



Cancer-Fighting Super Condiment

SciFinder®

Amy Christuk, Account Consultant®

ACS Fall 2010 National Meeting & Exposition

August 22-26, 2010

Boston, MA



SciFinder®

Let's be frank, baseball fans love their hot dogs

- 21,378,064 hot dogs served at Major League Baseball stadiums
- Equivalent of 29,691 times round the bases



Fenway Park is the top dog



Dress it up with yellow mustard

Basic Ingredients

- Mustard seed
- Water
- Vinegar or other liquids
- Other flavorings and spices



The spice in the classic yellow mustard is turmeric



SciFinder[®] supports the complete user experience

- Making your research easier to perform
- Helping you find information that is more responsive to your true intent
- Providing more relevant ways to view and digest your answers



SciFinder provides new options for locating (patent) references

SciFinder - Substance Answer Set - Mozilla Firefox

Substance Identifier "curcumin" > substances (1) > 458-37-7

Substances [Get References](#) [Get Reactions](#) [Get Commercial Sources](#) [Combine Answer Sets](#)

1 Substance 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number ↓

Answers per Page [15] View: [Icons]

1. Substance Detail
458-37-7

Double bond geometry as shown.

C₂₁ H₂₀ O₆

1,6-Heptadiene-3,5-dione, 1,7-bis(4-hydroxy-3-methoxyphenyl)-, (1E,6E)-

~5,610 References
Reactions
Commercial Sources
Regulatory Information
Link

Analysis [Refine](#)

Analyze by: [Substance Role](#)

Click bar to view only those substances within the current answer set

Analytical Study	1
Biological Study	1
Formation, Nonpreparative	1
Miscellaneous	1
Occurrence	1
Preparation	1
Process	1
Properties	1
Prophetic in Patents	1
Reactant or Reagent	1

Show More

Markush is part of Explore Substances

The screenshot shows the SciFinder web interface in a Mozilla Firefox browser window. The page title is "SciFinder - Explore Substances". The navigation bar includes "Explore References", "Explore Substances", and "Explore Reactions". A user is logged in as Jason Anderson. The breadcrumb trail is "Substance Identifier 'curcumin' > substances (1) > 458-37-7".

The main content area is titled "Explore Substances" and features a search interface. On the left, there is a sidebar with search options: "Chemical Structure", "Markush" (highlighted with a red arrow and a "NEW" badge), "Molecular Formula", and "Substance Identifier". The "Markush" option is selected, and a chemical structure of curcumin is displayed in the center. Below the structure, there is a "Search" button and search type options: "Substructure" (selected) and "Allow variability only as specified".

On the right side of the interface, there are three panels: "Saved Answer Sets" (with options "save" and "View All", and an "Import" button), "Keep Me Posted Results" (with "No profiles exist"), and "My Connections" (with "No invitations to connect", "No outstanding sent invitations", and "No connection with colleagues").

At the bottom of the page, there is a footer with "Contact Us | Copyrights and Trademarks" and "Copyright © 2010 American Chemical Society. All Rights Reserved."

Markush searches enable preliminary IP assessment

The screenshot displays the SciFinder Reference Answer Set interface in Mozilla Firefox. The search query is 'Markush substructure' with 101 references found. The interface includes navigation tools like 'Get Substances', 'Get Reactions', 'Get Cited', 'Get Citing', 'Get Full Text', and 'Combine Answer Sets'. The results are sorted by 'Accession Number' and displayed in a list format. The first three references are:

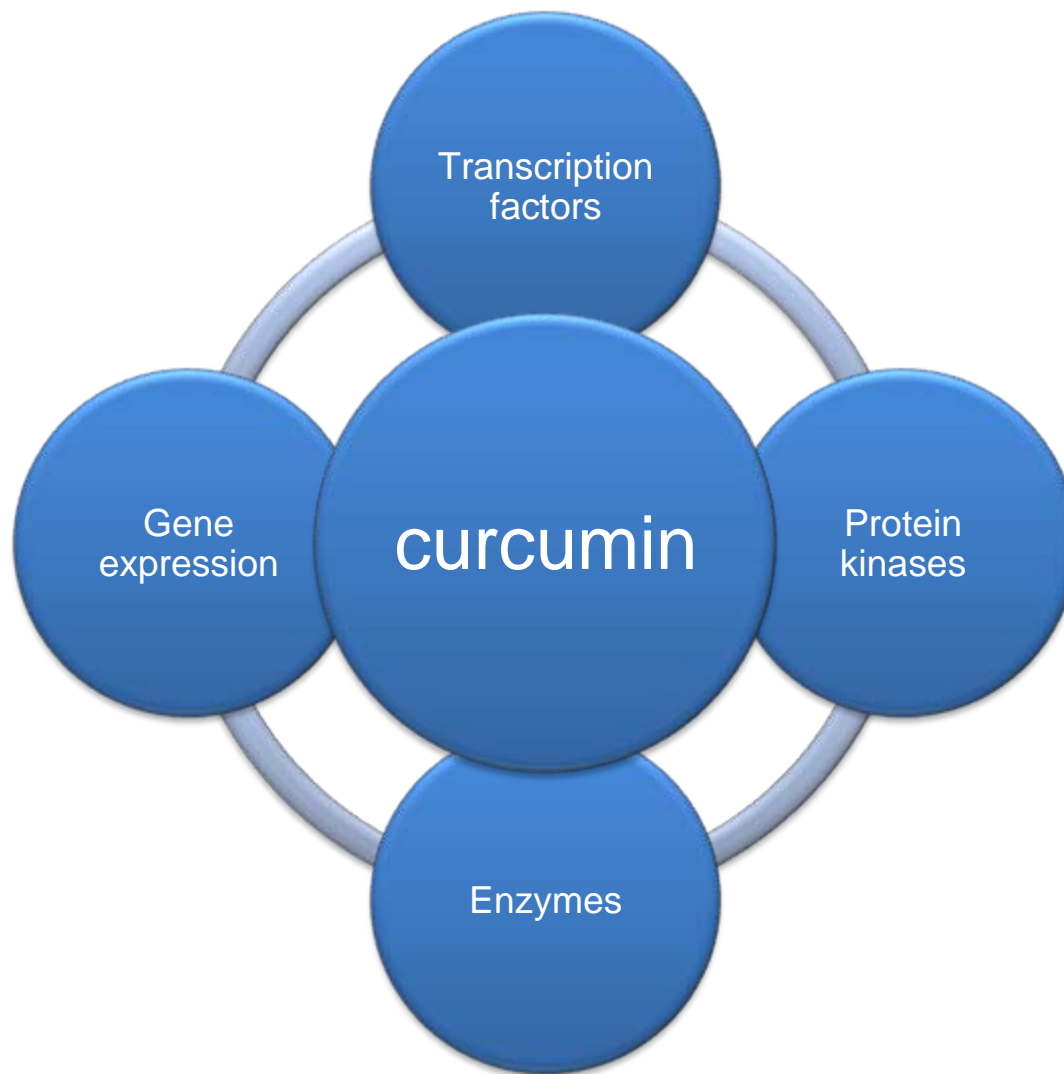
- 1. Curcumin analog compositions and related methods**
By Chen, Danyang
From PCT Int. Appl. (2010), WO 2010045395 A2 20100422. Language: English, Database: CAPLUS
Novel curcumin-analog compds. are disclosed that are antioxidants useful in inhibition of pro-inflammation, angiogenic, and vascular permeability factors and elimination of reactive oxygen species. The curcumin compds. specifically inhibit VEGF and are useful in treating various diseases that are mediated through the oxidative stress pathway, including those that are characterized by inflammation, angiogenesis, or vascular leakage.
+Substances ▲Reactions fCiting DFull Text 🔗Link 0 Comments 0 Tags
- 2. Method for preparation of long acting curcumin derivative and pharmaceutical application**
By Ku, Baoshan; Zhou, Weidong; Yu, Fenghua; Yao, Haiyan; Yao, Guangyin
From PCT Int. Appl. (2010), WO 2010025589 A1 20100311. Language: Chinese, Database: CAPLUS
A long acting curcumin deriv., its prepn. method, and pharmaceutical application is disclosed. The claimed long acting curcumin deriv. is shown in structure I (R1,R2 = H or MeO; R3,R4 = C1-50 alkyl or aryl). The claimed compd. was prepd. from curcuminoids via esterification with fatty acid, or salicylic acid, or the corresponding acyl chloride to provide the title product. The obtained delayed release effect of curcumin deriv. has better pharmaceutical effect than curcuminoids on the treatment of depression and cancer.
+Substances ▲Reactions fCiting DFull Text 🔗Link 0 Comments 0 Tags
- 3. Difluoroboron curcumin derivatives for amyloid-β plaque imaging in Alzheimer's disease diagnosis**
By Chongzhao, Ran; Moore, Anna
From PCT Int. Appl. (2010), WO 2010017094 A2 20100211. Language: English, Database: CAPLUS
The present invention provides curcumin-derived near IR (NIR) imaging probes. Upon interacting with amyloid β aggregates, these probes undergo a range of changes, qualifying them as "smart" probes. The inventors have demonstrated that probes of the invention have the capacity to monitor the progression of Alzheimer's disease in an in vivo animal model. In addn., the present invention encompasses probes useful as PET imaging agents, MRI imaging agents and multimodal imaging agents, as well as related methods of detecting and imaging amyloid β aggregates and plaques.
+Substances ▲Reactions fCiting DFull Text 🔗Link 0 Comments 0 Tags

The right sidebar shows an 'Analysis' section with a 'Refine' tab. The 'Analyze by:' dropdown is set to 'Author Name'. A table lists authors and their corresponding number of references:

Author Name	Count
Snow Alan D	6
Castillo Gerardo M	4
Kim Darrick S H L	4
Osawa Toshihiko	4
Sakai Yasushi	4
Cummings Joel	3
Kono Yasuhiro	3
Lake Thomas P	3
Larsen Lesley	3
Nguyen Beth P	3

A 'Show More' button is located at the bottom of the analysis sidebar.

Curcumin slows cancer growth



High-value patent information is complementary to CAS REGISTRYSM

SciFinder - Curcumin analog... - Mozilla Firefox

SciFinder - Curcumin analog...

Reference Detail [Get Substances](#) [Get Reactions](#) [Get Cited](#) [Get Citing](#) [Get Full Text](#)

Link Save Print Export

Return [Previous](#) | [Next](#)

1. Curcumin analog compositions and related methods

By: Chen, Danyang
Assignee: USA

Novel curcumin-analog compds. are disclosed that are antioxidants useful in inhibition of pro-inflammation, angiogenic, and vascular permeability factors and elimination of reactive oxygen species. The curcumin compds. specifically inhibit VEGF and are useful in treating various diseases that are mediated through the oxidative stress pathway, including those that are characterized by inflammation, angiogenesis, or vascular leakage.

Patent Information

Patent No.	Kind	Date	Application No.	Date
WO 2010045395	A2	Apr 22, 2010	WO 2009-US60726	Oct 14, 2009

Priority Application

US 2008-105284P	P	Oct 14, 2008
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Indexing

Pharmacology (Section 1-6) [ⓘ](#)

Section cross-reference(s): 26, 63

Concepts [ⓘ](#)

Angiogenesis inhibitors Antioxidants

Substances [ⓘ](#)

458-37-7DP Curcumin analogs

Quick Links

0 Tags, 0 Comments

Patent Information

Apr 22, 2010
WO 2010045395
A2

Application

Oct 14, 2009
WO 2009-US60726

Priority

Oct 14, 2008
US 2008-105284

Source

PCT Int. Appl.
31pp.
Patent
2010
CODEN: PIXXD2

Accession Number

2010:503879
CAN 152:470400
CAPLUS

Get Similar Reactions evaluates similar reactions and synthetic strategies

SciFinder - Reaction Answer Set - Mozilla Firefox

2. Reaction Detail [Link](#) [Similar Reactions](#)

Get Similar Reactions

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (4215)
- Medium - Reaction centers plus adjacent atoms and bonds (25)
- Narrow - Reaction centers plus extended atoms and bonds (10)

Get Reactions Cancel

R: N₂H₄, S: AcOH, 6 h.

NOTE: Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1

Curcumin analog compositions and related methods
By Chen, Danyang
From PCT Int. Appl., 2010045395, 22 Apr 2010

Enhanced reactions display shows similar transformations and highlighted relevant atoms/bonds

The screenshot displays the SciFinder web interface for a reaction set. The browser window title is "SciFinder - Reaction Answer Set - Mozilla Firefox". The address bar shows the path: "Create Keep Me Posted > Markush substructure > references (101) > get reactions (3) > similar reactions (25)".

The main content area shows a list of reactions. The first reaction is selected and expanded to show details. The reaction is: O=C(C=Cc1ccc(O)cc1OS(=O)(=O)N)C(=O)C=Cc2ccc(O)cc2OS(=O)(=O)N.NN>>O=C(C=Cc1ccc(O)cc1OS(=O)(=O)N)C1=NC=C(C=Cc2ccc(O)cc2OS(=O)(=O)N)N1. The reaction conditions are "s: AcOH, 6 h, 85 °C".

The reaction is displayed with a red box highlighting the atoms and bonds that are transformed during the reaction. A red arrow points to the carbonyl carbon of the starting material, which becomes the C4 position of the imidazole ring in the product. The text "Double bond geometry as shown." is present below both the starting material and the product.

On the right side of the interface, there is an "Analysis" panel with a "Refine" button. The "Analyze by:" dropdown is set to "Catalyst". Below this, a "Click bar" is shown with "ACOH" selected and a count of "4". A "Show More" button is located at the bottom of the panel.

It's also in the seeds



Selenium starves cancer cells?

SciFinder - Relationship of... - Mozilla Firefox

Research Topic "cancer prevention with seleniu..." > references (41) > remove 12 references (29) > Relationship of selenium intak...

Reference Detail [Get Substances](#) [Get Reactions](#) [Get Cited](#) [Get Citing](#) [Get Full Text](#)

[Return](#) [Link](#) [Save](#) [Print](#) [Export](#) [Previous](#) | [Next](#)

8. Relationship of selenium intake to cancer

By: Whanger, P. D.
Edited by Awad, Atif B.; Bradford, Peter G

A review. The article discusses the anticarcinogenic function of selenium. It discusses mechanisms for cancer prevention by selenium, including its effects on apoptosis, effects on DNA repair, its role in selenoenzymes, its effects on carcinogen metab., its effects on the immune system, selenium as an antiangiogenic agent, and its specific inhibition of tumor cell growth by certain selenium metabolites.

Indexing

Animal Nutrition (Section 18-0)

Section cross-reference(s): 1, 14

Concepts

Angiogenesis inhibitors	Antitumor agents
Apoptosis	Carcinogens
DNA repair	Human
Immune system	Neoplasm
Nutrition, animal	

relationship of selenium intake to cancer

Substances

7782-49-2 Selenium, biological studies

relationship of selenium intake to cancer

Biological study, unclassified; Drug mechanism of action; Pharmacological activity; Therapeutic use; Biological study; Uses

Quick Links

0 Tags, 0 Comments

Source

Nutrition and Cancer Prevention
Pages 189-219
Conference; General Review
2006
CODEN: 69HUM8
ISBN: 978-0-8493-3945-5

Company/Organization

Department Environmental and Molecular Toxicology
Oregon State University
Corvallis, OR, USA

Accession Number

2006:150314
CAN 145:488302
CAPLUS

Publisher

CRC Press LLC
Boca Raton, Fla

Language

English

DOI searching helps pinpoint documents

The screenshot displays the SciFinder web application interface within a Mozilla Firefox browser window. The page title is "SciFinder - Explore References - Mozilla Firefox". The main navigation bar includes "SciFinder - Explore References" and three primary search categories: "Explore References", "Explore Substances", and "Explore Reactions". A user is logged in as "Jason Anderson" with a "Sign Out" link. The "Explore References" section is active, showing a search form with a "Document Identifier(s)" field containing the text "10.1093/inci/djn512". A red arrow points to the "inci" portion of the DOI. Below the input field, instructions state "Enter one per line. Examples: 1983:4296, 107:12935, 10.1021/np050327j". A "Search" button is located to the right of the input field. On the right side of the interface, there are three utility panels: "Saved Answer Sets" (with options for "save", "View All", and "Import"), "Keep Me Posted Results" (stating "No profiles exist"), and "My Connections" (stating "No invitations to connect", "No outstanding sent invitations", and "No connection with colleagues"). The footer contains "Contact Us | Copyrights and Trademarks" and "Copyright © 2010 American Chemical Society. All Rights Reserved."

DOI is visible in detail display and breadcrumbs

SciFinder - Selenium and Vi... - Mozilla Firefox

SciFinder - Selenium and Vi...

Create Keep Me Posted Document ID "10.1093/jnci/djn512" > references (1) > Selenium and Vitamin E: Cell T...

Reference Detail [Get Substances](#) [Get Reactions](#) [Get Cited](#) [Get Citing](#) [Get Full Text](#)

[Return](#)

Selenium and Vitamin E: Cell Type- and Intervention-Specific Tissue Effects in Prostate Cancer

By: Tsavachidou, Dimitra; McDonnell, Timothy J.; Wen, Sijin; Wang, Xuemei; Vakar-Lopez, Funda; Pisters, Louis L.; Pettaway, Curtis A.; Wood, Christopher G.; Do, Kim-Anh; Thall, Peter F.; Stephens, Clifton; Efsthathiou, Eleni; Taylor, Robert; Menter, David G.; Troncoco, Patricia; Lippman, Scott M.; Logothetis, Christopher J.; Kim, Jeri

Background Secondary analyses of two randomized, controlled phase III trials demonstrated that selenium and vitamin E could reduce prostate cancer incidence. To characterize pharmacodynamic and gene expression effects assocd. with use of selenium and vitamin E, we undertook a randomized, placebo-controlled phase IIA study of prostate cancer patients before prostatectomy and created a preoperative model for prostatectomy tissue interrogation. Methods Thirty-nine men with prostate cancer were randomly assigned to treatment with 200 µg of selenium, 400 IU of vitamin E, both, or placebo. Laser capture microdissection of prostatectomy biopsy specimens was used to isolate normal, stromal, and tumor cells. Gene expression in each cell type was studied with microarray anal. and validated with a real-time polymerase chain reaction (PCR) and immunohistochem. An anal. of variance model was fit to identify genes differentially expressed between treatments and cell types. A beta-uniform mixt. model was used to analyze differential expression of genes and to assess the false discovery rate. All statistical tests were two-sided. Results The highest nos. of differentially expressed genes by treatment were 1329 (63%) of 2109 genes in normal epithelial cells after selenium treatment, 1354 (66%) of 2051 genes in stromal cells after vitamin E treatment, and 329 (56%) of 587 genes in tumor cells after combination treatment (false discovery rate = 2%). Validation of 21 representative genes across all treatments and all cell types yielded Spearman correlation coeffs. between the microarray anal. and the PCR validation ranging from 0.64 (95% confidence interval [CI] = 0.31 to 0.79) for the vitamin E group to 0.87 (95% CI = 0.53 to 0.99) for the selenium group. The increase in the mean percentage of p53-pos. tumor cells in the selenium-treated group (26.3%), compared with that in the placebo-treated group (5%), showed borderline statistical significance (difference = 21.3%; 95% CI = 0.7 to 41.8; P = .051). Conclusions We have demonstrated the feasibility and efficiency of the preoperative model and its power as a hypothesis-generating engine. We have also identified cell type- and zone-specific tissue effects of interventions with selenium and vitamin E that may have clin. implications.

Indexing

Quick Links
0 Tags, 0 Comments

Source
Journal of the National Cancer Institute
Volume 101
Issue 5
Pages 306-320
Journal
2009
CODEN: JNCIEQ
ISSN: 0027-8874
DOI: 10.1093/jnci/djn512

Company/Organization
Department of Cancer Biology
The University of Texas
College Station, TX, USA

Accession Number
2009:290435
CAPLUS

Publisher
Oxford University Press

Vinegar is another long-time food element and cancer-fighter

SciFinder - Antioxidants se... - Mozilla Firefox

SciFinder - Antioxidants se...

15. Antioxidants separated from vinegar for preventing carcinogenesis

By: Kaminakai, Kazuo; Kawabata, Hiroki; Nishikawa, Yasushi; Minamida, Kumiko; Shitaji, Yumi; Tamura, Yoshitaka
Assignee: Tamanoi Vinegar Co., Ltd., Japan

The antioxidants dihydroferulic acid and dihydrosinapic acid sepd. from vinegar are claimed as health foods for preventing carcinogenesis. The antitumor effect against human colon, lung, mammary, bladder, and prostate cancer cell lines were tested.

Patent Information

Patent No.	Kind	Date	Application No.	Date
JP 2003095976	A	Apr 3, 2003	JP 2001-288024	Sep 21, 2001

Priority Application

JP 2001-288024	Sep 21, 2001
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Indexing

Pharmacology (Section 1-6)

Section cross-reference(s): 17

Concepts

Antioxidants	Antitumor agents
Bladder, neoplasm	Human
Lung, neoplasm	Mammary gland, neoplasm
Prostate gland, neoplasm	Vinegar

antioxidants sepd. from vinegar for preventing carcinogenesis

Intestine, neoplasm

colon; antioxidants sepd. from vinegar for preventing carcinogenesis

Substances

1135-23-5P	Dihydroferulic acid
14897-78-0P	Dihydrosinapic acid

antioxidants sepd. from vinegar for preventing carcinogenesis

Pharmacological activity; Purification or recovery; Therapeutic use; Biological study; Preparation; Uses

Supplementary Terms

Apr 3, 2003
JP 2003095976
A

Application

Sep 21, 2001
JP 2001-288024

Source

Jpn. Kokai Tokkyo Koho
6 pp.
Patent
2003
CODEN: JKXXAF

Classifications

Main IPC A61K045-00
Secondary IPC A61K031-192;
A61P035-00; A61P039-06;
C09K015-08; C09K015-34

Accession Number

2003:257824
CAN 138:265626
CAPLUS

Language

Japanese



The next time you have a hot dog, be sure to dress it up with mustard!



If you have a SciFinder username and password, you can use the web version of SciFinder

The screenshot shows the SciFinder Sign In page in a Mozilla Firefox browser window. The browser title is "SciFinder - Sign In - Mozilla Firefox". The page features the SciFinder logo and the tagline "...Part of the process™".

Sign In

Username

Password

Remember my username

[Forgot Username or Password?](#)

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

Welcome to SciFinder!

With SciFinder, you can be more creative and productive in your research process. You significantly improve your productivity by:

- Accessing current, high-quality scientific information
- Linking to more relevant journal articles and patent documents than any other source
- Exploring substructures and reactions

China Leads All Nations in Publication of Chemical Patents According to CAS, the World's Most Authoritative Publisher of Chemical Information

Read the complete [article](#).

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scifinder.cas.org

The web version of SciFinder offers a number of advantages

Streamlined navigation to enable faster results and discoveries

Easier, single-screen access to powerful SciFinder features

More intuitive content layouts

No need to install desktop software

CAS events at the ACS Fall National Meeting & Exposition

“Exploring the Potential of World Traditional Medicine”

Monday, August 23, 2:30 p.m.,
Room 255 BCEC







@caschatter

