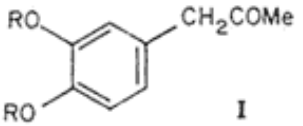
Part II, Chapters 2.11-13, App. D
ACS Style Guide, Chapter 14

References, Bibliography & Search

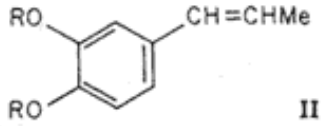
Search

Chemical Abstracts Vol. 82, 1975 Page 408

72640z **Phenylacetones from 1-phenylpropenes.** Kojima, Atsushi; Katagami, Tsutomu; Okubo, Ichiro (Mitsui Pharmaceuticals, Inc. and Mitsui Toatsu Chemicals, Inc.) **Japan. Kokai 74 100,044** (Cl. 16 C54), 20 Sep 1974, Appl. 73 12,622, 31 Jan 1973; 3 pp. Phenylacetones **I** (R = lower alkyl; or



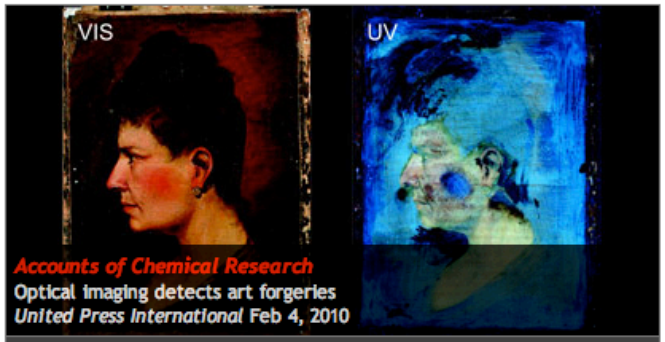
I



II

R_2 = CH_2) were prepd. by peracid oxidn. of 1-phenylpropenes **II** in a halohydrocarbon solvent in the presence of a carbonate salt, followed by heating with mineral acid. Thus, a peracid soln. was prepd. from 250 g 86% HCO_2H and 130 g 35% H_2O_2 and added at 30–40° to a stirred mixt. of 162.2 g isosafrole and 15 g Na_2CO_3 in 500 ml CH_2ClCH_2Cl. The mixt. was stirred at 35–40° for 6 hr and the solvent evapd. Heating the residue with 1.8 kg 15% aq. H_2SO_4 for 2 hr gave 73% **I** (R_2 = CH_2), 95.7% pure. Also prepd. was **I** (R = Me). Ikuo Matsumoto

ACS Journals in the News



Browse Our Journals

Journals A–Z | View by Subject Area

A

Accounts of Chemical Research
ACS Applied Materials & Interfaces
ACS Chemical Biology
ACS Chemical Neuroscience—New in 2010
ACS Medicinal Chemistry Letters—New in 2010
ACS Nano
Analytical Chemistry

C&EN Latest News

Genentech, Sanofi Ink Academic Pacts
Feb 23, 2010
Collaboration: Deals follow a trend of closer links between drug industry and academic research.

Anthrax Case Closed
Feb 23, 2010
Investigation: FBI concludes that government biodefense researcher Bruce Ivins was the culprit in the attacks.

Growing Piles Of Toxic Trash
Feb 22, 2010
Electronic Waste: Developing countries need to prepare for surge in domestic discards, UNEP says.

SNPE Announces Sale Of Isochem
Feb 22, 2010
Fine Chemicals: French company will be acquired by Aurelius, a German private equity firm.

C&EN Online | Current Issue | Latest News RSS Feed

Announcements

ACS Publications Response to Office of Science & Technology Policy RFI on Public Access Policies
On January 21, 2010, the society's Publications Division submitted to Dr. John P. Holdren, Director of the Office of Science & Technology Policy, a set of comments and recommendations in response to a request for information

Advertisements


Info for Advertisers

Stay Current
Sign up to get notices about the latest articles via e-mail and RSS feed.
Learn more

Authors & Reviewers
Contribute, Publish, and Review
- Resource Center
- Author Benefits
- Journals Information
- Books Information
- Copyright & Permissions

A division of the American Chemical Society

SciFinder® - Part of the Process™

SciFinder is the leading research tool used by scientists around the world. Scientists use SciFinder to access single- and multi-step reactions, experimental and predicted properties, and substance information from the CAS REGISTRY, the "gold standard" for chemical substance information. Its advanced search and analysis tools makes SciFinder a vital part of today's research process.

SciFinder®
Part of the process.™

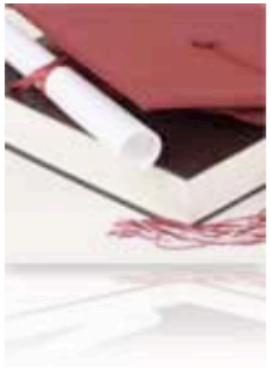
You can explore one single source for scientific information in journal and patent literature from around the world.

See a demo of SciFinder!

Chemistry

Biology

Biomass



Academia

Welcome to Spectral Database for Organic Compounds, SDBS.

This is a free site organized by National Institute of Advanced Industrial Science and Technology (AIST), Japan.

NMR: *T.Saito, K.Hayamizu, M.Yanagisawa and O.Yamamoto*
MS: *N.Wasada*
ESR: *K.Someno*
IR: *S.Kinugasa, K.Tanabe and T.Tamura*
Raman: *K.Tanabe and J.Hiraishi*

What's New

2010.01.07	New options are added to "compound search" and sort method for the "search results".
2009.11.05	Server will be down.(2009/12/01 10:00 - 2009/12/02 20:00)
2009.09.29	New data were updated.(584 Spectra)
2009.09.15	Server will be down.(2009/10/09 19:00 - 2009/10/13 10:00)

Disclaimer

We are doing our best to compile high quality databases. However, there are no such databases without any errors or mistakes. We make no warranties to those effects and shall not be liable for any damage that may result from errors in the database. When you find errors or mistakes, please inform us using the form which can be accessed from the Contact button shown above.

Access to this database is free of charge. However we request visitors to our database not to download more than 50 spectra and/or compound information in one day. All accesses are recorded. It is prohibited that you use any information of SDBS for profit-making or commercial use without obtaining proper permission from us. If more spectra are required for some specific purpose or commercial use, you should consult us and describe the intended usage or purpose of our SDBS.

We also request that when you use the data of our SDBS in your publication or presentation, a proper acknowledgement be given

- Please do not access or download data by using automated processes.
- Please check Javascript and Cookie settings if you can not proceed to search page. The settings have to be active in order to use SDBS.

We had a numerous access from one particular site.
We are investigating the details of the incident.

I agree the disclaimer and use SDBS.

MyPDB Login

A MEMBER OF THE PDB

RCSB PDB PROTEIN DATA BANK

An Information Portal to Biological Macromolecular Structures

As of **Tuesday Feb 23, 2010 at 4 PM PST** there are 63559 Structures | **PDB Statistics**

Home Hide
News & Publications
Policies
FAQ
Contact
Feedback
About Us

Deposition Hide
All Deposit Services
Electron Microscopy
NMR
Validation Server
BioSync Beamline
Related Tools

Search Hide
Advanced Search
Latest Release
Latest Publications
Sequence Search
Ligand Search
Unreleased Entries
Browse Database
Histograms

Tools Hide
File Downloads
FTP Services
File Formats
Services: RESTful | SOAP
Widgets
Compare Structures

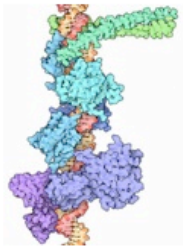
Education Hide
Looking at Structures
Molecule of the Month
Educational Resources

A Resource for Studying Biological Macromolecules

The PDB archive contains information about experimentally-determined structures of proteins, nucleic acids, and complex assemblies. As a member of the **wwPDB**, the RCSB PDB curates and annotates PDB data according to agreed upon standards.

The RCSB PDB also provides a variety of tools and resources. Users can perform simple and advanced searches based on annotations relating to sequence, structure and function. These molecules are visualized, downloaded, and analyzed by users who range from students to specialized scientists.

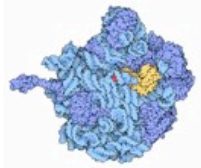
Molecule of the Month: Enhanceosome



Take a moment to ponder the form of your body: the shape of your face, the color of your eyes, the length of your fingers, the perfect articulation of your bones and muscles, the way your hair grows curly or straight. Now let your imagination travel inward, and think of the complex shapes and functions of your different cells, and the teeming molecular world inside each one. Remarkably, this amazing structure and form and function is specified by information in the genome, which encodes a mere 20,000-25,000 protein-coding genes. One of the great puzzles being pieced together by scientists is the mechanism by which these genes, and the methods used to control their expression, specify all of these different aspects of life. ■ **Read more**

... ■ **Previous Features**

PSI Featured Molecule: Antibiotics and Ribosome Function



A series of new structures reveal the atomic basis of antibiotics that attack bacterial ribosomes. The drugs wedge themselves in key loops of ribosomal RNA, inhibiting the motions needed for decoding and recycling.

■ **Read more from the Structural Genomics Knowledgebase** ■ **Previous Features**

New user? Try the browser **compatibility check** and information on **Getting Started**.

News

- **Complete News**
- **Newsletter**
- **Discussion Forum**
- **Job Listings**

wwPDB Statement on Retraction of PDB Entries

23-February-2010

Online Narrated Tutorial Demonstrates How to Use the RCSB PDB

Comprehensive training materials to introduce users to the features and functionality of the RCSB PDB are now freely available at **openhelix.com**. **More >>**

23-February-2010

Changes to the wwPDB Policy for Depositing Polypeptide Structures

The **wwPDB** now accepts polypeptide structure depositions of all gene products; all naturally-occuring, non-ribosomally synthesized peptides, such as antibiotics; and all peptidic repeat units of larger polymers, such as fibrous and amyloid polymers. **More >>**

FTP Archive

The up-to-date PDB archive is available at: **ftp.wwpdb.org**

Time-stamped yearly snapshots are available at: **ftp://snapshots.wwpdb.org**

ACS Publications Home Page

http://pubs.acs.org/

Apple Yahoo! .Mac Apple RG eBay News RG favs.

Subscriber access provided by UNIV OF MISSOURI COLUMBIA

ACS | Journals | C&EN | CAS

ACS Publications
High quality. High impact.

Publications A-Z | Home | Authors & Reviewers | Librarians | ACS Members | Help

Search | Citation | DOI | Advanced Search

Anywhere | Search

Personalize your experience: Log In | Register | Cart | Website Demos

Journals A-Z | Books | Authors & Reviewers | Librarians | ACS Members | About Us | e-Alerts | Help

ACS Journals in the News

Accounts of Chemical Research
Optical imaging detects art forgeries
United Press International Feb 4, 2010

1 2 3 4 5 6 7 8 9 10

Browse Our Journals

Journals A–Z View by Subject Area

A

Accounts of Chemical Research
ACS Applied Materials & Interfaces
ACS Chemical Biology
ACS Chemical Neuroscience—New in 2010
ACS Medicinal Chemistry Letters—New in 2010
ACS Nano
Analytical Chemistry

C&EN Latest News

Genentech, Sanofi Ink Academic Pacts
Feb 23, 2010
Collaboration: Deals follow a trend of closer links between drug industry and academic research.

Anthrax Case Closed
Feb 23, 2010
Investigation: FBI concludes that government biodefense researcher Bruce Ivins was the culprit in the attacks.

Growing Piles Of Toxic Trash
Feb 22, 2010
Electronic Waste: Developing countries need to prepare for surge in domestic discards, UNEP says.

SNPE Announces Sale Of Isochem
Feb 22, 2010
Fine Chemicals: French company will be acquired by Aurelius, a German private equity firm.

C&EN Online | Current Issue | Latest News RSS Feed

Announcements

ACS Publications Response to Office of Science & Technology Policy RFI on Public Access Policies

On January 21, 2010, the society's Publications Division submitted to Dr. John P. Holdren, Director of the Office of Science & Technology Policy, a set of comments and recommendations in response to a request for information

Advertisements

Info for Advertisers

Stay Current

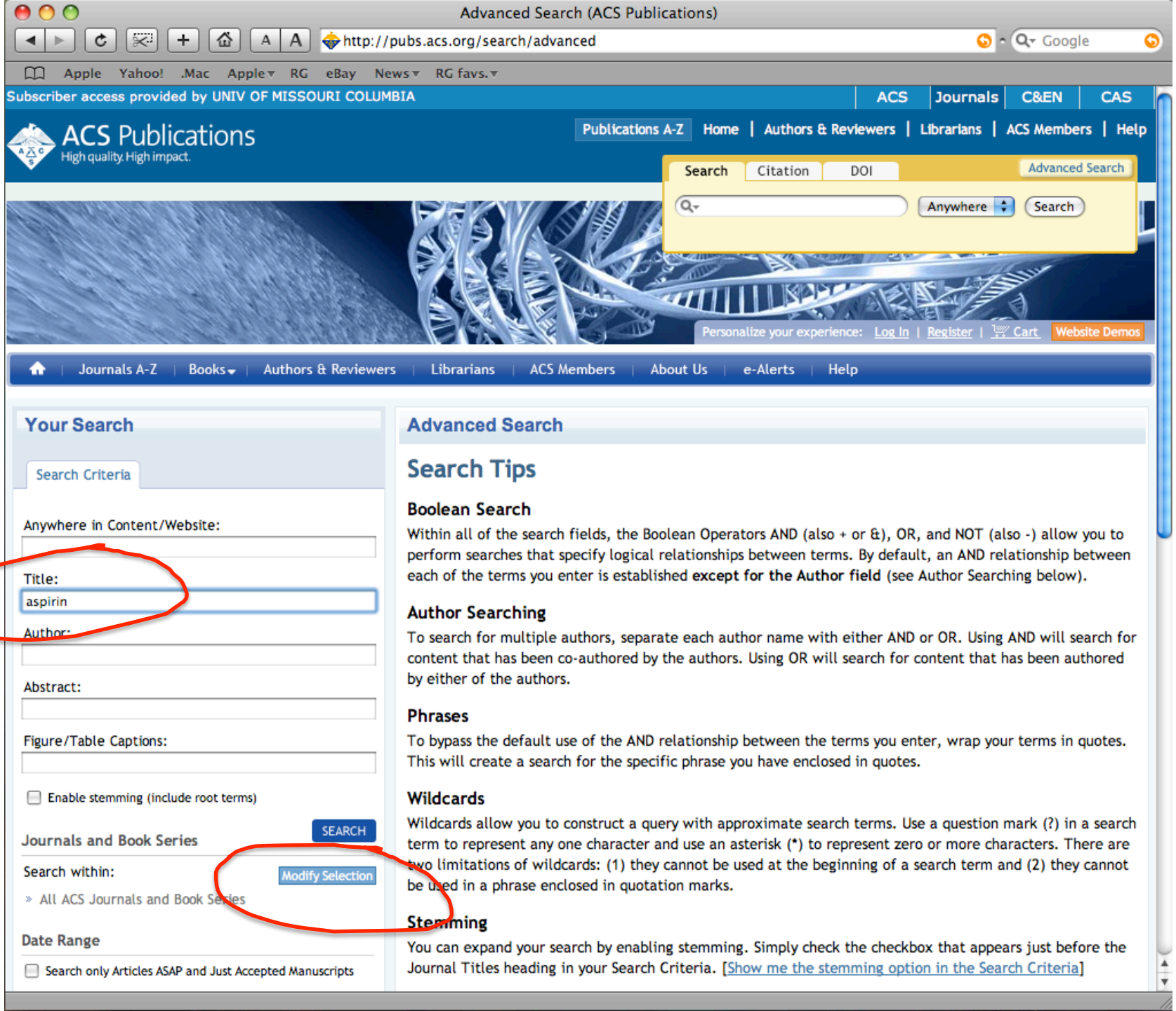
Sign up to get notices about the latest articles via e-mail and RSS feed.

Learn more

Authors & Reviewers

Contribute, Publish, and Review

- Resource Center
- Author Benefits
- Journals Information
- Books Information
- Copyright & Permissions


Advanced Search (ACS Publications)
http://pubs.acs.org/search/advanced
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
Subscriber access provided by UNIV OF MISSOURI COLUMBIA
ACS Journals C&EN CAS
ACS Publications
High quality. High impact.
Publications A-Z Home | Authors & Reviewers | Librarians | ACS Members | Help
Search Citation DOI Advanced Search
Anywhere Search
Personalize your experience: Log In | Register | Cart Website Demos
Journals A-Z | Books | Authors & Reviewers | Librarians | ACS Members | About Us | e-Alerts | Help
Your Search
Search Criteria
Anywhere in Content/Website:
Title:
aspirin
Author:
Abstract:
Figure/Table Captions:
Enable stemming (include root terms)
SEARCH
Journals and Book Series
Search within:
Modify Selection
» All ACS Journals and Book Series
Date Range
Search only Articles ASAP and Just Accepted Manuscripts
Advanced Search
Search Tips
Boolean Search
Within all of the search fields, the Boolean Operators AND (also + or &), OR, and NOT (also -) allow you to perform searches that specify logical relationships between terms. By default, an AND relationship between each of the terms you enter is established except for the Author field (see Author Searching below).
Author Searching
To search for multiple authors, separate each author name with either AND or OR. Using AND will search for content that has been co-authored by the authors. Using OR will search for content that has been authored by either of the authors.
Phrases
To bypass the default use of the AND relationship between the terms you enter, wrap your terms in quotes. This will create a search for the specific phrase you have enclosed in quotes.
Wildcards
Wildcards allow you to construct a query with approximate search terms. Use a question mark (?) in a search term to represent any one character and use an asterisk (*) to represent zero or more characters. There are two limitations of wildcards: (1) they cannot be used at the beginning of a search term and (2) they cannot be used in a phrase enclosed in quotation marks.
Stemming
You can expand your search by enabling stemming. Simply check the checkbox that appears just before the Journal Titles heading in your Search Criteria. [Show me the stemming option in the Search Criteria]

Your Search

Show Search Tips

Search Criteria | Search Filters | New Search

Filters Applied:
Title: aspirin [Remove]

Content Type
Book Chapter (2)
Journal Article (82)

Publication
ACS Symposium Series (ACS Book Series) (2)
Anal. Chem. (14)
Biochemistry (5)
Biomacromolecules (1)
Crystal Growth & Design (4)
J. Agric. Food Chem. (2)
J. Am. Chem. Soc. (8)
J. Chem. Educ. (26)
J. Chem. Eng. Data (1)
J. Med. Chem. (11)
J. Org. Chem. (3)
J. Phys. Chem. (1)
J. Phys. Chem. B (3)
J. Proteome Res. (1)
Langmuir (1)
Org. Process Res. Dev. (1)

Search Results

Sort By: Relevance

All (84) | Research (82) | News, Features, Commentary (1) | General Information (1)

Showing 1-20 of 84

Results per page: 20

Page: 1 2 3 4 5 | Next

Select All For Selected Content: View Abstracts Download Citations

Experiments with Aspirin

Abstract | Supporting Info

Edward Barry , Londa L. Borer

J. Chem. Educ., **2000**, *77* (3), p 354
Publication Date (Web): March 1, 2000 (Article)
DOI: 10.1021/ed077p354

Hi-Res PDF [34K]
PDF w/ Links [34K]
Subscriber Access

A series of experiments based on aspirin have been used in our high school chemistry laboratory. Experiments include (i) synthesis, purification, and characterization of aspirin by mp and TLC, (ii) percentage composition of a commercial aspirin tablet by ...

Aspirin and Prostaglandin Synthesis

Abstract

Ernest A. Harrison Jr.

J. Chem. Educ., **1979**, *56* (11), p 768
Publication Date: November 1979 (Letter)
DOI: 10.1021/ed056p768.2

Hi-Res PDF [1181K]
PDF w/ Links [1182K]
Sponsored Access

Aspirin inhibits the synthesis of prostaglandins.

Welcome to Spectral Database for Organic Compounds, SDBS.

This is a free site organized by National Institute of Advanced Industrial Science and Technology (AIST), Japan.

NMR: *T.Saito, K.Hayamizu, M.Yanagisawa and O.Yamamoto*
MS: *N.Wasada*
ESR: *K.Someno*
IR: *S.Kinugasa, K.Tanabe and T.Tamura*
Raman: *K.Tanabe and J.Hiraishi*

What's New

2010.01.07	New options are added to "compound search" and sort method for the "search results".
2009.11.05	Server will be down.(2009/12/01 10:00 - 2009/12/02 20:00)
2009.09.29	New data were updated.(584 Spectra)
2009.09.15	Server will be down.(2009/10/09 19:00 - 2009/10/13 10:00)

Disclaimer

We are doing our best to compile high quality databases. However, there are no such databases without any errors or mistakes. We make no warranties to those effects and shall not be liable for any damage that may result from errors in the database. When you find errors or mistakes, please inform us using the form which can be accessed from the Contact button shown above.

Access to this database is free of charge. However we request visitors to our database not to download more than 50 spectra and/or compound information in one day. All accesses are recorded. It is prohibited that you use any information of SDBS for profit-making or commercial use without obtaining proper permission from us. If more spectra are required for some specific purpose or commercial use, you should consult us and describe the intended usage or purpose of our SDBS.

We also request that when you use the data of our SDBS in your publication or presentation, a proper acknowledgement be given

- Please do not access or download data by using automated processes.
- Please check Javascript and Cookie settings if you can not proceed to search page. The settings have to be active in order to use SDBS.

We had a numerous access from one particular site.
We are investigating the details of the incident.

I agree the disclaimer and use SDBS.

SDBS Compounds and Spectral Search

Compound Name:
aspirin match partial

Molecular Formula:
C, H, then the other elements are alphabetical order, "%,*" for the wild card

Molecular Weight:
to
Numbers between left and right columns
Up to the first place of a decimal point

CAS Registry No.:
"%,*" for the wild card.

SDBS No.:
"%,*" for the wild card.

Atoms:

C(Carbon)		to	
H(Hydrogen)		to	
N(Nitrogen)		to	
O(Oxygen)		to	
F(Fluorine)		to	
Cl(Chlorine)		to	
Br(Bromine)		to	
I(Iodine)		to	
S(Sulfur)		to	
P(Phosphorus)		to	
Si(Silicon)		to	

Numbers between left and right columns.

Spectrum:
Check the spectra of your interest.
- ☐ MS
- ☐ IR
- ☐ ^{13}C NMR
- ☐ Raman
- ☐ ^{1}H NMR
- ☐ ESR

IR Peaks(cm^{-1}): Allowance
± 10
"," or space is the separator for multiple peaks.
Use "-", to set a range:. eg. 550-750,1650 3000-
Transmittance < 80 %

^{13}C NMR Shift(ppm): Allowance
± 2.0
"," is the separator for multiple shifts, eg. 129.3,18.4,...
No shift regions:
Range defined by two numbers separated by a space, eg. 110 78,...

^{1}H NMR Shift(ppm): Allowance
± 0.2
No shift regions:

MS Peaks and intensities:
Mass and its intensity are a set of data separated by a space, eg. 110 22,..

Search | Clear | Hit: 20hit | Sort by: Molecular Weight

(c) National Institute of Advanced Industrial Science and Technology (AIST)

SDBS Search Results: 1 - 2 out of 2 hits

SDBS No	Molecular Formula	Molecular Weight	MS	CNMR	HNMR	IR	Raman	ESR	Compound Name
532	C9H8O4	180.2	Y	Y	Y	Y	Y	N	2-acetoxybenzoic acid
6670	C10H10O4	194.2	Y	Y	Y	Y	Y	N	methyl acetylsalicylate

Return to Search

(c) National Institute of Advanced Industrial Science and Technology (AIST)

SDBS Information

SDBS No.: 532

Compound Name:
o-acetoxybenzoic acid

Molecular Formula: $C_9H_8O_4$

Molecular Weight: 180.2

CAS Registry No.:
50-78-2

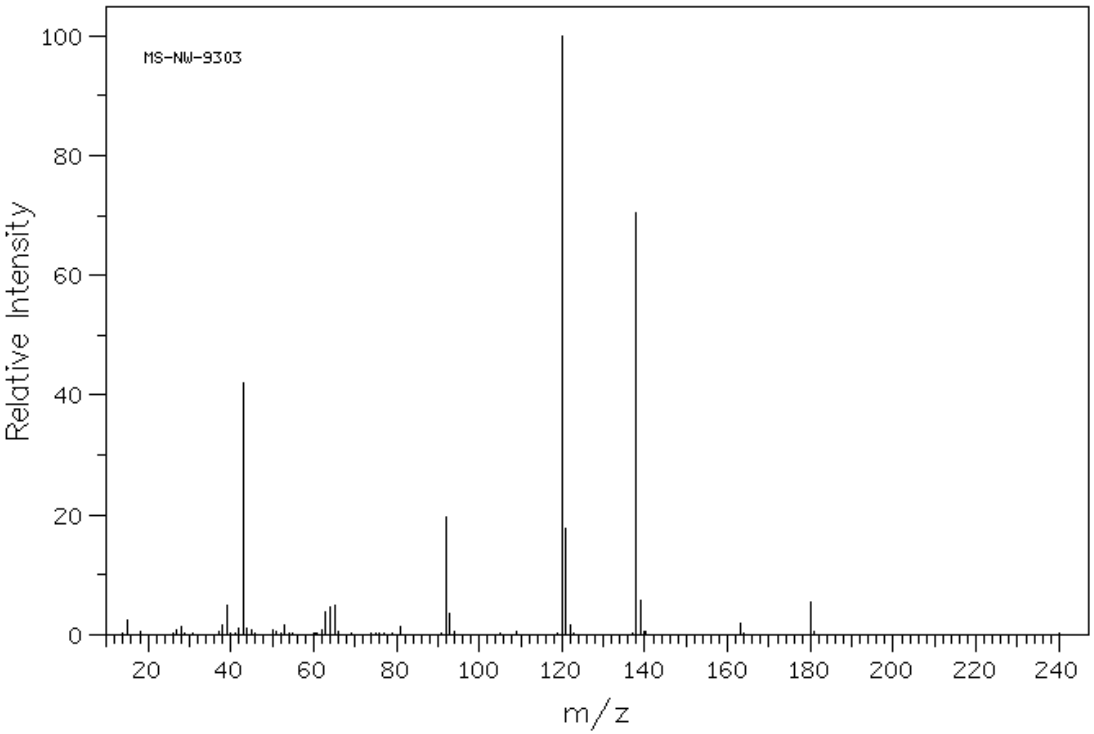
Spectral Code:
Mass :
^{13}C NMR : in $CDCl_3$
^{1}H NMR : 400 MHz in $CDCl_3$
IR : KBr disc
IR : nujol mull
Raman : 4880 A,200 M,powder

Chemical Information:

Return to Search:
Return to Result:

SDBS-Mass

```
MS-NW-9303          SDBS NO.   532
o-acetoxybenzoic acid
C9H8O4              (Mass of molecular ion:    180)
```




```
Source Temperature: 170 °C
Sample Temperature: 100 °C
DIRECT, 75 eV
```

peak data

MS-NW-9303 SDBS NO. 532

SDBS Information

SDBS No.: 532

Compound Name:
o-acetoxybenzoic acid

Molecular Formula: $C_9H_8O_4$

Molecular Weight: 180.2

CAS Registry No.:
50-78-2

Spectral Code:
Mass :
^{13}C NMR : in $CDCl_3$
^{1}H NMR : 400 MHz in $CDCl_3$
IR : KBr disc
IR : nujol mull
Raman : 4880 A,200 M,powder

Chemical Information:

Return to Search:
Return to Result:

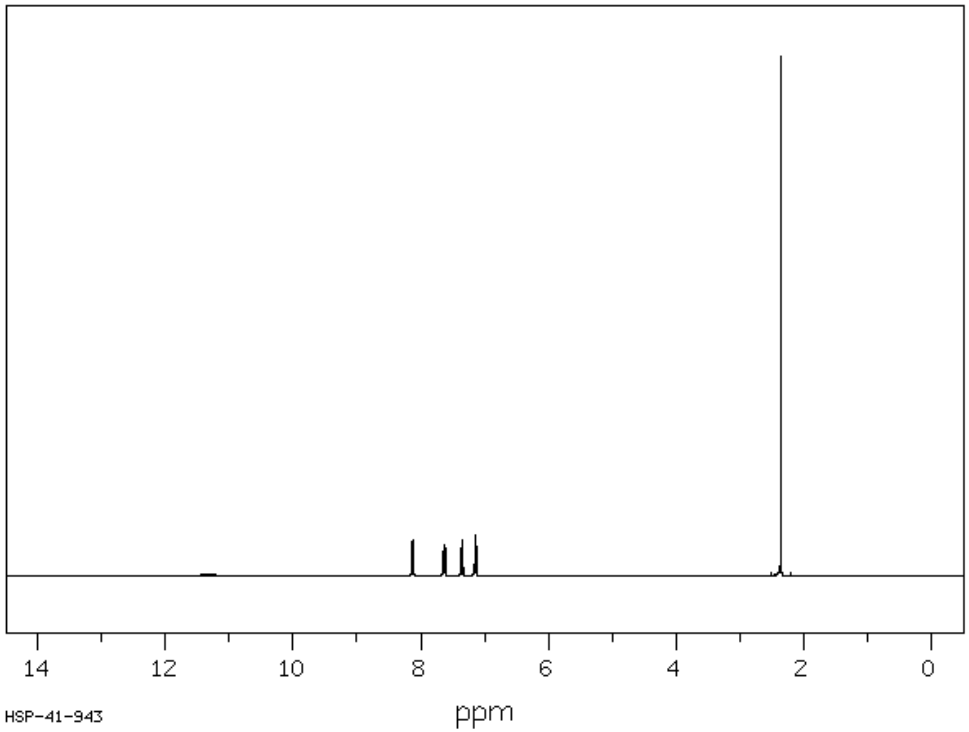
SDBS-^{1}H NMR SDBS No. 532HSP-41-943

399.65 MHz

C_9 H_8 O_4

0.039 g : 0.5 ml $CDCl_3$

o-acetoxybenzoic acid



A division of the American Chemical Society

SciFinder® - Part of the Process™

SciFinder is the leading research tool used by scientists around the world. Scientists use SciFinder to access single- and multi-step reactions, experimental and predicted properties, and substance information from the CAS REGISTRY, the "gold standard" for chemical substance information. Its advanced search and analysis tools makes SciFinder a vital part of today's research process.

SciFinder®
Part of the process.™

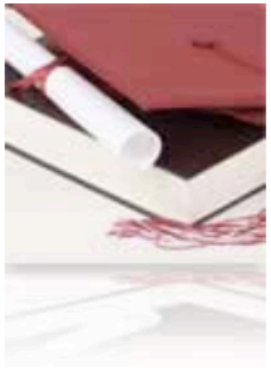
You can explore one single source for scientific information in journal and patent literature from around the world.

See a demo of SciFinder!

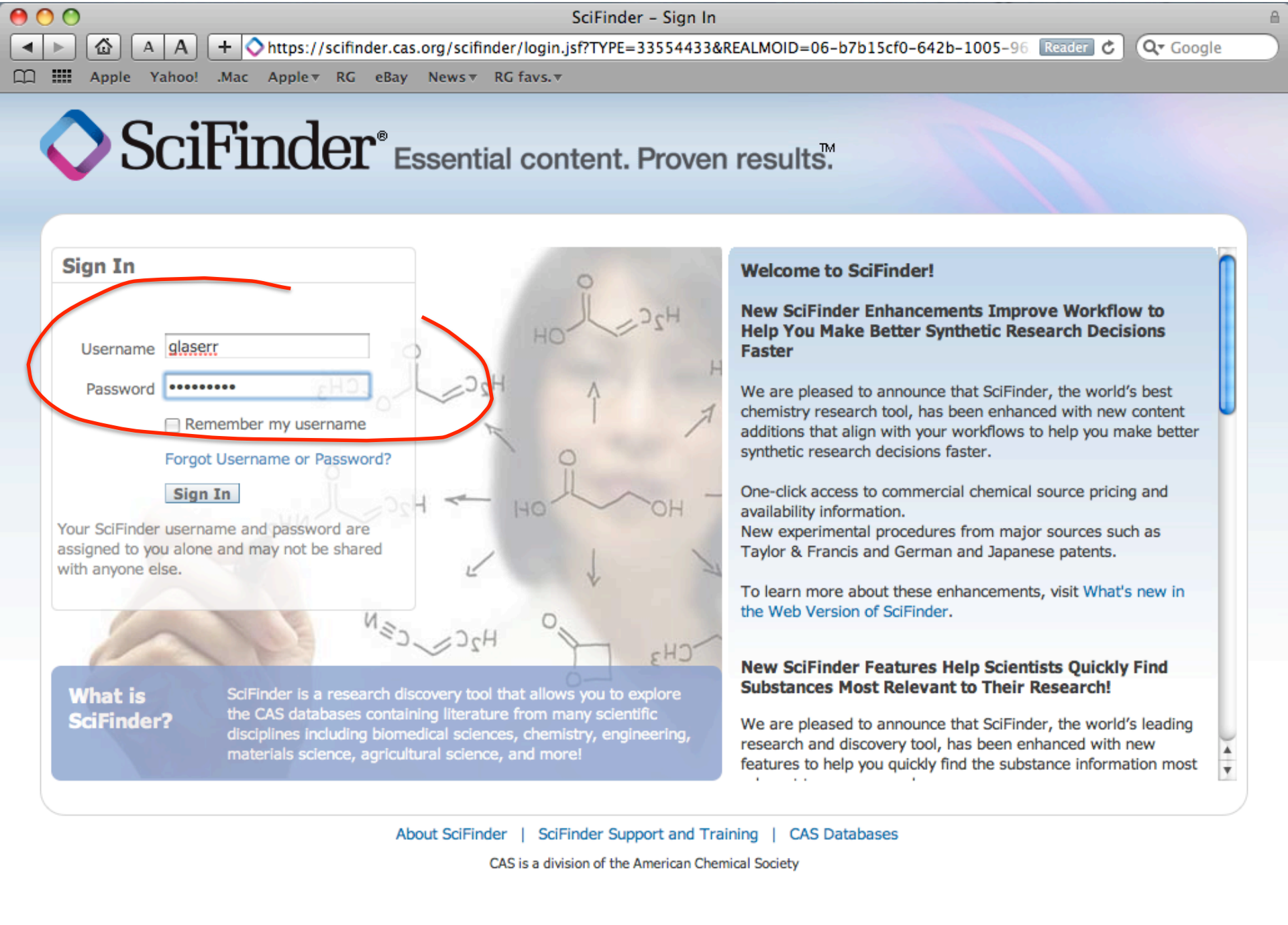
Chemistry

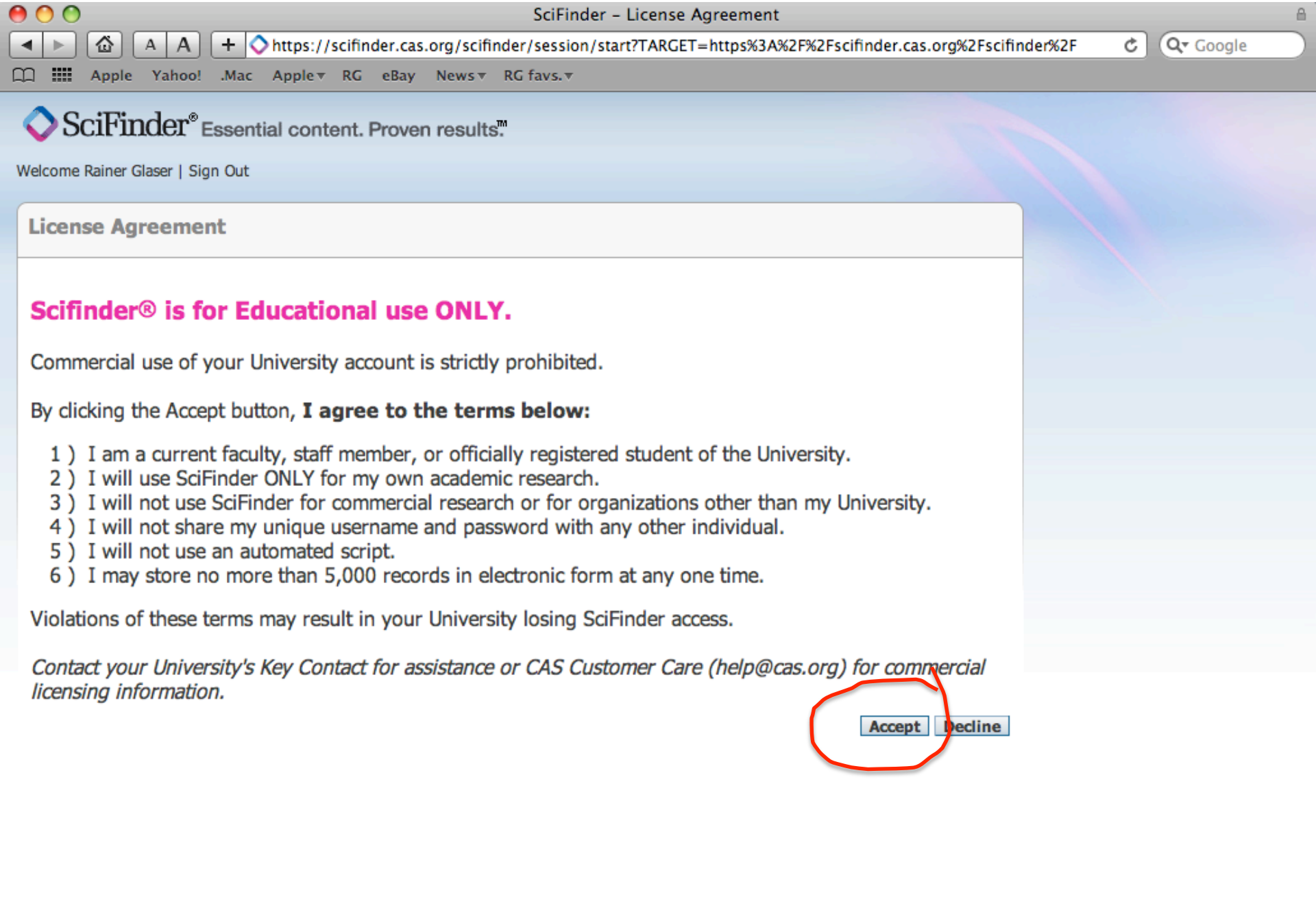
Biology

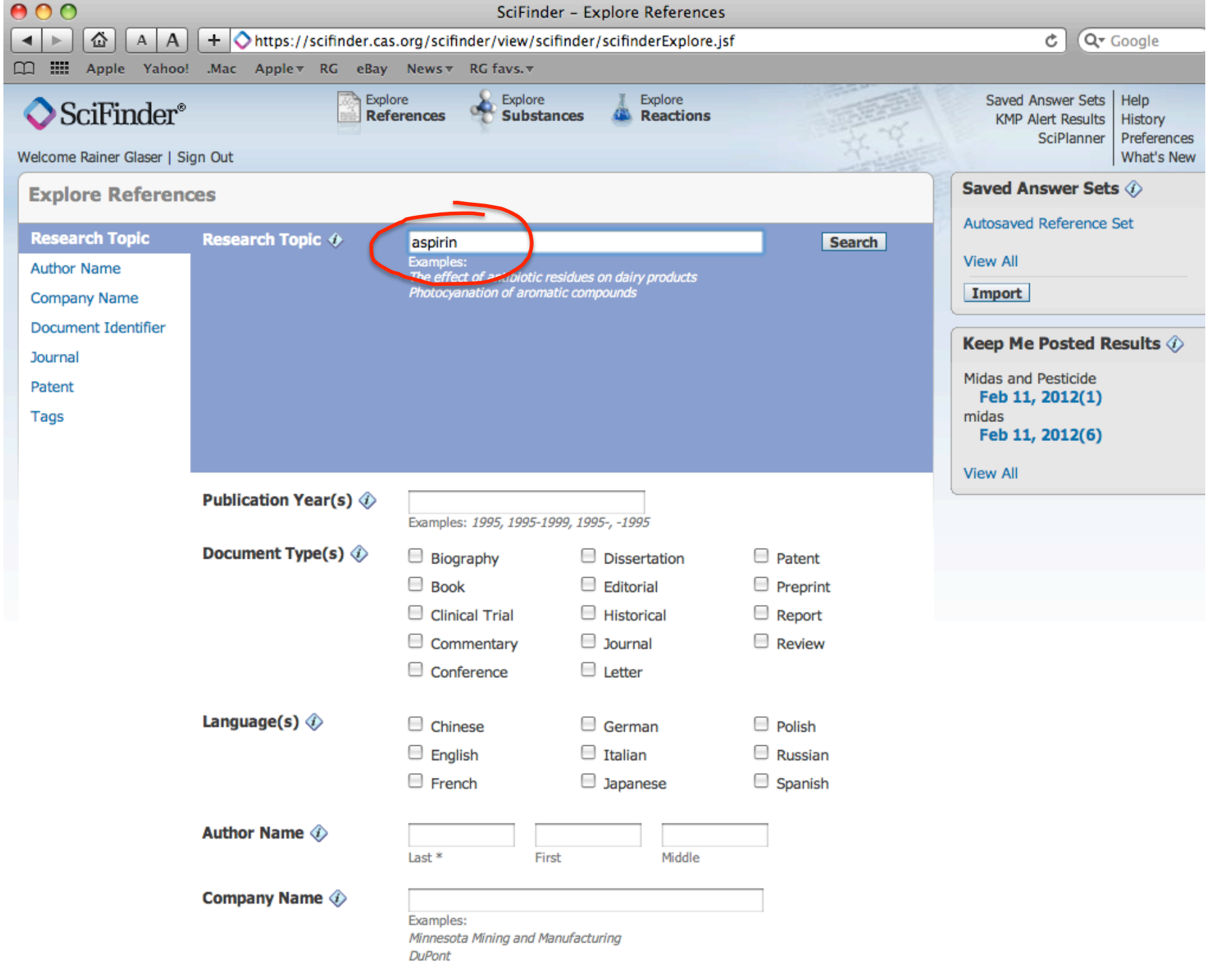
Biomass

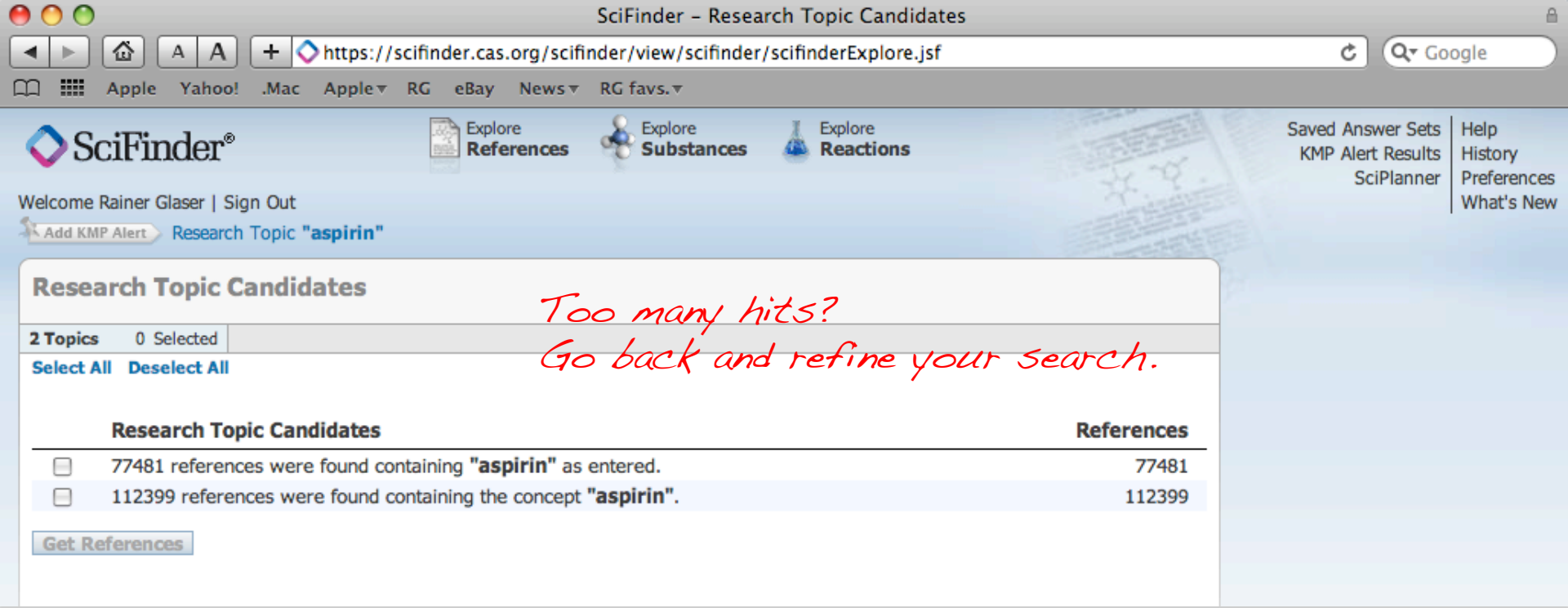


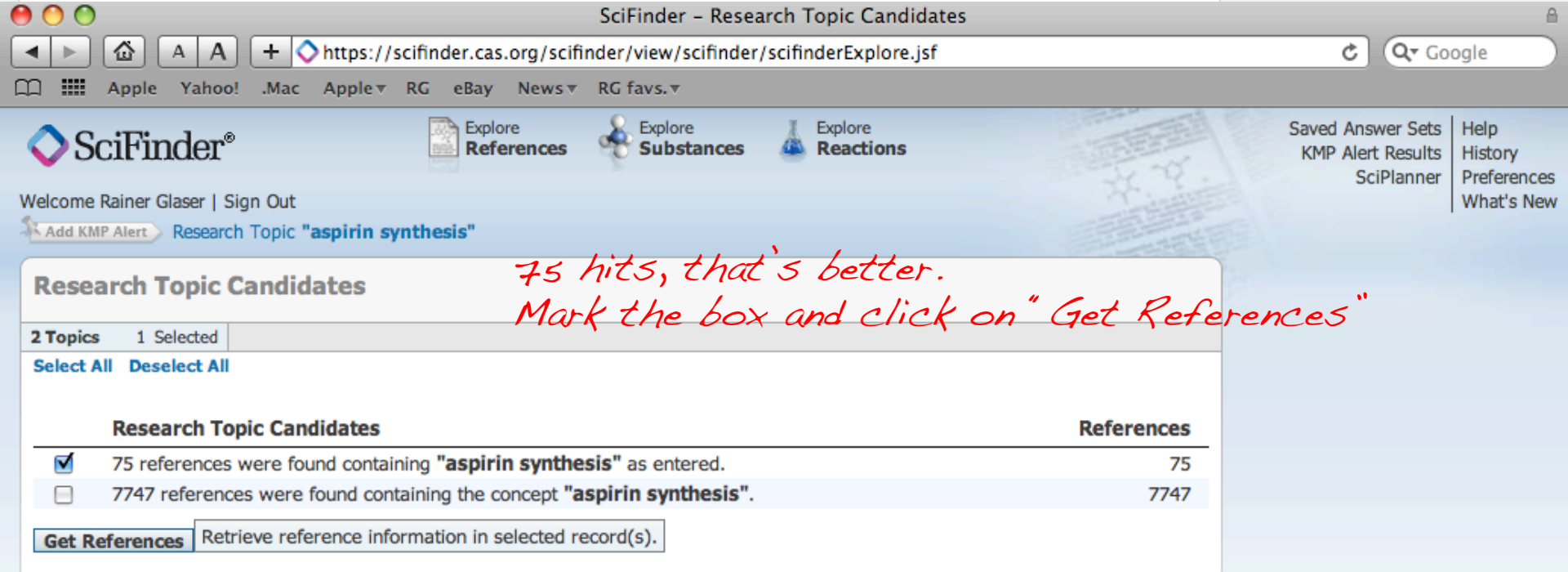
Academia


SciFinder – Sign In
https://scifinder.cas.org/scifinder/login.jsf?TYPE=33554433&REALMOID=06-b7b15cf0-642b-1005-96
Reader
Google
Apple
Yahoo!
.Mac
Apple
RG
eBay
News
RG favs.
SciFinder®
Essential content. Proven results.™
Sign In
Username
glaserr
Password
Remember my username
Forgot Username or Password?
Sign In
Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.
What is SciFinder?
SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!
Welcome to SciFinder!
New SciFinder Enhancements Improve Workflow to Help You Make Better Synthetic Research Decisions Faster
We are pleased to announce that SciFinder, the world's best chemistry research tool, has been enhanced with new content additions that align with your workflows to help you make better synthetic research decisions faster.
One-click access to commercial chemical source pricing and availability information.
New experimental procedures from major sources such as Taylor & Francis and German and Japanese patents.
To learn more about these enhancements, visit What's new in the Web Version of SciFinder.
New SciFinder Features Help Scientists Quickly Find Substances Most Relevant to Their Research!
We are pleased to announce that SciFinder, the world's leading research and discovery tool, has been enhanced with new features to help you quickly find the substance information most
About SciFinder | SciFinder Support and Training | CAS Databases
CAS is a division of the American Chemical Society


SciFinder – License Agreement
https://scifinder.cas.org/scifinder/session/start?TARGET=https%3A%2F%2Fscifinder.cas.org%2Fscifinder%2F
Google
Apple
Yahoo!
.Mac
Apple
RG
eBay
News
RG favs.
SciFinder® Essential content. Proven results.℠
Welcome Rainer Glaser | Sign Out
License Agreement
Scifinder® is for Educational use ONLY.
Commercial use of your University account is strictly prohibited.
By clicking the Accept button, I agree to the terms below:
1) I am a current faculty, staff member, or officially registered student of the University.
2) I will use SciFinder ONLY for my own academic research.
3) I will not use SciFinder for commercial research or for organizations other than my University.
4) I will not share my unique username and password with any other individual.
5) I will not use an automated script.
6) I may store no more than 5,000 records in electronic form at any one time.
Violations of these terms may result in your University losing SciFinder access.
Contact your University's Key Contact for assistance or CAS Customer Care (help@cas.org) for commercial licensing information.
Accept
Decline


SciFinder – Explore References
https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
SciFinder®
Explore References
Explore Substances
Explore Reactions
Saved Answer Sets
KMP Alert Results
SciPlanner
Help
History
Preferences
What's New
Welcome Rainer Glaser | Sign Out
Explore References
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
Research Topic
aspirin
Search
Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Saved Answer Sets
Autosaved Reference Set
View All
Import
Keep Me Posted Results
Midas and Pesticide
Feb 11, 2012(1)
midas
Feb 11, 2012(6)
View All
Publication Year(s)
Examples: 1995, 1995-1999, 1995-, -1995
Document Type(s)
Biography
Book
Clinical Trial
Commentary
Conference
Dissertation
Editorial
Historical
Journal
Letter
Patent
Preprint
Report
Review
Language(s)
Chinese
English
French
German
Italian
Japanese
Polish
Russian
Spanish
Author Name
Last *
First
Middle
Company Name
Examples:
Minnesota Mining and Manufacturing
DuPont


SciFinder – Research Topic Candidates
https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
SciFinder®
Explore References
Explore Substances
Explore Reactions
Saved Answer Sets
KMP Alert Results
SciPlanner
Help
History
Preferences
What's New
Welcome Rainer Glaser | Sign Out
Add KMP Alert
Research Topic "aspirin"
Research Topic Candidates
Too many hits?
Go back and refine your search.
2 Topics 0 Selected
Select All Deselect All
Research Topic Candidates
References
77481 references were found containing "aspirin" as entered. 77481
112399 references were found containing the concept "aspirin". 112399
Get References


SciFinder – Research Topic Candidates
https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
SciFinder®
Explore References
Explore Substances
Explore Reactions
Saved Answer Sets
KMP Alert Results
SciPlanner
Help
History
Preferences
What's New
Welcome Rainer Glaser | Sign Out
Add KMP Alert
Research Topic "aspirin synthesis"
Research Topic Candidates
75 hits, that's better.
Mark the box and click on "Get References"
2 Topics 1 Selected
Select All Deselect All
Research Topic Candidates
References
75 references were found containing "aspirin synthesis" as entered. 75
7747 references were found containing the concept "aspirin synthesis". 7747
Get References
Retrieve reference information in selected record(s).

References

Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

75 References | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [20] | 1 2 3 4

Display:

1. **Research progress in application of ionic liquids to aspirin synthesis** Full Text
By Wang, Zhan-jun; Xiao, Peng; Yang, Yue; Wang, Xiao-dan
From Dangdai Huagong (2011), 40(7), 762-764. | Language: Chinese, Database: CAPLUS
Structure, property, classification and **synthesis** of ionic liqs. were briefly reviewed. Research situation of ionic liqs. in **aspirin synthesis** at home in recent years was introduced; some development proposals were also put forward. Lastly, development trend of ionic liqs. in **aspirin synthesis** was prospected.

2. **Synthesis and evaluation of conjugates of non-steroidal anti-inflammatory drugs (NSAIDs) with valproic acid for antiproliferative properties and apoptosis induction** Full Text
By Mali, Sunil V.; Himaja, M.; Khanna, Amit; Periyasamy, Giridharan; Sikarwar, Mukesh
From Journal of Pharmacy Research (2011), 4(7), 2136-2139. | Language: English, Database: CAPLUS
Valproic acid, an antiepileptic drug showed anticancer effects by inhibition of histone deacetylase (HDAC inhibitor). In this study, we have synthesized conjugates of valproic acid-NSAID such as **aspirin**, indomethacin, naproxen and sulindac contg. Pro-Lys dipeptide linker. Their cytotoxicity was tested in different cancer cell lines. Sulindac-valproic acid conjugate 4c showed moderate cytotoxicity in various cancer cell lines. The pro-apoptotic genes were upregulated in the colorectal cell line treated with compd. 4c. These in vitro findings suggest that valproic acid - NSAID conjugates showed better efficacy by inducing apoptosis in colorectal cells.

3. **Discussion on selection of catalysts used in the synthesis of aspirin** Full Text
By Zhao, Zhixiong
From Huagong Shikan (2011), 25(2), 27-29. | Language: Chinese, Database: CAPLUS
During the **synthesis** of **aspirin** in org. chem. lab., concd. sulfuric acid is often used as catalyst. Concd. sulfuric acid catalyst has disadvantage of low yield, high corrosivity and heavy pollution to environment, and can not be recovered and reused, and side reactions are easily occurred. In this paper, sodium bisulfate as catalyst in the catalytic **synthesis** of **aspirin** is feasible by selecting three lab. common chems. as catalysts and comparing expt. results, environmental friendliness, consumption and so on.

4. **Synthesis of salicylic acid saccharide carboxylate and evaluation of their bioactivity** Full Text
By Wu, Xue-fen; Ma, Jin-gang; Hou, Yi-min; Cui, Xiao-ge; Sun, De-mei
From Zhongyi Xuebao (2011), 26(3), 333-335. | Language: Chinese, Database: CAPLUS
The objective of this paper is to prep. salicylic acid saccharide carboxylate, evaluate their irritation activity and biol. activity. The salicylic acid saccharide carboxylate were prepd. through carboxylic acid-org. alkali, and the acetylated salicylic glucopyranose tetraacetate was synthesized by sequential elution; the structure of the products were identified by 1H-NMR and IR. The anticoagulant activity and anti-inflammatory activities were resp. evaluated by the cutting tail in mice and the models of mice ear edema induced by xylene, and the irritation activity was obsd. by tissue slices. Results show that four beta-configuration salicylic acid saccharide carboxylate were prepd. and three

Analysis | Refine

Analyze by:

Author Name

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

An Shengji	2
Begaliev Sh S	2
Del Soldato Piero	2
Garcia Marilyn	2
Giustarini Daniela	2
Kiyashev D K	2
Knaus Edward E	2
Kong Xiangping	2
Liang Jiulai	2
Perrino Elena	2

Show More

Categorize

More detailed analysis based on CAS indexing

Categorize

References

Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

75 References | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Citing References | Answers per Page [20] | 1 2 3 4

Display:

1. **Synthesis of 5-(2-,3- and 4-methoxyphenyl)-4H-1,2,4-triazole-3-thiol derivatives exhibiting anti-inflammatory activity** Full Text
By Labanauskas, L.; Udrenaite, E.; Gaidelis, P.; Brukstus, A.
From Farmaco (2004), 59(4), 255-259. | Language: English, Database: CAPLUS ~61
New S-alkylated 5-(2-,3- and 4-methoxyphenyl)-4H-1,2,4-triazole-3-thiols and 5-(2-,3- and 4-methoxyphenyl)-4-phenyl-4H-1,2,4-triazole-3-thiols were synthesized by the alkylation of 3-(2-,3- and 4-methoxyphenyl)-4,5-dihydro-1H-1,2,4-triazole-5-thiones or 3-(2-,3- and 4-methoxyphenyl)-4-phenyl-4,5-dihydro-1H-1,2,4-triazole-5-thiones with 1-iodobutane or 1-(1,3-benzodioxol-5-yl)-2-bromo-1-ethanone, 2-bromo-1-(2,3-dihydro-1,4-benzodioxin-6-yl)-1-ethanone and 2-bromo-1-(3,4-dihydro-2H-1,5-benzodioxepin-7-yl)-1-ethanone. Many of the synthesized compds exhibited anti-inflammatory activity in rat model of carrageenin- and bentonite-induced paw edema. Structure activity relations are discussed.

2. **Synthesis, anticonvulsant, and anti-inflammatory evaluation of some new benzotriazole and benzofuran-based heterocycles** Full Text
By Dawood, Kamal M.; Abdel-Gawad, Hassan; Rageb, Eman A.; Ellithey, Mohey; Mohamed, Hanan A.
From Bioorganic & Medicinal Chemistry (2006), 14(11), 3672-3680. | Language: English, Database: CAPLUS ~52
Treatment of 2-bromoacetylbenzofuran with 1H-benzotriazole afforded 1-(benzofuran-2-yl)-2-(benzotriazol-1-yl) ethanone which reacted with phenylisothiocyanate to give the corresponding thioacetanilide derivs. Treatment of the latter ethanone and thioacetanilide derivs. with hydrazonoyl chlorides afforded the corresponding pyrazole and 1,3,4-thiadiazole derivs. The thioacetanilide deriv. reacted with α-haloketones and α-halodiketones to afford thiophene and thiazole derivs., resp. The newly synthesized compds. were found to possess anticonvulsant and anti-inflammatory activities with the same mechanism of action of selective COX-2 inhibitors.

3. **O2-Acetoxymethyl-protected diazeniumdiolate-based NSAIDs (NONO-NSAIDs): Synthesis, nitric oxide release, and biological evaluation studies** Full Text
By Velazquez, Carlos A.; Rao, P. N. Praveen; Citro, Michael L.; Keefer, Larry K.; Knaus, Edward E.
From Bioorganic & Medicinal Chemistry (2007), 15(14), 4767-4774. | Language: English, Database: CAPLUS ~31
A novel group of O2-acetoxymethyl-protected diazeniumdiolate-based nonsteroidal anti-inflammatory prodrugs (NONO-NSAIDs) were synthesized by esterifying the carboxylate group of **aspirin**, ibuprofen, or indomethacin with O2-acetoxymethyl 1-[N-(2-hydroxyethyl)-N-methylamino]diazeniumdiolate. The resulting nitric oxide (•>NO)-releasing prodrugs (7-9) did not exhibit in vitro cyclooxygenase (COX) inhibitory activity against the COX-1 and COX-2 isoenzymes (IC50s > 100 μM). In contrast, prodrugs 7 and 8 significantly decreased carrageenan-induced rat paw edema showing enhanced in vivo anti-inflammatory activities (ID50's = 552 and 174 μmol/kg, resp.) relative to those of the parent NSAIDs **aspirin** (ID50 = 714 μmol/kg) and ibuprofen (ID50 = 326 μmol/kg). The rate of porcine liver esterase-mediated •NO release from prodrugs 7-9 (2 mol of •NO/mol of test compd. in 0.6-6.5 min) was substantially higher compared to that obsd. without enzymic catalysis (about 1 mol of •NO/mol of test

Analysis | Refine

Analyze by:

Author Name

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

An Shengji	2
Begaliev Sh S	2
Del Soldato Piero	2
Garcia Marilyn	2
Giustarini Daniela	2
Kiyashev D K	2
Knaus Edward E	2
Kong Xiangping	2
Liang Jiulai	2
Perrino Elena	2

Show More

Categorize

More detailed analysis based on CAS indexing

Categorize

By Basudhar, Debashree; Ridnour, Lisa A.; Wink, David A.; Miranda, Katrina M.
From Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009 (2009), BIOL-014. | , Database: CAPLUS ~0

Aspirin belongs to the class of non-steroidal anti inflammatory drugs (NSAIDs), which are commonly used to relieve pain and inflammation. NSAIDs also inhibit proliferation of cancer cells and decrease risk of Alzheimer's disease in adults before the onset of age-assocd. inflammatory processes within the brain. Although NSAIDs has been shown to be effective against these conditions, they can have serious side effects, particularly gastrointestinal ulcers with chronic use. To improve the safety profile of these drugs, a second generation of NSAIDs (COXIBs) has been synthesized. Despite the initial success of COXIBs, long term cardiovascular side effects have led to withdrawal of several such drugs from the market. Nitric oxide (NO) and nitroxyl (HNO) are important modulators of numerous physiol. functions such as vasodilation, inhibition of platelet aggregation and tumor regression. In the central nervous system, NO is a neurotransmitter involved in memory function. In this regard, adducts of NSAIDs and COXIBs with NO have been synthesized that will allow retention of traditional analgesic properties and redn. of side effects. In this presentation, **synthesis** and NO and HNO release properties of new NO and HNO-**aspirin** adducts will be discussed. Also the effects of these mols. on different signaling pathways will be presented to understand the mechanism of action.

19. **One step method for synthesis of copper aspirin** Full Text
By Zhang, Jingdong; Wang, Sihong; Zhang, Xiaoyong; Yao, Yanhong; Piao, Yingai; Li, Donghao
From Faming Zhuanli Shenqing Gongkai Shuomingshu (2009), CN 101456816 A 20090617. | Language: Chinese, Database: CAPLUS ~0

The method comprises metathetic reaction of **aspirin** and copper salt aq. soln. in org. solvent to obtain copper **aspirin**. The org. solvent comprises acetone, 2-butanone, THF, dioxane or methanol. The copper salt comprises copper sulfate, copper nitrate, copper chloride or copper acetate. The yield is high and the purity is high.

20. **Dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin and ibuprofen: Synthesis, biological evaluation and nitric oxide release studies** Full Text
By Abdellatif, Khaled R. A.; Chowdhury, Morshed Alam; Dong, Ying; Das, Dipankar; Yu, Gang; Velazquez, Carlos A.; Suresh, Mavanur R.; Knaus, Edward E.
From Bioorganic & Medicinal Chemistry Letters (2009), 19(11), 3014-3018. | Language: English, Database: CAPLUS ~7

A new group of hybrid nitric oxide (NO) releasing anti-inflammatory (AI) ester prodrugs (NONO-NSAIDs) wherein a 1,3-dinitrooxy-2-Pr (12a-c), or O2-acetoxymethyl-1-[2-(methyl)pyrrolidin-1-yl]diazen-1-ium-1,2-diolate (14a-c), NO-donor moiety is directly attached to the carboxylic acid group of **aspirin**, indomethacin or ibuprofen were synthesized. NO release from the dinitrooxypropyl, or diazen-1-ium-1,2-diolate, ester prodrugs was increased substantially upon incubation in the presence of L-cysteine (12a-c) or rat serum (14a-c). The ester prodrugs (12a-c, 14a-c), which did not inhibit the COX-1 isoenzyme, exhibited modest inhibitory activity against the COX-2 isoenzyme. The NONO-NSAIDs 12a-c and 14a-c exhibited in vivo AI activity that was similar to that exhibited by the parent drug **aspirin**, indomethacin or ibuprofen when the same oral dose (μmol/kg) was administered. These similarities in oral potency profiles suggest these NONO-NSAIDs act as classical prodrugs that require metabolic activation by esterase-mediated hydrolysis. Hybrid NO-donor/anti-inflammatory prodrugs of this type (NONO-NSAIDs) offer a potential drug design concept targeted toward the development of anti-inflammatory drugs with reduced adverse gastrointestinal effects.

Contact Us | Copyrights and Trademarks
Copyright © 2012 American Chemical Society. All Rights Reserved.

SciFinder - Dinitroglyceryl...
https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
SciFinder®
Explore References
Explore Substances
Explore Reactions
Saved Answer Sets
KMP Alert Results
SciPlanner
Help
History
Preferences
What's New
Welcome Rainer Glaser | Sign Out
Add KMP Alert
Research Topic "aspirin synthesis" > references (75) > Dinitroglyceryl and diazen-1-i...
Reference Detail
Get Substances
Get Reactions
Get Cited
Get Citing
Get Full Text
Send to SciPlanner
Link
Save
Print
Export
Return
Previous
Next

20. Dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin and ibuprofen: Synthesis, biological evaluation and nitric oxide release studies

By: Abdellatif, Khaled R. A.; Chowdhury, Morshed Alam; Dong, Ying; Das, Dipankar; Yu, Gang; Velazquez, Carlos A.; Suresh, Mavanur R.; Knaus, Edward E.

A new group of hybrid nitric oxide (NO) releasing anti-inflammatory (AI) ester prodrugs (NONO-NSAIDs) wherein a 1,3-dinitrooxy-2-Pr (12a-c), or O2-acetoxymethyl-1-[2-(methyl)pyrrolidin-1-yl]diazen-1-ium-1,2-diolate (14a-c), NO-donor moiety is directly attached to the carboxylic acid group of aspirin, indomethacin or ibuprofen were synthesized. NO release from the dinitrooxypropyl, or diazen-1-ium-1,2-diolate, ester prodrugs was increased substantially upon incubation in the presence of L-cysteine (12a-c) or rat serum (14a-c). The ester prodrugs (12a-c, 14a-c), which did not inhibit the COX-1 isoenzyme, exhibited modest inhibitory activity against the COX-2 isoenzyme. The NONO-NSAIDs 12a-c and 14a-c exhibited in vivo AI activity that was similar to that exhibited by the parent drug aspirin, indomethacin or ibuprofen when the same oral dose (μmol/kg) was administered. These similarities in oral potency profiles suggest these NONO-NSAIDs act as classical prodrugs that require metabolic activation by esterase-mediated hydrolysis. Hybrid NO-donor/anti-inflammatory prodrugs of this type (NONO-NSAIDs) offer a potential drug design concept targeted toward the development of anti-inflammatory drugs with reduced adverse gastrointestinal effects.

Indexing

Pharmacology (Section1-7)

Section cross-reference(s): 26

Concepts

Structure-activity relationship

inflammation-inhibiting; synthesis, biol. evaluation, and nitric oxide release studies of dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin, and ibuprofen NSAIDS

Drug metabolism Nonsteroidal anti-

Substances

329900-75-6 Cyclooxygenase-2

inhibition; synthesis, biol. evaluation, and nitric oxide release studies of dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin, and ibuprofen NSAIDS

Biological study, unclassified; Biological study

Quick Links

0 Tags, 0 Comments

Source

Bioorganic & Medicinal Chemistry Letters
Volume19
Issue11
Pages3014-3018
Journal
2009
CODEN:BMCLE8
ISSN:0960-894X
DOI:10.1016/j.bmcl.2009.04.059

Company/Organization

Faculty of Pharmacy and Pharmaceutical Sciences
University of Alberta
Edmonton, AB, Can. T6G 2N8

Accession Number

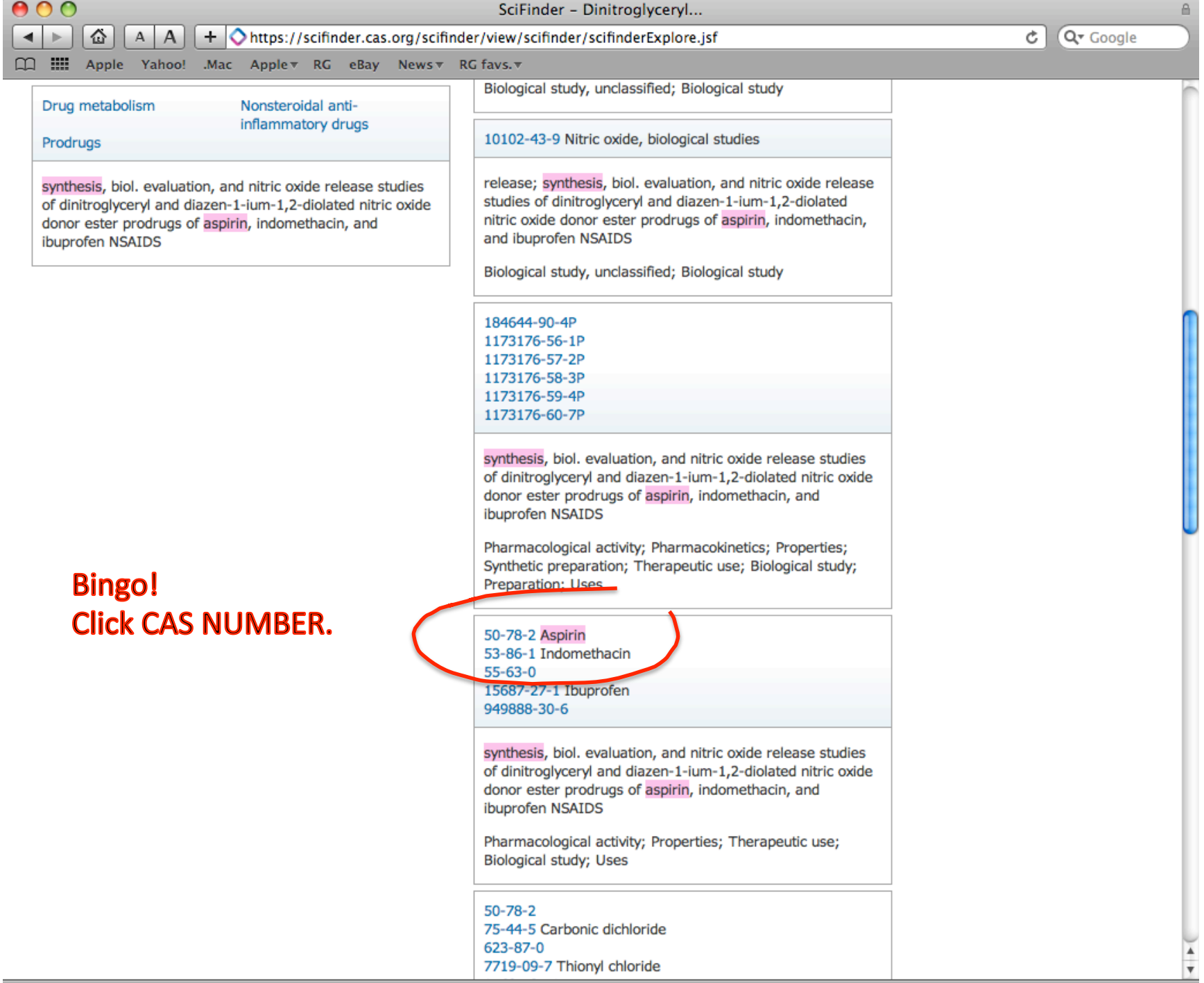
2009:603803
CAN151:163643
CAPLUS

Publisher

Elsevier B.V.

Language

English


SciFinder - Dinitroglyceryl...
https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
Drug metabolism
Nonsteroidal anti-inflammatory drugs
Prodrugs
synthesis, biol. evaluation, and nitric oxide release studies of dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin, and ibuprofen NSAIDS
Biological study, unclassified; Biological study
10102-43-9 Nitric oxide, biological studies
release; synthesis, biol. evaluation, and nitric oxide release studies of dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin, and ibuprofen NSAIDS
Biological study, unclassified; Biological study
184644-90-4P
1173176-56-1P
1173176-57-2P
1173176-58-3P
1173176-59-4P
1173176-60-7P
synthesis, biol. evaluation, and nitric oxide release studies of dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin, and ibuprofen NSAIDS
Pharmacological activity; Pharmacokinetics; Properties; Synthetic preparation; Therapeutic use; Biological study; Preparation; Uses
50-78-2 Aspirin
53-86-1 Indomethacin
55-63-0
15687-27-1 Ibuprofen
949888-30-6
synthesis, biol. evaluation, and nitric oxide release studies of dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin, and ibuprofen NSAIDS
Pharmacological activity; Properties; Therapeutic use; Biological study; Uses
50-78-2
75-44-5 Carbonic dichloride
623-87-0
7719-09-7 Thionyl chloride
Bingo!
Click CAS NUMBER.

Substance Detail

Get References | Get Reactions | Get Commercial Sources | Get Regulatory Info | Send to SciPlanner

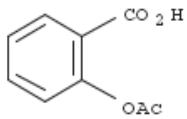
Link | Save | Print | Export

CAS Registry Number: 50-78-2

$C_9H_8O_4$

Benzoic acid, 2-(acetyloxy)-

Rhodine (7CI); Salicylic acid acetate (8CI); 2-(Acetyloxy)benzoic acid; 2-Acetoxybenzoic acid; 2-Carboxyphenyl acetate; A.S.A. Empirin; AC 5230; ASA; Acenterine; Acesal; Acesan; Acetard; Aceticyl; Acetilum acidulatum; Acetisal; Acetol; Acetonyl; Acetophen; Acetosal; Acetosalic acid; Acetosalin; Acetylin; Acetylsal; Acetylsalicylic acid; Acetyonyl; Acetysal; Acidum acetylsalicylicum; Acimetten; Acisal; Acylpyrin; Adiro; Albyl E; Anopyrin; Asaflow; Asagran; Asatard; Ascoden 30; Ascolong; Ascriptin; Aspalon; Aspergum; Aspirdrops; Aspirin; Aspirin Protect 100; Aspirin Protect 300; Aspirin-Direkt; Aspirina 03; Aspirine; Aspro; Aspro Clear; Aspropharm; Asteric; Astrix; Benaspir; Bialpirina; Bialpirinia; Caprin; Cardioaspirin; Cardioaspirina; Cardiomagnyl; Claradin; Colfarit; Colsprin; Contrheuma Retard; Coraspin; Coricidin; Coricidin D; Crystar; Darvon Compound; Dolean pH 8; Dominal; Doril; Duramax; ECM; Easprin; Ecopirin; Ecosprin; Ecotrin; Empirin; Endosprin; Endydol; Entericin; Enterophen; Enterosarine; Entrophen; Ewin; Extren; Gelprin; Globentyl; Globoid; Helicon; Idragin; Istopirin; Kapsazal; Lysoprin (pharmaceutical); Magnecyl; Measurin; Medisyl; Melhoral; Micristin; Miniasal; Mycropyrin; NSC 27223; NSC 406186; Neuronika; Novid; Nu-seals; O-Acetylsalicylic acid; Persistin; Polopiryna; Rheumintabletten; Rhodine 2312; Rhodine NC RP; Rhonal; SP 189; Salacetin; Salcetogen; Saletin; Salospir; Salycylacetylsalicylic acid; Solpyron; Supac; Temperal; ThromboASS; Toldex; Triple-sal; Trombyl; Xaxa; Yasta; Zorprin; o-(Acetyloxy)benzoic acid; o-Acetoxybenzoic acid; o-Carboxyphenyl acetate



Deleted CAS Registry Numbers: 2349-94-2, 11126-35-5, 11126-37-7, 26914-13-6, 98201-60-6

~29,039 References

~29,039 References

Document Types: Book, Conference, Dissertation, Journal, Patent, Preprint, Report

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Combinatorial Study	✓		✓	
Formation, Nonpreparative	✓	✓		✓
Miscellaneous	✓	✓		✓
Occurrence	✓	✓		✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓			
Reactant or Reagent	✓	✓	✓	✓
Uses	✓	✓	✓	✓

▸ **Bioactivity Indicators** NEW

▸ **Target Indicators** NEW

Predicted Properties: Biological Chemical Density Lipinski and Related Spectra Structure-related Thermal

Biological Properties	Value	Condition	Note
Bioconcentration Factor	6.79	pH 1 Temp: 25 °C	(94)
Bioconcentration Factor	6.60	pH 2 Temp: 25 °C	(94)
Bioconcentration Factor	5.13	pH 3 Temp: 25 °C	(94)
Bioconcentration Factor	1.59	pH 4 Temp: 25 °C	(94)
Bioconcentration Factor	1.0	pH 5 Temp: 25 °C	(94)
Bioconcentration Factor	1.0	pH 6 Temp: 25 °C	(94)
Bioconcentration Factor	1.0	pH 7 Temp: 25 °C	(94)
Bioconcentration Factor	1.0	pH 8 Temp: 25 °C	(94)
Bioconcentration Factor	1.0	pH 9 Temp: 25 °C	(94)
Bioconcentration Factor	1.0	pH 10 Temp: 25 °C	(94)

Top

Chemical Properties	Value	Condition	Note
Koc	137	pH 1 Temp: 25 °C	(94)
Koc	133	pH 2 Temp: 25 °C	(94)
Koc	103	pH 3 Temp: 25 °C	(94)
Koc	32.1	pH 4 Temp: 25 °C	(94)

Top

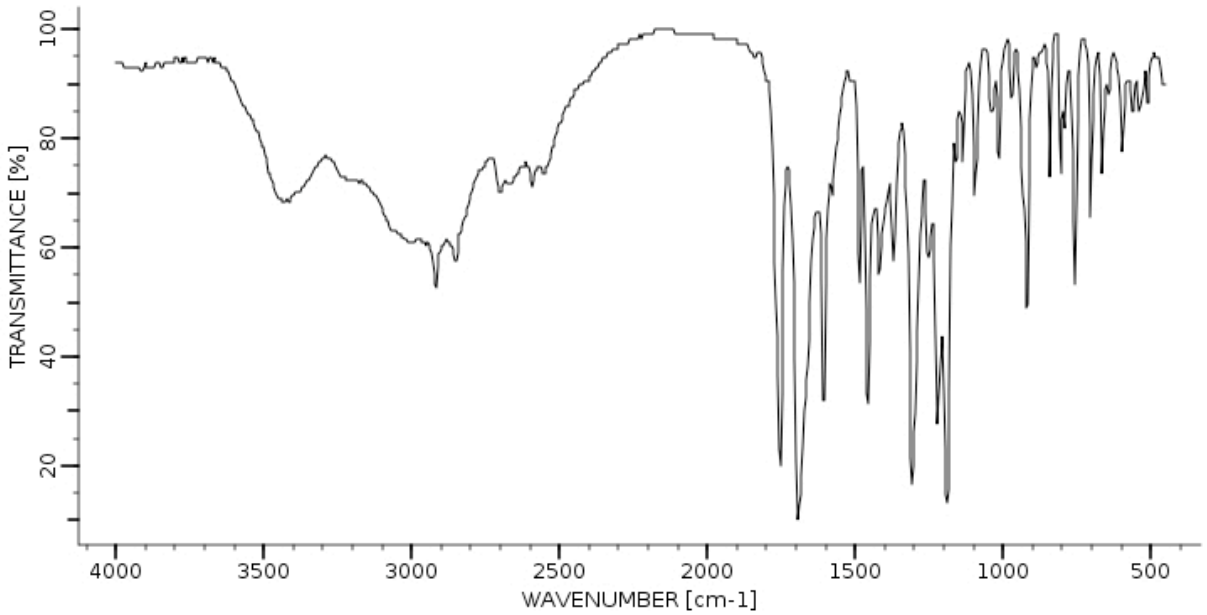
Refractive Index	1.652	Wavlen: 589.3 nm	(87)CAS
Refractive Index	1.640	Wavlen: 589.3 nm	(87)CAS
Refractive Index	1.502	Wavlen: 589.3 nm	(87)CAS
Refractive Index	1.4842-1.4936	Wavlen: 589.3 nm; Temp: 25 °C	(16)NLM

Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(5)AIST
Carbon-13 NMR Spectrum	See spectrum		(6)BIORAD
Carbon-13 NMR Spectrum	See spectrum		(7)WSS
Carbon-13 NMR Spectrum	See spectrum		(7)WSS
Carbon-13 NMR Spectrum	See spectrum		(8)WSS
Carbon-13 NMR Spectrum	See spectrum		(8)WSS
Carbon-13 NMR Spectrum	See full text	1 of 3	(9)CAS
Circular Dichroism Spectrum	See full text		(10)IC
Emission/Luminescence Spectrum	See full text		(21)CAS
IR Absorption Spectrum	See spectrum		(7)WSS
IR Absorption Spectrum	See spectrum		(7)WSS
IR Absorption Spectrum	See spectrum		(5)AIST
IR Absorption Spectrum	See spectrum		(5)AIST
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See spectrum		(28)BIORAD
IR Absorption Spectrum	See full text	1 of 16	(29)CAS
IR Reflectance Spectrum	See full text		(30)CAS
IR Spectrum	See full text	1 of 3	(31)CAS
Mass Spectrum	See spectrum		(35)BIORAD

Top

IR Absorption Spectrum

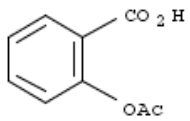
Print



CAS Registry Number: 50-78-2

$C_9H_8O_4$

Benzoic acid, 2-(acetyloxy)-



Spectrum ID

BR056823

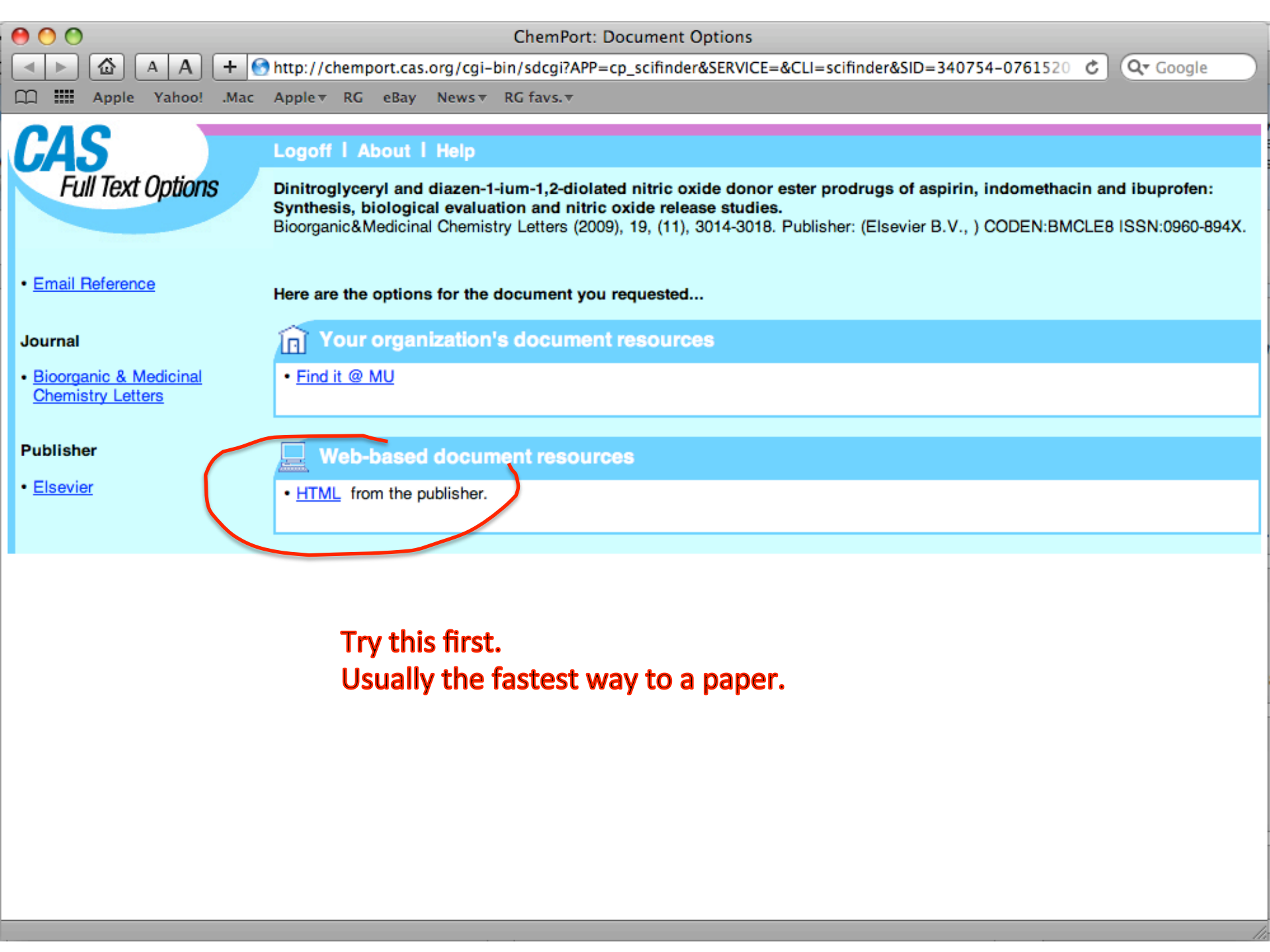
Spectrometer

BIO-RAD DIGILAB FT-IR OR EQUIVALENT

Source

Infrared spectral data from the Bio-Rad/Sadtler IR Data Collection was obtained from Bio-Rad Laboratories, Philadelphia, PA (US). Copyright © Bio-Rad Laboratories. All Rights Reserved.

Copyright © 2012 American Chemical Society. All Rights Reserved.


ChemPort: Document Options
http://chemport.cas.org/cgi-bin/sdcgi?APP=cp_scifinder&SERVICE=&CLI=scifinder&SID=340754-0761520
Google
Apple
Yahoo!
.Mac
Apple
RG
eBay
News
RG favs.
CAS Full Text Options
Logoff | About | Help
Dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin and ibuprofen: Synthesis, biological evaluation and nitric oxide release studies.
Bioorganic&Medicinal Chemistry Letters (2009), 19, (11), 3014-3018. Publisher: (Elsevier B.V.,) CODEN:BMCLE8 ISSN:0960-894X.
• Email Reference
Here are the options for the document you requested...
Journal
• Bioorganic & Medicinal Chemistry Letters
Your organization's document resources
• Find it @ MU
Publisher
• Elsevier
Web-based document resources
• HTML from the publisher.
Try this first.
Usually the fastest way to a paper.

Dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester pr...09.04.059 : Bioorganic & Medicinal Chemistry Letters | ScienceDirect.com
http://www.sciencedirect.com/science/article/pii/S0960894X09005150
Apple Yahoo! .Mac Apple RG eBay News RG favs.
SciVerse ScienceDirect
Hub | ScienceDirect | Scopus | Applications
Register | Login | Go to SciVal Suite
Home | Browse | Search | My settings | My alerts | Help
Export citation PDF (394 K) More options...
Search ScienceDirect Search

Bioorganic & Medicinal Chemistry Letters
Volume 19, Issue 11, 1 June 2009, Pages 3014–3018

Dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin and ibuprofen: Synthesis, biological evaluation and nitric oxide release studies

Khaled R.A. Abdellatif, Morshed Alam Chowdhury, Ying Dong, Dipankar Das, Gang Yu, Carlos A. Velázquez, Mavanur R. Suresh, Edward E. Knaus

Faculty of Pharmacy and Pharmaceutical Sciences, University of Alberta, Edmonton, Alta, Canada T6G 2N8

Received 24 March 2009. Revised 6 April 2009. Accepted 7 April 2009. Available online 20 April 2009.

http://dx.doi.org/10.1016/j.bmcl.2009.04.059, How to Cite or Link Using DOI
Permissions & Reprints

Abstract

A new group of hybrid nitric oxide (NO) releasing anti-inflammatory (AI) ester prodrugs (NONO-NSAIDs) wherein a 1,3-dinitrooxy-2-propyl (**12a–c**), or O^2-acetoxymethyl-1-[2-(methyl)pyrrolidin-1-yl]diazen-1-ium-1,2-diolate (**14a–c**), NO-donor moiety is directly attached to the carboxylic acid group of aspirin, indomethacin or ibuprofen were synthesized. NO release from the dinitrooxypropyl, or diazen-1-ium-1,2-diolate, ester prodrugs was increased substantially upon incubation in the presence of L-cysteine (**12a–c**) or rat serum (**14a–c**). The ester prodrugs (**12a–c, 14a–c**), which did not inhibit the COX-1 isozyme, exhibited modest inhibitory activity against the COX-2 isozyme. The NONO-NSAIDs **12a–c** and **14a–c** exhibited in vivo AI activity that was similar to that exhibited by the parent drug aspirin, indomethacin or ibuprofen when the same oral dose (μmol/kg) was administered. These similarities in oral potency profiles suggest these NONO-NSAIDs act as classical prodrugs that require metabolic activation by esterase-mediated hydrolysis.

Related articles
- Diazen-1-ium-1,2-diolated nitric oxide donor... *Bioorganic & Medicinal Chemistry*
- Diazen-1-ium-1,2-diolated and nitrooxyethyl ... *Bioorganic & Medicinal Chemistry*
- Diazen-1-ium-1,2-diolated nitric oxide donor... *Bioorganic & Medicinal Chemistry*
- Novel (E)-2-(aryl)-3-(4-methanesulfonylpheny... *Bioorganic & Medicinal Chemistry*
- O2-Acetoxymethyl-protected diazeniumdiolate-... *Bioorganic & Medicinal Chemistry*

View more related articles

Mendeley Readers
We are sorry. There is no related information available for the given article(s).

powered by MENDELEY

Table Download
Find HTML data tables from the current article to download.
Find Tables
About Table Download

MostDownloaded
Most downloaded articles from the last three months

Findit@MU Journal Article Finder

http://mulibraries.1cate.com/?sid=CAS%3ACAPLUS&issn=0960-894X&volume=19&issue=11&coden=BMCLE8&genre=

Google

Apple Yahoo! .Mac Apple RG eBay News RG favs.

MU Libraries
University of Missouri

Need Help? Ask A Librarian
Report Problems

Your article:

Author University of Alberta, Faculty of Pharmacy and Pharmaceutical Sciences

Author Abdellatif, Khaled ; Khaled R. A. Abdellatif

Title Dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin and ibuprofen: Synthesis, biological evaluation and nitric oxide release studies

Journal Title or ISSN: Bioorganic & Medicinal Chemistry Letters

Volume 19 **Issue** 11 **Year** 2009 **Pages** 3014

Bioorganic & Medicinal Chemistry Letters ISSN: 0960-894X

Full Text: 1998 — present available in *ScienceDirect - Freedom Collection (All)*

Request a copy (charges may apply if owned by MU Libraries)/ILL@MU

Journal Title or ISSN: Bioorganic & Medicinal Che

match exact title match start of title match every word in title

Find It @

or start a new search

Browse Very Long Lists of E-Journals ...

0-9 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 non-roman

SwetsWise Linker version 1.7.3b May 21, 2008

© 1999-2011, Swets

Copyright © 2011
MU Libraries, University of Missouri
104 Ellis Library, Columbia, MO 65201
Ph: (573) 882-4701

Contact Us
Report a problem with website
EEO/ADA

Dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester pr...09.04.059 : Bioorganic & Medicinal Chemistry Letters | ScienceDirect.com
http://www.sciencedirect.com/science/article/pii/S0960894X09005150
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
SciVerse ScienceDirect
Hub | ScienceDirect | Scopus | Applications
Register | Login | Go to SciVal Suite
Home | Browse | Search | My settings | My alerts | Help
Export citation PDF (394 K) More options...
Search ScienceDirect Search

ELSEVIER

Bioorganic & Medicinal Chemistry Letters

Volume 19, Issue 11, 1 June 2009, Pages 3014–3018

Dinitroglyceryl and diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of aspirin, indomethacin and ibuprofen: Synthesis, biological evaluation and nitric oxide release studies

Khaled R.A. Abdellatif, Morshed Alam Chowdhury, Ying Dong, Dipankar Das, Gang Yu, Carlos A. Velázquez, Mavanur R. Suresh, Edward E. Knaus

Faculty of Pharmacy and Pharmaceutical Sciences, University of Alberta, Edmonton, Alta, Canada T6G 2N8

Received 24 March 2009. Revised 6 April 2009. Accepted 7 April 2009. Available online 20 April 2009.

http://dx.doi.org/10.1016/j.bmcl.2009.04.059, How to Cite or Link Using DOI

Permissions & Reprints

Abstract

A new group of hybrid nitric oxide (NO) releasing anti-inflammatory (AI) ester prodrugs (NONO-NSAIDs) wherein a 1,3-dinitrooxy-2-propyl (**12a–c**), or O^2-acetoxymethyl-1-[2-(methyl)pyrrolidin-1-yl]diazen-1-ium-1,2-diolate (**14a–c**), NO-donor moiety is directly attached to the carboxylic acid group of aspirin, indomethacin or ibuprofen were synthesized. NO release from the dinitrooxypropyl, or diazen-1-ium-1,2-diolate, ester prodrugs was increased substantially upon incubation in the presence of L-cysteine (**12a–c**) or rat serum (**14a–c**). The ester prodrugs (**12a–c, 14a–c**), which did not inhibit the COX-1 isozyme, exhibited modest inhibitory activity against the COX-2 isozyme. The NONO-NSAIDs **12a–c** and **14a–c** exhibited in vivo AI activity that was similar to that exhibited by the parent drug aspirin, indomethacin or ibuprofen when the same oral dose (μmol/kg) was administered. These similarities in oral potency profiles suggest these NONO-NSAIDs act as classical prodrugs that require metabolic activation by esterase-mediated hydrolysis.

Related articles
- Diazen-1-ium-1,2-diolated nitric oxide donor... *Bioorganic & Medicinal Chemistry*
- Diazen-1-ium-1,2-diolated and nitrooxyethyl ... *Bioorganic & Medicinal Chemistry*
- Diazen-1-ium-1,2-diolated nitric oxide donor... *Bioorganic & Medicinal Chemistry*
- Novel (E)-2-(aryl)-3-(4-methanesulfonylpheny... *Bioorganic & Medicinal Chemistry*
- O2-Acetoxymethyl-protected diazeniumdiolate-... *Bioorganic & Medicinal Chemistry*

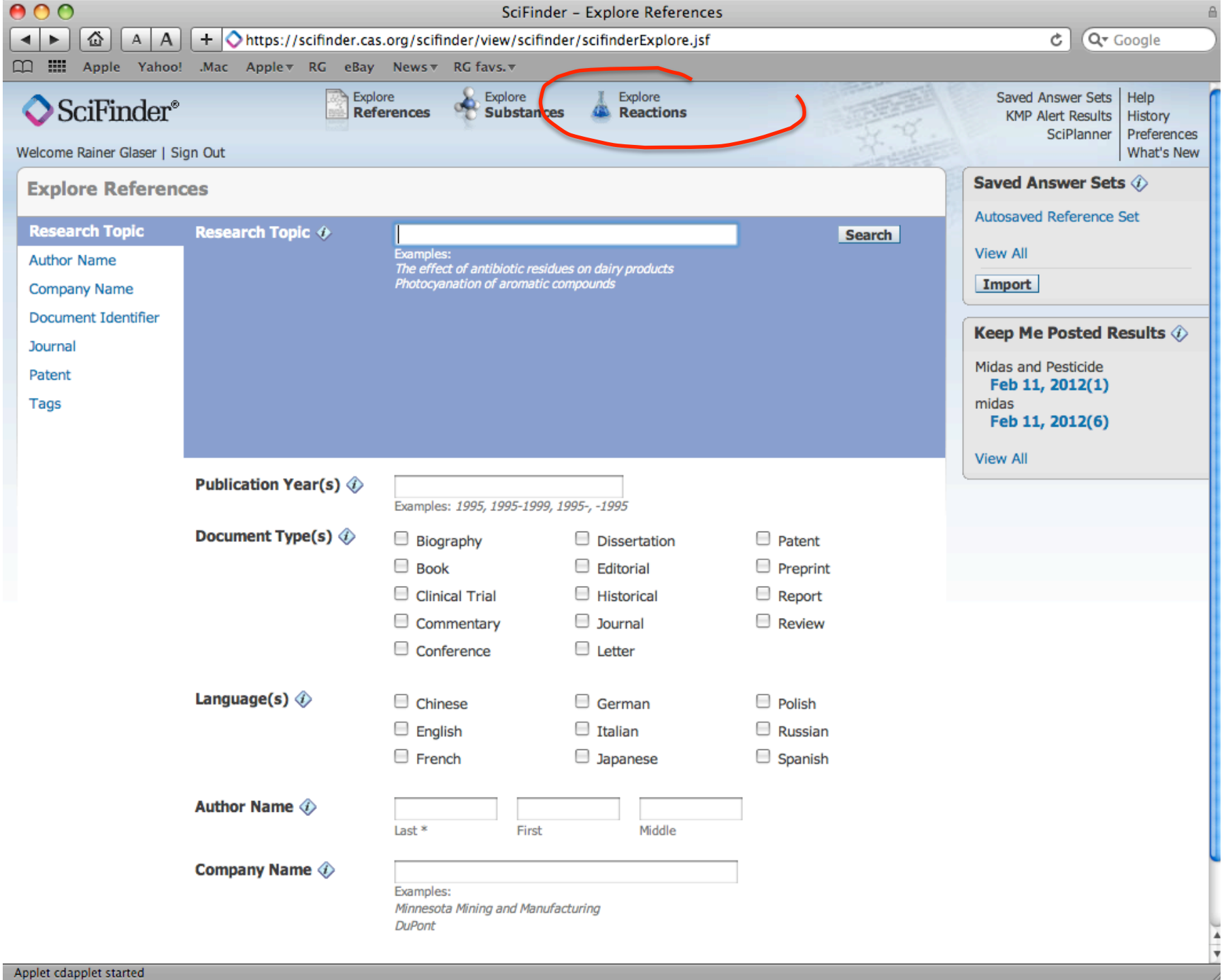
View more related articles

Mendeley Readers
We are sorry. There is no related information available for the given article(s).

powered by MENDELEY

Table Download
Find HTML data tables from the current article to download.
Find Tables
About Table Download

MostDownloaded
Most downloaded articles from the last three months


SciFinder – Explore References
https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
SciFinder®
Explore References
Explore Substances
Explore Reactions
Saved Answer Sets
KMP Alert Results
SciPlanner
Help
History
Preferences
What's New
Welcome Rainer Glaser | Sign Out
Explore References
Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags
Research Topic
Search
Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds
Publication Year(s)
Examples: 1995, 1995-1999, 1995-, -1995
Document Type(s)
Biography
Book
Clinical Trial
Commentary
Conference
Dissertation
Editorial
Historical
Journal
Letter
Patent
Preprint
Report
Review
Language(s)
Chinese
English
French
German
Italian
Japanese
Polish
Russian
Spanish
Author Name
Last *
First
Middle
Company Name
Examples:
Minnesota Mining and Manufacturing
DuPont
Saved Answer Sets
Autosaved Reference Set
View All
Import
Keep Me Posted Results
Midas and Pesticide
Feb 11, 2012(1)
midas
Feb 11, 2012(6)
View All
Applet cdapplet started

SciFinder – Explore Reactions

https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

Apple Yahoo! .Mac Apple RG eBay News RG favs.

SciFinder®

Explore References | Explore Substances | Explore Reactions

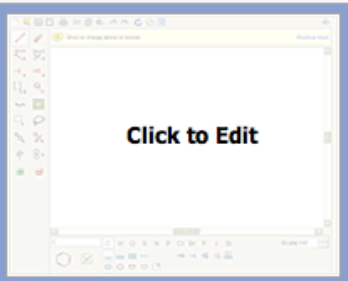
Saved Answer Sets | Help
KMP Alert Results | History
SciPlanner | Preferences
What's New

Welcome Rainer Glaser | Sign Out

Explore Reactions

Reaction Structure

Reaction Structure



Search

Solvent(s) Select Solvents

Non-participating Functional Group(s) Select Groups

Number of Steps

Examples: *1, 1-3, 1-, -3*

Classification(s)

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Source(s)

- Any source
- Patents only
- Sources other than patents

Publication Year(s)

Examples: *1995, 1995-1999, 1995-, -1995*

Saved Answer Sets

Autosaved Reference Set

View All

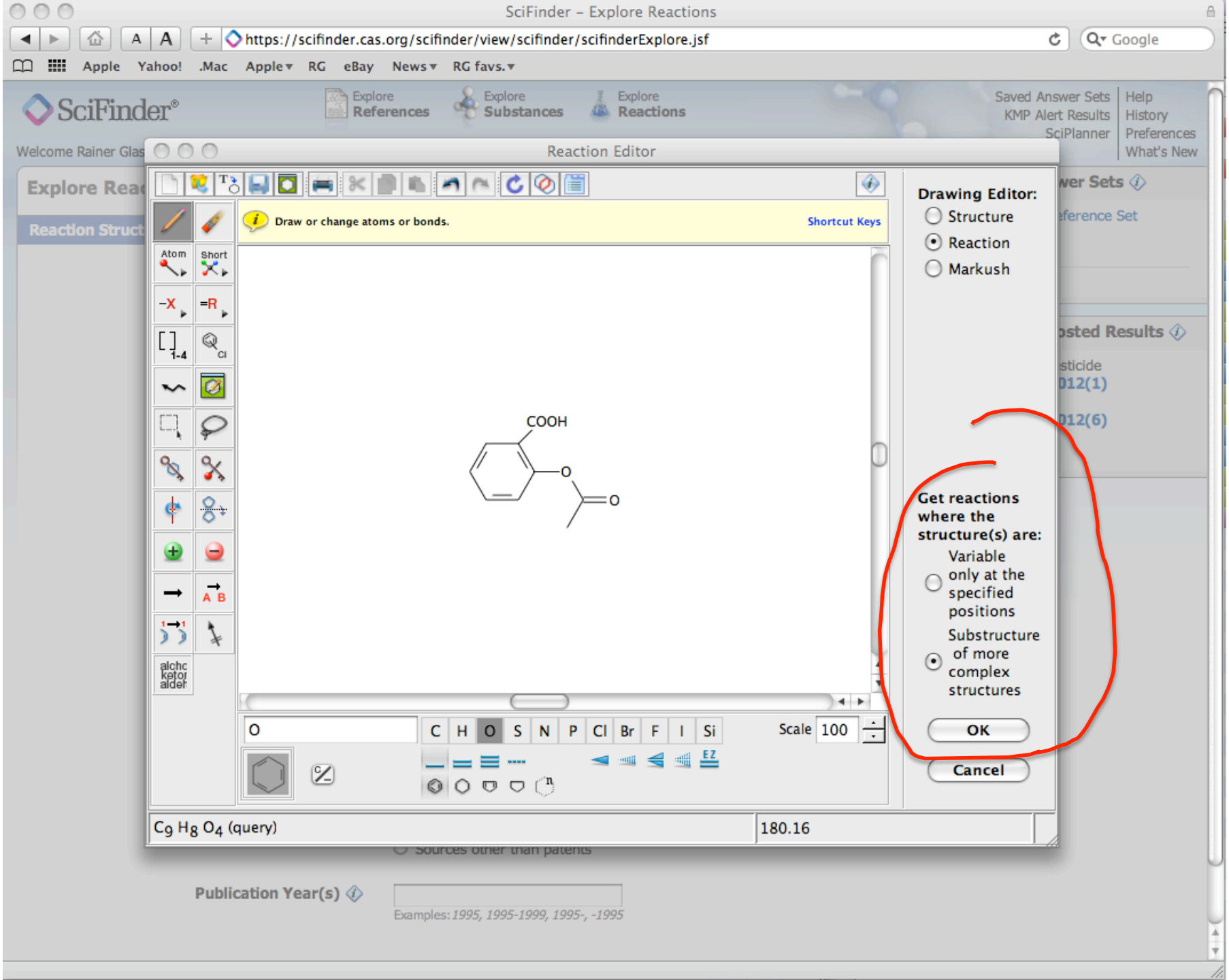
Import

Keep Me Posted Results

Midas and Pesticide
Feb 11, 2012(1)
midas
Feb 11, 2012(6)

View All

Run script ";"


SciFinder – Explore Reactions
https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf
Google
Apple Yahoo! .Mac Apple RG eBay News RG favs.
SciFinder®
Explore References
Explore Substances
Explore Reactions
Saved Answer Sets
KMP Alert Results
SciPlanner
Help
History
Preferences
What's New
Welcome Rainer Glas
Reaction Editor
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
COOH
O
O
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructure of more complex structures
OK
Cancel
C H O S N P Cl Br F I Si
Scale 100
C9 H8 O4 (query)
180.16
Publication Year(s)
Examples: 1995, 1995-1999, 1995-, -1995

SciFinder – Explore Reactions

https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

Apple Yahoo! .Mac Apple RG eBay News RG favs.

SciFinder®

Explore References | Explore Substances | Explore Reactions

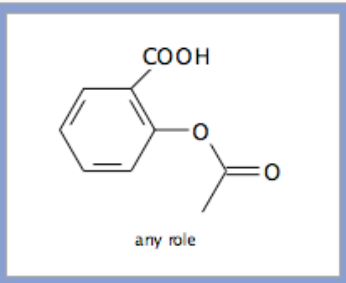
Saved Answer Sets | Help
KMP Alert Results | History
SciPlanner | Preferences
What's New

Welcome Rainer Glaser | Sign Out

Explore Reactions

Reaction Structure

Reaction Structure



Click image to change structure or view detail

Search

Search type: Allow variability only as specified
Substructure

Solvent(s) Select Solvents

Non-participating Functional Group(s) Select Groups

Number of Steps

Examples: *1, 1-3, 1-, -3*

Classification(s)

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Source(s)

- Any source
- Patents only
- Sources other than patents

Saved Answer Sets

Autosaved Reference Set

View All

Import

Keep Me Posted Results

Midas and Pesticide
Feb 11, 2012(1)
midas
Feb 11, 2012(6)

View All

Reactions

Get References | Tools | Send to SciPlanner

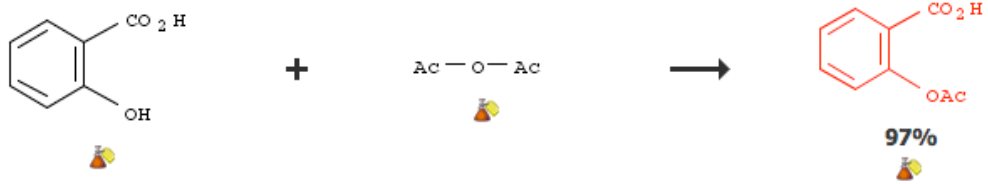
7515 Reactions 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Relevance | Answers per Page [15] | 1 2 3 4 5 6 ... 501

Display:

1. **View Reaction Detail** | **Link** | **Similar Reactions**

Single Step *Hover over any structure for more options.*



Overview

Steps/Stages

1.1 C:$ZnCl_2$, 1 h, 80-90°C
1.2 R:H_2O, cooled

Notes

green chemistry, solid acid catalyst loaded on bentonite used, optimization study, optimized on ZnCl2 concentration, reaction temperature, reaction time, amount of catalyst, Reactants: 2, Reagents: 1, Catalysts: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Solid acid catalyst loaded on bentonite and its catalysis of the synthesis of acetylsalicylate Full Text
By Wang, Hong-Bin et al
From Yingyong Huaxue, 26(2), 182-186; 2009

2. **View Reaction Detail** | **Link** | **Similar Reactions**

Single Step *Hover over any structure for more options.*

Analysis | Refine

Analyze by:

Catalyst

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

Pd	1408
Carbon	1052
4-DMAP	930
$Pd(PPh_3)_4$	755
DMF	358
Dicyclohexylborane	280
172222-30-9	190
C_5H_5N	147
72287-26-4	125
246047-72-3	108

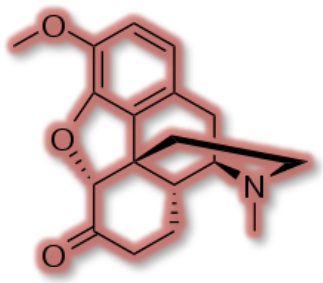
Show More

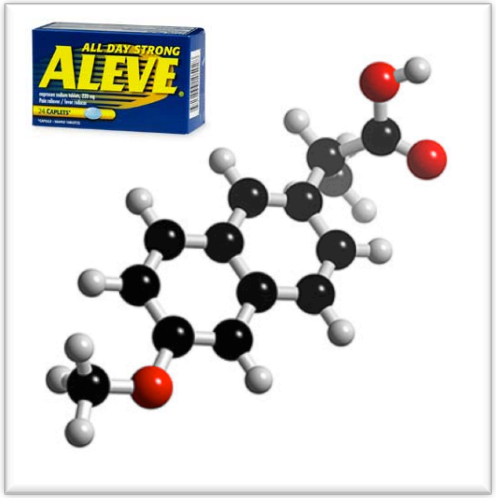
How to Search the Literature, How to Report Experimental Data, and How to Create Bibliography.

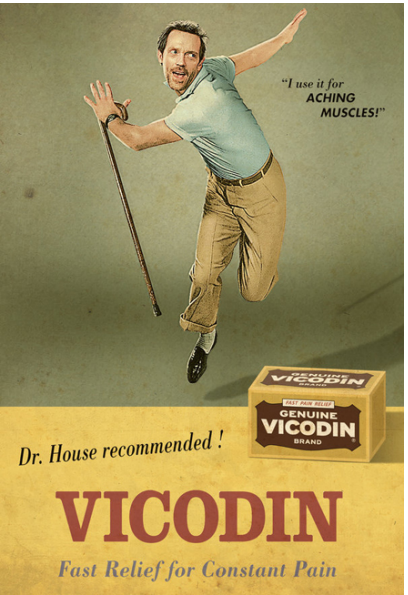
Example: Painkiller Nomenclature, Synthesis and Spectroscopic Analysis.

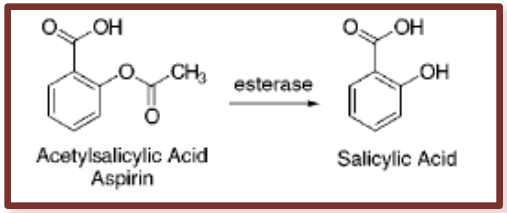
Assign. #5: Handout & online.

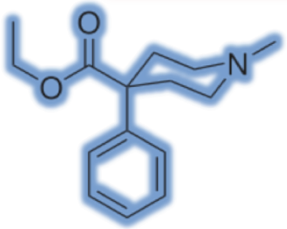
Project #1: Oral Presentation of A#5.



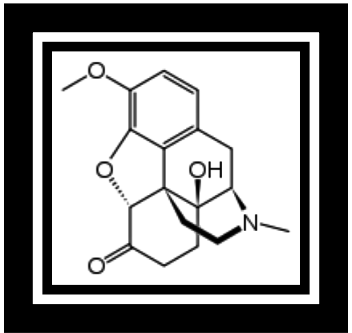








Demerol



Oxycodone

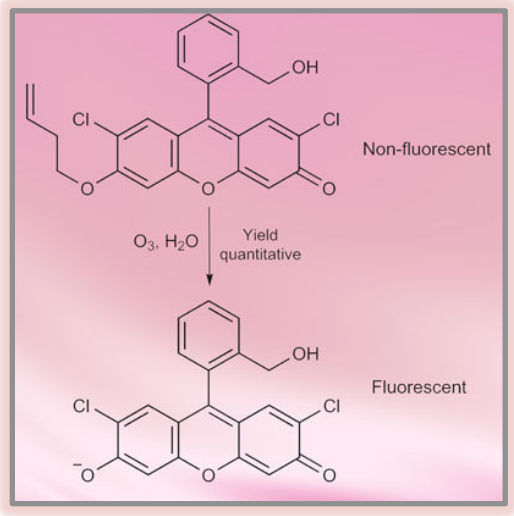
(5*R*,9*R*,13*S*,14*S*)-4,5α-epoxy-14-hydroxy-3-methoxy-17-methyl-morphinan-6-one

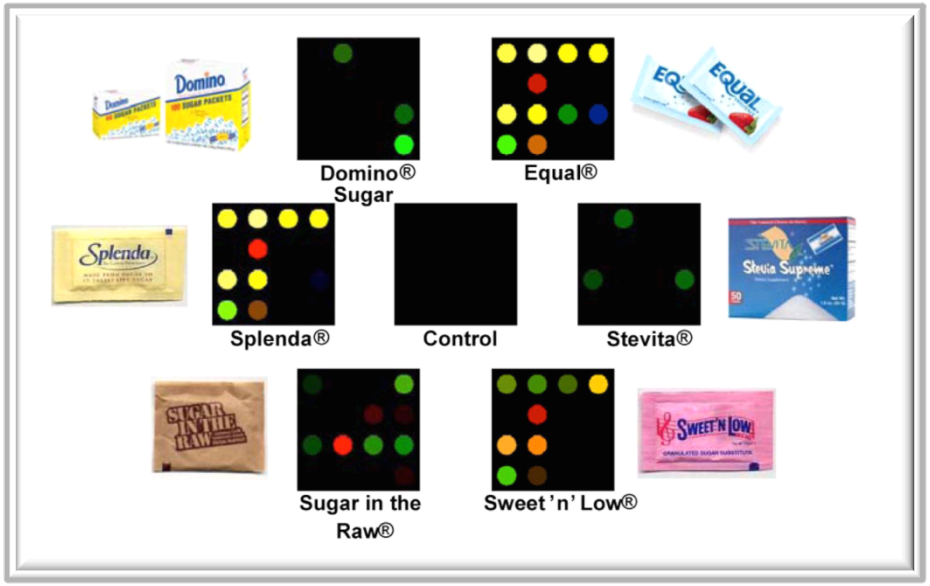
How to Search the Literature, How to Report Experimental Data, and How to Create Bibliography.

Colorimetric Indicator Dyes: Nomenclature, Synthesis and Spectroscopic Analysis.

Assign. #5: Handout & online.

Assign. #6: Oral Presentation of A#5.





Leading Reference

Iron-Catalyzed Direct Arylation through an Aryl Radical Transfer Pathway

Frédéric Vallée, James J. Mousseau, and André B. Charette*

Department of Chemistry, Université de Montréal, P.O. Box 6128, Station Downtown, Montréal, Québec, Canada, H3C 3J7

Received December 18, 2009; E-mail: andre.charette@umontreal.ca

Biaryl compounds are omnipresent in Nature as well as in numerous biologically active compounds, including antibiotics[1] and various receptor inhibitors, and have been used to treat hypertension as well as bipolar disorders. Consequently, they have attracted much pharmaceutical interest,[2] as well as in other areas including material and supramolecular sciences.[3,4]

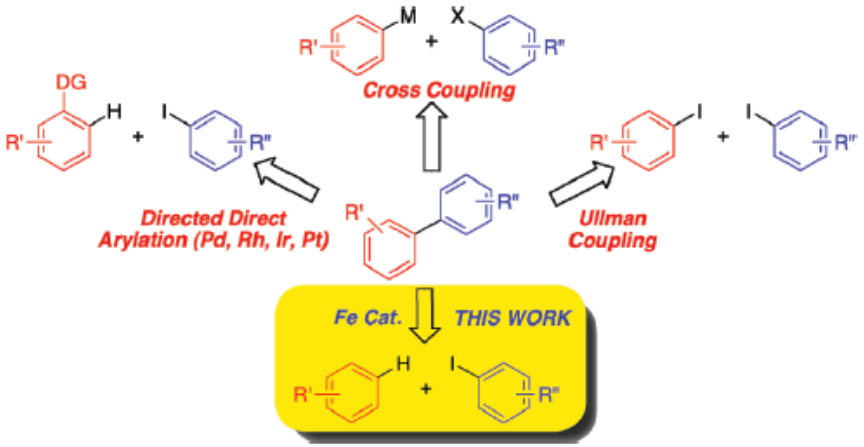


Figure 1. Various ways to prepare biaryl compounds.

Cite a few, "leading" references to describe context.

Cite all papers that report original work that is pertinent to the work you report.

Oral Presentation Organization

Each oral presentation session will have one chair and one co-chair.

Session Chair and co-Chair

Will make sure that all scheduled speakers are present.
Will make sure the presentations are ready for display.

Session Chair

Will briefly announce each talk (topic and presenters).
Will lead the discussion session.

Session co-Chair

Will keep track of time (9+2+1 format).
Organize clean transitions between talks.