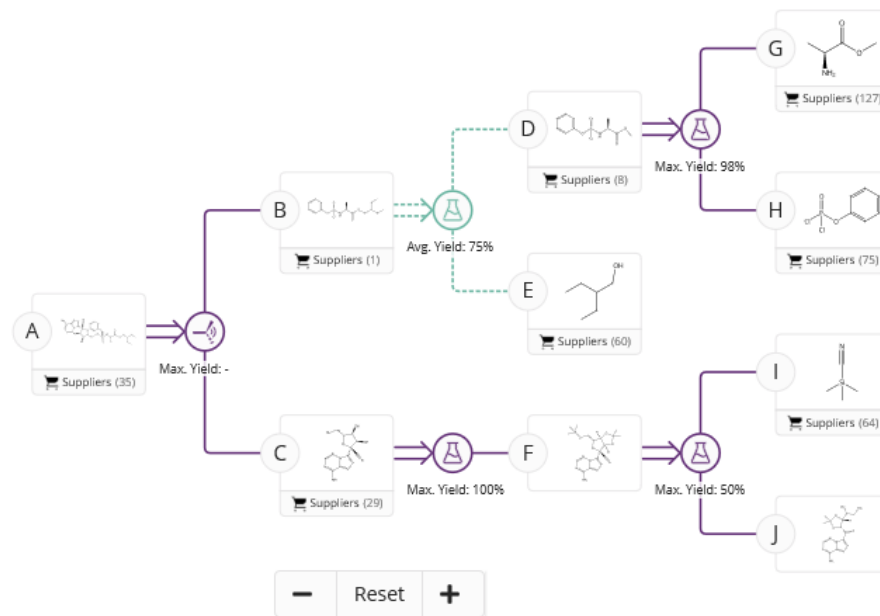
Evidence ⓘ

Yield ⓘ

Atom Efficiency ⓘ

Apply

Reset Scoring



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# Substances Detail Page

## Substance Detail (1 of 1)

References (488)

Reactions (325)

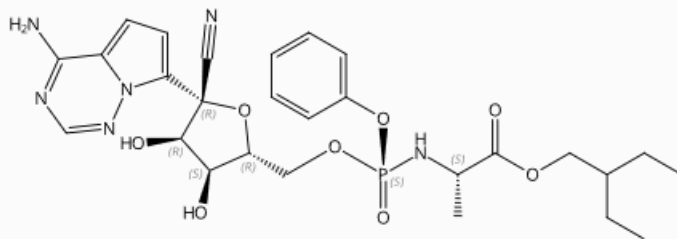
Suppliers (37)



Save

CAS Registry Number

1809249-37-3



Absolute stereochemistry shown

$C_{27}H_{35}N_6O_8P$

L-Alanine, N-[(S)-hydroxyphenoxyposphiny]l-, 2-ethylbutyl ester, 6-ester with 2-C-(4-aminopyrrolo[2,1-f][1,2,4]triazin-7-yl)-2,5-anhydro-D-altrnonitrile

Key Physical Properties	Value	Condition
<a href="#">Molecular Weight</a>	602.58	-
<a href="#">Density (Predicted)</a>	1.47±0.1 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
<a href="#">pKa (Predicted)</a>	12.00±0.70	Most Acidic Temp: 25 °C

Other Names and Identifiers

Predicted Properties

Predicted Spectra

Bioactivity Indicators

Anti-infective agents

[Antiviral agents \(183\)](#)

Target Indicators

Enzymes

[Alanine aminotransferase \(12\)](#)

[Angiotensin-converting enzyme 2 \(29\)](#)

[Proteinase 3CLpro \(11\)](#)

[RNA-dependent RNA polymerase \(30\)](#)

Glycoproteins

[Viral spike glycoproteins \(30\)](#)

Viral proteins

[Viral spike glycoproteins \(30\)](#)

Regulatory Information

Confidential Business Information: Public

Regulatory Synonyms (2)

Details by Country/International & Other Lists

Additional Details

Expand All

# Markush Detail Page

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Patent Markush Match

As Drawn (71)

Substructure (1,314)

Filter by

Patent Office

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- ☐ China (5)
- ☐ European Patent Organization (4)

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## Patent Markush (71)

Sort: Relevance ▾

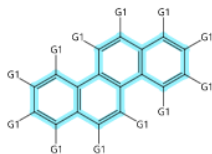
☐ References ▾



Save

☐ 1

US20130214259



Patent claim 29

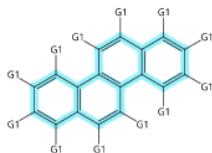
PATENTPAK ▾

Full Text ▾

There are no notes to display for this structure.

☐ 2

WO2009008352



Patent claim 1

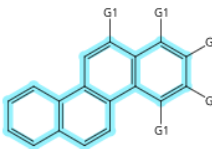
PATENTPAK ▾

Full Text ▾

There are no notes to display for this structure.

☐ 3

WO2002088025



Patent claim 2

PATENTPAK ▾

Full Text ▾

There are no notes to display for this structure.

PATENTPAK  
CONNECTION

PAGE

79

2100

Z00H1

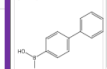
DOWNLOAD

PDF

PDF+

Key Substances in Patent

CAS RN  
6122-98-2

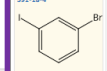


Analyzed Markup Locations (2)

Page 79

Page 82

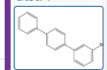
CAS RN  
595-58-4



Analyzed Markup Locations (1)

Page 79

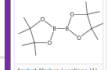
CAS RN  
17933-87-4



Analyzed Markup Locations (1)

Page 79

CAS RN  
73183-34-3



Analyzed Markup Locations (1)

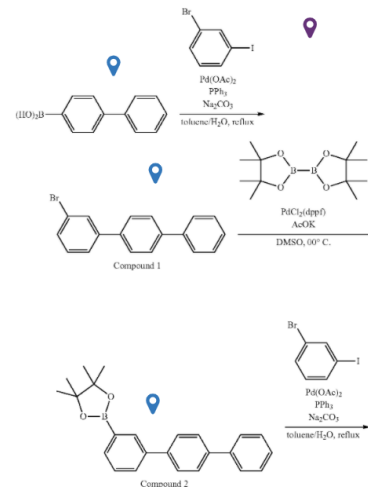
Page 79

CAS RN  
1483377-23-8

Page 79

dures, and the like shown in the following Examples can be appropriately modified so far as the gist of the present inven-

[0281] A compound (H-1) was synthesized according to the following scheme.



# New Content & Capabilities - Sequence Search

## Searching for...



All



Substances



Reactions



References



Suppliers



Biosequences

## 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...

BLAST CDR Motif Search

Sequence Type:

Nucleotide

Protein

Search Within:

☒ Nucleotides

☐ Proteins

Limit Total Sequence Results to:

100



Start Biosequence Search

[Advanced Biosequence Search ^](#)

[Reset All](#)

Alignment Identity % [?](#)

-

Match with Gaps?

☐ Yes

☒ No

Gap Costs [?](#)

Existence 11 Extension 1

Query Coverage % [?](#)

90

Word Size [?](#)

6

Scoring Matrix [?](#)

BLOSUM62

BLAST Algorithm

TBLASTn-fast

E-Value [?](#)

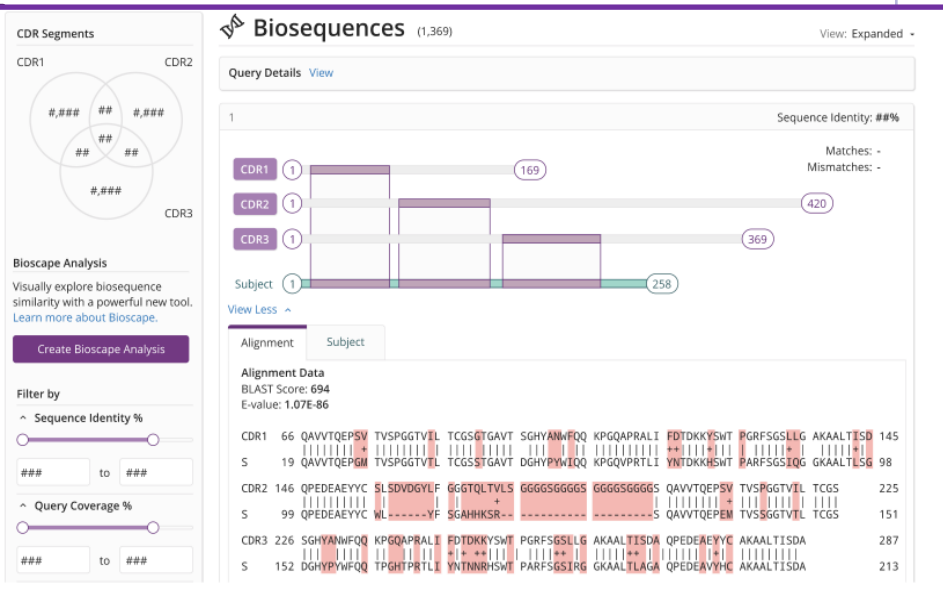
10

# New Content & Capabilities - Sequence Search

## BLAST Display



## CDR Display



**SciFinder<sup>n</sup>**  
A CAS SOLUTION



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Senior Account Consultant

tliu2@acs-i.org

# SciFinderN 文獻查詢



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# Find References

Find document references that match your query, which can be [search terms](#), a [chemical structure](#), or both:

- If you enter a search term **or** chemical structure query, SciFinder<sup>n</sup> retrieves associated references, such as journal articles and patents.
- If you enter **both** a search term query and a structure query, the search results must match both criteria (queries are joined by the logical AND).

Find ADVANCED **References** by:

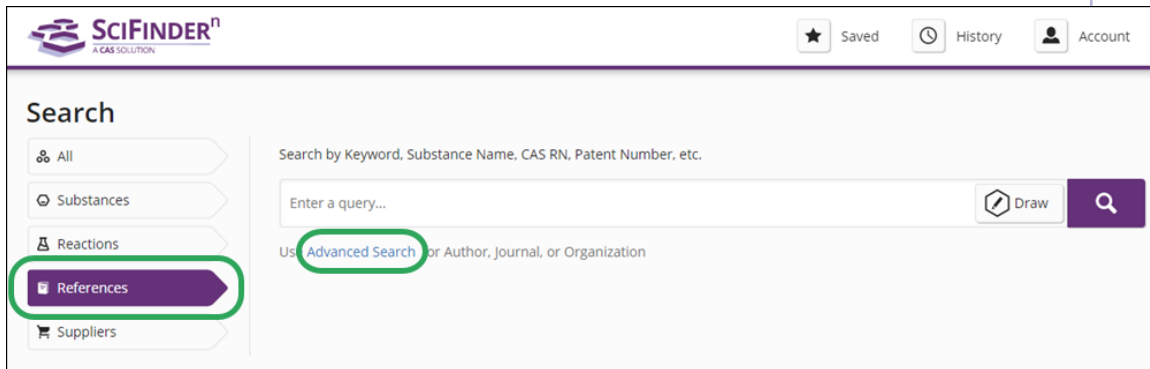
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[Find References Associated with a Company or Organization](#)

[Find a Reference Using Journal Information](#)

Find **Patent References** by:

- [Assignee](#)
- [Inventor](#)



## Find References Using Search Terms

Search terms may be:

- **Research Topic/Keyword/Concept** (e.g., analgesics)

- **Substance Name** (e.g., ibuprofen,  $\beta$ -amyloid)

**Note:** If your search term contains a Greek letter, see [Greek Letters Used in Searching](#) to insert the correct character.

- **CAS Registry Number** (with dashes, e.g., 51146-57-7)

- **Accession Number** (e.g., 1986:230471)

- **PubMed ID Number** (e.g., 15980585)

- **Digital Object Identifier (DOI)** (e.g., 10.1093/nar/gki470)

- **Patent Number** (no spaces, e.g., US4571400)

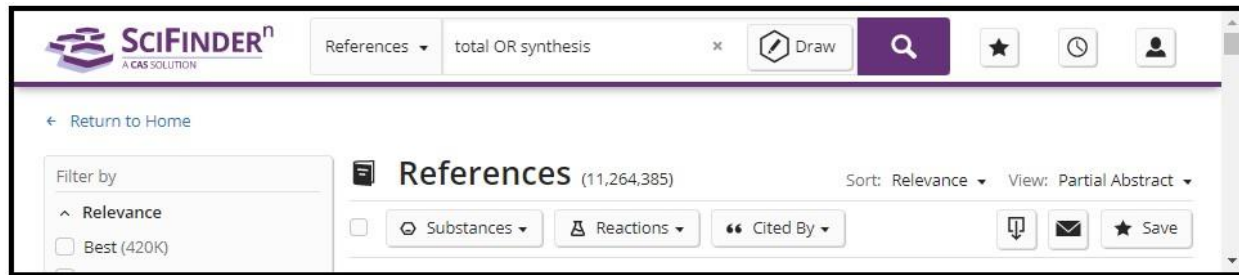
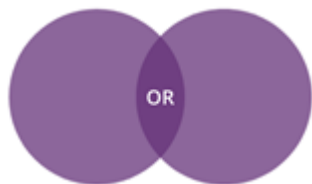
- **Patent Application Number** (with dash, e.g., US1984-682902)

**Note:** You may enter multiple numbers separated by a space, no commas or other punctuation. The search field has a 2000-character limit.

There are a total of five basic Boolean search operators:

•OR

- The OR operator will provide results that contain either of the keywords
- Will provide results that contain either of the terms
- This is the default search when no operators are present in the search query
- total OR synthesis



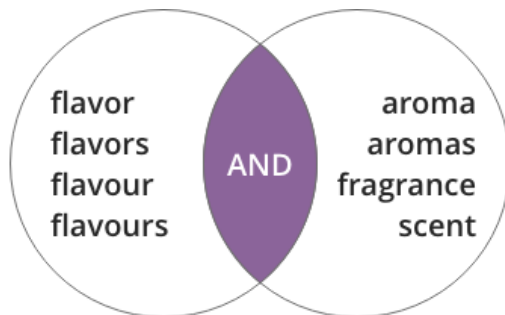
*Examples:*

- ("flavor" **or** "extract") and ("turmeric" **or** "curcumin")
- (flavor not dye) **or** extract
- 13463-67-7 **or** 7664-41-7

## •AND

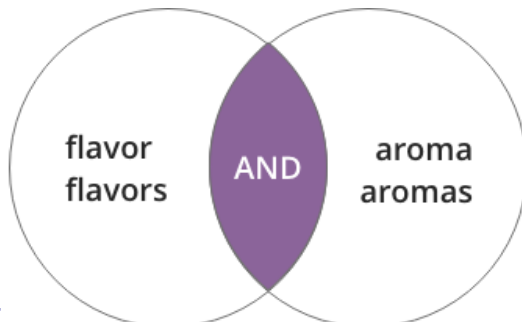
The **and** operator returns any combination of the terms' plurals, synonyms, or alternate spellings.

**Example:** The query **flavor and aroma** returns only results that **contain plurals/synonyms/alternate spellings of both terms**.



Entering [terms in quotation marks](#) to create a bound phrase **narrows the term to include**.

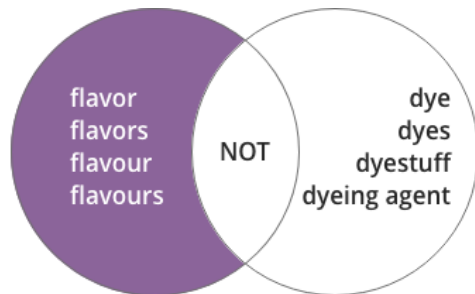
**Example:** The query **"flavor" and "aroma"** returns only results that **contain the exact spelling (includes plurals) of both terms**.



## •NOT

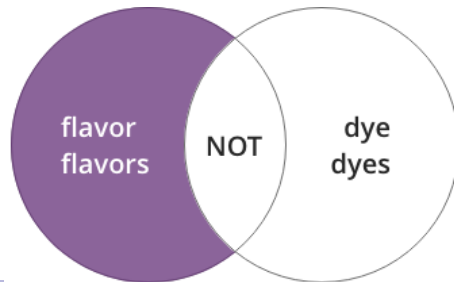
The **not** operator excludes any combination of the terms' plurals, synonyms, or alternate spellings.

**Example:** The query **flavor not dye** returns results that **contain plurals/synonyms/alternate spellings of flavor** but **excludes** those that **contain plurals/synonyms/alternate spellings of both flavor and dye**.



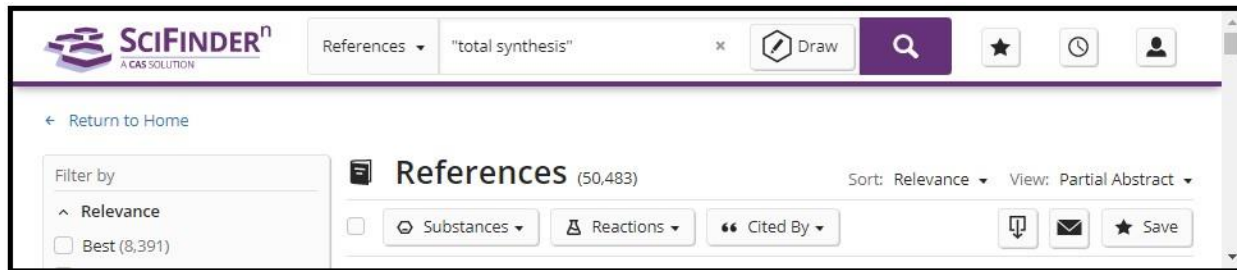
Entering [terms in quotation marks](#) to create a bound phrase **narrows the term to exclude**.

**Example:** The query **"flavor" not "dye"** returns results that **contain flavor(s)** but **excludes** those that **contain both flavor(s) and dye(s)**.



• “”

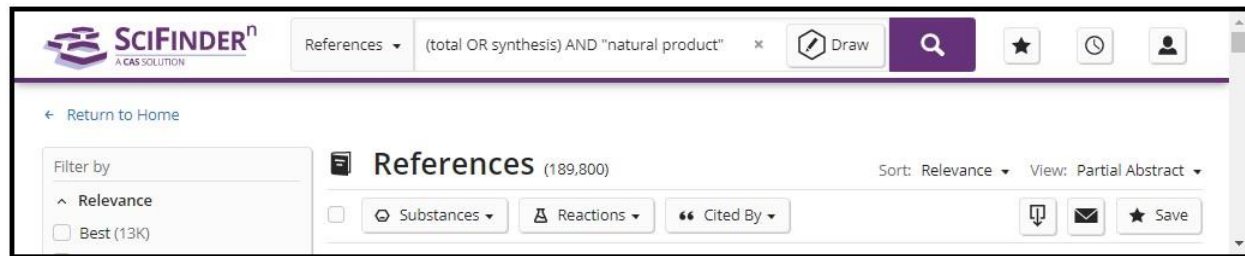
- Quotation marks means you are searching for a specific phrase
- Will provide results that contain the exact phrase and will not return references with uses of these keywords on their own
- “total synthesis”



Entering terms in **quotation marks** creates a bound phrase that specifies an exact spelling (plurals accepted, but no alternative spellings or synonyms) and side-by-side relationship.



- ()
- Parentheses can be added to allow the user to combine Boolean operators
- (total OR synthesis) AND "natural product"



Entering terms and operators in **parentheses** creates an **expression that functions as a single unit** that interacts with other terms.

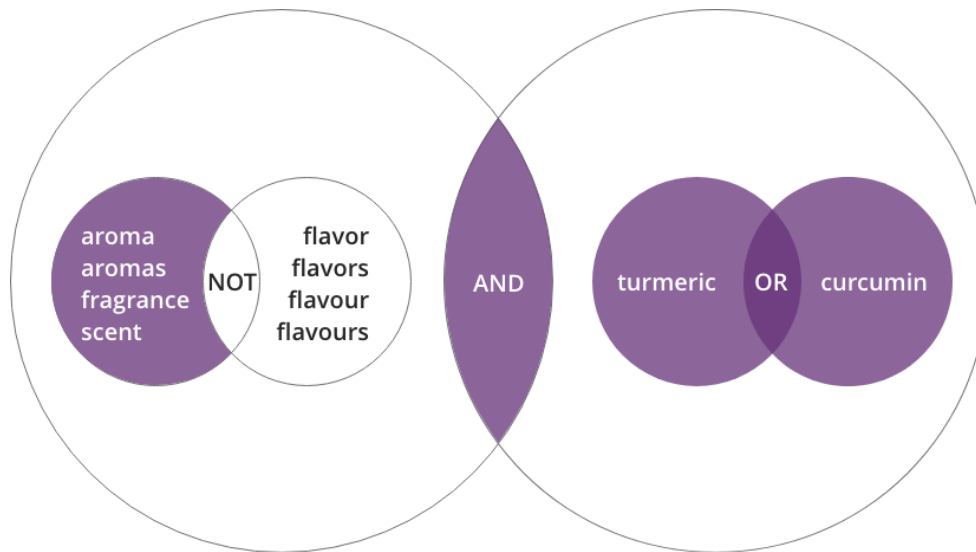
*Examples:*

- (extract not flavor) and ("turmeric" or "curcumin")
- ((turmeric or flavonoids) and immune cells) not inflammatory

## Boolean Modifier: ( )

Enclosing terms and a Boolean operator within parentheses creates a Boolean expression that functions as a **single unit/condition** that can interact with other terms, expressions, phrases, and operators.

Example: The query **(aroma not flavor) and ("turmeric" or "curcumin")** returns only results that **contain plurals/synonyms/alternate spellings of aroma, but not plurals/synonyms/alternate spellings of flavor and also contain turmeric, curcumin, or both.**



# Syntactic Reference Text Wildcard Searching \* ?

You may search references using the asterisk (\* - match 0 or more characters) and question mark (? - match 0 or 1 character) wildcard characters.

Wildcard queries search a reference's:

- Title
- Abstract
- Keywords
- Substances/Medline Chemicals
- Cplus Concepts

## Notes:

- Wildcards **contained within quotes are ignored.**
- Wildcards **do not find two terms that are separated by a space** (for example, *water?based* will find *water-based* but not *water based*).

The following wildcard characters will be supported:

- \* - Used to match 0 or more characters
- ? - Used to match 0 or 1 character

Wildcard characters can be used within a term (infix) or at the end of a term (terminal).

- Leading wildcard characters are not supported and will be ignored in a query.



## Examples

The query **Adsor\*** will match terms such as:

- Adsorbents
- Adsorbers
- Adsorption

SciFINDER<sup>n</sup>  
A CAS SOLUTION

References ▾ Adsor\* | x Draw 🔍 ★ ⌚ 👤

☐ 5

**Pore and solid diffusion models for fixed-bed adsorbers**  
By: Weber, Thomas W.; Chakravorti, Ranjit K.  
AIChE Journal (1974), 20(2), 228-38 | Language: English, Database: CAPlus

Most models for fixed bed adsorbers have used either the homogeneous-solid or pore diffusion model for the pellets. When the adsorption isotherm is linear, the models can lead to identical breakthrough curves. The conditions for this equivalence are given. One of the bulk flow factors that was included in the formulation of one pore diffusion model will be significant only for feedstreams containing a relatively high concentration of adsorbate. The porosity factor of the pore model is important, especially as the porosity decreases. The importance of the 2 diffusional models with respect to the predicted breakthrough curves is demonstrated. For comparable beds, the breakthrough curve based on the homogeneous model is delayed with respect to that based on the pore model at early times, regardless of the shape of the isotherm. The possible solutions for an irreversible isotherm are reviewed for each of the models, and a solution is presented for the general case of a pore model with an outside film resistance.  
[View Less ^](#)

Full Text ▾   Substances (0)   Reactions (0)   Cited By (1,356)   Citation Map

☐ 6

**Low-cost adsorbents for heavy metals uptake from contaminated water: a review**  
By: Babel, Sandhya; Kurniawan, Tonni Agustiono  
Journal of Hazardous Materials (2003), 97(1-3), 219-243 | Language: English, Database: CAPlus

A review covers the tech. feasibility of various low-cost adsorbents for heavy metal removal from contaminated water. Instead of using com. activated C, researchers have worked on inexpensive materials, such as chitosan, zeolites, and other adsorbents, which have high adsorption capacity and are locally available. The results of their removal performance are compared to that of activated C. It is evident from our literature survey of ~100 papers that low-cost adsorbents have demonstrated outstanding removal.

## Examples

The query `alumin?um` will hit on terms such as

- Aluminum
- Aluminium
- Etc.

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo and 'A CAS SOLUTION' tagline are visible. The search bar contains the query 'alumin?um'. Below the search bar, the 'References' section shows 22 results. The left sidebar provides filtering options: 'Filter by' (Relevance, Document Type, Substance Role, Language, Publication Year), 'Document Type' (Journal, Review, Conference), 'Substance Role' (Analytical Study, Biological Study, Process, Properties, Uses), 'Language' (English), and 'Publication Year' (1978 to 2018). The main content area lists two references. The first reference is titled 'Large-grained poly-silicon thin films by aluminium-induced crystallisation of microcrystalline silicon' by Ekanayake, G.; Quinn, T.; Reehal, H. S. The second reference is titled 'Effect of the titanium:boron ratio on the efficiency of aluminum grain-refining alloys' by Pearson, J.; Birch, M. E. J. Both references include an abstract and a 'Full Text' link. The interface also features a 'Draw' button and a 'Save' button.

SciFinder<sup>n</sup>  
A CAS SOLUTION

References | alumin?um

Return to Home

Filter by

- Relevance
  - Best (4)
  - Good (18)
  - Fair (0)
- Document Type
  - Journal (19)
  - Review (1)
  - Conference (3)
- Substance Role
  - Analytical Study (2)
  - Biological Study (1)
  - Process (4)
  - Properties (6)
  - Uses (5)
- Language
  - English (22)
- Publication Year
  - 1978 to 2018

Learn more about Relevance...

References (22)

Sort: Relevance | View: Full Abstract

Substances | Reactions | Cited By

1

**Large-grained poly-silicon thin films by aluminium-induced crystallisation of microcrystalline silicon**

By: Ekanayake, G.; Quinn, T.; Reehal, H. S.  
Journal of Crystal Growth (2006), 293(2), 351-358 | Language: English, Database: CAlplus  
[View Reference Detail](#)

**Abstract:** Al-induced crystallization of microcrystalline Si ( $\mu\text{-Si:H}$ ) thin films prepared by electron cyclotron resonance plasma-enhanced CVD (ECR-PECVD) on  $\text{SiO}_2$ -coated Si wafers was studied. The starting structure was substrate/ $\mu\text{-Si:H/Al}$ . Annealing this structure at a temperature of 520° resulted in successful layer exchange and the formation of a substrate/Al+Si layer/poly-Si geometry. Grain sizes exceeding ~60  $\mu\text{m}$  were achieved in films displaying a preferential (100) orientation. The length of time the samples are kept under ambient conditions before annealing plays a key role in controlling grain size and orientation. It is likely that this time delay influences the formation of the interface between the Si and Al layers and, hence, the crystallization process. These poly-Si layers exhibit an average surface roughness ( $R_a$ ) generally in the range ~7-12 nm.

Full Text | Substances (2) | Reactions (0) | Cited By (16) | Citation Map

2

**Effect of the titanium:boron ratio on the efficiency of aluminum grain-refining alloys**

By: Pearson, J.; Birch, M. E. J.  
Journal of Metals (1979), 31(11), 27-31 | Language: English, Database: CAlplus  
[View Reference Detail](#)

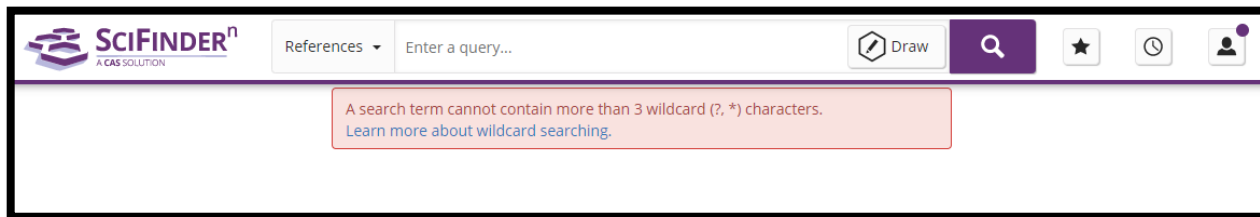
**Abstract:** Grain refinement of cast com. Al, AA3004 [37321-73-6], and AA7050 [37301-61-4] with Al master alloys containing 5-6 Ti and  $\leq 1.0\%$  B was investigated. The Al-5Ti-1% B addition gave the most efficient grain refinement, often to <200  $\mu\text{m}$  diameter, and Al-6% Ti the least. The grain size was generally finer for the alloys than for Al.

Full Text | Substances (4) | Reactions (0) | Cited By (11) | Citation Map

3

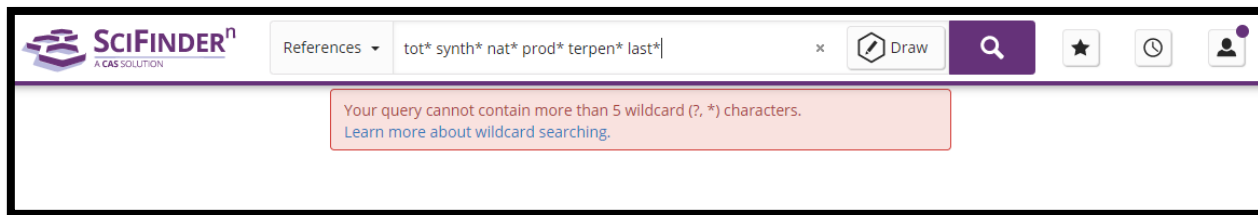
## Exceptions:

- A term must have at least 3 non-wildcard characters for a wildcard to be searched
  - If a term has less than 3 non-wildcard characters, any wildcard terms will be searched literally.
- A search term cannot contain more than 3 wildcard characters
  - Currently, searchers will be provided with an error message for this scenario.



- In a subsequent build, terms with more than 1 wildcard character will be searched literally and the user will be provided with an informational message.

A search cannot contain more than 5 wildcard terms.



Chuan-Che Liu Ph.D.

Senior Account Consultant

[tliu2@acs-i.org](mailto:tliu2@acs-i.org)

# Substance Searching

A world map with a light gray background. Numerous small blue dots are scattered across the map, representing various locations. Thin, light gray lines connect some of these dots, forming a network that spans across continents, suggesting global connectivity or data flow.

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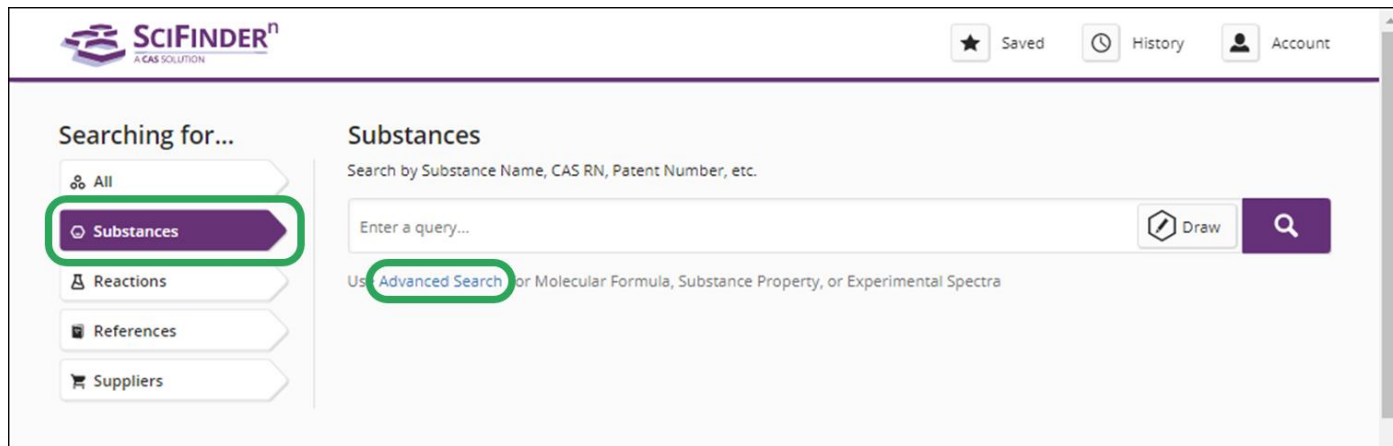
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- **Find Substances**

- Find substances that match your query, which can be substance names, CAS Registry Numbers, document identifiers, or a chemical structure:
- [Find Substances by Substance Name, Registry Number, or Document Identifier](#)
- [Find Substances by Chemical Structure](#)
- **Note:** If **both search term and chemical structure queries are present**, substances will **only match the chemical structure query** (search term query is ignored).
- Click [Advanced Search](#) to find substances by [molecular formula](#), [substance property](#), and [experimental spectra](#).



## Find Substances by Name, Registry Number, or Document Identifier

Search terms may be:

### •Substance Name:

- **Example:** benoxaprofen  
**Note:** Wildcard searching using an asterisk only works for single-search-term, single-word substance name searches (e.g., benoxa\*). Partial substance names without a wildcard character will not return results.
- **Example:** methyl ethyl ketone  
**Note:** For an exact match, use double quotes around the substance name. Searching multiple word substance names without quotes also returns results matching part of the name. For example, searching the above example without double quotes returns methyl ethyl ketone, methyl, ethyl ketone, and ethyl.
- **Example:**  $\beta$ -amyloid  
**Note:** If your search term contains a Greek letter, see [Greek Letters Used in Searching](#) to insert the correct character. to insert the correct character.

### •CAS Registry Number (with or without dashes, e.g., 51146-57-7, 51146577)

**Note:** Square brackets are accepted around RNs (e.g., [51146-57-7]), but not single or double quotes.

### •Document Identifier:

- **Patent Number** (no spaces, e.g., US4571400)
- **Accession Number** (e.g., 1986:230471)
- **PubMed ID Number** (e.g., 15980585)
- **CAS Accession Number (CAN):** document number in CA Plus (e.g., 148:486341)



# Wildcard searching for substance (Lactobacillus\* )

【常見益生菌乳酸菌中英文名對照表 / 市售益生菌乳酸菌中英文名對照】

乳酸桿菌屬 Lactobacillus	簡稱	關於
嗜酸乳桿菌 (Lactobacillus acidophilus)	A菌	如優格等發酵乳製品就含有豐富的嗜酸乳桿菌。這種益生菌能協助免疫系統保持腸道細菌的平衡。女性多攝食嗜酸乳桿菌有助於抑制白色念珠菌造成的陰道炎。嗜酸乳桿菌還能調節體內的膽固醇濃度，能在小腸中產生可對抗病原微生物的有益物質。
乾酪乳桿菌 (Lactobacillus casei)	C菌	相當耐酸，能有效地通過胃酸膽鹼的考驗，而有規模的進入腸道定殖。
約氏乳桿菌 (Lactobacillus johnsonii)	LJ菌	健康新生兒之消化道中分離純化，屬人體原生菌種。Salivarius意指“腺體型”最初是由人類腺體中被發現，是人體消化道中的原生菌種，亦是美國食品藥品監督管理局（FDA）表列安全菌種之一。
副乾酪乳桿菌 (Lactobacillus paracasei)	LP菌	耐胃酸及膽鹽，在腸道中定殖效果良好，能促進體內Th1細胞激素分泌，抑制Th2細胞所造成的敏感免疫反應，達到免疫系統平衡。對於異位性皮膚炎等過症狀可能有療效。
鼠李糖乳桿菌 GG株 (Lactobacillus rhamnosus GG)	LGG菌	是當前世界上研究最多的益生菌，也是首批被證實能夠在人體腸道存活並定殖的益生菌之一。可在血清中增加足夠的細胞間白素-10，降低引起局部性敏感免疫反應的細胞激素形成。能促進益菌生長、降低對乳品或食物的過敏、治療不明原因或急性腹瀉功能等。
洛德乳桿菌 (Lactobacillus reuteri)	R菌	是少數在成人與嬰兒體內皆可發現到的乳酸菌之一，可幫助實質腸道細胞的生長，促進益菌繁殖。



乳酸桿菌屬 Lactobacillus	簡稱	關於
發酵乳桿菌 (Lactobacillus Fermentum)	LF菌	常見於發酵動物和植物材料，用作益生菌的商品化發酵乳桿菌菌株包括PCC，ME-3 和 CECT5716。

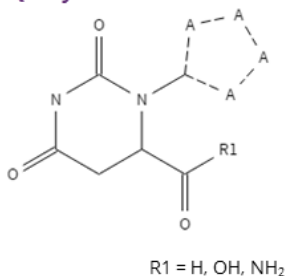
DER<sup>n</sup>

# Find Patent Markush Structures

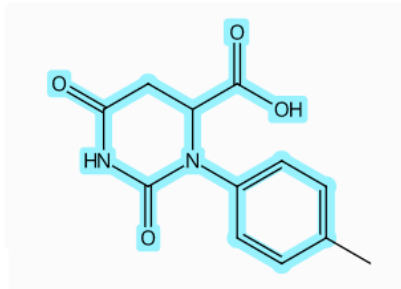
Use a **Patent Markush** search to find structures (including generic structures) matching your query within patent references.

For example:

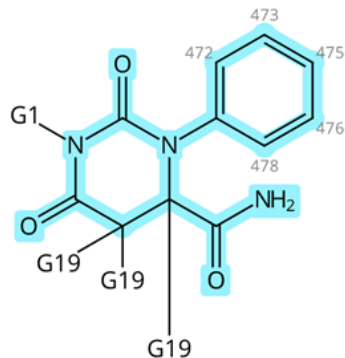
Query



Substructure Match

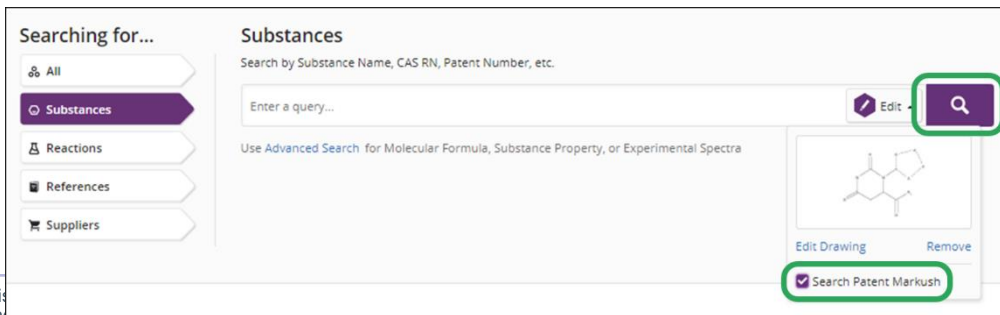


Markush Match



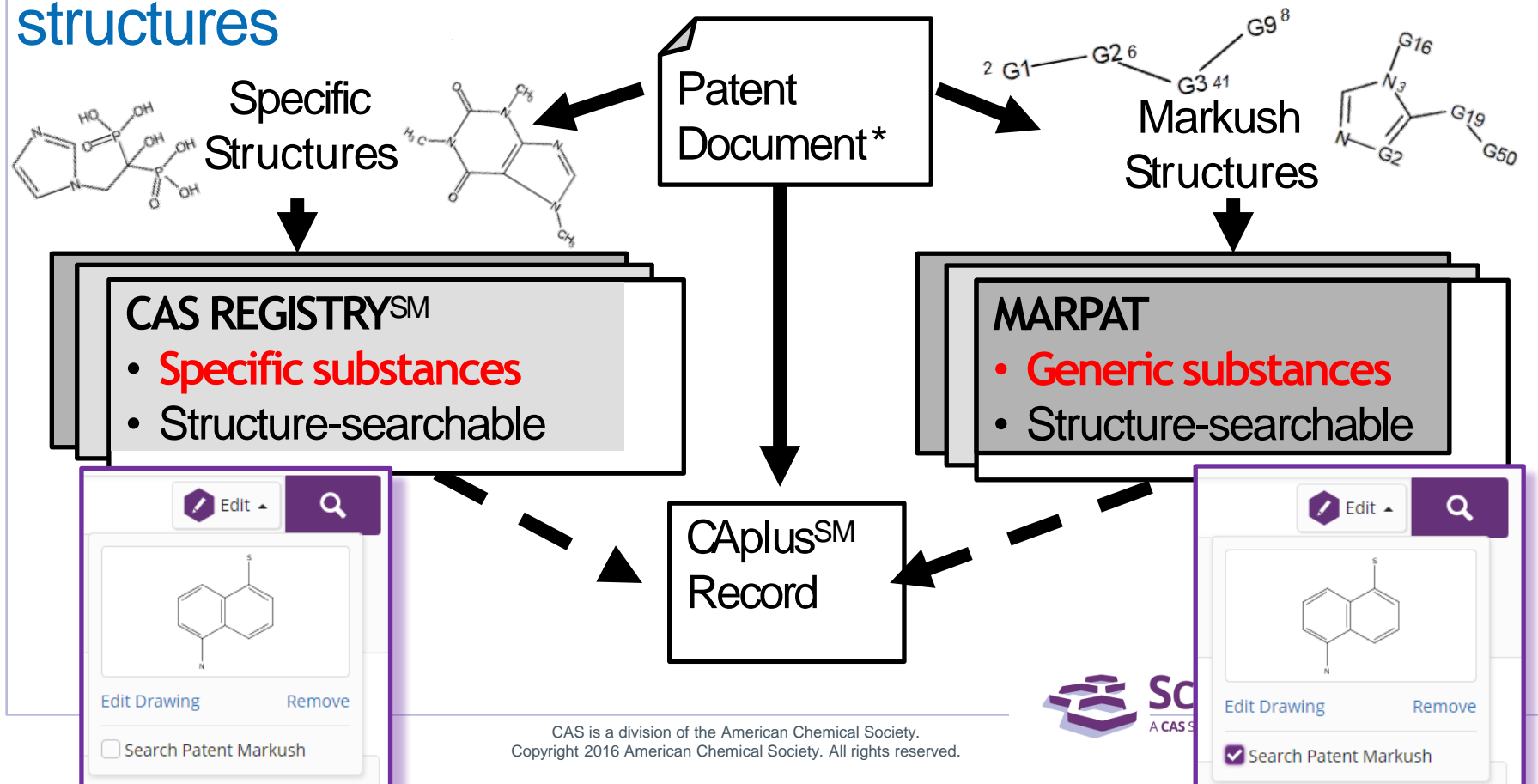
To conduct a Patent Markush search, click the **Substances** search type. [Draw the query](#) using a structure editor, and then check the box for **Search Patent Markush**.

Click the **magnifying glass** to submit the query.



A screenshot of a web-based search interface. On the left, a sidebar titled 'Searching for...' contains buttons for 'All', 'Substances' (highlighted), 'Reactions', 'References', and 'Suppliers'. The main area is titled 'Substances' and contains a search bar with the placeholder 'Enter a query...'. Below the search bar is a link to 'Use Advanced Search for Molecular Formula, Substance Property, or Experimental Spectra'. On the right, there is a preview of a chemical structure with 'Edit Drawing' and 'Remove' buttons. At the bottom right, there is a checkbox labeled 'Search Patent Markush' which is checked. A green box highlights a magnifying glass icon in the top right corner of the interface.

# Patent documents are evaluated for specific and Markush structures



# Find Reactions by Name, Registry Number, or Document Identifier

Search terms may be:

## •Substance Name:

- **Example:** benoxaprofen  
**Note:** Wildcard searching using an asterisk only works for single-search-term, single-word substance name searches (e.g., benoxa\*).
- **Example:** methyl ethyl ketone
- **Example:**  $\beta$ -amyloid  
**Note:** If your search term contains a Greek letter, see [Greek Letters Used in Searching](#) to insert the correct character.

## •CAS Registry Number (with or without dashes, e.g., 51146-57-7, 51146577)

### Notes:

- Square brackets are accepted around RNs (e.g., [51146-57-7]), but not single or double quotes.
- You may enter multiple CAS RNs separated by a space, no commas or other punctuation. The search field has a 2000-character limit.

## •Document Identifier:

- **Patent Number** (no spaces, e.g., US4571400)
- **Accession Number** (e.g., 1986:230471)
- **PubMed ID Number** (e.g., 15980585)
- **CAS Accession Number (CAN):** document number in CA Plus (e.g., 148:486341)



## Biosequence Searching: New Data, New Options

- New biosequence search option:
  - BLAST Search nucleotides and proteins
  - CDR: Search complementarity-determining regions of antibodies and T-Cell receptors and antibodies
  - Motif: sequence matching with wild cards and other features
- Over 550 M sequence-patent relationships and ~ 23 M sequences linked to non-patent literature
- Displays sequence alignment with filters and links to literature references
- Export sequence answer sets into Excel, including alignments
- Bioscape visualization tool provides additional analysis options

# Find Biosequences

There are three biosequence search types:

- **BLAST (Basic Local Alignment Search Tool)**: Search for proteins as well as nucleotides using a set of local alignment algorithms (BLASTn, MegaBlast, BLASTp, tBLASTn, BLASTx).
- **CDR (Complementarity-Determining Region)**: Search for antibody and t-cell receptors.
- **Motif**: Search for short patterns in DNA, RNA, or proteins with queries enabled for additional variability.



# Find Biosequences - BLAST

Find biosequences that match your query, which can be a protein/nucleotide string or a .txt/.fasta file.

1. Enter or copy and paste a protein/nucleotide string, or upload a sequence file:

- **Single sequence:** .txt file
- **Multiple sequences:** .fasta file

**Note:** The **maximum number** of sequences is **100**.

2. Select the appropriate **Sequence Type** based on your query.

3. Select the relevant **Search Within** option.

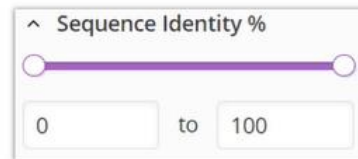
4. You may select **total sequence result limit** of 10 to 20,000 (default is 100).

5. Click the **Start Biosequence Search** button.

Click [Advanced Biosequence Search](#) to find sequences using parameters such as sequence identity percentage, gap costs, and BLAST algorithm.

The screenshot shows the SciFinder Biosequences search page. On the left, a sidebar lists search categories: All, Substances, Reactions, References, Suppliers, and Biosequences (highlighted). The main area is titled 'Biosequences' and contains a search box with the text 'Enter a protein or nucleotide string, or upload a .txt or .fasta file. Learn more about Biosequence Search.' Below this is a 'BLAST' tab and an 'Upload Sequence' button. A text area contains a protein sequence: '> pdb|1E57|C Chain C, Physalis Mottle Virus MDSEVVKVQASIPAPGSLSPQHTQSPAIVLPQFEATTFTGTAETAQVSLQTADPITKLTAPYRHAQIVECKAI LPTDVLAVSNPLTVLAWPANSPATPTQLRVYGGQSFVLGGISAATIEVPLNLDSVNRHLKDSVTYDTPKLLA YSRAPTNPSKIPTASISQISGRILSKPHILIAN'. Below the sequence is a 'Start Biosequence Search' button. On the right, there are options for 'Sequence Type' (Nucleotide or Protein), 'Search Within' (Nucleotides or Proteins), and a 'Limit Total Sequence Results to:' dropdown set to 100. At the bottom right is a 'Start Biosequence Search' button. Numbered callouts 1 through 5 point to the search box, the 'Upload Sequence' button, the 'Sequence Type' dropdown, the 'Search Within' dropdown, and the 'Start Biosequence Search' button respectively.

# Coverage and Sequence Identity percentages



Query Sequence    QQLLVVEEGG

Subject Sequence    QQLLVVEEIGS

Alignment

$$\text{Query Coverage (100\%)} = \frac{\text{Alignment Length}}{\text{Query Length}} = \frac{10}{10}$$

$$\text{Subject Coverage (91\%)} = \frac{\text{Alignment Length}}{\text{Subject Length}} = \frac{10}{11}$$

$$\text{Sequence Identity (90\%)} = \frac{\text{Number of Matches}}{\text{Alignment Length}} = \frac{9}{10}$$

# Find Biosequences - BLAST

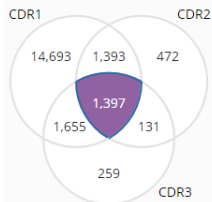
**Advanced Biosequence Search** has default values based on the selected **Sequence Type** and **Search Within** options.

Sequence Type / Search Within	Options (Default Value Shown)										
	Adjust Parameters for Short Sequences	Sequence Identity %	Match with Gaps	Gap Costs	Query Coverage %	Word Size	Reward for Match, Penalty for Mismatch	Scoring Matrix	BLAST Algorithm	E- Value	Exclude Low- Complexity Regions
Nucleotide / Nucleotides	Available	80	No	Existence 5, Extension 2	90	11	2, -3	—	BLASTn	10	No
Nucleotide / Proteins	N/A	—	No	Existence 11, Extension 1	90	6	—	BLOSUM62	BLASTx-fast	10	—
Protein / Nucleotides	N/A	—	No	Existence 11, Extension 1	90	6	—	BLOSUM62	TBLASTn-fast	10	—
Protein / Proteins	Available	—	No	Existence 11, Extension 1	90	3	—	BLOSUM62	BLASTp	10	No

# CDR Search

## CDR Complementarity-Determining Region

Select a segment below to view individual or intersecting CDR results.



Apply

Reset Segments

Bioscape Analysis

Visually explore sequence similarity with a new tool.  
[Learn more about Bioscape.](#)

Create Bioscape Analysis

Filter by

^ E-Value

0 to  $10^6$

^ Query Coverage %

0 to 100

^ Subject Coverage %

0 to 100

^ Alignment Identity %

Query Details [View Less](#)

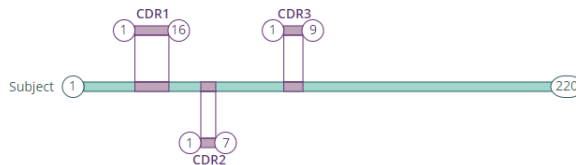
> CDR1  
KSSQSLLYTDGKTYLY

> CDR2  
LVSKLDS

> CDR3  
LQSTHFPHT

1

Alignment Identity: 100%



Matches: 32  
Mismatches: 0

[View Less](#) ▾

Alignment Subject References

References

Alignment Data  
BLAST Score: 79  
E-Value: 10.54998675038594

CDR1	1	KSSQSLLYTD	GKTYLY	16
S	25	KSSQSLLYTD	GKTYLY	40
CDR2	1	LVSKLDS		7
S	56	LVSKLDS		62
CDR3	1	LQSTHFPHT		9
S	95	LQSTHFPHT		103



# Find Biosequences - CDR

Find biosequences that match your query, which can be a protein string or a .txt/.fasta file.

**1. Enter, copy and paste, or upload a file for up to three CDRs.**

**2. You may select total sequence result limit of 10 to 20,000 (default is 100).**

**3. Click the Start Biosequence Search button.**

The screenshot shows the SciFinder Biosequences search page. On the left is a sidebar with navigation links: All, Substances, Reactions, References, Suppliers, and Biosequences (highlighted). The main area is titled 'Biosequences' and includes a search instruction: 'Enter a protein string, or upload a .txt or .fasta file. [Learn more about Biosequence Search.](#)'. Below this are three tabs: BLAST, CDR (selected), and Motif. A purple circle with the number '1' points to the 'Upload Sequence' button. The CDR section contains three input fields for CDR1, CDR2, and CDR3, each with a sequence (RASQGIRNYLA, AASTLQS, and QRYNRAPYT respectively) and a clear button (X). A purple circle with the number '2' points to the 'Limit Total Sequence Results to:' dropdown menu, which is set to 1000. A purple circle with the number '3' points to the 'Start Biosequence Search' button. The top right of the page has links for Saved, History, and Account.

# Find Biosequences - Motif

Find biosequences that match your query, which can be a protein/nucleotide string.

1. Enter or copy and paste a protein/nucleotide string.
2. Select the appropriate **Sequence Type** based on your query.
3. You may select **total sequence result limit** of 10 to 20,000 (default is 100).
4. Click the **Start Biosequence Search** button.

Click **Advanced Biosequence Search** to find sequences using query coverage % and e-value.

The screenshot shows the SciFinder Biosequences search page. On the left is a sidebar with search categories: All, Substances, Reactions, References, Suppliers, and Biosequences (highlighted). The main area is titled 'Biosequences' and includes a search input field with the example query '[LI][ALKV]G[FL][VI][D][AG]DG' (callout 1). Above the input are tabs for BLAST, CDR, and Motif. To the right of the input is a 'Clear Search' link. Below the input is a green-bordered button labeled 'Advanced Biosequence Search' (callout 4). On the right side, there are settings for 'Sequence Type' with 'Nucleotide' and 'Protein' buttons (callout 2), and 'Limit Total Sequence Results to:' with a dropdown set to '5000' (callout 3). At the bottom right is a purple 'Start Biosequence Search' button (callout 4). The top navigation bar includes 'Saved', 'History', and 'Account' links.

HSPAIR[AL]YLKTIRQLDNKSVIDEI[IVAL]EHLDKLIF

# Motif Search

## Motif Search Details

Sequence Type: Protein  
Query Coverage: 90%  
E-Value: 10

## Bioscape Analysis

Visually explore sequence similarity with a new tool.  
[Learn more about Bioscape.](#)

Create Bioscape Analysis

Filter by

^ E-Value

0 to  $10^6$

^ Query Coverage %

0 to 100

^ Subject Coverage %



## Biosequences (95)

View: Expand

Query Details [View More](#)

> Seq 1: 1 HSPAIRAYLKTIRQLDNKSVIDEIEHLDKLIF 33  
> Seq 1: 1 HSPAIRAYLKTIRQLDNKSVIDEIEHLDKLIF 33  
> Seq 2: 1 HSPAIRAYLKTIRQLDNKSVIDEVEHLDKLIF 33  
> Seq 3: 1 HSPAIRAYLKTIRQLDNKSVIDEAEHLDKLIF 33  
> Seq 4: 1 HSPAIRAYLKTIRQLDNKSVIDEIEHLDKLIF 33  
> Seq 5: 1 HSPAIRLYLKTIRQLDNKSVIDEIEHLDKLIF 33  
> Seq 6: 1 HSPAIRLYLKTIRQLDNKSVIDEVEHLDKLIF 33  
> Seq 7: 1 HSPAIRLYLKTIRQLDNKSVIDEAEHLDKLIF 33  
> Seq 8: 1 HSPAIRLYLKTIRQLDNKSVIDEIEHLDKLIF 33

[View Less](#)

Alignment

Subject

References

References

Alignment Data

BLAST Score: 252

E-Value: 8.71183e-28

Q	1	HSPAIRAYLK	TIRQLDNKSV	ID EIEHLDK	LIF	33
S	58	HSPAIRAYLK	TIRQLDNKSV	ID EIEHLDK	LIF	90

# Biosequence Motif Codes

Degenerate Code	Meaning
<b>X</b>	any amino acid
<b>B</b>	D or N (aspartic acid or asparagine)
<b>Z</b>	E or Q (glutamic acid or glutamine)
<b>J</b>	I or L (isoleucine or leucine)

Degenerate Code	Meaning
<b>N</b>	A or C or G or T
<b>R</b>	A or G
<b>Y</b>	C or T
<b>M</b>	A or C
<b>K</b>	G or T
<b>S</b>	C or G
<b>W</b>	A or T
<b>H</b>	A or C or T
<b>B</b>	C or G or T
<b>V</b>	A or C or G
<b>D</b>	A or G or T






## Biosequence Motif Codes


Degenerate Code	Meaning
[XYZ]	Any nucleotide or amino acid listed within the square brackets
{m,n}	at least m and maximum n residues length
{n}	exactly n length
^XYZ\$	Search for the exact sequence XYZ


# Thank you!

# High valued function – MethodesNow Search

CAS Solutions ▾


 **METHODSNow™**  
A CAS SOLUTION

 Saved

 Account

## Search

Enter keyword, matrix, analyte, etc.



[Advanced Search](#)

### Browse Method Categories

<a href="#">Agricultural Applications / Analysis</a>	<a href="#">Fuels / Geology / Biofuels</a>	<a href="#">Pharmacology / Toxicology</a>
<a href="#">Bioassays</a>	<a href="#">Historical Analysis / Dating</a>	<a href="#">Polymer Analysis</a>
<a href="#">Biomolecule Isolation</a>	<a href="#">Miscellaneous</a>	<a href="#">Water Analysis</a>
<a href="#">Environmental Analysis</a>	<a href="#">Organic Compound Analysis</a>	
<a href="#">Food Analysis</a>	<a href="#">Organometallics / Inorganics</a>	

### Recent Searches

# High valued function – MethodesNow Search

## Method Detail (1 of 43)

### Analysis of Gemcitabine hydrochloride in Blood plasma by RP-HPLC

CAS MN: 1-101-CAS-65250

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: Precipitation; Liquid chromatographic UV detectors; HPLC

Materials	Role	Image
Gemcitabine hydrochloride	analyte	<a href="#">View Structure</a>
Blood plasma	matrix	
Phenomenex C <sub>18</sub> (250 mm x 4.6 mm, 5 µm)	material	
Filter (0.4 µm)	material	
Methanol	reagent	<a href="#">View Structure</a>

## Source

Bioanalytical method development and validation of gemcitabine hydrochloride by RP-HPLC method

Rajesh, V.; Anupama, B.; Jagathi, V.; Varaprasad, K.

Asian Journal of Chemistry (2011), 23 (9), 3961 - 3963. Asian Journal of Chemistry

CODEN: AJCHEW | ISSN: 09707077

Full Text -



"gemcitabine hydrochloride"



Full Text -

#### Abstract ^

A simple, accurate, precise and sensitive HPLC method with UV detection was developed and validated to sep. and detect gemcitabine hydrochloride in human plasma using capecitabine hydrochloride as an internal standard. Gemcitabine hydrochloride and capecitabine hydrochloride (internal standard) were extracted from human plasma using methanol protein precipitation and were chromatographed on a phenomenex C<sub>18</sub> (250 mm x 4.6 mm, 5µm) column using 20 µl injection volume and detection at 270 nm. An isocratic mobile phase consisting of methanol: water (85:15 % volume/volume) was used to sep. these drugs. The retention times of gemcitabine hydrochloride and internal standard were 4.6 and 6.2 resp. The method was validated over the range of 406.10-4020.05 ng/mL. The limit of detection was 200 ng/mL and the limit of quantification was 400 ng/mL. Within and between-day precisions are less than 6.5 % for all quality control samples. The absolute recoveries of gemcitabine hydrochloride was greater than 90 % were achieved. The described method can be readily utilized for anal. of pharmaceutical products.

#### Equipment Used

High-performance liquid chromatography system, Shimadzu scientific instruments

#### Conditions

Chromatographic

Mobile phase, methanol and water (85:15% v/v); flow rate, 1.0 mL/min; total run time, 10 mins; detection wavelength, 270 nm.

#### Instructions

##### Preparation of standard solutions

1. Prepare stock standard solutions of gemcitabine hydrochloride and the (Capecitabine hydrochloride) internal standard by dissolving appropriate amounts of compounds in a known volume of methanol and water.
2. Store the prepared solutions at 4 °C.

##### Precipitation


1. Collect blank human blood with heparin from healthy and drug free volunteers.
2. Centrifuge the samples at 5000 rpm at room temperature.
3. Collect the plasma and store at -30 °C until analysis.
4. Prepare the blank plasma sample by adding 1 mL of plasma and 1 mL of methanol and vortex for 30 s.
5. Then centrifuge the solution at 4 °C, 5000 rpm for 5 min.
6. Take the supernatant liquid and transfer to HPLC vials.


##### High-performance liquid chromatography analysis


1. Perform the analysis on Shimadzu scientific instruments consisting of LC-20 AT pump and SPD-20 AT variable wavelength detector.
2. Carry out separation of compounds using a phenomenex C<sub>18</sub> (250 mm x 4.6 mm, 5 µm).
3. Use the mobile phase consisting of methanol and water (85:15% v/v).
4. Filter the mobile phase through 0.4 µm filter and then degas ultrasonically for 15 min.
5. Set the flow rate at 1.0 mL/min and total run time to 10 mins.
6. Monitor the eluent at a wavelength of 270 nm for gemcitabine hydrochloride.


#### Validation


# High valued function – Formulation Search



 Help & Support


 History


 Account




Formulation  
Designer

Search for

 Formulations



 Ingredients

Search for Formulations by Ingredient, Purpose, Form, Function, etc.



Use [Advanced Search](#) for Ingredient, Function, Purpose, Physical Form, Delivery Route, or Target

Recent Search History

March 26, 2021		
10:43 AM		
 Ingredients	Molidustat (1)	<div>Rerun Search</div> <div>Edit Search</div>
10:39 AM		
 Ingredients	Ponatinib (1)	<div>Rerun Search</div> <div>Edit Search</div>
March 11, 2021		

