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A CAS SOLUTION

ACS International Ltd
vhyttinen@acs-i..org

SciFinderⁿ

New premier CAS solutions to explore chemistry including
MethodsNow, PatentPak

Veli-Pekka Hyttinen

Budapest, September 19, 2018

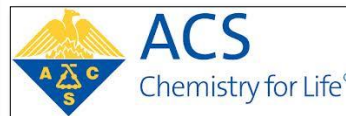


SciFINDER[®]
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CAS supports the mission of the ACS

ACS Mission

To improve people's lives through the transforming power of chemistry.



CAS Mission

To provide the world's best digital research environment to search, retrieve, analyze and link chemical information.



CAS indexing process

Source Selection



Document Indexing



RXN, Methods Formulations



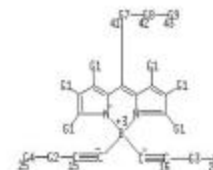
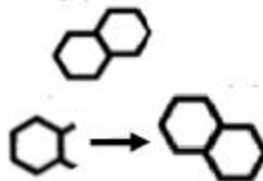
Markush Indexing



Authority Processing



1990
Smith, M.
anthracene



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

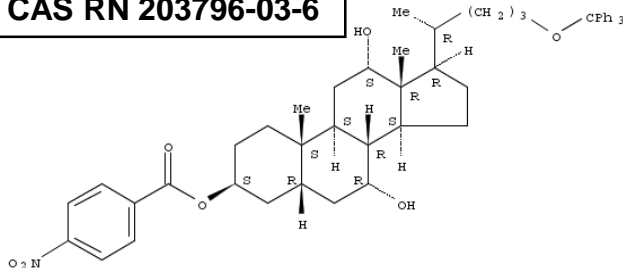
CAS scientists find the chemistry, and save you time!

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

Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding NaHCO₃ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na₂SO₄. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO₂ chromatography (Et₂O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529,1489, 1448, 1345 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m, 9 H) 5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); ¹³C NMR (CDCl₃, 75 MHz) δ 164.21, 150.56,

144.70, 136.79, 130.77, 64.22, 47.79, 46.79, 42.18, 28.74, 27.71, 26.85, 26.3 (thioglycerol+Na⁺ matrix)

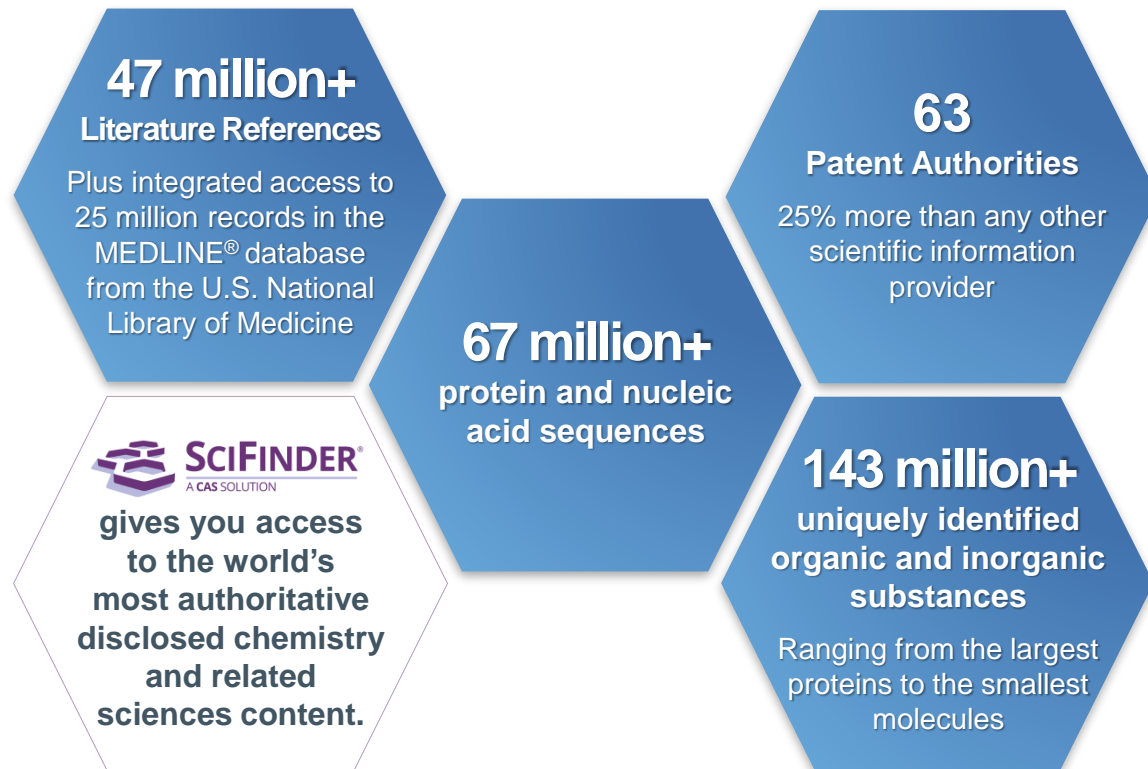
CAS RN 203796-03-6



Absolute stereochemistry.

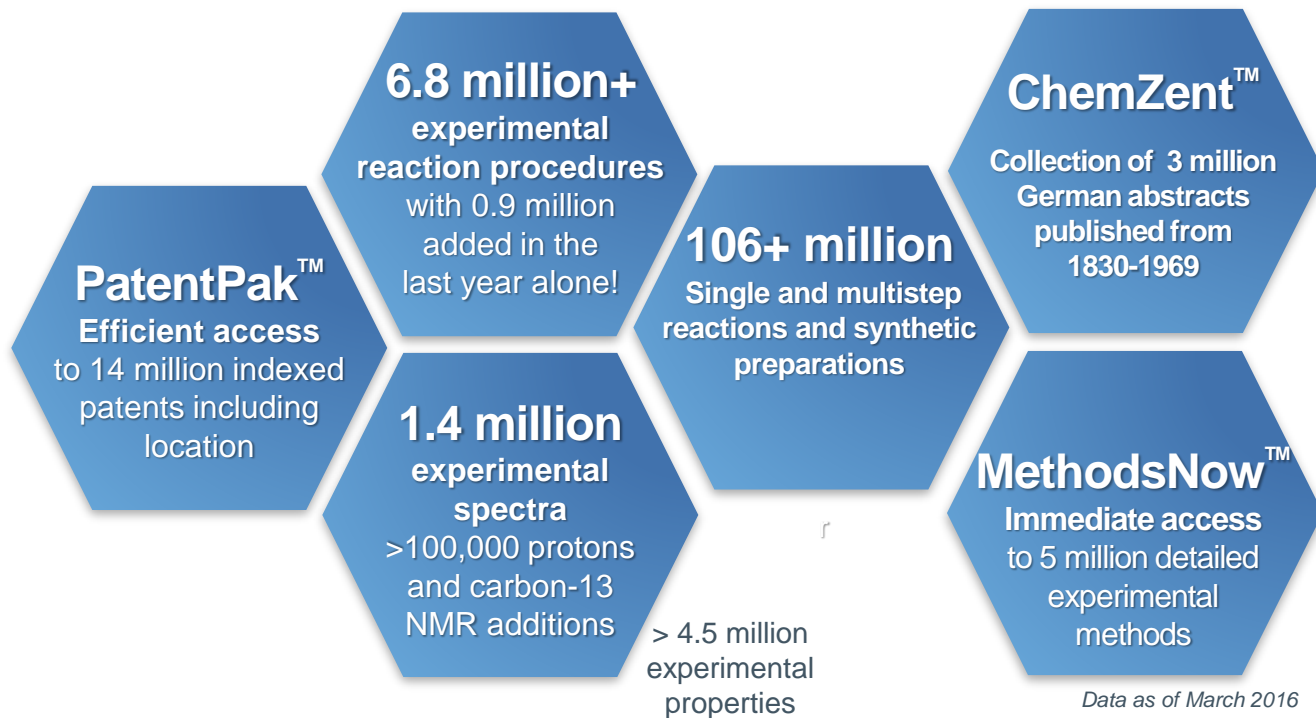


CAS analyzes the world's disclosed research to keep SciFinder the most valuable tool supporting your organization's research enterprise



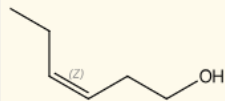
Data as of March 2016

SciFinder saves you time by delivering valuable information to advance your research





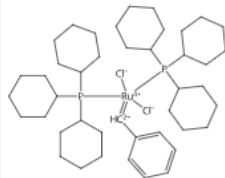
Key Substances in Patent

CAS RN
928-96-1

Analyst Markup Locations (2)

Page 14

Page 24

CAS RN
172222-30-9

Analyst Markup Locations (1)

Page 24

inert and a septum. The monomer was degassed under vacuum for one hour. The contents of the reaction vessel was then kept under an argon atmosphere. Distilled cis-3-hexen-1-ol (0.13 grams, 1.35 mmoles, 0.16 ml) was added by syringe. Methylene chloride (40 ml) was sparged for 15 minutes with a vigorous stream of argon and then cannula transferred into the resin kettle. The monomer / solvent solution was stirred vigorously. In an argon filled drybox, ruthenium catalyst, phenylmethylene bis(tricyclohexylphosphine) dichloride (0.11 grams, 0.141 mmoles), was weighed into a septum capped glass vial and dissolved in 10 ml of methylene chloride. The catalyst solution was injected via syringe into the reaction vessel. The reaction mixture was heated and maintained at 40°C while being vigorously stirred under an argon atmosphere for 24 hours. The reaction mixture was then cooled to ambient temperature. A mixture of ethyl vinyl ether (2.92 grams, 3.9 ml, 40.4 mmoles)



METHODSNOW™

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- Largest single collection of scientific method information
 - Addresses core chemistry markets, new standard: CAS Method Number
- CAS-quality indexing and new, value-add templating of key methods from important full-text sources
- Covers 4.5+ million synthetic step-by-step protocols from 2000 onwards, and 0.5+ million analytical methods focusing in Pharma, Ag, and chemicals
- Details for analytical researchers such as matrix, analyte, instrumentation and comparison capabilities



One product, two interfaces

- **Synthetic methods inside in SciFinder**

*Synthetic chemist looking for great methods?
They are in SciFinder.*

The screenshot shows the SciFinder interface with a chemical reaction scheme. Below the reaction, a procedure is listed:

Procedure

1. Stir the mixture of 7-ethyl-4-methoxy-ycarboxymethyl-2H-chromen-2-one (400 mg, 1.05 mmol), 1- azidoundecane (350 mg, 1.82 mmol), copper(II) sulfate pentahydrate (10 mg, 0.17 mmol), L-tyrosine L-ascorbate (300 mg, 1.82 mmol) in t-BuOH/water (15 mL/15 mL) at room temperature for 4 hours.
2. Add water to the mixture.

View more...

Attributes and Data

¹H NMR, ¹³C NMR, IR, MS, Mass Spec, ...

View with MethodsNow

- **Analytical methods in separate database: www.MethodsNow.com**

*Analytical scientist just looking for great methods?
A new, easy to use interface just for you.*

The screenshot shows the MethodsNow interface with a search bar and a list of method categories:

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

Browse Method Categories

Agricultural Applications / Analysis	Fuels / Geology / Biofuels	Pharmacology / Toxicology
Bioassays	Historical Analysis / Dating	Polymer Analysis
Biomolecule Isolation	Miscellaneous	Water Analysis
Environmental Analysis	Organic Compound Analysis	
Food Analysis	Organometallics / Inorganics	

Recent Searches

Browse: Pesticide Residue Analysis

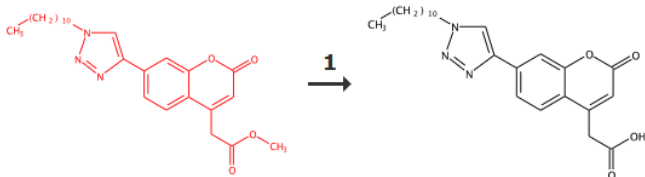


MethodsNow

7-Triazolylcoumarin-based fluorescent tag system for stepwise, comparative assessment of small molecule mic

By Jeon, Moon-Kook; Kang, Myoung-Ku; Park, Koon Ha
From Tetrahedron, 68(30), 6038-6053; 2012
Published by Elsevier Ltd.

Reaction Steps **1** 2 3 4



Products	2H-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1H-1,2,3-triazol-4-yl)-, 75%, CAS RN 1384966-77-1
Reactants	2H-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1H-1,2,3-triazol-4-yl)-, methyl ester, 1384966-75-9
Reagents	Hydrochloric acid, CAS RN: 7647-01-0 Lithium hydroxide, CAS RN: 1310-65-2
Solvents	Water, CAS RN: 7732-18-5 Tetrahydrofuran, CAS RN: 109-99-9

Print

MethodsNow

Procedure	<ol style="list-style-type: none">1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H-1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg, 0.780 mmol) in THF/water(25 mL/25 mL) at room temperature.2. Stir the reaction mixture for 3 hours at room temperature.3. Adjust pH 3-4 to the reaction mixture by adding 1 N hydrochloric acid.4. Partition the reaction mixture between ethyl acetate and water.5. Extract the aqueous layer with ethyl acetate.6. Dry the combined organic layer over magnesium sulfate.
Scale	milligram
¹H NMR	¹ H NMR (300 MHz, acetone- <i>d</i> ₆): δ = 7.83 (s, 1H), 8.58 (s, 1H), 7.92 (d, <i>J</i> = 8.1 Hz, 1H), 7.84 (d, <i>J</i> = 8.1 Hz, 1H), 6.47 (s, 1H), 4.50 (t, <i>J</i> = 7.2 Hz, 2H), 3.99 (s, 2H), 2.00 (quintet, <i>J</i> = 7.2 Hz, 2H), 1.32-1.43 (m, 4H), 1.22-1.32 (m, 12H), 0.87 ppm (t, <i>J</i> = 6.8 Hz, 3H).
¹³C NMR	¹³ C NMR (125 MHz, DMF- <i>d</i> ₂ , 60 °C): δ = 161.0, 155.1, 154.2, 146.5, 136.0, 127.2, 123.7, 122.1, 120.4, 115.3, 113.5, 51.1, 32.8, 29.9, 27.3, 23.5, 18.7, 14.7 ppm (decarboxylation occurred to give the corresponding 4-methyl derivative).
IR	IR (ATR, neat): ν = 3423, 2922, 2851, 1702 (2C=O, overlapped), 1619, 1561, 1375, 1154, 936, 852, 809 cm ⁻¹ .
HRMS	HRMS (EI): <i>m/z</i> calculated for C ₂₄ H ₃₁ N ₃ O ₄ : 425.2315 [M ⁺]; found: 425.2315.
Mass Spec	MS (ESI): <i>m/z</i> : 426 [M+H ⁺].
MP	235.5±0.8 °C.
CAS Method Number	3-352-CAS-78415

Print/Export

Close



MethodsNow – Analytical Scientist Interface

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Search

Enter keyword, matrix, analyte, etc.

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[Biomolecule Isolation](#)



[Environmental Analysis](#)

[Food Analysis](#)

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[hplc lycopene analysis](#)

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[← Return to Home](#)

Advanced Search

Publication Name

Keyword

Analyte

Matrix

Method Category

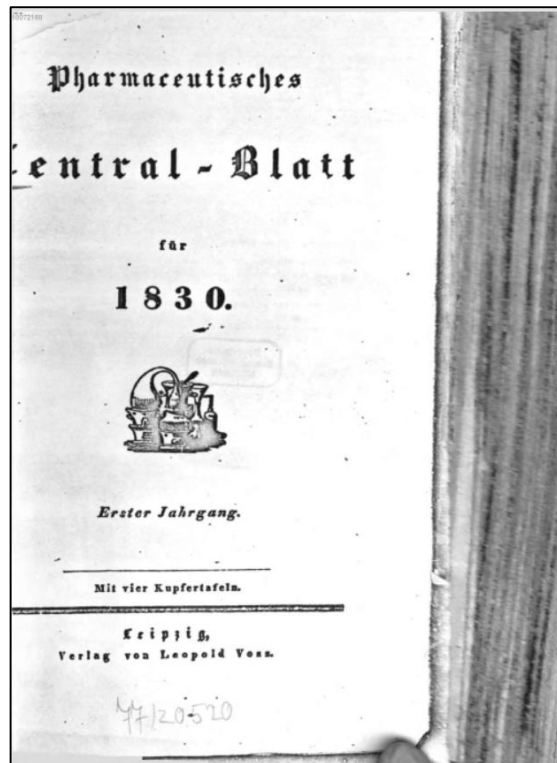
Technique

CAS Method Number

Publication Name

Chemisches Zentralblatt predates the introduction of Chemical Abstracts by almost 80 years

- Published German language abstracts from 1830-1969
- Chronicles the birth of chemistry as a science
 - Before 1800, chemistry was more alchemy (i.e. how to turn lead into gold) than actual science
- Searchable substance structures in 3 million machine translated abstracts



First Issue:
Note, the name changed several times before 1856

Categorize and analyze options make it easy to find relevant information

Categorize

1. Select a heading and category. 2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in biology (221)	Select All Deselect All	
General chemistry	Animal pathology (69)	<input type="checkbox"/> Interferons 7	
Biotechnology	Animal pathology (69)	<input type="checkbox"/> Antibodies and Immunoglobulins 5	
Synthetic chemistry	Immunology (72)	<input type="checkbox"/> Interferons, α 5	
Genetics & protein chemistry	Processes & systems (44)	<input type="checkbox"/> Vaccines 5	
Physical chemistry	Endocrinology (48)	<input type="checkbox"/> Interleukin 2 3	
Polymer chemistry	Anatomy (27)	<input type="checkbox"/> Interleukin 4 3	
Biology	Substances in adverse effects (16)	<input type="checkbox"/> Leukotriene B4 3	
Technology		<input type="checkbox"/> RANTES (chemokine) 3	
Analytical chemistry		<input type="checkbox"/> Spleen 3	
Environmental chemistry		<input type="checkbox"/> Tumor necrosis factor α 3	
		<input type="checkbox"/> Anti-HIV agents, vaccines 2	
		<input type="checkbox"/> CD4 antigens 2	
		<input type="checkbox"/> CXC chemokines 2	
		<input type="checkbox"/> Etanercept 2	
		<input type="checkbox"/> High throughput screening 2	

Biology > Immunology

SUBSTANCES

Get References Get Reactions Get Commercial Sources

Analyze Refine

Sort by: CAS Registry Number

0 of 1 Substance Selected

Analyze by:

- Target Indicators
- Bioactivity Indicators**
- Commercial Availability
- Elements
- Reaction Availability
- Substance Role

Transport proteins (all) 1

Show More

1. **28911-01-5**

~2061 ~34

C₁₇ H₁₂ Cl₂ N₄
4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-(2-chlorophenyl)-1-methyl-

Regulatory Information
Spectra
Experimental Properties

SciFinder-n Get to actionable results more quickly with a streamlined new interface

Streamlined search navigation saves you clicks

Immediately run past searches

The screenshot displays the SciFinder-n search interface. At the top, there are navigation links for 'Saved', 'History', and 'Account'. The main search area includes a search bar with the text 'treatment of cancer' and a search button. Below the search bar, there are options for 'Advanced Search' and a chemical structure drawing. The 'References' menu item is highlighted. The 'Recent Searches' section shows a search for 'high temperature low density plasma' and another for 'Advanced Search'.

More conveniently search structures and text

SciFinder-n Information presented to facilitate rapid understanding

Powerful filtering capabilities allow rapid focus

The screenshot displays the SciFinder-n interface for a reaction search. On the left, a 'Structure Match' sidebar offers filtering options: 'As Drawn (5)', 'Substructure (18)', and 'Filter by' categories including Substance Role (Product, Reactant), Yield (90-100%, 80-89%, 70-79%, 50-69%, 30-49%), Number of Steps (1), Experimental Protocols (MethodsNow Available, Procedure Available), Reaction Type, Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes, Source Reference, Publication Year, Document Type, and Language. The main area, titled 'Reactions (13)', shows 'Scheme 1 (2 Reactions) View' with a chemical reaction scheme. Below the scheme are 'Suppliers (3)' and 'Suppliers (6)' buttons. Two 'Reaction Summary' sections are visible, each detailing reagents (Sodium acetate, Acetic acid, manganese(3+) salt (3:1)), catalysts, solvents (Acetic acid), and conditions. Both summaries indicate 1 step and a 92% yield. A 'Full Text' button is provided for each summary. The right side of the interface includes a 'View - Select -' dropdown and 'Print', 'Email', and 'Save' icons.

Intuitive information layouts fosters quick comprehension

One idea can lead you to another - SciFinderⁿ has you covered!

The screenshot displays the SciFinder web application interface. At the top, a browser window shows five tabs, all labeled 'SciFinder', which are circled in purple. Below the browser, the SciFinder logo and navigation menu are visible. The search results page is titled 'References (3,103)' and shows a list of search results. The first result is 'Multikinase inhibitors: a new option for the treatment of thyroid cancer' by Gild, Matti L.; Bullock, Martyn; Robinson, Bruce G.; Clifton-Bligh, Roderick. The second result is 'sorafenib for the treatment of renal cancer' by Strumberg, Dirk. The interface includes filters for 'Structure Match', 'Document Type', 'Language', and 'Publication Year'. A purple arrow points from the text 'Simultaneous searches can be performed in new browser/windows' to the multiple browser tabs.

Simultaneous searches can be performed in new browser/windows

SciFinder-n Citation Mapping helps you understand where to go next in your literature review

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References ▾ Enter a query... Draw Search Star Clock User

Citation Map

Identification and characterization of a *Pantoea citrea* gene encoding glucose dehydrogenase that is essential for causing pink disease of pineapple

By: Cha, Jae-Soon; Pujol, Catherine; Kado, Clarence I. Applied and Environmental Microbiology (1997), 63(1), 71-76 | Language: English, Database: CAPUS

View Reference Detail View More ▾

References This Document Cites

Basic local alignment search tool	Basic local alignment search tool.
34K Citations	34K Citations
DNA sequencing with chain-terminating inhibitors	DNA sequencing with chain-terminating inhibitors.
16K Citations	16K Citations
A simple method for displaying the hydrophobic character of a protein.	A simple method for displaying the hydrophobic character of a protein.

References Citing This Document

The commercial production of chemicals using pathway engineering	The biochemistry, physiology and genetics of PQQ and PQQ-containing enzymes
155 Citations	131 Citations
Gluconobacter oxydans: its biotechnological applications	Immune evasion of the human pathogenic yeast <i>Candida albicans</i> : Pra1 is a Factor H, FHL-1 and plasminogen binding surface protein
42 Citations	42 Citations
The periplasmic serine protease inhibitor ecotin protects bacteria against neutrophil elastase	The periplasmic serine protease inhibitor ecotin protects bacteria against neutrophil elastase
120 Citations	40 Citations
Multigene editing in the Escherichia coli genome via the CRISPR-Cas9 system	Quinoprotein ethanol dehydrogenase of <i>Pseudomonas aeruginosa</i> is a homodimer. Sequence of the gene and deduced structural properties of the enzyme
39 Citations	26 Citations
Genetic and biochemical characterization of the pathway in <i>Pantoea citrea</i> leading to pink disease of pineapple	The epidemiology and management of seedborne bacterial disease...
	18 Citations
	Mathematical modeling of in vitro enzymatic

Interactive map allows speedy identification of important research (maybe even that one paper you wouldn't otherwise find!)

A product portfolio that emphasizes investment in AI and scalability – with a focus on speed and cost

The screenshot displays the SciFinder web interface with search results for 'treatment of cancer'. The interface is divided into several sections:

- Search Panel (Left):** Includes filters for Substances, Reactions, and Suppliers. The 'References' filter is selected. Recent searches are listed for March 28, 2017 (11:55 AM and 10:14 AM) and March 27, 2017 (5:33 PM).
- Structure Match Panel (Top Left):** Shows 'As Drawn (5)' and 'Substructure (18)' results. Filter by options include Substance Role (Product, Reactant), Yield (90-100%, 80-89%, 70-79%, 50-69%, 30-49%), Number of Steps (1-13), Experimental Protocols (Methods Now Available, Procedure Available), Reaction Type, Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes, Source Reference (Publication Year, Document Type, Language), and Suppliers.
- Reaction Scheme Panel (Middle Left):** Displays 'Scheme 1 (2 Reactions)' with a chemical structure and options for Reagents, Catalysts, Solvents, Conditions, and View Reaction.
- References Panel (Right):** Shows 'References (3,103)' for 'treatment of cancer'. Filter by options include Document Type (Journal, Patent, Review, Conference, Dissertation) and Language (English, Chinese, Japanese, Korean, French). A 'Publication Year' bar chart shows a peak in 2017. Two reference entries are visible:
 - Multikinase inhibitors: a new option for the treatment of thyroid cancer** (Nature Reviews Endocrinology, 2011). Abstract: A review. Preclin. models have shown that inhibition of kinases in mitogenic and angiogenic signaling pathways can have antitumoral effects. Starting with a brief synopsis of a malignancy that responds well to kinase inhibition (chronic myeloid leukemia) compared with one with less durable responses as yet (melanoma), this Review highlights challenges that must be overcome in order to successfully translate small-mol. therapies to thyroid cancer. In the future, Thyroid cancer typically has a good outcome following standard treatment, which include surgery, radiotherapy, iodine ablation, and TSH...
 - sorafenib for the treatment of renal cancer** (Expert Opinion on Pharmacotherapy, 2012). Abstract: A review. Introduction: was the first oral antiangiogenic multikinase inhibitor (Raf kinases, VEGF receptors 1 - 3, PDGF-beta, Flt-3, c-kit) for advanced renal cell carcinoma (RCC) to be approved. Since 2005, a total of six drugs have been approved for the treatment of RCC. Areas covered: The preclin. and clin. development of sorafenib that led to its approval for advanced RCC is reviewed in this paper. Its safety, tolerability and efficacy are summarized and compared with other approved treatment...

Questions?

CAS is a global team of scientists helping scientists

For more than 110 years, CAS has been the leader in developing cutting-edge information solutions to advance innovation across the spectrum of science and technology.

Every day at CAS hundreds of scientists analyze the world's disclosed scientific discoveries and, leveraging the latest technologies, infuse insights to deliver answers.



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