



SciFinder®

Universidad de SALAMANCA

17 de Noviembre de 2009



SciFinder®

CAS is a division of the American Chemical Society

Dra. Míriam Plana

CAS/STN Regional Marketing Manager

mplana@cas.org

Agenda

- Bases de datos de CAS: ¡más contenido!
- La versión web de SciFinder: ¡Novedades!
- SciFinder: registro
- Ejemplos de búsquedas:
 - Por tema
 - Por estructura
 - Por reacción

Agenda

- **Bases de datos de CAS: ¡más contenido!**
- La versión web de SciFinder: ¡Novedades!
- SciFinder: registro
- Ejemplos de búsquedas:
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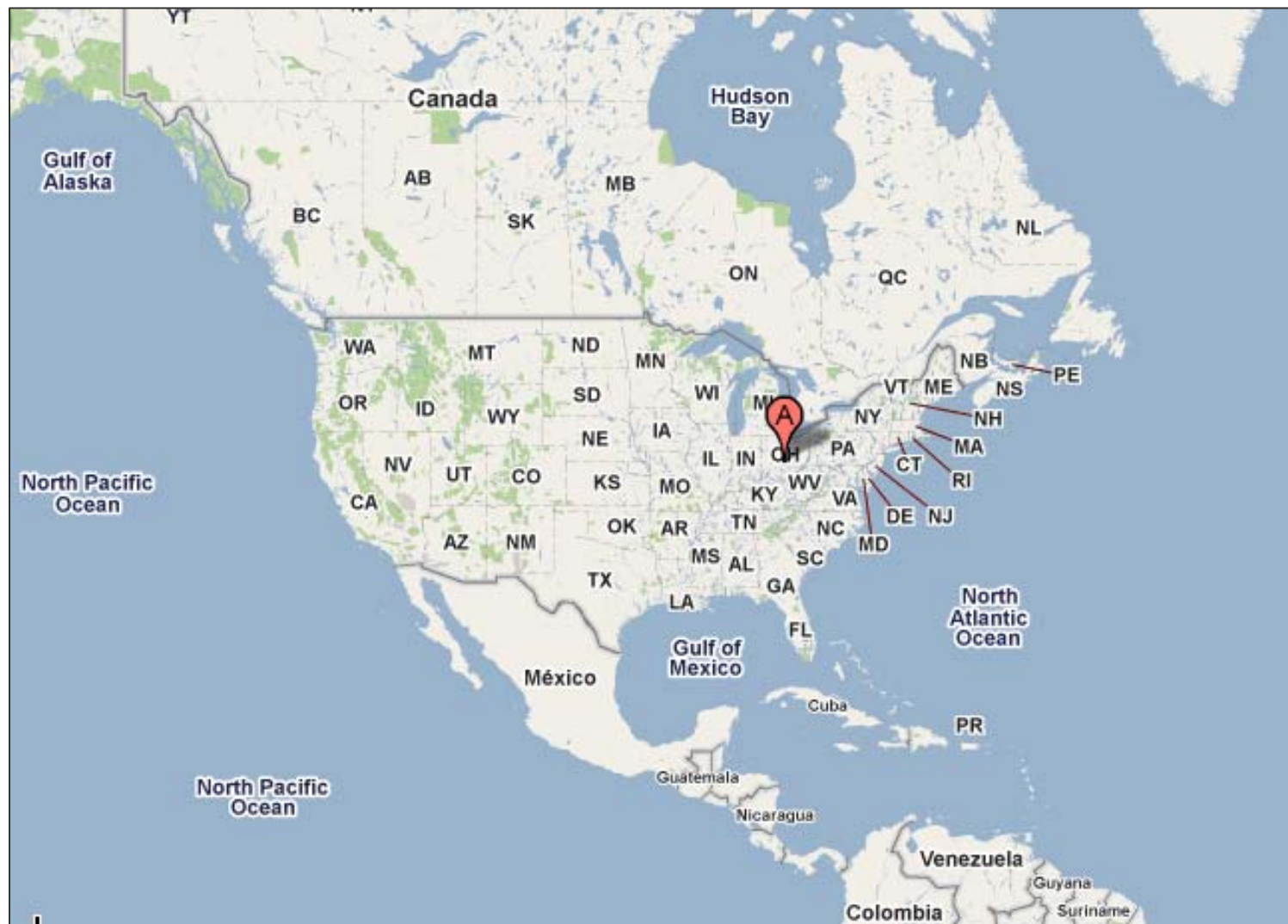
Contenido: bases de datos

CAplusSM	CAS REGISTRYSM	CASREACT[®]
• >31M bibliographic records • >10K journals covered • Patents from 59 patent offices • Updated daily (~3K daily) • Links to almost 400 publishers and 9 patent offices • Literature back to early 1800s • Cited articles from 1997 onward	• >51M small molecules • >61M sequences • Updated daily (>12K daily) • Substances reported comprehensively in literature back to 1957 • Includes nomenclature, spectra, and properties (experimental and predicted)	• >19M single and multi-step reactions • Extracted from patents and journal articles • Updated weekly (~30K weekly) • Reactions back to 1840 • Reaction conditions starting in 2003

Contenido: bases de datos

CHEMCATS®	CHEMLIST®	MEDLINE®
• >35M commercially available compounds • >900 suppliers • >1000 chemical catalogs • Updated when new or revised catalogs are available • Contact/ordering information including quantity and pricing (when available)	• >248K inventoried / regulated substances • >100 inventories & regulated lists from 1979 to present • Updated weekly (~50 additions) • Contains regulatory requirements for substances	• >18M bibliographic records • 4,800 biomedical journals • Updated 4 times per week • 1950 -1966 from OLDMEDLINE database

SciFinder ofrece información biomédica adicional a través de MEDLINE® producida por la National Library of Medicine



CAS Headquarters: Columbus, OHIO



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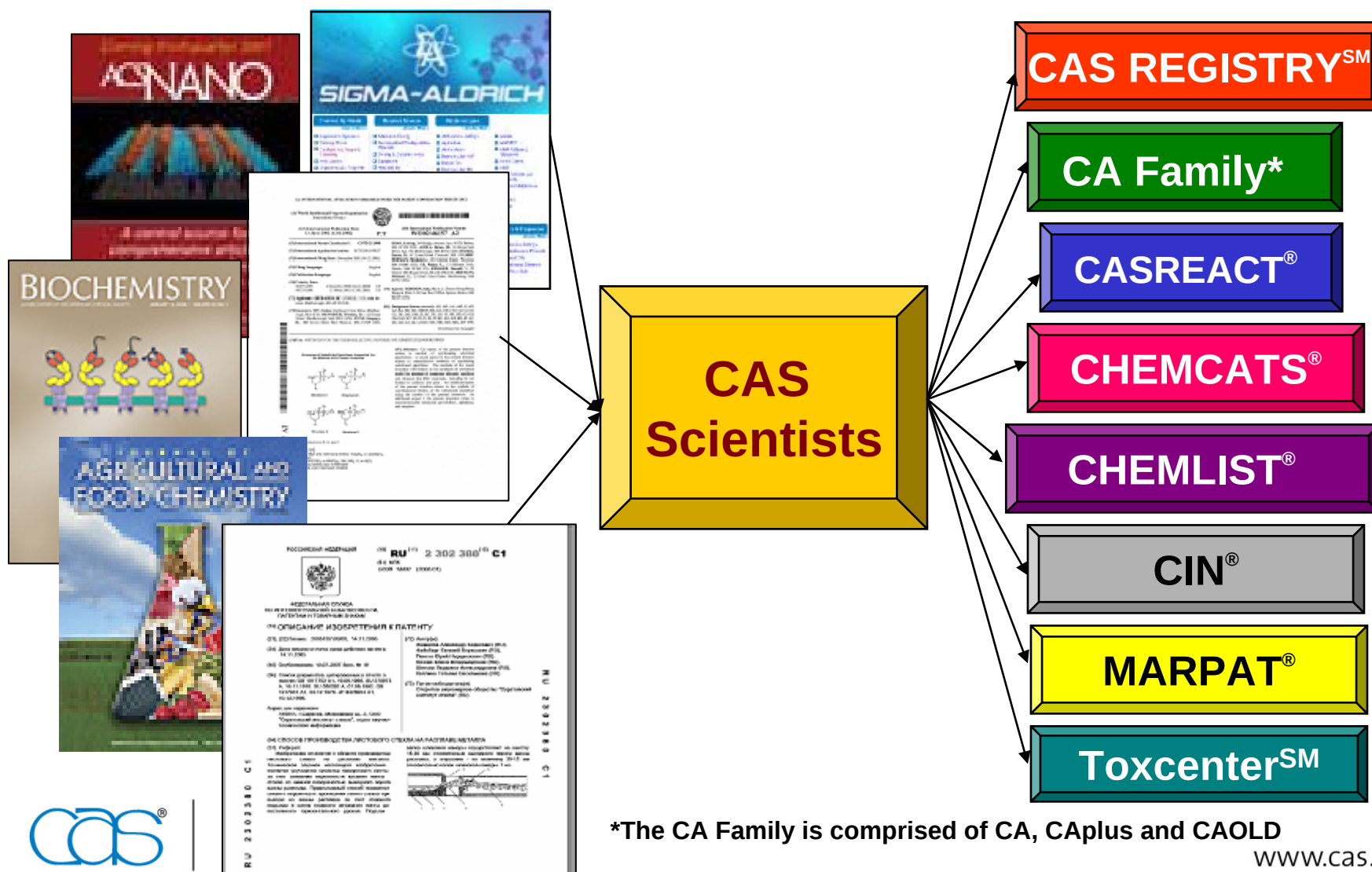
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CAS Editorial: más de 600 científicos!!!



CAS resume e indiza los contenidos de muchas fuentes produciendo bases de datos de gran calidad



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La última actualización ofrece nuevas funcionalidades y contenidos, sólo disponibles en la versión web!



- Búsqueda de reacciones
- Propiedades
- Herramientas de colaboración
- Nuevas opciones de trabajo
- Nuevas funciones

¿Una reacción a explorar?

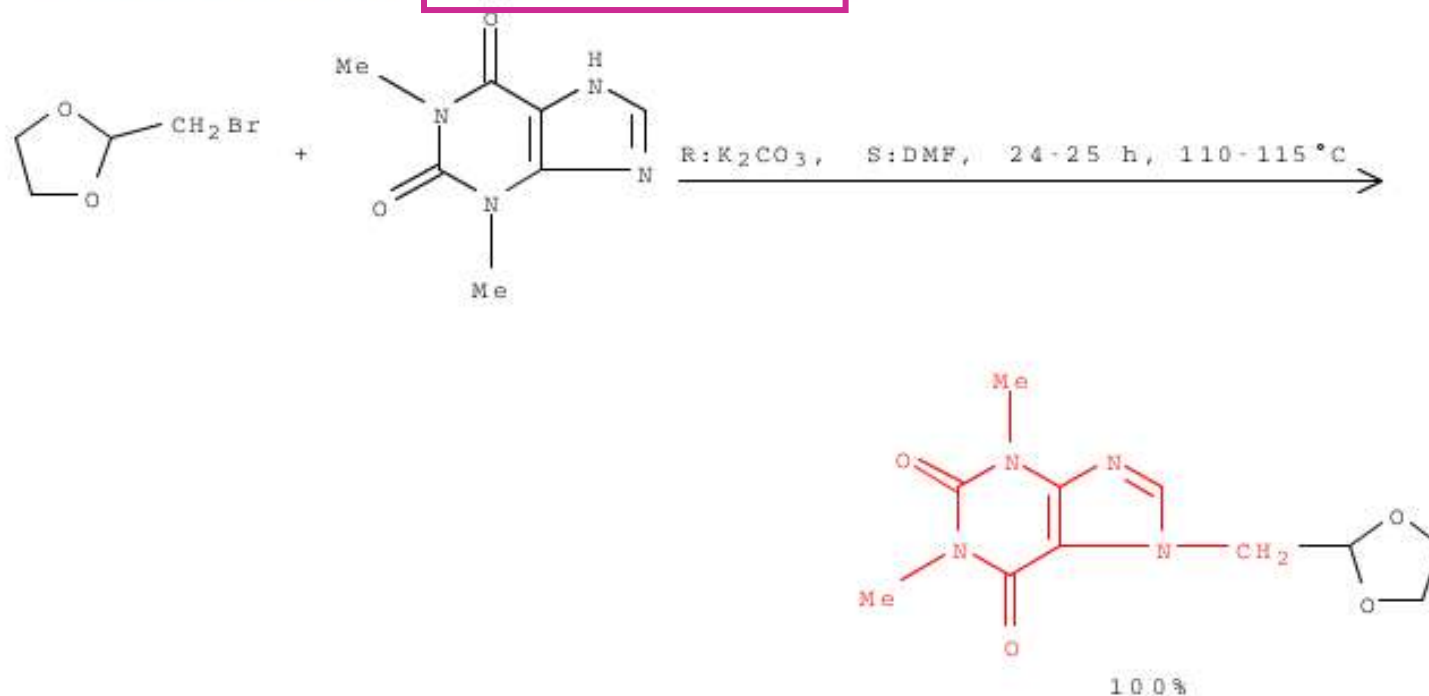


1. Reaction Detail



Similar Reactions

NEW



NOTE: Reactants: 2, Reagents: 1, Solvents: 1,
Steps: 1, Stages: 1

Process for preparation of pure doxofylline

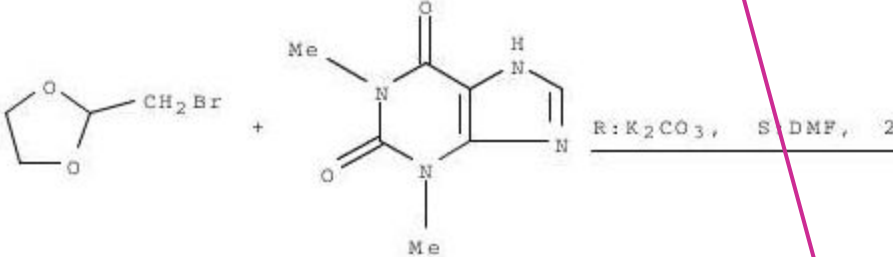
By Rajendra, Agarwal et al

From Indian Pat. Appl., 2007MU01019, 27 Mar 2009

www.cas.org

Búsqueda de reacciones similares

1. Reaction Detail [Link](#) **Similar Reactions** NEW



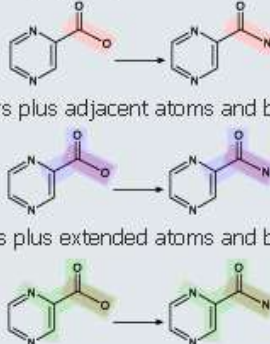
Get Similar Reactions 

Retrieve similar reactions from:

- ☒ All reactions
- ☐ Current answer set

Include this level of similarity:

- ☒ Broad - Reaction centers only (3924)
- ☐ Medium - Reaction centers plus adjacent atoms and bonds (324)
- ☐ Narrow - Reaction centers plus extended atoms and bonds (4)



[Get Reactions](#) [Cancel](#)

- Búsqueda similar usando centros de reacción.
- La búsqueda puede ser en todas las reacciones o sólo en el “answer set”.
- Se pueden escoger entre 3 niveles de precisión.

Nueva jerarquía de disolventes desarrollada por los científicos de CAS.



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La nueva opción “Sort” permite a los investigadores conseguir rápidamente referencias/estructuras/reacciones relevantes

The screenshot displays the SciFinder Reactions interface. At the top, there are tabs for 'Reactions' and 'Get References'. Below this, a header bar shows '138 Reactions', '0 Selected', and buttons for 'Keep Selected' and 'Remove Selected'. On the right of this bar are 'Save', 'Print', and 'Export' buttons. A 'Sort by:' dropdown menu is open, showing options: 'Similarity' (highlighted), 'Accession Number', 'Number of Steps', 'Percent Yield', 'Publication Year', and 'Similarity'. The main area shows a chemical reaction between a pyridine derivative and a substituted benzene derivative. The reaction conditions are 'R:Et₃N, S:Dioxane, 100°C'. The product is a complex molecule with a pyridine ring, a benzene ring, and a carboxylic acid group. Below the reaction, there is a 'NOTE' section with details: 'Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1'. At the bottom, there is a citation: 'N-Hydroxy-1,2-disubstituted-1H-benzimidazol-5-yl acrylamides as novel histone deacetylase inhibitors: Design, synthesis, SAR studies, and in vivo antitumor activity. By Wang, Haishan et al. From Bioorganic & Medicinal Chemistry Letters, 19(5), 1403-1408; 2009'.

- Etapas
- Rendimiento
- Año de publicación
- Similaridad

Los investigadores pueden añadir su propio contenido...

3. Heteroaryl substituted pyrrolo[2,3-b]pyridines and pyrrolo[2,3-b]pyrimidines as Janus kinase inhibitors and their preparation and use in the treatment of diseases

By Rodgers, James D.; Shepard, Stacey; Maduskuie, Thomas P., Jr.; Wang, Haisheng; Falahatpisheh, Nikoo; Rafalski, Maria; Arvanitis, Argvrios G.; Storace, Louis; Jalluri, Ravi Kumar; Fridman, Jordan S.; et al

From U.S. Pat. Appl. Publ. (2009), US 2009181959 A1 20090716. Language: English, Database: CAPLUS

The invention provides heteroaryl substituted pyrrolo[2,3-b]pyridines and heteroaryl substituted pyrrolo[2,3-b]pyrimidines of formula I that modulate the activity of Janus **kinases** and are useful in the **treatment** of diseases related to activity of Janus **kinases**. Comps. of formula I wherein A1 and A2 are independently C and N; T, U and V are independently O, S, N, CR5 and NH and derivs.; dotted lines are single and double bond forming an arom. 5-membered ring; X is N and CR4; Y is C1-8 alkylene, C2-8 alkenylene, C2-8 alkynylene, etc.; Z is H, halo, C1-8 alkyl, C2-8 alkenyl, C2-8 alkynyl, etc.;...

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [1 Comment](#) [2 Tags](#)

Comments **BETA**

Unconventional liquid-liquid extraction in undergraduate laboratories: cloud-point separation and preconcentration

1 Comment Sort by: [Newer First](#) | [Older First](#)

we should try this technique in the lab

Marie Sparks

Posted August 31, 2009 9:54 AM
Last Modified August 31, 2009 9:54 AM

Add Comment:

Maximum of 1024 characters per comment; 50 comments per post
Reminder: Your comments and tags can be viewed by you

2 Tags | [Edit Tags](#)

janus inhibitors(1); project x competitive patents(1)

[Save](#)

Characters Remaining: 1024

[Close](#)

....y ¡compartirlo!

3. Heteroaryl substituted pyrrolo[2,3-b]pyridines and pyrrolo[2,3-b]pyrimidines as Janus kinase inhibitors and their preparation and use in the treatment of diseases

Create Keep Me Posted Explore Tag "laboratory experiments"

My Connections **BETA** Invite Colleagues To Connect

Connections

Invitations

6 Connections 0 Selected Remove

My Connections allows you to share comments and tags with these colleagues.

Connected Colleagues	E-mail	Profile
☐ Perry, James	jperry@cas.org	CAS

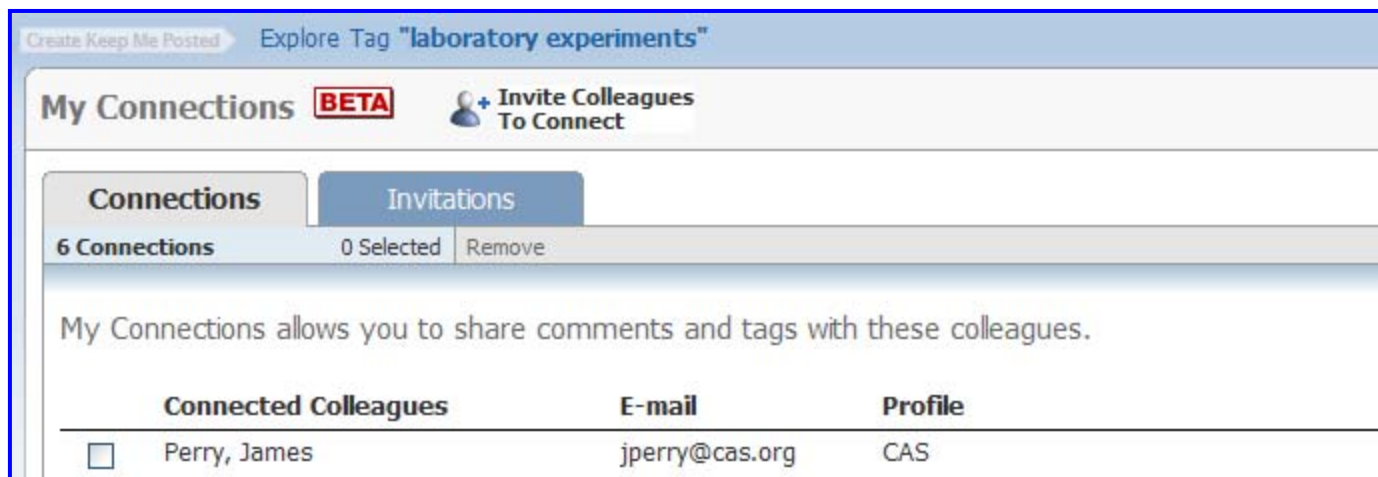
janus inhibitors(1); project x competitive patents(1)

Add Comment: Maximum of 1024 characters per comment; 50 comments per user.
Reminder: Your comments and tags can be viewed by your connected colleagues.

Save

Characters Remaining: 1024

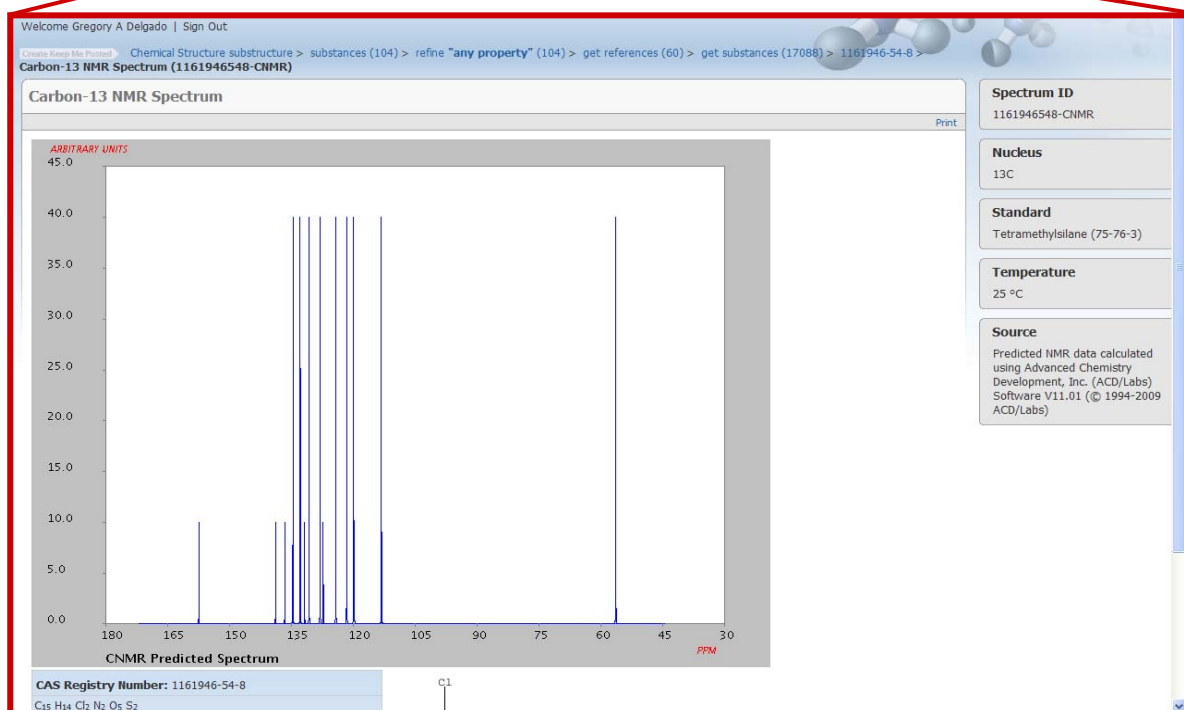
La flexibilidad de la Web permite a CAS probar y desarrollar nuevas funcionalidades para satisfacer las necesidades de los usuarios



- CAS quiere compartir con los usuarios los nuevos desarrollos
- *Software is production quality*
- El uso y los *feedbacks* conducen a desarrollo de más funcionalidades y opciones

^{13}C -NMR espectros teóricos de más de 28 millones de sustancias

Molecular Weight	437.32	(1)		
Spectra Properties	Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum NEW	See spectrum		(2)	
Proton NMR Spectrum	See spectrum		(2)	



- New **predicted** spectral data is being added to CAS REGISTRYSM as an ongoing project
- Predicted spectra available through an agreement with ACD/Labs



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Los investigadores pueden centrar sus búsquedas estructurales con las características más importantes para ellos

Refine by Property Value

1. Select one or more properties. Click each property to display value options.

2. Specify values and limits.

Properties - 1 selected

- ☐ H Acceptors
- ☐ H Donors
- ☒ **Molecular Weight**
- ☐ logP
- ☐ Freely Rotatable Bonds
- ☐ Bioconcentration Factor
- ☐ Boiling Point
- ☐ Density
- ☐ Enthalpy of Vaporization
- ☐ Flash Point
- ☐ H Acceptor/Donor Sum
- ☐ Koc
- ☐ logD
- ☐ Mass Intrinsic Solubility
- ☐ Mass Solubility
- ☐ Molar Intrinsic Solubility
- ☐ Molar Solubility
- ☐ Molar Volume
- ☐ pKa
- ☐ Polar Surface Area
- ☐ Vapor Pressure

Values - Predicted Molecular Weight

Specify range:

400 to 600

Min: 0.0 Max:

☐ Include substances with no value for the specified properties

- SciFinder now provides access to over 2.5 billion chemical property values across over 37 million substances!
- Researchers can leverage this for focused search results to save time and increase productivity

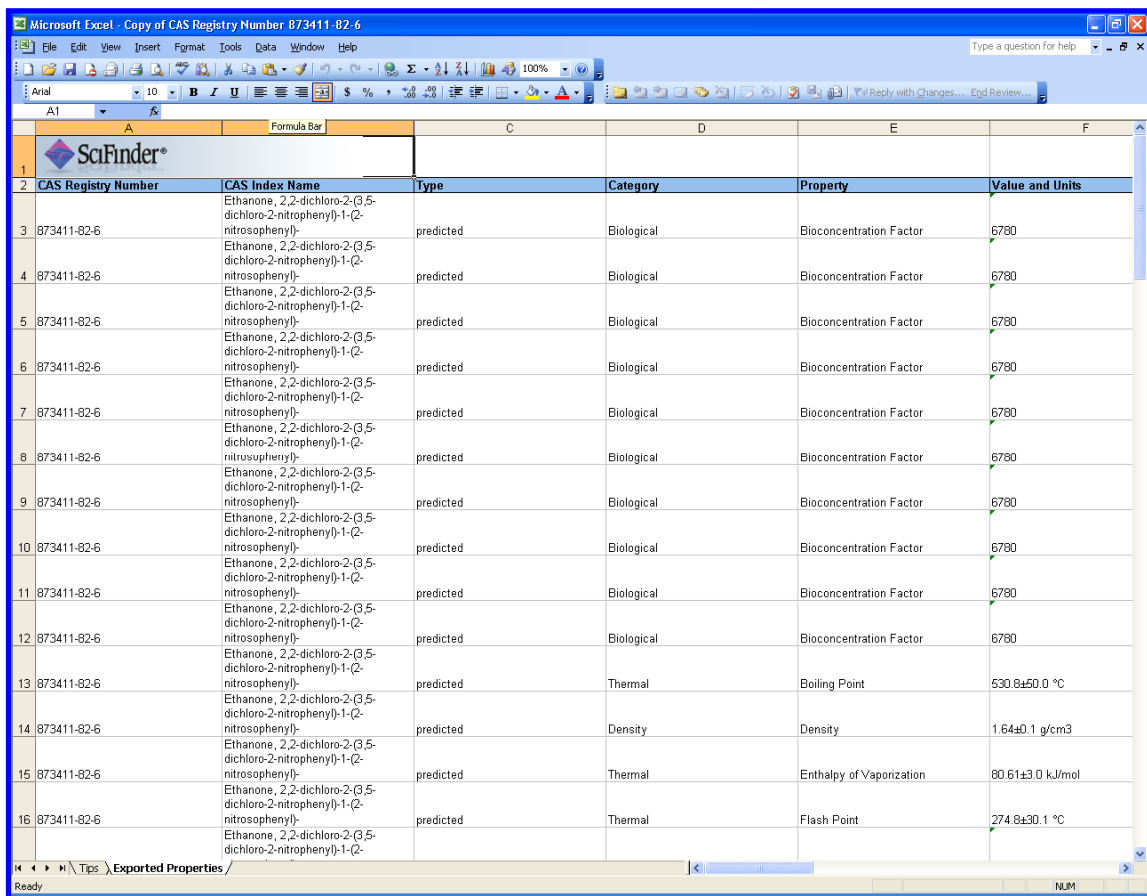


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Posibilidad de esportar a Microsoft® Excel® las propiedades de una sustancia. Permote revisar y analizar las porpiedades químicas.



CAS Registry Number	CAS Index Name	Type	Category	Property	Value and Units
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Biological	Bioconcentration Factor	6780
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Biological	Bioconcentration Factor	6780
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Biological	Bioconcentration Factor	6780
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873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Biological	Bioconcentration Factor	6780
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Biological	Bioconcentration Factor	6780
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873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Biological	Bioconcentration Factor	6780
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873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Biological	Bioconcentration Factor	6780
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Biological	Bioconcentration Factor	6780
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Thermal	Boiling Point	530.8±50.0 °C
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Density	Density	1.64±0.1 g/cm3
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Thermal	Enthalpy of Vaporization	80.61±3.0 kJ/mol
873411-82-6	Ethanone, 2,2-dichloro-2-(3,5-dichloro-2-nitrophenyl)-1-(2-nitrosophenyl)-	predicted	Thermal	Flash Point	274.8±30.1 °C

- Similar al Commercial Availability report
- Para manipular datos, usar Excel
- Añadir/eliminar columnas
- Ordenar y filtrar por valores específicos

Los usuarios pueden escoger cómo ver sus resultados...

SciFinder - Reference Answer Set - Windows Internet Explorer

https://scifinder-beta.cas.org/scifinder/view/text/refList.jsf?nav=r00ABXQAAWF0ACQx00UzNDEyNl04NkYzLTUwQUYtNlUy3Qy00M0EzQThBRjhFM

File Edit View Favorites Tools Help

SciFinder - Referenc... x Poison Ivy Treatments, ...

SciFinder®

Explore References Explore Substances Explore Reactions

Welcome Jonathan W Taylor | Sign Out

Create Keep Me Posted Research Topic "poison ivy treatment" > references (143)

References Get Substances Get Reactions Get Cited Get Citing

143 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags

Select All Deselect All Sort by: Accession Number

Save Print Export

Analysis Refine

Analyze by:

Change number of answers per page

Answers per Page [20]

Select the number of answers to show per page.

15 | 20 | 25 | 50 | 75 | 100

Displaying more answers per page may increase page-loading time.

1. **Poly(urea-urethane) compositions useful as topical medicaments and methods of using the same**
By Chesson, Jerry; Romack, Timothy J.; Swick, Lance L.; Terry, David R.
From PCT Int. Appl. (2009), WO 2009051648 A2 20090423. Language: English, Database: CAPLUS
The present invention provides a method of **treating** a skin ailment including administering to a subject in need thereof, a therapeutically effective amt. of a compn. including (i) a primary diamine; (ii) a secondary arom. diamine; (iii) a polyisocyanate; and (iv) optionally, a polyol. The present invention also provides a method of forming a skin bandage.
Substances Reactions Citing Full Text Link Comments Tags

2. **Poly(urea-urethane) compositions useful as topical medicaments and methods of using the same**
By Chesson, Jerry; Romack, Timothy J.; Swick, Lance L.; Terry, David R.
From U.S. Pat. Appl. Publ. (2009), US 2009098194 A1 20090416. Language: English, Database: CAPLUS
The present invention provides a method of **treating** a skin ailment, including administering to a subject in need thereof, a therapeutically effective amt. of a compn. including (i) a primary diamine; (ii) a secondary arom. diamine; (iii) a polyisocyanate; and (iv) optionally, a polyol. The present invention also provides a method of forming a skin bandage. Acetone 850 mL, Me Et ketone 100 mL, polyetheramine D-2000 60.0 mL, secondary diamine UOP 4200 15.0 mL, polyether polyol Multanol 4012 20.0 mL, ethylene glycol 5.0 mL, and MDI Lupranate 5143 32.0 mL were added sequentially with stirring to make a clear off white soln. The poly(urea-urethane) formulation formed a film that allowed transport of hydrocortisone. When the formulation was applied to a severe sunburn of the scalp, pain and discomfort subsided and the polymer film formed a protective coating over the burned skin.
Substances Reactions Citing Full Text Link Comments Tags

3. **Preparation of triazolo[1,5-a]quinolines as adenosine A3 receptor ligands for treating disease**
By Susan, Edit; Boer, Kinga; Kapui, Zoltan; Timari, Geza; Batori, Sandor; Szlavik, Zoltan; Mikus, Endre; Vargane Szeredi, Judit; Finet, Michel; Urban Szabo, Katalin; et al
From PCT Int. Appl. (2008), WO 2008149168 A1 20081211. Language: English, Database: CAPLUS
The present invention relates to the adenosine A3 receptor ligands of the general formula I (wherein R1, R2 are H or straight or branched C1-4 alkyl; R3,R5 are H, straight or branched C1-4 alkyl, etc.; R4 is Ph, benzyl, thienyl, etc.; R13 is CN, aminocarbonyl, etc.; X is CH2, NH, S, etc.; n = 0-2) and to their salts, solvates, N-oxides and isomers, to pharmaceutical compns. contg. I, to their therapeutic uses, and to a process for prepg. I. Example compd. II was prepd. by reacting 1,2-diamino-3-cyano-4-benzylamino-6-(morpholin-4-yl)quinolinium tosylate (prepn. given) with 3-methoxybenzaldehyde. II had an IC50 of 38 nM in

Name	Count
Addeeton Donald Stuart	5
Arr Teresa Leigh	4
Batori Sandor	4
Boer Kinga	4
Kapui Zoltan	4
Meadows Sandra Dora	4
Mikus Endre	4
Timari Geza	4
Urban Szabo Katalin	4
Aranyi Peter	3

...si lo quieren ver muy detallado...

The image displays three overlapping screenshots of the SciFinder web interface, illustrating the search results for the topic "poison ivy treatment".

The top screenshot shows the search results list, with the first result highlighted:

- 1. Poly(urea-urethane) compositions useful as topical medicaments

The middle screenshot shows a detailed view of the first result, including the abstract and references:

By Chesson, Jerry; Romack, Timothy J.; Swick, Lance L.; Terry, David R.
From PCT Int. Appl. (2009), WO 2009/01648 A2 20090423. Language: English, Database: CAPLUS

The bottom screenshot shows a detailed view of the second result, including the abstract and references:

By Chesson, Jerry; Romack, Timothy J.; Swick, Lance L.; Terry, David R.
From U.S. Pat. Appl. Publ. (2009), US 2009/098194 A1 20090416. Language: English, Database: CAPLUS

A callout box labeled "View:" with three icons (list, table, detailed) points to the interface elements, indicating the different ways to view the search results.

Esta opción, también está para las sustancias...

The screenshot displays the SciFinder web interface in a Windows Internet Explorer browser. The URL bar shows the address: <https://scifinder-test.cas.org:90/scifinder/view/substance/substanceList.jsf?nav=r00ABXQAAWFOAC>. The page header includes the SciFinder logo and navigation links: Explore References, Explore Substances, and Explore Reactions. A user is logged in as Jonathan W Taylor. The main content area shows a list of substances, with two details expanded. The first substance is 110862-48-1, and the second is 110979-23-2 (Component: 110862-48-1). Both substances have chemical structures and a list of references. A red box highlights the 'View' options (1, 2, 3, 4) for the second substance detail.

1. Substance Detail
110862-48-1

2. Substance Detail
110979-23-2
(Component: 110862-48-1)

View: 1 2 3 4

View: 1 2 3 4

Eficiencia en la búsqueda.

SciFinder®

Welcome Jonathan W Taylor | Sign Out

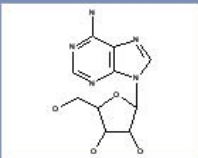
Explore References | Explore Substances | Explore Reactions

Explore Substances

Chemical Structure | Chemical Structure

Molecular Formula

Substance Identifier



Click image to change structure or view detail

Search type: ☒ Exact Structure ☐ Substructure ☐ Similarity

☐ Show precision analysis

Characteristic(s)

☐ Single component

☐ Commercially available

☐ Included in reference(s)

Class(es)

☐ Alloys

☐ Mixtures

Los *links* hacen que “navegar” a través de los resultados sea mucho más rápido

SciFinder - CAS Registry Number 944585-79-9 - Windows Internet Explorer

https://scifinder-beta.cas.org/scifinder/view/substance/substanceDetail.jsf?nav=r00ABXQAAWF0ACQyMDREREQ0RI04NkYzLTUwQjA4NDJGRi0zNjk2MTYxRjheQ

File Edit View Favorites Tools Help

SciFinder - Explore Sub... SciFinder - CAS Regi...

SciFinder®

Explore References Explore Substances Explore Reactions

Welcome Jonathan W Taylor | Sign Out

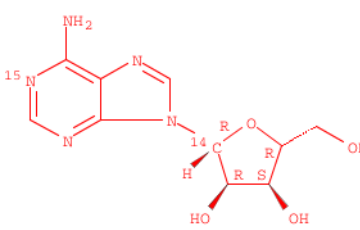
Create Keep Me Posted Chemical Structure exact > substances (345) > 944585-79-9

Substance Detail Get References Get Reactions Get Commercial Sources Get Regulatory Information

Link Save Print Export

8.

CAS Registry Number: 944585-79-9
C₁₀ H₁₃ N₅ O₄
Adenosine-1'-14C-1-15N (9CI)



Absolute stereochemistry.

Source of Registration: CA

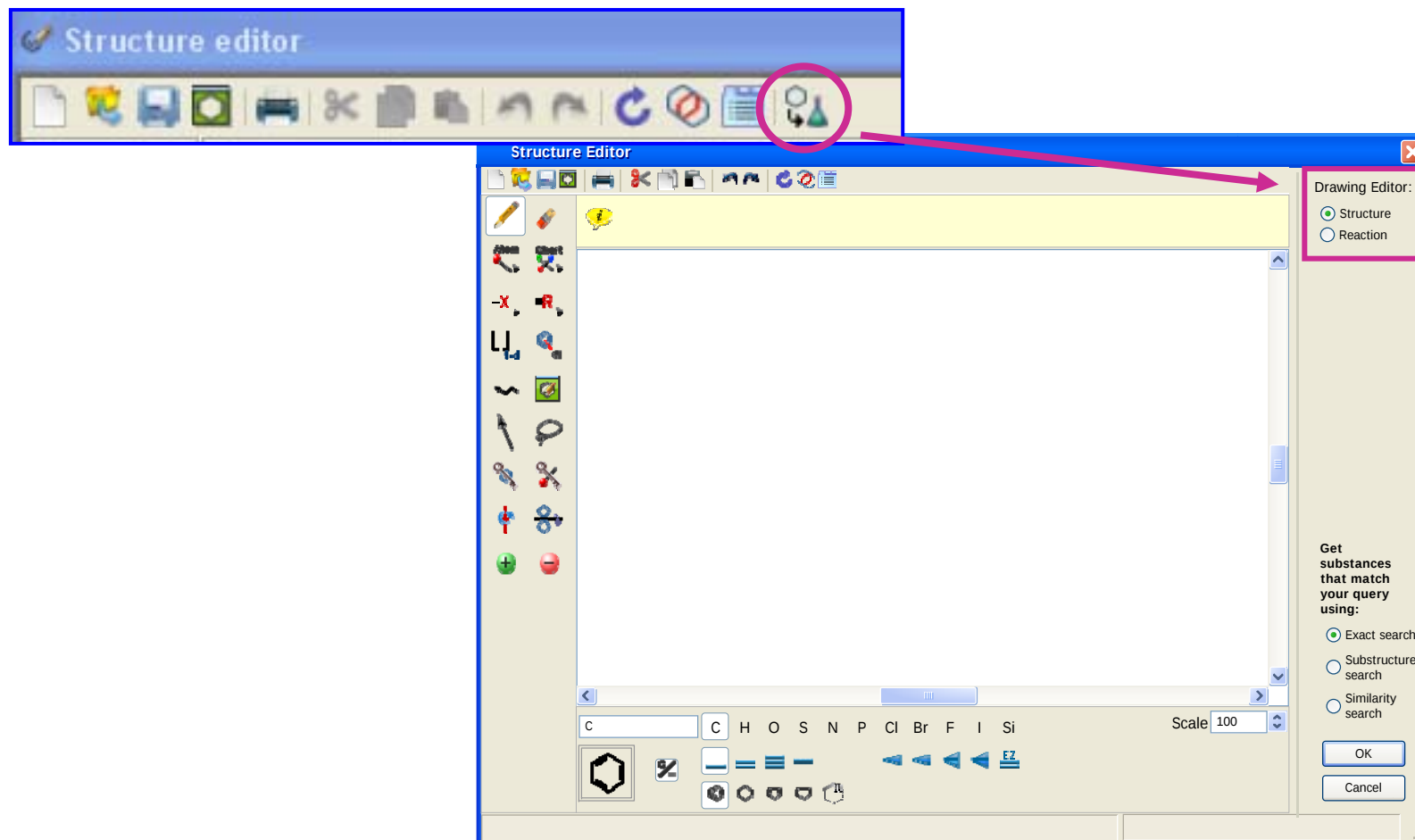
Document Type: Journal

Role	Nonpatents
Biological study	✓
Preparation	✓

Previous Next

Role	Nonpatents
Biological study	✓
Preparation	✓

Cambio flexible y rápido entre las búsquedas por estructura y por reacción



Próximos SciFinder e-Seminars

- “Exploring What’s New with SciFinder” e-Seminar scheduled for November 11th, 2009 with rebroadcasts dates on November 17th and 18th
 - Focus on new enhancements and content
 - Register at: <http://casevents/webex.com>

Clicar en el seminario al que queremos asistir...

All e-Seminars


 Product: Category: Language:

All event times in: [Europe DT](#)

Date & Time	Event	Category	Subcategory
November 2009			
November 18, 2009 3:00 - 4:00 Europe ST	SciFinder®: Exploring What's New with SciFinder®!	Search Techniques,Miscellaneous Topics	Intermediate Enroll
November 17, 2009 15:00 - 16:00 Europe ST	SciFinder®: Exploring What's New with SciFinder®!	Search Techniques,Miscellaneous Topics	Intermediate Enroll
November 17, 2009 12:00 - 13:00 Europe ST	SciFinder®: Exploring What's New with SciFinder®!	Search Techniques,Miscellaneous Topics	Intermediate Enroll
November 11, 2009 20:00 - 21:00 Europe ST	SciFinder®: Exploring What's New with SciFinder®!	Search Techniques,Miscellaneous Topics	Intermediate Enroll

Total: 20 recordings Page: 1 2

Topic	Category	Subcategory	Date	Size	Duration	Format
SciFinder® Tutorial: Navigating the Web Version of SciFinder SciFinder® offers a variety of ways to search and retrieve information. Understanding the navigatio...	Basic Orientation,Search Techniques	Basic	March 23, 2009	13.9 MB	23 mins	WRF
SciFinder®: Finding "Greener" Research Processes SciFinder has a wealth of green chemistry technologies and innovative research developments that wil...	Miscellaneous Topics	Intermediate	May 13, 2009	56.2 MB	62 mins	WRF
Advanced Reaction Searching in the Web Version of SciFinder In this tutorial, you will learn how to use advanced reaction search features using the web version ...	Reactions	Advanced	November 4, 2008	9.1 MB	16 mins	WRF
Intermediate Reaction Searching in the Web Version of SciFinder In this tutorial, you will learn more advanced reaction search techniques using the web version of S...	Reactions	Intermediate	November 4, 2008	8.0 MB	13 mins	WRF

... y completar el formulario.

Enroll for SciFinder®: Exploring What's New with SciFinder®!

Please provide the following information to complete your enrollment. An asterisk (*) indicates a required field.

Please answer the following questions.

* First Name:		* Last Name:	
* Email Address:		Phone Number:	
* Confirm Email Address:			
* Company:			
Address 1:			
Address 2:			
City:		State/Province:	
ZIP/Postal code:			
Country/Region:	United States of America		
* Would you like to receive information about future CAS e-Seminars at your email address?:			
☒ Yes			
☐ No			
* SciFinder Login ID (Academics: Please list name of University or College):			
* Job Title:			

Done



Más información...

SciFinder®

CAS Customer Care

Web: www.cas.org

E-mail: help@cas.org

Training and Support: www.cas.org/support/scifi/



SciFinder®

CAS is a division of the American Chemical Society

www.cas.org

Agenda

- Bases de datos de CAS: ¡más contenido!
- La versión web de SciFinder: ¡Novedades!
- **SciFinder: registro**
- Ejemplos de búsquedas:
 - Por tema
 - Por estructura
 - Por reacción

 **SciFinder® ...Part of the process™**

Welcome to User Registration for SciFinder®!

Click Next to begin registration as a new user.

[Next>>](#)

 **SciFinder® ...Part of the process™**

Please provide the following information:
(bold* = required)

--CONTACT INFORMATION--

First Name*:

Last Name*:

Email*:

Confirm Email*:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username*: [Tips](#)

Password*:

Re-enter Password*:

--SECURITY INFORMATION--

Security Question*:

Answer*: [Why?](#)

[Register>>](#) [Clear All](#)

- Introducir datos de contacto
- Crear User Name y Password
- Pregunta de seguridad

¡Ayuda!

Username and Password: Tips

Q. How long does my username need to be?

A. Your username must contain a minimum of 5 characters and a maximum of 15 characters.

Q. What types of characters can my username include?

A. Your username can be all letters. It can optionally contain numbers and the following special characters:

-	dash
_	underscore
.	period
@	at symbol

Q. How long does my password need to be?

A. Your password must contain a minimum of 7 and a maximum of 15 characters.

Q. Can my password be the same as my username?

A. At least 2 of the characters in your password must be different from your username.

Q. What types of characters does my password have to include?

A. Your password must include at least three (3) of the following:

- Letters
- Mixed upper and lowercase letters
- Numbers
- Non-alphanumeric characters (e.g., @, #, %, &, *)

Q. When I change my password, how different does it need to be from my old password?

A. A new password must differ from your old password by at least 2 characters.

Additional questions may be directed to [CAS Customer Care](#).



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 SciFinder® ...Part of the process™

Please provide the following information:
(**bold*** = required)

--CONTACT INFORMATION--	
First Name*:	
Last Name*:	
Email*:	
Confirm Email*:	
Phone Number:	
Fax Number:	
Area of Research:	Select one
Job Title:	Select one

--USERNAME AND PASSWORD--	
Username*:	
Password*:	
Re-enter Password*:	

--SECURITY INFORMATION--	
Security Question*:	Select one
Answer*:	

 SciFinder® ...Part of the process™

Almost Finished

Thank you for completing the initial step in registering to use SciFinder®! You will receive an e-mail message from CAS with instructions for completing the registration process.

To complete your SciFinder registration, you must click the link provided below. By clicking the link, you agree to all of the following terms and conditions:

- I will not share my username and password with any other person.
- I will search only for myself and not for others or other organizations.
- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
- I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.
- My organization's SciFinder License and the CAS Information Use Policies (<http://www.cas.org/legal/infopolicy.html>) apply to my use of SciFinder.
- I will contact my SciFinder Key Contact if I have questions.

If you do not accept these terms and conditions, do not click the link and delete this e-mail message.

<https://scifinder.cas.org/registration/completeRegistration.html?respKey=D948E32D-86F3-F00A-11E0-D28193AFA95D>

If you need assistance at any time, consult the key contact at your organization.



Registration for SciFinder® is Complete

You have successfully completed the registration process.

To sign in to SciFinder®, click the link below.

<https://scifinder.cas.org/scifinder>



<https://scifinder.cas.org/scifinder>



SciFinder®

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ACS Journals C&EN CAS

Advanced Search

Site Search

Home About CAS Our Expertise Solutions Products & Services Support & Training News & Events

The world's most
authoritative and
comprehensive
source of chemical substance information

RESEARCHERS
Learn about  SciFinder®

PROFESSIONAL SEARCHERS
Learn about **STN**®

Current Customers
Find all your product resources in SciFinder and STN Support & Training.
 

CAS offers the **CAS REGISTRY**™ - the largest collection of substance information - as well as indexed references from more than 10,000 major scientific journals and 59 patent authorities around the world. **CAS databases** are:

- ▶ Updated daily
- ▶ Built and quality controlled by CAS scientists
- ▶ Accessed via **SciFinder** and **STN** - award-winning search and analysis tools
- ▶ A single resource for both patents and journal articles

SUBSTANCES
50,856,889
organic and inorganic

Content Corner
▶ 50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY

Colors of Chemistry
Yellow-dyed silk robes were so precious to ancient Chinese emperors that they permitted no one else to wear them. These emperors also



ACS Journals C&EN CAS

Advanced Search

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Home About CAS Our Expertise Solutions Products & Services Support & Training News & Events

The world's most **authoritative** and **comprehensive** substance information

Select a Quick Link

- Sign in to SciFinder
- Sign in to STN on the Web
- Sign in to STN Easy
- CAS Databases
- CAS Registry System
- SciFinder Support & Training
- SciFinder Content at a Glance
- SciFinder Training Calendar
- STN Support & Training
- STN Database Summary Sheets
- STN Training Calendar
- Select a Quick Link

RESEARCHERS
Learn about  SciFinder®

PROFESSIONAL SEARCHERS
Learn about  STN®

SUBSTANCES
50,856,889
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CAS offers the **CAS REGISTRY**™ - the largest collection of substance information - as well as indexed references from more than 10,000 major scientific journals and 59 patent authorities around the world. **CAS databases** are:

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- ▶ A single resource for both patents and journal articles

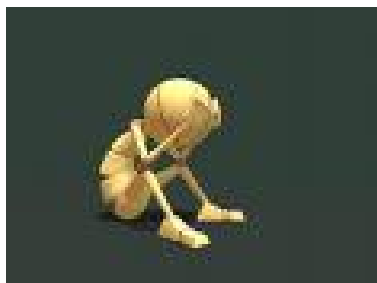
Content Corner

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Colors of Chemistry
Yellow-dyed silk robes were so precious to ancient Chinese emperors that they permitted no one else to wear them. These emperors also



Cuando surgen problemas...



He olvidado el Password...

No encuentro lo que busco...

SciFinder se me cierra...

E-mail a : mplana@cas.org ←

- “He perdido/no recuerdo el **password**...”

Opción: “Forgot username or Password?”

The image shows a screenshot of the SciFinder website's login interface. At the top, the SciFinder logo is followed by the tagline "...Part of the process™". Below this is a "Sign In" section with input fields for "Username" and "Password", a "Remember my username" checkbox, and a "Forgot Username or Password?" link. A pink rectangular box highlights the "Forgot Username or Password?" link, and a pink arrow points from it to a large white text box with a pink border that contains the text "Forgot Username or Password?". To the right of the login form, there is a "Welcome to SciFinder!" message and a list of benefits. At the bottom of the page, there are links for "About SciFinder", "SciFinder Support and Training", and "CAS Databases", along with the text "CAS is a division of the American Chemical Society".

SciFinder® ...Part of the process™

Sign In

Username

Password

☐ Remember my username

[Forgot Username or Password?](#)

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

What is SciFinder?

SciFinder is a... the CAS data... disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

Welcome to SciFinder!

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

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

50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY

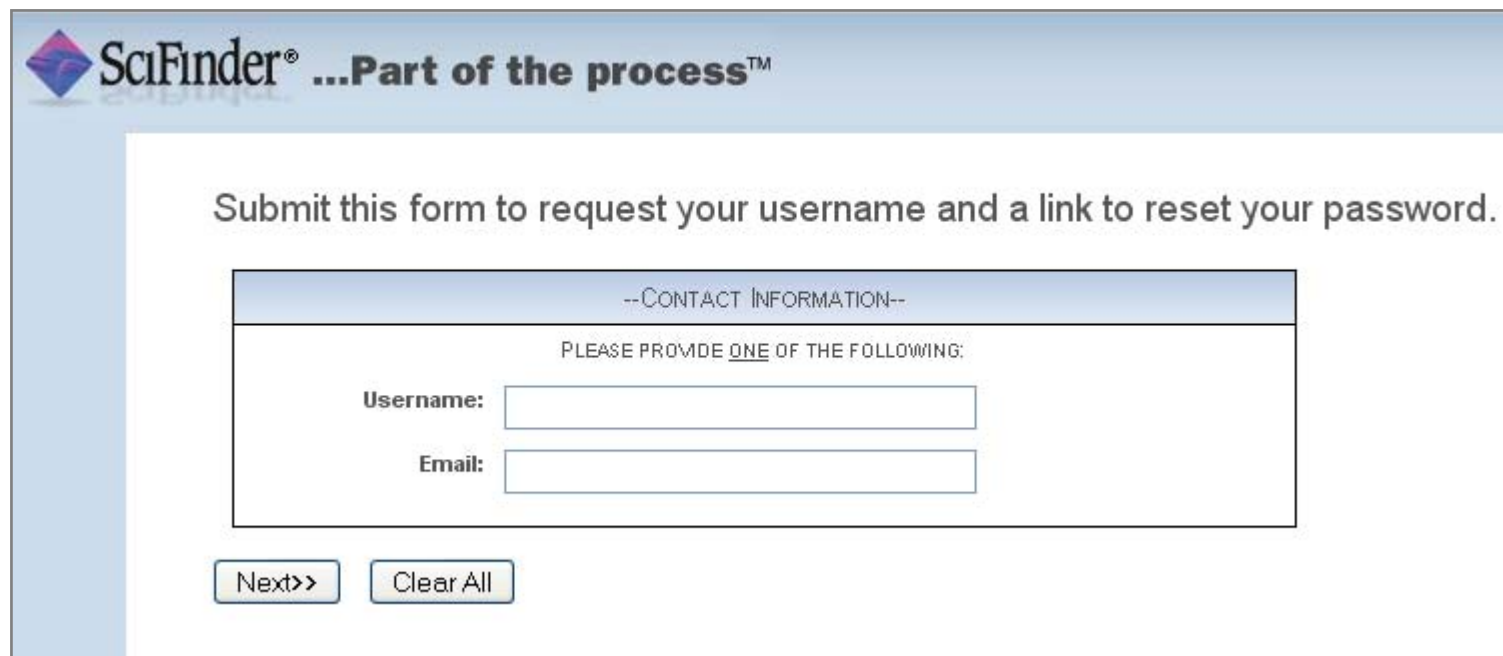
Columbus, Ohio (September 8, 2009) - Chemical Abstracts Service (CAS), a division of the American Chemical Society,...

substance just nine months ago - in contrast, it took 33 years for CAS to register the 10 millionth compound in 1990.

About SciFinder | SciFinder Support and Training | CAS Databases

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www.cas.org



The screenshot shows the SciFinder login page with a password reset form. The header includes the SciFinder logo and the tagline "...Part of the process™". The form is titled "Submit this form to request your username and a link to reset your password." and contains a section for contact information. Below this, it asks the user to provide either a username or an email address. There are two input fields: one for the username and one for the email. At the bottom of the form, there are two buttons: "Next>>" and "Clear All".

SciFinder® ...Part of the process™

Submit this form to request your username and a link to reset your password.

--CONTACT INFORMATION--

PLEASE PROVIDE ONE OF THE FOLLOWING:

Username:

Email:

Next>> Clear All

Responder al formulario.

En breve CAS os envía el username o password

- “SciFinder me da un error...”

The screenshot shows the SciFinder login interface. At the top, the SciFinder logo is followed by the text "...Part of the process™". Below this is a "Sign In" section with a red error message box that reads: "Username and/or password is invalid. Try again, or contact CAS for assistance." This message is repeated in a larger box below the login fields. The login fields include "Username", "Password", a "Remember my username" checkbox, and a "Forgot Username" link. A "Sign In" button is also present. To the right of the login section, there is a "Welcome to SciFinder!" message followed by a list of benefits: "With SciFinder, you can be more creative and productive in your research process. You significantly improve your productivity by:"

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

Below the list, there is a section titled "Once Recorded in CAS" which mentions the 50 millionth substance in CAS REGISTRY. At the bottom of the page, there are links for "About SciFinder", "SciFinder Support and Training", and "CAS Databases".

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!

SCIFINDER

CAS is a division of the American Chemical Society

- “SciFinder me da un error...”

E-mail a **mplana@cas.org** con un
“pantallazo” del problema.



¡Ayuda a resolver el problema con rapidez!

Agenda

- Bases de datos de CAS: ¡más contenido!
- La versión web de SciFinder: ¡Novedades!
- SciFinder: registro
- **Ejemplos de búsquedas:**
 - Por tema
 - Por estructura
 - Por reacción



SciFinder[®]

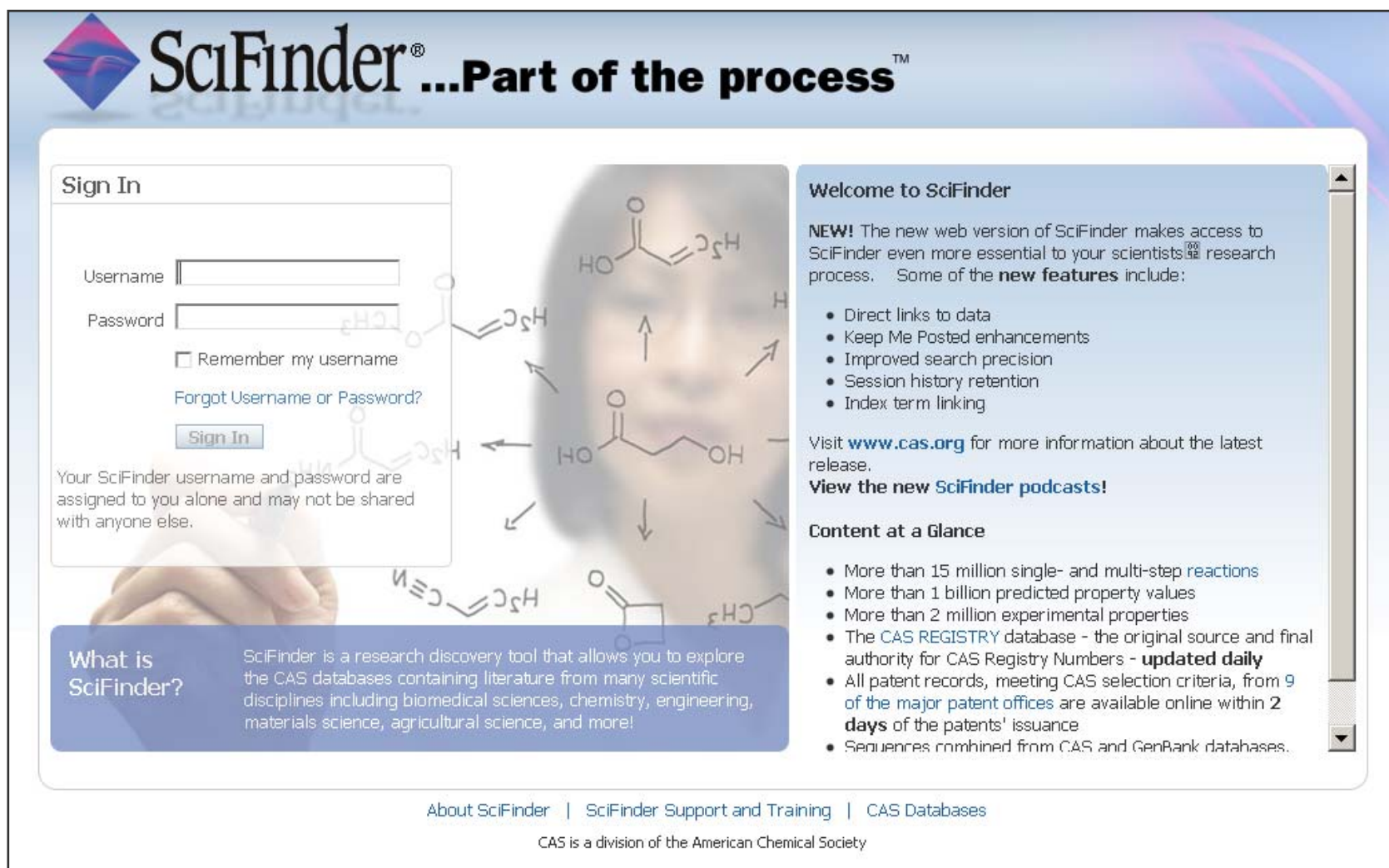
SciFinder[®]

EJEMPLOS DE BÚSQUEDAS



SciFinder[®]

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SciFinder® ...Part of the process™

Sign In

Username

Password

☐ Remember my username

[Forgot Username or Password?](#)

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

Welcome to SciFinder

NEW! The new web version of SciFinder makes access to SciFinder even more essential to your scientists' research process. Some of the **new features** include:

- Direct links to data
- Keep Me Posted enhancements
- Improved search precision
- Session history retention
- Index term linking

Visit www.cas.org for more information about the latest release.

View the new SciFinder podcasts!

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!

Content at a Glance

- More than 15 million single- and multi-step **reactions**
- More than 1 billion predicted property values
- More than 2 million experimental properties
- The **CAS REGISTRY** database - the original source and final authority for CAS Registry Numbers - **updated daily**
- All patent records, meeting CAS selection criteria, from **9 of the major patent offices** are available online within **2 days** of the patents' issuance
- Sequences combined from CAS and GenBank databases.

[About SciFinder](#) |
 [SciFinder Support and Training](#) |
 [CAS Databases](#)

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Welcome to SciFinder

 Please wait while your session starts...



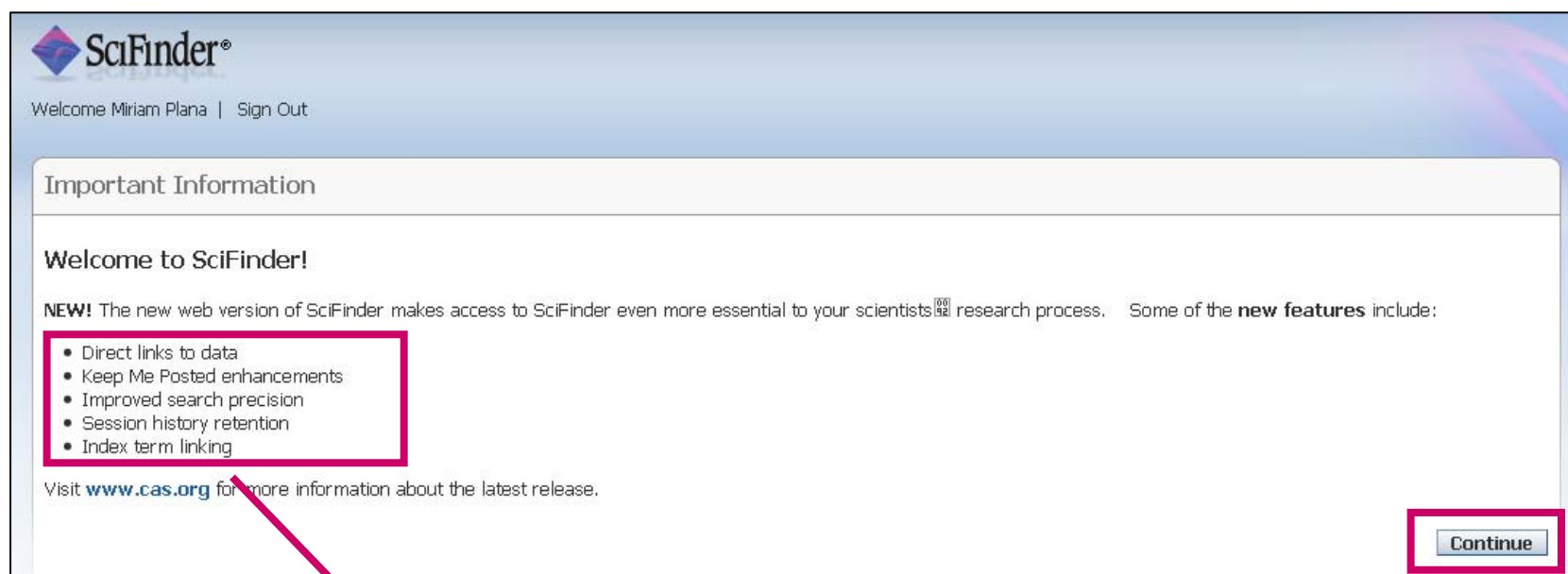
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Part of the process.™

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https://scifinder.cas.org



- Direct links to data
- Keep Me Posted enhancements
- Improved search precision
- Session history retention
- Index term linking

Barra de Herramientas

SciFinder®

Welcome Miriam Plana | Sign Out

Explore References | Explore Substances | Explore Reactions

red Answer Sets | Help
Keep Me Posted Results | History
NEW My Connections | Preferences

Explore References

Research Topic

Author Name
Company Name
Document Identifier
Journal
Patent
Tags **NEW**

Research Topic

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

Search

Refs. guardadas,
alertas (KMP),
conexiones

Opciones de
búsqueda

Publication Year(s)

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

Document Type(s)

☐ Biography ☐ Dissertation ☐ Patent
☐ Book ☐ Editorial ☐ Preprint
☐ Clinical Trial ☐ Historical ☐ Report
☐ Commentary ☐ Journal ☐ Review
☐ Conference ☐ Letter

Language(s)

☐ Chinese ☐ German ☐ Polish
☐ English ☐ Italian ☐ Russian
☐ French ☐ Japanese ☐ Spanish

Author Name

Last * First Middle

Company Name

Examples:
Minnesota Mining and Manufacturing
DuPont

¡Ayuda!

Saved Answer Sets

prova
climatic change
Autosaved Substance Set

View All

Import

Keep Me Posted Results

Cambio climatico
Oct 17, 2009 (6)
Oct 10, 2009 (4)
Oct 03, 2009 (9)

View All

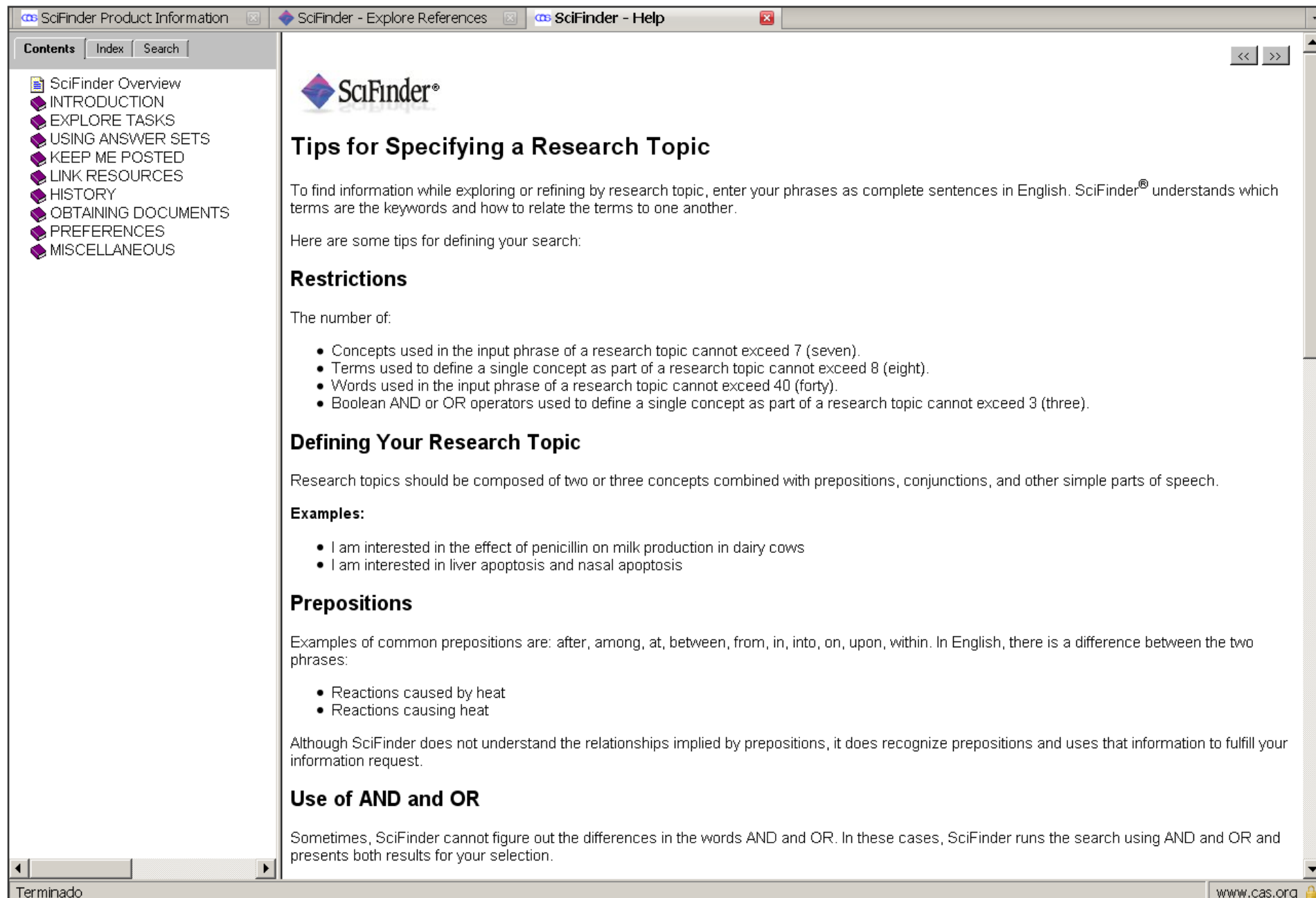
My Connections

No invitations to connect

You have 1 outstanding sent invitation

No connections in your network

Para limitar
la búsqueda



The screenshot displays the SciFinder Web interface. At the top, there are three browser tabs: 'SciFinder Product Information', 'SciFinder - Explore References', and 'SciFinder - Help'. The main content area is titled 'Contents' and includes a sidebar with a list of links: 'SciFinder Overview', 'INTRODUCTION', 'EXPLORE TASKS', 'USING ANSWER SETS', 'KEEP ME POSTED', 'LINK RESOURCES', 'HISTORY', 'OBTAINING DOCUMENTS', 'PREFERENCES', and 'MISCELLANEOUS'. The main content area features the SciFinder logo and the title 'Tips for Specifying a Research Topic'. Below the title, there is a paragraph explaining that users should enter phrases as complete sentences in English. This is followed by a section titled 'Restrictions' which lists four bullet points regarding the number of concepts, terms, words, and Boolean operators allowed. Next is a section titled 'Defining Your Research Topic' which explains that research topics should be composed of two or three concepts combined with prepositions, conjunctions, and other simple parts of speech. This is followed by an 'Examples' section with two bullet points. Then, there is a section titled 'Prepositions' which provides examples of common prepositions and explains that SciFinder recognizes them. Finally, there is a section titled 'Use of AND and OR' which explains that SciFinder runs the search using both AND and OR and presents both results for your selection. The bottom of the interface shows a status bar with the text 'Terminado' and the URL 'www.cas.org'.

SciFinder Product Information | SciFinder - Explore References | SciFinder - Help

Contents | Index | Search

SciFinder Overview
INTRODUCTION
EXPLORE TASKS
USING ANSWER SETS
KEEP ME POSTED
LINK RESOURCES
HISTORY
OBTAINING DOCUMENTS
PREFERENCES
MISCELLANEOUS

SciFinder®

Tips for Specifying a Research Topic

To find information while exploring or refining by research topic, enter your phrases as complete sentences in English. SciFinder® understands which terms are the keywords and how to relate the terms to one another.

Here are some tips for defining your search:

Restrictions

The number of:

- Concepts used in the input phrase of a research topic cannot exceed 7 (seven).
- Terms used to define a single concept as part of a research topic cannot exceed 8 (eight).
- Words used in the input phrase of a research topic cannot exceed 40 (forty).
- Boolean AND or OR operators used to define a single concept as part of a research topic cannot exceed 3 (three).

Defining Your Research Topic

Research topics should be composed of two or three concepts combined with prepositions, conjunctions, and other simple parts of speech.

Examples:

- I am interested in the effect of penicillin on milk production in dairy cows
- I am interested in liver apoptosis and nasal apoptosis

Prepositions

Examples of common prepositions are: after, among, at, between, from, in, into, on, upon, within. In English, there is a difference between the two phrases:

- Reactions caused by heat
- Reactions causing heat

Although SciFinder does not understand the relationships implied by prepositions, it does recognize prepositions and uses that information to fulfill your information request.

Use of AND and OR

Sometimes, SciFinder cannot figure out the differences in the words AND and OR. In these cases, SciFinder runs the search using AND and OR and presents both results for your selection.

Terminado | www.cas.org

BÚSQUEDA TEMÁTICA:

**“Interactions of drugs (pharmaceuticals)
with grapefruit juice”**



 Explore References  Explore Substances  Explore Reactions

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Explore References

Research Topic  Interactions of drugs (pharmaceuticals) with grapefruit juice 

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

Research Topic  Interactions of drugs (pharmaceuticals) with grapefruit juice

Publication Year(s) 
Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s) 

☐ Biography	☐ Dissertation	☐ Patent
☐ Book	☐ Editorial	☐ Preprint
☐ Clinical Trial	☐ Historical	☐ Report
☐ Commentary	☐ Journal	☐ Review
☐ Conference	☐ Letter	

Language(s) 

☐ Chinese	☐ German	☐ Polish
☐ English	☐ Italian	☐ Russian
☐ French	☐ Japanese	☐ Spanish


[Explore References](#)
[Explore Substances](#)
[Explore Reactions](#)

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Create Keep Me Posted Research Topic "Interactions of drugs (pharmac..."

Research Topic Candidates

25 Topics 0 Selected

Select All Deselect All

Research Topic Candidates	References
☐ 357 references were found containing both of the concepts "Interactions" and "grapefruit juice", and either the concept "drugs" or the concept "pharmaceuticals". The concepts found were closely associated with one another.	357
☐ 701 references were found containing both of the concepts "Interactions" and "grapefruit juice", and either the concept "drugs" or the concept "pharmaceuticals". The concepts found were present anywhere (perhaps widely separated) within the reference.	701
☐ 357 references were found containing all of the concepts "Interactions", "drugs" and "grapefruit juice" closely associated with one another.	357
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☐ 701 references were found where all of the concepts "Interactions", "pharmaceuticals" and "grapefruit juice" were present anywhere in the reference.	701
☐ 170916 references were found containing the concept "Interactions", and either the concept "drugs" or the concept "pharmaceuticals". The concepts found were closely associated with one another.	170916
☐ 360957 references were found containing the concept "Interactions", and either the concept "drugs" or the concept "pharmaceuticals". The concepts found were present anywhere (perhaps widely separated) within the reference.	360957
☐ 170916 references were found containing the two concepts "Interactions" and "drugs" closely associated with one another.	170916
☐ 360957 references were found where the two concepts "Interactions" and "drugs" were present anywhere in the reference.	360957
☐ 170916 references were found containing the two concepts "Interactions" and "pharmaceuticals" closely associated with one another.	170916
☐ 360957 references were found where the two concepts "Interactions" and "pharmaceuticals" were present anywhere in the reference.	360957
☐ 479 references were found containing the two concepts "Interactions" and "grapefruit juice" closely associated with one another.	479
☐ 741 references were found where the two concepts "Interactions" and "grapefruit juice" were present anywhere in the reference.	741
☐ 542 references were found containing the concept "grapefruit juice", and either the concept "drugs" or the concept "pharmaceuticals". The concepts found were closely associated with one another.	542

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Create Keep Me Posted Research Topic "Interactions of drugs (pharmac..."

Explore References Explore Substances Explore Reactions

Research Topic Candidates

25 Topics 1 Selected

Select All Deselect All

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SciFinder®

Welcome Miriam Plana | Sign Out

Create Keep Me Posted Research Topic "Interactions of drugs (pharmac..." > references (357)

References Get Substances Get Reactions Get Cited Get Citing

357 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 18 View: [icon]

References Get Substances Get Reactions Get Cited Get Citing

simvastatin (20 and 80 mg/kg, resp.). Both **juices** did not have a significant effect on the pharmacokinetic parameters of either simvastatin lactone (SVL) or its active metabolite simvastatin hydroxy acid (SVA).

2. **Grapefruit juice interaction with oral budesonide**
By Seidegaard, J.; Randvall, G.; Nyberg, L.; Borgaa, O.
From Pharmazie (2009), 64(7), 461-465. Language: English.
Grapefruit juice (GFJ) inhibits CYP3A activity in men participated in this open crossover study. Three mg budesonide as ER capsules or plain capsules was swallowed with or without previous intake of GFJ. Regular-strength GFJ 200 mL was given three times a day for four days. Budesonide was administered immediately after the...

3. **Influence of grapefruit juice on the pharmacokinetics of diltiazem in wistar rats upon single and multiple dosage regimens**
By Boddu, S. P.; Yamsani, M. Rao; Potharaju, S.; Veeraraghavan, S.; Rajak, S.; Kumar V. V. S. S.; Avery, B. A.; Repka, M. A.; Varanasi, V. S. K. Kiran
From Pharmazie (2009), 64(8), 525-531. Language: English, Database: CAPLUS
Drug efflux by intestinal P-glycoprotein (P-gp) is recognized as a significant biochem. barrier affecting oral absorption for a no. of **drugs** apart from the cytochrome P 450 3A enzyme. Various conflicting reports have been published regarding the effects of **grapefruit juice** (GFJ) on P-gp mediated **drug** efflux, in which GFJ has been shown to have no effect, as an inhibitor effect or activation of the enzyme. Therefore the present study's objective was to provide clarification of previous findings, adopting a two-way approach, involving both single dose and multiple dosage regimens. Diltiazem (...)

Información relacionada con las referencias

Neuvonen Pertti J 13
Lilja Jari J 11
Paine Mary F 10
Uesawa Yoshihiro 10
Bailey D G 9
Mohri Kiminori 9
Watkins Paul B 9
Dresser George K 8
Spence J David 8

Show More

SciFinder®

Welcome Miriam Plana | Sign Out

Create Keep Me Posted Research Topic "Interactions of drugs (pharmac..." > references (357)

References Get Substances Get Reactions Get Cited Get Citing

357 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 18 View: [icon]

1. Toxicity of grapefruit juice
By Butterweck, Veronika; Zurojewski, Immo; Galloway, Cheryl; Frye, Regina; Derendon, Harriet
From Planta Medica (2009), 75(11), 1196-1202. Language: English, Database: CAPLUS
Since data concerning the toxicity and pharmacokinetics of compounds performed a chronic study in rats over a 4-wk period using 2 simvastatin (20 and 80 mg/kg, resp.). Both juices did not have active metabolite simvastatin hydroxy acid (SVA) when administered. [Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)

2. Grapefruit juice interaction with oral budesonide: equal effect
By Seidegaard, J.; Randvall, G.; Nyberg, L.; Borgaa, O.
From Pharmazie (2009), 64(7), 461-465. Language: English, Database: CAPLUS
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3. Influence of grapefruit juice on the pharmacokinetics of diltiazem in wistar rats upon single and multiple dosage regimens
By Boddu, S. P.; Yamsani, M. Rao; Potharaju, S.; Veeraraghavan, S.; Rajak, S.; Kumar V. V. S. S.; Avery, B. A.; Repka, M. A.; Varanasi, V. S. K.; Kiran
From Pharmazie (2009), 64(8), 525-531. Language: English, Database: CAPLUS
Drug efflux by intestinal P-glycoprotein (P-gp) is recognized as a significant biochem. barrier affecting oral absorption for a no. of drugs apart from the cytochrome P 450 3A enzyme. Various conflicting reports have been published regarding the effects of grapefruit juice (GFJ) on P-gp mediated drug efflux, in which GFJ has been shown to have no effect, as an inhibitor effect or activation of the enzyme. Therefore the present study's objective was to provide clarification of previous findings, adopting a two-way approach, involving both single dose and multiple dosage regimens. Diltiazem (... [Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)

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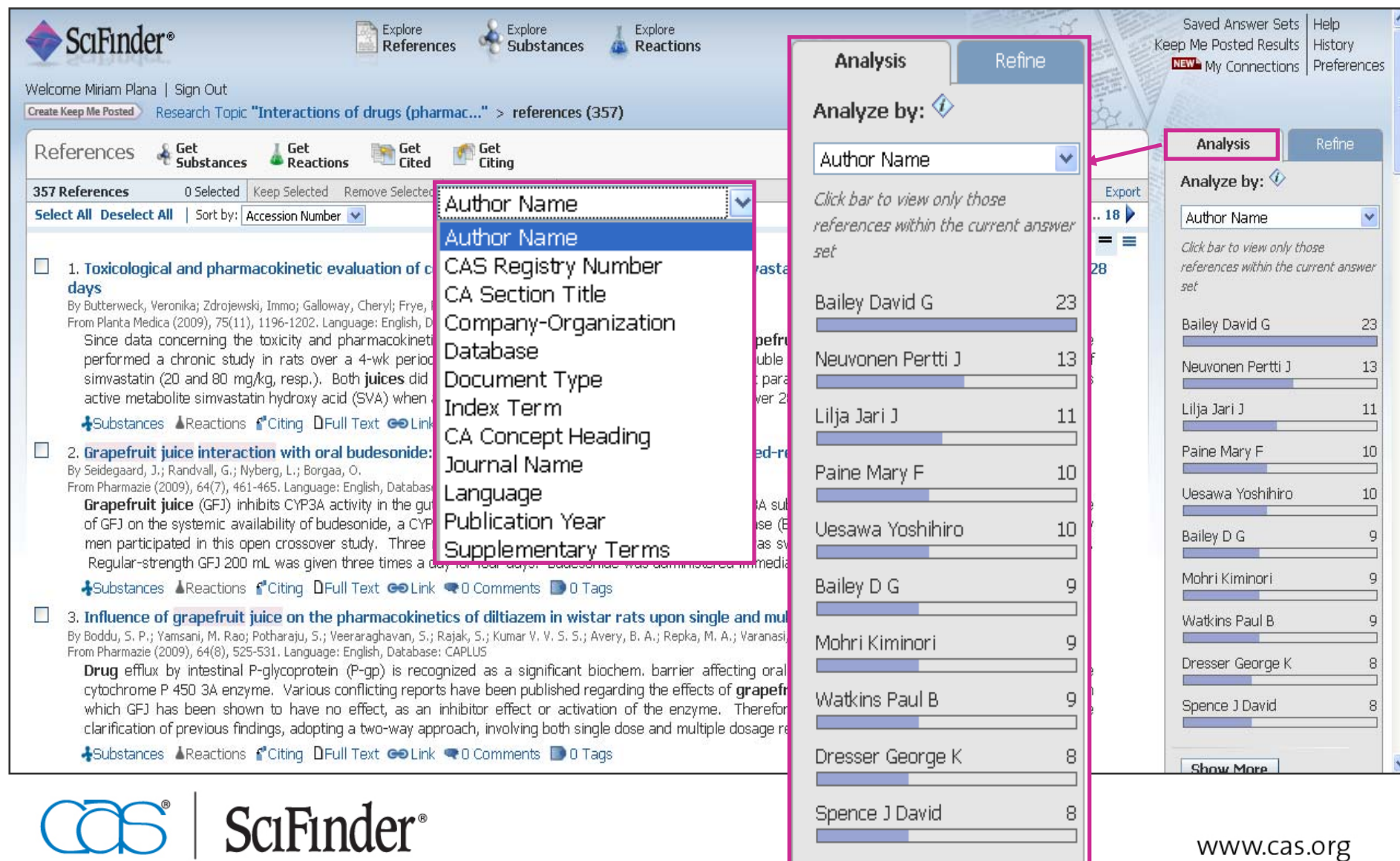
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81. The grapefruit juice effect is not limited to cytochrome P450 (P450) 3A4: Evidence for covalent binding to protein in P450s 2B6 and 3A5
By Lin, Hsia-lien; Kent, Ute M.; Hollenberg, Paul F.
From Journal of Pharmacology and Experimental Therapeutics (2005), 313(1), 154-164. Language: English, Database: CAPLUS
Bergamottin (BG), a component of **grapefruit juice**, is a mechanism-based inactivator of cytochrome P450 3A4. The inactivation of both P450s was NADPH-dependent and irreversible. The kinetic constants for the deethylation activity of P 450 2B6 were: K_i , 5 μ M; k_{inact} , 0.09 min⁻¹; and $t_{1/2}$, 8 min. The kinetic constants for the hydroxylation activity of P 450 3A4 were: K_i , 20 μ M; k_{inact} , 0.045 min⁻¹; and $t_{1/2}$, 15 min. Incubation of P 450 3A4 with BG resulted in a time-dependent decrease in enzyme activity.

82. Grapefruit juice-drug interaction issues
By Bailey, David G.
Edited by Boullata, Joseph I.; Arment, Vincent T.; Malone, Margaret
From Handbook of Drug-Nutrient Interactions (2004), 175-194. Language: English, Database: CAPLUS
A review discusses the basic science of **grapefruit juice-drug interactions**, their clinical evidence, and their management.

83. Two major grapefruit juice components differ in time to onset of intestinal CYP3A4 inhibition
By Paine, Mary F.; Criss, Anne B.; Watkins, Paul B.
From Journal of Pharmacology and Experimental Therapeutics (2005), 312(3), 1151-1160. Language: English, Database: CAPLUS
Grapefruit juice elevates blood levels of some **drugs** taken orally, primarily by inhibiting intestinal CYP3A4. Two major components of **grapefruit juice**, 6',7'-dihydroxybergamottin (DHB) and bergamottin (BG), have been demonstrated to inhibit CYP3A4. Using CYP3A4-expressing Caco-2 cells and representative probes from distinct CYP3A4 substrates, we compared the time-dependent inhibitory properties of DHB and BG. DHB rapidly inhibited CYP3A4 activity, whereas BG required a longer time to inhibit CYP3A4 activity.

84. Effect of grapefruit juice volume on the reduction of fexofenadine bioavailability: Possible mechanism of action
By Dresser, George K.; Kim, Richard B.; Bailey, David G.
From Clinical Pharmacology and Therapeutics (New York, NY: United States) (2005), 77(3), 170-177. Language: English, Database: CAPLUS
Fexofenadine is a second-generation antihistamine that is not metabolized by CYP3A4. However, the bioavailability of fexofenadine is reduced when it is administered with **grapefruit juice**. The purpose of this study was to determine the effect of **grapefruit juice** volume on the reduction of fexofenadine bioavailability and to identify the possible mechanism of action.

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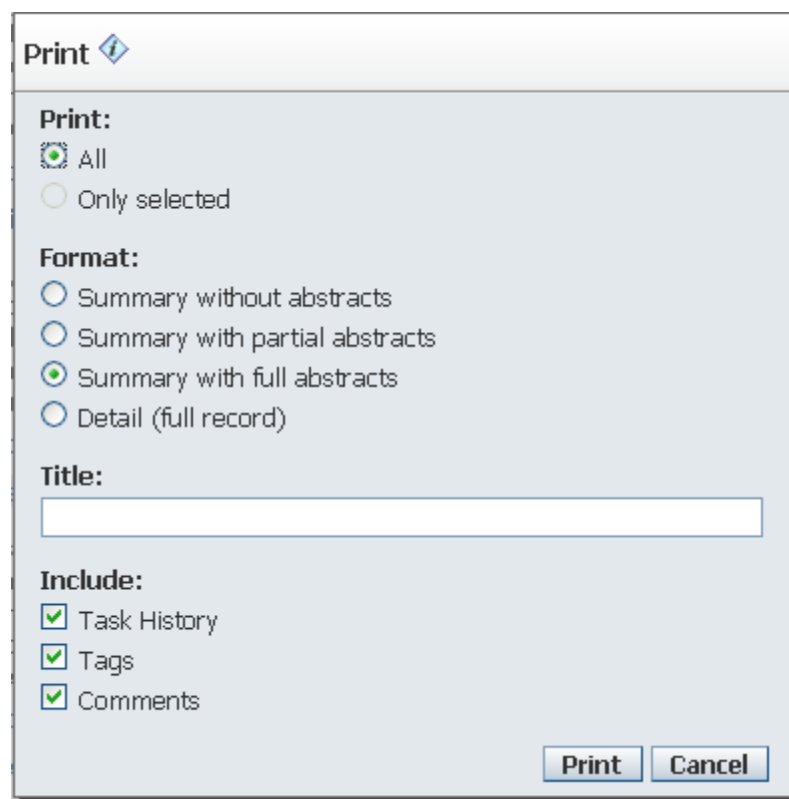
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25. Further characterization of a furanocoumarin-free grapefruit juice on drug disposition: studies with cyclosporine
By Paine, Mary F.; Widmer, Wilbur W.; Pusek, Susan N.; Beavers, Kimberly L.; Criss, Anne B.; Snyder, Jennifer; Watkins, Paul B.
From American Journal of Clinical Nutrition (2008), 87(4), 863-871. Language: English, Database: CAPLUS
Background: We previously established furanocoumarins as mediators of the **interaction** between **grapefruit juice** (GFJ) and the model CYP3A4 substrate felodipine in healthy volunteers using a GFJ devoid of furanocoumarins. It remains unclear whether furanocoumarins mediate **drug-GFJ interactions** involving CYP3A4 substrates that are also P-glycoprotein substrates. Objective: The effects of furanocoumarin-free GFJ on **drug** disposition were further characterized by using the dual CYP3A4/P-glycoprotein substrate cyclosporine. Design: By randomized crossover design, 18 healthy volunteers received cyclosporine...
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42. Clinical relevance of the small intestine as an organ of drug elimination: drug-fruit juice interactions
By Paine, Mary F.; Oberlies, Nicholas H.
From Expert Opinion on Drug Metabolism & Toxicology (2007), 3(1), 67-80. Language: English, Database: CAPLUS
A review. Most **drugs** are taken orally. For those intended to act systemically, a significant fraction of the dose can be eliminated during its first passage through a sequence of organs before entry into the general circulation. For some **drugs**, the degree of first-pass elimination can be large enough such that oral bioavailability is significantly reduced, with the consequent potential for a reduced clin. response. Of these first-pass eliminating organs, the small intestine and liver are the most commonly implicated, in part because they express the highest levels of **drug**-metabolizing enzymes...
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55. A furanocoumarin-free grapefruit juice establishes furanocoumarins as the mediators of the grapefruit juice-felodipine interaction. [Erratum to document cited in CA145:137286]
By Paine, Mary F.; Widmer, Wilbur W.; Hart, Heather L.; Pusek, Susan N.; Beavers, Kimberly L.; Criss, Anne B.; Brown, Sherri S.; Thomas, Brian F.; Watkins, Paul B.
From American Journal of Clinical Nutrition (2006), 84(1), 264. Language: English, Database: CAPLUS
On page 1101, numerous values in Table 1 were incorrectly listed as P values. The cor. table is given.
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62. A furanocoumarin-free grapefruit juice establishes furanocoumarins as the mediators of the grapefruit juice-felodipine interaction
By Paine, Mary F.; Widmer, Wilbur W.; Hart, Heather L.; Pusek, Susan N.; Beavers, Kimberly L.; Criss, Anne B.; Brown, Sherri S.; Thomas, Brian F.; Watkins, Paul B.

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Neuvonen Pertti J	13
Lilja Jari J	11
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Uesawa Yoshihiro	10
Bailey D G	9
Mohri Kiminori	9
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Dresser George K	8
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1. Toxicological and pharmacokinetic evaluation of concomitant intake of grapefruit juice and simvastatin days
By Butterweck, Veronika; Zdrojewski, Immo; Galloway, Cheryl; Frye, Reginald; Derendorf, Hartmut
From Planta Medica (2009), 75(11), 1196-1202. Language: English, Database: CAPLUS
Since data concerning the toxicity and pharmacokinetics of concomitant repeated administration of grapefruit juice performed a chronic study in rats over a 4-wk period using 2 different strengths (regular [RS] and double strength [DS] simvastatin (20 and 80 mg/kg, resp.). Both juices did not have a significant effect on the pharmacokinetic parameters of simvastatin hydroxy acid (SVA) when administered concomitantly in a dose of 20 mg/kg over 28 days.

2. Grapefruit juice interaction with oral budesonide: equal effect on immediate-release and delayed-release formulations
By Seidegaard, J.; Randvall, G.; Nyberg, L.; Borgaa, O.
From Pharmazie (2009), 64(7), 461-465. Language: English, Database: CAPLUS
Grapefruit juice (GFJ) inhibits CYP3A activity in the gut wall, thereby decreasing first-pass metabolism of CYP3A substrates. In this study, the effect of GFJ on the systemic availability of budesonide, a CYP3A-metabolized drug, both from an extended-release (ER) and immediate-release (IR) formulation was evaluated. Ten healthy men participated in this open crossover study. Three mg budesonide as ER capsules or plain capsules was swallowed with or without GFJ. Regular-strength GFJ 200 mL was given three times a day for four days. Budesonide was administered immediately after the last GFJ intake.

3. Influence of grapefruit juice on the pharmacokinetics of diltiazem in wistar rats upon single and multiple dosing
By Boddu, S. P.; Yamsani, M. Rao; Potharaju, S.; Veeraraghavan, S.; Rajak, S.; Kumar V. V. S. S.; Avery, B. A.; Repka, M. A.; Varanasi, V.
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Term	Count
Drug interactions	262
Grapefruit juice	235
Human	106
pharmacokinetics	87
Humans	78
Beverages	71
Drug bioavailability	61
*Beverages	60
Food-Drug Interactions	56
Citrus paradisi	53

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1. Toxicological and pharmacokinetic evaluation of concomitant intake of grapefruit juice and simvastatin in rats after repeated treatment over 28 days
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☐ 1. **Toxicological and pharmacokinetic evaluation of concomitant intake of grapefruit juice and simvastatin in rats after repeated treatment over 28 days**
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☐ 3. **Influence of grapefruit juice on the pharmacokinetics of diltiazem in wistar rats upon single and multiple dosage regimens**
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Drug interactions	97
Grapefruit juice	91
Human	69
Pharmacokinetics	50
Citrus paradisi	42
Humans	37
Beverages	35
Drug bioavailability	35
*Citrus paradisi	31
Food-Drug Interactions	30

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1. **Toxicol days**
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From Planta...
Since d... of **grapefruit juice** (GFJ) and simvastatin are lacking, we performed a chronic study in rats over a 4-wk period using 2 different strengths (regular [RS] and double strength [DS]) of GFJ and 2 different doses of simvastatin (20 and 80 mg/kg, resp.). Both **juices** did not have a significant effect on the pharmacokinetic parameters of either simvastatin lactone (SVL) or its active metabolite simvastatin hydroxy acid (SVA) when administered concomitantly in a dose of 20 mg/kg over 28 days. However, when ...
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1. Toxicological and pharmacokinetic studies
By Butterweck, Veronika; Zdrojewski, Im...
From Planta Medica (2009), 75(11), 1196-1201.
Since data concerning the toxicity of simvastatin, a hydrophilic statin, performed a chronic study in rats. Simvastatin (20 and 80 mg/kg, active metabolite simvastatin hydroxyacid) was administered daily for 14 days.

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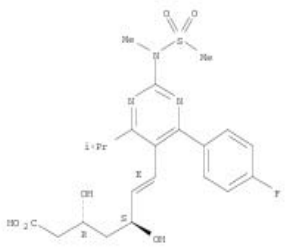
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Substances | Get References | Get Reactions | Get Commercial Sources

64 Substances | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | Answers per Page [15] | 1 2 3 4 5 | View: [Icons]

☐ 1. Substance Detail
287714-41-4



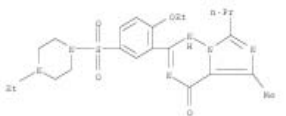
Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,362 References
Reactions

☐ 2. Substance Detail
224785-90-4

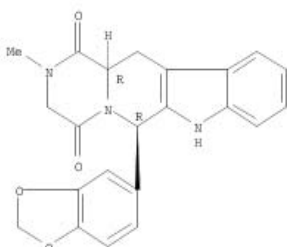


C₂₃ H₃₂ N₆ O₄ S

Imidazo[5,1-f][1,2,4]triazin-4(1H)-one, 2-[2-ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-

~571 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 3. Substance Detail
171596-29-5



Absolute stereochemistry.
Rotation (+).

C₂₂ H₁₉ N₃ O₄

Pyrazino[1',2':1,6]pyrido[3,4-b]indole-1,4-dione, 6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-, (6R,12aR)-

~732 References
Reactions

Analysis | Refine

Analyze by: Substance Role

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

Biological Study	64
Preparation	64
Uses	64
Process	63
Properties	63
Reactant or Reagent	63
Analytical Study	62
Occurrence	52
Formation, Nonpreparative	45
Miscellaneous	39

Show More

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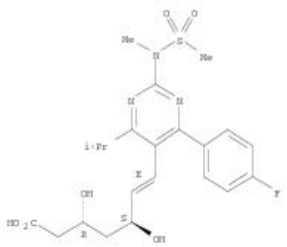
Create Keep Me Posted | Research Topic "Interactions of drugs (pharmac..." > reference

Substances [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

64 Substances 0 Selected Keep Selected Remove Selected

Select All Deselect All Sort by: CAS Registry Number

☐ 1. Substance Detail 287714-41-4



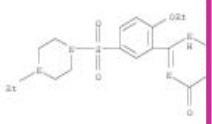
Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,362 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 2. Substance Detail 224785-90-4

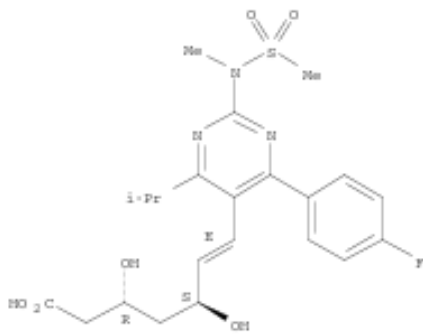


C₂₃ H₃₂ N₆ O₄ S

Imidazo[5,1-f][1,2,4]triazole, 4-ethyl-1-piperazinylsulfonylpropyl-

~571 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 1. Substance Detail 287714-41-4



Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,362 References
Reactions
Commercial Sources
Regulatory Information
Link

Analysis

Analyze by: Substance Role

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

Category	Count
Biological Study	64
Preparation	64
Uses	64
Process	63
Properties	63
Reactant or Reagent	63
Analytical Study	62
Occurrence	52
Formation, Nonpreparative	45
Miscellaneous	39

Show More

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Create Keep Me Posted Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > 287714-41-4

Substance Detail

Get References Get Reactions Get Commercial Sources Get Regulatory Information

Link Save Print Export

Previous Next

1.

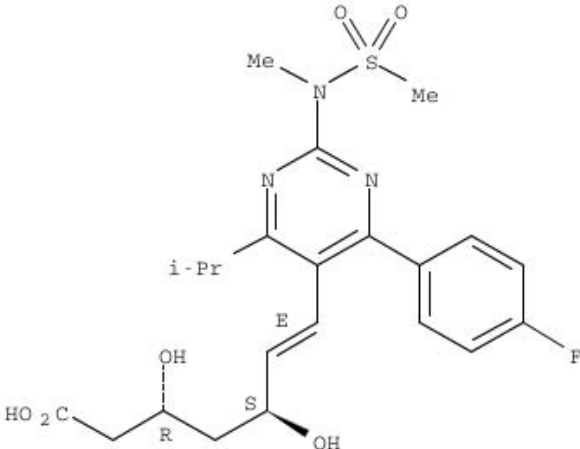
CAS Registry Number: 287714-41-4

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

(E)-(3R,5S)-7-[4-(4-Fluorophenyl)-6-isopropyl-2-[(methylsulfonyl)(methyl)amino]pyrimidin-5-yl]-3,5-dihydroxyhept-6-enoic acid; Rosuvastatin; ZD 4522

Component



Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

Source of Registration: CA

~1,362 References

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

CAplus Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical study		✓		
Biological study	✓	✓	✓	✓
Miscellaneous	✓	✓		
Preparation	✓	✓	✓	✓
Process	✓	✓		
Properties	✓	✓	✓	
Prophetic in patents	✓		✓	
Reactant or reagent	✓	✓	✓	
Uses	✓	✓	✓	

Predicted Properties: [Biological](#) [Chemical](#) [Density](#) [Lipinski and Related](#) [Spectra](#) [Structure-related](#) [Thermal](#)

Biological Properties	Value	Conditions	Notes	Top
Bioconcentration Factor	1.20	pH 1 Temp: 25 °C	(11)	
Bioconcentration Factor	1.22	pH 2 Temp: 25 °C	(11)	
Bioconcentration Factor	1.17	pH 3 Temp: 25 °C	(11)	
Bioconcentration Factor	1.0	pH 4 Temp: 25 °C	(11)	
Bioconcentration Factor	1.0	pH 5 Temp: 25 °C	(11)	
Bioconcentration Factor	1.0	pH 6 Temp: 25 °C	(11)	
Bioconcentration Factor	1.0	pH 7 Temp: 25 °C	(11)	
Bioconcentration Factor	1.0	pH 8 Temp: 25 °C	(11)	
Bioconcentration Factor	1.0	pH 9 Temp: 25 °C	(11)	
Bioconcentration Factor	1.0	pH 10 Temp: 25 °C	(11)	



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Chemical Properties	Value	Conditions	Notes	Top
Koc	39.3	pH 1 Temp: 25 °C	(11)	
Koc	40.0	pH 2 Temp: 25 °C	(11)	
Koc	38.2	pH 3 Temp: 25 °C	(11)	
Koc	25.8	pH 4 Temp: 25 °C	(11)	
Koc	6.09	pH 5 Temp: 25 °C	(11)	
Koc	1.0	pH 6 Temp: 25 °C	(11)	
Koc	1.0	pH 7 Temp: 25 °C	(11)	
Koc	1.0	pH 8 Temp: 25 °C	(11)	
Koc	1.0	pH 9 Temp: 25 °C	(11)	
Koc	1.0	pH 10 Temp: 25 °C	(11)	
logD	0.41	pH 1 Temp: 25 °C	(11)	
logD	0.42	pH 2 Temp: 25 °C	(11)	
logD	0.40	pH 3 Temp: 25 °C	(11)	
logD	0.23	pH 4 Temp: 25 °C	(11)	
logD	-0.40	pH 5 Temp: 25 °C	(11)	
logD	-1.33	pH 6 Temp: 25 °C	(11)	
logD	-2.29	pH 7 Temp: 25 °C	(11)	
logD	-3.03	pH 8 Temp: 25 °C	(11)	
logD	-3.29	pH 9 Temp: 25 °C	(11)	
logD	-3.32	pH 10 Temp: 25 °C	(11)	
logP	0.422±0.850	Temp: 25 °C	(11)	
Mass Intrinsic Solubility	Sparingly Soluble (0.33 g/L)	Temp: 25 °C	(11)	
Mass Solubility	Sparingly Soluble (0.34 g/L)	pH 1 Temp: 25 °C	(11)	
Mass Solubility	Sparingly Soluble (0.33 g/L)	pH 2 Temp: 25 °C	(11)	
Mass Solubility	Sparingly Soluble (0.35 g/L)	pH 3 Temp: 25 °C	(11)	
Mass Solubility	Sparingly Soluble (0.53 g/L)	pH 4 Temp: 25 °C	(11)	
Mass Solubility	Slightly Soluble (2.2 g/L)	pH 5 Temp: 25 °C	(11)	
Mass Solubility	Soluble (19 g/L)	pH 6 Temp: 25 °C	(11)	
Mass Solubility	Very Soluble (170 g/L)	pH 7 Temp: 25 °C	(11)	
Mass Solubility	Very Soluble (925 g/L)	pH 8 Temp: 25 °C	(11)	

Density Properties	Value	Conditions	Notes	Top
Density	1.368±0.06 g/cm ³	Temp: 20 °C Press: 760 Torr	(11)	
Molar Volume	351.8±3.0 cm ³ /mol	Temp: 20 °C Press: 760 Torr	(11)	
Lipinski and Related Properties	Value	Conditions	Notes	Top
Freely Rotatable Bonds	12		(11)	
H Acceptors	9		(11)	
H Donors	3		(11)	
H Donor/Acceptor Sum	12		(11)	
logP	0.422±0.850	Temp: 25 °C	(11)	
Molecular Weight	481.54		(11)	
Spectra Properties	Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum NEW	See spectrum		(12)	
Proton NMR Spectrum	See spectrum		(12)	
Structure-related Properties	Value	Conditions	Notes	Top
Polar Surface Area	149 Å ²		(11)	
Thermal Properties	Value	Conditions	Notes	Top
Boiling Point	745.6±70.0 °C	Press: 760 Torr	(11)	
Enthalpy of Vaporization	114.08±3.0 kJ/mol	Press: 760 Torr	(11)	
Flash Point	404.7±35.7 °C		(11)	
(11) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 for Solaris (© 1994-2009 ACD/Labs)				
(12) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V9.07 (© 1994-2009 ACD/Labs)				
Experimental Properties: Biological Spectra Thermal				
Biological Properties	Value	Conditions	Notes	Top
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(1) CAS	
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(2) CAS	



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Half-Life (Biological)	See full text	(5) CAS	
Half-Life (Biological)	See full text	(6) CAS	
Spectra Properties	Value	Conditions	Notes Top
Carbon-13 NMR Spectrum	See full text		(7) CAS
IR Absorption Spectrum	See full text		(7) CAS
Mass Spectrum	See full text		(8) CAS
Mass Spectrum	See full text		(9) CAS
Proton NMR Spectrum	See full text		(7) CAS
Two-Dimensional NMR Spectrum	See full text		(7) CAS
UV and Visible Absorption Spectrum	See full text		(7) CAS
UV and Visible Absorption Spectrum	See full text		(10) CAS
Thermal Properties	Value	Conditions	Notes Top
Melting Point	161.9 °C		(10) CAS

[\(1\) Verhulst, Anja; Molecular Pharmacology 2008, V74\(4\), P1084-1091 CAPLUS](#)
[\(2\) Schneck, Dennis W.; Clinical Pharmacology & Therapeutics \(St. Louis, MO, United States\) 2004, V75\(5\), P455-463 CAPLUS](#)
[\(3\) Simonson, Steven G.; Clinical Pharmacology & Therapeutics \(St. Louis, MO, United States\) 2004, V76\(2\), P167-177 CAPLUS](#)
[\(4\) Hinton, Laura K.; Pharmaceutical Research 2008, V25\(5\), P1063-1074 CAPLUS](#)
[\(5\) Peng, Sean X.; Journal of Pharmaceutical Sciences 2009, V98\(5\), P1877-1884 CAPLUS](#)
[\(6\) Obach, R. Scott; Drug Metabolism and Disposition 2008, V36\(7\), P1385-1405 CAPLUS](#)
[\(7\) Astarita, Anna; Journal of Photochemistry and Photobiology, A: Chemistry 2007, V187\(2-3\), P263-268 CAPLUS](#)
[\(8\) Xu, Dong-Hang; Rapid Communications in Mass Spectrometry 2006, V20\(16\), P2369-2375 CAPLUS](#)
[\(9\) Gao, Jun; Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences 2007, V856\(1-2\), P35-40 CAPLUS](#)
[\(10\) Hojjati, Mohammad; Journal of Supercritical Fluids 2007, V41\(2\), P187-194 CAPLUS](#)

[◀ Previous](#) | [Next ▶](#)

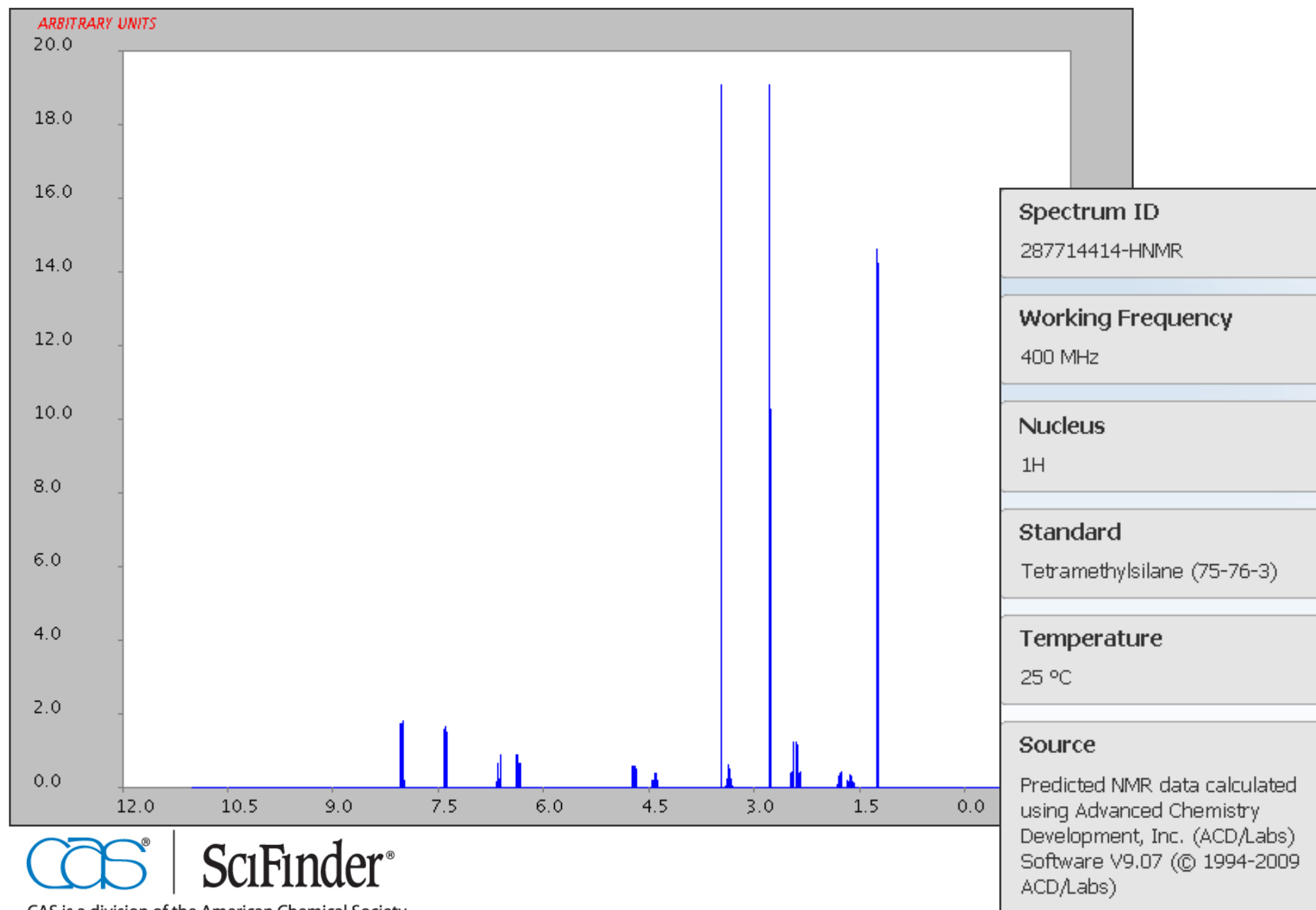
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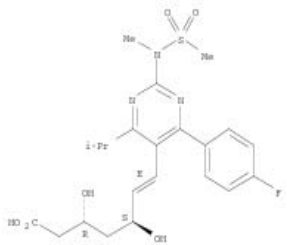
Welcome Miriam Plana | Sign Out
Create Keep Me Posted Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > 287714-41-4 > Proton NMR Spectrum (287714414-HNMR)

Substances [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

64 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [15] 1 2 3 4 5 View: [Icons]

☐ 1. Substance Detail
287714-41-4



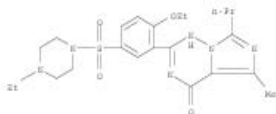
Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,362 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 2. Substance Detail
224785-90-4

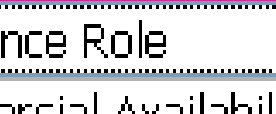


C₂₃ H₃₂ N₆ O₄ S

Imidazo[5,1-f][1,2,4]triazin-4(1H)-one [(4-ethyl-1-piperazinyl)sulfonyl]phenylpropyl-

~571 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 3. Substance Detail
171596-29-5



C₂₂ H₁₉ N₃ O₄

Pyrazino[1',2':1,6]pyrido[3,4-b]indole-1,4-dione, 6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-, (6R,12aR)-

~732 References
Reactions
Commercial Sources
Regulatory Information
Link

Substance Role
Commercial Availability
Elements
Reaction Availability
Substance Role

Biological Study 64
Preparation 64
Uses 64
Process 63
Properties 63
Reactant or Reagent 63
Analytical Study 62
Occurrence 52
Formation, Nonpreparative 45
Miscellaneous 39

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Create Keep Me Posted | Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > 287714-41-4 > Proton NMR Spectrum (287714414-HNMR)

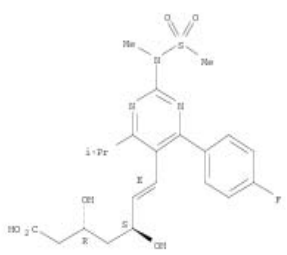
Substances | Get References | Get Reactions | Get Commercial Sources

64 Substances | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

61 substances with Reaction Availability **Referenced in a Reaction** are displayed | Keep Analysis | Clear Analysis

Select All | Deselect All | Sort by: CAS Registry Number | Answers per Page [15] | 1 2 3 4 5 | View: [Icons]

☐ 1. Substance Detail
287714-41-4



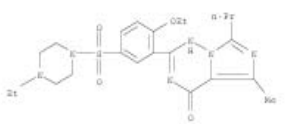
Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,362 References

☐ 2. Substance Detail
224785-90-4

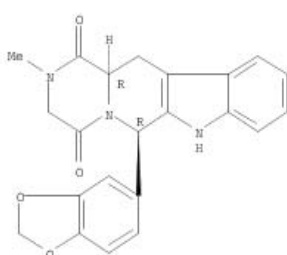


C₂₃ H₃₂ N₆ O₄ S

Imidazo[5,1-f][1,2,4]triazin-4(1H)-one, 2-[2-ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-

~571 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 3. Substance Detail
171596-29-5



Absolute stereochemistry.
Rotation (+).

C₂₂ H₁₉ N₃ O₄

Pyrazino[1',2':1,6]pyrido[3,4-b]indole-1,4-dione, 6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-, (6R,12aR)-

~732 References

Analysis | Refine

Analyze by: [Icon]

Reaction Availability [Dropdown]

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

Referenced in a Reaction 61

Not Referenced in a Reaction 3

Show More

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Explore References | Explore Substances | Explore Reactions

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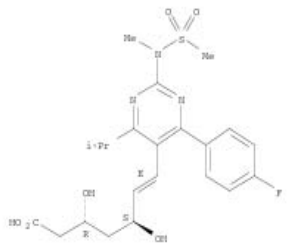
Create Keep Me Posted | Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61) ←

Substances | Get References | Get Reactions | Get Commercial Sources

61 Substances | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | Answers per Page [15] | 1 2 3 4 5 | View: [Icons]

☐ 1. Substance Detail
287714-41-4



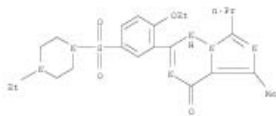
Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,362 References
Reactions

☐ 2. Substance Detail
224785-90-4

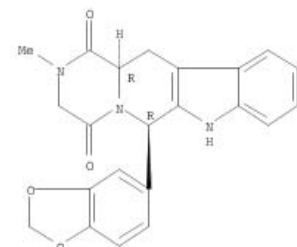


C₂₃ H₃₂ N₆ O₄ S

Imidazo[5,1-f][1,2,4]triazin-4(1H)-one, 2-[2-ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-

~571 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 3. Substance Detail
171596-29-5



Absolute stereochemistry.
Rotation (+).

C₂₂ H₁₉ N₃ O₄

Pyrazino[1',2':1,6]pyrido[3,4-b]indole-1,4-dione, 6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-, (6R,12aR)-

~732 References
Reactions

Analysis | Refine

Analyze by: Reaction Availability

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

Referenced in a Reaction 61

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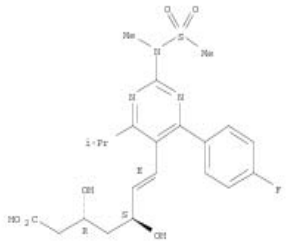
Create Keep Me Posted Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61)

Substances Get References Get Reactions **Get Commercial Sources**

61 Substances 5 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [15] 1 2 3 4 5 View: [Icons]

☒ 1. Substance Detail
287714-41-4



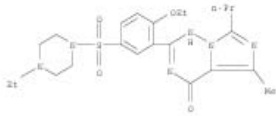
Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,362 References
Reactions

☒ 2. Substance Detail
224785-90-4

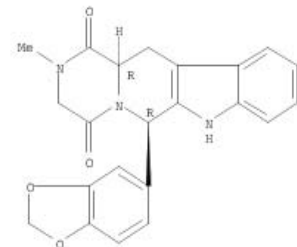


C₂₃ H₃₂ N₆ O₄ S

Imidazo[5,1-f][1,2,4]triazin-4(1H)-one, 2-[2-ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-

~571 References
Reactions
Commercial Sources
Regulatory Information
Link

☒ 3. Substance Detail
171596-29-5



Absolute stereochemistry.
Rotation (+).

C₂₂ H₁₉ N₃ O₄

Pyrazino[1',2':1,6]pyrido[3,4-b]indole-1,4-dione, 6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-, (6R,12aR)-

~732 References
Reactions

Analysis Refine

Analyze by: Reaction Availability

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

Referenced in a Reaction 61

Show More

The screenshot displays the SciFinder web interface. At the top, there are navigation links: "Explore References", "Explore Substances", and "Explore Reactions". A user is logged in as "Miriam Plana". The search path is: Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61) > commercial sources (180).

The main section is titled "Commercial Sources" and shows 180 results. A disclaimer states: "This chemical supplier information is provided on an 'as is' basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this information."

Results are sorted by "Catalog Name" and shown in a list with checkboxes. The first five results are:

- 3B Scientific Corporation Product List**
Company Name: 3B Scientific Corporation, Publication Date: 8 Sep 2009
Order Number: 3B3-035269, Quantity: N/A
158876-82-5 Rupatadine fumarate
[Link](#)
- 3B Scientific Corporation Product List**
Company Name: 3B Scientific Corporation, Publication Date: 8 Sep 2009
Order Number: 3B2-1912, Quantity: 0.5g
171596-29-5 Tadalafil
[Link](#)
- 3B Scientific Corporation Product List**
Company Name: 3B Scientific Corporation, Publication Date: 8 Sep 2009
Order Number: 3B2-1047, Quantity: 1g
224785-90-4 Vardenafil
[Link](#)
- 3B Scientific Corporation Product List**
Company Name: 3B Scientific Corporation, Publication Date: 8 Sep 2009
Order Number: 3B2-1955, Quantity: N/A
287714-41-4 Rosuvastatin
[Link](#)
- Acanthus Research Product List**
Company Name: Acanthus Research, Publication Date: 10 Feb 2009
Order Number: TAD-08-001, Quantity: 75mg, 375mg
171596-29-5 (6R-trans)-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino [1', 2':1,6] pyrido[3,4-b]indole-1,4-dione
[Link](#)

On the right side, there is an "Analyze by:" section with a dropdown menu for "Catalog Name". Below it, a list of commercial sources is shown with their respective counts:

- ACC Corp. Chemical Compounds Catalog 7
- Atomax Chemicals Product List 7
- Advanced Technology Product List 6
- Amfinecom Product List 6
- Shanghai FWD Chemicals Product List 6
- Bepharm Product List 5
- Carbone Scientific Product List 5
- China Hallochem Pharma Co., Ltd. Product List 5
- Finechemie & Pharma Product List 5
- Waterstone Technology

The screenshot displays the SciFinder web interface. At the top, there are navigation links: "Explore References", "Explore Substances", and "Explore Reactions". The user is logged in as "Miriam Plana". The search path is: Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61) > commercial sources (180).

The main content area shows a list of commercial sources. The first five items are:

1. 3B Scientific Corporation Product List
Company Name: 3B Scientific Corporation, Publication Date: 8 Sep
Order Number: 3B3-035269, Quantity: N/A
158876-82-5 Rupatadine fumarate
[Link](#)
2. 3B Scientific Corporation Product List
Company Name: 3B Scientific Corporation, Publication Date: 8 Sep
Order Number: 3B2-1912, Quantity: 0.5g
171596-29-5 Tadalafil
[Link](#)
3. 3B Scientific Corporation Product List
Company Name: 3B Scientific Corporation, Publication Date: 8 Sep
Order Number: 3B2-1047, Quantity: 1g
224785-90-4 Vardenafil
[Link](#)
4. 3B Scientific Corporation Product List
Company Name: 3B Scientific Corporation, Publication Date: 8 Sep
Order Number: 3B2-1955, Quantity: N/A
287714-41-4 Rosuvastatin
[Link](#)
5. Acanthus Research Product List
Company Name: Acanthus Research, Publication Date: 10 Feb 2009
Order Number: TAD-08-001, Quantity: 75mg, 375mg
171596-29-5 (6R-trans)-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino [1', 2':1,6] pyrido[3,4-b]indole-1,4-dione
[Link](#)

An "Export" dialog box is open, showing the following options:

- Export: ☐ All answers, ☒ Only selected answers
- File Name: *
Grapefruit
- File Type:
Portable Document Format (*.pdf)
Portable Document Format (*.pdf)
Rich Text Format (*.rtf)
Microsoft Excel Worksheet (*.xls) **(Selected)**
Quoted Format (*.txt)
Tagged Format (*.txt)
- Include: ☒ Task History

The dialog box has "Export" and "Cancel" buttons.

On the right side, there is a section "Analyze by:" with a dropdown menu "Catalog Name". Below it, a list of commercial sources is shown with their respective counts:

- ACC Corp. Chemical Compounds Catalog 7
- Atomax Chemicals Product List 7
- Advanced Technology Product List 6
- Amfinecom Product List 6
- Shanghai FWD Chemicals Product List 6
- Bepharm Product List 5
- Carbone Scientific Product List 5
- China Hallochem Pharma Co., Ltd. Product List 5
- Finechemie & Pharma Product List 5
- Waterstone Technology

Microsoft Excel - Grapefruit.xls [Read-Only]

File Edit View Insert Format Tools Data Window Help Adobe PDF

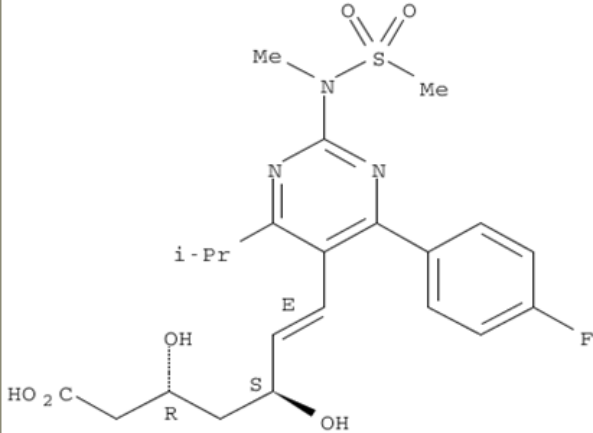
Type a question for help

A1 fx

1 SciFinder®

2 CAS Registry Number: 287714-41-4

3



HO₂C-CH(OH)-CH₂-S-CH=CH-C₆H₄-N(Me)-SO₂-Me

4 Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

Chemical Name	Catalog Name	Company Name	Street Address	City	State or Province
Rosuvastatin	3B Scientific Corporation Product List	3B Scientific Corporation	1840 Industrial Drive, Suite 160	Libertyville	IL
Rosuvastatin-D3 sodium salt	ACC Corp. Chemical Compounds Catalog	American Custom Chemicals Corp.	P O Box 262527	San Diego	CA

Ready

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome Miriam Plana | Sign Out

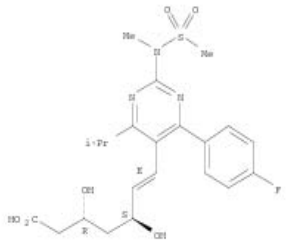
Create Keep Me Posted | Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61) > 287714-41-4

Substances | Get References | Get Reactions | Get Commercial Sources

61 Substances | 1 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | Answers per Page [15] | 1 2 3 4 5 | View: [Icons]

☒ 1. Substance Detail
287714-41-4



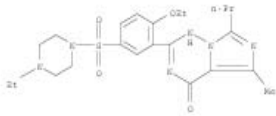
Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,366 References
Reactions

☐ 2. Substance Detail
224785-90-4

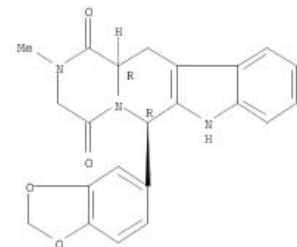


C₂₃ H₃₂ N₆ O₄ S

Imidazo[5,1-f][1,2,4]triazin-4(1H)-one, 2-[2-ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-

~571 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 3. Substance Detail
171596-29-5



Absolute stereochemistry.
Rotation (+).

C₂₂ H₁₉ N₃ O₄

Pyrazino[1',2':1,6]pyrido[3,4-b]indole-1,4-dione, 6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-, (6R,12aR)-

~732 References
Reactions

Analysis | Refine

Analyze by: [Icon]

Reaction Availability

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

Referenced in a Reaction 61

Show More

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. The main search bar shows a sequence of filters: 'Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61) > 287714-41-4'. Below this, a 'Substances' section shows '61 Substances' with options to 'Get References', 'Get Reactions', and 'Get Compounds'. A 'Get References' dialog box is open, allowing users to select retrieval options. The dialog box has two main sections: 'Retrieve references for:' and 'For each substance, retrieve:'. The 'Retrieve references for:' section has two radio buttons: 'All substances' and 'Selected substances' (which is selected). The 'For each substance, retrieve:' section has a list of checkboxes for various types of references, including 'Adverse Effect, including toxicity', 'Analytical Study', 'Biological Study', 'Combinatorial Study', 'Crystal Structure', 'Formation, nonpreparative', 'Miscellaneous', 'Occurrence', 'Prophetics in Patents', 'Preparation', 'Process', 'Properties', 'Reactant or Reagent', 'Spectral Properties', and 'Uses'. The 'Additional related references, e.g., activity studies, disease studies.' checkbox is also present. The 'Get References' button is highlighted. In the background, the 'Substance Detail' for '287714-41-4' is visible, showing a chemical structure and the name '6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-'. The 'Analysis' section on the right shows 'Analyze by: Reaction Availability' and a 'Show More' button.

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Create Keep Me Posted Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61) > 287714-41-4

Substances Get References Get Reactions Get Compounds

61 Substances 1 Selected Keep Selected Remove Selected

Select All Deselect All Sort by: CAS Registry Number

1. Substance Detail
287714-41-4

Absolute stereochemistry.
Rotation (+).
Double bond geometry as shown.

C₂₂ H₂₈ F N₃ O₆ S

6-Heptenoic acid, 7-[4-(4-fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)-

~1,366 References

Reactions

Get References

Retrieve references for:

☐ All substances ☒ Selected substances

For each substance, retrieve:

☒ Adverse Effect, including toxicity ☐ Prophetics in Patents

☐ Analytical Study ☐ Preparation

☐ Biological Study ☐ Process

☐ Combinatorial Study ☐ Properties

☐ Crystal Structure ☐ Reactant or Reagent

☐ Formation, nonpreparative ☐ Spectral Properties

☐ Miscellaneous ☐ Uses

☐ Occurrence

For each sequence, retrieve:

☐ Additional related references, e.g., activity studies, disease studies.

Get References Cancel

Save Print Export

1 2 3 4 5

View: [Icons]

Analyze by: Reaction Availability

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

Referenced in a Reaction 61

Show More

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user is logged in as 'Miriam Plana'. The search path is: Research Topic "Interactions of drugs (pharmac..." > references (357) > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61) > get references (316).

The main content area shows a list of references. The first three are visible:

- 1. Pharmaceutically active compounds with novel medical uses and method of identifying such compounds**
By Kuhn, Michael; Campillos, Monica; Bork, Peer; Jensen, Lars Juhl; Gavin, Anne-Claude; Petsalaki, Evangelia; Garcia Urdales, Eduardo; Russel, Rob
From PCT Int. Appl. (2009), WO 2009124755 A1 20091015. Language: English, Database: CAPLUS
The invention provides a method for identifying a novel medical indication of a pharmaceutically active compd. The invention further provides novel medical indications for several pharmaceutically active compds. Specifically, compds. are provided for the prevention and treatment of a disease or disorder treatable with a serotonin-norepinephrine reuptake inhibitor (SNRI), a serotonin receptor antagonist, an estazolam, a dopamine receptor antagonist, a dopamine receptor agonist, an L-type calcium channel blocker, a selective estrogen receptor modulator (SERM), and an antihistamine. Also provi...
+Substances +Reactions +Citing +Full Text +Link +0 Comments +0 Tags
- 2. Compositions and methods for reducing hepatotoxicity associated with drug administration and treating non-alcoholic fatty liver disease, non-alcoholic steatohepatitis and associated cirrhosis**
By Mehal, Wajahat; Avlin, Imada
From U.S. Pat. Appl. Publ. (2009), US 2009239831 A1 20090924. Language: English, Database: CAPLUS
The present invention relates to the discovery that acetylsalicylic acid (ASA or aspirin), salicylic acid (SA) and related salicylate esters and their pharmaceutically acceptable salts, when coadministered in effective amts. with a drug or other bioactive agent which typically (in the absence of the salicylate compd.) produces significant hepatotoxicity as a secondary indication, will substantially reduce or even eliminate such hepatotoxicity. Favorable therapeutic intervention results from the use of the present invention having the effect of reducing hepatotoxicity assocd. with the administ...
+Substances +Reactions +Citing +Full Text +Link +0 Comments +0 Tags
- 3. Pharmaceutical composition comprising racetam and carnitine for the treatment of mitochondrial and/or metabolic disturbance**
By Perreira, Jose Roberto Da Costa; Falcí, Marcio; Alario, Mauricio Matteis
From PCT Int. Appl. (2009), WO 2009105853 A2 20090903. Language: English, Database: CAPLUS
The present invention refers to a pharmaceutical compn. comprising a compd. of the racetam class of nootropics having a pyrrolidine nucleus, such as piracetam, and carnitine. The pharmaceutical compn. may further comprise coenzyme Q10 and/or agent assocd. with mitochondrial and/or metabolic disturbance, such as hypocholesterolemic agent of the statins group, a hypoglycemic agent, or an antiepileptic agent. The invention also includes a method of treatment for mitochondrial disturbances, for example, myopathy and a neurodegenerative dysfunction comprising administration of the pharmaceutical ...
+Substances +Reactions +Citing +Full Text +Link +0 Comments +0 Tags

On the right side, there is an 'Analysis' panel with a table of authors and their counts:

Author Name	Count
Davidson Michael H	13
Anonymous	12
Stein Evan A	9
Jones Peter H	8
Mckenney James M	8
Milionis Haralampos J	8
Shepherd James	8
Ballantyne Christie M	7
Kastelein John J P	7
Miller Elinor	7


[Explore References](#)
[Explore Substances](#)
[Explore Reactions](#)

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[Research Topic "Interactions of drugs \(pharmac..."](#)
[references \(357\)](#)
[refine "2004-2009" \(149\)](#)
[get substances \(64\)](#)
[keep analysis "Reaction Availability" \(61\)](#)
[get references \(316\)](#)

> **Compositions and methods for r...**

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

Link Save Print Export

◀ Previous Next ▶

2. Compositions and methods for reducing hepatotoxicity associated with drug administration and treating non-alcoholic fatty liver disease, non-alcoholic steatohepatitis and associated cirrhosis

By: Mehal, Wajahat; Avlin, Imaeda

Assignee: Yale University, USA

The present invention relates to the discovery that acetylsalicylic acid (ASA or aspirin), salicylic acid (SA) and related salicylate esters and their pharmaceutically acceptable salts, when coadministered in effective amts. with a drug or other bioactive agent which typically (in the absence of the salicylate compd.) produces significant hepatotoxicity as a secondary indication, will substantially reduce or even eliminate such hepatotoxicity. Favorable therapeutic intervention results from the use of the present invention having the effect of reducing hepatotoxicity assocd. with the administration of certain drugs and other bioactive agents and in certain instances of allowing the administration of higher doses of a compd. which, without the coadministration, would produce hepatotoxicity which limits or even negates the therapeutic value of the compd. The invention also relates to methods of reducing the likelihood of a patient at risk for non-alc. fatty liver diseases (NAFLD), including non-alc. steatohepatitis (NASH), or treating NAFLD or NASH including primary NASH, NASH secondary to liver transplantation (NASH post-liver transplantation) or cirrhosis represent alternative aspects of the present invention. Thus, aspirin inhibited the caspase-1 pathway and protected from acetaminophen (APAP)-induced mortality in mice. A two signal requirement for initiation of APAP induced liver toxicity was identified, TLR9, providing a signal for the transcription of pro-IL-1 β and pro-IL-18, and the NALP3 inflammasome, providing the signal for cleavage and activation of these pro-cytokines.

Patent Information

Patent No.	Kind	Date	Application No.	Date
US 20090239831	A1	Sep 24, 2009	US 2009-386412	Apr 17, 2009
WO 2009051840	A2	Apr 23, 2009	WO 2008-US11945	Oct 20, 2008
WO 2009051840	A3	Aug 6, 2009		

Priority Application

Quick Links

0 Tags, 0 Comments

Patent Information

Sep 24, 2009
US 2009239831
A1

Application

Apr 17, 2009
US 2009-386412

Priority

Oct 18, 2007
US 2007-999413
Oct 20, 2008
WO 2008-US11945

Source

U.S. Pat. Appl. Publ.
34pp.
Patent
2009
CODEN: USXXCO

Classifications



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(1 of 1)

United States Patent Application

20090239831

Kind Code

A1

Mehal; Wajahat ; et al.

September 24, 2009

Compositions and methods for reducing hepatotoxicity associated with drug administration and treating non-alcoholic fatty liver disease, non-alcoholic steatohepatitis and associated cirrhosis

Abstract

The present invention relates to the discovery that acetylsalicylic acid (ASA or aspirin), salicylic acid (SA) and related salicylate esters and their pharmaceutically acceptable salts, when coadministered in effective amounts with a drug or other bioactive agent which typically (in the absence of the salicylate compound) produces significant hepatotoxicity as a secondary indication, will substantially reduce or even eliminate such hepatotoxicity. Favorable therapeutic intervention results from the use of the present invention having the effect of reducing hepatotoxicity associated with the administration of certain drugs and other bioactive agents and in certain instances of allowing the administration of higher doses of a compound which, without the coadministration, would produce hepatotoxicity which limits or even negates the therapeutic value of the compound. The invention also relates to methods of reducing the likelihood of a patient at risk for non-alcoholic fatty liver diseases (NAFLD), including non-alcoholic steatohepatitis (NASH), or treating NAFLD or NASH including primary NASH, NASH secondary to liver transplantation (NASH post-liver transplantation) or cirrhosis represent alternative aspects of the present invention.

SciFinder®

Explore References | Explore Substances | Explore Reactions

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Create Keep Me Posted | Research Topic "Interactions of drugs (pharmac..." > **references (357)** > refine "2004-2009" (149) > get substances (64) > keep analysis "Reaction Availability" (61) > get references (316) > Compositions and methods for ...

References | Get Substances | Get Reactions | Get Cited | Get Citing

357 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Add Tags | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [20] | 1 2 3 4 5 6 ... 18 | View: [icon]

☐ 1. Toxicological and pharmacokinetic evaluation of concomitant intake of grapefruit juice and simvastatin in rats after repeated treatment over 28 days

By Butterweck, Veronika; Zdrojewski, Immo; Galloway, Cheryl; Frye, Reginald; Derendorf, Hartmut
From Planta Medica (2009), 75(11), 1196-1202. Language: English, Database: CAPLUS

Since data concerning the toxicity and pharmacokinetics of concomitant repeated administration of grapefruit juice (GFJ) and simvastatin are lacking, we performed a chronic study in rats over a 4-wk period using 2 different strengths (regular [RS] and double strength [DS]) of GFJ and 2 different doses of simvastatin (20 and 80 mg/kg, resp.). Both juices did not have a significant effect on the pharmacokinetic parameters of either simvastatin lactone (SVL) or its active metabolite simvastatin hydroxy acid (SVA) when administered concomitantly in a dose of 20 mg/kg over 28 days. However, when ...

+Substances | Reactions | Citing | Full Text | Link | Comments | Tags

☐ 2. Grapefruit juice interaction with oral budesonide: equal effect on immediate-release and delayed-release formulations

By Seidegaard, J.; Randvall, G.; Nyberg, L.; Borgaa, O.
From Pharmazie (2009), 64(7), 461-465. Language: English, Database: CAPLUS

Grapefruit juice (GFJ) inhibits CYP3A activity in the gut wall, thereby decreasing first-pass metab. of CYP3A substrates. In this study be evaluated the influence of GFJ on the systemic availability of budesonide, a CYP3A-metabolised drug, both from an extended-release (ER) formulation and plain capsules. Eight healthy men participated in this open crossover study. Three mg budesonide as ER capsules or plain capsules was swallowed with or without previous intake of GFJ. Regular-strength GFJ 200 mL was given three times a day for four days. Budesonide was administered immediately after the...

+Substances | Reactions | Citing | Full Text | Link | Comments | Tags

☐ 3. Influence of grapefruit juice on the pharmacokinetics of diltiazem in wistar rats upon single and multiple dosage regimens

By Boddu, S. P.; Yamsani, M. Rao; Potharaju, S.; Veeraghavan, S.; Rajak, S.; Kumar V. V. S. S.; Avery, B. A.; Repka, M. A.; Varanasi, V. S. K. Kiran
From Pharmazie (2009), 64(8), 525-531. Language: English, Database: CAPLUS

Drug efflux by intestinal P-glycoprotein (P-gp) is recognized as a significant biochem. barrier affecting oral absorption for a no. of drugs apart from the cytochrome P 450 3A enzyme. Various conflicting reports have been published regarding the effects of grapefruit juice (GFJ) on P-gp mediated drug efflux, in which GFJ has been shown to have no effect, as an inhibitor effect or activation of the enzyme. Therefore the present study's objective was to provide clarification of previous findings, adopting a two-way approach, involving both single dose and multiple dosage regimens. Diltiazem (...)

+Substances | Reactions | Citing | Full Text | Link | Comments | Tags

Analysis | Refine

Analyze by: [icon]

Author Name [v]

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

Bailey David G	23
Neuvonen Pertti J	13
Lilja Jari J	11
Paine Mary F	10
Uesawa Yoshihiro	10
Bailey D G	9
Mohri Kiminori	9
Watkins Paul B	9
Dresser George K	8
Spence J David	8

Categorize

More detailed analysis based on CAS indexing

Categorize

By Boddu, S. P.; Yamsani, M. Rao; Potharaju, S.; Veeraraghavan, S.; Rajak, S.; Kumar V. V. S. S.; Avery, B. A.; Repka, M. A.; Varanasi, V. S. K.; Kiran
From Pharmazie (2009), 64(8), 525-531. Language: English, Database: CAPLUS

Drug efflux by intestinal P-glycoprotein (P-gp) is recognized as a significant biochem. barrier affecting oral absorption for a no. of **drugs** apart from the cytochrome P-450 3A enzyme. Various conflicting reports have been published regarding the effects of **grapefruit juice** (GFJ) on P-gp mediated **drug** efflux, in which GFJ has been shown to have no effect, as an inhibitor effect or activation of the enzyme. Therefore the present study's objective was to provide clarification of previous findings, adopting a two-way approach, involving both single dose and multiple dosage regimens. Diltiazem (...)

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

☐ 4. **Grapefruit juice-based bev**
By Widmer, Wilbur W.; Stinson, William
From U.S. (2009), US 7550167 B1 2009
A **grapefruit juice**-based bev includes the steps of clarifying coumarins and furanocoumarins

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

☐ 5. **In vitro interactions with r**
By Brill, Shlomo; Zimmermann, Christian
From Planta Medica (2009), 75(4), 332
Interactions of acutely adr established. In this study, we naringenin and the furanocou than in the fruit, we compared

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

☐ 6. **Interactions between grap**
By Hayashibara, Masakazu
From Yonago Acta Medica (2009), 52(1)
The extent of **interaction** b antagonists with **grapefruit j** lower bioavailability is likely efondipine, felodipine, manidi

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

☐ 7. **Interaction of statins with**
By Wen, Wenbing; Cheng, Huoqing; Li
From Zhongguo Yiyuan Yaoxue Zazhi (2009), 29(1)
A review. **Interaction** of s infective agents, cisapride, **grapefruit juice** and androstammines was discussed.

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

☐ 8. **Food-drug interaction: the case of grapefruit juice**

Categorize

1. Select a heading and category.

Category Heading	Category	Index Terms	Selected Terms
All	Topics (345)		
General chemistry	Substances (397)		
Biology			
Biotechnology			
Genetics & protein chemistry			
Physical chemistry			
Polymer chemistry			
Analytical chemistry			
Technology			
Synthetic chemistry			
Environmental chemistry			
Catalysis			

All

[Refine](#) [Cancel](#)

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Categorize

More detailed analysis based on CAS indexing

[Categorize](#)

Categorize ⓘ

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

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Topics (345)		
General chemistry	Substances (397)		
Biology			
Biotechnology			
Genetics & protein chemistry			
Physical chemistry			
Polymer chemistry			
Analytical chemistry			
Technology			
Synthetic chemistry			
Environmental chemistry			
Catalysis			

All

Categorize ⓘ

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

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Substances in biology (276)		
General chemistry	Organisms (52)		
Biology	Processes & systems (42)		
Biotechnology	Anatomy (39)		
Genetics & protein chemistry	Substances in adverse effects (68)		
Physical chemistry	Animal pathology (20)		
Polymer chemistry	Immunology (11)		
Analytical chemistry	Endocrinology (10)		
Technology			
Synthetic chemistry			
Environmental chemistry			
Catalysis			

Biology

Refine Cancel

Categorize ⓘ

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

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Substances in biology (276)	Select All Deselect All	
General chemistry	Organisms (52)	☐ Bergamottin 7	
Biology	Processes & systems (42)	☐ 6',7'-Dihydroxybergamottin 6	
Biotechnology	Anatomy (39)	☐ Furocoumarins 6	
Genetics & protein chemistry	Substances in adverse effects (68)	☐ Felodipine 5	
Physical chemistry	Animal pathology (20)	☐ Naringenin 4	
Polymer chemistry	Immunology (11)	☐ Nisoldipine 4	
Analytical chemistry	Endocrinology (10)	☐ Naringin 3	
Technology		☐ Terfenadine 3	
Synthetic chemistry		☐ Atorvastatin 2	
Environmental chemistry		☐ Bergapten 2	
Catalysis		☐ Cisapride 2	
		☐ Cyclosporin A 2	
		☐ Nifedipine 2	
		☐ Nimodipine 2	
		☐ Simvastatin 2	
		☐ Amiodarone 1	
		☐ Amlodipine 1	
		☐ Desipipine 1	

Biology > Substances in adverse effects

Refine **Cancel**

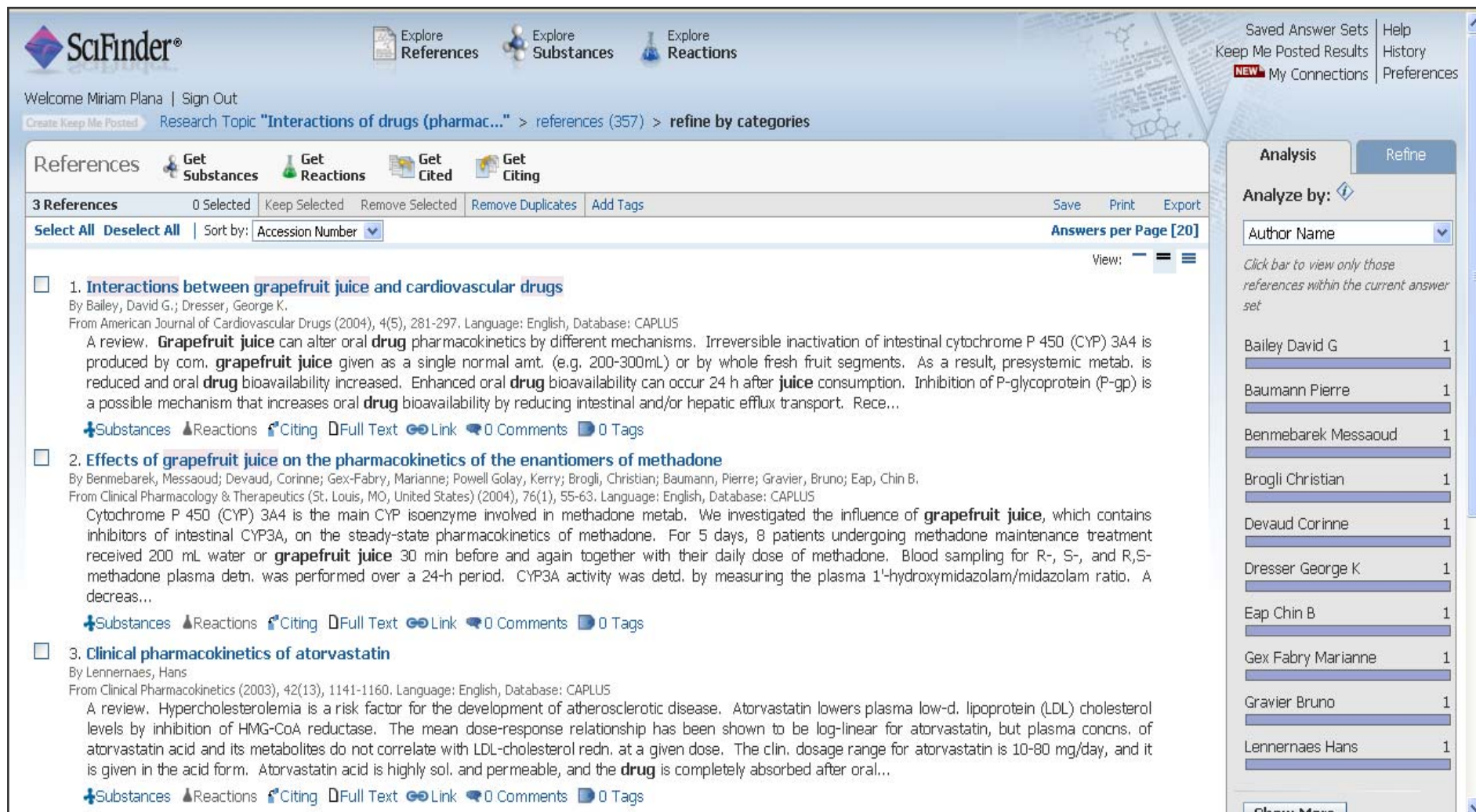
Categorize ⓘ

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

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Substances in biology (276)	Select All Deselect All	Click 'X' to remove the term or entire category from 'Selected Terms'
General chemistry	Organisms (52)	☐ Bergamottin 7	*Biology > Substances in adverse effects(3)
Biology	Processes & systems (42)	☐ 6',7'-Dihydroxybergamottin 6	☒ Opioids
Biotechnology	Anatomy (39)	☐ Furocoumarins 6	☒ Sildenafil
Genetics & protein chemistry	Substances in adverse effects (68)	☐ Felodipine 5	☒ Atorvastatin
Physical chemistry	Animal pathology (20)	☐ Naringenin 4	
Polymer chemistry	Immunology (11)	☐ Nisoldipine 4	
Analytical chemistry	Endocrinology (10)	☐ Naringin 3	
Technology		☐ Terfenadine 3	
Synthetic chemistry		☒ Atorvastatin 2	
Environmental chemistry		☐ Bergapten 2	
Catalysis		☐ Cisapride 2	
		☐ Cyclosporin A 2	
		☐ Nifedipine 2	
		☐ Nimodipine 2	
		☐ Simvastatin 2	
		☐ Amiodarone 1	
		☐ Amlodipine 1	
		☐ Desidipine 1	

Biology > Substances in adverse effects > 3 Index Term(s) Selected

 **Refine** **Cancel**



The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user is logged in as 'Miriam Plana'. The search topic is 'Interactions of drugs (pharmac...'. The results are categorized under 'References' and show 3 references. The first reference is titled 'Interactions between grapefruit juice and cardiovascular drugs' by Bailey, David G.; Dresser, George K. The second reference is 'Effects of grapefruit juice on the pharmacokinetics of the enantiomers of methadone' by Benmebarek, Messaoud; Devaud, Corinne; Gex-Fabry, Marianne; Powell Golay, Kerry; Brogli, Christian; Baumann, Pierre; Gravier, Bruno; Eap, Chin B. The third reference is 'Clinical pharmacokinetics of atorvastatin' by Lennernaes, Hans. On the right side, there is an 'Analysis' panel with a table showing the number of references for each author.

SciFinder®

Welcome Miriam Plana | Sign Out

Research Topic "Interactions of drugs (pharmac..." > references (357) > refine by categories

References | Get Substances | Get Reactions | Get Cited | Get Citing

3 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Add Tags | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [20]

View: [icon] [icon] [icon]

☐ 1. Interactions between grapefruit juice and cardiovascular drugs

By Bailey, David G.; Dresser, George K.
From American Journal of Cardiovascular Drugs (2004), 4(5), 281-297. Language: English, Database: CAPLUS

A review. **Grapefruit juice** can alter oral **drug** pharmacokinetics by different mechanisms. Irreversible inactivation of intestinal cytochrome P 450 (CYP) 3A4 is produced by com. **grapefruit juice** given as a single normal amt. (e.g. 200-300mL) or by whole fresh fruit segments. As a result, presystemic metab. is reduced and oral **drug** bioavailability increased. Enhanced oral **drug** bioavailability can occur 24 h after **juice** consumption. Inhibition of P-glycoprotein (P-gp) is a possible mechanism that increases oral **drug** bioavailability by reducing intestinal and/or hepatic efflux transport. Rece...

+Substances | Reactions | Citing | Full Text | Link | Comments | Tags

☐ 2. Effects of grapefruit juice on the pharmacokinetics of the enantiomers of methadone

By Benmebarek, Messaoud; Devaud, Corinne; Gex-Fabry, Marianne; Powell Golay, Kerry; Brogli, Christian; Baumann, Pierre; Gravier, Bruno; Eap, Chin B.
From Clinical Pharmacology & Therapeutics (St. Louis, MO, United States) (2004), 76(1), 55-63. Language: English, Database: CAPLUS

Cytochrome P 450 (CYP) 3A4 is the main CYP isoenzyme involved in methadone metab. We investigated the influence of **grapefruit juice**, which contains inhibitors of intestinal CYP3A, on the steady-state pharmacokinetics of methadone. For 5 days, 8 patients undergoing methadone maintenance treatment received 200 mL water or **grapefruit juice** 30 min before and again together with their daily dose of methadone. Blood sampling for R-, S-, and R,S-methadone plasma detn. was performed over a 24-h period. CYP3A activity was detd. by measuring the plasma 1'-hydroxymidazolam/midazolam ratio. A decreas...

+Substances | Reactions | Citing | Full Text | Link | Comments | Tags

☐ 3. Clinical pharmacokinetics of atorvastatin

By Lennernaes, Hans
From Clinical Pharmacokinetics (2003), 42(13), 1141-1160. Language: English, Database: CAPLUS

A review. Hypercholesterolemia is a risk factor for the development of atherosclerotic disease. Atorvastatin lowers plasma low-d. lipoprotein (LDL) cholesterol levels by inhibition of HMG-CoA reductase. The mean dose-response relationship has been shown to be log-linear for atorvastatin, but plasma concns. of atorvastatin acid and its metabolites do not correlate with LDL-cholesterol redn. at a given dose. The clin. dosage range for atorvastatin is 10-80 mg/day, and it is given in the acid form. Atorvastatin acid is highly sol. and permeable, and the **drug** is completely absorbed after oral...

+Substances | Reactions | Citing | Full Text | Link | Comments | Tags

Analysis | Refine

Analyze by: [icon]

Author Name [v]

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

Bailey David G	1
Baumann Pierre	1
Benmebarek Messaoud	1
Brogli Christian	1
Devaud Corinne	1
Dresser George K	1
Eap Chin B	1
Gex Fabry Marianne	1
Gravier Bruno	1
Lennernaes Hans	1

Show More



 Explore
References

 Explore
Substances

 Explore
Reactions

Welcome Miriam Plana | Sign Out

Create Keep Me Posted | Research Topic "Interactions of drugs (pharmac..." > references (357) > refine by categories > Interactions between grapefrui...

Reference Detail  Get
Substances  Get
Reactions  Get
Cited  Get
Citing  Get
Full Text

Link Save Print Export

Previous Next

1. Interactions between grapefruit juice and cardiovascular drugs

By: Bailey, David G.; Dresser, George K.

A review. Grapefruit juice can alter oral drug pharmacokinetics by different mechanisms. Irreversible inactivation of intestinal cytochrome P 450 (CYP) 3A4 is produced by com. grapefruit juice given as a single normal amt. (e.g. 200-300mL) or by whole fresh fruit segments. As a result, presystemic metab. is reduced and oral drug bioavailability increased. Enhanced oral drug bioavailability can occur 24 h after juice consumption. Inhibition of P-glycoprotein (P-gp) is a possible mechanism that increases oral drug bioavailability by reducing intestinal and/or hepatic efflux transport. Recently, inhibition of org. anion transporting polypeptides by grapefruit juice was obsd. in vitro; intestinal uptake transport appeared decreased as oral drug bioavailability was reduced. Numerous medications used in the prevention or treatment of coronary artery disease and its complications have been obsd. or are predicted to interact with grapefruit juice. Such interactions may increase the risk of rhabdomyolysis when dyslipidemia is treated with the HMG-CoA reductase inhibitors atorvastatin, lovastatin, or simvastatin. Potential alternative agents are pravastatin, fluvastatin, or rosuvastatin. Such interactions might also cause excessive vasodilatation when hypertension is managed with the dihydropyridines felodipine, nifedipine, nisoldipine, or nitrendipine. An alternative agent could be amlodipine. In contrast, the therapeutic effect of the angiotensin II type I receptor antagonist losartan may be reduced by grapefruit juice. Grapefruit juice interacting with the antidiabetic agent repaglinide may cause hypoglycemia, and interaction with the appetite suppressant sibutramine may cause elevated BP and HR. In angina pectoris, administration of grapefruit juice could result in atrioventricular conduction disorders with verapamil or attenuated antiplatelet activity with clopidogrel. Grapefruit juice may enhance drug toxicity for antiarrhythmic agents such as amiodarone, quinidine, disopyramide, or propafenone, and for the congestive heart failure drug, carvediol. Some drugs for the treatment of peripheral or central vascular disease also have the potential to interact with grapefruit juice. Interaction with sildenafil, tadalafil, or vardenafil for erectile dysfunction, may cause serious systemic vasodilatation esp. when combined with a nitrate. Interaction between ergotamine for migraine and grapefruit juice may cause gangrene or stroke. In stroke, interaction with nimodipine may cause systemic hypotension. If a drug has low inherent oral bioavailability from presystemic metab. by CYP3A4 or efflux transport by P-gp and the potential to produce serious overdose toxicity, avoidance of grapefruit juice entirely during pharmacotherapy appears mandatory. Although altered drug response is variable among individuals, the outcome is difficult to predict and avoiding the combination will guarantee toxicity is prevented. The elderly are at particular risk, as they are often prescribed medications and frequently consume grapefruit juice.

Indexing

Pharmacology (Section 1-0) 

Saved Answer Sets
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Help
History
Preferences

Quick Links

0 Tags, 0 Comments

Source

American Journal of Cardiovascular Drugs
Volume 4
Issue 5
Pages 281-297
Journal; General Review
2004
CODEN: AJCDDJ
ISSN: 1175-3277

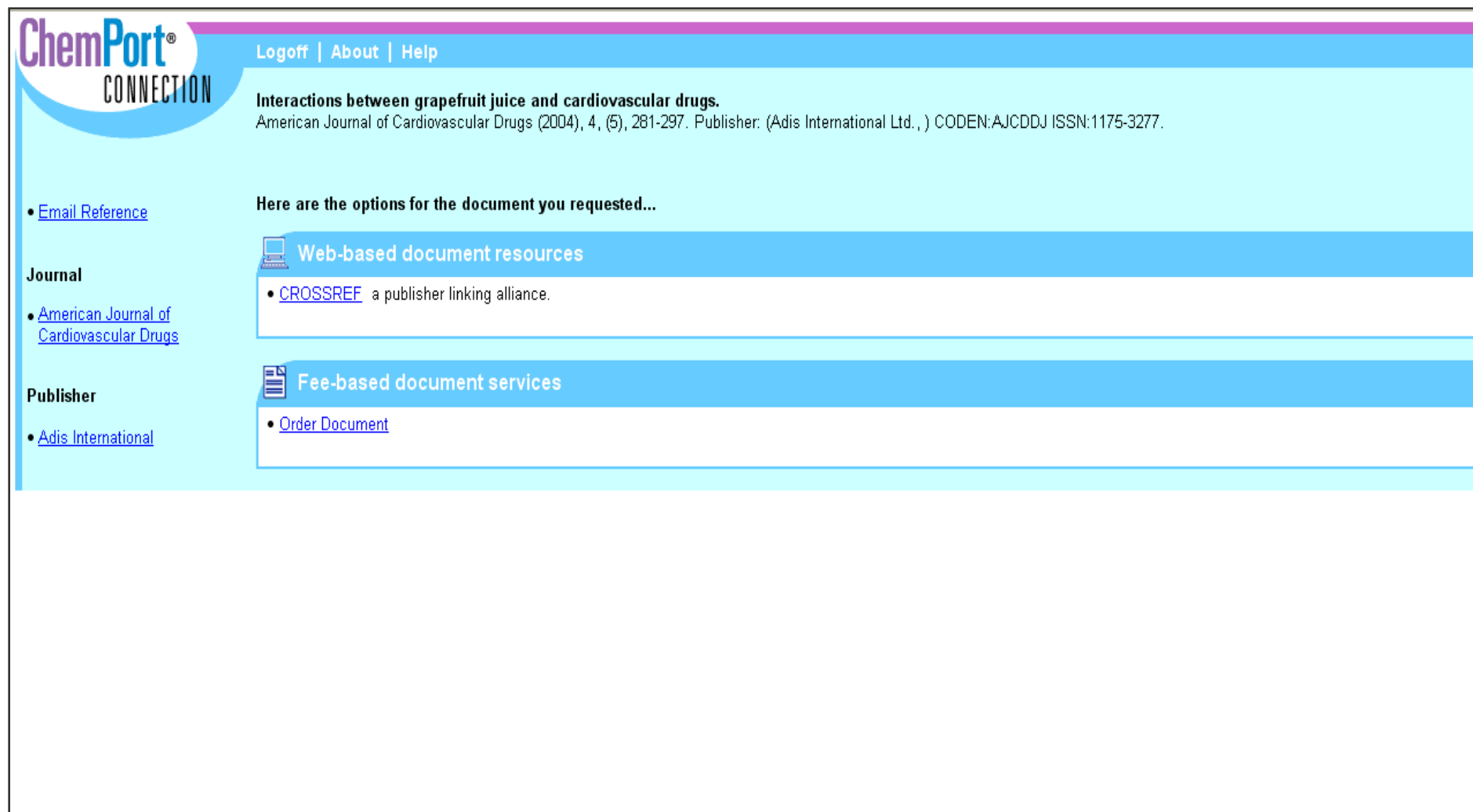
Company/Organization

Department of Medicine and
Lawson Health Research
Institute
London Health Sciences Centre
London, ON, Can.

Accession Number

2004:1002661
CAN 142:347731
CAPLUS

Publisher



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Interactions between grapefruit juice and cardiovascular drugs.
American Journal of Cardiovascular Drugs (2004), 4, (5), 281-297. Publisher: (Adis International Ltd.,) CODEN:AJCDDJ ISSN:1175-3277.

• [Email Reference](#)

Journal

• [American Journal of Cardiovascular Drugs](#)

Publisher

• [Adis International](#)

Here are the options for the document you requested...

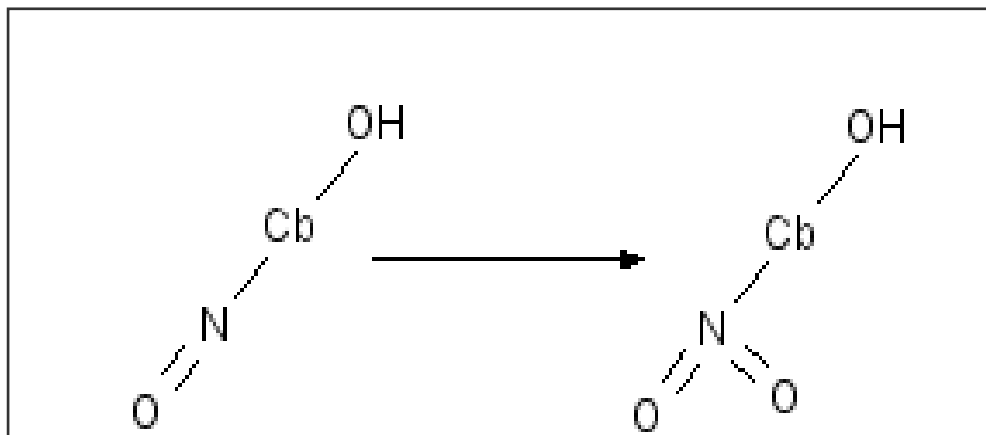
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BÚSQUEDA POR REACCIÓN:





 Explore References

 Explore Substances

 Explore Reactions

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Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags **NEW**

Research Topic

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

Search

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

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prova

climatic change

Autosaved Reference Set

View All

Import

Keep Me Posted Results

Cambio climatico

Nov 07, 2009 (7)

Oct 31, 2009 (7)

Oct 24, 2009 (12)

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 Explore
References

 Explore
Substances

 Explore
Reactions

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Explore Reactions

Reaction Structure

Reaction Structure 



Click image to draw or import structure

Search 

Solvents 

Select Solvents 

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 

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Keep Me Posted Results

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CAS is a division of the American Chemical Society

www.cas.org

The screenshot displays the SciFinder Reaction editor interface. The main window shows a chemical reaction between a reactant and a product. The reactant is a chiral amine with a hydroxyl group, and the product is a chiral amine with a hydroxyl group. The reaction is shown with a reaction arrow pointing from the reactant to the product. The interface includes a toolbar with various chemical editing tools, a sidebar with navigation options, and a right panel with saved answer sets and connections.

Reaction editor

Drag the reaction arrow to specify reaction direction.
Default role assignments may be changed using the Reaction role tool.

reactant/reagent → product

Get reactions where the structure(s) are:

- ☐ Variable only at the specified positions
- ☒ Substructures of more complex structures

Acceptar
Cancelar

Formula not available

Sources other than patents

Explore Reactions
Reaction Structure
Reaction

Welcome Miriam Piana | Sign Out

Solvent
Number
Classific
Source

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Autosaved Reference Set
View All
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Keep Me Posted Results
Cambio climatico
Nov 07, 2009 (7)
Oct 31, 2009 (7)
Oct 24, 2009 (12)
View All

My Connections
No invitations to connect
No outstanding sent invitations
You have 4 connections

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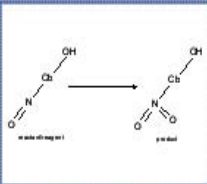
Welcome Miriam Plana | Sign Out

Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help | Keep Me Posted Results | History | **NEW** My Connections | Preferences

Explore Reactions

Reaction Structure | Reaction Structure ⓘ



Click image to change structure or view detail

Search

Search type: ⓘ ☐ Allow variability only as specified ☒ Substructure

Solvents ⓘ **Select Solvents** **NEW**

Number of Steps ⓘ
Examples: 1, 1-3, 1-3

Classification(s) ⓘ

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

Source(s) ⓘ ☐ Any source

Saved Answer Sets ⓘ

prova
climatic change
Autosaved Reference Set

View All

Import

Keep Me Posted Results ⓘ

Cambio climatico
Nov 07, 2009 (7)
Oct 31, 2009 (7)
Oct 24, 2009 (12)

View All

My Connections ⓘ

No invitations to connect
No outstanding sent invitations
You have 4 connections

SciFinder®

Explore References | Explore Substances | Explore Reactions

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Create Keep Me Posted | Reaction Structure substructure > reactions (8658)

Reactions **Get References**

8658 Reactions 0 Selected | Keep Selected | Remove Selected

Select All Deselect All | Sort by: Accession Number

Answers per Page [15] 1 2 3 4 5 6 ... 578

Display: [Icons]

☐ 1. Reaction Detail [Link](#) [Similar Reactions](#) **NEW**

NOTE: Reactants: 2, Solvents: 1, Steps: 1, Stages: 1

4-(Benzimidazol-2-yl)-1,2,5-oxadiazol-3-ylamine derivatives: Potent and selective p70S6 kinase inhibitors
By Bandarage, Upul et al
From Bioorganic & Medicinal Chemistry Letters, 19(17), 5191-5194; 2009

☐ 2. Reaction Detail [Link](#)

Analysis | Refine

Sample Analysis

Catalyst

Pd

4-PyNMe₂

CsH₅N

Pd(OH)₂

Piperidine

H₂SO₄

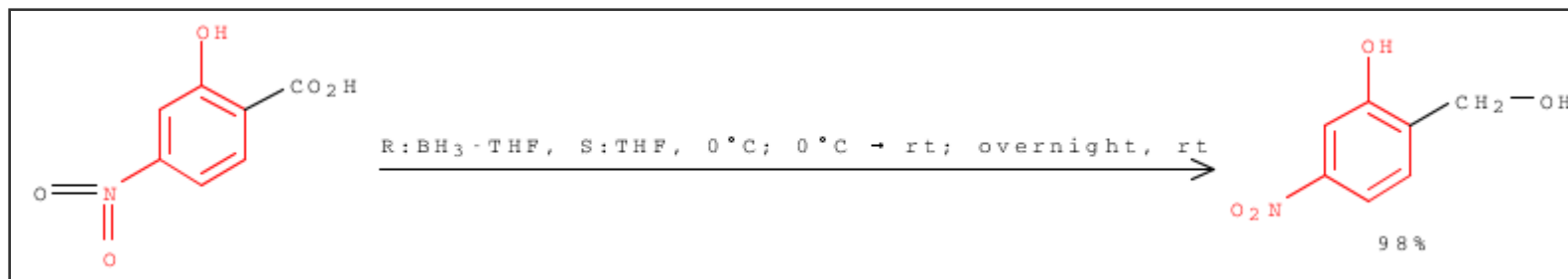
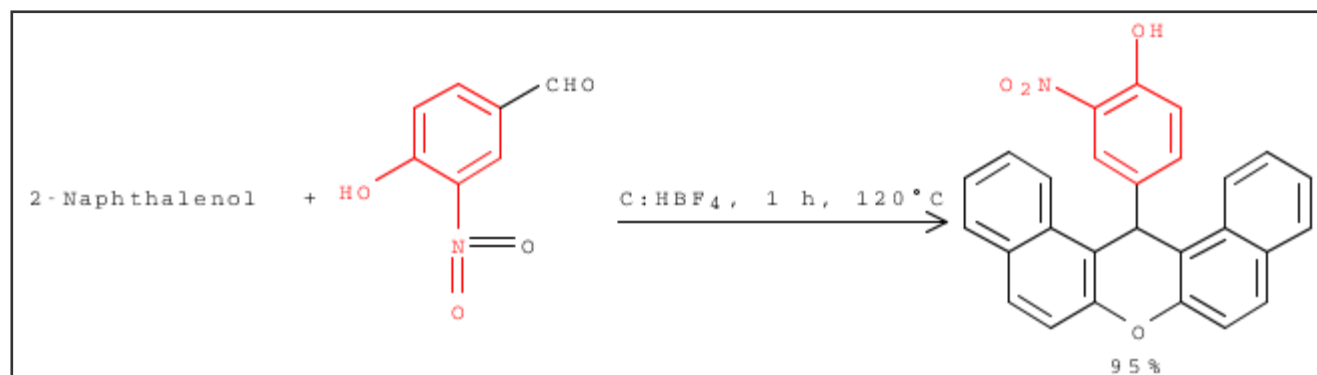
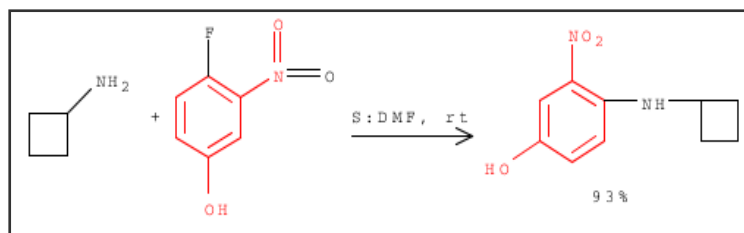
AcOH

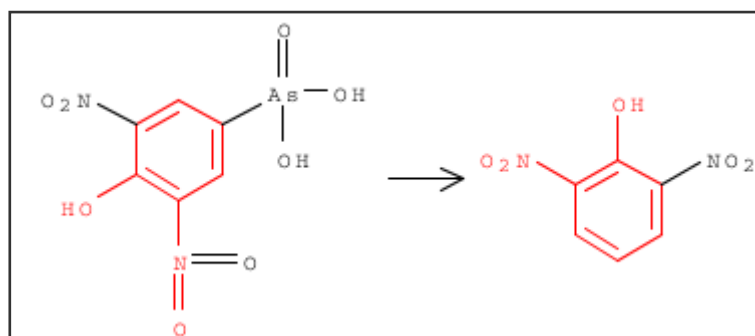
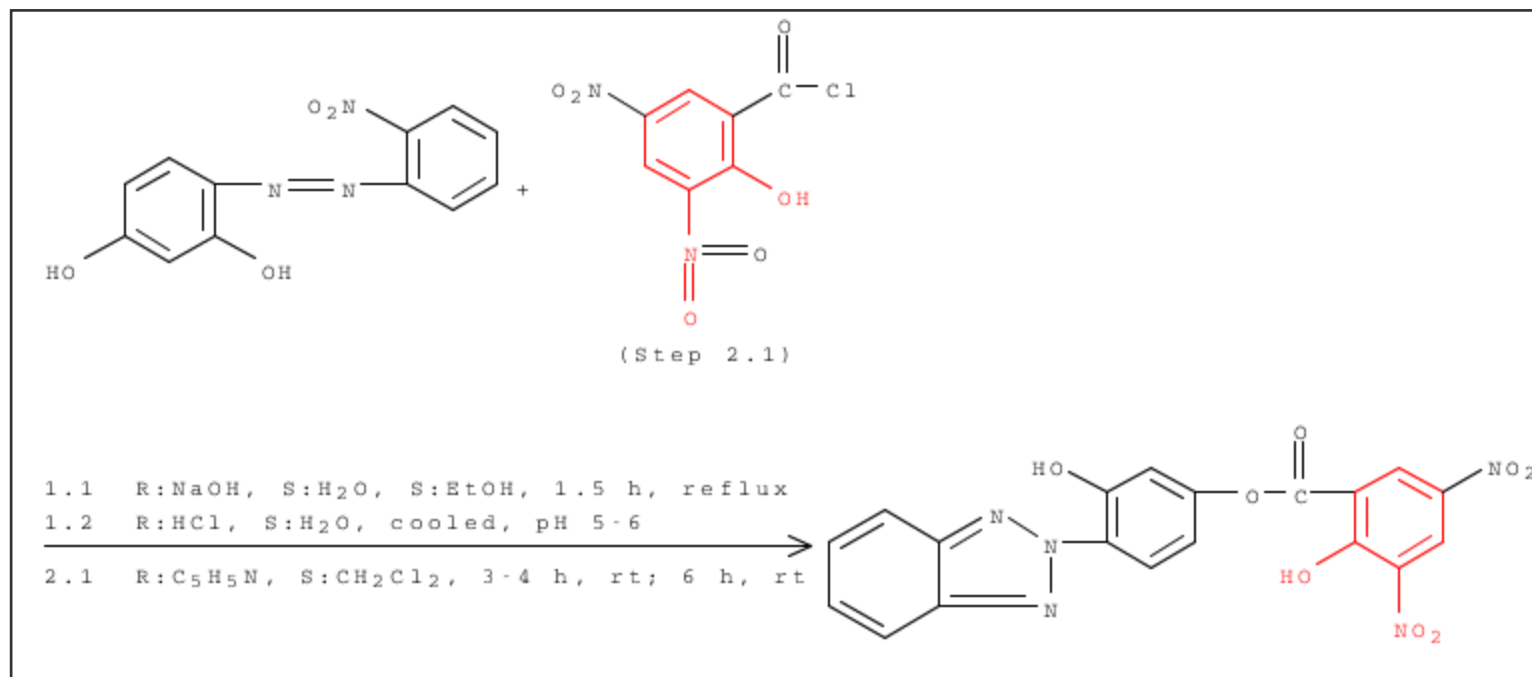
DMF

Pd(PPh₃)₄

Pd(OAc)₂

Show Full Analysis





The screenshot displays the SciFinder web interface with the "Reaction editor" window open. The editor shows a chemical reaction where a reactant (a benzene ring with a nitro group and a hydroxyl group) reacts to form a product (a benzene ring with a nitro group and a hydroxyl group). A pink arrow points from the reactant to the product. The interface includes a left sidebar with navigation options like "Explore Reactions", "Reaction Structure", "Solvents", "Number", and "Classification". The top right corner has links for "Saved Answer Sets", "Keep Me Posted Results", and "My Connections". The bottom right corner has buttons for "Aceptar" and "Cancelar".

Reaction editor

Click an atom to block substitution.

reactant/reagent

product

Get reactions where the structure(s) are:

- ☐ Variable only at the specified positions
- ☒ Substructures of more complex structures

Scale 100

Formula not available

Saved Answer Sets

Keep Me Posted Results

NEW! My Connections

Help History Preferences

Saved Answer Sets

prova

climatic change

Autosaved Reference Set

View All

Import

Keep Me Posted Results

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Oct 31, 2009 (7)

Oct 24, 2009 (12)

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SciFinder®

Explore References | Explore Substances | Explore Reactions

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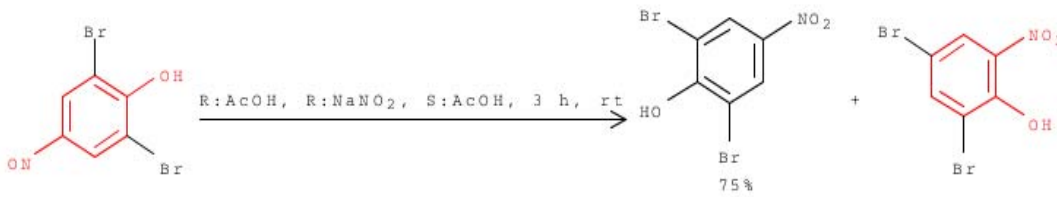
Create Keep Me Posted | Reaction Structure substructure > reactions (47)

Reactions **Get References**

47 Reactions 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All Deselect All | Sort by: Accession Number | Answers per Page [15] 1 2 3 4 | Display: [Icons]

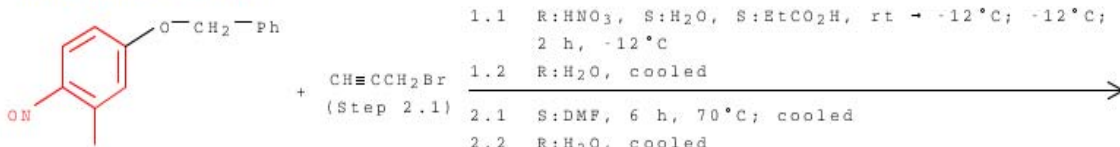
☐ 1. Reaction Detail [Link](#) [Similar Reactions](#) **NEW**



NOTE: Reactants: 1, Reagents: 2, Solvents: 1, Steps: 1, Stages: 1

Rearrangements during nitrosodecarboxylation of isomeric dibromohydroxybenzoic acids
By Shishkin, V. N. and Fadin, M. V.
From Russian Journal of Organic Chemistry, 44(5), 688-692; 2008

☐ 2. Reaction Detail [Link](#)



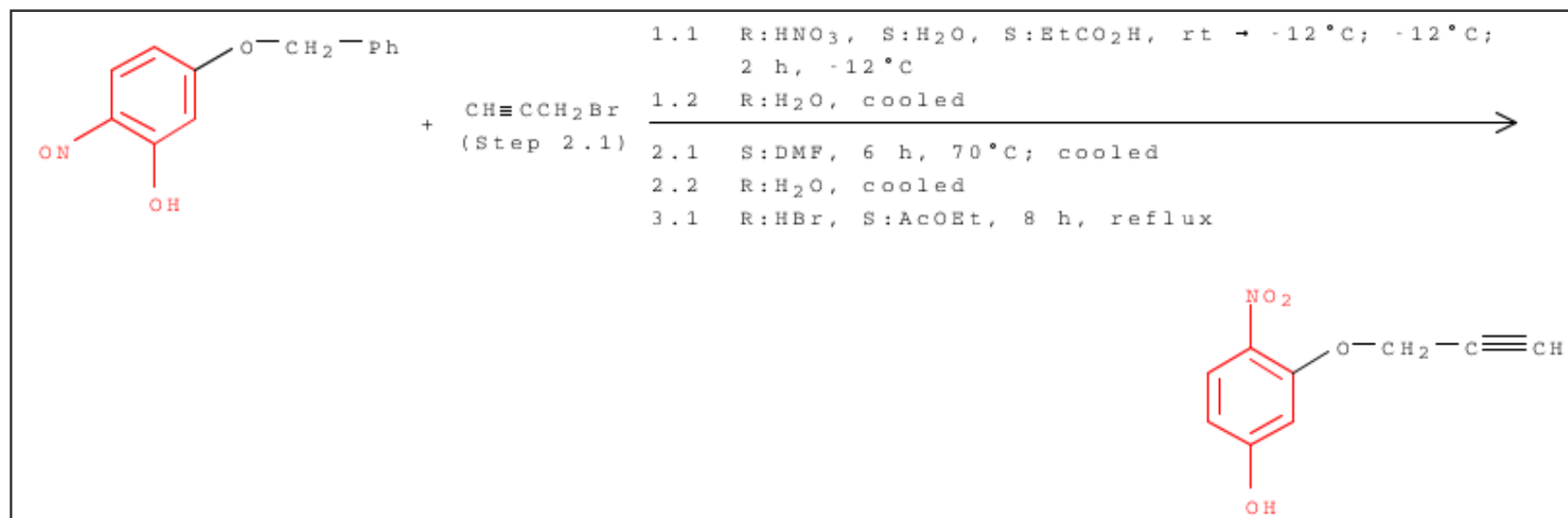
Analysis | Refine

Analyze by: Catalyst

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

HNO3	1
Na2CO3	1
Ni	1

Show More



The screenshot displays the SciFinder Reaction editor interface. The main window shows a chemical reaction between a reactant and a product. The reactant is a chiral amine derivative, and the product is a corresponding amine derivative. The reaction is shown with a pink arrow indicating the transformation. The interface includes a toolbar with various chemical editing tools, a search bar, and a sidebar with navigation options. The sidebar also displays a list of saved answer sets and connections.

Reaction editor

Click an atom in the reactant and its corresponding atom in the product.

reactant: reagent

product

Get reactions where the structure(s) are:

- ☐ Variable only at the specified positions
- ☒ Substructures of more complex structures

Acceptar

Cancelar

Formula not available

SciFinder®

Explore References | Explore Substances | Explore Reactions

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Create Keep Me Posted | Reaction Structure substructure > reactions (45)

Reactions **Get References**

45 Reactions 0 Selected | Keep Selected | Remove Selected

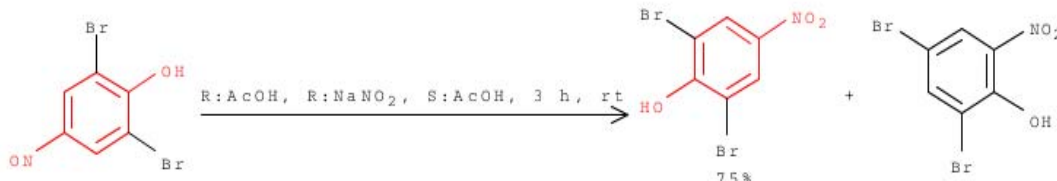
Select All Deselect All | Sort by: Accession Number

Save Print Export

Answers per Page [15] 1 2 3

Display:

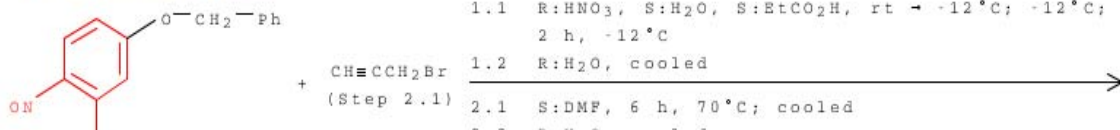
☐ 1. Reaction Detail [Link](#) [Similar Reactions](#) **NEW**



NOTE: Reactants: 1, Reagents: 2, Solvents: 1, Steps: 1, Stages: 1

Rearrangements during nitrosodecarboxylation of isomeric dibromohydroxybenzoic acids
By Shishkin, V. N. and Fadin, M. V.
From Russian Journal of Organic Chemistry, 44(5), 688-692; 2008

☐ 2. Reaction Detail [Link](#)

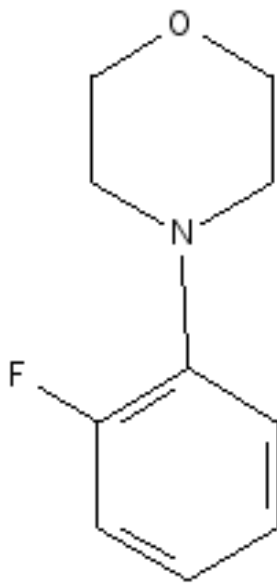


1.1 R:HNO3, S:H2O, S:EtCO2H, rt → -12°C; -12°C; 2 h, -12°C
1.2 R:H2O, cooled
2.1 S:DMF, 6 h, 70°C; cooled
2.2 R:H2O, cooled



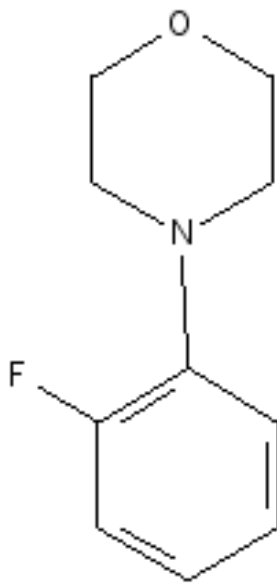
BÚSQUEDA POR SUSTANCIA:

- Buscar $\text{InAs}_x\text{Sb}_{1-x}/\text{InAs}$
- Buscar estructuras similares a:



BÚSQUEDA POR SUSTANCIA:

- **Buscar InAsxSb1-x/InAs**
- **Buscar estructuras similares a:**





 Explore
References

 Explore
Substances

 Explore
Reactions

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Explore References

Research Topic

Research Topic ⓘ

Search

Author Name

Company Name

Document Identifier

Journal

Patent

Tags **NEW**

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

Publication Year(s) ⓘ

Document Type(s) ⓘ

Language(s) ⓘ

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

☐ Biography

☐ Book

☐ Clinical Trial

☐ Commentary

☐ Conference

☐ Dissertation

☐ Editorial

☐ Historical

☐ Journal

☐ Letter

☐ Patent

☐ Preprint

☐ Report

☐ Review

☐ Chinese

☐ English

☐ French

☐ German

☐ Italian

☐ Japanese

☐ Polish

☐ Russian

☐ Spanish

Saved Answer Sets ⓘ

Keep Me Posted Results ⓘ

My Connections ⓘ

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Autosaved Reaction Set

View All

Import

Cambio climatico
Nov 07, 2009 (7)
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View All

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No outstanding sent invitations
You have 4 connections

Waiting for scifinder.cas.org...  scifinder.cas.org

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with the SciFinder logo and links to 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user greeting 'Welcome Miriam Plana | Sign Out' is visible. The main content area is titled 'Explore Substances' and features a search bar with a 'Search' button. Below the search bar, there are several filter categories with checkboxes:

- Chemical Structure**
 - Chemical Structure (selected)
 - Molecular Formula
 - Substance Identifier
- Characteristic(s)**
 - ☐ Single component
 - ☐ Commercially available
 - ☐ Included in reference(s)
- Class(es)**
 - ☐ Alloys
 - ☐ Coordination compounds
 - ☐ Incompletely defined
 - ☐ Mixtures
 - ☐ Polymers
 - ☐ Organics, and others not listed
- Studies**
 - ☐ Analytical
 - ☐ Biological
 - ☐ Preparation
 - ☐ Reactant or reagent

On the right side, there is a sidebar with three sections:

- Saved Answer Sets**: Includes links for 'prova', 'climatic change', and 'Autosaved Reaction Set', with a 'View All' link and an 'Import' button.
- Keep Me Posted Results**: Shows a list of results for 'Cambio climatico' with dates and counts: 'Nov 07, 2009 (7)', 'Oct 31, 2009 (7)', and 'Oct 24, 2009 (12)', with a 'View All' link.
- My Connections**: Displays 'No invitations to connect', 'No outstanding sent invitations', and 'You have 4 connections'.

SciFinder®

Welcome Miriam Plana | Sign Out

Explore References | Explore Substances | Explore Reactions

Explore Substances

Chemical Structure | Molecular Formula ⓘ | Substance Identifier

Al.In.As

Examples:
H4SiO4
H4O4Si
H4SiO4

Search

Molecular Formula ⓘ

Al.In.As

Saved Answer Sets ⓘ

prova
climatic change
Autosaved Reaction Set

View All

Import

Keep Me Posted Results ⓘ

Cambio climatico
Nov 07, 2009 (7)
Oct 31, 2009 (7)
Oct 24, 2009 (12)

View All

My Connections ⓘ

No invitations to connect
No outstanding sent invitations
You have 4 connections

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Create Keep Me Posted | Molecular Formula "Al . As . In" > substances (186)

Explore References | Explore Substances | Explore Reactions

Get References | Get Reactions | Get Commercial Sources

186 Substances | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | Answers per Page [15] | 1 2 3 4 5 6 ... 13 | View: [Icons]

☐ 1. Substance Detail
1191906-25-8

Component	Component Ratio
In	0.2 - 0.8
As	1
Al	0.2 - 0.8

Al . As . In

INDEX NAME NOT YET ASSIGNED

~1 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 2. Substance Detail
1160728-70-0

Component	Component Ratio
In	1
As	1
Al	0.48

Al . As . In

Aluminum indium arsenide (Al_{0.48}InAs)

~1 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 3. Substance Detail
1147780-61-7

Component	Component Ratio
In	0.15- 0.5
As	1
Al	0.5 - 0.85

Al . As . In

Aluminum indium arsenide (Al_{0.5-0.85}In_{0.15-0.5}As)

~1 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 4. Substance Detail
1089731-05-4

☐ 5. Substance Detail
1052696-53-3

☐ 6. Substance Detail
1052696-52-2

Analysis | Refine

Analyze by: [Icon]

Substance Role [Dropdown]

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

Uses 164

Properties 131

Process 108

Preparation 29

Analytical Study 15

Reactant or Reagent 10

Formation, Nonpreparative 6

Miscellaneous 4

Biological Study 1

Combinatorial Study 1

Show More

Get References

Retrieve references for:

☒ All substances ☐ Selected substances

For each substance, retrieve:

☒ All references

☐ References associated with:

- ☐ Adverse Effect, including toxicity
- ☐ Analytical Study
- ☐ Biological Study
- ☐ Combinatorial Study
- ☐ Crystal Structure
- ☐ Formation, nonpreparative
- ☐ Miscellaneous
- ☐ Occurrence
- ☐ Prophetics in Patents
- ☐ Preparation
- ☐ Process
- ☐ Properties
- ☐ Reactant or Reagent
- ☐ Spectral Properties
- ☐ Uses

For each sequence, retrieve:

☐ Additional related references, e.g., activity studies, disease studies.

Get References **Cancel**

Substances 186 Substances 0 Selected Keep Selected Remove Selected

Select All Deselect All Sort by: CAS Registry Number

1. Substance Detail 1191906-25-8

Component	Component Ratio
In	0.2 - 0.8
As	1
Al	0.2 - 0.8

Al . As . In

INDEX NAME NOT YET ASSIGNED

~1 References

Reactions

Commercial Sources

Regulatory Information

Link

4. Substance Detail 1089731-05-4

5. Substance Detail 1052696-53-3

6. Substance Detail 1052696-52-2

Analysis Refine

Analyze by: Substance Role

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

Uses	164
Properties	131
Process	108
Preparation	29
Analytical Study	15
Reactant or Reagent	10
Formation, Nonpreparative	6
Miscellaneous	4
Biological Study	1
Combinatorial Study	1

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user is logged in as 'Miriam Plana'. The search criteria are 'Molecular Formula "Al . As . In" > substances (186) > get references (7274)'. The main section shows a list of references, with the first three visible. Each reference entry includes a checkbox, a title, author information, a brief abstract, and a set of icons for 'Substances', 'Reactions', 'Citing', 'Full Text', 'Link', 'Comments', and 'Tags'. The right sidebar contains a 'Sample Analysis' section with a list of authors and their corresponding progress bars, and a 'Show Full Analysis' button. The bottom of the interface shows the CAS logo and the SciFinder logo, along with the text 'CAS is a division of the American Chemical Society'.

SciFinder®

Welcome Miriam Plana | Sign Out

Create Keep Me Posted Molecular Formula "Al . As . In" > substances (186) > get references (7274)

References Get Substances Get Reactions Get Cited Get Citing

7274 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 364 View: [icon]

☐ 1. Semiconductor photo detector
By Makita, Kikuo; Nakada, Takeshi
From Jpn. Kokai Tokkyo Koho (2009), JP 2009252769 A 20091029. Language: Japanese, Database: CAPLUS
The invention relates to a semiconductor photo detector equipped with the mesa structure which sticks out from the semiconductor substrate, and can control temporal deterioration of the light absorption layer in which it causes by oxidn. etc. The semiconductor photo detector is prepd. with the semiconductor substrate and the mesa structure which sticks out from the semiconductor substrate. The mesa structure has a light absorption layer; a multiplication layer of an electronic multiplication type; a contact layer narrowed from the multiplication layer laminated with a contact layer from the ...
+Substances +Reactions +Citing +Full Text +Link +Comments +Tags

☐ 2. Semiconductor substrates having multilayer semiconductor layers showing different lattice constant from base plates
By Nagase, Kazuhiro; Geka, Hirotsuka
From Jpn. Kokai Tokkyo Koho (2009), JP 2009242124 A 20091022. Language: Japanese, Database: CAPLUS
The title substrates, useful for transistors, etc., comprise base plates having lattice const. x, Sb-contg. first semiconductor layers and having lattice const. y, second semiconductor layers (graded buffer layers) having lattice const. changing from y to z, and third semiconductor layers having lattice const. z in this order (x < z < y). Preferably, the substrates are characterized by (1) first semiconductor layers comprising AlGaAsSb or InAlGaAsSb, (2) base plates comprising GaAs or InP, (3) third semiconductor layers comprising InxAl1-xAs (0.2 < x < 0.8) or InAlGaAsSb. The first semicondu...
+Substances +Reactions +Citing +Full Text +Link +Comments +Tags

☐ 3. Thin InP spacer layer in a high speed laser for reduced lateral current spreading
By Verma, Ashish K.; Thiagarajan, Sumesh Mani K.; Young, David Bruce; Ha, Yuk Lung; Dimitrov, Roman
From U.S. (2009), US 7606279 B1 20091020. Language: English, Database: CAPLUS
A high speed laser (e.g., DFB laser) is described that comprises a substrate, an active region positioned above the substrate, a mesa positioned above the active region, and one or more layers disposed between the active region and the mesa, wherein the thickness of at least one of the one or more layers is implemented to at least partially minimize the distance between the mesa and active region such that lateral current spreading between the mesa and the active region is at least partially minimized. A transmitter optical subassembly comprising the laser is also described.
+Substances +Reactions +Citing +Full Text +Link +Comments +Tags

☐ 4. Semiconductor substrate, semiconductor device and semiconductor device manufacturing method

Analysis Refine

Sample Analysis

Author Name

Capasso Federico

Cho Alfred Y

Sivco Deborah L

Faist Jerome

Cho A Y

Gmachl Claire

Sirtori Carlo

Del Alamo Jesus A

Hutchinson Albert L

Kawamura Yuichi

Show Full Analysis

Categorize

SciFinder®

Welcome Miriam Plana | Sign Out

Create Keep Me Posted Molecular Formula "Al . As . In" > substances (186) > get references (7274)

References **Get Substances** **Get Reactions** **Get Cited** **Get Citing**

7274 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 364 View: [icon]

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+Substances **+Reactions** **+Citing** **+Full Text** **+Link** **+Comments** **+Tags**

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+Substances **+Reactions** **+Citing** **+Full Text** **+Link** **+Comments** **+Tags**

☐ 4. **Semiconductor substrate, semiconductor device and semiconductor device manufacturing method**

Analysis **Refine**

Refine by: **Research Topic**
☐ Author Name
☐ Company Name
☐ Document Type
☐ Publication Year
☐ Language
☐ Database

Research Topic

Examples:
The effect of antibiotic residues in dairy products
Photocyanation of aromatic compounds
Refine

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user is logged in as 'Miriam Plana'. The search path is: Molecular Formula "Al . As . In" > substances (186) > get references (7274) > refine "Quantum dots" (446). The main results area shows 446 references, sorted by Accession Number. The first three references are listed with their titles, authors, and abstracts. On the right, there is an 'Analysis' sidebar with a table of authors and their corresponding number of references.

References | [Get Substances](#) | [Get Reactions](#) | [Get Cited](#) | [Get Citing](#)

446 References | 0 Selected | [Keep Selected](#) | [Remove Selected](#) | [Remove Duplicates](#) | [Add Tags](#) | [Save](#) | [Print](#) | [Export](#)

[Select All](#) [Deselect All](#) | Sort by: [Accession Number](#) | [Answers per Page \[20\]](#) | [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) ... [23](#) | View: [List](#) [Grid](#)

☐ 1. **Vertical-cavity surface-emitting semiconductor laser with large-aperture light extraction from substrate**
By Zhang, Yan; Ning, Yongqiang; Qin, Li; Liu, Yun; Wang, Lijun; Li, Te
From Faming Zhuanli Shenqing Gongkai Shuomingshu (2009), CN 101510667 A 20090819. Language: Chinese, Database: CAPLUS
The title vertical-cavity surface-emitting semiconductor laser with large-aperture light extrn. from substrate comprises a contact layer, an upper reflector, an active region, a lower reflector, a substrate, a small-aperture electrode, a large-aperture light extrn. window, an insulating film, and a substrate electrode. The insulating film encloses and is connected with the small-aperture electrode, and the substrate electrode encircles and is connected with the large-aperture light extrn. window. With simple prepn. process, the invention not only enlarges the light extrn. aperture of a vertical-...

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

☐ 2. **Immersion layer in columnar quantum dash structure as a polarization insensitive light emitter at 1.55 μm**
By Sek, Grzegorz; Podemski, Pawel; Andrzejewski, Janusz; Misiewicz, Jan; Hein, Sebastian; Hofling, Sven; Forchel, Alfred
From Applied Physics Express (2009), 2(6), 061102/1-061102/3. Language: English, Database: CAPLUS
The authors report on polarization independent 1.55 μm room temp. edge emission from an InGaAs immersion layer, being a quasi-two-dimensional surrounding of columnar quantum dashes formed during the close stacking self assembled growth. Calcns. performed in an 8 band k

model revealed that the in-plane strain distribution across the immersion layer induces a significant heavy hole-light hole valence states mixing leading to equal transverse elec. and transverse magnetic components of the optical transition intensity.

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

☐ 3. **Nonvolatile memory and three-state FETs using cladded quantum dot gate structure**
By Jain, Faquir C.
From U.S. Pat. Appl. Publ. (2009), US 2009184346 A1 20090723. Language: English, Database: CAPLUS
The present invention discloses structures and method of fabricating cladded quantum dot gate nonvolatile memory and three-state field-effect transistor devices that can be scaled down to sub-22 nm dimensions and embedded along side with other functional circuits. Another innovation is the design of transport channel, which comprises an asym. coupled well structure comprising two or more wells. This structure enhances the retention time in nonvolatile memory by increasing the effective sepn. between channel charge and the quantum dots located in the floating gate. The cladded quantum dot ga...

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [Comments](#) [Tags](#)

☐ 4. **Short-wavelength (760-920 nm) AlGaInAs quantum dot lasers**

Analysis | [Refine](#)

Analyze by: [Author Name](#)

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

Wang Z G	41
Xu B	35
Sasakura H	27
Adachi S	26
Gendry M	26
Muto S	26
Fafard S	24
Ustinov V M	20
Brault J	19
Ledentsov N N	19

[Show More](#)

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user is logged in as 'Miriam Plana'. The search path is: Molecular Formula "Al . As . In" > substances (186) > get references (7274) > refine "quantum dots" (446). The main results area shows 446 references, sorted by Accession Number. The first three references are listed with their titles, authors, and abstracts. The right sidebar shows an 'Analysis' section with a dropdown menu set to 'Company-Organization'. Below this, a list of organizations and their corresponding number of references is displayed.

References

446 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 23 View: [icon]

1. **Vertical-cavity surface-emitting semiconductor laser with large-aperture light extraction from substrate**
By Zhang, Yan; Ning, Yongqiang; Qin, Li; Liu, Yun; Wang, Lijun; Li, Te
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4. **Short-wavelength (760-920 nm) AlGaInAs quantum dot lasers**

Analysis Refine

Analyze by: [icon]

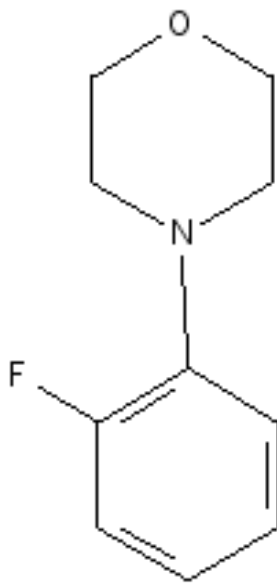
Company-Organization

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

Chinese Academy of Sciences, Peop Rep China	55
Hokkaido University, Japan	32
University of Michigan, USA	10
University of Sheffield, UK	10
National Central University, Taiwan	9
National Research Council, Can	9
Russian Academy of Sciences, Russia	8
University of Illinois at Urbana Champaign, USA	7
Boston University, USA	6

BÚSQUEDA POR SUSTANCIA:

- Buscar InAsxSb1-x/InAs
- Buscar estructuras similares a:





 Explore
References

 Explore
Substances

 Explore
Reactions

Welcome Miriam Plana | Sign Out

Explore References

Research Topic

Research Topic 

Search

Author Name

Company Name

Document Identifier

Journal

Patent

Tags 

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

Saved Answer Sets 

prova
climatic change
Autosaved Reaction Set

View All

Import

Keep Me Posted Results 

Cambio climatico
Nov 07, 2009 (7)
Oct 31, 2009 (7)
Oct 24, 2009 (12)

View All

My Connections 

No invitations to connect
No outstanding sent invitations
You have 4 connections

Waiting for scifinder.cas.org...  scifinder.cas.org

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with the SciFinder logo, a welcome message for 'Miriam Plana', and links to 'Sign Out', 'Explore References', 'Explore Substances', and 'Explore Reactions'. On the right side of the top bar are links for 'Saved Answer Sets', 'Keep Me Posted Results', 'NEW My Connections', 'Help', 'History', and 'Preferences'. The main content area is titled 'Explore Substances' and features a sidebar with search criteria: 'Chemical Structure' (selected), 'Molecular Formula', and 'Substance Identifier'. The central area contains a 'Search' button and a placeholder for a chemical structure image with the text 'Click image to draw or import structure'. Below this, there are three sections of filters: 'Characteristic(s)' with checkboxes for 'Single component', 'Commercially available', and 'Included in reference(s)'; 'Class(es)' with checkboxes for 'Alloys', 'Coordination compounds', 'Incompletely defined', 'Mixtures', 'Polymers', and 'Organics, and others not listed'; and 'Studies' with checkboxes for 'Analytical', 'Biological', 'Preparation', and 'Reactant or reagent'. On the right side of the main area, there are three panels: 'Saved Answer Sets' showing 'prova', 'climatic change', and 'Autosaved Reaction Set' with a 'View All' link and an 'Import' button; 'Keep Me Posted Results' showing 'Cambio climatico' with dates and counts (Nov 07, 2009 (7), Oct 31, 2009 (7), Oct 24, 2009 (12)) and a 'View All' link; and 'My Connections' showing 'No invitations to connect', 'No outstanding sent invitations', and 'You have 4 connections'.

Structure editor

Draw or change atoms or bonds.

Atom Short

-X =R

[] 1-4 Cl

Scale 100

C H O S N P Cl Br F I Si

C₁₀H₁₂FNO (query) 181,21

Get substances that match your query using:

- ☐ Exact search
- ☐ Substructure search
- ☒ Similarity search

Acceptar Cancelar

Saved Answer Sets

Keep Me Posted Results

NEW My Connections

Help History Preferences

Saved Answer Sets

prova
climatic change
Autosaved Reaction Set

View All

Import

Keep Me Posted Results

Cambio climatico
Nov 07, 2009 (7)
Oct 31, 2009 (7)
Oct 24, 2009 (12)

View All

My Connections

No invitations to connect
No outstanding sent invitations
You have 4 connections

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Welcome Miriam Plana | Sign Out

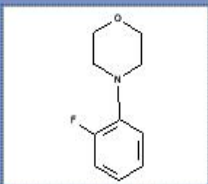
Explore References | Explore Substances | Explore Reactions

Explore Substances

Chemical Structure | Chemical Structure ⓘ

Molecular Formula

Substance Identifier



Click image to change structure or view detail

Search type: ⓘ

- ☒ Exact Structure
- ☐ Substructure
- ☒ Similarity

☐ Show precision analysis

Search

Characteristic(s)

- ☐ Single component
- ☐ Commercially available
- ☐ Included in reference(s)

Class(es) ⓘ

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

Saved Answer Sets ⓘ

Keep Me Posted Results

NEW My Connections

Help
History
Preferences

prova
climatic change
Autosaved Reaction Set

View All

Import

Keep Me Posted Results ⓘ

Cambio climatico
Nov 07, 2009 (7)
Oct 31, 2009 (7)
Oct 24, 2009 (12)

View All

My Connections ⓘ

No invitations to connect
No outstanding sent invitations
You have 4 connections

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome Miriam Plana | Sign Out

Create Keep Me Posted | Chemical Structure similarity

Saved Answer Sets | Help
Keep Me Posted Results | History
NEW My Connections | Preferences

Similarity Candidates

8 Candidates | 3 Selected

Select All | Deselect All

Similarity Candidates	Substances
☒ ≥ 99 (most similar)	1
☐ 95-98	0
☒ 90-94	3
☒ 85-89	13
☐ 80-84	71
☐ 75-79	137
☐ 70-74	342
☐ 65-69	1017
☐ 60-64 (least similar)	2540

Get Substances

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SciFinder®

Explore References | Explore Substances | Explore Reactions

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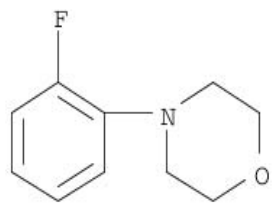
Create Keep Me Posted | Chemical Structure similarity > substances (17)

Substances | Get References | Get Reactions | Get Commercial Sources

17 Substances | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: Similarity Score | Answers per Page [15] | 1 2 | View: [Icons]

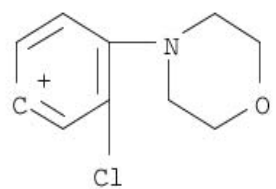
☐ 1. Substance Detail
384344-17-6 | Score: ≥ 99



C₁₀ H₁₂ F N O
Morpholine, 4-(2-fluorophenyl)-

~4 References
Reactions
Commercial Sources
Regulatory Information
Link

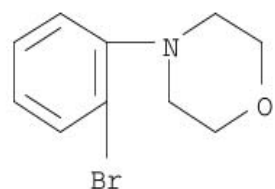
☐ 2. Substance Detail
72472-49-2 | Score: 92



C₁₀ H₁₁ Cl N O
Phenylum, 3-chloro-4-(4-morpholinyl)- (9Cl)

~1 References
Reactions
Commercial Sources
Regulatory Information
Link

☐ 3. Substance Detail
87698-82-6 | Score: 92



C₁₀ H₁₂ Br N O
Morpholine, 4-(2-bromophenyl)-

~7 References
Reactions
Commercial Sources
Regulatory Information
Link

Analysis | Refine

Analyze by: Substance Role

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

Preparation	13
Reactant or Reagent	8
Properties	2
Analytical Study	1
Formation, Nonpreparative	1
Process	1
Prophetic in Patents	1

Show More

Export

Export:

- ☒ All answers
- ☐ Only selected answers

File Name: *

propiedades

File Type:

Microsoft Excel Worksheet (*.xls)

Properties to Export:

- ☒ All property values
- ☐ Only experimental property values
- ☐ Only predicted property values
- ☐ Select property values...

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1. Substance Detail 384344-17-6

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Reactant or Reagent 8

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2	CAS Registry Number	CAS Index Name	Type	Category	Property	Value and Units
3	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted	Biological	Bioconcentration Factor	1.0
4	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted	Biological	Bioconcentration Factor	1.0
5	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted	Biological	Bioconcentration Factor	1.0
6	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted	Biological	Bioconcentration Factor	1.11
7	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted	Biological	Bioconcentration Factor	5.97
8	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted	Biological	Bioconcentration Factor	10.9
9	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted		Bioconcentration Factor	11.8
10	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted		Bioconcentration Factor	11.9
11	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted		Bioconcentration Factor	12.0
12	384344-17-6	Morpholine, 4-(2-fluorophenyl)-	predicted		Bioconcentration Factor	12.0

Property

- Bioconcentration Factor
- Boiling Point
- Density
- Enthalpy of Vaporization
- Flash Point
- Freely Rotatable Bonds
- H Acceptors
- H Donor/Acceptor Sum
- H Donors
- Koc
- logD
- logP
- Mass Intrinsic Solubility
- Mass Solubility
- Melting Point
- Molar Intrinsic Solubility
- Molar Solubility
- Molar Volume
- Molecular Weight
- pKa



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