



**Web version of SciFinder[®]: New features
and improved performance**

November 16, 2008

www.cas.org



A division of the American Chemical Society

New features at a glance...

- **Features you know and love...**
 - **Categorize**
 - **Combine answer sets**
 - **Duplicate removal**
 - **Analyze / Refine options**
 - **CHEMLIST®**
 - **.rtf export**
 - **Sorting**
 - **Structure Drawing Editor options**
 - **Substructure moduling**
 - **Improved reaction displays**
 - **Search shortcuts**
 - **CHEMCATS® export**
- **Features you've never seen...**
 - **Direct links to data**
 - **Keep Me Posted enhancements**
 - **Improved search precision**
 - **Session history retention**
 - **Index Term linking**
 - **New layouts**
- **And new content...**
 - **New experimental data**
 - **New predicted data**
 - **Sources of Registration**
 - **“Prophetic” substance indicators**
 - **New reaction data**

Removing duplicates is easy.

The screenshot shows the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below this, a 'Welcome' message and a 'Sign Out' link are visible. A status bar indicates 'Opened saved answer set "SciFinder" (156)'. The main content area is titled 'References' and shows a list of 156 references. The 'Remove Duplicates' button is highlighted with a red box. The first two references are visible:

- 1. The prospects of antagonizing the growth hormone secretagogue receptor to treat obesity**
By Zhao, Hongyu; Serby, Michael D.; Liu, Bo
From Expert Opinion on Therapeutic Patents (2008), 18(9), 989-998. Language: English, Database: CAPLUS
Background: Ghrelin is an endogenous ligand of the growth hormone secretagogue receptor (GHS-R) that functions as a short-term meal initiator and a long-term energy balance regulator. Antagonizing GHS-R could be a method to treat obesity. Objective: To review the published in vivo characterization of GHS-R antagonists between 2005 and 2008 and evaluate the validity of antagonizing GHS-R as a therapeutic strategy for obesity. Methods: Primary literature was searched using SciFinder and Google Scholar. Patents were searched using the European Patent Office and SciFinder. Results/conclusion:...
- 2. Enhancements to CAS' predicted properties coverage**
By Schenck, Roger; Drotleff, Elizabeth
From Abstracts of Papers, 236th ACS National Meeting, Philadelphia, PA, United States, August 17-21, 2008 (2008), (), CINF-070. Language: English, Database: CAPLUS
Mol. properties have gained in importance as more chem. is being performed in silico. While exptl. properties are valued, predicted property algorithms have been greatly improved and the resulting data has steadily gained acceptance in the scientific community. It is crit. for information platforms to deliver this data in an efficient and comprehensive manner. CAS' STN and SciFinder products are well-known delivery vehicles with approx. 1.6 B predicted properties in the flagship CAS Registry database. CAS plans to focus on augmenting their existing collection with the inclusion of addnl. p...

Shortcuts let you quickly create a new query based on a structure diagram.

Features you know...

SciFinder® Explore References Explore Substances Explore Reactions

Welcome | Sign Out

Create Keep Me Posted Substance Identifier "lipitor" > substances (1) > 134523-03-8

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

Share Save Print Export

CAS Registry Number: 134523-03-8
(Component: 134523-00-5)

C₃₃ H₃₅ F N₂ O₅ · 1/2 Ca

1H-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1), (βR,δR)-

1H-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1), [R-(R*,R*)]- ; Atorvastatin calcium ; Atorvastatin hemicalcium ; Atorvastatin hemicalcium salt ; CI 981 ; Lipitor ; Sortis ; Tahor ; YM 548

Deleted CAS Registry Numbers: 334757-04-9

Source of Registration: CA

Document Types: Conference, Journal, Patent

Role **Patents** **Nonpatents** **Nonspecific Derivatives from Patents**

| | | | |
|------------------|---|---|--|
| Analytical study | ✓ | ✓ | |
|------------------|---|---|--|

Chemical Structure: A chemical structure diagram of Atorvastatin calcium salt. The structure features a central pyrrole ring with a 4-fluorophenyl group at position 2, a 1-methylethyl group at position 3, and a phenyl group at position 5. A side chain at position 4 includes a carbonyl group attached to a phenylamino group (PhNH-), and a heptanoic acid chain with hydroxyl groups at the β and δ positions. The calcium salt is indicated by the 'Ca' label. A red box highlights the 'Explore by Chemical Structure' button below the structure.

Absolute stereochemistry.

Combine now offers more options.

Combine Answer Sets

Select an option for combining the two selected saved answer sets:

- Combine - Include all references from both sets
- Intersect - Include only references that appear in both sets
- Exclude - Include only references that appear in one set but not the other
- Exclude - Include only references that appear in the other set but not this one
- Remove duplicate references

Combine Answer Sets

Select an option for combining the selected saved answer sets:

- Combine - Include all references from all selected answers
- Intersect - Include only references that appear in all selected sets
- Remove duplicate references

Combine multiple answer sets

Refine by Atom Attachment is now available.

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome | Sign Out

Create Keep Me Posted | Chemical Structure substructure > substances (3092)

Substances 3092 Substances

Select All Deselect All

1. 1044140-88

C26 H29 N5 O6

INDEX NAME NOT YET

~1 References

Reactions

Commercial Source

Regulatory Informa

Share

4. 1041692-51

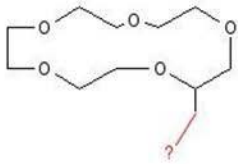
C42 H70 Cl2 N4 O16

INDEX NAME NOT YET

Refine by Atom Attachment

1. Click an atom to display the attachments present at that site. 2. Select attachment(s) of interest.

Substructure



Atom Attachments

Select All Deselect All

| | |
|---|------|
| <input type="checkbox"/> H or None | 55 |
| <input type="checkbox"/> C | 2137 |
| <input type="checkbox"/> O | 685 |
| <input type="checkbox"/> N | 242 |
| <input type="checkbox"/> S | 22 |
| <input type="checkbox"/> Br | 13 |
| <input type="checkbox"/> Cl | 3 |
| <input type="checkbox"/> F | 2 |
| <input type="checkbox"/> I | 1 |
| <input type="checkbox"/> Other | 30 |
| <input type="checkbox"/> A - Any (not H) | 3007 |
| <input checked="" type="checkbox"/> Q - Any (not C,H) | 961 |
| <input type="checkbox"/> Hy - Heterocycle | 42 |
| <input type="checkbox"/> X - Halogen | 19 |
| <input type="checkbox"/> Ak - Alkyl chain | 16 |
| <input type="checkbox"/> Cb - Carbocycle | 10 |

? = Q

Refine Cancel

Analysis Refine

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Reference Availability
- Atom Attachment

Select Attachments

Keep Me Posted now displays steps in your search.

The screenshot shows the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below this is a 'Welcome' message and a 'Sign Out' link. A red box highlights the 'Create Keep Me Posted' button in the top left. The main content area shows search results for 'Research Topic "cell signaling pathways" with limiters > references (34)'. A 'References' section is visible with options like 'Get Substances', 'Get Reactions', 'Get Cited', and 'Get Citing'. A '34 References' summary bar includes '0 Selected', 'Keep Selected', 'Remove Selected', and 'Remove Duplicates'. Below this is a 'Select All Deselect All' bar and a 'Sort by: Accession Number' dropdown. The 'Create Keep Me Posted Profile' dialog box is open, containing the following fields and options:

- Title: *** (Required): A text input field.
- Description:** A text area with scrollbars.
- Status:** Radio buttons for 'Enabled' (selected) and 'Disabled'.
- Exclude previously retrieved references.
- Expiration Date:** A date picker set to 'Sep 4, 2009'.
- Buttons:** 'Create' and 'Cancel'.

On the right side of the dialog, there is a 'Search:' section with the following details:

- Explore references by research topic: **cell signaling pathways**
- Limiters:**
 - Document Types** - Dissertation, Conference, Journal, Clinical Trial
 - Languages** - Japanese, German, Chinese, English
 - Company Name** - pfizer
- Candidates Selected:** References which contain the concept "cell signaling pathways".

Up to 10 previous sessions are available for download.

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, with a 'Welcome' message and a 'Sign Out' link. The main search area shows a breadcrumb trail: 'Research Topic "transposition and gene regulat..." > references (1364) > refine "2008" (34)'. Below this is a 'History' section with a 'Print' and 'Export' option. The history is divided into two sessions. The first session, dated September 4, 2008 at 3:16 PM, details the exploration of references by research topic, the selection of candidates, and the refinement of an answer set by company. The second session, dated September 4, 2008 at 3:20 PM, details the exploration of references by research topic, the selection of candidates, and the refinement of an answer set by publication year. On the right side, a 'Previous Sessions' sidebar is highlighted with a red border, listing ten downloadable session files with their respective IDs.

History Print Export

Session began September 4, 2008 at 3:16 PM

Explore references by research topic: transposable elements initiated, resulting in 2 candidates September 4, 2008 3:17 PM

Explore complete
Candidates Selected
 19907 references were found containing "transposable elements" as entered.

Explore results
 Answer set 1 created with
 2656 answers from CAPLUS
 17251 answers from MEDLINE

Refine Answer set 1 by company
 cold spring harbor laboratories
 Answer set 2 created with
 33 answers from CAPLUS
 49 answers from MEDLINE

Explore references by research topic: transposition and gene regulation initiated, resulting in 5 candidates September 4, 2008 3:20 PM

Explore complete
Candidates Selected
 1364 references were found containing both of the concepts "transposition" and "gene regulation".

Explore results
 Answer set 3 created with
 635 answers from CAPLUS
 729 answers from MEDLINE

Refine Answer set 3 by publication year
 2008
 Answer set 4 created with
 17 answers from CAPLUS
 17 answers from MEDLINE

Previous Sessions

- SFSessionHistory-2008-09-04_151635.rtf
- SFSessionHistory-2008-09-04_151534.rtf
- SFSessionHistory-2008-09-04_151453.rtf
- SFSessionHistory-2008-09-04_150745.rtf
- SFSessionHistory-2008-09-04_150703.rtf
- SFSessionHistory-2008-09-04_150516.rtf
- SFSessionHistory-2008-09-04_150417.rtf
- SFSessionHistory-2008-09-04_145528.rtf
- SFSessionHistory-2008-09-04_145242.rtf
- SFSessionHistory-2008-09-04_145136.rtf

Links to data make organizing and collaborating easier.

SciFinder®

Welcome | Sign Out

Explore References | Explore Substances | Explore Reactions

Create Keep Me Posted | Research Topic "cell signaling pathways" with limiters > references (34)

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

34 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number

1. **Cartilage preservation by inhibition of Janus kinase 3 in two rodent models of rheumatoid arthritis**
 By Milici, Anthony J.; Kudlacz, Elizabeth M.; Audoly, Laurent; Zwillich, Samuel; Changelian, Paul
 From Arthritis Research & Therapy (2008), 10(1), No pp. given. Language: English, Database: CAPLUS
 Introduction: CP-690550 is a small mol. inhibitor of Janus kinase 3 (JAK3), a crit. enzyme in the signaling pathway of several cytokines (interleukin (IL)-2, -7, -15 and -21) that are important in various T cell functions and immune homeostasis. The purpose of this study was to evaluate CP-690550 in murine collagen-induced arthritis (CIA) models of rheumatoid arthritis (RA). Methods: CIA and AA were induced using std. protocols in mice via osmotic mini-pump infusion at doses ranging from 1.5-15 mg/kg/day followin...

Substances Reactions Citing Full Text **Share**

2. **FMRFamide-like peptides encoded on the G-protein-coupled receptor Y58G8A.4 heterologous to Caenorhabditis elegans**
 By Kubiak, Teresa M.; Larsen, Martha J.; Bowman, Jerry
 From Biopolymers (2008), 90(3), 339-348. Language: English
 Two alternatively spliced variants of an orthologous G-protein-coupled receptor (GPCR) were cloned and functionally expressed in Chinese hamster ovary (CHO) cells. The Y58G8A.4a and Y58G8A.4b proteins (397 and 433 amino acid residues, resp.) differ both in amino acid sequence and length of the C-terminal tail of the receptor. A calcium mobilization assay was used as a read-out for receptor function. Both receptors were activated, with nanomolar potencies, by putative peptides encoded by the flp-18 precursor gene, leading to their designation as F...

Substances Reactions Citing Full Text **Share**

Copy and paste link for quick access to this reference.
https://scifinder-beta.cas.org/scifinder/view/link_v1/reference.jsf?
 Create a bookmark, save in a document, or e-mail to a colleague.

Create links to answers, saved answer sets, and alerts.

Supplier information for multiple compounds can be exported to Excel.

Microsoft Excel - Phosphoric Acid & Similar.xls [Read-Only]

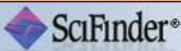
File Edit View Insert Format Tools Data Window Help Adobe PDF

Type a question for help

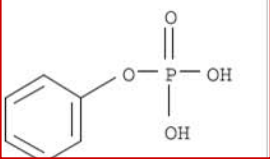
100%

Arial 10

A1

1 

2 CAS Registry Number: 701-64-4


3 

| 4 | Chemical Name | Catalog Name | Company Name | Street Address | City | State or Province |
|---|-----------------------------------|--|---|--|----------------|-------------------|
| 5 | Phenylphosphoric acid | 3B Scientific Corporation Product List | 3B Scientific Corporation | 1840 Industrial Drive, Suite 160 | Libertyville | IL |
| 6 | Phenylphosphoric acid | ABCR Product List | ABCR GmbH KG | Im Schleher 10 | Karlsruhe | |
| 7 | PHENYLPHOSPHORIC ACID | Advanced Technology Product List | Advanced Technology & Industrial Co | Unit B, 1/F., Cheong Shing Building Cheong Shing Bldg., 17 Walnut St. | Tai Kok Tsui | Kln |
| 8 | Phosphoric acid, monophenyl ester | Ambinter Stock Screening Collection | Ambinter | 50, avenue de Versailles | Paris | |
| 9 | Phenylphosphoric acid | Aminecom Product List | Aminecom Inc. | 824 Bollingbrook Street | St. Petersburg | VA |

All Substances / Tips / 52331-30-3 / 13388-86-8 / 2310-89-6 / 701-64-4 /

Index Terms are linked for faster exploring.

Indexing

Pharmaceuticals (Section 63-6) 

Section cross-reference(s): 1, 2, 62

Concepts

Nail(anatomical)

- strengthening agents; method for treatment of nail inflammatory diseases with chitosans

Alcohols

C16-18; method for treatment of nail inflammatory diseases with chitosans
Cosmetic use; Modifier or additive use; Therapeutic use; Biological study; Uses

Drugs

antipsoriatic; method for treatment of nail inflammatory diseases with chitosans

Topical drug delivery systems

applied to nail surface under semi-occlusive or occlusive medication; method for treatment of nail inflammatory diseases with chitosans

Alopecia

areata; method for treatment of nail inflammatory diseases with chitosans

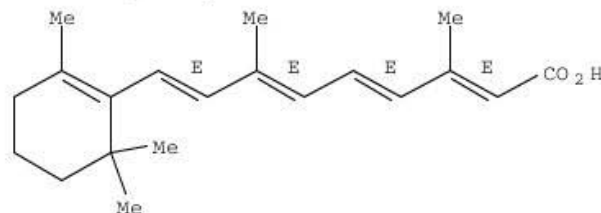
Substances

57-13-6 Urea
57-55-6 Propylene glycol
64-17-5 Ethanol
67-63-0 Isopropanol
67-71-0
111-77-3 Diethyleneglycol monomethylether
141-78-6 Ethyl acetate
25322-68-3

method for treatment of nail inflammatory diseases with chitosans

Cosmetic use; Modifier or additive use; Therapeutic use; Biological study; Uses

50-78-2 Aspirin
65-85-0 Benzoic acid
69-72-7 Salicylic acid
302-79-4 Tretinoin
Double bond geometry as shown.



378-44-9

Content in SciFinder keeps expanding.

- **New experimental data**
Thousands of new NMR, IR, and MS spectra as well as experimental physical properties now appear in Substance Details.
- **New predicted data**
Millions of NMR spectra are coming soon. Predicted properties now total more than 1.7 million.
- **Sources of registration**
Substance Details now show all source of registration data including nontraditional sources.
- **“Prophetic” substance indicators**
A new role for substances indexed as prophetics (in patents) has been added.
- **New reaction content**
Thousands of evaluated reactions from reaction encyclopedias continue to be added, giving you access to important older reactions.