

Your SciFinderⁿ team

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SCIFINDERⁿ
A CAS SOLUTION

What SciFinderⁿ can and SciFinder_{web} never could do
hbz Meeting 2020



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Agenda

1. Search without limits for virus (in general) and SARS-CoV-2

- By text
- By structure
- For Syntheses & Retrosyntheses

2. Important to know about SciFinderⁿ

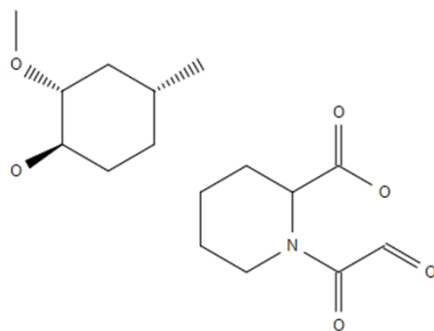
- Live history
- Combine answer sets
- Move from SciFinder_{web} to SciFinderⁿ
- Alerts
- Help in SciFinderⁿ

3. Specific training materials for all areas

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

SciFinderⁿ permits searching without limits

Features that are exclusively available in SciFinderⁿ are highlighted in blue!



Do my structural components on the left hand side help to fight a virus infection?

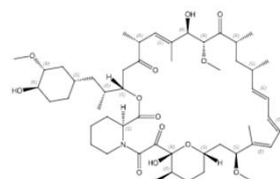
1. Search virus in SciFinderⁿ = 1.5 M references
2. Search my components in SciFinderⁿ = 6737 substructure hit substances

It is not possible to combine both hit sets in SciFinder_{web}. Combined in SciFinderⁿ 2867 references are retrieved that intersect.

SciFinderⁿ permits searching without limits

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

53123-88-9



Absolute stereochemistry shown
Double bond geometry shown

C₅₁H₇₉NO₁₃
Rapamycin

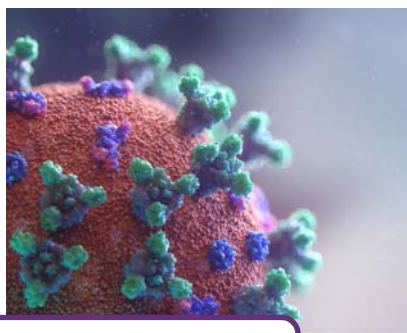


Photo by Fusion Medical
Animation on [Unsplash!](#)

Which compound can be of help?

- From 2862 references **518 611 substances are retrieved**
- The **first one in my list is Rapamycin – the best hit to my search** (and not the latest addition to the database)
- Rapamycin blocks the production of ribosomes that are critical for protein production. As the Virus needs to amplify proteins massively that can be of help.

Let's have a look at the search in detail!

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The combined text-structure search in SciFinderⁿ: Do the structural components help to fight a virus infection?

The screenshot displays the SciFinderⁿ search interface. On the left, a 'Search' sidebar lists categories: All, Substances, Reactions, References (highlighted), and Suppliers. The main search area contains a search bar with the text 'virus'. Below the search bar, a callout box with a red pointer to the search input area contains the text: 'Combine text terms with structural components. You can even draw fragments of a one-component substance in one window of the structure editor.' To the right of the search bar, there is a 'Use Advanced Search for Author, Journal, or Organization' link. Below this, a 'Structure Editor' window is visible, showing two chemical structures and buttons for 'Edit Drawing' and 'Remove'. The top navigation bar includes 'Saved', 'History', and 'Account' options.

Combined references: Which compound can help in my case?

The screenshot displays the SciFinder interface with a search for "virus" in the References section. The search results show 2,862 references. A callout box points to the search bar area, stating "The search retrieved 2862 references". Another callout box points to the "Substances" button in the left sidebar, stating "Click on „Substances“ to open the result selection". A third callout box points to the "Get Substances from References" button in the results area, stating "With SciFinderⁿ substances from all these results can be retrieved at a time".

Structure Match

AS D

Subs

Filter by

Document Type

Journal (2,203)

Patent (654)

References (2,862)

Sort: Relevance View: Partial Abstract

Substances

Substances

Re

Save

Get Substances from References

Targeting Human Myxoma Virus Is I All Results Selected Results

By: Lun, Xue Qing; Zho... /ang, Limei; Barrett, John W.; Stanford, Marianne M.; McFadden, Grant; Bell, John; Senger, Donna L.; et al
Cancer Research (2007), 67(18), 8818-8827 | Language: English, Database: CPlus

Get related substances: Rapamycin is displayed on top

The screenshot displays the SciFinder search interface. At the top, the SciFinder logo is on the left, followed by a search bar containing 'Substances' and 'Enter a query...'. To the right of the search bar are icons for 'Draw', a search magnifying glass, a star, a clock, and a user profile. Below the search bar, a 'Return to Home' link is visible. The main content area is titled 'Substances (518,611)' and includes a 'Sort: Relevance' dropdown and a 'View Partial' dropdown. Below this are buttons for 'References', 'Reactions', and 'Suppliers', along with icons for a document, an envelope, and a star labeled 'Save'. On the left side, there is a 'Filter by' section with two expandable categories: 'Commercial Availability' (with options for 'Available (17K)' and 'Not Available (501K)') and 'Reaction Role' (with options for 'Product (30K)', 'Reactant (13K)', 'Reagent (3,259)', 'Catalyst (2,636)', and 'Solvent (1,000)'). Below these is a 'Reference Role' section with an option for 'Adverse Effect (10K)'. The search results are displayed in three columns. The first column shows result 1: '53123-88-9' with a chemical structure of Rapamycin, the formula $C_{51}H_{79}NO_{13}$, and the name 'Rapamycin'. The second column shows result 2: '171715-28-9' with the text 'Image Not Available', 'Unspecified', and 'Protein kinase FRAP'. The third column shows result 3: '59865-13-3' with a chemical structure of Cyclosporin A, the formula $C_{62}H_{111}N_{11}O_{12}$, and the name 'Cyclosporin A'. Each result card includes a checkbox at the top and a zoom icon on the right.

Helpful hints

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

- Use as many SciFinderⁿ-tabs in parallel as you like
 - Open a new SciFinderⁿ tab by
 - Clicking on the SciFinderⁿ logo while holding the „Ctrl“ key – new ScFinderⁿ search page
 - Clicking on a Registry number while holding the „Ctrl“ key – details on the substance in new tab
 - Clicking on a reference title while holding the „Ctrl“ key – document details in new tab
- Use browser navigation without issues (Back/Forward button)
- Use SciFinderⁿ on your tablet with all search options

We are interested in the Virus SARS-CoV-2

- What is known so far about this new Corona virus?
- What is the most important publication, and how is a key publication linked to other publications?
- What is discussed in the context of SARS-CoV-2 globally?
- One specific reference about fast detection of the virus infection by PCR
- Helpful hint

What is known so far about this new Corona virus?: Search for the new Corona virus SARS-CoV-2



Saved



History



Account

Search

All

Substances

Reactions

References

Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

"novel coronavirus" or "severe acute respiratory syndrome"

x



Draw



Use [Advanced Search](#) for Author, Journal, or Organization



Work with the answer set :

The screenshot displays the SciFinder search results page. At the top, the search bar contains the query "novel coronavirus" or "severe acute respiratory syndrome". The results are filtered to 13,250 references. A callout box points to the search bar, stating: "The query terms are highlighted in the retrieved reference hits." The left sidebar shows filters for Document Type (Journal, Patent, Review, Biography, Book), Language (English, Chinese, Japanese, French, German), and Publication Year (1953 to 2020). A callout box points to the Publication Year filter, stating: "Refine by publication year, while being able to see when the most references were published in this area." The main content area shows two reference hits. The first hit is titled "Identification of a novel coronavirus in patients with severe acute respiratory syndrome" and includes the text: "The severe acute respiratory syndrome (SARS) has recently been identified as a new clin. entity. SARS is thought to be caused by an unknown infectious agent. Clin. specimens from patients with SARS were searched for unknown viruses with the use of cell cultures and mol. techniques. A novel coronavirus was identified in patients with SARS. The virus was isolated in cell culture, and a sequence 300 nucleotides in length was obtained by a PCR (PCR)-based random-amplification procedure. Genetic characterization indicated that the virus is only distantly related to known coronaviruses (Identical in...". The second hit is titled "A novel coronavirus associated with severe acute respiratory syndrome" and includes the text: "By: Ksiazek, Thomas G.; Erdman, Dean; Goldsmith, Cynthia S.; Zaki, Sherif R.; Peret, Teresa; Emery, Shannon; Tong, Suxiang; Urbani, Carlo; Comer, James A.; Lim, Wilina; et al".

What is the most relevant publication?

The screenshot shows the SciFinder search results page. At the top, the SciFinder logo is on the left, and the search bar contains the query "novel coronavirus" or "severe acute respiratory". The search results are displayed under the heading "References (678)". The results are sorted by "Relevance". A callout box on the right side of the page states: "References will be ordered by relevance by default, so that you can find the most relevant reference on top." The first result is a paper titled "A novel coronavirus from patients with pneumonia in China, 2019" by Zhu, Na; Zhang, Dingyu; Wang, Wenling; Li, Xingwang; Yang, Bo; Song, Jingdong; Zhao, Xiang; Huang, Baoying; Shi, Weifeng; Lu, Roujian; et al. The abstract text is partially visible, starting with "In Dec. 2019, a cluster of patients with pneumonia of unknown cause was linked to a seafood wholesale market in Wuhan, China. A previously unknown betacoronavirus was discovered through the use of unbiased sequencing in samples from patients with pneumonia. Human airway epithelial cells were used to isolate a novel coronavirus, named 2019-nCoV, which formed a clade within the subgenus sarbecovirus, Orthocoronavirinae subfamily. Different from both MERS-CoV and SARS-CoV, 2019-nCoV is the seventh member of the family of coronaviruses that infect humans. Enhanced surveillance and further investig...". Below the abstract, there are buttons for "Full Text", "Substances (0)", "Reactions (0)", "Cited By (16)", and "Citation Map". On the left side, there are filter options for "Document Type" (Journal, Patent, Review, Commentary, Editorial) and "Language" (English, Chinese, Korean, Spanish, German).

How is this publication linked to others? – Citation Map I

3

A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster
By: Chan, Jasper Fuk-Woo; Yuan, Shuofeng; Kok, Kin-Hang; To, Kelvin Kai-Wang; Chu, Hin; Yang, Jin; Xing, Fanfan; Liu, Jieling; Yip, Cyril Chik-Yan; Poon, Rosana Wing-Shan; et al
Lancet (2020), 395(10223), 514-523 | Language: English, Database: CAplus

An ongoing outbreak of pneumonia associated with a novel coronavirus was reported in Wuhan city, Hubei province, China. Affected patients were geog. linked with a local wet market as a potential source. No data on person-to-person or nosocomial transmission have been published to date. In this study, we report the epidemiol., clin., laboratory, radiol., and microbiol. findings of five patients in a family cluster who presented with unexplained pneumonia after returning to Shenzhen, Guangdong province, China, after a visit to Wuhan, and an addnl. family member who did not travel to Wuhan. Phylogenetic anal. of genetic sequences from these patients were done. From Jan 10, 2020, we enrolled a family of six patients who travelled to Wuhan from Shenzhen between Dec 29, 2019 and Jan 4, 2020. Of six family members who travelled to Wuhan, five were identified as infected with the novel coronavirus. Addnl., one family member, who did not travel to Wuhan, became infected with the virus after several days of contact with four of the family members. None of the family members had contacts with Wuhan markets or animals, although two had visited a Wuhan hospital. Five family members (aged 36-66 years) presented with fever, upper or lower respiratory tract symptoms, or diarrhea, or a combination of these 3-6 days after exposure. They presented to our hospital (The University of Hong Kong-Shenzhen Hospital, Shenzhen) 6-10 days after symptom onset. They and one asymptomatic child (aged 10 years) had radiol. ground-glass lung opacities. Older patients (aged >60 years) had more systemic symptoms, extensive radiol. ground-glass lung changes, lymphopenia, thrombocytopenia, and increased C-reactive protein and lactate dehydrogenase levels. The nasopharyngeal or throat swabs of these six patients were neg. for known respiratory microbes by point-of-care multiplex RT-PCR, but five patients (four adults and the child) were RT-PCR pos. for genes encoding the internal RNA-dependent RNA polymerase and surface Spike protein of this novel coronavirus, which were confirmed by Sanger sequencing. Phylogenetic anal. of these five patients' RT-PCR amplicons and two full genomes by next-generation sequencing showed that this is a novel coronavirus, which is closest to the bat severe acute respiratory syndrome (SARS)-related coronaviruses found in Chinese horseshoe bats. Our findings are consistent with person-to-person transmission of this novel coronavirus in hospital and family settings, and the reports of infected travelers in other geog. regions. The Shaw Foundation Hong Kong, Michael Seak-Kan Tong, Respiratory Viral Research Foundation Limited, Hui Ming, Hui Hoy and Chow Sin Lan Charity Fund Limited, Marina Man-Wai Lee, the Hong Kong Hainan Com. Association South China Microbiol. Research Fund, Sanming Project of Medicine (Shenzhen), and High Level-Hospital Program (Guangdong Health Commission).

[View Less ^](#)

Full Text ▾

Substances (0) Reactions (0) Cited By (15) Citation Map

The Citation map provides a quick overview of cited and citing references.



How is one publication linked with others? – Citation Map II

Citation Map

A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster

By: Chan, Jasper Fuk-Woo; Yuan, Shuofeng; Kok, Kin-Hang; To, Kelvin Kai-Wang; Chu, Hin; Yang, Jin; Xing, Fanfan; Liu, Jieling; Yip, Cyril Chik-Yan; Poon, Rosana Wing-Shan; et al
Lancet (2020), 395(10223), 514-523 | Language: English, Database: CPlus

Full Text

Abstract: An ongoing outbreak of pneumonia associated with a novel coronavirus was reported in Wuhan city, Hubei province, China. Affected patients were geog. linked with a local wet market as a potential source. No data on person-to-person or nosocomial transmission have been published to date. In this study, we report the epidemiol., clin., laboratory, radiol., and microbiol. findings of five patients in a family cluster who presented with unexplained pneumonia after returning to Shenzhen, Guangdong province, China, after a visit to Wuhan, and an addnl. family member who did not travel to Wuhan. Phylo...

[View More](#)

Filter by

Document Type

- Journal (46)
- Review (6)

Author

- Lau, Susanna K. P. (9)
- Woo, Patrick C. Y. (9)
- Yuen, Kwok-Yung (9)
- Chan, Kwok-Hung (5)
- Chan, K H (4)

[View All](#)

Concept

- Homo sapiens (10)
- Human (10)
- Female (8)
- Humans (8)
- Male (8)

[View All](#)

References This Document Cites

- Coronavirus as a possible cause of severe acute respiratory syndrome. Lancet (London, England) (2003)
Cited By 1,515 [Map](#)
- Bats are natural reservoirs of SARS-like coronaviruses. Science (Washington, DC, United States) (2005)
Cited By 996 [Map](#)
- Severe acute respiratory syndrome coronavirus-like virus in Chinese. [Map](#)
- Clinical progression and viral load in a community outbreak of coronavirus-associated SARS pneumonia: a prospective study. Lancet (London, England) (2003)
Cited By 732 [Map](#)
- Discovery of seven novel mammalian and avian coronaviruses in the genus Deltacoronavirus supports bat coronaviruses as the gene source of...

References Citing This Document

- Pattern of early human-to-human transmission of Wuhan 2019 novel coronavirus (2019-nCoV), December 2019 to January 2020. Euro surveillance : bulletin Europeen sur les maladies transmissibles = European communicable disease bulletin (2020)
Citing 5 [Map](#)
- Incubation period of 2019 novel coronavirus (2019-nCoV) infections among travellers from Wuhan, China, 20-28 January 2020. Euro surveillance : bulletin Europeen sur les maladies transmissibles = European communicable disease bulletin (2020)
Citing 3 [Map](#)
- Pathogenicity and transmissibility of 2019-nCoV-A quick overview and comparison with other emerging viruses. Microbes and Infection (Date unavailable)
Citing 2 [Map](#)
- Phase-adjusted estimation of the number of Coronavirus Disease 2019 cases in Wuhan, China. Cell Discovery (2020)
Citing 1 [Map](#)
- China coronavirus: Six questions scientists are asking. Nature (London, United Kingdom) (2020)
Citing 1 [Map](#)
- An interim review of the epidemiological characteristics of 2019 novel...

Citations can be filtered by concepts. Click on „View All“ to review all concepts.

View all concepts and select Disease outbreaks

Concept

Top Count | Alphanumeric

2 Selected

<input type="checkbox"/> Female (8)	<input type="checkbox"/> COVID-19 (2)	<input type="checkbox"/> Child (1)
<input type="checkbox"/> Humans (8)	<input type="checkbox"/> Diagnosis (2)	<input type="checkbox"/> Child, Preschool (1)
<input type="checkbox"/> Male (8)	<input type="checkbox"/> Diarrhea (2)	<input type="checkbox"/> China Rattus coronavirus HKU24 (1)
<input type="checkbox"/> Homo sapiens (7)	<input type="checkbox"/> Disease Progression (2)	<input type="checkbox"/> Colonoscopy (1)
<input type="checkbox"/> Human (7)	<input type="checkbox"/> DNA sequences (2)	<input type="checkbox"/> Dexamethasone (1)
<input type="checkbox"/> Severe acute respiratory syndrome (7)	<input type="checkbox"/> Hong Kong (2)	<input type="checkbox"/> Diagnostic biomarkers (1)
<input type="checkbox"/> Adult (6)	<input type="checkbox"/> Molecular epidemiology (2)	
<input type="checkbox"/> Middle Aged (6)		
<input checked="" type="checkbox"/> Disease Outbreaks (5)		
<input type="checkbox"/> Aged (4)	<input type="checkbox"/> Viral envelope E proteins (2)	<input type="checkbox"/> Follow-Up Studies (1)
<input type="checkbox"/> China (4)	<input type="checkbox"/> Viral hemagglutinins, HE (hemagglutinin-esterase) (2)	<input type="checkbox"/> Genome (1)
<input type="checkbox"/> Microbial gene (4)	<input type="checkbox"/> Viral matrix M proteins (2)	<input type="checkbox"/> Genome, Viral (1)
<input type="checkbox"/> Molecular evolution (4)	<input type="checkbox"/> Viral proteins (2)	<input type="checkbox"/> Genotypes (1)
<input type="checkbox"/> Protein sequences (4)	<input type="checkbox"/> Viral RNA sequences (2)	<input type="checkbox"/> Global Health (1)
<input type="checkbox"/> SARS Virus (4)		<input type="checkbox"/> Human coronavirus (1)
<input type="checkbox"/> Severe acute respiratory		

[Apply](#) [Cancel](#)

Let's have a look at citations discussing Disease Outbreaks



How is one publication linked with others? – Citation Map results

Citation Map

A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster

By: Chan, Jasper Fuk-Woo; Yuan, Shuofeng; Kok, Kin-Hang; To, Kelvin Kai-Wang; Chu, Hin; Yang, Jin; Xing, Fanfan; Liu, Jieling; Yip, Cyril Chik-Yan; Poon, Rosana Wing-Shan; et al

Lancet (2020), 395(10223), 514-523 | Language: English, Database: CPlus

Abstract: An ongoing outbreak of pneumonia associated with a novel coronavirus was reported in Wuhan city, Hubei province, China. Affected patients were geog. linked with a local wet market as a potential source. No data on person-to-person or nosocomial transmission have been published to date. In this study, we report the epidemiol., clin., laboratory, radiol., and microbiol. findings of five patients in a family cluster who presented with unexplained pneumonia after returning to Shenzhen, Guangdong province, China, after a visit to Wuhan, and an addnl. family member who did not travel to Wuhan. Phylo...

[View More](#)

Full Text

Filter by

Document Type

Journal (5)

Author

Chan, K H (3)

Chan, K S (3)

Cheng, V C C (3)

Chu, C M (3)

Hung, I F N (3)

[View All](#)

Concept

Homo sapiens (10)

Human (10)

Female (8)

Humans (8)

Male (8)

Disease Outbreaks (5)

[View All](#)

References This Document Cites

Clinical progression and viral load in a community outbreak of coronavirus-associated SARS pneumonia: a prospective study.

Lancet (London, England) (2003)

Cited By 732

[Map](#)

Viral load in patients infected with pandemic H1N1 2009 influenza A virus.

Journal of medical virology (2010)

Cited By 132

[Map](#)

Viral loads in clinical specimens and SARS manifestations.

Emerging infectious diseases (2004)

Cited By 76

[Map](#)

Viral replication in the nasopharynx is associated with diarrhea in patients with severe acute respiratory syndrome.

Clinical infectious diseases : an official publication of the Infectious Diseases Society of America (2004)

Cited By 38

[Map](#)

A patient with asymptomatic severe acute respiratory syndrome (SARS) and antigenemia from the 2003-2004 community outbreak of SARS in Guangzhou, China.

Clinical infectious diseases : an official publication of the Infectious Diseases Society of America (2006)

Cited By 12

[Map](#)

References Citing This Document

There are no references available in SciFinderⁿ that cite this document.

By refining citations with concepts, you reduce the number of cited/citing documents you need to review. This can save you a lot of time!

The concepts have been assigned by CAS scientists during the intellectual indexing process.



What has been discussed in the context of SARS-CoV-2 globally?

- Concepts

Use the concept filter to refine precisely.
In SciFinderⁿ this filter is not limited to any number of references.

Publication Year

2020

Apply

View Larger

Organization

Publication Name

Concept

CAS Solutions

Formulation Purpose

Database

Search Within Results

SciFinderⁿ

References

novel coronavirus or severe acute respiratory syndrome

Search

Results: 1678

Sort: Relevance

View: Partial Abstract

Filter by

Document Type

Journal (610)

Patent (54)

Review (57)

Commentary (1)

Editorial (33)

View All

Language

English (554)

Chinese (113)

Korean (8)

Spanish (4)

German (1)

View All

Publication Year

2019 to 2020

Apply

View Larger

Available at My Institution

Author

Organization

Publication Name

Concept

CAS Solutions

Formulation Purpose

References (1678)

Sort: Relevance

View: Partial Abstract

Substances (0)

Reactions (0)

Cited By (16)

Citation Map

1

A novel coronavirus from patients with pneumonia in China, 2019

By: Zhu, Na; Zhang, Dongyi; Wang, Wending; Li, Jingwang; Yang, Bin; Song, Jingdong; Zhao, Xiang; Huang, Shaoying; Shi, Wenfang; Li, Ruijiao, et al.

New England Journal of Medicine (2020), 382(8), 727-733 | Language: English, Database: CAPUS

In Dec. 2019, a cluster of patients with pneumonia of unknown cause was linked to a seafood wholesale market in Wuhan, China. A previously unknown betacoronavirus was discovered through the use of unbiased sequencing in samples from patients with pneumonia. Human airway epithelial cells were used to isolate a novel coronavirus, named 2019-nCoV, which formed a clade within the subgenus sarbecovirus, Orthocoronavirinae subfamily. Different from both MERS-CoV and SARS-CoV, 2019-nCoV is the seventh member of the family of coronaviruses that infect humans. Enhanced surveillance and

View More

Full Text

Substances (0)

Reactions (0)

Cited By (16)

Citation Map

2

Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China

By: Huang, Changlin; Wang, Yeming; Li, Jingwang; Ren, Lik; Zhao, Jieping; Hu, Yi; Zhang, Li; Fan, Guohua; Xu, Jieping; Gu, Xiaoping, et al.

Lancet (2020), 395(10223), 497-506 | Language: English, Database: CAPUS

A recent cluster of pneumonia cases in Wuhan, China, was caused by a novel betacoronavirus, the 2019 novel coronavirus (2019-nCoV). We report the epidemiological, clinical, laboratory, and radiological characteristics and treatment and clinical outcomes of these patients. All patients with suspected 2019-nCoV were admitted to a designated hospital in Wuhan. We prospectively collected and analyzed data on patients with laboratory-confirmed 2019-nCoV infection by real-time RT-PCR and next-generation sequencing. Data were obtained with standardized data collection forms shared by the International Severe Acute Respiratory and Emerging Infection Consortium. Data were obtained with standardized data collection forms shared by the International Severe Acute Respiratory and Emerging Infection Consortium.

View More

Full Text

Substances (11)

Reactions (0)

Cited By (18)

Citation Map

3

A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster

Concepts - Concept Filter I

^ Concept

- Homo sapiens (82)
- Human (82)
- Severe acute respiratory syndrome (77)
- Humans (59)
- Severe acute respiratory syndrome coronavirus (58)

[View All](#)

Concept is the principal filter for refining with CAS keyword indexing.

The 5 most abundant concepts are displayed, more options are available via „View All“

Concepts - Concept Filter II

Concept ×

Top Count | Alphanumeric | Search

1 Selected

<input type="checkbox"/> Homo sapiens (82)	<input type="checkbox"/> Influenza A virus (13)	<input type="checkbox"/> Human herpesvirus 4 (9)
<input type="checkbox"/> Human (82)	<input type="checkbox"/> Rotavirus (13)	<input type="checkbox"/> Leukemia (9)
<input checked="" type="checkbox"/> Severe acute respiratory syndrome (77)	<input type="checkbox"/> Antibodies and Immunoglobulins (12)	<input type="checkbox"/> Molecular epidemiology (9)
<input type="checkbox"/> Humans (59)	<input type="checkbox"/> Betacoronavirus (12)	<input type="checkbox"/> Molecular evolution (9)
<input type="checkbox"/> Severe acute respiratory syndrome coronavirus (58)	<input type="checkbox"/> Human papillomavirus (12)	<input type="checkbox"/> Nipah virus (9)
<input type="checkbox"/> Antiviral agents (48)	<input type="checkbox"/> Marburgvirus (12)	<input type="checkbox"/> Rhinovirus (9)
<input type="checkbox"/> Coronavirus (42)	<input type="checkbox"/> Pharmaceutical carriers (12)	<input type="checkbox"/> Swine (9)
<input type="checkbox"/> Viral infection (42)	<input type="checkbox"/> Pharmaceutical excipients (12)	<input type="checkbox"/> Viral spike glycoproteins (9)
<input type="checkbox"/> Coronavirus Infections (34)	<input type="checkbox"/> Pneumonia (12)	<input type="checkbox"/> Bacterial infection (8)
<input type="checkbox"/> Middle East respiratory syndrome coronavirus (32)	<input type="checkbox"/> Respiratory syncytial virus (12)	<input type="checkbox"/> Cardiovascular disease (8)
<input type="checkbox"/> Influenza virus (26)	<input type="checkbox"/> Anti-inflammatory agents (11)	<input type="checkbox"/> Chronic obstructive pulmonary disease (8)
<input type="checkbox"/> Animals (25)	<input type="checkbox"/> Chiroptera (11)	<input type="checkbox"/> Combination chemotherapy (8)
<input type="checkbox"/> Severe acute respiratory syndrome coronavirus 2 (23)	<input type="checkbox"/> Female (11)	<input type="checkbox"/> Coronaviridae (8)
<input type="checkbox"/> Zika virus (22)	<input type="checkbox"/> Genome, Viral (11)	<input type="checkbox"/> DNA sequences (8)
	<input type="checkbox"/> Lassa virus (11)	<input type="checkbox"/> Filoviridae (8)
	<input type="checkbox"/> Mumps virus (11)	

Apply Cancel

„View All“ contains further filter options:

- Analyse by **Top Count**, **Alphanumeric** or **Search**
- **Search** allows you to query any concept, internal and right-hand truncation is allowed
- All entries on a page can be selected
- The system will memorize checkmarked concepts when entering different terms

Concepts - Concept Filter III

Concept

Top Count Alphanumeric Search

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

1 Selected

- Sabia virus (1)
- Saccharomyces (2)
- Saccharomyces cerevisiae (1)
- Saimiriine herpesvirus (1)
- Saline waters (1)
- Saliva (5)
- Salivary gland neoplasm (1)
- Salmon (1)
- Salmonella (5)
- Salmonella bongori (1)
- Salmonella choleraesuis arizonae (1)
- Salmonella dublin (1)
- Salmonella enterica (3)
- Schistosoma
- Schistosoma
- Schistosoma
- Schistosoma mansoni (1)
- Schistosoma mekongi (1)
- Schistosomatidae (1)
- Schistosomiasis (4)
- Schistosomicides (1)
- Schizosaccharomyces pombe (1)
- Schmallenberg virus (1)
- Schmidt syndrome (1)
- Schnitzler syndrome (1)
- Scleritis (1)
- Severe acute respiratory syndrome (77)
- Severe acute respiratory syndrome coronavirus (58)
- Severe acute respiratory syndrome coronavirus 2 (23)
- Severe acute respiratory syndrome-related coronavirus (1)
- Sex (2)
- Sezary syndrome (1)
- Sheep (1)
- β -Sheet (1)

← Prev 1 2 3 Next →

Apply Cancel

SciFinderⁿ memorizes what was selected. Selected concepts will be combined with „OR“.

Concept

Top Count Alphanumeric Search

Concept Name

Severe Search

1 Selected

- Severe acute respiratory syndrome (77)
- Severe acute respiratory syndrome coronavirus 2 (23)
- Severe acute respiratory syndrome coronavirus (58)
- Severe acute respiratory syndrome-related coronavirus (1)

Apply Cancel

A specific reference from Prof. Christian Drosten, Charité Berlin



References

"novel coronavirus" or "Severe acute respiratory syndro



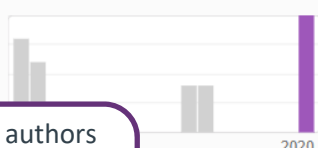
Filter by

Document Type

Journal (5)

Editorial (2)

Publication Year



No Max

Apply

View Larger

Selection of specific authors is possible in the respective filter. Special character in the name can lead to multiple entries.

At My Institution

2019

2020

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

2019

Author

Nishiura, Hiroshi (10)

Akhmetzhanov, Andrei R (8)

Linton, Natalie M (8)

Jung, Sung-Mok (7)

Kinoshita, Ryo (7)

Drosten, Christian (5)

View All

References (5)

Sort: Relevance

View: Full Abstract

Substances

Reactions

Cited By



Save

1

[Detection of 2019 novel coronavirus \(2019-nCoV\) by real-time RT-PCR.](#)

By: Corman, Victor M; Landt, Olfert; Kaiser, Marco; Molenkamp, Richard; Meijer, Adam; Chu, Daniel K W; Bleicker, Tobias; Brünink, Sebastian; Schneider, Julia; Schmidt, Marie Luisa; et al

Euro surveillance : bulletin Europeen sur les maladies transmissibles = European communicable disease bulletin (2020), 25(3) | Language: English, Database: MEDLINE

BACKGROUND: The ongoing outbreak of the recently emerged novel coronavirus (2019-nCoV) poses a challenge for public health laboratories as virus isolates are unavailable while there is growing evidence that the outbreak is more widespread than initially thought, and international spread through travellers does already occur. AIM: We aimed to develop and deploy robust diagnostic methodology for use in public health laboratory settings without having virus material available. METHODS: Here we present a validated diagnostic workflow for 2019-nCoV, its design relying on close genetic relatedness of 2019-nCoV with SARS coronavirus, making use of synthetic nucleic acid technology. RESULTS: The workflow reliably detects 2019-nCoV, and further discriminates 2019-nCoV from SARS-CoV. Through coordination between academic and public laboratories, we confirmed assay exclusivity based on 297 original clinical specimens containing a full spectrum of human respiratory viruses. Control material is made available through European Virus Archive - Global (EVAg), a European Union infrastructure project. CONCLUSION: The present study demonstrates the enormous response capacity achieved through coordination of academic and public laboratories in national and European research networks.

Full Text

Substances (0)

Reactions (0)

Cited By (2)

Citation Map



Helpful hint I



The screenshot shows the NDR website interface. At the top, there is a navigation bar with the NDR logo and various menu items: Nachrichten, Niedersachsen, Schleswig-Holstein, Mecklenburg-Vorpommern, Hamburg, Sport, Ratgeber, Kultur, Geschichte, and Verkehr. Below this is a secondary navigation bar with 'NDR Info', Sendungen, NDR Info Spezial, Die Redaktion, and App. The main content area features a large image of a coronavirus particle on the left. To its right, the text reads: 'Je weiter sich das Coronavirus in Europa ausbreitet, desto mehr wollen die Menschen darüber wissen. Auf dieses Informationsbedürfnis reagiert NDR Info mit einem neuen Coronavirus-Podcast, der jeden Tag ein Update zur Situation liefert. Montags bis freitags beantwortet Prof. Dr. Christian Drosten (Leiter der [Virologie an der Berliner Charité](#)) in Interviews Fragen zur aktuellen Situation, erklärt Zusammenhänge und schildert, wie er persönlich diese Tage'. To the right of the article, there is a 'MEHR NACHRICHTEN' section with three items: 'Tödliche Verfolgungsjagd: Sieben Jahre Haft', 'Coronavirus: Live-Ticker zur Lage in Norddeutschland', and 'Corona: Neue Vorkehrungen für Kitas und Schulen'. A 'Übersicht' button is located below these items.

Please feel free to review the daily report of Prof. Drosten on the Corona virus update – it is most helpful!

Helpful hint II

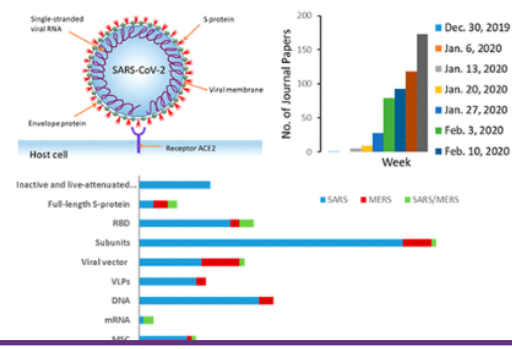
Background

ARTICLE SECTIONS

Jump To ▾

The outbreak of the novel coronavirus disease, COVID-19, caused by the new coronavirus 2019-nCoV that is now officially designated as severe acute respiratory syndrome-related coronavirus SARS-CoV-2, represents a pandemic threat to global public health.^(1,2) Although the epicenter of the COVID-19 outbreak in December of 2019 was located in Wuhan, China, this disease has spread to more than 100 countries (Figure 1) with over 100 000 confirmed cases and over 3,800 confirmed deaths worldwide (Figure 2) as of March 9, 2020.⁽³⁾ In addition, millions of people's lives have been affected as a result of mandatory isolations/quarantines. The ripple effect of the COVID-19 outbreak could potentially bring major challenges to worldwide health systems and have far-reaching consequences on the global economy if the spread of the virus is not effectively controlled.^(1,2,4)

Abstract



Publication of CAS on Data about
SARS-CoV-2 in [ACS central science](#)
open access

Reference searching in more detail: Boolean operators

Use parentheses to group logical expressions such as OR'ed synonyms:
(fungicide OR pesticide) AND strobilurin

AND Requires both terms or phrases to be present within the document



OR Requires either one or both terms or phrases to be present
Connect synonyms with OR



NOT excludes documents from an answer set
Be careful when using the NOT operator, you cannot always
assess the context of document texts



Wildcards and phrase search

Wildcards and the phrase search allow for more comprehensive and precise retrieval | Use in reference and substance name searches

Internal and right-hand truncation is available

- * Replaces 0 to any number of characters polymorph* | immunoglobulin conjugate*
- ? Replaces 0 or 1 character benzonorbornen?

Terms masked with double quotes will be searched as a phrase,
e.g.: "Liquid crystal display"

General advice for text queries

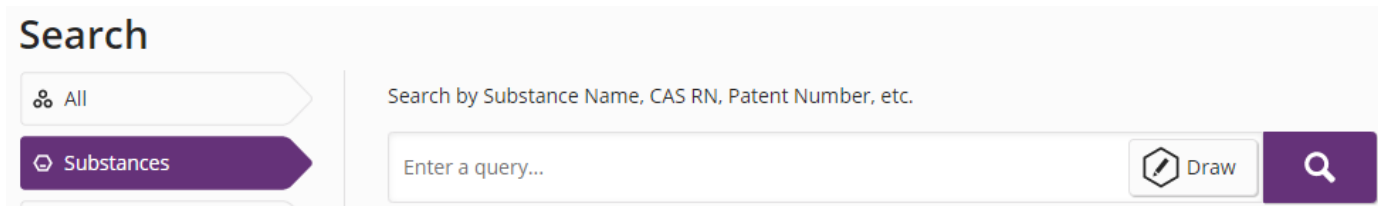
- Use noun phrases and/or Boolean operators
- Look up indexed concepts and use them in your text queries for precise searching
- Combine synonyms in parentheses

novel coronavirus disease
"novel coronavirus" **and** disease

"Severe acute respiratory syndrome coronavirus 2" or "COVID-19"

coronavirus **and** (sciuridae **or** squirrel)

Substance searching in the text field I



The screenshot shows the SciFinder search interface. On the left, under the heading "Search", there are two filter buttons: "All" (with a grid icon) and "Substances" (with a magnifying glass icon and highlighted in purple). To the right of the filters, the text "Search by Substance Name, CAS RN, Patent Number, etc." is displayed above a search input field. The input field contains the placeholder text "Enter a query...". To the right of the input field are two buttons: "Draw" (with a pencil icon) and a search button (with a magnifying glass icon).

- allows input of up to 2000 characters
- Input can be chemical names, Trade names, Acronyms, CAS Registry Numbers, DOIs and Patent Numbers

Substance searching in the text field II

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

Search with one or more substance names, identifiers or document IDs

Geraniol	Finds geraniol record
106-24-1	Finds geraniol record, uses CAS Registry number as identifier
Geraniol acetate	Finds 3 records: geraniol acetate, geraniol and acetate ion
"Geraniol acetate" geraniol	Finds 2 records: Geraniol acetate and geraniol
Geraniol*	Finds all names with the stem geraniol
WO2018027202	Finds all indexed substances for patent WO2018027202

Internal and right-hand truncation is available

E.g.: aspirin* | copper*alloy* | immunoglobulin*conjugate*

Chemical name search examples

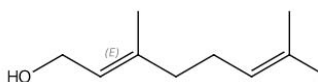
Substances ▾ "Geraniol acetate" geraniol × Draw

Substances (2)

References ▾ Reactions ▾ Suppliers ▾

1

106-24-1



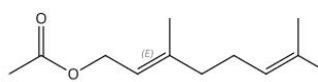
Double bond geometry shown

$C_{10}H_{18}O$
Geraniol

20K References 4,134 Reactions 92 Suppliers

2

105-87-3



Double bond geometry shown

$C_{12}H_{20}O_2$
Geraniol acetate

7,985 References 935 Reactions 72 Suppliers

Substances ▾ copper*alloy* × Draw

Substances (111,435)

References ▾ Reactions ▾ Suppliers ▾

1

12668-36-9

Component	Percent
Cu	x
Sn	x

Cu.Sn
Components: 2
Copper-tin alloy

3,836 References 9 Reactions 0 Suppliers

2

11143-56-9

Component	Percent
Zn	x
Cu	x

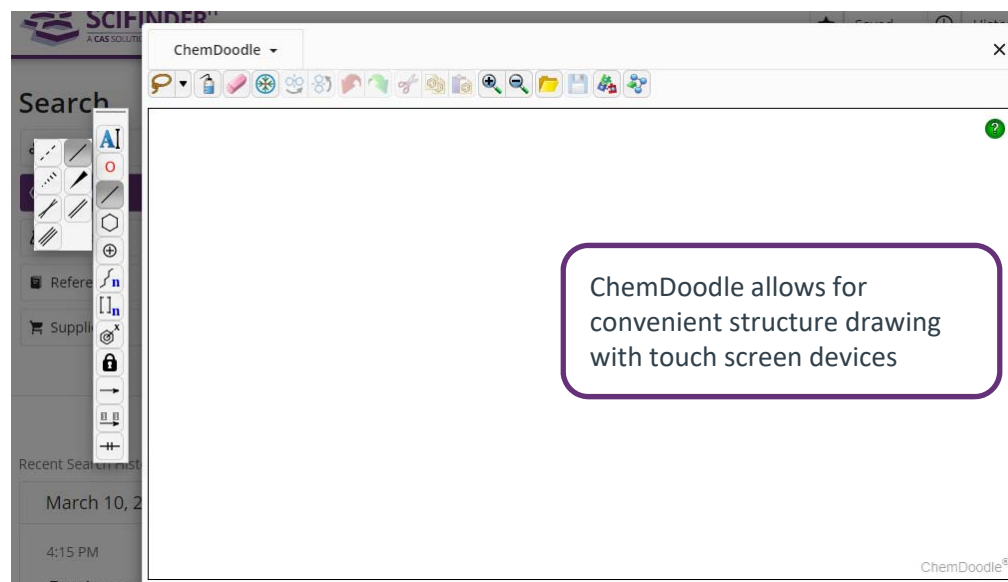
Cu.Zn
Components: 2
Copper zinc alloy

3,313 References 768 Reactions 1 Supplier

Substance structure search

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

- The CAS Draw structure editor is the same as in SciFinder_{web}
- The ChemDoodle editor is new in SciFinderⁿ



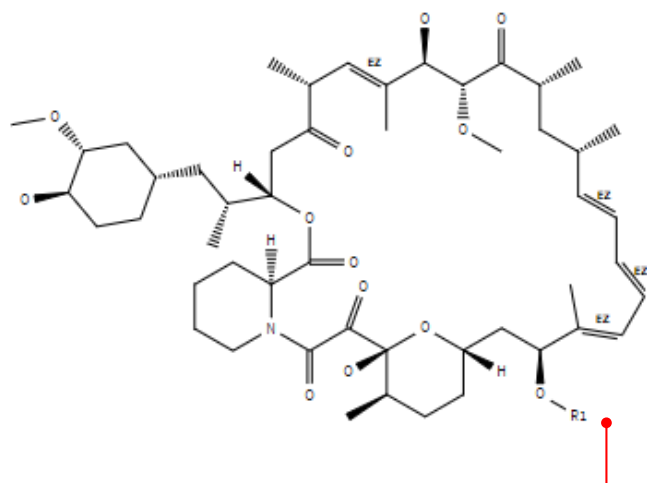
Substance structure search

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

- The three different structure search types run simultaneously:
 - As Drawn, Substructure, Similarity Result
- The Exact/As Drawn structure search is different in SciFinderⁿ:

SciFinder _{web}	SciFinder ⁿ
Exact structure, mixtures or salts or labeled versions of the exact structure were retrieved	The exact part of the substance answer retrieves: Exact structure, mixtures or salts or labeled version
Structure with variables cannot be searched as exact	Structure with variables can be searched exactly – as “As Drawn”

Substance structure search: Rapamycin: As Drawn



Variability was introduced by using R1 for any hetero- or carbocycle

SciFinderⁿ
A CAS SOLUTION

Substances ▾ Enter a query... Edit ▾ 🔍

← Return to Home

Structure Match

- As Drawn (2)
- Substructure (6)
- Similarity (9,448)

Analyze Structure Precision

Filter by

- Commercial Availability
 - Not Available (2)
- Reaction Role
 - Product (2)
- Reference Role
 - Biological Study (2)

Substances (2) Sort: Rel

- References ▾
- Reactions ▾
- Suppliers ▾

1	2
328059-92-3	328059-91-2
Absolute stereochemistry shown Double bond geometry shown	Absolute stereochemistry shown Double bond geometry shown
C₅₆H₈₁NO₁₃ Rapamycin, 7-O-demethyl-7-O-phenyl-, (7R,31S)-	C₅₆H₈₁NO₁₃ Rapamycin, 7-O-demethyl-7-O-phenyl-, (31S)-
1 Reference 1 Reaction 0 Suppliers	1 Reference 1 Reaction 0 Suppliers

substance answer set: Rapamycin I

Structure Match

- As Drawn (218)
- Substructure (3,010)
- Similarity (9,448)

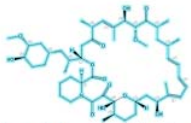
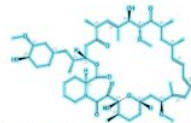
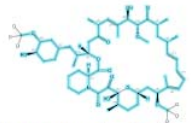
Analyze Structure Precision

Filter by

- Commercial Availability
 - Available (4)
 - Not Available (192)
- Reaction Role
 - Product (13)
 - Reactant (6)
 - Reagent (1)

Substances (196) Sort: Relevance View Partial

References Reactions Suppliers Save

1	2	3
151519-50-5	53123-88-9	392711-23-8
		
Absolute stereochemistry shown Double bond geometry shown	Absolute stereochemistry shown Double bond geometry shown	Absolute stereochemistry shown Double bond geometry shown
C₅₀H₇₇NO₁₃ Novolimus	C₅₁H₇₉NO₁₃ Rapamycin	C₅₁H₇₃D₆NO₁₃ Rapamycin, 7,41-di-O-demethyl-7,41-di-O-(methyl- <i>d</i> ₃)-
155 References 9 Reactions 13 Suppliers	37K References 2,175 Reactions 134 Suppliers	3 References 4 Reactions 0 Suppliers

Analysis for the substance answer set for Rapamycin II

Classes

- Alloys
- Coordination compounds
- Incompletely defined
- Mixtures
- Polymers
- Organics, and others not listed

In SciFinder_{web} you can refine by substance classes before retrieving the corresponding references

SciFinder_{web}

^ Number of Components

- 1 (135)
- 2 (47)
- 3 (12)
- 4 (2)

In SciFinderⁿ you can refine by a specific number of components within the substance answer set.

^ Substance Class

- Organic/Inorganic Small Molecule (135)
- Mixture (55)
- Salt and Compound With (5)
- Protein/Peptide Sequence (2)
- General Derivative (1)
- Polymer (1)

In SciFinderⁿ you can refine by substance classes within the reference answer set while reviewing the reference hits.

SciFinderⁿ



Helpful hints for substance searching

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

- Search for Deuterium and Tritium using the structure editor
- Analyze by precision can be applied in the answer set to differentiate local charges or to divide an aromatic ring from a singular double bond in a ring
- See all literature entries when you review substance properties in CAS Registry (not only the latest one)

Not Rapamycin, but Remdesivir (Tradenname Sirolimus from Gilead) is a hot candidate to treat SARS-CoV-2

But Gilead faces a problem

www.bloomberg.com/.../chinese-company-says-it-can-make-gilead-s-... ▼

Chinese Company Says It Can Make Gilead's Coronavirus Drug

Feb 12, 2020 - Chinese Firm Makes **Gilead Drug** in Virus Fight, Raising IP Fears. Bloomberg News. February 11, 2020, 6:51 PM PST Updated on February 12, ...

Suzhou-based BrightGene Bio-Medical Technology Co. said it has developed technology to synthesize the active pharmaceutical ingredients of Gilead's remdesivir. A leading candidate to treat the virus that's killed more than 1,000 people, the drug isn't licensed or approved anywhere in the world. BrightGene rose 20% Wednesday in Shanghai.

How to prepare Remdesivir? I



Reactions

1809249-37-3

Draw



Start the reaction search with the CAS Registry Number of Remdesivir

Return to Home

Filter by

Substance Role

Product (294)

Reactant (1)

Yield

50-69% (3)

30-49% (3)

10-29% (1)

No Yield Available (287)

Number of Steps

Reactions (294)

View Expanded

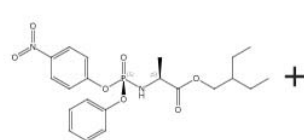
References



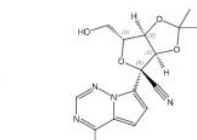
Save

Scheme 1 (5 Reactions)

Steps: 1-2 Yield: 69%



Absolute stereochemistry shown



Absolute stereochemistry shown



Absolute stereochemistry shown

Supplier (1)

Suppliers (18)

This is the final step in the synthesis

How to prepare Remdesivir? II

<input type="checkbox"/>	Reaction Summary	Steps: 1 Yield: 69%	Discovery and Synthesis of a Phosphoramidate Prodrug of a Pyrrolo[2,1-f][triazin-4-amino] Adenine C-Nucleoside (GS-5734) for the Treatment of Ebola and Emerging Viruses
	1.1 Reagents: Diisopropylethylamine, Magnesium chloride Solvents: Tetrahydrofuran; 50 °C		By: Siegel, Dustin; et al Journal of Medicinal Chemistry (2017), 60(5), 1648-1661
	1.2 Reagents: Hydrochloric acid Solvents: Water; 0 °C		
	View Reaction Detail Experimental Protocols		Full Text ▾
<input type="checkbox"/>	Reaction Summary	Steps: 2	Preparation of amino acid-containing nucleosides for treating flaviviridae virus infections
	1.1 Reagents: Magnesium chloride Solvents: Acetonitrile; 15 min, rt		By: Clarke, Michael O'Neil Hanrahan; et al World Intellectual Property Organization, WO2017184668 A1 2017-10-26
	1.2 Reagents: Diisopropylethylamine; 4 h, rt		
	2.1 Reagents: Sulfuric acid Solvents: Tetrahydrofuran; 0 °C; 0 °C → rt		
	View Reaction Detail		PATENTPAK ▾ Full Text ▾
<input type="checkbox"/>	Reaction Summary	Steps: 2	Preparation of nucleosides and methods for treating Filoviridae virus infections
	1.1 Reagents: Magnesium chloride Solvents: Acetonitrile; 15 min, rt		By: Chun, Byoung Kwon; et al United States, US20160122374 A1 2016-05-05
	1.2 Reagents: Diisopropylethylamine; 4 h, rt		
	1.3 Solvents: Ethyl acetate; rt → 0 °C		
	2.1 Reagents: Hydrochloric acid Solvents: Tetrahydrofuran, Water; rt → 0 °C; 0 °C → rt		
	View Reaction Detail		PATENTPAK ▾ Full Text ▾

These three options to prepare Remdesivir are from Gilead

Experimental Protocols

MethodsNow™

Products	L-Alanine, <i>N</i> -[(<i>S</i>)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester with 2-C-(4-aminopyrrolo[2,1- <i>f</i>] [1,2,4]triazin-7-yl)-2,5-anhydro-D-altroneitrile, Yield: 69%
Reactants	2-C-(4-Aminopyrrolo[2,1- <i>f</i>][1,2,4]triazin-7-yl)-2,5-anhydro-3,4- <i>O</i> -(1-methylethylidene)-D-altroneitrile L-Alanine, <i>N</i> -[(<i>S</i>)-(4-nitrophenoxy)phenoxyphosphinyl]-, 2-ethylbutyl ester
Reagents	Diisopropylethylamine Magnesium chloride Hydrochloric acid
Solvents	Tetrahydrofuran Water
Procedure	<ol style="list-style-type: none">1. Dissolve (2<i>S</i>)-2-ethylbutyl 2-((((((2<i>R</i>,3<i>S</i>,4<i>R</i>,5<i>R</i>)-5-(4-aminopyrrolo[2,1-<i>f</i>][1,2,4]triazin-7-yl)-5-cyano-3,4-dihydroxytetrahydrofuran-2-yl)methoxy)(phenoxy)phosphoryl)amino) propanoate in acetonitrile.2. Load the resulting solution onto a Lux Cellulose-2 chiral column.3. Equilibrate the resulting solution in acetonitrile.4. Elute the product with isocratic acetonitrile/methanol (95:5 (v/v)).
Transformation	Hydrolysis of Acetals/ Orthoesters/ Enol Ethers and Similar Compounds Preparation of Inorganic Esters from Alcohols

Characterization Data

^ L-Alanine, *N*-[(*S*)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester with 2-*C*-(4-aminopyrrolo[2,1-*f*][1,2,4]triazin-7-yl)-2,5-anhydro-D-altroneitrile

Proton NMR Spectrum (400 MHz, methanol- d_4): δ 8.05 (s, 1H), 7.36 (d, J = 4.8 Hz, 1H), 7.29 (br t, J = 7.8 Hz, 2H), 7.19-7.13 (m, 3H), 7.11 (d, J = 4.8 Hz, 1H), 4.73 (d, J = 5.2 Hz, 1H), 4.48-4.38 (m, 2H), 4.37-4.28 (m, 1H), 4.17 (t, J = 5.6 Hz, 1H), 4.08-3.94 (m, 2H), 3.94-3.80 (m, 1H), 1.48 (sep, J = 12.0, 6.1 Hz, 1H), 1.34 (p, J = 7.3 Hz, 4H), 1.29 (d, J = 7.2 Hz, 3H), 0.87 (t, J = 7.4 Hz, 6H).

Phosphorous-31 NMR (162 MHz, methanol- d_4): δ 3.71 (s).

Optical Rotatory Power $[\alpha]_D^{21}$ -46 (c 1.0, MeOH).

Mass Spectrum MS m/z : 603.1 [M + 1].

CAS Method Number 3-006-CAS-16999368

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Reaction file in SciFinderⁿ

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

- This is an entire new File you use
- Reactions are organized into Reaction Schemes - no longer per document
- You can create reaction alerts for automatic delivery
- You can search for stereospecific reactions
- You get experimental procedures (1:1 out of publications/patents)
- You get experimental protocols (intellectually indexed from the publication/patent and the supplementary information)
 - here for the Remdesivir synthesis

Helpful hints for reaction searching: Working with the reaction answers

- You have additional filters available:
 - Substance filters – list substance names no longer RNs (for reagents, solvents, reactants, catalysts)
 - Reaction type (Full, Product only, Failed reactions)
 - Reaction notes (about the reaction mechanism, reaction details)
 - Commercial availability of products; starting materials

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

^ Reagent

- Boron trichloride (234)
- Trimethylsilyl triflate (194)
- Hydrochloric acid (169)
- Chlorotrimethylsilane (168)
- Magnesium chloride (157)

[View All](#)

^ Reaction Type

- Full (293)
- Product Only (1)

^ Reaction Notes

- Thermal (136)
- Stereoselective (118)

^ Commercial Availability

- Products (170)
- All Starting Materials (51)

How else can Remdesivir be prepared?

Reactions 1809249-37-3 Draw

CAS RN
1809249-37-3

CAS Name
L-Alanine, *N*-[(*S*)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester with 2...

Substance Detail

Reactions (295)

Synthesize (294)

Create Retrosynthesis Plan

References (28)

Suppliers (18)

Absolute stereochemistry shown

Edit Structure - Reset +

Is there a way to see the full synthesis immediately, and maybe also the Chinese way to bypass Gilead's patent?

Use the Retrosynthesis plan

Retrosynthesis – experimental plan (for existing substances)

Retrosynthesis Edit Plan Options Powered by ChemPlanner®

Overview Steps 📄 ✉ ★ Save

Step Key

⇒ A Experimental

⇨ B Predicted OFF

Plan Information

Estimated Yield: 23%

Overall Price: \$6,432.43
(USD per 100 grams)

Commercially Available:
A, C, D, E, F, H, I, K

All reactions have been published. The Retrosynthesis plan is created based on multiple references (cross-reference search).

Feedback

Retrosynthesis – reference reactions

Overview Steps

- A ⇒ B + C**
Maximum Yield: -
Evidence (2)
Alternative Steps (44)
- B ⇒ D + E + F**
Maximum Yield: -
Evidence (2)
Alternative Steps (11)
- C ⇒ G**
Maximum Yield: 74%
Evidence (2)
Alternative Steps (35)
- E ⇒ H + I**
Maximum Yield: 91%
Evidence (20,481)
Alternative Steps (20)
- G ⇒ J + K**
Maximum Yield: 90%
Evidence (5)
Alternative Steps (48)

In the reaction steps tab you see:

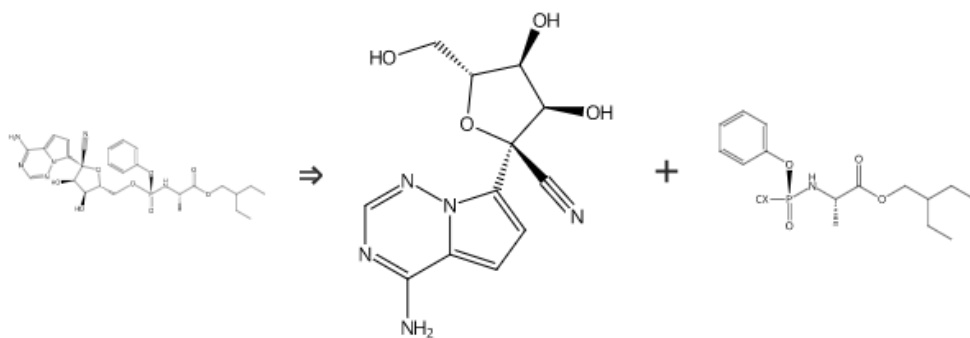
1. The number of Evidence Publications for the step selected
2. Alternative reactions that can be used for the step of interest
 1. If you select alternative steps you see that the other disconnections are changed accordingly
 2. The plan information as well changes

Retrosynthesis – predictive plan (for existing and new substances)

- Shows transformations applied to the target, that were not reported, yet
- The target can be existing or new
- The shown transformations were selected based on rules that fit to the target molecule
- The predicted disconnection provides a link to all existing reactions that fit to the rule applied

Retrosynthesis – predictive plan (for Remdesivir)

9 of 44



Select

 Predicted Step

Evidence (2,495)

Average Yield: 37%

Reaction searching is a big part of the hbz meeting in June.
Please come and see the predictive steps there! For a preview:
<https://www.cas.org/hbz/scifinder-n-predictive-retrosynthesis>

Agenda

1. Search without limits for virus (in general) and SARS-CoV-2

- By text
- By structure
- For Syntheses & Retrosyntheses

2. Important to know about SciFinderⁿ

- Live history
- Combine answer sets
- Move from SciFinder_{web} to SciFinderⁿ
- Alerts
- Help in SciFinderⁿ

3. Specific training materials for all areas

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

SciFinderⁿ - live History I

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

- History is automatically saved
- Searches can be re-run and/or edited
- Filter options allow to retrieve specific searches easily

SciFinderⁿ - live History II



References - Enter a query...



Filter by

Result Type

- All (50)
- Patent Markush (47)
- Reactions (164)
- References (848)
- Retrosynthesis (70)

[View All](#)

Date

Start Date to End Date
mm/dd/yyyy to mm/dd/yyyy

March, 2020						
SU	MO	TU	WE	TH	FR	SA
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	31				

Search History (1,663)

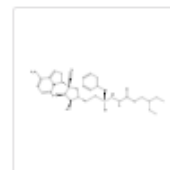
Select the Result type you like to see

Every session is saved automatically

3:17 PM

Retrosynthesis

Synthetic Depth: 3
Rules Supporting Predicted Reactions: Common
Break & Protect Bonds: No



Open Plan

Edit Options

Complete

The Retrosynthesis plan can be opened or edited

Retrosynthesis Plan will expire on Jun 9, 2020.

3:10 PM

Substances

Remdesivir (1)

Rerun Search

Edit Search

The Substance search can be opened or edited



SciFinderⁿ just like SciFinder_{web} permits to combine answer sets

- Save the answer sets to combine (no upper limit to the size of the saved set)
- Combine with “AND” up to 5 answer sets
- Combine with “OR” up to 5 answer sets
- Combine with “NOT” 2 answer sets

Combine answer sets – save answer sets first

References (28)

Substances Reactions Cited By

Save Search

Name
Remdesivi

Tags (optional)

Ruthenium catalysts
 esterification transesterification

New Tag (optional)

Therapeutic efficacy of the small molecule GS-5734 against coxsackievirus in rhesus monkeys
By: Warren, Travis K.; Jordan, Robert; Lo, Michael K.; Ray, Adrian S.; Mackman, Richard L.; Soloveva, Veronica; Siegel, Dustin; Perron, Michel; Bannister, Roy; Hui, Hon C.; et al
Nature (London, United Kingdom) (2016), 531(7594), 381-385 | Language: English, Database: CPlus

Sort: Relevance View: Partial Abstract

References (740)

Substances Reactions Cited By

1

A novel coronavirus from patients with pneumonia in China
By: Zhu, Na; Zhang, Dingyu; Wang, Wenling; Li, Xingwang; Lu, Roujian; et al
New England Journal of Medicine (2020), 382(8), 727-733
In Dec. 2019, a cluster of patients with pneumonia of unknown etiology was reported in Wuhan, China. A previously unknown betacoronavirus was discovered in the patients. Human airway epithelial cells were found to be susceptible to the virus. Whole-genome sequencing revealed that the virus formed a clade within the subgenus sarbecovirus. Orthogonal subtyping and phylogenetic analysis showed that 2019-nCoV is the seventh member of the family of coronaviruses.
[Investigate](#)
[View More](#)

2

Save Search

Name
novel coronavirus" or "sev. ac. respiratory syn.

Tags (optional)

Ruthenium catalysts
 esterification transesterification

New Tag (optional)



Combine answer sets I

The screenshot displays the SciFinder web interface. At the top, a search bar contains the query "novel coronavirus" or "severe acute respiratory syndro" with a search icon and a "Draw" button. Below the search bar, a "Saved" section (173 items) lists two saved searches:

- novel coronavirus" or "sev. ac. respiratory syn."
March 11, 2020, 6:16 PM
References "novel coronavirus" or "severe acute respiratory syndrome"
+ Filters
- Remdesivir references
March 11, 2020, 6:11 PM
References Reference Results from Substances

A "Combine Saved Results" dialog box is overlaid on the right side of the screen. It features a progress indicator with steps 1, 2, and 3, where step 1 is active. The dialog asks to "Select a Result Type:" and offers three options:

- Substances (with a "Select" button)
- Reactions (with a "Select" button)
- References (with a "Select" button, circled in red)

A "Learn More About Combine" link is located at the bottom right of the dialog. In the background, a filter sidebar is visible with sections for "Result Type" (Reactions: 42, References: 60, Retrosynthesis: 1, Substances: 70), "Alerts" (Unviewed: 9), and "Tags" (esterification transesterification: 1, Ruthenium catalysts: 1). A red arrow points from a callout box to the "Combine" button in the background interface.

Combine the answer sets

Combine answer sets II

Combine Saved Reference Results

Select a Combine Option:

- Add
- Intersect**
- Subtract

[Learn More About Combine](#)

Combine Saved Reference Results: Intersect

Select Up to 5 Saved Items:

Item	Date
<input checked="" type="checkbox"/> novel coronavirus" or "sev. ac. respiratory syn."	March 11, 2020
<input checked="" type="checkbox"/> Remdesivir references	March 11, 2020
<input type="checkbox"/> Seema Agarwal Bayreuth	January 20, 2020
<input type="checkbox"/> Knoelker, H-J	November 19, 2019
<input type="checkbox"/> all best	November 19, 2019
<input type="checkbox"/> best patents	November 19, 2019
<input type="checkbox"/> Wiebke Fischer	November 17, 2019
<input type="checkbox"/> andrea-lilian.morger@charite.de	1 Selected Result November 4, 2019
<input type="checkbox"/> rachel-leanne.nicholls@cec.mpg.de	November 3, 2019
<input type="checkbox"/> text only	October 25, 2019

[View Results](#) [Cancel](#) [Learn More About Combine](#)

References (4)

Sort: Publication Year: Newest View: Partial Abstract

Substances Reactions Cited By Save

1

Learning from the past: possible urgent prevention and treatment options for severe acute respiratory infections caused by 2019-nCoV

By: Morse, Jared S.; Lalonde, Tyler; Xu, Shiqing; Liu, Wenshe R.
ChemRxiv (2020), 1-23 | Language: English, Database: CAplus

With the current trajectory of the 2019-nCoV outbreak unknown, public health and medicinal measures will both be needed to contain spreading of the virus and to optimize patient outcomes. While little is known about the virus, an examination of the genome sequence shows strong homol. with its more well-studied cousin, SARS-CoV. The spike protein used for host cell infection shows key nonsynonymous mutations which may hamper efficacy of previously developed therapeutics but remains a viable target for the development of biologics and macrocyclic peptides. Other key drug targets, including RdRp...

[View More](#)

Full Text

Substances (19)

Reactions (0)

Cited By (0)

Citation Map

2

Prediction of the 2019-nCoV 3C-like protease (3CLpro) structure: virtual screening reveals velpatasvir, ledipasvir, and other drug repurposing candidates

By: Chen, Yu Wai; Yiu, Chin-Pang Benu; Wong, Kwok-Yin
ChemRxiv (2020), 1-15 | Language: English, Database: CAplus

We prepared the three-dimensional model of the 2019-nCoV 3C-like protease (3CLpro) using the crystal structure of the highly-similar (96% identity) ortholog from the SARS-CoV. All residues involved in the catalysis, substrate binding and dimerization are 100% conserved. Comparison of the polyprotein PP1AB sequences showed 86% identity. The 3C-like cleavage sites on the coronaviral polyproteins are highly conserved. Based on the near-identical substrate specificities and high sequence identities, we are in the opinion that some of the previous progress of specific inhibitors development for the...

[View More](#)

Full Text

Substances (15)

Reactions (0)


Cited By (0)

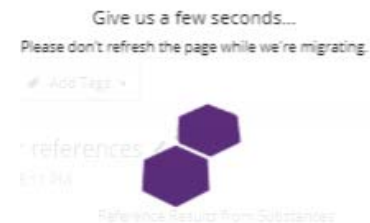
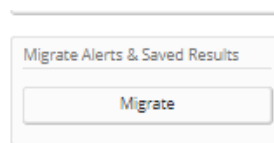
Citation Map

The combination result

How to move saved answer sets over to SciFinderⁿ

Features that are exclusively available in SciFinderⁿ are highlighted in blue!

- Start in Saved answers 
- Move your answer sets by clicking on the “Migrate” button
- Alerts will be migrated, as well
- Note: the moved answers and alerts will be in:
 - SciFinderⁿ and
 - SciFiner_{web}



Alerts in SciFinderⁿ –included in saved answers

- See in your saved answers on which searches you are running Alerts



reaction example

December 18, 2018, 9:46 AM

Reactions + Filters
As Drawn

[Rerun Search](#)

Alerts Add Tags

Indication that an Alert
retrieved new results

Alerts in SciFinderⁿ – delivered in SciFinderⁿ

All Results were not reviewed

Frequency

No Alerts As Available **Weekly** Monthly

Results [Mark All As Viewed](#)

- February 25, 2020 (5)
- January 25, 2020 (41)
- October 7, 2019 (10)
- September 30, 2019 (17)
- September 23, 2019 (8)
- September 16, 2019 (1)
- September 9, 2019 (5)
- April 28, 2019 (1)
- April 21, 2019 (12)

First result was reviewed

Alerts Add Tags

Frequency

No Alerts As Available **Weekly** Monthly

Results [Mark All As Viewed](#)

- February 25, 2020 (5)
- January 25, 2020 (41)
- October 7, 2019 (10)
- September 30, 2019 (17)
- September 23, 2019 (8)
- September 16, 2019 (1)
- September 9, 2019 (5)
- April 28, 2019 (1)
- April 21, 2019 (12)

Reactions + Filters
AS Drawn

Alerts in SciFinderⁿ –delivered by e-mail

Alert results arrive per mail one time a week



SciFinder-n Alert Processing <no-reply@cas.org>

□ Faerber, Karin

SciFinder-n Alert Results for References

Click here to download pictures. To help protect your privacy, Outlook prevented automatic download of some pictures in this message.

□ **antibiotica resistance (695)**

The first 5 Results are listed. [View Results in SciFinderⁿ](#)

Live link to SciFinderⁿ

Isolation, identification and drug resistance analysis of bacterial etiology in new neonatal piglets diarrhea in Gansu area

By: Huang, Meizhou; Liu, Yongming; Wang, Hui; Wang, Shengyi; Cui, Dong-an; Li, Shengkun
Xibei Nongye Xuebao (2015) | Chinese

Live link to SciFinderⁿ

Bacterial spectrum and analysis of drug resistance in peritoneal dialysis-related peritonitis

By: Li, Can-ming; Chen, Yan-ru; Ye, Zeng-chun; Peng, Hui; Lou, Tan-qi
Shiyong Yaowu Yu Linchuang (2015) | Chinese

Analysis of treatment strategy on drug resistance of ICU pneumonia patients infected by extensively drug resistant acinetobacter baumannii

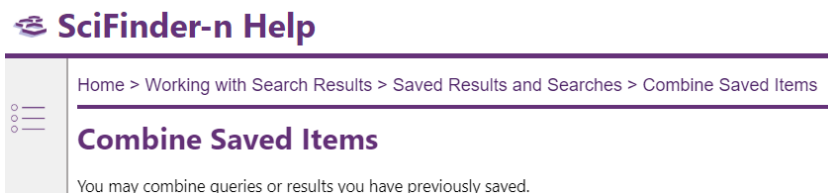
By: Jiang, Le; Yu, Guo-feng; Zhang, Yi-ting; Lu, Di



Where to find help on SciFinderⁿ

- This presentation is available for you to use on site, it links to detailed resources on the next slides
- The help menu in SciFinderⁿ (bottom right corner of the screen - scroll down)

Help Contact Us



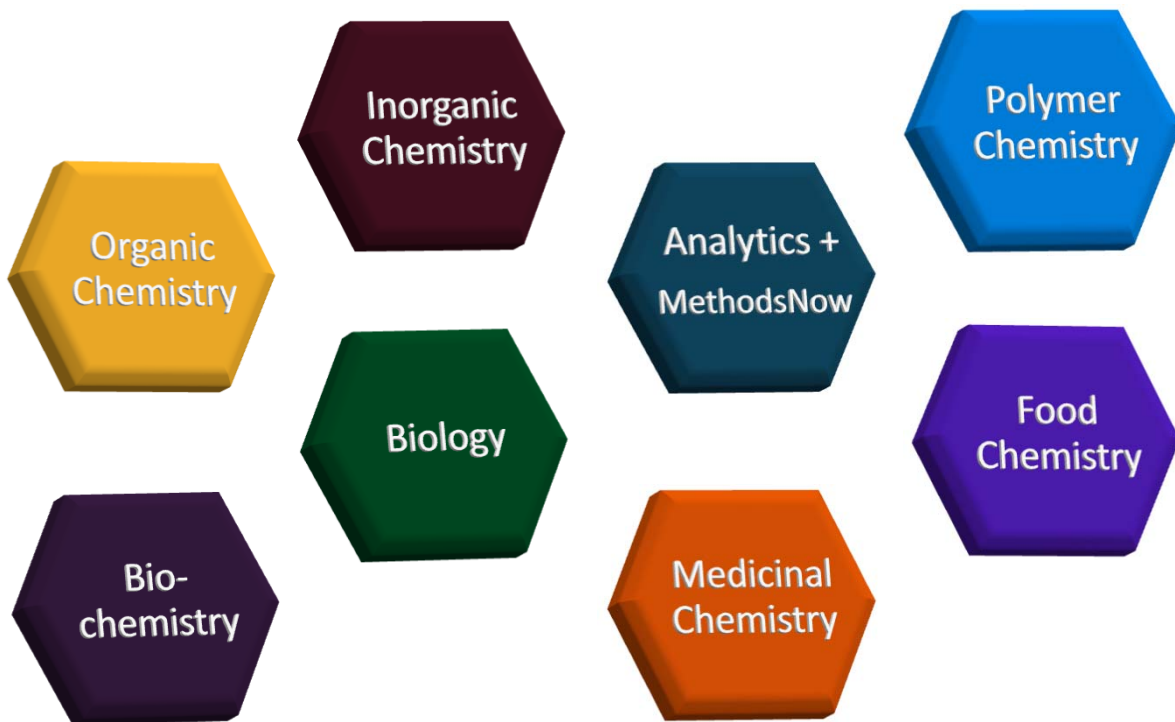
- hbz SciFinderⁿ training page: <https://www.cas.org/hbz/schulungseite>
- CAS SciFinderⁿ training pages: <https://www.cas.org/support/training/scifinder-n>
- Your trainer team in Germany – please connect: kfaerber@acs-i.org

Agenda

1. Search without limits for virus (in general) and SARS-CoV-2
 - By text
 - By structure
 - For Syntheses & Retrosyntheses
2. Important to know about SciFinderⁿ
 - Live history
 - Combine answer sets
 - Move from SciFinder_{web} to SciFinderⁿ
 - Alerts
 - Help in SciFinderⁿ
3. Specific training materials for all areas

Research Areas included in SciFinderⁿ

Please click on the topics to get to the specific resources.



Linking page – Biology in SciFinderⁿ

Click [here](#) to get back to the research area overview slide.

1. The specific protection mechanism of the Monarch Butterfly against parasites when raised on Milkweed plants ➡ [PDF](#)
 - Reference search, Latin names used, use quotation marks for connected terms
 - Analyse answers by concepts, intellectually assigned by CAS
 - Get related substances
 - View related sequences
 - The citation map for related publications
2. Overall literature on Monarch Butterflies and their use of secondary metabolites of Milkweed leaves for parasite protection ➡ [Video](#)
 - Reference search, (operators: AND, OR, NOT, use wildcards)
 - Analyse answers by concepts, intellectually assigned by CAS
 - Safe answer sets, combine answer sets
 - Create your weekly Alert

Linking page – Analytics in SciFinderⁿ

Click [here](#) to get back to the research area overview slide.

Quantification of Glyphosate intake in the body ➡ [PDF](#)

- Reference search
 - Analyze answers by concepts, intellectually assigned by CAS, and other filters
 - Retrieving analytical information - with and without access to MethodsNow Analysis
- Search within MethodsNow Analysis
 - Analyze answers by various filters
 - Download method details
 - Compare results side by side

Linking page – Food Chemistry in SciFinderⁿ

Click [here](#) to get back to the research area overview slide.

Low caloric sugars in cocktails and alcoholic beverages in general ➡ [PDF](#)

- Reference search (boolean operators, truncation, brackets)
 - Analyze answers by concepts intellectually assigned by CAS and other filters
 - Reference detail and full text of patents with PatentPak
 - View substance details
- Reaction search
 - Analyze answers by various filters
 - View reaction details
 - View experimental details and MethodsNow Synthesis

Linking page – Biochemistry in SciFinderⁿ

Click [here](#) to get back to the research area overview slide.

Biosynthetic preparation of vanillin ➡ [PDF](#)

- Simultaneous text and structure search
 - Structure search for 'vanillin' and text search for 'fermentation'
 - View substructure results sorted by relevance
 - Limit to substance roles and indexed concepts
- Reaction search
 - Analyze indexed reactions and limit with reaction notes and publication filters
 - Analyze reaction schemes
 - View reaction details and download experimental protocols with MethodsNow

Linking page – Medicinal Chemistry in SciFinderⁿ

Click [here](#) to get back to the research area overview slide.

Identify checkpoint inhibitors of apoptosis-regulating protein PD-1 ➡ [PDF](#)

- Reference search
 - Use logical operators, phrase search and search history
 - Make use of relevance sorting and 'Search' function of concept filter
- Substance analysis
 - Analyze substances by relevance
 - Use substance-related filters, bioactivity and target Indicators
 - Look up location of indexed substances in patent full-text with PatentPak

Gold Nanoparticles used as therapeutic agents against cancer ➡ [Video](#)

- Simultaneous text and generic structure search
 - Refine with concepts
 - Work in multiple tabs
 - Access full-text

Linking page – Polymer Chemistry in SciFinderⁿ

Click [here](#) to get back to the research area overview slide.

Searching bifunctional PEGs used to produce conjugates with biomaterials such as antibodies ➡ [Video](#)

- Structure editor and structure search
 - Define structure incl. repeating units and lock atoms
 - Sort substance answers by number of references to identify polymeric forms
- Analyze reference results
 - Analyze concepts by count and use 'Search' option
 - Refine by adding a free text search
 - Show location of compound in patent full-text with PatentPak

Linking page – Organic Chemistry in SciFinderⁿ

Click [here](#) to get back to the research area overview slide.

1. Metall organic complexes ➡ [Video](#)
 - Substance search using the structure editor
 - Recieve and analyze reference answer set
2. Predictive retrosynthesis of an oxetan derivative ➡ [Video](#)
 - Create retrosynthesis plan
 - Review evidence reactions to select appropriate reaction
3. Carbenes ➡ [Video](#)
 - Substance search using the structure editor
 - Refine answer set
4. Isotope isomer of tetrabenzene ➡ [Video](#)
 - Substance search using the structure editor
 - Specify search for isotope loaction

Linking page – Inorganic Chemistry in SciFinderⁿ

Click [here](#) to get back to the research area overview slide.

Queries on different uses of Zirconium ➡ [PDF](#)

1. Pre-catalyst for the intramolecular hydroamination of alkenes

- Reference search with text
 - Refine results via „Search Within Results“
 - Reference search with chemical formula of complex

2. Part of alloys

- Reference search as a combined text and structure search
- Get related substances
 - Analyze substance answer set
 - Use of structure editor

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org



SCIFINDERⁿ
A CAS SOLUTION

Inorganic searching – without limits – in the world of Zirconium

CAS is a division of the American Chemical Society.
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Click [here](#) to get back to the research area overview slide.

Search Question

1. Zirconium – pre-catalyst for the intramolecular hydroamination of alkenes
2. Zirconium – part of alloys

Click [here](#) to get back to the research area overview slide.

1. Zirconium – pre-catalyst for the intramolecular hydroamination of alkenes – Text search I

The screenshot shows the SciFinder search results page. At the top, the SciFinder logo is on the left, and the search bar contains the query "hydroamination of alkenes". Below the search bar, there are navigation icons for "Draw", search, star, clock, and user profile. The main content area is titled "References (185)" and includes a "Return to Home" link. A callout box points to the search bar with the text "Search for hydroamination of alkenes". On the left, a sidebar offers a "Load More Results" button and a "Filter by" section with "Document Type" options: Journal (144), Patent (1), Review (32), Conference (28), Dissertation (11), and Preprint (1). The main results list shows a single entry: "Rhodium- and iridium-catalyzed hydroamination of alkenes" by Hesp, Kevin D.; Stradiotto, Mark, published in ChemCatChem (2010), 2(10), 1192-1207. The abstract text is partially visible, mentioning "hydroamination of alkenes" and "atom-economical strategy". At the bottom of the result card, there are buttons for "Full Text", "Substances (0)", "Reactions (0)", "Cited By (150)", and "Citation Map".

Click [here](#) to get back to the research area overview slide.

1. Zirconium – pre-catalyst for the intramolecular hydroamination of alkenes – Text search II

The screenshot shows the SciFinder search results page for the query "hydroamination of alkenes". The search bar at the top contains the query and a search icon. Below the search bar, there are navigation options like "Return to Home" and a "References" section with 185 results. The results are sorted by Relevance and shown as Partial Abstracts. The first result is "Rhodium- and iridium-catalyzed hydroamination of alkenes" by Hesp, Kevin D.; Stradiotto, Mark, published in ChemCatChem (2010), 2(10), 1192-1207. The second result is "Copper Hydride-Catalyzed Hydroamination of Alkenes and Alkynes" by Pirnot, Michael T.; Wang, Yi-Ming; Buchwald, Stephen L., published in Angewandte Chemie, International Edition (2016), 55(1), 48-57. On the left side, there is a filter panel with options for Document Type, Language, Publication Year, Available at My Institution, Author, Organization, Publication Name, Concept, and Database. At the bottom of the filter panel, there is a "Search Within Results" section with a text input field containing "intramolecular" and a "Find" button.

Refine with intramolecular

A dialog box titled "Search Within Results" is shown. It contains a text input field with the word "intramolecular" and a "Find" button.

Click [here](#) to get back to the research area overview slide.

1. Zirconium – pre-catalyst for the intramolecular hydroamination of alkenes – Text search III

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#) [Load More Results](#)

Return to Home

References - "hydroamination of alkenes" x Draw

References (65)

Substances Reactions Cited By

1

Rhodium- and iridium-catalyzed hydroamination of alkenes
By: Hesp, Kevin D.; Stradiotto, Mark
ChemCatChem (2010), 2(10), 1192-1207 | Language: English, Database: CPlus

A review. The **hydroamination of alkenes** represents an atom-economical strategy for the synthesis of nitrogen-containing moieties from readily available components. In recent years, the application of Group 9 transition metal catalysts in this reaction enabled significant progress to be made toward addressing several major challenges within the field of metal-mediated hydroamination. Using Rh- and Ir-based catalysts for the intermolecular hydroamination reaction, advances were made in the regioselective addition of amines to olefins in an anti-Markovnikov fashion producing industrially relevant linear amine products, as well as the concise synthesis of chiral amines by asymmetric hydroamination. The **intramolecular** addition of a variety of amine groups to pendant alkenes was also studied in the context of developing expedient routes to nitrogen-containing heterocycles; using simple Rh- and Ir-based catalysts, a wide range of substrates including those that contain functional groups that are poised for further synthetic elaboration are readily cyclized. Extension of these catalyst systems to include the asymmetric synthesis of a variety of functionalized 1-methylpyrrolidine compounds was recently achieved. To complement these catalytic investigations, thorough stoichiometric and kinetic studies unveiled diverse mechanistic pathways that originate from either initial amine or olefin activation. The understanding gained through these mechanistic investigations provides the framework for the design of increasingly effective alkene hydroamination catalysts.

Full Text Substances (0) Reactions (0)

2

Rhodium Phosphine- π -Arene Intermediates in the Hydroamination of Alkenes
By: Liu, Zhijian; Yamamichi, Hideaki; Madrahimov, Sherzod T.; Hartwig, John F.
Journal of the American Chemical Society (2011), 133(8), 2772-2782 | Language: English, Database: CPlus

A detailed mechanistic study of the **intramolecular hydroamination of alkenes** with amines catalyzed by Rh complexes of a biaryldialkylphosphine is reported. The active catalyst contains the phosphine ligand bound in a κ^1, η^5 form in which the arene is π -bound to Rh. Addition of deuterated amine to an internal olefin showed that the reaction occurs by trans addition of the N-H bond across the C-C bond, and this stereochemistry implies that the reaction occurs by nucleophilic attack of the amine on a coordinated alkene. Indeed, the cationic

Full Text Substances (0) Reactions (0) Cited By (150) Citation Map

Search Within Results
Intramolecular

SCIFINDERⁿ
A CAS SOLUTION

Intramolecular is part of the title or abstract or concept terms

Click [here](#) to get back to the research area overview slide.

Publication of Prof. Peter Roeskys team on $[(S)\text{-PEBA}]_2\text{Zr}(\text{NMe}_2)_2$ as possible catalyst – How to search this? – SciFinderⁿ



[Return to Home](#)

Filter by

Document Type

- Journal (14M)
- Patent (3.8M)
- Review (605K)
- Biography (6,559)
- Book (29K)

[View All](#)

Language

- English (12.6M)
- Chinese (1.6M)
- Japanese (1.5M)
- Undetermined (955K)

References (18,477,876) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

1

Synthesis of enantiomeric pure zirconium and hafnium benzamidinate complexes
By: Brunner, Tobias S.; Hartenstein, Larissa; Roesky, Peter W.
Journal of Organometallic Chemistry (2013), 730, 32-36 | Language: English, Database: CAplus

Two enantiomerically pure group 4 amidinate complexes $[(S)\text{-PEBA}]_2\text{Zr}(\text{NMe}_2)_2$ (1) and $[(S)\text{-PEBA}]_2\text{Hf}(\text{NMe}_2)_2$ (2) containing the chiral amidinate N,N'-bis-((S)-1-phenylethyl)benzamidinate ((S)-PEBA, 5) were synthesized and structurally characterized. Both compounds were obtained as all (S)-A-diastereomers being chiral at the ligand and chiral at metal. $[(S)\text{-PEBA}]_2\text{Zr}(\text{NMe}_2)_2$ was used as precatalyst for the intramol. hydroamination of alkenes and one alkyne. Although good conversions were observed at higher temperatures, only very low enantioselectivities were obtained.

Full Text Substances (13) Reactions (6) Cited By (5) Citation Map

One described catalyst for the reaction is $[(S)\text{-PEBA}]_2\text{Zr}(\text{NMe}_2)_2$

The search for $[(S)\text{-PEBA}]_2\text{Zr}(\text{NMe}_2)_2$ is a reference search in SciFinderⁿ: text search on the term – use the first answer – sorted to the top

Click [here](#) to get back to the research area overview slide.

Publication of Prof. Peter Roeskys team on $[(S)\text{-PEBA}]_2\text{Zr}(\text{NMe}_2)_2$ as possible catalyst – How to search this? – SciFinder_{web}

Research Topic "[{(S)-PEBA}2Zr(NMe2)2] "

REFERENCES ?

Select All Deselect All

0 of 31 Research Topic Candidates Selected

References

<input type="checkbox"/>	No References were found containing the concept "{".	0
<input type="checkbox"/>	459 references were found containing both of the concepts "{ and "2", and either the concept "[PEBA]2Zr" or the concept "NMe2". The concepts found were closely associated with one another.	459
<input type="checkbox"/>	635 references were found containing both of the concepts "{ and "2", and either the concept "[PEBA]2Zr" or the concept "NMe2". The concepts found were present anywhere (perhaps widely separated) within the reference.	635
<input type="checkbox"/>	1 reference was found containing both of the concepts "{ and "2", and either the concept "[PEBA]2Zr".	1
<input type="checkbox"/>	1163 references were found containing both of the concepts "S" and "2", and either the concept "[PEBA]2Zr" or the concept "NMe2". The concepts found were closely associated with one another.	1163
<input type="checkbox"/>	3841 references were found containing both of the concepts "S" and "2", and either the concept "[PEBA]2Zr" or the concept "NMe2". The concepts found were present anywhere (perhaps widely separated) within the reference.	3841
<input type="checkbox"/>	1 reference was found containing all of the concepts "S", "[PEBA]2Zr" and "2" closely associated with one another.	1
<input type="checkbox"/>	1 reference was found containing both of the concepts "S" and "2", and either the concept "[PEBA]2Zr".	1
<input type="checkbox"/>	1163 references were found containing all of the concepts "S", "NMe2" and "2" closely associated with one another.	1163
<input type="checkbox"/>	3841 references were found where all of the concepts "S", "NMe2" and "2" were present anywhere in the reference.	3841

REFERENCES: RESEARCH TOPIC ?

[{(S)-PEBA}2Zr(NMe2)2]

Examples:

The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

Search

This search for $[(I)\text{-PEBA}]_2\text{Zr}(\text{NMe}_2)_2$ is impossible in SF_{Web}

Click [here](#) to get back to the research area overview slide.

2. Zirconium – Part of alloys – Used for tubes in chemical plants, because of corrosion resistance



Search

All

Substances

Reactions

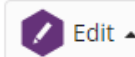
References

Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

"corrosion resistance"

x



Edit



Use [Advanced Search](#) for Author, Journal, or Organization

Combine text terms with structural components. You can even draw fragments of a one-component substance in one window of the structure editor.

Zr

Edit Drawing

Remove



Click [here](#) to get back to the research area overview slide.

2. Zirconium – Part of alloys – Which alloys are used? I

The screenshot shows the SciFinder search results page for the query "corrosion resistance". The interface includes a search bar at the top with the query and a "References" dropdown. Below the search bar, there are navigation options like "Return to Home" and "Structure Match" filters. The main content area displays a list of references, with the first one highlighted. A callout box points to the "Substances" filter button with the text "Which Alloys are used?".

Structure Match

- As Drawn (13K)
- Substructure (18K)

Filter by

- Document Type
- Substance Role
- Language
 - English (4,782)
 - Chinese (3,986)
 - Japanese (2,981)
 - Russian (800)
 - German (344)

References (13,797) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

Corrosion resistance of ZrN films on AISI 304 stainless steel substrate
By: Chou, Wen-Jun; Yu, Ge-Ping; Huang, Jia-Hong
Surface and Coatings Technology (2003), 167(1), 59-67 | Language: English, Database: CAplus

The **corrosion resistance** of ion-plated Zr, ZrN, and ZrN/Zr films on com. AISI 304 stainless steel has been investigated by electrochem. measurement. The electrolyte, 0.5 M H₂SO₄ containing 0.05 M KSCN, was used for the potentiodynamic polarization. The potentiodynamic scan was conducted from -800 to 800 mV (SCE) with scan rate ranging from 10 to 600 mV/min. The N/Zr ratios of the ZrN films determined by XPS were essentially stoichiometric. The composition depth profiles measured by secondary ion mass spectrometry (SIMS) indicated that the compositions in the ZrN films were uniform from the fil...

[View More](#)

Click [here](#) to get back to the research area overview slide.

2. Zirconium – Part of alloys – Which alloys are used? II



Substances ▾

Enter a query...



← Return to Home

Filter by

▾ Commercial Availability

▾ Reaction Role

▾ Reference Role

▾ Stereochemistry

▾ Number of Components

▾ Substance Class

Alloy (45K)

Tabular Inorganic (2,332)

Organic/Inorganic Small Molecule (2,137)

Manual Registration (1,520)

Polymer (1,320)

View All

▾ Isotopes

Substances (53,996)

Sort: Relevance ▾ View Partial ▾

References ▾

Reactions ▾

Suppliers ▾



Save

1

7440-67-7

Zr

Zr
Zirconium

2

25658-42-8

Zr≡N

NZr
Zirconium nitride (ZrN)

3

11109-50-5

Component Percent

Fe	66-74
Cr	18.00-20.00
Ni	8.00-10.50
Mn	0-2.00
Si	0-1.00
C	0-0.08
P	0-0.045
S	0-0.030

Refine to substance classes - use alloys and tabular inorganics

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Click [here](#) to get back to the research area overview slide.

2. Zirconium – Part of alloys – Which alloys are used? III

Substances (58,552) Sort: Relevance View: Partial

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
 - 1 (4,501)
 - 2 (5,865)
 - 3 (8,303)
 - 4 (7,602)
 - 5 or more (30K)
- Substance Class

References Reactions Suppliers Save

1 7440-67-7 Zr Zirconium

2 25658-42-8 Zr≡N Zirconium nitride (ZrN)

3 11109-50-5

Component	Percent
Fe	66-74
Cr	18.00-20.00
Ni	8.00-10.50
Mn	0-2.00
Si	0-1.00
C	0-0.08

Get 58 552 substances from the **substructure answer set**

refine to substance classes use alloys and tabular inorganics

2. An alloy of Zr Zn Fe (Cr or Ni) helps against corrosion – How to find those?

1. Use the answer set with extracted substances from the search:
“corrosion resistance” (text) and Zr (substance)
2. Limit to alloys and tabular inorganics
3. Refine search with other elements needed
4. Limit the number of components to your needs

Click [here](#) to get back to the research area overview slide.

Use answer set with extracted substances from the search: “corrosion resistance” (text) and Zr (substance). Then refine to alloys and tabular inorganics.

Substances (49,810) Sort: Relevance View Partial

References Reactions Suppliers Save

1 2 3

Component	Percent
Fe	66-74
Cr	18.00-20.00
Ni	8.00-10.50
Mn	0-2.00
Si	0-1.00
C	0-0.08

Component	Ratio
N	2
Zr	2
O	1

N.O.Zr
Components: 3
Zirconium nitride oxide (Zr₂)

Component	Ratio
Zr	1
N	0.91
O	0.26

N.O.Zr
Components: 3
Zirconium nitride oxide (Zr)

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Number of Components
- Substance Class
 - Alloy (47K)
 - Organic/Inorganic Small Molecule (3,182)
 - Tabular Inorganic (2,680)
 - Polymer (2,060)
 - Manual Registration (2,018)

View All

Get 58552 substances from the substructure answer set

Get 49810 substances – by refinement to alloy and tabular inorganics. Alloys and tabular inorganics were described in these documents.

Refine to substance classes - use alloys and tabular inorganics

Click [here](#) to get back to the research area overview slide.

Refine search - Other elements needed Zn Fe (Cr or Ni) I

Substances - Enter a query... Draw

Return to Home

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Number of Components
- Substance Class
 - Alloy (47K)
 - Organic/Inorganic Small Molecule (3,182)
 - Tabular Inorganic (2,680)
 - Polymer (2,060)
 - Manual Registration (2,018)
- View All
- Isotopes
- Metals
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator
- Target Indicator
- Search Within Results
 - Draw

Substances (49,810) Sort: Relevance View: Partial

References Reactions Suppliers Save

1	2	3																																		
11109-50-5	12163-96-1	831196-74-8																																		
<table border="1"><thead><tr><th>Component</th><th>Percent</th></tr></thead><tbody><tr><td>Fe</td><td>66-74</td></tr><tr><td>Cr</td><td>18.00-20.00</td></tr><tr><td>Ni</td><td>8.00-10.50</td></tr><tr><td>Mn</td><td>0-2.00</td></tr><tr><td>Si</td><td>0-1.00</td></tr><tr><td>C</td><td>0-0.08</td></tr><tr><td>P</td><td>0-0.045</td></tr><tr><td>S</td><td>0-0.030</td></tr></tbody></table>	Component	Percent	Fe	66-74	Cr	18.00-20.00	Ni	8.00-10.50	Mn	0-2.00	Si	0-1.00	C	0-0.08	P	0-0.045	S	0-0.030	<table border="1"><thead><tr><th>Component</th><th>Ratio</th></tr></thead><tbody><tr><td>N</td><td>2</td></tr><tr><td>Zr</td><td>2</td></tr><tr><td>O</td><td>1</td></tr></tbody></table> <p>N.O.Zr Components: 3 Zirconium nitride oxide (Zr₂N₂O)</p>	Component	Ratio	N	2	Zr	2	O	1	<table border="1"><thead><tr><th>Component</th><th>Ratio</th></tr></thead><tbody><tr><td>Zr</td><td>1</td></tr><tr><td>N</td><td>0.91</td></tr><tr><td>O</td><td>0.26</td></tr></tbody></table> <p>N.O.Zr Components: 3 Zirconium nitride oxide (ZrN_{0.91}O_{0.26})</p>	Component	Ratio	Zr	1	N	0.91	O	0.26
Component	Percent																																			
Fe	66-74																																			
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Component	Ratio																																			
N	2																																			
Zr	2																																			
O	1																																			
Component	Ratio																																			
Zr	1																																			
N	0.91																																			
O	0.26																																			
<p>C,Cr,Fe,Mn,Ni,P,S,Si Components: 8 AISI 304</p> <p>39K References 28 Reactions 0 Suppliers</p>	<p>53 References 0 Reactions 0 Suppliers</p>	<p>3 References 0 Reactions 0 Suppliers</p>																																		
4	5	6																																		
		831196-75-9																																		
		<table border="1"><thead><tr><th>Component</th><th>Ratio</th></tr></thead><tbody><tr><td>Zr</td><td>1</td></tr></tbody></table>	Component	Ratio	Zr	1																														
Component	Ratio																																			
Zr	1																																			

Refine with other elements needed: Zn Fe (Cr or Ni)

Click [here](#) to get back to the research area overview slide.

Refine search - Other elements needed Zn Fe (Cr or Ni) II

The screenshot shows the CAS Draw software interface. On the left is a toolbar with various drawing tools. The main workspace contains a periodic table with three elements highlighted: Zr, Zn, and Fe. A callout box points to these elements with the text "Zr, Zn, Fe selected from the periodic table". On the right, the "R-group Definitions" panel is open, showing a list of R-groups (R1 to R10). R1 is selected and its definition is shown as "Cr, Ni". A callout box points to this definition with the text "Cr and Ni build an R group". Below the R-group definitions is a smaller periodic table with the same elements highlighted. At the bottom of the interface, there is a search bar containing "Fe" and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si, D, T.

Cr and Ni build an R group

Refine with other elements needed: Zn & Fe were selected from the periodic table
Cr & Ni form an R-group; click with the R-group on the drawing pad

Click [here](#) to get back to the research area overview slide.

Refine search - other elements needed Zn Fe (Cr or Ni) III

Search Within Results

SCIFINDERⁿ
A CAS SOLUTION

Substances ▾ Enter a query... Draw 🔍 ★ 🕒

← Return to Home

Filter by

- Commercial Availability
 - Available (1)
 - Not Available (703)
- Reaction Role
 - Reagent (1)
- Reference Role
 - Analytical Study (11)
 - Biological Study (14)
 - Formation (6)
 - Miscellaneous (32)
 - Nanoscale (13)
 - [View All](#)

Substances (704) Sort: Relevance ▾ View

References ▾ Reactions ▾ Suppliers ▾

1 **783345-27-7**

Component	Percent
Mg	93-96
Nd	2.6-3.1
Gd	1.0-1.7
Zr	0.40-1.0
Zn	0.20-0.50
Misch metal	0-0.4

2 **54938-66-8**

Component	Percent
Al	88-91
Zn	5.7-6.7
Mg	2.1-2.6
Cu	1.5-2.0
Zr	0.11-0.17
Fe	0-0.15

3 **58904-05-5**

Component	Percent
Al	86-99
Zn	1-7.7
Mg	0-3
Cu	0-2.3
Mn	0-0.6
Zr	0-0.4

[Edit Drawing](#)

As Drawn

Substructure

Use as drawn

Click [here](#) to get back to the research area overview slide.

Refine search - Number of components



Substances ▾

Enter a query...

[← Return to Home](#)

Filter by

▾ Commercial Availability

▾ Reference Role

▾ Number of Components

4 (1)

5 or more (703)

Tabular Inorganic (0)

▾ Isotopes

▾ Metals

▾ Regulatory Information

▾ Search Within Results

Substances (1)

References ▾

Reactions ▾

Suppliers ▾

1

118501-78-3

Component	Percent
Zr	99
Zn	0.5
Fe	0.4
Cr	0.1

Cr.Fe.Zn.Zr

Components: 4

Zirconium alloy, base, Zr 99,Zn 0.5,Fe 0.4,Cr 0.1

This is our substance

Refine the search to a specific number of components



Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org

Click [here](#) to get back to the
research area overview slide.

Inorganic searching – without limits – in the world of Zirconium

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org



Retrieving analytical methods from publications



Search Question

Quantification of glyphosate intake in the body

- In order to be able to assess whether an injury or illness is caused by the herbicide glyphosate, it is necessary to determine its uptake into the body.
- A quantitative analysis method of glyphosate in blood or other body parts is necessary.

Click [here](#) to get back to the research area overview slide.

Start and refine query in Scifinderⁿ



References ▾

Glyphosate

×

Draw



^ Concept

- Herbicides (202)
- Pesticides (129)
- Food analysis (127)
- HPLC (83)
- Soil analysis (61)
- Blood analysis (33)
- Blood serum (9)
- Blood (8)
- Blood plasma (5)
- Blood serum albumins (5)
- Skin (4)
- Lung (2)
- Eye disease, irritation (1)
- Lung neoplasm (1)
- Skin rash (1)

[View All](#)

^ Substance Role

- Adverse Effect (1,585)
- Analytical Study (919)
- Biological Study (15K)
- Formation (20)
- Miscellaneous (69)

[View All](#)

References (52)

Sort: Relevance ▾ View: Partial Ab

Substances ▾ Reactions ▾ Cited By ▾



1

Determination of **glyphosate**, **glyphosate** metabolites, and glufosinate in human serum by gas chromatography-mass spectrometry

By: Motojyuku, Megumi; Saito, Takeshi; Akieda, Kazuki; Otsuka, Hiroyuki; Yamamoto, Isotoshi; Inokuchi, Sadaki
Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2008) 875(2) 509-514 | | Analis

Query and refinement gives 52 results with promising titles.
But blood and body related concepts and the substance glyphosate don't have to be related.



Click [here](#) to get back to the research area overview slide.

Reference details

Reference Detail (1 of 52)

← Prev Next →

Substances (3) Reactions (0) Cited By (62) Citation Map



Journal

Source

Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences
Volume: 875
Issue: 2
Pages: 509-514
Journal
2008
DOI:

Determination of glyphosate, glyphosate metabolites, and glufosinate in human serum by gas chromatography-mass spectrometry

By: Motojyuku, Megumi; Saito, Takeshi; Akieda, Kazuki; Otsuka, Hirovuki; Yamamoto, Isotoshi; Inokuchi, Sadaki

Abstract: This paper describes an assay for the determination of [phosphonic acid] (AMPA), and glufosinate (GLUF) in human serum. After extraction, serum samples were derivatized and analyzed by gas chromatography-mass spectrometry. The concentration range of 3-100.0 µg/mL for GLYP, AMPA, and GLL and interday variations were <15%. Precision and accuracy were <15%. This method can quantify the GLYP and AMPA content in the serum of a GLYP-pc determination of GLYP and its metabolite AMPA in serum obtained from human.

Concepts

Blood analysis

Forensic analysis

Homo sapiens

Human

Mass spectrometry

Gas chromatography-mass spectrometry

Poisoning, biological

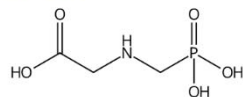
Solid phase extraction

Substances

D
A
C
C

Substances (3)

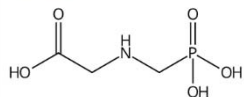
1071-83-6



C₃H₈NO₅P
Glyphosate

Role: Analyte, Analytical Study
Notes: metabolites

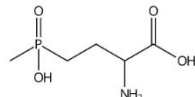
1071-83-6



C₃H₈NO₅P
Glyphosate

Role: Adverse Effect, Including Toxicity, Analyte, Biological Study, Analytical Study

51276-47-2



C₅H₁₂NO₄P
Glufosinate

Role: Analyte, Analytical Study



Click [here](#) to get back to the research area overview slide.

Analytical information

Conventional way:
Review the full text for description of analytical procedure

Full Text ▾

DOI

View all Sources

MethodsNow: Analysis

Title	CAS Method Number
Analysis of Glyphosate in Blood serum by Solid phase extraction	1-125-CAS-60678 ↗

Alternative:
Use the MethodsNow: Analysis opportunity to receive all information directly

Opens new tab to MethodsNow: Analysis record.
Only accessible with MNA subscription

Click [here](#) to get back to the research area overview slide.

Different platform, possibly new login necessary

The screenshot shows the 'METHODSNow' interface. At the top, there is a search bar and navigation icons. The main heading is 'Method Detail (1 of 1)'. Below this, the title of the method is 'Analysis of Glyphosate in Blood serum by Solid phase extraction'. The CAS number is 'CAS MN: 1-125-CAS-60678'. The method category is 'Forensic Analysis' and the technique is 'Gas chromatography-mass spectrometry; Solid phase extraction'. A table lists the materials used in the method, including (Aminomethyl)phosphonic acid, Glyphosate, Glufosinate, Blood serum, a 30 m x 0.25 mm HP-5MS fused-silica capillary column, Sorbent (265 mg, 11 mm o.d. x 20 mm length), and Acetonitrile. Each material has a role (analyte, matrix, or reagent) and a 'View Structure' link, except for Blood serum. CAS RN numbers are provided for the analytes and reagent.

Materials	Role	Image	CAS RN
(Aminomethyl)phosphonic acid	analyte	View Structure	1066-51-9
Glyphosate	analyte	View Structure	1071-83-6
Glufosinate	analyte	View Structure	51276-47-2
Blood serum	matrix		
30 m x 0.25 mm HP-5MS fused-silica capillary column with a film thickness of 0.25 μ m obtained	material		
Sorbent (265 mg, 11 mm o.d. x 20 mm length)	material		
Acetonitrile	reagent	View Structure	75-05-8

Title of method, not publication

All materials with standardized roles indexed

Click [here](#) to get back to the research area overview slide.

CAS Solutions

METHODSNOW
A CAS SOLUTION

Method Detail (1 of 1) ← Prev Next →

Analysis of Glyphosate in Blood serum by Solid phase extraction

CAS MN: 1-125-CAS-60678

Source

Determination of glyphosate, glyphosate metabolites, and glufosinate in human serum by gas chromatography-mass spectrometry

Motojyuku, Megumi; Saito, Takeshi; Akieda, Kazuki; Otsuka, Hiroyuki; Yamamoto, Isotoshi; Inokuchi, Sadaki

Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2008), 875 (2), 509 - 514. Elsevier B.V.

CODEN: JCBAAI | ISSN: 15700232 | DOI: 10.1016/j.jchromb.2008.10.003

Full Text

Equipment Used

This paper describes the determination of glyphosate and glufosinate in human serum by gas chromatography-mass spectrometry (GC-MS). The method involves solid phase extraction (SPE) of the analytes from serum samples onto a C18 sorbent (265 mg, Acetonitrile) followed by elution with water. The eluate is then dried and reconstituted in water. The resulting solution is injected into a GC-MS system equipped with a gas chromatograph system, 6890, Agilent, Palo Alto, CA, USA and a mass spectrometer (MS), 5975B, Agilent.

Conditions

Instrument

carrier gas: helium, flow rate rate: 0.6 ml/min, injection volume: 1 µL, injection temperature: 250 °C, oven programme: 100 - 3000 °C at 20 °C/min, quadrupole temperature: 150 °C

ion source temperature: 230 °C, mass-selective detector interface temperature: 280 °C

Bibliographic information of publication

Used equipment and applied conditions

Click [here](#) to get back to the research area overview slide.

Detailed step by step instruction for the analysis – manually extracted from the publication and supplementary data

Method Detail (1 of 1) ← Prev Next →

Instructions

A Sample Preparation

1. Inject 400 ml of Rundup (41% glyphosateisopropylammonium) into the healthy human volunteers..
2. Collect the serum sample after 1.5 hours of ingestion.
3. Select the individual with heart rate of 96 beats/min, systolic blood pressure of 100 mmHg,

Extraction

1. Extract the calibration curves and the QC and clinical serum samples by employing a solid-p
2. Utilize a Sep-Pak Plus PS-2 sorbent, obtained from Waters Corporation, along with a styrene
3. Add 0.2 ml of serum and 0.2 ml acetonitrile to centrifuge tubes and vortex the mixture.
4. Centrifuge the tubes at 3000 rpm for 5 min.
5. Add 10 µl (100 ug/ml) of the internal standard to the 0.2 ml sample.
6. Purify the sample extracts using Sep-Pak® Plus PS-2 (265 mg, 11 mm o.d. x 20 mm length).
7. Load them onto SPE cartridges conditioned with acetonitrile (4 ml) and distilled water (4 ml)
8. Dry the cartridges at 5 psi for 3 min and elute with 2 ml of acetonitrile.
9. Reduce the eluates to dryness under nitrogen at 50 °C.
10. Reconstitute the samples in 50 µl each of *N*-methyl-*N*-(tert-butyl(dimethylsilyl) trifluoroacetar (TBBMCS) and acetonitrile.
11. Vortex the mixture for 15 min.

GC - MS

1. Perform gas chromatographic analyses using an Agilent 6890 quadrupole gas chromatograp mass spectrometer (MS).
2. Carry out the separation on a 30 m x 0.25 mm HP-5MS fused-silica capillary column with a fi
3. Use helium in the place of a carrier gas with a flow rate of 0.6 ml/min.
4. Inject 1 µl of the extract in a split-less mode at an injection temperature of 250 °C.
5. Programme the oven temperature to increase from an initial temperature of 100 °C (held for 5 min) to 300 °C (held for 5 min) at 20 °C/min.
6. Set the temperature of the oven to 300 °C and increase the temperature to 450 °C at 20 °C/min.

Validation

Limit of Detection	0.25 µg/ml, (ami 0.25 µg/ml, Glyphosate (GLYP) 0.05 µg/ml, Glufosinate (GLUF)
Limit of Quantitation	3 µg/ml, AMPA 3 µg/ml, GLYP 3 µg/ml, GLUF
Recovery	20.8, 22.1, 22.3% for 3, 30 and 90 µg/ml 37.5, 37.6, 38.8% for 3, 30 and 90 µg/ml 38.8, 39.3, 41.6% for 3, 30 and 90 µg/ml
Accuracy	93.5, 91.6, 94.7% (Intraday); 93.1, 92.0, 9 95.5, 103.0, 98.3% (Intraday); 95.3, 101.7 92.9, 88.2, 91.7% (Intraday); 93.7, 88.6, 9
Precision	7.5, 6.9, 10.6% RSD for 3, 30 and 90 µg/n 7.2, 8.5, 10.6% RSD for 3, 30 and 90 µg/n 6.4, 7.9, 8.8% RSD for 3, 30 and 90 µg/ml

Validation and also calibration data listed if indicated in the publication

Click [here](#) to get back to the research area overview slide.

Start and refine query in MethodsNow: Analysis



Glyphosate



Specify glyphosate as analyte

^ Analyte

- Glyphosate (404)
- (Aminomethyl)phosphonic acid (180)
- Glufosinate (89)
- Maleic hydrazide (37)
- Mepiquat (30)

[View All](#)

Define the blood and body related terms as matrix

^ Matrix

- Drinking waters (50)
- Blood serum (10)
- Blood (3)
- Blood plasma (3)
- Skin (1)

[View All](#)

Additional refinement options

^ Method Category

^ Technique

^ Year



Click [here](#) to get back to the research area overview slide.

Results (17)

Sort Relevance ▾

The references are sorted by relevance



Compare (0/3)

Analysis of Glyphosate in Blood serum by Solid phase extraction

CAS MN: 1-125-CAS-60678

[View Details & Instructions](#)

[Add to Compare](#)

Up to 3 methods can be compared in tabellar view side by side

Analyte (Aminomethyl)phosphonic acid; Glyphosate; Glufosinate

Matrix Blood serum

Other Materials Reagent: Acetonitrile

Material: 30 m x 0.25 mm HP-5MS fused-silica capillary column with a film thickness of 0.25 um obtained: Sorbent (265 mg, 11 mm o.d. x 20 mm length)
[View All](#) ▾

Method Category Forensic Analysis

Technique Gas chromatography-mass spectrometry; Solid phase extraction

Equipment Used Gas chromatograph system; Mass spectrometer (MS)

Click [here](#) to get back to the research area overview slide.

Start and refine query in MethodsNow: Analysis

You can also use the Advanced Search to define roles in the beginning

Search

Enter keyword, matrix, or

[Advanced Search](#)

Advanced Search

Keyword

Analyte

AND

Keyword

Matrix

Method Category

Technique

CAS Method Number

Publication Name

Glyphosate immediately is defined as Analyte

Results (19)

Analyte

- Glyphosate (19)
- Glufosinate (11)
- (Aminomethyl)phosphonic acid (7)
- Fenitrothion (3)
- Malathion (3)

View All

Matrix

- Blood serum (10)
- Urine (5)
- Blood (3)
- Blood plasma (3)
- Soils (2)

View All

Method Category

- Analysis of M

CAS MN: 1-125-1

View Details &

Technique

Equipment User

Source

Terms containing „blood“ are assigned as Matrix



Click [here](#) to get back to the research area overview slide.

Method details

Method Detail (1 of 19)

Analysis of Methyl viologen in Blood by Atmospheric precipitation

CAS MN: 1-125-CAS-286197

Method Category

Technique:

Title of Method		
A	B	C
1	Title of Method	Analysis of Methyl viologen in Blood by Atmospheric precipitation
2	CAS Method Number	1-125-CAS-286197
3	Method Category	Forensic Analysis; Toxin Assay; Herbicide Analysis
4	Technique	HPLC-tandem mass spectrometry; Atmospheric precipitation
5		
6	Materials	Role CAS RN
7	Methyl viologen	analyte 1910-42-5
8	Glyphosate	analyte 1071-83-3
9	Glufosinate	analyte 51276-47-2
10	Diquat	analyte 2764-72-9
11	Urine	matrix
12	Blood	matrix
13	ZORBAX SB-Aq column (100 mm x 2.1 mm, 1.8 µm particle)	material
14	Dichloromethane	reagent 75-09-2
15	Acetonitrile	reagent 75-05-8
16		
17	Equipment Used	Liquid chromatography system, 1200 series, Agilent Technologies, Inc., Palo Alto, CA, USA Triple quadrupole mass spectrometer, 6410, Agilent Technologies, Inc., Palo Alto, CA, USA
18	Conditions	Instrument Conditions Column: ZORBAX SB-Aq column (100 mm x 2.1 mm, 1.8 µm particle); column temperature: 40 °C; mobile phase: 15 mM heptafluorobutyric acid (HFBA) (mobile phase A) and acetonitrile (mobile phase B); flow rate: 0.3 mL/min; injection volume: 5 µL
19		Nebulizer pressure: 40 psi; drying gas flow: 10 L/min at 350 °C; HV capillary voltage: 4000 V; fragmentation voltage: 131 V (for paraquat), 144 V (for diquat), 88 V (for glufosinate) and 65 V (for glyphosate); collision energy: 48 V (for paraquat), 24 V (for diquat), 8 V (for glufosinate) and 4 V (for glyphosate)

← Prev Next →

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- XLS

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You can download method details as PDF or XLS file

MethodsNow™

Page 1

Title of Method	Analysis of Methyl viologen in Blood by Atmospheric precipitation Link to Details
CAS Method Number	1-125-CAS-286197
Method Category	Forensic Analysis; Toxin Assay; Herbicide Analysis
Technique	HPLC-tandem mass spectrometry; Atmospheric precipitation

	Role	CAS RN
Methyl viologen	analyte	1910-42-5
Glyphosate	analyte	1071-83-3
Glufosinate	analyte	51276-47-2
Diquat	analyte	2764-72-9
Urine	matrix	
Blood	matrix	
ZORBAX SB-Aq column (100 mm x 2.1 mm, 1.8 µm particle)	material	
Dichloromethane	reagent	75-09-2
Acetonitrile	reagent	75-05-8

Equipment Used	Liquid chromatography system, 1200 series, Agilent Technologies, Inc., Palo Alto, CA, USA Triple quadrupole mass spectrometer, 6410, Agilent Technologies, Inc., Palo Alto, CA, USA
Conditions	Instrument Conditions Column: ZORBAX SB-Aq column (100 mm x 2.1 mm, 1.8 µm particle); column temperature: 40 °C; mobile phase: 15 mM heptafluorobutyric acid (HFBA) (mobile phase A) and acetonitrile (mobile phase B); flow rate: 0.3 mL/min; injection volume: 5 µL; Nebulizer pressure: 40 psi; drying gas flow: 10 L/min at 350 °C; HV capillary voltage: 4000 V; fragmentation voltage: 131 V (for paraquat), 144 V (for diquat), 88 V (for glufosinate) and 65 V (for glyphosate); collision energy: 48 V (for paraquat), 24 V (for diquat), 8 V (for glufosinate) and 4 V (for glyphosate)
Source	Simultaneous determination and quantitation of paraquat, diquat, glufosinate and glyphosate in postmortem blood and urine by LC-MS-MS



Click [here](#) to get back to the research area overview slide.

Compare Methods

Compare (0/3)

Compare

Add to Compare

Select Results to Download

Sort Relevance

Compare Results

Compare (3/3)

Remove from Compare

Atmospheric precipitation

Compare Methods

Select up to three methods to compare with each other

As soon as some methods are selected, the compare button will be activated. Click on this button to review the selected methods

You can download the compared methods as PDF or XLS file

	1	2	3
Title	Analysis of Methyl viologen in Blood by Atmospheric precipitation	Analysis of 1-(3,4-Dichlorophenyl)-3-methylurea in Blood by Liquid chromatography-mass spectrometry	Analysis of Glyphosate in Blood by Solid phase extraction
Id Number	1-125-CAS-286197	1-125-CAS-122738	1-125-CAS-297318
Id Category	Forensic Analysis; Toxin Assay; Herbicide Analysis	Forensic Analysis	Forensic Analysis
Technique	HPLC-tandem mass spectrometry; Atmospheric precipitation	Liquid chromatography-mass spectrometry; Extraction; Solid phase extraction	Atmospheric precipitation; Electrospray ionization mass spectrometry; Hydrophilic interaction View All
Analyte	Methyl viologen; Glyphosate ; Glufosinate; Diquat	Naled; Pyrimethanil; Dinocap; Azoxystrobin; Metoxuron; Terbufos; Dialifos; Epoxiconazole; 4-Nitrophenol;	Glyphosate ; (Aminomethyl)phosphonic acid

Retrieving analytical methods



- Refine by Substance Role: Analytical Study
- Retrieve method from full text



- Separate compendium specifically for analytical methods
- Define Substance Role in queries or refinements
- Export detailed instructions directly
- Very good coverage for various areas like organic chemistry, food science, cosmetics, environmental chemistry



Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org

Click [here](#) to get back to the
research area overview slide.

Retrieving analytical methods from publications

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org



SCIFINDERⁿ
A CAS SOLUTION

Food Chemistry in SciFinderⁿ



Click [here](#) to get back to the research area overview slide.

Search Question

Compositions of low caloric sugars in cocktails and alcoholic beverages in general

Click [here](#) to get back to the research area overview slide.

Low caloric sugars in cocktails and alcoholic beverages in general

Young people increasingly consider their calorie intake, even on their nights out. How to compose tasty sweet drinks that respect their wish for reduced calorie content?

Search

- All
- Substances
- Reactions
- References**
- Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

("low calorie" OR low-calorie) AND (sugar OR sweeten*)

Use [Advanced Search](#) for Author, Journal, or Organization

Click [here](#) to get back to the research area overview slide.



References ▾

("low calorie" OR low-calorie) AND (sugar OR sweeten*) ×



Review the search or start a new one from the top search bar

The references are ordered by relevance

References (63,028)

Sort: Relevance ▾ View: Partial Abstract ▾

Substances ▾ Reactions ▾ Cited By ▾



Terms that match the query are highlighted

1

Low-calorie sweeteners and other sugar substitutes: A review of the safety issues

By: Kroger, Manfred; Meister, Kathleen; Kava, Ruth

Comprehensive Reviews in Food Science and Food Safety (2006), 5(2), 35-47 | Language: English, Database: CPlus

A review. Sugar-free or reduced-sugar foods and beverages are very popular in the United States and other countries, and the sweeteners that make them possible are among the most conspicuous ingredients in the food supply. Extensive scientific research has demonstrated the safety of the low-calorie sweeteners currently approved for use in foods in the United



Click [here](#) to get back to the research area overview slide.

Refine the answer set

Standardized concepts are assigned according to the novelty or innovation of the publication.

Filter by

- Document Type
- Substance Role
- Language
- Publication Year
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
- CAS Solutions
- Formulation Purpose
- Database
- Search Within Results

All filters and refinement options can be found on the left hand side

^ Concept

- Carbohydrates (35K)
- Proteins (12K)
- Fats and Glyceridic oils (6.662)
- Homo sapiens (6.132)
- Human (6.132)

[View All](#)

„View all“ expands the list or opens a fly-out window as necessary

Find relevant concepts quickly by using the „Search“ option

Concept

Top Count | Alphanumeric | **Search**

Concept Name

beverage

Select All on Page

- Alcoholic beverages (494)
- Alcoholic beverages, low-calorie (9)
- Canned beverages, canned carbonated beverages (2)
- Canned beverages, canned coffee beverages (2)

Click [here](#) to get back to the research area overview slide.

The screenshot displays the SciFinder search interface with the following elements:

- Document Type:** Journal (45K) and Patent (16K) are selected. Other options include Review (2.527), Biography (1), and Book (5). A "View All" link is present.
- Substance Role:** A list of roles with checkboxes, including Adverse Effect (5), Analytical Study (16), Biological Study (847), Miscellaneous (1), Nanoscale (1), Occurrence (2), Preparation (33), Process (54), Properties (6), Prophetic in Patents (1), Reactant or Reagent (6), and Uses (588). A "View Fewer" link is at the bottom.
- Publication Year:** A histogram showing a sharp increase in publications starting around 2010. Input fields are set to "2010" to "2020" with an "Apply" button. "Reset" and "View Larger" links are also available.
- Search Within Results:** A search box containing the text "alcohol" and a "Find" button.

Filter options within each category are OR combined, the categories themselves are combined with AND:

(Journal OR Patent) AND
Uses AND (2010-2020) AND
alcohol

Multiple „Search Within Results“ are combined with AND

Click [here](#) to get back to the research area overview slide.

Reference details

Reference Detail (1 of 159)

Bibliographic data

Substances (36)

Reactions (0)

Cited By (1)

Citation Map



Save

Patent

Patent Information

Patent Number
US20110244094

Publication Date
2011-10-06

Application Number
US2010-12750720

Low calorie composite sweetener as sugar alternative and methods for producing the same

By: Markosyan, Avetik; Purkayastha, Siddhartha

Abstract: The invention provides a process for producing a low calorie composite sweetener as a sugar alternative. The invention further provides a low calorie composite sweetener that can be used in many products. The low calorie composite sweetener is

PATENTPAK Viewer

Full Text

View full text of patents with PatentPak

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
US20110244094	English	A1	PDF PDF+ Viewer	2011-10-06	US2010-12750720	2010-03-31
US8357417	English	B2	PDF	2013-01-22	US2010-12750720	2010-03-31

Click [here](#) to get back to the research area overview slide.

^ Concepts

Alcoholic beverages Food

Atomization, physical Glycosides

^ Substances

Bakery cakes

Bakery products

Beverages

Bread

Carbohydrates

Substances (36)

64-17-5 1405-86-3 1405-86-3

^ Formulations

C2H6O
Alcohol
PATENTPAK

Concepts, Substances and additional Information - here Formulations - are extracted manually from the publications and made available in Scifinderⁿ

^ Formulations

Diet Cookies: Sweetener

[View Formulus® Detail](#)

Location: example 14
Purpose: Sweetening agents

Component	Function	Amount Reported
Flours and Meals	active agent	50 %
Margarine	-	30 %
Milk	-	1 %

Click [here](#) to get back to the research area overview slide.

PatentPak

PAGE 1 /10 ZOOM - + DOWNLOAD PDF | PDF+

Full text available, searchable via browser or pdf viewer



US 20110244094A1

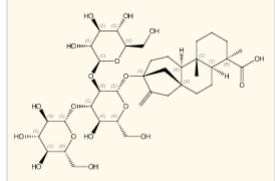
(19) **United States**
(12) **Patent Application Publication** (10) **Pub. No.: US 2011/0244094 A1**
MARKOSYAN et al. (43) **Pub. Date: Oct. 6, 2011**

(54) **LOW CALORIE COMPOSITE SWEETENER AS SUGAR ALTERNATIVE AND METHODS** **Publication Classification**

PATENTPAK
A CAS SOLUTION

Key Substances in Patent

CAS RN
58543-17-2



Analyst Markup Locations (1)
Page 6

...of the
id minimizes
ses when the
ed by direct
ersion. The
etener to be
of the granu-

distributed to form a layer with thickness of 3 mm on a vibratory tray. 10.03 g Reb-A 97 (containing stevioside 31%, rebaudioside C 0.21%, rebaudioside A 98.56%, rebaudioside B 0.22%) was dissolved in 15.04 g of solvent mixture containing 4 volumes of water per 1 volume of ethyl alcohol to make rebaudioside A 40% (w/w) solution. The

Substances hyperlinked in text.



Click [here](#) to get back to the research area overview slide.

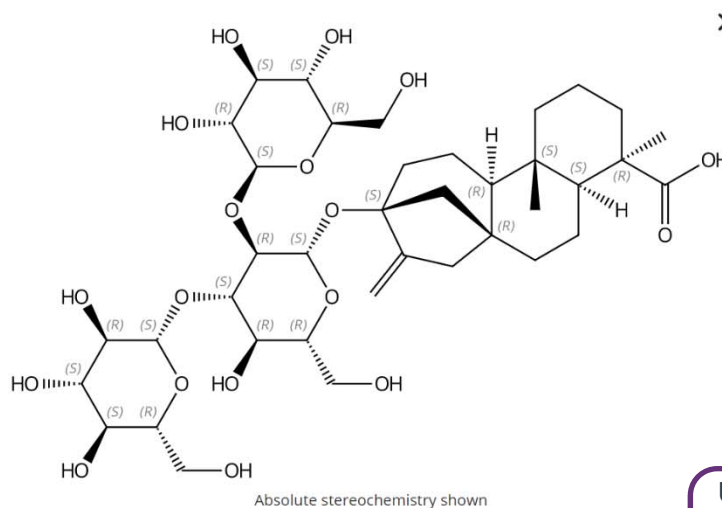
Substances in Scifinderⁿ

Open substance details (via clicking on CAS registry number or "Substance Detail") from reference or search for name, structure, chemical formula, etc.

Find reactions with the substance in any role or as the product
Refine the search afterwards

CAS RN	58543-17-2
CAS Name	Rebaudioside B
Substance Detail	
Reactions (30)	
Synthesize (22)	
Create Retrosynthesis Plan	
References (622)	
Suppliers (29)	

Find known and new ways to synthesize the substance



Use the structure as template for a new structure or reaction search

Edit Structure - Reset +

Click [here](#) to get back to the research area overview slide.

Reactions in Scifinderⁿ

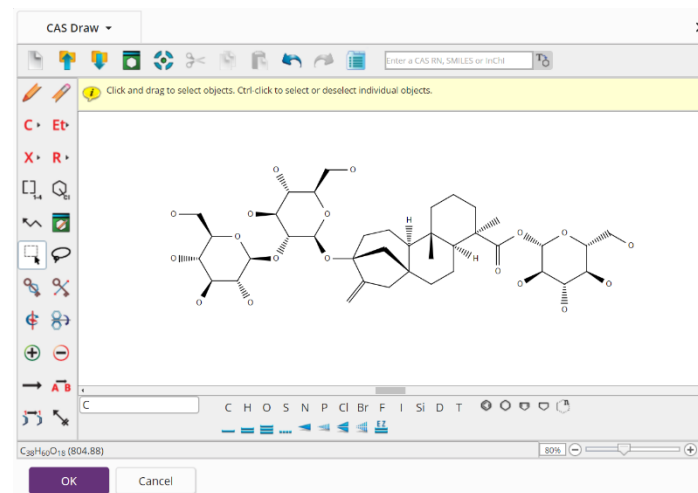
How can a particular Stevioside be synthesized?

Start reaction search from substance details via structure or text search



Reactions 57817-89-7 Draw

Reactions (30)
Synthesize (22)



Click [here](#) to get back to the research area overview slide.

Use filters to refine answer set

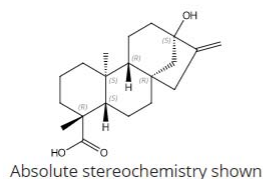
Filter by

- ^ Substance Role
 - Product (3)
 - Reactant (11)
- ^ Yield
- ^ Number of Steps
- ^ Experimental Protocols
- ^ Reaction Type
- ^ Stereochemistry
- ^ Catalyst
- ^ Commercial Availability
- ^ Reaction Notes
- ^ Search Within Results

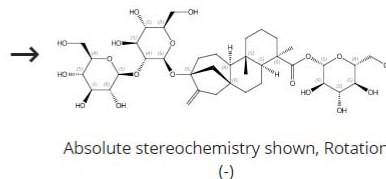
Reactions with the same scheme are summarized

Scheme 2 (1 Reaction)

Steps: 3



Suppliers (40)



Suppliers (86)



Reaction Summary

Steps: 3

- 1.1 Catalysts: UDP-glycosyltransferase
- 2.1 Catalysts: UDP-glycosyltransferase
- 3.1 Catalysts: UDP-glycosyltransferase

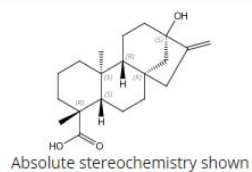
Development of Photoaffinity Probe for the Discovery of Steviol Glycosides Biosynthesis Pathway in Stevia rebaudiana and Rapid Substrate Screening

By: Li, Weichao; et al
ACS Chemical Biology (2018), 13(8), 1944-1949

[View Reaction Detail](#) | [Experimental Protocols](#)

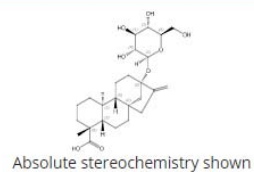
Full Text ▾

Click [here](#) to get back to the research area overview slide.



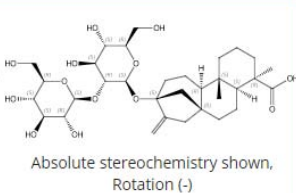
🛒 Suppliers (40)

1 →



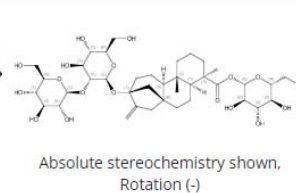
🛒 Suppliers (6)

2 →



🛒 Suppliers (36)

3 →



🛒 Suppliers (86)

Step 1 **Step 2** Step 3

↔ Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	UDP-glycosyltransferase	-	-
CAS Reaction Number: Not assigned				

Notes

biotransformation, enzymic, UDP-glycosyltransferase UGT91D2 used

Refer

Develop
Probe for
Glycosyl
in Stevia

Different reaction steps can be visualized. All given information from publication and supplemental content is extracted.

Comp:

Click [here](#) to get back to the research area overview slide.

Experimental Protocols

MethodsNow™

Products [Steviolbioside](#)

Reactants [Steviolmonoside](#)

Catalysts [UDP-glycosyltransferase](#)

Procedure

1. Perform the reaction in a total volume of 100 mL containing 100 mM Tris-HCl buffer (pH 8.0), 3 mM MgCl₂, 10 mg/mL BSA, 1 mM UDP-glucose along with 1 mM of steviolmonoside, and 20 μM recombinant UGT for 4 hours at 30 °C.
2. Terminate the reaction by adding 200 mL of water saturated n-butanol.
3. Extract the mixture three times with 200 mL of water-saturated n-butanol.
4. Evaporate the combined organic phase completely by a rotary evaporator.
5. Dissolve the residue in MeOH/H₂O (50%/50%, v/v) to obtain 19-O-β-glucopyranosol steviol.

Characterization Data

^ Steviolbioside

Proton NMR Spectrum (400 MHz, MeOD) δ 5.41 (1H, d, *J*= 8.2 Hz), 3.83 (1H, dd, *J*= 1.9, 12.2 Hz), 3.69 (1H, dd, *J*= 4.5, 12.2 Hz), 3.37 (4H, m), 2.67 (1H, dd, *J*= 3.1, 17.1 Hz), 2.22 (1H, d, *J*= 13.1), 1.91 (4H, m), 1.72 (3H, m), 1.45 (6H, m), 0.96 (3H, s), 0.85 (3H, s)

Carbon-13 NMR (100 MHz, MeOD) δ 223.90, 176.65, 94.17, 77.31, 77.25, 72.62, 69.62, 60.92, 57.18, 54.37, 53.71, 48.23, 48.02, 43.62, 41.09, 39.49, 39.36, 37.91, 37.53, 37.09, 27.63, 21.34, 20.06, 18.82, 18.55, 12.68

The detailed reaction protocol is given in the reaction details if available.

It is extracted manually from publication and supplemental information.

The reaction answer set can be refined for results that include MethodsNow reaction protocols or general experimental procedures. [Compare Filters on slide 11]

^ Experimental Protocols

- MethodsNow: Synthesis (3)
- Experimental Procedure (1)

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org

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research area overview slide.

Food Chemistry in SciFinderⁿ

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org



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Medicinal Chemistry in SciFinderⁿ



Click [here](#) to get back to the research area overview slide.

Search Question

- Identify relevant protein checkpoint inhibitors of apoptosis-regulating protein PD-1 with a special focus on antibodies
- Obtain recent patents related to these inhibitors and locate the substance information

Click [here](#) to get back to the research area overview slide.

The Search History allows for a quick start



Filter by

Result Type

- All (49)
- Patent Markush (40)
- Reactions (378)
- References (2,554)
- Retrosynthesis (172)

[View All](#)

Date

Start Date to End Date

March, 2020

SU	MO	TU	WE	TH	FR	SA
	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30	31	1	2	3
4						

Search History (5,002)

March 11, 2020

2:23 PM

Substances Amisulpride (1)

[Rerun Search](#)

[Edit Search](#)

12:24 PM

References pd or "Programmed cell death protein" or "programmed cell death ligand" (608K)

[Rerun Search](#)

[Edit Search](#)

Boolean and Phrase Search allow for customized precise searches

Rerun Search from history



Click [here](#) to get back to the research area overview slide.

More than 600k results are retrieved

Filter by

- Document Type
 - Journal (470K)
 - Patent (116K)
 - Review (34K)
 - Biography (26)
 - Book (265)
 - [View All](#)
- Substance Role
 - Adverse Effect (74)
 - Analytical Study (1,877)
 - Biological Study (4,531)
 - Combinatorial Study (6)
 - Formation (1,310)
 - [View All](#)
- Language

References (608,921)

Sort: Relevance ▾ View: Full Abstract ▾

Substances ▾ Reactions ▾ Cited By ▾ Save

1

Biomarkers for predicting efficacy of pd-1/ pd-l1 inhibitors

By: Yi, Ming; Jiao, Dechao; Xu, Hanxiao; Liu, Qian; Zhao, Weiheng; Han, Xinwei; Wu, Kongming
Molecular Cancer (2018), 17, 129/1-129/14 | Language: English, Database: CAplus

A review. **Programmed cell death protein 1/programmed cell death ligand 1 (PD-1/PD-L1)** is a neg. modulatory signaling pathway for activation of T cell. It is acknowledged that **PD-1/PD-L1** axis plays a crucial role in the progression of tumor by altering status of immune surveillance. As one of the most promising immune therapy strategies, **PD-1/ PD-L1** inhibitor is a breakthrough for the therapy of some refractory tumors. However, response rate of **PD-1/PD-L1** inhibitors in overall patients is unsatisfactory, which limits the application in clin. practice. Therefore, biomarkers which could effectively predict the efficacy of **PD-1/PD-L1** inhibitors are crucial for patient selection. Biomarkers reflecting tumor immune microenvironment and tumor cell intrinsic features, such as **PD-L1** expression, d. of tumor infiltrating lymphocyte (TIL), tumor mutational burden, and mismatch-repair (MMR) deficiency, have been noticed to associate with treatment effect of anti-**PD-1**/anti-**PD-L1** therapy. Furthermore, gut microbiota, circulating biomarkers, and patient previous history have been found as valuable predictors as well. Therefore establishing a comprehensive assessment framework involving multiple biomarkers would be meaningful to interrogate tumor immune landscape and select sensitive patients.

Most relevant results appear at the top



Click [here](#) to get back to the research area overview slide.

Using the search function in the concept filter allows us to focus on keywords related to 'programmed cell death protein 1'

Concept

Top Count Alphanumeric Search

Concept Name

programmed cell death

5 Selected

All concepts are shown which contain the query terms

<input type="checkbox"/> Programmed cell death (46)	<input type="checkbox"/> Programmed cell death 6-interacting proteins (40)	<input type="checkbox"/> Programmed cell death protein 4 (429)
<input type="checkbox"/> Programmed Cell Death 1 Ligand 2 Protein (388)	<input checked="" type="checkbox"/> Programmed cell death protein 1 (15K)	<input type="checkbox"/> Programmed cell death protein 5 (79)
<input type="checkbox"/> Programmed cell death 1 ligand 2 proteins (1,401)	<input type="checkbox"/> Programmed cell death protein 10 (95)	<input type="checkbox"/> Programmed cell death protein 6 (128)
<input checked="" type="checkbox"/> Programmed cell death 1 ligand protein inhibitors (51)	<input type="checkbox"/> Programmed cell death protein 11 (23)	<input type="checkbox"/> Programmed cell death protein 8 (194)
<input checked="" type="checkbox"/> Programmed cell death 1 ligand proteins (44)	<input checked="" type="checkbox"/> Programmed cell death protein 1 inhibitors (845)	<input type="checkbox"/> Programmed cell death proteins (716)
<input checked="" type="checkbox"/> Programmed Cell Death 1 Receptor (4,763)	<input type="checkbox"/> Programmed cell death protein 2 (45)	

Apply Cancel

Additional concepts might be selected subsequently

Click [here](#) to get back to the research area overview slide.

Analyze all indexed substances, even if based on large answer sets

The screenshot shows a SciFinder search results page for 'References' (20,432). The page includes a filter sidebar on the left with categories like Document Type, Substance Role, and Language. The main content area displays a list of references, with the first one highlighted. A callout box points to the 'Substances' filter button, indicating that all substances indexed for these 20k documents can be analyzed.

References (20,432) Sort: Relevance View: Full Abstract

Substances Reactions Cited By Save

Effectiveness of pd-1/ pd-l1 inhibitors

By: Yi, Ming; Jiao, Dechao; Xu, Hanxiao; Liu, Qian; Zhao, Weiheng; Han, Xinwei; Wu, Kongming
Molecular Cancer (2018), 17, 129/1-129/14 | Language: English, Database: CAplus

A review. Programmed cell death protein 1/programmed cell death ligand 1 (PD-1/PD-L1) is a neg. modulatory signaling pathway for activation of T cell. It is acknowledged that PD-1/PD-L1 axis plays a crucial role in the progression of tumor by altering status of immune surveillance. As one of the most promising immune therapy strategies, PD-1/ PD-L1 inhibitor is a breakthrough for the therapy of some refractory tumors. However, response rate of PD-1/PD-L1 inhibitors in overall patients is unsatisfactory, which limits the application in clin. practice. Therefore, biomarkers which could effectively predict the efficacy of PD-1/PD-L1 inhibitors are crucial for patient selection. Biomarkers reflecting tumor immune microenvironment and tumor cell intrinsic features, such as PD-L1 expression, d. of tumor infiltrating lymphocyte (TIL), tumor mutational burden, and mismatch-repair (MMR) deficiency, have been noticed to associate with treatment effect of anti-PD-1/anti-PD-L1 therapy. Furthermore, gut microbiota, circulating biomarkers, and patient previous history have been found as valuable predictors as well. Therefore establishing a comprehensive assessment framework involving multiple biomarkers would be meaningful to interrogate tumor immune landscape and select sensitive patients.

Full Text Substances (5) Reactions (0) Cited By (49) Citation Map

Click [here](#) to get back to the research area overview slide.

Indexed substance set of any size can be effectively filtered to limit to PD-1 antagonists

Relevance ranking brings substances of interest to the top

Filter by

- Commercial Availability
 - Available (27K)
 - Not Available (681K)
- Reaction Role
 - Product (77K)
 - Reactant (32K)
 - Reagent (4,555)
 - Catalyst (3,616)
 - Solvent (1,369)
- Reference Role
 - Adverse Effect (13K)
 - Analytical Study (188K)
 - Biological Study (483K)

Substances (709,308) Sort: Relevance View Partial

References Reactions Suppliers

<input type="checkbox"/> 1 946414-94-4 Image Not Available Notes: A fully human IgG4 antibody blocking the programmed cell death-1 receptor Unspecified Nivolumab Protein/Peptide Sequence Sequence Length: 1308 5,104 References 1 Reaction 8 Suppliers	<input type="checkbox"/> 2 1374853-91-4 Image Not Available Unspecified Pembrolizumab 3,995 References 0 Reactions 10 Suppliers	<input type="checkbox"/> 3 1380723-44-3 Image Not Available Unspecified Atezolizumab 1,448 References 1 Reaction 6 Suppliers
--	--	---

Substance Class, Bioactivity and Target Indicator filters help us to focus on most relevant compounds

^ Substance Class

- Protein/Peptide Sequence (570K)
- Manual Registration (123K)
- Organic/Inorganic Small Molecule (72K)
- Nucleic Acid Sequence (53K)

We focus on antibodies and peptides and limit the substances accordingly

^ Bioactivity Indicator

- Antitumor agents (37K)
- Pharmaceutical im agents (28K)
- Biopharmaceuticals
- Anti-infective agents (10K)
- Vaccines (8,708)
- Receptor antagonists (3,733)

[View All](#)

^ Target Indicator

- Proteinaceous antigens
- proteins (5,196)
- checkpoint molecules (4,108)
- Apoptosis-regulating proteins (3,733)
- Membrane proteins (3,665)

[View All](#)

Bioactivity and Target Indicators are available as filters, also for large answer sets. Filtering restricts our answer set to 3,733 substances

Click [here](#) to get back to the research area overview slide.

The Bioactivity Indicators in the detailed record of Nivolumab show the target of interest

Substances (3,733)

CTRL+Click to open detailed record in a new tab

[946414-94-4](#)

Image Not Available

Notes: A fully human IgG4 antibody blocking the programmed cell death-1 receptor

Unspecified
Nivolumab

Protein/Peptide Sequence
Sequence Length: 1308

5,104
References

1
Reaction

8
Suppliers

Substance Detail (1 of 3,733)

References (5,104)

Reaction (1)

Suppliers (8)

← Prev Next →



★ Save

Unspec
Pembr
CAS Registry Number
016111 01 1

3,9
Refere
Nivolumab

Notes: A fully human IgG4 antibody blocking the programmed cell death-1 receptor

Bioactivity Indicators

Receptor antagonists

[Programmed cell death protein 1 inhibitors \(322\)](#)

Vaccines (119)

[Cancer vaccines \(171\)](#)

'Programmed cell death protein 1 inhibitors' is what we were looking for, click the blue text to go to the respective references

Click [here](#) to get back to the research area overview slide.

We explore Nivolumab related patents and determine the location of Nivolumab in the full-text with PatentPak

Filter by

- Document Type
 - Journal (70)
 - Patent (252)
 - Review (18)
- Language
 - English (241)
 - Japanese (6)
 - Chinese (4)
 - Korean (1)
- Publication Year
 - 2010
 - 2020
 - No Min to No Max Apply

References (252) Sort: Publication Year: Newest View: Full Abstract

Substances Reactions Cited By Save

1

Compositions and methods for treating cancer with a combination of programmed death receptor (PD-1) antibodies and vicriviroc

By: Giranda, Vincent L.; Pinheiro, Elaine M.; Li, Anlong
World Intellectual Property Organization, WO2020033283 A1 2020-02-13 | Language: English, Database: CAplus

The present invention relates to methods of treating a cell proliferation disorder (e.g., cancer) comprising administering: (a) vicriviroc, or a pharmaceutically acceptable salt thereof; (b) nivolumab or antigen binding fragment thereof to a subject in need thereof; and (c) such agents for the treatment of the subject.

PATENTPAK Full Text Citation Map

2

Use of interleukin-7 and chimeric antigen receptor (CAR)-bearing immune effector cells for treating tumors

By: Park, Jaehan; Lee, Byung Ha; Choi, Dong Hoon
World Intellectual Property Organization, WO2020020206 A1 2020-02-06 | Language: English, Database: CAplus

center in a subject in need thereof, comprising administering to the subject a composition comprising: (a) a CAR-bearing immune effector cell and an IL-7 protein (e.g., modified IL-7 protein).

Patent: WO2020028400 Language: English Kind Code: A1 PatentPak Options: PDF | PDF+ | **Viewer**

PATENTPAK Full Text Substances (24) Reactions (0) Cited By (0) Citation Map

Either open the PatentPak Viewer from the summary page (shown here) or open the detailed substance record and click the PatentPak link of the substance of interest



Click [here](#) to get back to the research area overview slide.

PatentPak directly shows us where Nivolumab is present in the patent full-text

WO2020028400

The screenshot displays the PatentPak interface for patent WO2020028400. At the top, there are navigation controls for PAGE (90/120), ZOOM (minus and plus icons), and DOWNLOAD (PDF and PDF+). On the left, a sidebar titled 'Key Substances in Patent' lists two entries: Nivolumab (CAS RN 946414-94-4) and Immunoglobulin G4, anti-(human protein PD-1) (CAS RN 1374853-91-4). A callout box points to the Nivolumab entry with the text 'Click icon/link to go to the location in the patent'. The main text area shows patent claims 67, 68, and 69. Claim 69 includes a list of checkpoint inhibitors: nivolumab, pembrolizumab, ipilimumab, atezolizumab, durvalumab, avelumab, and tremelimumab. A callout box points to this list with the text 'This method patent claims the use of one or more of the listed checkpoint inhibitors'. Blue location pins are placed above each name in the list, and a red line connects the top pin (nivolumab) to the sidebar entry.

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org

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research area overview slide.

Medicinal Chemistry in SciFinderⁿ

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org



SCIFINDERⁿ
A CAS SOLUTION

Biosearching in SciFinderⁿ



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Search Question

The protection mechanism of the Monarch Butterfly against parasites when raised on Milkweed plants

- Which substance in Milkweed (their caterpillar host plant) protects the Monarch Butterfly against parasites?
- Do proteins play a role in this defense mechanism?
- What is known about these proteins?

Click [here](#) to get back to the research area overview slide.

Which substances from Milkweed protect the Monarch Butterfly against parasites? – The Start I

The Monarch Butterfly is indexed with his genus in CAS data:

- Danaus, more precise Danaus Plexippus – how to know that?

The screenshot shows the SCIFINDER search interface. At the top, the search bar contains the query "Monarch Butterfly". A red box highlights the search bar with the text "Search for „Monarch Butterfly“". Below the search bar, the page displays "References (752)". On the left, there is a filter panel titled "Filter by" with a sub-section "Document Type" containing checkboxes for Journal (701), Patent (11), Review (49), Commentary (5), and Conference (15). The main content area shows a list of references, with the first one highlighted: "The Monarch butterfly genome yields insights into long-distance migration" by Zhan, Shuai; Merlin, Christine; Boore, Jeffrey L.; Reppert, Steven M. The abstract text is partially visible, mentioning the draft 273-Mb genome of the migratory monarch butterfly (Danaus plexippus) and a set of 16,866 protein-coding genes. At the bottom of the reference card, there are buttons for "Full Text", "Substances (3)", "Reactions (3)", "Cited By (358)", and "Citation Map".

Click [here](#) to get back to the research area overview slide.

Which substances from Milkweed protect the Monarch Butterfly against parasites? – The Start II

Reference Detail (1 of 2,525) + Prev Next →

Substances (0) Reactions (0) Cited By (358) Citation Map Download Email Save

Journal
Source: Cell (Cambridge, MA, United States)
Volume: 147
Issue: 5
Pages: 1171-1185
Journal: 2011
DOI: 10.1016/j.cell.2011.09.052

Database Information
AN: 2011:1531071
CAN: 155:675930
CAplus

The Monarch butterfly genome yields insights into long-distance migration

By: Zhan, Shuai; Merlin, Christine; Boore, Jeffrey L.; Reppert, Steven M.

Abstract: This report presents the draft 273-Mb genome of the migratory monarch butterfly (*Danaus plexippus*) and a set of 16,866 protein-coding genes. Orthol. properties suggest that the Lepidoptera are the fastest evolving insect order yet examined. Compared to the silkworm *Bombyx mori*, the monarch genome shares prominent similarity in orthol. content, microsynteny, and protein family sizes. The monarch genome reveals a vertebrate-like opsin whose existence in insects is widespread; a full repertoire of mol. components for the monarch circadian clockwork; all members of the juvenile hormone biosynthetic pathway whose regulation shows unexpected sexual dimorphism; addnl. mol. signatures of oriented flight behavior; microRNAs that are differentially expressed between summer and migratory butterflies; monarch-specific expansions of chemoreceptors potentially important for long-distance migration; and a variant of the sodium/potassium pump that underlies a valuable chem. defense mechanism. The monarch genome enhances our ability to better understand the genetic and mol. basis of long-distance migration. A host of factors contribute to the amazing migration behavior of the monarch butterfly, including sensory perception, a time-compensated compass mechanism, and seasonally regulated gene expression. The full genome sequence of this organism yields tantalizing mol. insights into the processes that likely underlie migration. The draft genome sequence is deposited in GenBank/EMBL/DBJ with project accession numbers AGBW01000001-AGBW01014067 and JH379599-JH392916 (WGS contigs).

Full Text ▾ Expand All | Collapse All

Concepts

Chemoreceptors Modifier: genes assocd. with	Molecular evolution
Role: Biological Study, Unclassified	Olfactory receptors Modifier: genes assocd. with
Circadian rhythm Modifier: genes assocd. with	Role: Biological Study, Unclassified
Danaus plexippus	Protein sequences

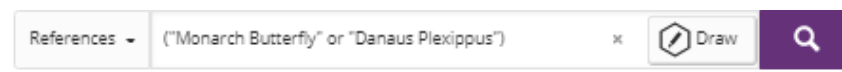
Open the first reference, ranked as the most relevant one by the SciFinderⁿ algorithm

Open the indexed concepts – review the highlighted terms



Which substances from Milkweed protect the Monarch Butterfly against parasites? – The Start III

- In CAS data the Monarch Butterfly is linked to Danaus Plexippus - for Medline data that may not be the case
- To collect all documents in both SciFinderⁿ databases use:



- Use „ “ for connected words
- Results in Detail:
 - 752 „Monarch Butterfly“
 - 459 „Danaus Plexippus“
 - 771 = („Monarch Butterfly“ or „Danaus Plexippus“)

Click [here](#) to get back to the research area overview slide.

Which substances from Milkweed protect the Monarch Butterfly against parasites?

Search as: („Monarch Butterfly“ or „Danaus Plexippus“) and Milkweed
-> 179 references

Search as: („Monarch Butterfly“ or „Danaus Plexippus“) and (Milkweed or Asclepias)
-> 228 references

The screenshot shows the SciFinder search results page. At the top, the SciFinder logo is on the left, and navigation icons (References, Draw, search, star, clock, user) are on the right. The search query is "Monarch Butterfly" or "D". Below the search bar, there's a "Return to Home" link. A message box says "Based on your query, we've returned the most relevant results. Would you like to load the entire result set? Learn about result relevance. Load More Results". A filter section titled "Filter by" has a "Document Type" dropdown with options: Journal (215), Patent (2), Review (9), Conference (7), Dissertation (4), Letter (1). The main results section is titled "References (228)" with "Sort: Relevance" and "View: Partial Abstract". Below this are buttons for "Substances", "Reactions", "Cited By", and "Save". The first result is "Milkweeds, monarch butterflies and the ecological significance of cardenolides" by Malcolm, Stephen B. (1995), with a snippet mentioning 139 references and the role of cardenolides in monarch butterfly defense.

Click [here](#) to get back to the research area overview slide.

Which substances from Milkweed protect the Monarch Butterfly against parasites?

Substances (253) Sort: Relevance View Partial

Filter by

- Commercial Availability
 - Available (162)
 - Not Available (91)
- Reaction Role
 - Product (144)
 - Reactant (115)
 - Reagent (75)
 - Catalyst (56)
 - Solvent (39)
- Reference Role
 - Adverse Effect (140)
 - Analytical Study (161)

1 29565-36-4
Absolute stereochemistry shown
 $C_{23}H_{34}O_2$
Cardenolide

2 71-63-6
Absolute stereochemistry shown

3 143-62-4
Absolute stereochemistry shown

Substances are ranked according to the relevance of the references – in this case, Cardenolide is displayed first

Click [here](#) to get back to the research area overview slide.

Do proteins play a role in the defense mechanism? I

The screenshot displays the SciFinder search results page. The search query is "Monarch Butterfly" or "Danaus Plexippus" and "Milkweed". The left sidebar contains filters for Document Type, Language, and Publication Year. The main content area shows three search results:

- Result 1:** "Milkweeds, monarch butterflies and the ecological significance of cardenolides" by Malcolm, Stephen B. (1995). Abstract: A review with 139 references. The contribution of Miriam Rothschild to the "monarch cardenolide story" is reviewed in the light of the 1914 challenge by the evolutionary biologist, E. B. Poulton for North American chemists to explain the chem. basis of unpalatability in monarch butterflies and their milkweed host plants. This challenge had lain unaccepted for nearly 50 yr until Miriam Rothschild took up the gauntlet and showed with the help of many able colleagues that monarchs are aposematically colored because they sequester toxic cardenolides from milkweed host plants for use as a defense.
- Result 2:** "Cardenolide fingerprint of monarch butterflies reared on common milkweed, *Asclepias syriaca* L." by Malcolm, Stephen B.; Cockrell, Barbara J.; Brower, Lincoln P. (1989). Abstract: Monarch butterfly, *Danaus plexippus*, larvae were collected during August 1983 from the common milkweed, *A. syriaca*, across its extensive North American range from North Dakota, east to Vermont, and south to Virginia. This confirms that the late summer distribution of breeding monarchs in eastern North America coincides with the range of this extremely abundant milkweed resource. Plant cardenolide concentrations, assayed by spectrophotometry in 158 samples from 27 collection sites, were biased towards plants with low cardenolide, and ranged from 4 to 229 µg/0.1 g dry weight, with a mean of 50 µg.
- Result 3:** "Plant-determined variation in the cardenolide content, thin-layer chromatography profiles, and emetic potency of monarch butterflies, *Danaus plexippus* reared on the milkweed, *Asclepias eriocarpa* in California" by Brower, L. P.; Seiber, J. N.; Nelson, C. J.; Lynch, S. P.; Tuskes, P. M. (1982). Abstract: TLC profiles of cardenolides were analyzed for individual plant-butterfly pairs; total cardenolide content was determined by

Review the Concepts to find relevant Substance Classes.

Click [here](#) to get back to the research area overview slide.

Do proteins play a role in the defense mechanism? II

The screenshot displays the SciFinder search interface. At the top, there are three tabs: 'Top Count', 'Alphanumeric', and 'Search'. A red dot points to the 'Search' tab with a callout box that says: "Use the „Search“ option to find relevant concepts quickly." Below the tabs is a list of concepts with checkboxes. A second callout box points to a '7 Selected' indicator, stating: "SciFinderⁿ remembers what was selected". Below this, a list of selected concepts is shown with checkboxes: Bacterial proteins (4), CLOCK Proteins (1), Hemolysin Proteins (4), insecticidal crystal protein, Bacillus Thuringiensis (4), Insect Proteins (2), Proteins (3), Protein sequences (4), and Peptide Hydrolases (1). A third callout box points to a 'Search' button in the 'Concept Name' field, which contains the text 'Protein'. Another 'Search' button is visible below it, next to the 'Concept Name' field containing 'Peptides'.

Click [here](#) to get back to the research area overview slide.

Do proteins play a role in the defense mechanism? III

The screenshot shows the SciFinder search results page. The search query is "Monarch Butterfly" or "Danaus Plexippus" and "Milkweed". The results are sorted by Relevance and show 15 references. The first reference is titled "Stepwise evolution of resistance to toxic cardenolides via genetic substitutions in the Na⁺/K⁺-ATPase of milkweed butterflies (Lepidoptera: Danaini)" by Petschenka, Georg; Fandrich, Steffi; Sander, Nils; Wagschal, Vera; Bopppe, Michael; Dobler, Susanne. The abstract mentions that monarchs are largely insensitive to cardenolides due to amino acid substitutions in the sodium pump (Na⁺/K⁺-ATPase). The second reference is titled "Community-wide convergent evolution in insect adaptation to toxic cardenolides by substitutions in the Na,K-ATPase" by Dobler, Susanne; Dalla, Safaa; Wagschal, Vera; Agrawal, Anurag A. The abstract discusses the extent of convergent molecular evolution and the role of the sodium pump in insect adaptation to cardenolides.

Unlike most other animal species, monarchs are largely insensitive to cardenolides, because their target site, the sodium pump (Na⁺/K⁺-ATPase), has evolved amino acid substitutions, that reduce cardenolide binding (so-called target site insensitivity, TSI)

Click [here](#) to get back to the research area overview slide.

What is known about the sodium-potassium pump ($\text{Na}^+/\text{K}^+-\text{ATPase}$) of *Danaus Plexippus*

Note: Limiting the search to this exact phrase („“) will be very specific, but not comprehensive

Retrieve the substances to find the protein

The screenshot shows the SciFinder interface with a search query: "sodium pump (Na+/K+-ATPase)" of "Danaus Plexippus". The search results are displayed in a list format, showing two entries:

- 1**
Community-wide convergent evolution in insect adaptation to toxic cardenolides by substitutions in the Na,K-ATPase
By: Dobler, Susanne; Dalla, Safaa; Wagschal, Vera; Agrawal, Anurag A.
Proceedings of the National Academy of Sciences of the United States of America (2012), 109(32), 13040-13045, S13040/1-S13040/3 | Language: English, Database: CAlplus
The extent of convergent mol. evolution is largely unknown, yet is critical to understanding the genetics of adaptation. Target site insensitivity to cardenolides is a prime candidate for studying mol. convergence because herbivores in 6 orders of insects have specialized on these plant poisons, which gain their toxicity by blocking an essential transmembrane carrier, the **sodium pump (Na, K-ATPase)**. We investigated gene sequences of the Na,K-ATPase α -subunit in 18 insects feeding on cardenolide-containing plants (spanning 15 genera and 4 orders) to screen for amino acid substitutions that might...

Below the first entry, there are filters for Substances (51), Reactions (0), Cited By (105), and Citation Map.

- 2**
Stepwise evolution of resistance to toxic cardenolides via genetic substitutions in the Na+/K+-ATPase of milkweed butterflies (Lepidoptera: Danaini)
By: Petschenka, Georg; Fandrich, Steffi; Sander, Nils; Wagschal, Vera; Boppre, Michael; Dobler, Susanne
Evolution (Hoboken, NJ, United States) (2013), 67(9), 2753-2761 | Language: English, Database: CAlplus
Despite the **monarch butterfly (Danaus plexippus)** being famous for its adaptations to the defensive traits of its milkweed host plants, little is known about the macroevolution of these traits. Unlike most other animal species, monarchs are largely...



Click [here](#) to get back to the research area overview slide.

What is known about the sodium-potassium pump (Na^+/K^+ -ATPase) of *Danaus Plexippus*

The screenshot displays the SciFinder search results page. The search query is 'Substances'. The results are sorted by Relevance and are displayed in a grid of 6 items. A filter on the left side is set to 'Substance Class', which is highlighted with a red arrow. The results include chemical structures for L-Glutamine and (-)-Asparagine, and protein/peptide sequences for Cytochrome oxidase subunit 1 from *Liriomyza SD-2012* mitochondria.

Item ID	Chemical Name	References	Reactions	Suppliers
56-85-9	L-Glutamine	76K	1,386	169
70-47-3	(-)-Asparagine	36K	1,316	95
9000-83-3	Unspecified Adenosine triphosphatase	93K	23	11
1418079-56-7	Unspecified Cytochrome oxidase (Liriomyza SD-2012 mitochondria gene COI subunit 1)			
1418079-55-6	Unspecified DNA (Liriomyza SD-2012 mitochondria gene COI cytochrome oxidase subunit 1)			
1418079-54-5	Unspecified Cytochrome oxidase (Liriomyza asclepiadis mitochondria gene COI subunit 1)			

Click [here](#) to get back to the research area overview slide.

What is known about the sodium-potassium pump (Na⁺/K⁺-ATPase) of Danaus Plexippus

Click on the CAS Registry Number to display detailed substance information

9
1418079-28-3
Image Not Available
Unspecified
Sodium-potassium pump (Danaus plexippus gene Na⁺/K⁺ ATPase α -subunit)
Protein/Peptide Sequence
Sequence Length: 717
1 Reference 0 Reactions 0 Suppliers

Click on the „References“ button to retrieve references mentioning the substance.

Substance Detail (9)
Reference (1)
CAS Registry Number
1418079-28-3
Image Not Available
Unspecified
Sodium-potassium pump (Danaus plexippus gene Na⁺/K⁺ ATPase α -subunit)
Protein/Peptide Sequence
Sequence Length: 717
Other Names
3 Other Names for this Substance
GenBank CQ05450
GenBank CQ05450 (Translated from: GenBank HE956755)
Na⁺/K⁺ ATPase (Danaus plexippus gene Na⁺/K⁺ ATPase α -subunit)
Sequence Details
Sequence: linear
1 LFGGFALLLM IGATLCFIAY GIVASTVEEP SDDHLVLTGV LAAVVIVTGT
51 FSYVQESKSS KINESFKNMV POFATVIREG EKLTIRAEDL VLDGVVEVKF
101 GDRPADIRI IEARGKVDN SSLTGESERQ SRGPEFTNEN PLETKNLAFF
151 STNAVEGTAK GIVICCGDNT VNGRZAGLAS GLDTGETPIA KEIHFTHLE
201 TOAVFLQVT FFTIAFILGY HMDAVFLI GITVANPEG LLATVTVCLT
251 LTAIRMASKN CLVKNLEAVE TLGSTSTICS DKYGTLTQNR MIVAMPFDN
References
351 EVAGDASEAA LLKCMELALG DVL SIRKRNK KVCEIPFNST NKYQVSIHES
401 DOPSDPRHLL VMKGAPERIL ERCSTIFIGG KEKVLDEEMK EAFNNAYLEL
451 GGLGERVLGF CDLQLPSDKY PIGYKFNDD PNFPLDNLRF VGLMSIDPP
501 RAAVPOAVAK CRSAGIKVIM VTGDHPITAK ATIAKSVGIIS EGNETVEDIA
551 ARLNIPVSEV NPREAKAAVW HGTDLRLNS DQLDEILKFH TEIVFARTSP
601 QQKLIIVEGC QRLGAIIVAVT GOGVNDSPAL KKADIGVAMG IAGSDVSKQA
Additional Details
Document Types
Journal
Source of Registration
GenBank
Substance Classes
Manual Registration, Protein Peptide Sequence

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Click [here](#) to get back to the research area overview slide.

One reference and its landscape – Citation Map I

References (1) View: Partial Abstract ▾

Substances ▾ Reactions ▾ Cited By ▾ Save

1

Community-wide convergent evolution in insect adaptation to toxic cardenolides by substitutions in the Na,K-ATPase

By: Dobler, Susanne; Dalla, Safaa; Wagschal, Vera; Agrawal, Anurag A.
Proceedings of the National Academy of Sciences of the United States of America (2012), 109(32), 13040-13045, S13040/1-S13040/3 | Language: English, Database: C4plus

The extent of convergent mol. evolution is largely unknown, yet is critical to understanding the genetics of adaptation. Target site insensitivity to cardenolides is a prime candidate for studying mol. convergence because herbivores in 6 orders of insects have specialized on these plant poisons, which gain their toxicity by blocking an essential transmembrane carrier, the sodium pump (Na,K-ATPase). We investigated gene sequences of the Na,K-ATPase α -subunit in 18 insects feeding on cardenolide-containing plants (spanning 15 genera and 4 orders) to screen for amino acid substitutions that might

[View More ▾](#)

Full Text ▾ Substances (51) Reactions (0) Cited By (105) Citation Map

Click on the „Citation Map“ button to review Cited and Citing References

Click [here](#) to get back to the research area overview slide.

One reference and its landscape – Citation Map II

Citation Map

Community-wide convergent evolution in insect adaptation to toxic cardenolides by substitutions in the Na,K-ATPase

By: Döbler, Susanne; Dalla, Safaa; Wagschal, Vera; Agrawal, Anurag A.
Proceedings of the National Academy of Sciences of the United States of America (2012), 109(32), 13040-13045, S13040/1-S13040/3 | Language: English, Database: CAlplus

Full Text ▾

Abstract: The extent of convergent mol. evolution is largely unknown, yet is critical to understanding the genetics of adaptation. Target site insensitivity to cardenolides is a prime candidate for studying mol. convergence because herbivores in 6 orders of insects have specialized on these plant poisons, which gain their toxicity by blocking an essential transmembrane carrier, the sodium pump (Na,K-ATPase). We investigated gene sequences of the Na,K-ATPase α -subunit in 18 insects feeding on cardenolide-containing plants (spanning 15 genera and 4 orders) to screen for amino acid substitutions that might...

[View More ▾](#)

Filter by

- Document Type
 - Journal (127)
 - Review (23)
 - Commentary (1)
 - Conference (1)
 - Editorial (1)
 - Preprint (1)
- Author
- Concept

References This Document Cites

- MEGAS: Molecular Evolutionary Genetics Analysis Using Maximum Likelihood, Evolutionary Distance, and Maximum Parsimony Methods
Molecular Biology and Evolution (2011)
Cited By 30K [Map](#)
- Insecticide resistance in insect vectors of human disease
Annual Review of Entomology (2000)
Cited By 757 [Map](#)
- A Single Amino Acid Mutation Contributes to Adaptive Beach Mouse Color Pattern
Science (Washington, DC, United States) (2006)
Cited By 423 [Map](#)
- Structure-function relationships in the sodium-potassium ATPase α subunit: site-directed mutagenesis of glutamine-111 to asparagine and asparagine-122

References Citing This Document

- The genetic causes of convergent evolution
Nature Reviews Genetics (2013)
Citing 307 [Map](#)
- Causes of molecular convergence and parallelism in protein evolution
Nature Reviews Genetics (2016)
Citing 91 [Map](#)
- Experimental interrogation of the path dependence and stochasticity of protein evolution using phage-assisted continuous evolution.
Proceedings of the National Academy of Sciences of the United States of America (2013)
Citing 81 [Map](#)
- Mechanisms and ecological consequences of plant defence induction and suppression in herbivore communities.

Filter Citations
by Concepts

Click [here](#) to get back to the research area overview slide.

One reference and its landscape – Citation Map III

Citation Map

Community-wide convergent evolution in insect adaptation to toxic cardenolides by substitutions in the Na,K-ATPase

By: Dobler, Susanne; Dalla, Safaa; Wagschal, Vera; Agrawal, Anurag A.
Proceedings of the National Academy of Sciences of the United States of America (2012), 109(32), 13040-13045, S13040/1-S13040/3 | Language: English, Database: Caplus

Abstract: The extent of convergent mol. evolution is largely unknown, yet is critical to understanding the genetics of adaptation. Target site insensitivity to cardenolides is a prime candidate for studying mol. convergence because herbivores in 6 orders of insects have specialized on these plant poisons, which gain their toxicity by blocking an essential transmembrane carrier, the sodium pump (Na,K-ATPase). We investigated gene sequences of the Na,K-ATPase α -subunit in 18 insects feeding on cardenolide-containing plants (spanning 15 genera and 4 orders) to screen for amino acid substitutions that might...

View More ▾

Full Text ▾

Concept

Top Count | Alphanumeric

1 Selected

- Molecular evolution (16)
- Animal gene (14)
- Adaptation, animal (12)
- Protein sequences (12)
- Mutation (11)
- Danaus plexippus (10)
- Drosophila melanogaster (10)
- Animals (9)
- Cardenolides (9)
- Sodium-potassium pumps (9)
- Evolution (8)
- Toxins (8)
- Cardiac glycosides (7)
- cDNA sequences (7)
- Genomics (7)
- Larva (7)
- Molecular evolution (16)
- Amino acids (4)
- Asclepias incarnata (4)
- Asclepias syriaca (4)
- Cell membrane (4)
- Convergent evolution (4)
- Evolution, Molecular (4)
- Heart (4)
- Hemolymph (4)
- Herbivory (4)
- Leaf (4)
- Nervous system (4)
- Plants (4)
- Sodium-Potassium-Exchanging ATPase (4)
- Amino Acid Sequence (3)
- Asclepias perennis (3)
- Bufadienolides (3)

Filter by

- Document Type
 - Journal (11)
 - Review (3)
- Author
- Concept
 - Molecular evolution (16)
 - Animal gene (14)
 - Adaptation, animal (12)
 - Protein sequences (12)
 - Mutation (11)

View All

References This Document Cites

- A Single Amino Acid Mutation Contributes to Adaptive Beach Mouse Color Pattern
Science (Washington, DC, United States) (2006)
Cited By 423 [Map](#)
- The molecular and population genetics of cyclodiene insecticide resistance
Insect Biochemistry and Molecular Biology (1994)
Cited By 74 [Map](#)
- Kinetic analysis of ouabain binding to native and mutated forms of sodium-potassium-ATPase and identification of a new region involved in cardiac glycoside interactions
Journal of Biological Chemistry (1993)
Cited By 50 [Map](#)
- Molecular adaptation of *Chrysochus* leaf beetles to toxic compounds in their food plants
Molecular Biology and Evolution (2004)
Cited By 30 [Map](#)

References Citing This Document

- The genetic causes of convergent evolution
Nature Reviews Genetics (2013)
Citing 307 [Map](#)
- Causes of molecular convergence and parallelism in protein evolution
Nature Reviews Genetics (2016)
Citing 91 [Map](#)
- Toxin-resistant isoforms of Na⁺/K⁺-ATPase in snakes do not closely track dietary specialization on toads
Proceedings of the Royal Society B: Biological Sciences (2016)
Citing 6 [Map](#)
- Mutations to the cardiotonic steroid binding site of Na⁺/K⁺-ATPase are associated with high level of resistance to gambufoulin in a natriuretic snake
Toxicon (2016)
Citing 6 [Map](#)
- Contingency in the convergent evolution of a regulatory network: dosage compensation in *Drosophila*
PLoS Biology (2019)
Citing 3 [Map](#)
- Mechanism of Resistance to Camptothecin, a Cytotoxic Plant Secondary Metabolite, by *Lymantria* sp. Larvae

Apply | Cancel

Search Question

The protection mechanism of the Monarch Butterfly against parasites when raised on Milkweed plants

- Which substance in Milkweed (their caterpillar host plant) protects the Monarch Butterfly against parasites? - **Cardenolide**
 - SciFinderⁿ offers more information about the compound of interest: see substance searching for related compounds
 - see substance details for physical properties
- Do proteins play a role in this defense mechanism? – **yes – the sodium pump-potassium (Na⁺/K⁺-ATPase) (of the Monarch Butterfly)**
 - SciFinderⁿ offers more information about many proteins of interest: see substance details and related references
 - SciFinderⁿ offers a structure search for sequences with less than 248 non-H atoms
- What is known about these proteins? – **A specific mutation of the enzyme enables the process**

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org

Click [here](#) to get back to the
research area overview slide.

Biosearching in SciFinderⁿ

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org



SCIFINDERⁿ
A CAS SOLUTION

Biochemistry Searching in SciFinderⁿ



Click [here](#) to get back to the research area overview slide.

Search Question

- Look for publications discussing the biosynthetic preparation of vanillin and close derivatives by *Streptomyces* bacteria
- Identify a typical starting material and investigate its possible biosyntheses including reaction pathways and used bacteria

Click [here](#) to get back to the research area overview slide.

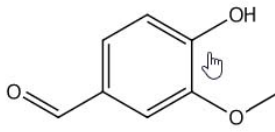
Search vanillin and prepare structure search

Substances ▾ Vanillin

Search for vanillin to use its structure for the derivative search

1

121-33-5



$C_8H_8O_3$
Vanillin

37K References 14K Reactions 131 Suppliers

Click on the structure to open the flyout window

CAS RN
121-33-5
CAS Name
Vanillin

Substance Detail

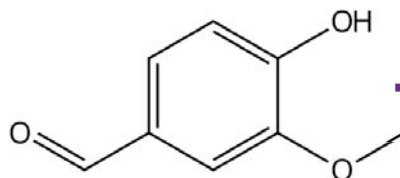
Reactions (14K)

Synthesize (1,309)

Create Retrosynthesis Plan

References (37K)

Suppliers (131)

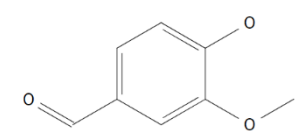


Edit Structure - Reset + ↕

Edit Structure

CAS Draw

Draw or change atoms or bonds



OK Cancel

Click OK to go back to the main interface

Click [here](#) to get back to the research area overview slide.

Search for 'fermentation' and the structure simultaneously

The screenshot shows the SciFinder search interface. At the top, there is a search bar with 'fermentation' entered and a search icon. Below the search bar, there is a 'Substances (1)' section with a chemical structure overlay. The structure is a benzene ring with a methoxy group (-OCH3) at the 3-position and an aldehyde group (-CHO) at the 4-position. Below the structure, there are buttons for 'Edit Drawing' and 'Remove'. To the left of the structure, there are buttons for 'References', 'Reactions', and 'Suppliers'. Below the structure, there is a 'References (3,476)' section with a 'Sort: Relevance' and 'View: Full Abstract' dropdown. The first result is titled 'Biotechnological production of vanillin' by Priefert, H.; Rabenhorst, J.; Steinbuchel, A. The abstract text is visible. Below the abstract, there are buttons for 'Full Text', 'Substance (1)', 'Reactions (0)', 'Cited By (384)', and 'Citation Map'. On the left side, there is a 'Structure Match' section with 'As Drawn (1,356)' and 'Substructure (3,476)' options. Below that, there is a 'Filter by' section with 'Document Type' filters: Journal (2,420), Patent (1,029), Review (50), Clinical Trial (2), and Conference (25). A red arrow points from the 'Substructure (3,476)' option to the 'References (3,476)' section.

A simultaneous text and structure search will be performed

As Drawn and Substructure results sets are created at the same time

The relevance algorithm brings suitable hit documents to the top of the result set



Click [here](#) to get back to the research area overview slide.

Limit to documents describing preparations of vanillin and focus on *Streptomyces* as biotechnologically used genus of bacteria

Substance Role

- Adverse Effect (17)
- Analytical Study (199)
- Biological Study (2,712)
- Formation (58)
- Miscellaneous (2)
- Preparation (777)

[View All](#)

Concept

- Fermentation (505)
- Microbial gene (105)
- Escherichia coli (88)
- Saccharomyces cerevisiae (76)
- Culture media (75)

[View All](#)

Substance roles allow us to limit to prepared vanillin derivatives

,View all' opens the concepts detail page

Concept

Top Count | Alphanumeric | Search

Concept Name

Streptomyces

34 Selected

We select all *Streptomyces* species in the 'Search' facet of the concept filter

<input checked="" type="checkbox"/> Streptomyces (38)	<input checked="" type="checkbox"/> Streptomyces filipinensis (1)	<input checked="" type="checkbox"/> Streptomyces psammoticus (2)
<input checked="" type="checkbox"/> Streptomyces achromogenes tomaymyceticus (2)	<input checked="" type="checkbox"/> Streptomyces griseovariabilis (1)	<input checked="" type="checkbox"/> Streptomyces roseochromogenes (1)
<input checked="" type="checkbox"/> Streptomyces albus (4)	<input checked="" type="checkbox"/> Streptomyces griseus (12)	<input checked="" type="checkbox"/> Streptomyces roseolus (3)
<input checked="" type="checkbox"/> Streptomyces antibioticus (1)	<input checked="" type="checkbox"/> Streptomyces halstedii (1)	<input checked="" type="checkbox"/> Streptomyces sakaiensis (1)
<input checked="" type="checkbox"/> Streptomyces aureus (1)	<input checked="" type="checkbox"/> Streptomyces hygrosopicus (1)	<input checked="" type="checkbox"/> Streptomyces sannanensis (4)
<input checked="" type="checkbox"/> Streptomyces bingchengensis (1)	<input checked="" type="checkbox"/> Streptomyces lavendulae (1)	<input checked="" type="checkbox"/> Streptomyces tendae (1)
<input checked="" type="checkbox"/> Streptomyces carzinostaticus neocarzinostaticus (1)	<input checked="" type="checkbox"/> Streptomyces lividans (1)	<input checked="" type="checkbox"/> Streptomyces threomyceticus (1)
<input checked="" type="checkbox"/> Streptomyces clavuligerus (1)	<input checked="" type="checkbox"/> Streptomyces morookaensis (1)	<input checked="" type="checkbox"/> Streptomyces varius (1)
<input checked="" type="checkbox"/> Streptomyces coelicolor (3)	<input checked="" type="checkbox"/> Streptomyces peucetius (2)	<input checked="" type="checkbox"/> Streptomyces violaceusniger (1)
<input checked="" type="checkbox"/> Streptomyces cvaneogriseus	<input checked="" type="checkbox"/> Streptomyces phage ϕ C31 (2)	

Click [here](#) to get back to the research area overview slide.

Ferulic acid appears as starting material in several reactions

Substances Reactions Cited By

Get Reactions from Reference

1

Towards a
By: Muheim, A.

All Results Selected Results

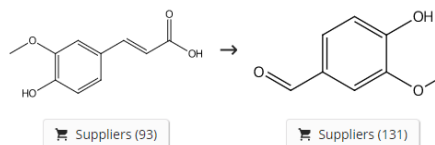
Easily move to the indexed reactions for all retrieved documents

Reaction Notes

- Biotransformation (69)
- Fermentation (43)
- Regioselective (23)
- Enzymic (21)
- Solid State (1)
- Solid-Supported Catalyst (1)

Reaction Notes facilitate finding relevant biotransformation or fermentation preparation methods

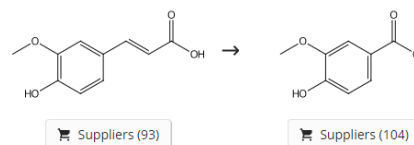
Scheme 2 (4 Reactions) Steps: 1 Yield: 75-81%



A reaction scheme contains reactions with identical reactants and products.

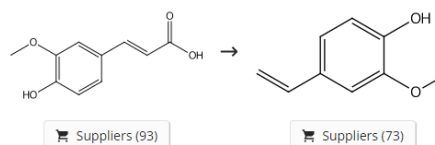
Expand Scheme

Scheme 4 (1 Reaction) Steps: 2



Expand Scheme

Scheme 31 (1 Reaction) Steps: 1



Expand Scheme

Click [here](#) to get back to the research area overview slide.

We can limit to specific journals with a biochemical focus and check the reaction summaries

- ^ Publication Name
- ChemBioChem (117)
 - Germany (42)
 - Chemistry & Biology (Cambridge, MA, United States) (14)
 - World Intellectual Property Organization (8)
 - Journal of the American Chemical Society (6)
 - Journal of Industrial Microbiology & Biotechnology (3)
 - Enzyme and Microbial Technology (2)
 - Applied and Environmental Microbiology (1)
 - Asian Journal of Microbiology, Biotechnology & Environmental Sciences (1)

Scheme 3 (1 Reaction) Steps: 1

Suppliers (93) Suppliers (104) Suppliers (131)

<input type="checkbox"/> Reaction Summary	Steps: 1	Microbial transformation of ferulic acid to vanillic acid by <i>Streptomyces sannanensis</i> MTCC 6637
1.1 Reagents: Ammonium nitrate, Sulfuric acid magnesium salt (1:1), Disodium phosphate, Sodium chloride, Monopotassium phosphate, Calcium chloride Solvents: Water; 20 d, pH 7.0, 28 °C		Enzyme and Microbial Technology (2007),
View Reaction Detail Experimental Protocols		

Colla

We can eye-screen reagents, catalysts, solvents and conditions with the reaction summaries

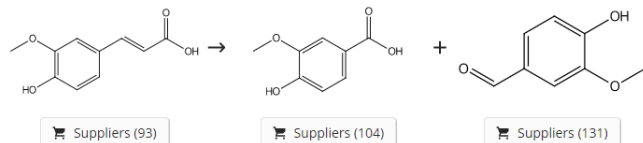
Open the Reaction Detail or Experimental protocols to access the detailed procedure



Click [here](#) to get back to the research area overview slide.

The reaction details contain the experimental protocol, which can be downloaded easily

Reaction Detail (Scheme 3, Reaction 1 of 1)



Step 1

Alternative Steps (5)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Ammonium nitrate Sulfuric acid magnesium salt (1:1) Disodium phosphate Sodium chloride Monopotassium phosphate Calcium chloride	-	Water	20 d, pH 7.0, 28 °C

CAS Reaction Number: 31-486-CAS-14011965

Notes

biotransformation, described medium, whole cell suspension of *Streptomyces sannanensis* MTCC6637 used, alternate reaction with crude cell extract of *Streptomyces sannanensis* MTCC6637 shown

Experimental Protocols

MethodsNow™ Experimental Procedure

Products	Vanillin Vanillic acid
Reactants	Ferulic acid
Reagents	Ammonium nitrate Sulfuric acid magnesium salt (1:1) Disodium phosphate Sodium chloride Monopotassium phosphate Calcium chloride

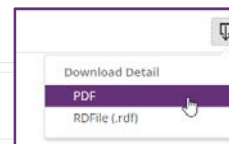
Solvents Water

Procedure

1. Prepare the minimal medium by the addition of basal inorganic salts, NH_4NO_3 (3.0 g/l) as a nitrogen source, $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ (0.2 g/l), NaCl (0.2 g/l), KH_2PO_4 (1.0 g/l), Na_2HPO_4 (4.0 g/l) and CaCl_2 (0.05 g/l).
2. Adjust the pH of the medium to 7.0.
3. Filter all the carbon sources sterilized through 0.2 μm nylon filter.
4. Add the mixture to minimal medium.
5. After growth on arginine glycerol salt broth for 7 days, transfer 1 ml cell suspension of *S. sannanensis* aseptically into 100 ml flask containing 25 ml of minimal medium with ferulic acid as a sole carbon source.
6. Carry out the microbial transformation.
7. Incubate the mixture for interval.
8. Repeat the procedure at least twice.

Transformation Ozonolysis

CAS Method Number 3-486-CAS-14011965



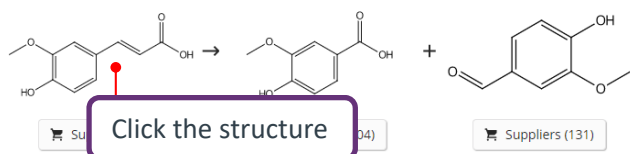
Download the details including the preparation

A step-by-step procedure is extracted from the journal or the supplement

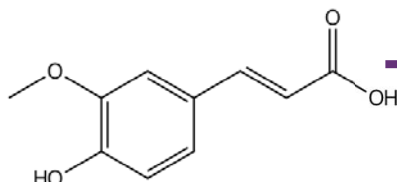
Click [here](#) to get back to the research area overview slide.

Can we also identify biotransformations to prepare ferulic acid?

Reaction Detail (Scheme 3, Reaction 1 of 1)



CAS RN
1135-24-6
CAS Name
Ferulic acid



Substance Detail
Reactions (2,099)
Synthesize (189)
Create Retrosynthesis Plan
References (27K)
Suppliers (93)

Edit Structure - Reset +

Reaction Notes

By Count Alphanumeric

2 Selected

- Biotransformation (54)
- Enzymic (42)
- Regioselective (14)
- Microwave Irradiation (9)
- Green Chemistry (8)
- Fermentation (6)
- Solid-Supported Catalyst (6)

Apply

Cancel

Restrict to appropriate reactions

Reactions (54)

References

Get References for Reactions

All Results

Selected Results

Move to bibliographic results



Click [here](#) to get back to the research area overview slide.

Concepts help us understand which bacteria play a role in biotransformations to produce ferulic acid

Concept

Top Count | Alphanumeric

3 Selected

- Fermentation (9)
- Pseudomonas, Streptomyces and Escherichia genera appear frequently
- Michaelis constant (4)
- Pseudomonas (4)
- Saccharomyces cerevisiae (4)
- Streptomyces griseus (4)
- Escherichia coli (3)

References (7)

Substances Reactions

1

[Highly efficient biotransformation of vanillin in recombinant strains of E. coli](#)

By: Overhage, Joerg; Steinbuechel, Alexander; Priefert, Horst

Abstract: The vaoA gene from Penicillium simplicissimum CBS 170.90, encoding vanillyl alc. oxidase, which also catalyzes the conversion of eugenol to coniferyl alc., was expressed in Escherichia coli XL1-Blue under the control of the lac promoter, together with the genes calA and calB, encoding coniferyl alc. dehydrogenase and coniferyl aldehyde dehydrogenase of Pseudomonas sp. strain HR199, resp. Resting cells of the corresponding recombinant strain E. coli XL1-Blue(pSKvaomPcalAmcalB) converted eugenol to ferulic acid with a molar yield of 91% within 15 h on a 50-mL scale, reaching a ferulic acid concentration of 8.6 g liter⁻¹. This biotransformation was scaled up to a 30-L fermentation volume. The maximum production rate for ferulic acid at that scale was 14.4 mmol per h per L of culture. The maximum concentration of ferulic acid obtained was 14.7 g liter⁻¹ after a total fermentation time of 30 h, which corresponded to a molar yield of 93.3% with respect to the added eugenol. For the establishment of a continuous culture of E. coli XL1-Blue(pSKvaomPcalAmcalB) was used to produce ferulic acid to vanillin (J. Overhage, H. Priefert, and H. Steinbuechel, Appl. Environ. Microbiol. 65:4837-4847, 1999). This process led to 0.3 g vanillin liter⁻¹, besides 0.1 g of vanillyl alcohol liter⁻¹ in a 30-L fed-batch culture. The genes ehyA and ehyB of Pseudomonas sp. strain HR199, and azuA and azuB of Escherichia coli XL1-Blue(pSKvaomPcalAmcalB) were shown to be unsuitable for establishing eugenol bioconversion in a fed-batch culture.

Full Text

Full Text

Expand All | Collapse All

Concepts

- DNA sequences
- Escherichia coli
- Fed-batch fermentation
- Microbial gene
- Modifier: vaoA
- Role: Biological Study, Unclassified
- Molecular cloning

Pseudomonas, Streptomyces and Escherichia genera appear frequently

CTRL+click to open the detailed record in a new tab

The transformation of eugenol to ferulic acid in a fed-batch culture is described

Your SciFinderⁿ team

Team contact:
kfaerber@acs-i.org

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research area overview slide.

Biochemistry Searching in SciFinderⁿ