



# SciFinder-Anleitung

**Teil 1: Einführung**

**Teil 2: Weitere Funktionen in SciFinder + Hilfen**

**Teil 3: Suche von Strukturen und Reaktionen**

**Teil 4: Markush-Strukturen und Patente**

**Achtung! Dieses Material wird von uns nicht mehr aktualisiert,  
da wir bereits mit SF-n arbeiten.**

Stand: 1.2.2019

**SciFinder**

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Heike Göbel, IVS der Chemisch-Geowissenschaftlichen Fakultät



# Teil 1: Einführung

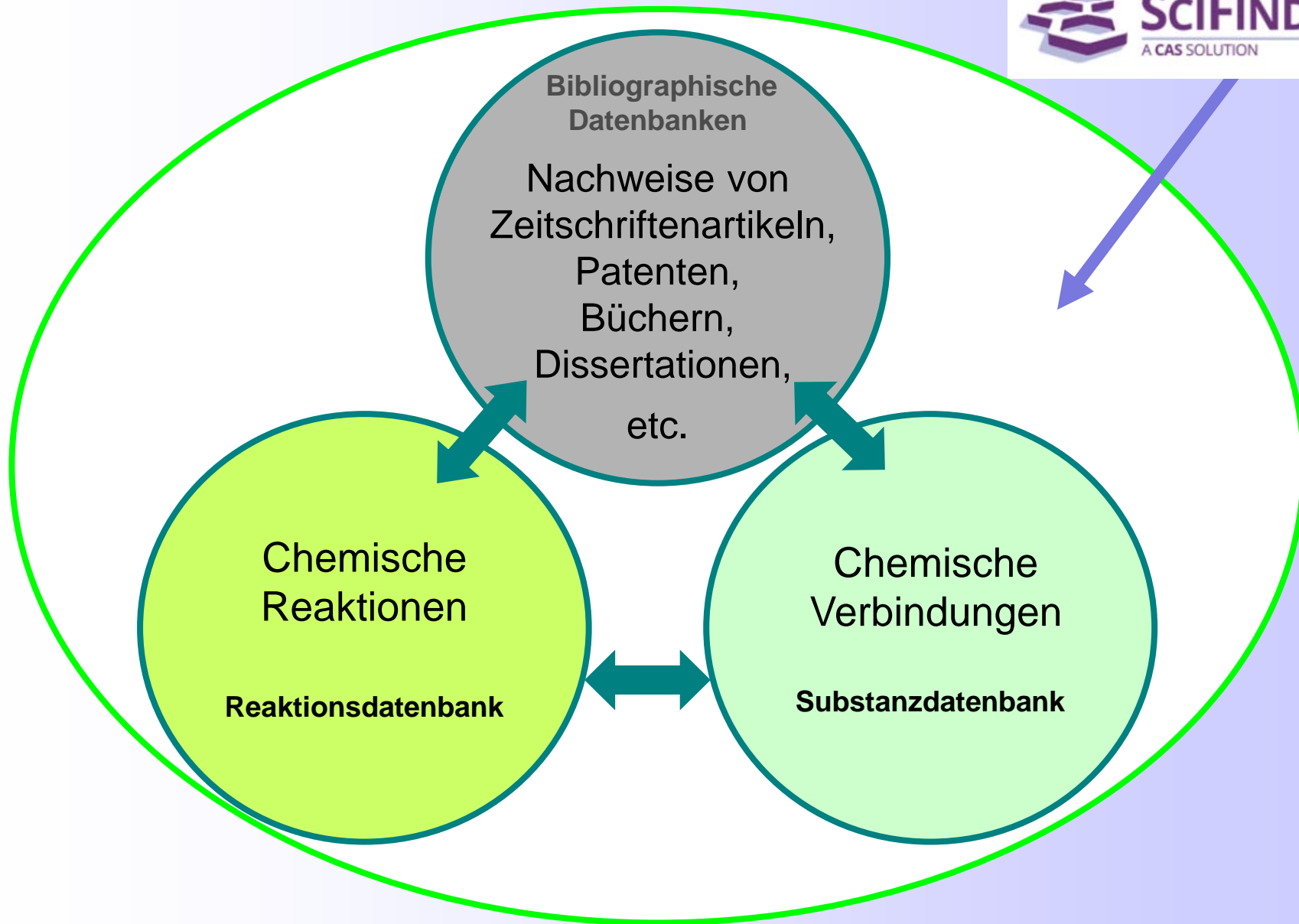
- Die Datenbanken in SciFinder
- Datenbanken und Suchmöglichkeiten in SciFinder
- SciFinder-Updates
- Zugang mit VPN-Client der Uni
- Registrierung bei CAS
- Benutzername oder Passwort vergessen?
- Gleichzeitiger Zugriff auf SciFinder/Timeout
- Einstellungen vor Recherchebeginn, History-Button
- Tipps zu Recherchestrategien
- Thematische Recherchen (References/ Research Topic)
- Auswahl passender Konzepte
- Dubletteneliminierung
- Suchverlauf: Breadcrumbs, History und Previous Sessions
- Zugriffe auf Volltexte in SciFinder
- Refine
- Suche nach Autoren
- Link-Button in SciFinder
- Speichern der Suchergebnisse, Exportformate, Drucken, Keep Me Posted



# Die Datenbanken in SciFinder

- **CAplus** Bibliografische Datenbank > 40 Mio. Einträge ab ca.1800 (inkl. Patente)
- **MEDLINE** Biomedizinische Informationen > 24 Mio Einträge ab 1809
- **CASreact** > 77 Mio. Reaktionen ab 1840
- **Registry** > 91 Mio. organische und anorganische Verbindungen  
> 65 Mio. Sequenzen
- **Chemcats** > 99 Mio Käufliche Substanzen > 980 Kataloge,  
> 870 Händler
- **Chemlist** Regulated **CHEM**icals **LIST**ing > 312.000,  
Informationen zu chemischen Substanzen aus nationalen,  
US-amerikanischen und internationalen Verzeichnissen und  
Regelwerken

# Datenbanken und Suchmöglichkeiten in



# SciFinder-Updates

- Die aktuellen Neuerungen kann man sich jederzeit über den Link “SciFinder Help/ What’s New” ansehen.

CAS Solutions

SCIFINDER<sup>®</sup>  
A CAS SOLUTION

Explore ▼ Saved Searches ▼ SciPlanner

Link Save

Preferences | SciFinder Help ▼ Sign Out

Help  
Training  
What's New  
Contact Us

CAS<sup>®</sup>  
A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

ACS | Journals | C&EN | CAS | Languages

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SciFinder  
STN  
Science IP  
MethodsNow  
PatentPak

NCI Global  
Other CAS Products  
Coming Soon

Home > Products > SciFinder

## What's New in SciFinder

**Patents from 20 Additional Patent Offices Enhance PatentPak™ Comprehensiveness (December 2015)**

Twenty more patent offices have been added to PatentPak, expanding the global coverage and comprehensiveness of this collection which now includes 31 patent authorities.

The following patent offices have been added to the PatentPak collection:

Austria	Estonia	Luxembourg	Slovenia
Australia	Greece	Monaco	Spain
Belgium	Ireland	Portugal	Sweden
Brazil	Latvia	Romania	Switzerland
Croatia	Lithuania	Slovakia	Turkey

These country authorities supplement the information already available from the following major patent offices:

- WIPO – World Intellectual Property Organization (WO)
- USPTO – United States Patent and Trademark Office (US)
- EPO – European Patent Office (EP)
- JPO – Japan Patent Office (JP)
- SIPO – State Intellectual Property Office of the Peoples Republic of China (CN)
- DPMA – German Patent and Trade Mark Office (DE)
- INPI – French Patent Office (FR)
- IPO – Intellectual Property Office (GB)
- KIPO – Korean Intellectual Property Office (KR)
- ROSPATENT – Federal Service for Intellectual Property (RU)

# Zugang zu SciFinder über das Internet

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

...weil es so schön aussieht:



## Sign In

Username

Password

Remember me  
(Do not use on a shared computer)

[Forgot Username or Password?](#)

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

## New to SciFinder?

[Learn more about gaining access to SciFinder.](#)



## News & Updates

### Welcome to SciFinder

**Did you notice our new look?**  
Our new branding will also be phased into training and other support materials in the coming months. If you are a Key Contact and have questions, or need assistance updating logos on any of your organization's websites, please contact the CAS Customer Center.

**Apply for the 2016 SciFinder Future Leaders Program!**  
Build your career, help shape the future of research information and attend one of the most respected scientific meetings in the world. [Apply for the 2016 SciFinder Future Leaders program by April 10!](#)

**A New Way to Explore Synthetic Preparations in SciFinder!**  
[Learn more about this new solution from CAS and try 5 free samples of MethodsNow today!](#)

**CHEMCATS Chemical Supplier Program**  
Chemical supplier? Be part of the world's preferred chemistry research solution. [Learn more now.](#)

**Introducing the PatentPak Interactive Patent Chemistry Viewer**  
The new PatentPak interactive patent chemistry viewer significantly reduces the time spent locating the important chemistry in a patent by using CAS scientists' direct links to key substances in the source patent.

**New Commercial Source Logos**  
You may notice supplier logos in [Commercial Sources Listings](#).

## What is SciFinder?

SciFinder<sup>®</sup> is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.

CAS is a division of the American Chemical Society

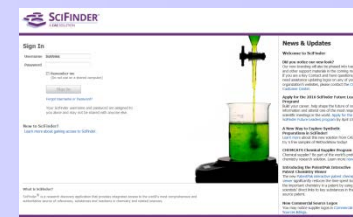
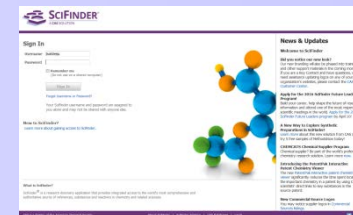
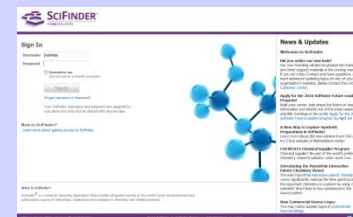
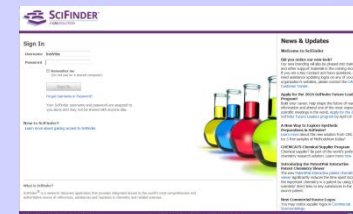
[About SciFinder](#) | [SciFinder Training](#) | [CAS Databases](#) | [Legal](#)



## Sign Out

Are you sure you want to sign out?

Abmeldung über  
Sign Out



# Registrierung bei CAS

**Dieser Link führt zur Registrierung bei CAS:**

Hier bitte den jeweiligen Link der Einrichtung eintragen!



Welcome to User Registration for SciFinder®

Click Next to begin registration

Next >>

Die fettgedruckten Felder müssen ausgefüllt werden.

Für Username und Password bitte keine Umlaute verwenden!

Bitte die Sicherheitsfrage und die Antwort darauf unbedingt notieren oder merken!

**Registration Information**

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?](#)

# Registrierung bei CAS (2)



## Registration Information

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

Password requirements:

- 7-15 characters
- Not too similar to the username
- Not too similar to the previous password
- Includes at least three of the following:
  - Lowercase letters
  - Uppercase letters
  - Numbers
  - Non-alphanumeric characters  
(Examples: @, #, %, &, \*)

Try again, or [contact us](#) for assistance.



## Almost Finished

Thank you for completing the initial step in registering to use SciFinder®!

You will receive an email message from CAS that includes a link and instructions for completing the registration process. ***You must click the link within 48 hours.*** If not, you will need to begin the registration process again.

Die **Registrierung** und die anschließende **Verifizierung** (nach Erhalt eines E-Mail-Links) müssen innerhalb von 48 h und **am selben PC** gemacht werden!



## 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>





# Benutzername oder Passwort vergessen?

Link auf der Startseite anklicken und den Anweisungen folgen...

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



### Sign In

Username

Password

Remember me  
(Do not use on a shared computer)

[Forgot Username or Password?](#)

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

**New to SciFinder?**  
[Learn more about gaining access to SciFinder.](#)



### Forgot Username or Password

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

#### Contact Information

Please provide one of the following:

Username:

Email:



### Forgot Username or Password

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

#### Security Information

Security Question: What is your favorite color?

Answer\*:  [Why?](#)



### Request Has Been Processed

You will receive an email message from CAS with instructions regarding your username and password.



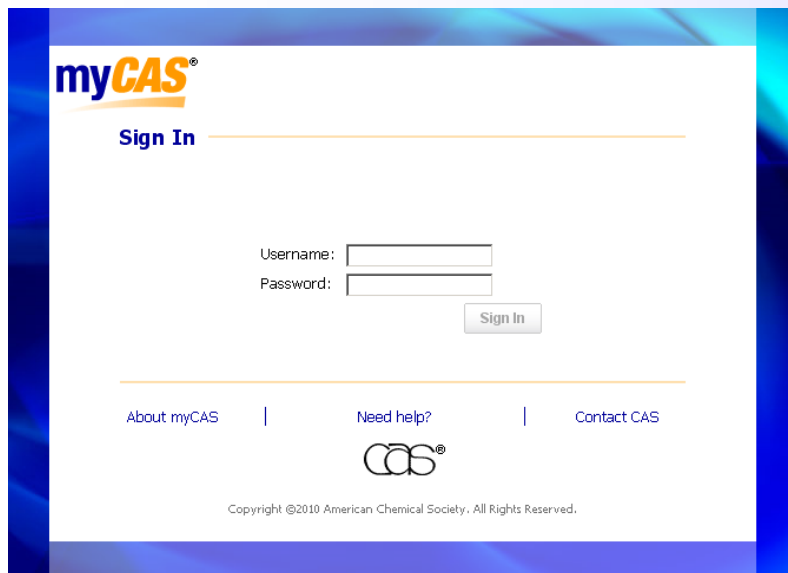
### Enter and confirm your new password

Password\*:

Re-enter Password\*:

# Benutzerdaten mit myCAS verwalten

<https://my.cas.org>



The image shows the myCAS Sign In page. It features the myCAS logo at the top left. Below the logo is a horizontal line with the text "Sign In" to its left. Underneath, there are two input fields: "Username:" and "Password:". To the right of the "Password:" field is a "Sign In" button. At the bottom of the page, there are three links: "About myCAS", "Need help?", and "Contact CAS". Below these links is the CAS logo and the text "Copyright ©2010 American Chemical Society. All Rights Reserved."

Mit dem Benutzernamen und dem Passwort für SciFinder kann man seine Benutzerdaten verwalten und z.B. das Passwort ändern.

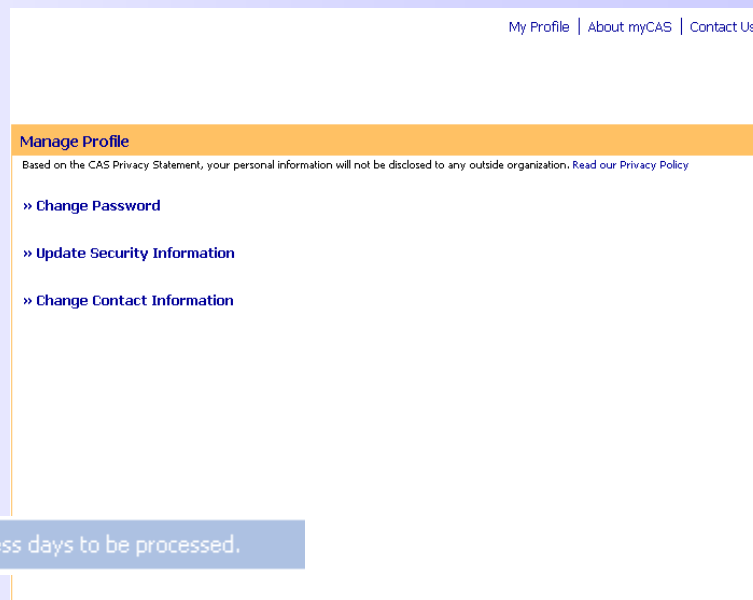


The image shows the myCAS Profile Details page. It features the myCAS logo at the top left. Below the logo is the text "Welcome SFoW Training | Sign Out". The page is divided into two main sections: "My Account" and "Profile Details". The "My Account" section is highlighted in orange and contains a link to "My Profile". The "Profile Details" section is also highlighted in orange and contains two sub-sections: "Personal Information" and "Contact Information".

Personal Information		
<b>Username:</b>	sfsweb110	
<b>First Name:</b>	SFoW	<a href="#">Edit</a>
<b>Last Name:</b>	Training	<a href="#">Edit</a>
<b>E-mail:</b>		<a href="#">Edit</a>

Contact Information		
<b>Company:</b>	CAS	
<b>Address:</b>	CAS SFoW Scholar Training 1	
<b>City:</b>	COLUMBUS	
<b>State/Region:</b>	OH	
<b>Country:</b>	US	
<b>Postal Code:</b>	43210	
<b>Phone Number:</b>		<a href="#">Edit</a>
<b>Fax Number:</b>		<a href="#">Edit</a>



The image shows the myCAS Manage Profile page. It features the myCAS logo at the top left. Below the logo is the text "My Profile | About myCAS | Contact Us". The page is divided into two main sections: "Manage Profile" and "Manage Profile". The "Manage Profile" section is highlighted in orange and contains a link to "Change Password". Below this link are two other links: "Update Security Information" and "Change Contact Information".


Based on the CAS Privacy Statement, your personal information will not be disclosed to any outside organization. [Read our Privacy Policy](#)

- [» Change Password](#)
- [» Update Security Information](#)
- [» Change Contact Information](#)

Your Change Contact Information request has been submitted and may take up to 2 business days to be processed.



# Timeout



Your session has ended due to inactivity. Sign in again to SciFinder.

### Sign In

Username

Password

Remember me  
(Do not use on a shared computer)

[Forgot Username or Password?](#)

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



## SciFinder Session Ended

Your session has ended due to inactivity.

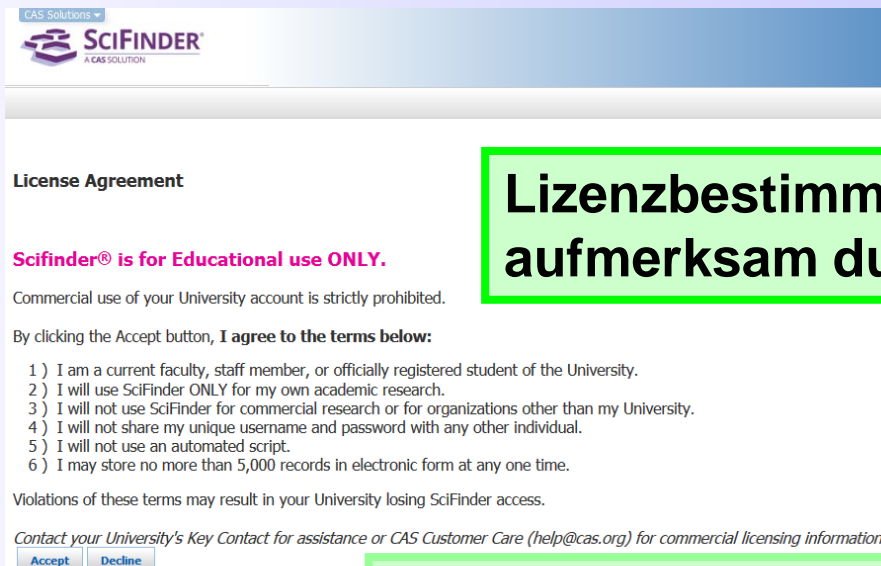
Wenn man bei **SciFinder** eingeloggt ist, aber einige Zeit nicht mit dem Programm arbeitet, dann erfolgt ein **Timeout**.



One Moment Please...

Please wait while we retrieve information on the document you've selected.

# Start der Suche / Einstellungen vor Recherchebeginn



Lizenzbestimmungen bitte aufmerksam durchlesen!

Die Einstellungen bleiben für den jeweiligen Nutzer permanent erhalten!



Research Topic "use of strophanthin" > references (307)

PREFERENCES

## Password and Account Information

Change password or account information (Opens in a new window)

## Keep Me Posted

Receive e-mail notification of Keep Me Posted results

Add or update e-mail address (Opens in a new window)

## My Commercial Sources

You have 0 preferred sources and 0 non-preferred sources.

[Review commercial source preferences](#)

## Remove Duplicate References

Automatically remove duplicate MEDLINE answers

If selected, response time may be affected.

## Starting Page

Select the default starting page:

- Explore References
- Explore Substances
- Explore Reactions

OK Cancel

## Voreinstellungen:

Man kann jederzeit sein Passwort ändern bei **Password and Account Information**.

Die Benachrichtigung per E-Mail für **Keep Me Posted-Ergebnisse** ist **voreingestellt**, man kann sie aber ausschalten.

Mit **My Commercial Sources** kann man sich bevorzugte Lieferanten auswählen.

Es kann das **automatische Entfernen von Duplikaten aus Medline** permanent eingestellt werden

Festlegen der zukünftigen **Startseite**.



# Stellen Sie die richtigen Fragen bei der Suche mit SciFinder „References/Research Topic“

Man kann in SciFinder (im Gegensatz zu anderen Datenbanken!) mit nahezu natürlichsprachigen Suchanfragen arbeiten.

## Recherchetipps:

- Thema in einzelne **Komponenten** (Hauptgedanken) zerlegen
- **Begriffe** durch **geeignete Präpositionen (of, in, with, by) trennen**.
- redundante und zu **allgemeine Worte** (wie z.B. **control, analysis, determination, examination, test, detection, search, study**) besser weglassen:  
**statt:** steroid analysis with hplc    **besser:** hplc of steroids
- mit einer mehr **allgemeinen/umfassenden Suche** starten und anschließend mit **Refine by** verfeinern
- (Eingeben weiterer oder speziellerer Suchworte)  
**Schrittweise Suchen!**



# Automatismen bei der Wortsuche in SciFinder

SciFinder sucht automatisch nach Synonymen, alternativen Schreibweisen, Pluralformen und verwendet

Trunkierungen:

- **Vorteile: einfach**
- **„Nachteile“: Kenntnisse der Regeln sind notwendig**

<b>Synonyme</b>	cancer, neoplasm, carcinoma, tumor, carcinogenesis
<b>Alternative Wortformen</b>	freeze, froze, frozen, freezing
<b>Irreguläre Pluralformen</b>	woman, women mice, mouse, mouses
<b>CAS Standard-abkürzungen</b>	oxidation, oxidn preparation, prep
<b>Amerikanische und britische Schreibweisen</b>	synthesize, synthesise color, colour
<b>Trunkierung bei bestimmten Wortstämmen</b>	Wörter mit mindestens 5 Buchstaben, die auf <b>-tion</b> enden: depletion = deple... Wörter mit der Nachsilbe (Suffix <b>-able, -ed, -ing</b> ): solvable = solv... Wörter, die mit <b>-e</b> enden: game = gam... (daraus wird dann z.B. gamma)



# Häufige Fehler bei Suche mit SciFinder

## „References/Research Topic“

- Beim Suchstart werden **zu spezielle Fragen** gestellt.
- **Zu viele Begriffe** (Konzepte) werden eingegeben.
- Nutzer kann die große Vielfalt der möglichen Suchworte für sein Suchthema nicht richtig einschätzen und sucht folglich nicht mit genügend Synonymen.
- **Adjektive in der Suchanfrage, die für mehrere Substantive gelten sollen, werden nur einmal eingegeben.**  
(falsch: *I am interested in chiral reduction or hydrogenation*)  
(richtig: *I am interested in chiral reduction or chiral hydrogenation*)
- **Suchworte werden mit AND verknüpft, obwohl eigentlich OR gemeint ist**  
(HPLC of steroids and alkaloids statt HPLC of steroids or alkaloids)
- Formulieren von Fragestellungen zu Patenten, Firmen, Zeiträumen, Dokumententypen schon bei der Start-Suchfrage  
(*I am interested in Patente zum Thema A von Autor B*)
- Zu frühes Einschränken “ anstatt bei großer Treffermenge mit **Analysis** bzw. **/Refine by** zu arbeiten

# Start einer thematischen Suche („References/Research Topic“) und „Advanced Search“

CAS Solutions

SCIFINDER<sup>®</sup>  
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "use of strophanthin" > references (307)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

REFERENCES: RESEARCH TOPIC ⓘ

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

Search

[Advanced Search](#)  Always Show

Publication Years

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

Document Types

<input type="checkbox"/> Biography	<input type="checkbox"/> Historical
<input type="checkbox"/> Book	<input type="checkbox"/> Journal
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Letter
<input type="checkbox"/> Commentary	<input type="checkbox"/> Patent
<input type="checkbox"/> Conference	<input type="checkbox"/> Preprint
<input type="checkbox"/> Dissertation	<input type="checkbox"/> Report
<input type="checkbox"/> Editorial	<input type="checkbox"/> Review

Languages

<input type="checkbox"/> Chinese	<input type="checkbox"/> Japanese
<input type="checkbox"/> English	<input type="checkbox"/> Polish
<input type="checkbox"/> French	<input type="checkbox"/> Russian
<input type="checkbox"/> German	<input type="checkbox"/> Spanish
<input type="checkbox"/> Italian	

Author

Last Name \*  First  Middle

Company

Examples:  
Minnesota Mining and Manufacturing  
DuPont

Das Logo fungiert gleichzeitig als Link zum Start einer neuen Suche.

Die Pfeiltasten des Browsers sollte man dagegen möglichst **nicht** benutzen!

Die Suche kann gleich am Anfang eingeschränkt werden.

Das wird allerdings als **Advanced Search** bezeichnet...

Mehrfachangaben sind möglich!



# Auswahl passender Konzepte

The screenshot shows the SciFinder interface with the search topic "modeling of the circadian clock...". The results are displayed in a table with columns for selection, description, and the number of references. The first row is highlighted in light blue and has a yellow box around the search phrase and a green box around the description. Below the table is a "Get References" button.

	References
<input type="checkbox"/> 19 references were found containing "modeling of the circadian clock" as entered.	19
<input type="checkbox"/> 1307 references were found containing the two concepts "modeling" and "circadian clock" closely associated with one another.	1307
<input type="checkbox"/> 4003 references were found where the two concepts "modeling" and "circadian clock" were present anywhere in the reference.	4003
<input type="checkbox"/> 7599335 references were found containing the concept "modeling".	7599335
<input type="checkbox"/> 18444 references were found containing the concept "circadian clock".	18444

**As entered:** eingegebene **Suchphrase** wurde genauso gefunden.

**Closely associated:** Suchworte kommen **in einem Satz zusammen** vor (enthält „as entered“) und sind **maximal 25 Wörter voneinander entfernt**.

**Anywhere in the reference:** Suchworte kommen **irgendwo** im Dokument vor (enthält „closely associated“).

# Trefferliste der Suche mit „Research Topic“

CAS Solutions | SCIFINDER | A CAS SOLUTION | Preferences | SciFinder Help | Sign Out | Access provided by FSU Jena | Welcome Ina Weiss

Explore | Saved Searches | SciPlanner | Save | Print | Export

Research Topic "glucosinolate in crop plant" > references (279)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | View Only CHEMZENT | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize | Sort by: Accession Number | Display Options

Analyze by: Author Name

Author Name	Count
Velasco Pablo	20
Cartea Maria Elena	19
Francisco Marta	10
Kirkegaard J A	6
Li Genyi	6
Wittstock Ute	6
Augustine Rehna	5
Bennett Richard N	5
Bisht Naveen C	5
Chen Sixue	5

2 of 279 Reference Selected

- Select All
- Deselect All
- Keep Selected
- Remove Selected

...s in the glucosinolate molecular network revealed by proteomics and metabolomics of Arabidopsis myb28/29 and cyp79B2/B3 glucosinolate mutants

...; Yoo, Mi-Jeong; Balmant, Kelly M.; Misra, Biswapriya B.; Dufresne, Craig; Abou-Hashem, Maged; Chen, Sixue; El-Domiaty, Maher (2016), 138, 1-19. | Language: English, Database: CAPLUS

...s in Brassicales are important for human health and plant defense against insects and pathogens. Here we investigate the proteomes and metabolomes of Arabidopsis myb28/29 and cyp79B2/B3 mutants deficient in aliph. glucosinolates and indolic glucosinolates, resp. Quant. proteomics of the myb28/29 and cyp79B2/B3 mutants led to the identification of 2785 proteins, of which 142 proteins showed significant changes in the two mutants compared to wild type (WT). By mapping the differential proteins using STRING, we detected 59 new edges in the glucosinolate metabolic network. These connections can be classified as primary with direct roles in glucosinolate metab., secondary related to plant stress responses, and tertiary involved in other biol. processes. Gene Ontol. anal. of the differential proteins showed high level of enrichment in the nodes belonging to metabolic process including glucosinolate biosynthesis and response to stimulus. Using metabolomics, we quantified 292 metabolites covering a broad spectrum of metabolic pathways, and 89 exhibited differential accumulation patterns between the mutants and WT. The changing metabolites (e.g.,  $\gamma$ -glutamyl amino acids, auxins and glucosinolate hydrolysis products) complement our proteomics findings. This study contributes toward engineering and breeding of glucosinolate profiles in plants in efforts to improve human health, crop quality and productivity. Glucosinolates in Brassicales constitute an important group of natural metabolites important for plant defense and human health. Its biosynthetic pathways and transcriptional regulation have been well-studied. Using Arabidopsis mutants of important genes in glucosinolate biosynthesis, quant. proteomics and metabolomics led to identification of many proteins and metabolites that are potentially related to glucosinolate metab. This study provides a comprehensive insight into the mol. networks of glucosinolate metab., and will facilitate efforts toward engineering and breeding of glucosinolate profiles for enhanced crop defense, and nutritional value.

2. Methodology for the determination of hormetic heat treatment of broccoli florets using hot humidified air: Temperature-time relationships

Quick View | Other Sources

By Duarte-Sierra, Arturo; Corcuff, Ronan; Arul, Joseph  
From Postharvest Biology and Technology (2016), 117, 118-124. | Language: English, Database: CAPLUS

Broccoli (*Brassica oleracea*) is one of the most consumed produce among Brassica crops because of its content in bioactive compds. such as glucosinolates and flavonoids. Preservation of this vegetable is a challenging task because of its rapid senescence, manifested as floret yellowing. In order to delay this undesirable aspect, several postharvest treatments have been explored including ... though heat treatments using arbitrary combinations of temp. and time have been found effective in slowing down the yellowing of broccoli florets, temp.-time variables for heat application. The objective of this work was to establish a temp.-time relationship using membrane electrolyte leakage ... oli florets were treated with hot humidified air at temps. from 32 to 52 °C for periods ranging from 5 to 1440 min. Electrolyte leakage was detd. by ... tems in 0.4 M mannitol soln. The percentage of electrolyte leakage increased with exposure time at each temp. test following zero order kinetics. The ... t the Arrhenius plot showed a clear broken linear pattern with a break with a transition or crit. temp. zone of 42-45 °C. Although equiv. times for ... kinetics of electrolyte leakage, the selection of treatment temp. needed to be below 42 °C, where the florets stored at 10 °C/95% RH for 10 days, ... sence without causing excessive anaerobic conditions and/or tissue damage. Heat treatment of florets at temps. in the crit. zone led to excessive ... spiration, while treatments with temps. above the crit. zone (>45 °C) led to severe anaerobic conditions as well as tissue damage, despite enhanced ... ps. above 42 °C. Heat treatment at 41 °C for 180 min as hormetic heat dose for broccoli florets is suggested. The results of this work suggest that ... sideration for heat treatment of fresh produce.

...aracterization of Brassica crops grown with different fertilizer application

...shinano, Takuro; Oka, Norikuni  
...ish, Database: CAPLUS

Show More

Mit Keep Selected kann man sich eine Trefferliste mit ausgewählten Dokumenten erstellen.

# Trefferliste (2)

CAS Solutions | SciFINDER<sup>®</sup> A CAS SOLUTION | Preferences | SciFinder Help | Sign Out

Access provided by FSU Jena  
Welcome Ina Weiss

Explore | Saved Searches | SciPlanner | Save | Print | Export

660 duplicates were automatically removed.

Research Topic "nano cellulose (nanocellulose)" with limiters > references (5913)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | View Only CHEMZENT | Tools | Create Keep Me Posted Alert | **Send to SciPlanner**

Analyze | Refine | Categorize

Sort by: Accession Number | 0 of 5913 References Selected

Analyze by: Author Name

Bras Julien	37
Rojas Orlando J	37
Isogai Akira	34
Oksman Kristina	27
Saito Tsuguyuki	25
Liu Yong	23
Park Jong Cheol	23
Dufresne Alain	20
Mathew Aji P	20
Tammelin Tekla	20

Show More

1. **Preparation of dialdehyde cellulose nanocrystal as an adsorbent for creatinine**  
Quick View | Other Sources  
By Huang, Rjin; Liu, Zehua; Sun, Bo; Fatehi, Pedram  
From Canadian Journal of Chemical Engineering (2016), Ahead of Print. | Language: English, Database: CAPLUS

In this work, dialdehyde cellulose nanocrystals (DCNCs) were prepd. via oxidizing cellulose nanocrystals (CNCs) with sodium permanganate. The results showed that the adsorption capacity of DCNCs increased with the increase in its aldehyde content. The results revealed that the adsorption isotherm of DCNCs agreed with the Freundlich process followed a second-order kinetic model. Overall, the max. adsorption of creatinine on DCNCs (with 4.41 mmol/g aldehyde under the adsorption conditions of 100 mg/L initial creatinine concn., 8 h treatment time, and pH 7. The results suggest that the dialdehyde cellulose nanocrystal is a promising adsorbent for creatinine to treat chronic renal failure.

2. **Preparation of a visual pH-sensing film based on tara gum incorporating cellulose and extracts from grape skins**  
Quick View | Other Sources  
By Ma, Qianyun; Wang, Lijuan  
From Sensors and Actuators, B: Chemical (2016), Ahead of Print. | Language: English, Database: CAPLUS

Exts. from grape skins (EGS) were incorporated into tara gum (TG)/cellulose nanocrystal (CNC) matrix to prep. a colorimetric pH-sensing film. The UV-vis spectra of EGS in the pH range of 1-10 were studied and the color clearly changed from bright red to dark green. Fourier transform-IR spectroscopy, SEM and thermal anal. were used to characterize TG/CNC/EGS films, and the effects of EGS addn. on mech. properties, oxygen permeability and optical properties were also tested. The results revealed that EGS was successfully introduced into the TG/CNC matrix without obvious interactions. The EGS addn. decreased the compact and continuous structure, thermal stability and barrier properties of the films. With EGS addn. from 0 to 15 g/100 g TG, the tensile strength and light transmittance of films gradually decreased from 65.50 to 44.32 MPa and from 65.11 to 41.71% at 660 nm, resp.; however, the elongation at break of films increased significantly from 30.10 to 54.80%. The films were also immersed in different buffers to evaluate the response to pH changes. The color range of TG/CNC/EGS film varied from red (in acid pH) to slightly green (in alkali pH). The pH-sensing film was also evaluated by an activation test on milk, with evident change in the coloration of the film, indicating that the film could be applied in food packaging for information concerning the packaged food.

3. **Genipin cross-linked antimicrobial nanocomposite films and gamma irradiation to prevent the surface growth of bacteria in fresh meats**  
Quick View | Other Sources  
By Khan, Avik; Gallah, Hejer; Riedl, Bernard; Bouchard, Jean; Safrany, Agnes; Lacroix, Marie-Claude  
From Innovative Food Science & Emerging Technologies (2016), Ahead of Print. | Language: English, Database: CAPLUS

A 125 µg/mL of nisin and 30 mM of disodium ethylenediaminetetraacetate (EDTA) were immobilized on the surface of the nanocrystal (CNC)/chitosan nanocomposite films by using genipin as cross-linker. The films were evaluated for antimicrobial activity against Listeria monocytogenes and Escherichia coli. The films showed good antimicrobial activity and stability during storage at 37 °C for 14 days. The films restricted the growth of L. monocytogenes and E. coli for more than 5 wk. The films were also evaluated for their stability in simulated gastric juice. The results showed that the films were responsible for the reduction of bacterial growth in fresh meats, and that the films could be applied in food packaging for information concerning foodborne illness.

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REFERENCE DETAIL | Get Related Citations | Link to Other Sources | Send to SciPlanner

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## 12. Nanocomposites of PBAT and cellulose nanocrystals modified by "in situ" polymerization and melt extrusion

By: Morelli, Carolina L.; Belgacem, Mohamed N.; Branciforti, Marcia C.; Salon, Marie C. B.; Bras, Julien; Bretas, Rosario E. S.

Cellulose nanocrystals (CNC) were successfully grafted with a low mol. wt. poly(butylene glutarate) through an "in situ" polymn. procedure. The grafting treatment decreased the CNC hydrophilic character and increased the onset of their thermal degridn. by approx. 20°C, thus increasing the possibilities of CNC application. Composites of grafted and nongrafted CNC with a poly(butylene-adipate-co-terephthalate) (PBAT) matrix were prepd. by melt extrusion. The CNC addn. led to an increase of 50% of the tensile elastic modulus of the PBAT. In addn., dynamic mech. thermal anal. showed that the composite with CNC retained its high modulus even at temps. far above the glass transition temp. of PBAT. At 60°C the storage modulus of the composite with CNC was approx. 200% higher than that of the pure PBAT. Thus, in this work, nanocomposites of improved properties were obtained through a combination of "in situ" polymn. and melt extrusion. POLYM. ENG. SCI., 2016. © 2016 Society of Plastics Engineers.

Indexing  
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# Dubletteneliminierung - Remove Duplicates:automatisch

Dubletteneliminierung als Voreinstellung bei Preferences:

## Remove Duplicate References

Automatically remove duplicate MEDLINE answers

If selected, response time may be affected.

The screenshot displays the SciFinder interface. At the top left, the SciFinder logo is visible. Below it, a notification box states: "10 duplicates were automatically removed". A central pop-up window provides details: "Candidates Selected: 307 references were found containing the two concepts 'use' and 'strophanthin' closely associated with one another. Automatically removed 10 duplicate MEDLINE answer(s). Answer set 2 created with 153 answers from CAPLUS and 144 answers from MEDLINE". The main interface shows a search for "Research Topic 'use of strophanthin' > references (297)". The "REFERENCES" section is active, with a toolbar containing options like "Get Substances", "Get Reactions", "Get Related Citations", "Get Full Text", and "Tools". The results are sorted by "Accession Number" and show 0 of 297 references selected. The first three results are:

- 1. Personalized Chemotherapy Profiling Using Cancer Cell Lines from Selectable Mice**  
By Kamiyama, Hirohiko; Rauenzahn, Sherri; Shim, Joong Sup; Karikari, Collins A.; Feldmann, Georg; Hua, Li; Kamiyama, Mihoko; Schuler, F. William; Lin, Ming-Tseh; Beaty, Robert M.; et al  
From Clinical Cancer Research (2013), 19(5), 1139-1146. | Language: English, Database: CAPLUS  
Purpose: High-throughput chemosensitivity testing of low-passage cancer cell lines can be **used** to prioritize agents for personalized chemotherapy. However, generating cell lines from primary cancers is difficult because contaminating stromal cells overgrow the malignant cells. Exptl. Design: We produced a series of hypoxanthine phosphoribosyl transferase (hprt)-null immunodeficient mice. During growth of human cancers in these mice, hprt-null murine stromal cells replace their human counterparts. Results: Pancreatic and ovarian cancers explanted from these mice were grown in selection media to produce pure human cancer cell lines. We screened one cell line with a 3,131-drug panel and identified 77 U.S. Food and Drug Administration (FDA)-approved drugs with activity, and two novel drugs to which the cell line was uniquely sensitive. Xenografts of this carcinoma were selectively responsive to both drugs. Conclusion: Chemotherapy can be personalized **using** patient-specific cell lines derived in biochem. selectable mice. Clin Cancer Res; 19(5); 1139-46. ©2012 AACR.
- 2. Treatment of hyperproliferative disorders using cardiac glycosides**  
By Oronsky, Bryan T.; Langecker, Peter  
From PCT Int. Appl. (2010), WO 2010036973 A1 20100401. | Language: English, Database: CAPLUS  
Provided are methods and compns. for treating and preventing hyperproliferative disorders such as psoriasis by administration of a cardiac glycoside alone or in combination locally or systemically with a calciotropic agents and/or a diffusion-limiting component, such as vasoconstrictor or collagen barrier. A patient with severe psoriasis was treated with digoxin and vitamin D.
- 3. Antiarrhythmic medicinal preparation prepared from blood-red hawthorn, nettle and lily-of-the-valley**  
By Bogdarin, Yuri A.; Orlova, Natalya A.  
From Russ. (1997), RU 21000401.1  
An antiarrhythmic preparation for preventing development of arrhythmia consists of extract of blood-red hawthorn, nettle and lily-of-the-valley.

The bottom of the screenshot is overlaid with a text box containing the following text:

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# Dubletteneliminierung - Remove Duplicates: manuell

The screenshot shows the SciFinder interface. At the top, there's a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. Below that, a search topic is displayed: 'Research Topic "nano cellulose (nanocellulose)..." with limiters > references (2102) > Nanocomposites of PBAT and cel...'. The main area has a 'REFERENCES' section with various tools like 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'View Only CHEMZENT'. A 'Tools' dropdown menu is open, showing options: 'Remove Duplicates', 'Combine Answer Sets', and 'Add Tag'. The 'Remove Duplicates' option is highlighted. Below the menu, it says 'Sort by: Accession Number' and '0 of 2102 References Selected'.

The screenshot shows the SciFinder interface with a notification message highlighted in a green box. The message reads: '259 duplicates were removed. To remove duplicates automatically, visit Preferences.' The notification is located below the navigation bar and above the main content area.

- Entfernung doppelter Treffer bei den Textstellennachweisen.
- Doppelte Einträge in den Antwortsätzen können bei **bis zu 10000 Dokumenten** entfernt werden.

Auch bei „**Keep Me Posted**“ können Dubletten vermieden werden.

The screenshot shows the 'Edit Keep Me Posted Profile' form. The form has a title field with the value 'nanocellulose'. Below it is a description field. The status is set to 'Enabled'. The duration is 'Expires On: Jan 28, 2014'. The frequency is 'Send updates once every Week'. A checkbox labeled 'Exclude previously retrieved references.' is checked. The form also shows 'Characters Remaining: 1024' and buttons for 'Edit' and 'Cancel'.

# Trefferliste: Ansichtsmöglichkeit „Quick View“

## 18. Characterization and Application of Nanostructured Films Containing Au and TiO<sub>2</sub> Nanoparticles Supported in Bacterial Cellulose

Quick View

Other Sources

By Dal'Acqua, Nicolle; Mattos, Alessandra Batista de; Krindges, Israel; Pereira, Marcelo Barbalho; Barud, Hernane da Silva; Ribeiro, Sidney Jose Lima; Duarte, Gian Carlos Silva; Radtke, Claudio; Almeida, Luciano Costa; Giovanela, Marcelo; et al  
From Journal of Physical Chemistry C (2015), 119(1), 340-349. | Language: English, Database: CAPLUS

### Quick View

#### Characterization and Application of Nanostructured Films Containing Au and TiO<sub>2</sub> Nanoparticles Supported in Bacterial Cellulose

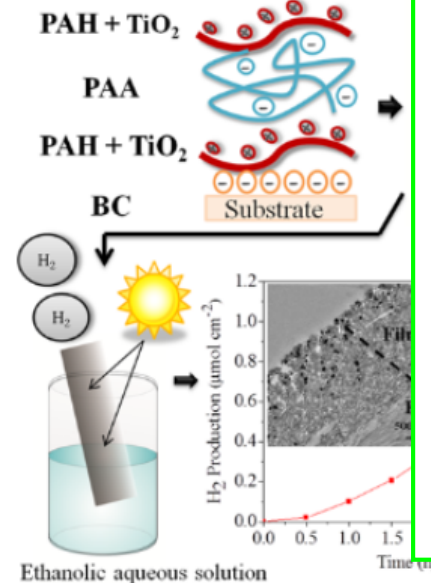
Other Sources

By Dal'Acqua, Nicolle; Mattos, Alessandra Batista de; Krindges, Israel; Pereira, Marcelo Barbalho; Barud, Hernane da Silva; Ribeiro, Sidney Jose Lima; Duarte, Gian Carlos Silva; Radtke, Claudio; Almeida, Luciano Costa; Giovanela, Marcelo; et al  
From Journal of Physical Chemistry C (2015), 119(1), 340-349. | Language: English, Database: CAPLUS

In the last several years, the use of renewable energy sources has increased; consequently, the no. of studies regarding their efficiency has also increased. It is well known that fossil and at. fuels will not last forever and that their use contributes to environmental pollution. Thus, nanostructured thin films have attracted attention due to numerous applications, including construction of photovoltaic energy generating and photoluminescence materials. Therefore, in this study, we prepd. and characterized thin films supported on bacterial cellulose that were produced using the layer-by-layer (LbL) technique. The weak polyelectrolytes, such as poly(allylamine hydrochloride) (PAH) and poly(acrylic acid) (PAA), combined with titanium dioxide (TiO<sub>2</sub>) and gold nanoparticles (Au NPs) were used to produce flexible devices capable of producing hydrogen gas (H<sub>2</sub>) by photocatalysis. The presence of the Au NPs and TiO<sub>2</sub> in the films was confirmed using UV-vis spectroscopy, Rutherford backscattering spectrometry, and X-ray diffraction. SEM was used to evaluate the surface morphol. of the films, and the distribution and av. size of the Au NPs were analyzed using transmission electron microscopy, which revealed sizes in the nanometer range. Finally, the thin films were analyzed using gas chromatog. to evaluate the H<sub>2</sub> prodn. by photocatalysis. Overall, the system with (PAH + TiO<sub>2</sub>) and PAA solns. at pH = 4.0 in the presence of gold salt that were reduced with UV light were more efficient due to their greater interactions with the TiO<sub>2</sub> during multilayer deposition.

Reference Images

Substance Images



Images

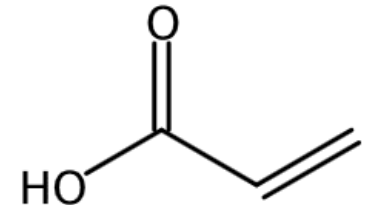
Substance Images

(acrylic acid)

1 2 3 4

79-10-7

C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>



## Was bedeuten „cf. preceding abstr.“ bzw. „cf. following abstr.“?

- Diese Aussagen beziehen sich auf die gedruckten Chemical Abstracts.
- cf.: von confer (lat.)= compare, vergleiche

### AN 1971:136574

#### 1. Combined mutagenic action of ethylenimine and EDTA. 2. Horse bean generations M2 and M3

[Quick View](#) [Other Sources](#)

By Rancelis, V.; Luksa, R.

From Lietuvos TSR Aukstuju Mokyklu Mokslo Darbai, Biologija (1969), 9, 189-203. | Language: Russian, Database: CAPLUS

Seeds of the M1 generation of the broad bean plants (cf. preceding abstr.) were germinated and grown sep. The M2 generation seeds were similarly selected, germinated, and grown for 2 months. The seed treatment with ethylenimine and (or) di-Na EDTA induced qual. as well as quant. chlorophyll mutations in the M2 generation plants. With application of both compds., the chlorophyll mutation frequency considerably increased in plants of the M3 generation. The M2 generation plants consisted of albina, Xantha, chlorina, and variegata mutants, whereas plants of the M3 generation consisted also of viridis, and chloronervis types. Many other mutations were obsd. in the M3 generation plants. EDTA may delay the appearance of mutants in the M2 generation.

### AN 1971:136573

#### 1. Combined mutagenic action of ethylenimine and EDTA. 1. Modification of the spectrum of chromosome aberrations in the root tips of horse beans

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
By Rancelis, V.; Baskakovaite, A.

From Lietuvos TSR Aukstuju Mokyklu Mokslo Darbai, Biologija (1969), 9, 177-88. | Language: Russian, Database: CAPLUS




Vicia faba (broad bean) seeds were soaked in 0.02 or 0.04% ethylenimine (I) and 0.20 or 0.02% di-Na EDTA for 15 hr, sep. or combined. After washing thoroughly with distd. H<sub>2</sub>O, they were grown in Koch flasks at 25°. The 1.6 cm rootlets of germinating seeds were fixed with HOAc-EtOH (1:3), 59, 69, 86, 111, 134, and 158 hr after planting, for cytol. anal. [V. N. Yurtsev method (1961)]. I and EDTA considerably decreased the mitotic activity of the cells, and increased the frequency of chromosome aberrations during anaphase and early telophase. In seeds germinating slowly, such aberrations were much less frequent. I induced more sep. and pair fragments, whereas EDTA formed chromosome aberrations. Simultaneous application of the compds. considerably increased the frequency of bridges owing to the EDTA capability to intensify restoration. The relinkage of the broken ends of chromosomes was done in the presence of EDTA, which removed di- and trivalent metals ions from them.




# Reference Details: In process



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REFERENCE DETAIL    

## 2. MWCNTs-like protection layer formation on bacterial cellulose bundles as a potential material for suspended resonator

Yin Tung Lee; Xing Qiu; Pun To Yung

Suspended carbon nanotubes (CNTs) resonator is a sensitive detector for chemical and biological applications. Small sizes of CNTs can enhance sensitivity, but increase complexity for fabrication. In order to overcome the challenges, a novel technique has been developed to produce a long, sensitive and high tensile strength carbon nanotubes (CNT) coated bacterial cellulose (BC) bundle. This study demonstrates the use of ultrasonication to perform carboxyl functionalized multi-walled carbon nanotubes (MWCNTs-COOH) self-assembling on the surface of BC bundles (BC/MWCNTs) via hydrogen bonds. Ultrasonication can disrupt dense cellulose network and produce the long BC/MWCNTs bundles ranging from 30 to 100 μm. Raman spectroscopy shows a drop at peak of hydroxyl (-OH, 3700 m(-1)) and carbonyl (C=O, 1600 cm(-1)). This indicates the formation of the continuous MWCNTs-like protection layer on BC surface. Electrical properties of the BC/MWCNTs bundles showed linearity from -6 V to +6 V. Composites with BC treated by higher ultrasonic powers, 100 W, show higher conductivity comparing to 80 W. Sensitivity from 10(-7) to 10(-9) A of long BC/MWCNTs composite bundles is reported in this paper. This technique may be competitive to the current state of carbon nanotubes resonator.

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
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# Zitierungen in Medline-Einträgen

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**Molecular characterization of a novel Ljungan virus (Parechovirus; Picornaviridae) reveals a fourth genotype and indicates ancestral recombination**

Toll Conny; Gullberg Maria; Johansson E Susanne; Tebb Robert B; Andersson Bjorn; Lindberg A Michael

Ljungan virus (LV) was discovered 20 years ago in Swedish bank voles (*Myodes glareolus*, previously referred to as *Clethrionomys glareolus*) during the search for an infectious agent causing lethal myocarditis in young athletes. To date, the genomes of four LV isolates, including the prototype 87-012 strain, have been characterized. Three of these LV strains were isolated from bank voles trapped in Sweden. Sequence analysis of an American virus (M1146), isolated from a montane vole (*Microtus montanus*) in western USA, indicates that this strain represents a genotype that is different from the Swedish strains. Here, we present genomic analyses of a fifth LV strain (64-7855) isolated from a southern red-backed vole (*Myodes gapperi*) trapped during arbovirus studies in New York state in the north-eastern USA in the 1960s. Sequence analysis of the 64-7855 genome showed an LV-like genome organization and sequence similarity to other LV strains. Genetic and phylogenetic analyses of the evolutionary relationship between the 64-7855 strain and other viruses within the family Picornaviridae, including previously published LV strains, demonstrated that the 64-7855 strain constitutes a new genotype within the LV species. Analyses also showed that different regions of the 64-7855 genome have different phylogenetic relationships with other LV strains, indicating that previous recombination events have been involved in the evolution of this virus.

Indexing

Concepts

Check Tags:

3' Untranslated Regions: OL, chemistry  
5' Untranslated Regions: GE, genetics  
Arvicolinae: VL, virology  
Evolution, Molecular  
Molecular Sequence Data  
Parechovirus: CL, classification  
Parechovirus: 3' Untranslated Regions: GE, genetics  
Phylogeny  
Picornaviridae Infections: VL, virology  
Recombination, Genetic  
Sequence Analysis, DNA

Substances

Chemical Names

3' Untranslated Regions: OL, chemistry  
5' Untranslated Regions: GE, genetics  
Arvicolinae: VL, virology  
Evolution, Molecular  
Molecular Sequence Data  
Parechovirus: CL, classification  
Parechovirus: 3' Untranslated Regions: GE, genetics  
Picornaviridae Infections: VL, virology  
Polymerase: GE, genetics  
Rodent Diseases: VL, virology  
Sequence Analysis, DNA

Other Sources

GENBANK:EU854568

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ACCESSION NUMBER

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PubMed ID: 19264646  
MEDLINE

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- 34) Lindberg, A Michael; *J Gen Virol* 2003, 84, 1223
- 35) Martin, D P; *AIDS Res Hum Retroviruses* 2005, 21, 98
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- 37) Mathews, David H; *J Mol Biol* 2002, 317, 191
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1 Gen Virol. 2009 Apr;80(4):845-53. Epub 2009 Mar 4.

**Molecular characterization of a novel Ljungan virus (Parechovirus; Picornaviridae) reveals a fourth genotype and indicates ancestral recombination.**

Toll C, Gullberg M, Johansson ES, Tebb RB, Andersson B, Lindberg AM

School of Pure and Applied Natural Sciences, University of Kalmar, SE-39182 Kalmar, Sweden.

**Abstract**

Ljungan virus (LV) was discovered 20 years ago in Swedish bank voles (*Myodes glareolus*, previously referred to as *Clethrionomys glareolus*) during the search for an infectious agent causing lethal myocarditis in young athletes. To date, the genomes of four LV isolates, including the prototype 87-012 strain, have been characterized. Three of these LV strains were isolated from bank voles trapped in Sweden. Sequence analysis of an American virus (M1146), isolated from a montane vole (*Microtus montanus*) in western USA, indicates that this strain represents a genotype that is different from the Swedish strains. Here, we present genomic analyses of a fifth LV strain (64-7855) isolated from a southern red-backed vole (*Myodes gapperi*) trapped during arbovirus studies in New York state in the north-eastern USA in the 1960s. Sequence analysis of the 64-7855 genome showed an LV-like genome organization and sequence similarity to other LV strains. Genetic and phylogenetic analyses of the evolutionary relationship between the 64-7855 strain and other viruses within the family Picornaviridae, including previously published LV strains, demonstrated that the 64-7855 strain constitutes a new genotype within the LV species. Analyses also showed that different regions of the 64-7855 genome have different phylogenetic relationships with other LV strains, indicating that previous recombination events have been involved in the evolution of this virus.

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Molecular characterization of M1146, an American isolate of Ljungan virus [J Gen Virol. 2003]

Molecular analysis of three Ljungan virus isolates reveals a new, blue-toe [J Virol. 2002]

Molecular characterization of a Canadian human parechovirus (HPeV)-3 isolate [J Med Virol. 2005]

Ljungan virus detected in bank voles (*Myodes glareolus*) and yellow-necked mice (*Peromyscus leucopus*) [Virus Res. 2006]

Identification of a contemporary human parechovirus type 1 by whole-genome sequencing [J Virol. 2008]

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## 1. Metabolic control analysis

By: Fell, David A.

A review. Metabolic Control Anal. (MCA) is a theor. fram metabolic systems to the kinetic characteristics of the co some of which is generic and is reviewed here. It is arg integrative biol. and the linking of genome to phenotype.

Eine Thematische Suche mit dem Index Term Metabolic Pathways

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Page: 1 of 104

1. **Manufacture of myo-inositol and myo-inositol derivative with recombinant microorganism**

By Konishi, Kazunobu; Imazu, Shinichi; Sato, Mayumi  
From PCT Int. Appl. (2013), WO 2013073483 A1 20130523. | Language: Japanese, Database: CAPLUS

[Problem] To impart significantly improved myo-inositol producing capability, suitable for use in recombinant DNA techniques and synthetic biol. methods, to a host microorganism that does not possess an endogenous myo-inositol biosynthesis pathway, such as Escherichia coli. [Soln.] Inositol monophosphatase activity is strengthened in a transformant obtained by introducing a myo-inositol biosynthesis pathway into a host microorganism that does not possess an endogenous myo-inositol biosynthesis pathway.

2. **Recombinant microorganism capable of fixing carbon dioxides and method for preparing useful material using same**

By Lee, Sang-Yuop; Jang, Yu-Sin; Im, Jung-Ae  
From PCT Int. Appl. (2013), WO 2013073860 A1 20130523. | Language: Korean, Database: CAPLUS

The present invention relates to a recombinant microorganism having genes introduced therein to code an acetyl-CoA synthases/carbon monoxide dehydrogenase complex (ACS/CODH) involved in a Wood-Ljungdahl pathway. The recombinant microorganism according to the present invention is capable of fixing carbon dioxides, and therefore is effective in producing useful material such as alc. and org. acid at high concns. and a high yield rate from CO2.



3. **Label-free quantitative proteomics of the lysine acetylome in mitochondria identifies substrates of SIRT3 in metabolic pathways**

By Rardin, Matthew J.; Newman, John C.; Held, Jason M.; Cusack, Michael P.; Sorensen, Dylan J.; Li, Biao; Schilling, Birgit; Mooney, Sean D.; Kahn, C. Ronald; Verdin, Eric; et al  
From Proceedings of the National Academy of Sciences of the United States of America (2013), 110(16), 6601-6606, S6601/1-56601/7. | Language: English, Database: CAPLUS

Large-scale proteomic approaches have identified numerous mitochondrial acetylated proteins; however in most cases, their regulation by acetyltransferases and deacetylases remains unclear. Sirtuin 3 (SIRT3) is an NAD+-dependent mitochondrial protein deacetylase that has been shown to regulate a limited no. of enzymes in key metabolic pathways. Here, we use a rigorous label-free quant. MS approach (called MS1 Filtering) to analyze changes in lysine acetylation from mouse liver mitochondria in the absence of SIRT3. Among 483 proteins, a total of 2,182 unique sites of lysine acetylation were identified after affinity

Concepts

Enzyme kinetics  
Metabolic pathways

Genome  
Phenotypes

application of metabolic control anal. in control and regulation of metab

Enzymes, biological studies

application of metabolic control anal. in control and regulation of metab

Biological study, unclassified; Biological study

Supplementary Terms

review metabolic control analysis enzyme kinetics

Citations

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- HISTORY:**
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  - Explore results
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  - Detailed display from Answer set 1 of Molecular characterization of a novel Ljungan virus (Parechovirus; Picornaviridae) reveals a fourth genotype and indicates ancestral recombination
  - Explore references by research topic metabolic control analysis initiated, resulting in 2 candidates (May 31, 2013 2:47 AM)
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  - Detailed display from Answer set 2 of Metabolic control analysis
  - Explore references by index term: Metabolic pathways initiated (May 31, 2013 2:50 AM)
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  - May 30 2013, 06:04 AM
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  - May 30 2013, 03:54 AM
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  - May 30 2013, 03:22 AM
  - May 30 2013, 03:14 AM
  - May 30 2013, 03:13 AM

**History:** Ausführlicher Überblick über alle Aktivitäten im Laufe der **gegenwärtigen** Suchsession

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# Zugriffe auf Volltexte in SciFinder

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1. **Metabolic control analysis** Quick View **Other Sources**  
By Fell, David A.  
From Topics in Current Genetics (2005), 13(Systems Biology), 69-80. | Language: English, Database: CAPLUS

A review. **Metabolic Control Anal.** (MCA) is a theor. framework for investigating and understanding **control** and regulation of metab. In particular, it relates the properties of **metabolic** systems to the kinetic characteristics of the component enzymes. However, not all of the properties of enzymes strongly influence the behavior of **metabolic** systems, some of which is generic and is reviewed here. It is argued that MCA is an important component of systems biol. that still has much to offer in the development of predictive and integrative biol. and the linking of genome to phenotype.

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**Optimization-Based Metabolic Control Analysis**  
Korkut Uygun, Basak Uygun, Howard W. T. Matthew, and Yinfun Huang  
Dept. of Chemical Engineering and Materials Science, Wayne State University, Detroit, MI 48202

DOI 10.1002/hprr.482  
Published online October 22, 2010 in Wiley Online Library (wileyonlinelibrary.com).

*In this work, a novel optimization-based metabolic control analysis (OMCA) method is introduced for reducing data requirement for metabolic control analysis (MCA). It is postulated that using the optimal control approach, the fluxes in a metabolic network are correlated to metabolite concentrations and enzyme activities as a state-feedback control system that is optimal with respect to a homeostasis objective. It is then shown that the optimal feedback gains are directly related to the elasticity coefficients (ECs) of MCA. This approach requires determination of the relative "importance" of metabolites and fluxes for the system, which is possible with significantly reduced experimental data, as compared with typical MCA requirements. The OMCA approach is applied to a top-down control model of glycolysis in hepatocytes. It is statistically demonstrated that the OMCA model is capable of predicting the ECs observed experimentally with few exceptions. Further, an OMCA-based model reconciliation study shows that the modification of four assumed stoichiometric coefficients in the model can explain most of the discrepancies, with the exception of elasticities with respect to the NADH/NAD ratio. © 2010 American Institute of Chemical Engineers Biotechnol. Prog., 26: 1567–1579, 2010*

Keywords: elasticity coefficients, optimal control, metabolic flux analysis, dynamic flux balance, metabolic homeostasis assumption, in silico models

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1. **Comprehensive profiling of the complex dendrimeric contrast agent Gadomer using a combined approach of CE, MS, and CE-MS**  
By Vetterlein, Kai; Bergmann, Ulf; Bueche, Karlo; Walker, Martina; Lehmann, Jochen; Linscheid, Michael W.; Scriba, Gerhard K. E.; **Hildebrand, Michael**  
From *Electrophoresis* (2007) 28(17) 2989-2999. | Language: English. Database: CAPLUS

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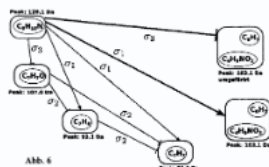
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1. Method for the identification of unknown substances by mass spectrometry

By Boecker, Sebastian; Scheubert, Kerstin; Rasche, Florian; Hufsky, Franziska  
From PCT Int. Appl. (2012), WO 2012126451 A2 20120927. | Language: German, Database: CAPLUS



A method for the identification of unknown substances by mass spectrometry includes the following steps: (a) recording at least two mass spectrometric fragmentation spectra (daughter ion spectra) for the substance to be identified, (b) detn. of a spectrum graph of the substance from the at least two mass spectrometric fragmentation spectra by calcg. possible sum formulas for the measured masses, detg. a derivation relation between these sum formulas, and evaluating the direct, as well as the indirect derivation relations on the basis of the mass intensities of the peaks in the spectrum, (c) detg. an optimal fragmentation graph of the substance by selecting the most likely relations from the relation pool under consideration of the evaluation, and (d) comparing the data of the complete or partial fragmentation graph chem. properties.

2. Method for the identification of unknown substances by mass spec

By Boecker, Sebastian; Scheubert, Kerstin; Rasche, Florian; Hufsky, Franziska  
From Ger. Offen. (2012), DE 102011014805 A1 20120920. | Language: German, Datab

A method for the identification of unknown substances by mass spe fragmentation spectra (daughter ion spectra) for the substance to be spectrometric fragmentation spectra by calcg. possible sum formulas; evaluating the direct, as well as the indirect derivation relations on fragmentation graph of the substance by selecting the most likely relat data of the complete or partial fragmentation graph with ref. data to ide

3. Method for identifying unknown substances by mass spectrometry

By Boecker, Sebastian; Rasche, Florian; Zichner, Thomas  
From PCT Int. Appl. (2010), WO 2010083811 A1 20100729. | Language: German, Datab

A method for the identification of unknown substances by mass spe fragmentation spectrum (daughter ion spectrum) of the substance to b spectrometric fragmentation spectrum, whereby the fragments of the s links in the fragmentation graph, and (c) comparing the data of the con structure, substance class, and/or chem. properties. The fragmenta tandem mass spectrometer. The fragmentation spectrum is produced A sepn. process by chromatog. or capillary electrophoresis is carried o

4. Method for identifying unknown substances by mass spectrometry

By Boecker, Sebastian; Rasche, Florian; Zichner, Thomas  
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A method for the identification of unknown substances by mass spe fragmentation spectrum (daughter ion spectrum) of the substance to b spectrometric fragmentation spectrum, whereby the fragments of the s

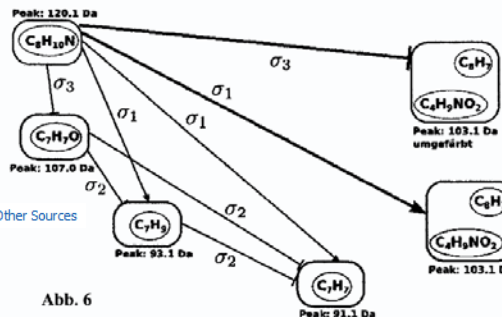


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1. Method for the identification of unknown substances by mass spectrometry

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Assignee: Germany

A method for the identification of unknown substances by mass spectrometry includes the following steps: (a) recording at least two mass spectrometric fragmentation spectra (daughter ion spectra) for the substance to be identified, (b) detn. of a spectrum graph of the substance from the at least two mass spectrometric fragmentation spectra by calcg. possible sum formulas for the measured masses, detg. a derivation relation between these sum formulas, and evaluating the direct, as well as the indirect derivation relations on the basis of the mass intensities of the peaks in the spectrum, (c) detg. an optimal fragmentation graph of the substance by selecting the most likely relations from the relation pool under consideration of the evaluation, and (d) comparing the data of the complete or partial fragmentation graph with ref. data to identify the substance based on their structure, substance class, and/or chem. properties.

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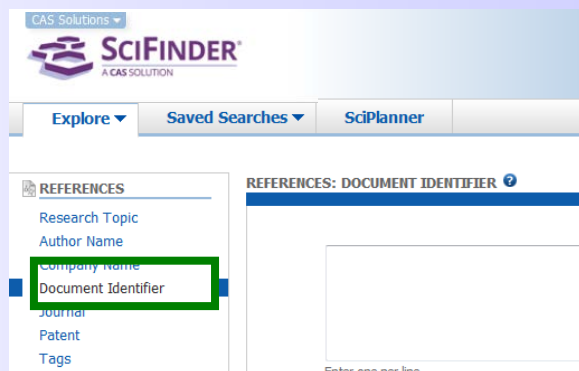




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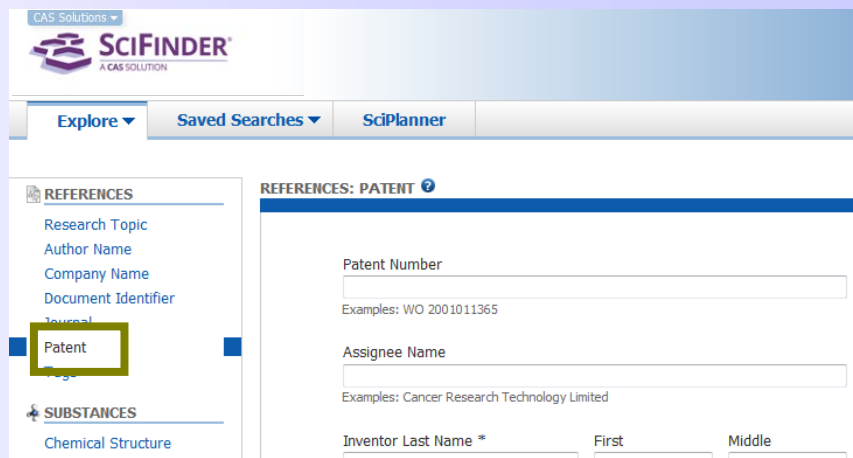
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**Beispiel: Publikationen von Stefan Schuster**

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**1. Medical sterile container and process for determining the sterilisation status of a medical sterile container**  
By Schuster, Stefan  
From Ger. Offen. (2013), DE 102011054827 A1 20130502. | Language: German, Database: CAPLUS

[Machine Translation of Descriptors]. In order to thus improve a medical sterile container with a container interior for taking up sterilizing objects, that the reliability is improved when allocating the sterilisation status "sterile", is suggested, planning a druckaktivierbare sterilisation status detection installation for detecting a sterilisation status of the sterile container. Furthermore an improved process for the determination of the sterilisation status of a medical sterile container is suggested.

**2. Agent-based modeling approach of immune defense against spores of opportunistic human pathogen**  
By Tokarski, Christian; Hummert, Sabine; Mech, Franziska; Figge, Marc Thilo; Germerodt, Sebastian; Schroeter, Anja; Schuster, Stefan  
From Frontiers in Microbial Immunology (2012), 3(April), 129. | Language: English, Database: CAPLUS

Opportunistic human pathogenic fungi like the ubiquitous fungus *Aspergillus fumigatus* are a major threat to system renders the body vulnerable to invasive mycoses that often lead to the death of the patient. While the medical progress, the process and dynamics of defense against invaded and ready to germinate fungal macrophages, neutrophil granulocytes form an important line of defense in that they clear conidia. Live imconidia as a dynamic process of touching, dragging and phagocytosis. To unravel strategies of phagocyte approach is used, implemented in NetLogo. Different modes of movement of phagocytes are tested regarding persistence in their recent direction, chemotaxis of chemokines excreted by conidia and communication between hunting strategy turned out to be superior to the simple random walk, following a gradient of chemokine advantage of communication between neutrophilic agents showed a strong dependency on the spatial sepathogens.

**3. The combinatorial multitude of fatty acids can be described by Fibonacci numbers**  
By Schuster, Stefan  
From arXiv.org, e-Print Archive, Quantitative Biology (2013), 1-14, arXiv:1303.7189v1 [q-bio.BM]. | Language: English, Database: CAPLUS

The famous series of Fibonacci nos. is defined by a recursive equation saying that each no. is the sum of its first two nos. are equal to unity. Here, we show that the nos. of fatty acids (straight-chain aliph. monocarb the Fibonacci nos. Thus, by investing one more carbon atom into extending a fatty acid, an organism can in factor of the Golden section, 1.618. As the Fibonacci series grows asymptotically exponentially, our res generally in biol. We also outline potential extensions of the calcns. to modified (e.g., hydroxylated) fatty ac interest for lipidomics, combinatorial chem., synthetic biol. and the theory of evolution (including prebiotic evo

**4. Correlation between sequence, structure and function for trisporoid processing proteins in the model**  
By Ellenberger, Sabrina; Schuster, Stefan; Woestemeyer, Johannes  
From Journal of Theoretical Biology (2013), 320, 66-75. | Language: English, Database: CAPLUS

Terpenoids, steroids, carotenoids, phytoenes and other chem. related substance groups fulfill multiple functi focuses on trisporoids that operate as pheromones in the phylogenetically ancient fungal group of mucoralea recognizing complementary mating partners and for inducing the differentiation program towards sexua

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## 2. The combinatorial multitude of fatty acids can be described by Fibonacci numbers

By: Schuster, Stefan

The famous series of Fibonacci nos. is defined by a recursive equation saying that each no. is the sum of its two predecessors, with the initial condition that the first two nos. are equal to unity. Here, we show that the nos. of fatty acids (straight-chain aliph. monocarboxylic acids) with n carbon atoms is exactly given by the Fibonacci nos. Thus, by investing one more carbon atom into extending a fatty acid, an organism can increase the variability of the fatty acids approx. by the factor of the Golden section, 1.618. As the Fibonacci series grows asymptotically exponentially, our results are in line with combinatorial complexity found generally in biol. We also outline potential extensions of the calcns. to modified (e.g., hydroxylated) fatty acids. The presented enumeration method may be of interest for lipidomics, combinatorial chem., synthetic biol. and the theory of evolution (including prebiotic evolution).

### Indexing

General Biochemistry (Section6)

### Citations

Berg, J; Biochemistry, 5th edn 2002  
Bicknell, M; Fibonacci Quart 1975, 13, 345

### QUICK LINKS

0 Tags, 0 Comments

### SOURCE

arXiv.org, e-Print Archive, Quantitative Biology  
Pages1-14,  
arXiv:1303.7189v1  
[q-bio.BM]  
Preprint  
2013  
CODEN:AQBRAY

### COMPANY/ORGANIZATION

Dept. of Bioinformatics  
Friedrich Schiller University  
Jena, Germany 07743

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- per E-Mail versenden und untereinander austauschen.

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# „Link“ zu Ergebnissen

CAS Solutions

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Explore Saved Searches

The combinatorial multitude of...

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- To access your active task, click a link in the breadcrumb above.
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CAS Solutions

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Welcome Ina Weiss

Explore Saved Searches SciPlanner Link Save Print Export

The combinatorial multitude of...

REFERENCE DETAIL Get Related Citations Link to Other Sources Send to SciPlanner

## The combinatorial multitude of fatty acids can be described by Fibonacci num

By: Schuster, Stefan

The famous series of Fibonacci nos. is defined by a recursive equation saying that each no. is the sum of its two preceding ones, equal to unity. Here, we show that the nos. of fatty acids (straight-chain aliph. monocarboxylic acids) with  $n$  carbons, by investing one more carbon atom into extending a fatty acid, an organism can increase the variability of the fatty acid series. The Fibonacci series grows asymptotically exponentially, our results are in line with combinatorial complexity four orders of magnitude to modified (e.g., hydroxylated) fatty acids. The presented enumeration method may be of interest for the study of evolution (including prebiotic evolution).

### Indexing

General Biochemistry (Section6)

Man kommt direkt zum Treffer (Antwortsatz/Substanz/Reaktion), der mit dem Link verknüpft ist.

**Wichtig!** Den Link kann man nur bei einem bestehenden Antwortsatz aktivieren.

Wenn der Antwortsatz gelöscht wird, dann bekommt man einen entsprechenden Hinweis.

CODEN:AQBRAY

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The requested link is invalid or incomplete. Ensure that the URL has not been edited or truncated. To access your default page, click OK.

OK

# Konvertierung von Antwortsätzen .sfr zu .akx

- Für die Konvertierung von Antwortsätzen aus der SciFinder-Client-Version zur SciFinder-Webversion gibt es ein Programm: <https://scifinder.cas.org/utils/sfr2akx/>
- Siehe: <http://www.cas.org/support/scifi/index.html>

**SciFinder® sfr to akx Conversion Tool**

**File Selection**

Username:

Filename:

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

**Öffnen von game.akx**

Sie möchten folgende Datei herunterladen:

**game.akx**

Vom Typ: AKX-Datei  
Von: <https://scifinder.cas.org>

Wie soll Firefox mit dieser Datei verfahren?

Öffnen mit

Datei speichern

Für Dateien dieses Typs immer diese Aktion ausführen

**sfr to akx Conversion Tool**

Follow these steps to convert SciFinder client files (.sfr) to the new web format (.akx).

1. In the File Selection box enter your Username.
2. Click the Browse button to locate and select the .sfr file or .zip collection of multiple .sfr files you wish to convert.
3. After you have finished making your selection click the "Convert to akx" button.
4. After the conversion to akx format has completed you will be prompted to either Save the resulting .akx file (or .zip file containing multiple .akx files) or choose a program to Open it. **Select the Save option.**
5. If problems are encountered in the conversion process, you will receive either, an on-screen alert in the case of a single .sfr file conversion, or a .zip file containing a Readme file with details of successful or failed conversions if a .zip collection was used originally. The conversion tool will ask you to save or open this file.
6. To import the .akx file into SciFinder, login and then click the Import button which is located in the Saved Answer Sets area on the right side of any Explore page. When the Import Answer Set dialog box appears, click Browse to locate the .akx file you wish to import and then click OK to import the file.

Note: .zip is the only compression format supported by this tool. ([More information on working with .zip files.](#))

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**SAVED ANSWER SETS ?**

[StammzellenAsEntered](#)

[aspergillus1966](#)

[Struktursuche](#)

[Reaction4](#)

[roetelmaus](#)

[GeranylKaffeatGetReferencesRN](#)

[View All](#) |

**Import Answer Set**

File Name:

Only .akx file format is supported.

# Export und Save: Speichern der Suchergebnisse


Save answers to the CAS server. To save answers to the your computer, use Export.

Save

Print

Export

**SAVE:** Pro Login-ID können maximal 50 Antwortsätze für die Verwendung in späteren Recherchen bzw. für ein „Combine“ bei CAS gespeichert werden.

Export 

\* Required

<b>Export:</b> <ul style="list-style-type: none"><li><input type="radio"/> All</li><li><input type="radio"/> Selected</li><li><input checked="" type="radio"/> Range</li></ul> <input type="text" value="2-4"/> <p>Example: 2-20</p>	<b>For:</b> <p><b>Citation Manager</b></p> <ul style="list-style-type: none"><li><input checked="" type="radio"/> Citation export format (*.ris)</li><li><input type="radio"/> Quoted Format (*.txt)</li><li><input type="radio"/> Tagged Format (*.txt)</li></ul> <p><b>Offline review</b></p> <ul style="list-style-type: none"><li><input type="radio"/> Portable Document Format (*.pdf)</li><li><input type="radio"/> Rich Text Format (*.rtf)</li><li><input type="radio"/> Answer Keys (*.txt)</li></ul> <p><b>Saving locally</b></p> <ul style="list-style-type: none"><li><input type="radio"/> Answer Key eXchange (*.akx)</li></ul>	<b>Details:</b> <p>File Name: *</p> <input type="text" value="Reference_09_12_2011_115307"/>
--	--	--

Export Cancel

**EXPORT** dient zum **lokalen Speichern** von Suchergebnissen auf dem **eigenen Rechner** (zum Import in Textverarbeitungsprogramme, zur Weiterverwendung in Texten usw.).

Dabei gibt es unterschiedliche Export-Formate.

# Export-Formate

Export ⌵

\* Required

Export:

- All
- Selected
- Range

Example: 2-20

For:

**Citation Manager**

- Citation export format (\*.ris)
- Quoted Format (\*.bt)
- Tagged Format (\*.bt)

Offline review

- Portable Document Format (\*.pdf)
- Rich Text Format (\*.rtf)
- Answer Keys (\*.bt)

Saving locally

- Answer Key eXchange (\*.akx)

Details:

File Name: \*

Export Cancel

Export ⌵

Only 500 answers can be exported at one time.

\* Required

Export:

- All
- Selected
- Range

Example: 2-20

For:

**Citation Manager**

- Citation export format (\*.ris)
- Quoted Format (\*.bt)
- Tagged Format (\*.bt)

Offline review

- Rich Text Format (\*.rtf)
- Answer Keys (\*.bt)

Saving locally

- Answer Key eXchange (\*.akx)

Details:

File Name: \*

Format:

- Summary without abstracts
- Summary with partial abstracts
- Summary with full abstracts
- Detail (full record)

Include:

- Task History
- Tags
- Comments

Export Cancel

**Citation Manager:** bei allen hier aufgeführten Formaten kann man maximal **100** Dokumente in einer Datei speichern.

**Offline review:** Im Summary-Format kann man höchstens **500** Dokumente als rtf oder pdf auf einmal in einer Datei speichern, im Detail-Format sind es dagegen nur maximal **100** Treffer.

Export ⌵

Only 100 answers can be exported at one time.

\* Required

Export:

- All
- Selected
- Range

Example: 2-20

For:

**Citation Manager**

- Citation export format (\*.ris)
- Quoted Format (\*.bt)
- Tagged Format (\*.bt)

Offline review

- Portable Document Format (\*.pdf)
- Rich Text Format (\*.rtf)
- Answer Keys (\*.bt)

Saving locally

- Answer Key eXchange (\*.akx)

Details:

File Name: \*

Format:

- Summary without abstracts
- Summary with partial abstracts
- Summary with full abstracts
- Detail (full record)

Include:

- Substances
- Concepts
- Task History
- Tags
- Comments

Export Cancel



# Drucken der Suchergebnisse im Summary-Format

## Print

### Print to PDF:

- All  
 Selected  
 Range

Example: 2-20

### Format:

- Summary without abstracts  
 Summary with partial abstracts  
 Summary with full abstracts  
 Detail (full record)

### Title:

### Include:

- Task History  
 Tags  
 Comments

Print

Cancel

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Page 1

### Task History

Task Began May 31, 2013 05:17 AM

#### Explore references by research topic: **mink oil (mustela oil)**

Research Topic: mink oil (mustela oil)  
Result Count: 3

#### Candidates Selected (ID 1)

232 references were found containing either the concept "mink oil" or the concept "mustela oil".

Answer Type: References  
Result Count: 232

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Page 2

### 1. Novel hair oil and its manufacture method thereof

By Chen, Yonglin

From [Faming Zhuanli Shenqing \(2013\), CN 103054772 A 20130424](#), Language: Chinese, Database: CAPLUS

The invention discloses a novel hair oil and its manuf. method. The invention is composed of following components by wt. part: aloin: 3~5, almond Oil: 10~20, Flos Osmanthi Fragrantis essence: 0.3~0.5, lanolin: 8~16, petrolatum: 20~30, bis(2-ethylhexyl) phthalate: 1~3, Span -60: 3~5, Pr hydroxybenzoate: 2~5, **mink oil**: 10~20, and is manufd. by mixing all raw materials except for vaseline and essence, stirring, adding vaseline, mixing, adding essence, stirring. Compared with prior art, the invention has the following beneficial effects: (1) good effect of improving hair lubricity, adhesion force and gloss; (2) wide application range, no deterioration in the course of product storage.

#### ~0 Citings

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### 2. Cosmetic lotion containing mink oil

By Wang, Yan

From [Faming Zhuanli Shenqing \(2013\), CN 103040653 A 20130417](#), Language: Chinese, Database: CAPLUS

The title skin care soln. is composed of glyceryl monostearate 20-40, stearic acid 6-12, octadecanol 10-20, **mink oil** 5-10, water-sol. lanolin 4-8, glycerol 20-30, menthol 10-20, iso-Pr myristate 30-50, essence 0.2-0.4 and deionized water 300-500 wt. parts. The skin care soln. is prepd. by (1) mixing stearic acid, glyceryl monostearate, water-sol. lanolin, iso-Pr myristate and glycerol, stirring at 60-80°C, (2) mixing other materials except for essence, stirring at 50-70°C, (3) adding the mixt. of step (1) into the mixt. of step (2), stirring, emulsifying, (4) cooling to room temp., adding the essence and stirring. The skin care soln. can make skin telangiectasia, promote blood circulation, improve skin nutrition state, moisturize skin and treat acne and other skin diseases.

#### ~0 Citings

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# Drucken der Suchergebnisse im Detail-Format

**Print**

**Print to PDF:**

All

Selected

Range

Example: 2-20

**Format:**

Summary without abstracts

Summary with partial abstracts

Summary with full abstracts

Detail (full record)

**Title:**

**Include:**

Substances

Concepts

Task History

Tags

Comments

Drucken bedeutet:  
Drucken als pdf!

SciFinder® Page 1

**10. Final amended report on the safety assessment of mink oil**

By: Andersen, F. Alan

Source: International Journal of Toxicology, Volume: 24, Issue: Suppl. 3, Pages: 57-64, Journal: General Review, 2005, CODEN: IJTOFN, ISSN: 1091-5818, DOI: 10.1080/10915810500257154

Company/Organization: USA

Accession Number: 2005:1252722, CAN 144:494776, CAPLUS

Publisher: Taylor & Francis, Inc.

Language: English

**Abstract**

A review. **Mink Oil**, obtained from the fatty tissues of minks, is a mixt. of the natural glycerides of 14 to 20 carbon chain fatty acids. There are 100 current reported uses as a hair-conditioning agent, an occlusive skin-conditioning agent, and as a surfactant; up to a max. concn. of 3%. **Mink Oil** is manuf. by harvesting animal hides and scraping the fat layer from the hide. It is rendered and refined using high temp. processes (230°F to 240°F) and sapon. to reduce free fatty acids. Analyses demonstrate that **Mink Oil** can be substantially free of impurities, including pesticides. **Mink Oil** does not absorb significant UVA or UVB radiation. In a clin. test of skin penetration, 1 h after application, **Mink Oil** was detected on the skin surface of all five panelists; it was detected within the stratum corneum in 2/5 panelists. **Mink Oil** has an oral LD<sub>50</sub> of >64.0 cc/kg in albino rats. No erythema or edema was noted after refined **Mink Oil** was applied for 24 h to intact and scarified area of albino rabbits. A 50% diln. of a **Mink Oil** cream did not sensitize guinea pigs in a maximization test. **Mink Oil** was not an ocular irritant to albino rabbits. Clin. studies using single occlusive patches found no irritation with up to 2.8% **Mink Oil**, although transient mild to no irritation was noted in two exaggerated-use studies. **Mink Oil** is used in aerosols and sprays. Although there are no inhalation toxicity data available on **Mink Oil**, the available data on particle sizes of cosmetic aerosols and sprays indicates diams. more than an order of magnitude larger than the diam. of respirable particles. Most of the glycerides in **Mink Oil** are triglycerides (glyceryl triesters), the safety of which has been substantiated in previous safety assessments; e.g., dermal absorption is nil to slight; there is little or no acute, subchronic, or chronic oral toxicity; dermal application was not assocd. with significant irritation or sensitization; ocular exposures were, at most, mildly irritating; most of the genotoxicity test systems are neg.; use as vehicles in carcinogenicity testing of other chems. has produced no adverse reaction; and clin. tests produce no irritation or sensitization reactions-but, they may enhance the of penetration of other chems. Formulators should be aware of the possible penetration-enhancing properties of **Mink Oil**. Although pesticide residues have been analyzed and found to be below levels of detection, the Panel is concerned that the available data suggesting the absence of pesticide residues in **Mink Oil** are limited. The Panel advised the industry that the total polychlorinated biphenyl (PCB)/pesticide contamination should be limited to not more than 40 ppm, with not more than 10 ppm for any specific residue.

**Indexing**

Essential Oils and Cosmetics (Section 62-0)

**Supplementary Terms**

review **mink oil** safety cosmetic hair

**Citations**

1)Bio-Toxicology Laboratories Inc; Unpublished data submitted by CTFA on August 5, 1994 1974

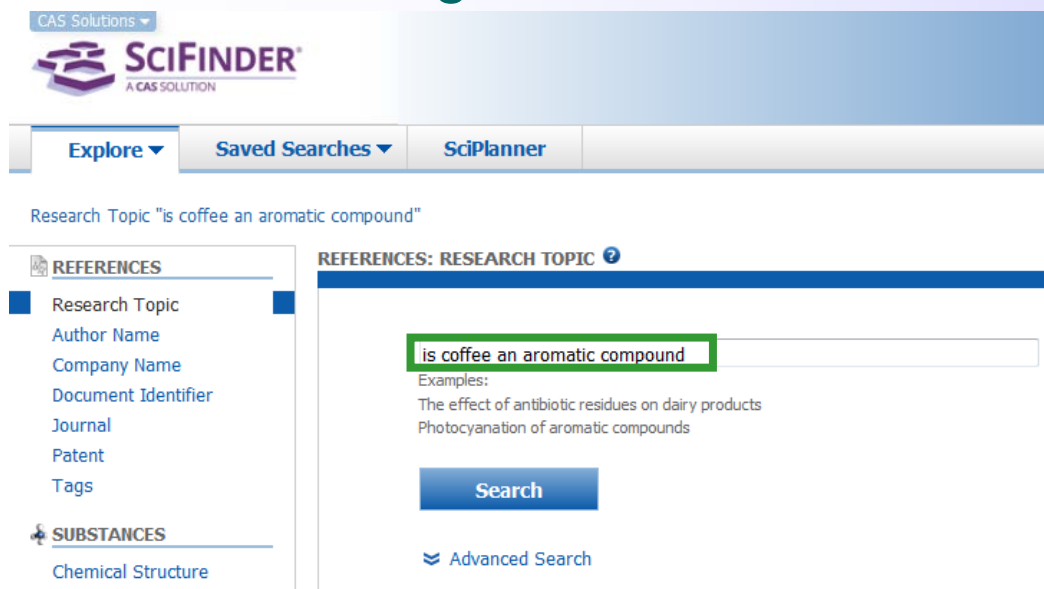
2)Bower, D; Minutes of the September 9, 1999 meeting of the CIR Expert Panel 1999

3)Complete Analysis Laboratories Inc; Unpublished data submitted by CTFA September 14, 2001 1996

# Keep Me Posted Alert

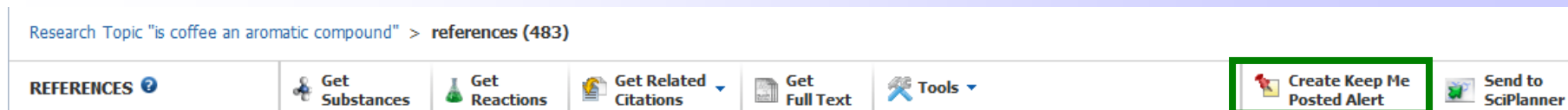
In SciFinder gibt es die Möglichkeit Keep Me Posted-Profile zu erstellen.

## 1. Suchanfrage stellen



The screenshot shows the SciFinder search interface. At the top left, there is a 'CAS Solutions' dropdown menu and the SciFinder logo. Below the logo is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. The main search area contains the text 'Research Topic "is coffee an aromatic compound"'. On the left side, there is a sidebar with 'REFERENCES' and 'SUBSTANCES' sections. The 'REFERENCES' section is active, showing a list of search criteria: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. The 'SUBSTANCES' section shows 'Chemical Structure'. The main search area has a search box containing 'is coffee an aromatic compound', a 'Search' button, and an 'Advanced Search' link. Below the search box, there are examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'.

## 2. Keep Me Posted einrichten



The screenshot shows the search results page for the query 'Research Topic "is coffee an aromatic compound" > references (483)'. The page has a navigation bar with several buttons: 'REFERENCES', 'Get Substances', 'Get Reactions', 'Get Related Citations', 'Get Full Text', 'Tools', 'Create Keep Me Posted Alert', and 'Send to SciPlanner'. The 'Create Keep Me Posted Alert' button is highlighted with a green box.

# Keep Me Posted erstellen (1)

Create Keep Me Posted Profile [?](#)

**Title:** \* \* Required

**Description:**

Characters Remaining: 1024

**Duration**  
Expires On: Jun 03, 2014 [Change](#)

**Frequency**  
Send updates once every Week  Exclude previously retrieved

**Search:**  
Explore references by research topic: **is coffee an aromatic compound**  
**Candidates Selected:**  
References which contain the two concepts "coffee" and "aromatic compound" closely associated with one another

**Create** **Cancel**

Beim Profilnamen sind auch Umlaute erlaubt.

Man kann wählen, ob man wöchentlich oder monatlich KMP-Ergebnisse erhalten möchte.

**KEEP ME POSTED** [?](#)

Roetelmaus  
Jun 08, 2013(7)

Rötelmaus  
Jun 08, 2013(7)

Aktivierung der Benachrichtigung über **Keep Me Posted-Ergebnisse** per E-Mail bei „Preferences“ im Startbildschirm einstellen.

SciFinder®

Explore **Saved Searches** SciPlanner

Research Topic "myodes glareolus (clothionomy..." > references (1483)

**PREFERENCES** [?](#)

**Keep Me Posted Notification**  
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Please ensure that CAS has your current e-mail address. Visit [myCAS](#) to add or change your address.

**My Suppliers**  
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**Remove Duplicate References**  
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**Starting Page**  
Select the default starting page:  
 Explore References  
 Explore Substances  
 Explore Reactions

**OK** **Cancel**

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Explore | Saved Searches | SciPlanner | Save | Print | Export

Author Name "scriba, g" > references (257)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools

**Create Keep Me Posted Alert** | Send to SciPlanner

Analyze | Refine | Categorize | Sort by: Accession Number | Answers per Page [100] Display: [ ] [ ] [ ]

0 of 257 References Selected

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können nicht nur beim  
ersten Schritt einer  
Suchanfrage erstellt  
werden, sondern auch  
z.B. von Antworten die  
aus einem Refine  
resultieren!

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Explore | Saved Searches | SciPlanner

Author Name "scriba, g" > references (257) > refine "Book" (2)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools

**Create Keep Me Posted Alert** | Send to SciPlanner

Analyze | Refine | Categorize | Sort by: Accession Number | Answers per Page [100] Display: [ ] [ ] [ ]

0 of 2 References Selected

1. **Special Issue: Pharmaceutical Analysis 2008. [In: Electrophoresis, 2008; 29(17)]** | Quick View | Other Sources  
By Watzig, Hermann; Scriba, Gerhard; Editors  
No Corporate Source data available | (2008), 225 pp.. | Language: English, Database: CAPLUS
2. **Special Issue: Pharmaceutical Analysis. [In: Electrophoresis; 2006, 27(12)]** | Quick View | Other Sources  
By Watzig, Hermann; Scriba, Gerhard; Editors  
No Corporate Source data available | (2006), 265 pp.. | Language: English, Database: CAPLUS

# Ergebnisse eines Keep Me Posted (1)

metabolic pathway analysis (21 answers)  
First 10 answers are listed

- Transcriptome alteration in a rice introgression line with enhanced alkali tolerance
- Salmonella enterica Typhimurium infection causes metabolic changes in chicken muscle involving AMP
- Plasma metabolomics identifies lipid abnormalities linked to markers of inflammation, microbial trans
- Network analysis of the MVA and MEP pathways for isoprenoid synthesis
- Distinct relationships of intramuscular and subcutaneous fat with cortical bone: findings from a cross-
- The effects of sapropterin on urinary monoamine metabolites in phenylketonuria
- A community-based study on determinants of circulating markers of cellular immune activation and kyr
- Screening method for drugs for insulin resistance and/or glucose intolerance by determining the inhibi
- Glyoxalase enzymes in trypanosomatids
- Metabolism and breeding of phytic acid in maize (Zea mays)

Neben dem Link zum KMP-Profil werden die Titel der ersten 10 Antworten angezeigt.

Nach Anklicken des Links in der E-Mail kommt man zum Anmeldebildschirm von SciFinder.

Nach der Anmeldung wird der Link aktiviert.



**RETRIEVING LINK**



Explore Saved Searches

Global proteome analysis of gl...

**CONFIRM VIEW REFERENCE**

You have an active task.

- To access your active task, click a link in the breadcrumb above.
- To leave your active task and view the requested reference, click **OK**.

Note: For best results, ensure that SciFinder is open in only one window or tab. Close any other window or tab that appears to be running SciFinder.

OK

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# Ergebnisse eines Keep Me Posted (2)

metabolic reconstruction

Search Strategy:

Select All Deselect All

Results

- Jun 1, 2013 (1)
- May 18, 2013 (1)
- May 11, 2013 (1)

Keep Me Posted-Ergebnisse, die noch nicht angesehen wurden, sind fett markiert.

Saved Searches

- Saved Answer Sets
- Keep Me Posted**
- History

Über Saved Searches/Keep Me Posted kann man sich jederzeit die Keep Me Posted-Ergebnisse ansehen.

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Explore Saved Searches SciPlanner

Microbial domestication signat...

KEEP ME POSTED Delete Selected

SAVED SEARCHES 1 of 11 Profiles Selected

- Saved Answer Sets
- Keep Me Posted**
- History

Roetelmaus

Search Strategy:

CAS Solutions

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Preferences | SciFinder Help | Sign Out

Welcome Ina Weiss

Explore Saved Searches SciPlanner Save Print Export

Keep Me Posted "metabolic reconstruction"[Jun 01, 2013] (1)

REFERENCES

Get Substances Get Reactions Get Related Citations Get Full Text Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

Answers per Page [100] Display: [List Icon]

0 of 1 Reference Selected


1. **Genomic reconstruction of transcriptional regulatory networks in lactic acid bacteria** Quick View Other Sources

By Ravcheev, Dmitry A.; Best, Aaron A.; Sernova, Natalia V.; Kazanov, Marat D.; Novichkov, Pavel S.; Rodionov, Dmitry A.  
From BMC Genomics (2013), 14, 94. | Language: English, Database: CAPLUS

Background: Genome scale annotation of regulatory interactions and reconstruction of regulatory networks are the crucial problems in bacterial genomics. The Lactobacillales order of bacteria collates various microorganisms having a large economic impact, including both human and animal pathogens and strains used in the food industry. Nonetheless, no systematic genome-wide anal. of transcriptional regulation has been previously made for this taxonomic group. Results: A comparative genomics approach was used for reconstruction of transcriptional regulatory networks in 30 selected genomes of lactic acid bacteria. The inferred networks comprise regulons for 102 orthologous transcription factors (TFs), including 47 novel regulons for previously uncharacterized TFs. Numerous differences between regulatory networks of the Streptococcaceae and Lactobacillaceae groups were described on several levels. The two groups are characterized by substantially different sets of TFs encoded in their genomes. Content of the inferred regulons and structure of their cognate TF binding motifs differ for many orthologous TFs between the two groups. Multiple cases of non-orthologous displacements of TFs that control specific metabolic pathways were reported. Conclusions: The reconstructed regulatory networks substantially expand the existing knowledge of transcriptional regulation in lactic acid bacteria. In each of 30 studied genomes the obtained regulatory network contains on av. 36 TFs and 250 target genes that are mostly involved in carbohydrate metab., stress response, metal homeostasis and amino acids biosynthesis. The inferred networks can be used for genetic expts., functional annotations of genes, metabolic reconstruction and evolutionary anal. All reconstructed regulons are captured within the Streptococcaceae and Lactobacillaceae collections in the RegPrecise database available at online.

Show More

# Bearbeitung von „Keep Me Posted“-Profilen

Edit Keep Me Posted Profile 

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**Title: \***  
Roetelmaus

**Description:**

Characters Remaining: 1024

**Status:**  Enabled  Disabled


**Duration**  
Expires On: Jul 19, 2013 [Change](#)

**Frequency**  
Send updates once every

Exclude previously retrieved references.

**Search:**  
Explore references by research topic: **myodes glareolus (clethrionomys glareolus, bank vole or bank voles)**  
**Candidates Selected:**  
References which contain at least one of the concepts "myodes glareolus", "clethrionomys glareolus", "bank vole" or "bank voles"

Die Laufzeit eines Profils ist über **Change** auf 1, 3, 6 und 12 Monate einstellbar.

**KEEP ME POSTED** 

Roetelmaus  
No results

---

Rötelmaus  
No results

---

Dynamic optimization  
May 25, 2013(1)  
May 18, 2013(1)  
Apr 27, 2013(3)

---

[View All](#)

**KEEP ME POSTED** 

Roetelmaus

 Expires in 14 days

Jun 15, 2013(4)  
Jun 08, 2013(7)

---

2 Wochen vor Ablauf eines Profils wird man in SciFinder an das Ablaufdatum erinnert und bekommt eine E-Mail.

In den „**Keep Me Posted Results**“ kann man die Laufzeit des Profils durch 1 Klick **um 1 Jahr verlängern**.



# Verlängerung von KMP-Profilen

MPAPalsson Edit  
This Keep Me Posted profile will expire in 10 days. [Extend 12 Months](#)  
▶ Search Strategy:

Kurz vor Ablauf eines Profils wird man in SciFinder an das Ablaufdatum erinnert. In den **Keep Me Posted** - Profilen kann man die Laufzeit des Profils durch 1 Klick **um 1 Jahr verlängern**.

The following Keep Me Posted profile(s) for inaweiss will be expiring soon:

Signal Transduction Model (Bioinformatic)  
Apr 06, 2011  
[Extend 12 months](#)

Wenn man der Erinnerungs-E-Mail auf „**Extend 12 month**“ klickt, dann wird nach der Anmeldung bei SciFinder das Profil automatisch um 1 Jahr verlängert.

Profile expiration has been extended.

**Signal Transduction Model (Bioinformatic)** Edit Enabled Apr 7, 2010 Mar 30, 2012  
▶ Search Strategy:  
**Select All** **Deselect All**  
Results Selected Results: [Combine](#) [Delete](#)

<input type="checkbox"/>	<a href="#">Mar 19, 2011 (1)</a>	<a href="#">Link</a>
<input type="checkbox"/>	<a href="#">Feb 26, 2011 (1)</a>	<a href="#">Link</a>



## Teil 2: Weitere Funktionen in SciFinder + Hilfen

- Analyze
- Combine
- Categorize
- Comments und Tags
- Import von Daten aus SciFinder in Literaturverwaltungsprogramme  
(Beispiele: Endnote, Endnote Web)
- Materialien und Hilfeseiten von CAS
- Zugang zu SciFinder mit dem Smartphone (iPod)

# Analyze: Show More

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Ina Weiss

Explore | Saved Searches | SciPlanner | Save | Print | Export

Research Topic "metabolic pathway analysis" > references (153)

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Accession Number

Answers per Page [100] Display: [ ] [ ] [ ]

0 of 153 References Selected

Page: 1 of 2

1. **Metabolic pathway analysis and kinetic studies for production of nattokinase in *Bacillus subtilis***  
By Unrean, P  
From Bioproc

We have anal. (EM fibrinolyti under dif model pr were the the most max. the condition

2. **Identifica**  
By Sharma, A  
From Europea

Sporadic call for a target ca Further modeled potential

3. **Characte**  
By Heekin, A  
No Corporate

4. **Compara cells**  
By Rengaraj,  
From Therioge

**Analyze - Author Name**

462 Items | 5 Selected | Export

Sort by: Frequency | Page: 1 of 10

Select bars to view only those references within the current answer set.

Author Name	Count
<input checked="" type="checkbox"/> Schuster Stefan	18
<input checked="" type="checkbox"/> Kaleta Christoph	9
<input checked="" type="checkbox"/> De Figueiredo Luis F	7
<input checked="" type="checkbox"/> Klamt Steffen	6
<input type="checkbox"/> Cakir Tunahan	4
<input type="checkbox"/> Nguyen Nhung H A	4
<input type="checkbox"/> Srienc Friedrich	4
<input type="checkbox"/> Unrean Pornkamol	4
<input checked="" type="checkbox"/> Dandekar Thomas	3
<input type="checkbox"/> Ding Dewu	3

Show More

Apply | Cancel

pathway anal. tool called elementary mode altered culturing conditions on the prodn. of a max. theor. yield for NK synthesis in *B. subtilis* on for NK prodn. was identified. To confirm NK activity. The optimal culturing conditions ed for engineering *B. subtilis* metab. towards sion that enable the cell to produce NK at the EMA being used to rationally design culture

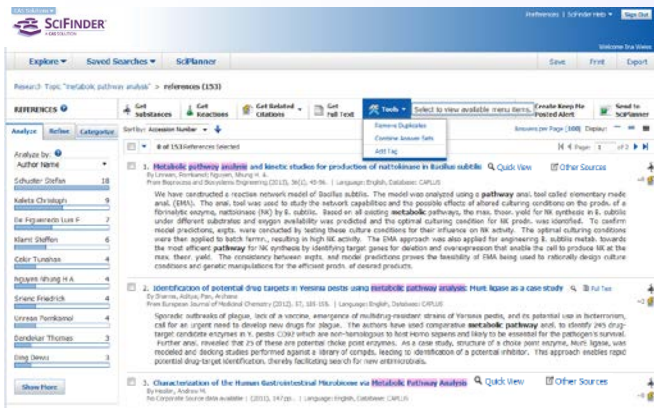
re ligase as a case study

a pestis, and its potential use in bioterrorism, **metabolic pathway** anal. to identify 245 drug- ally to be essential for the pathogen's survival. re of a choke point enzyme, MurE ligase, was tential inhibitor. This approach enables rapid

ed genes in chicken primordial germ

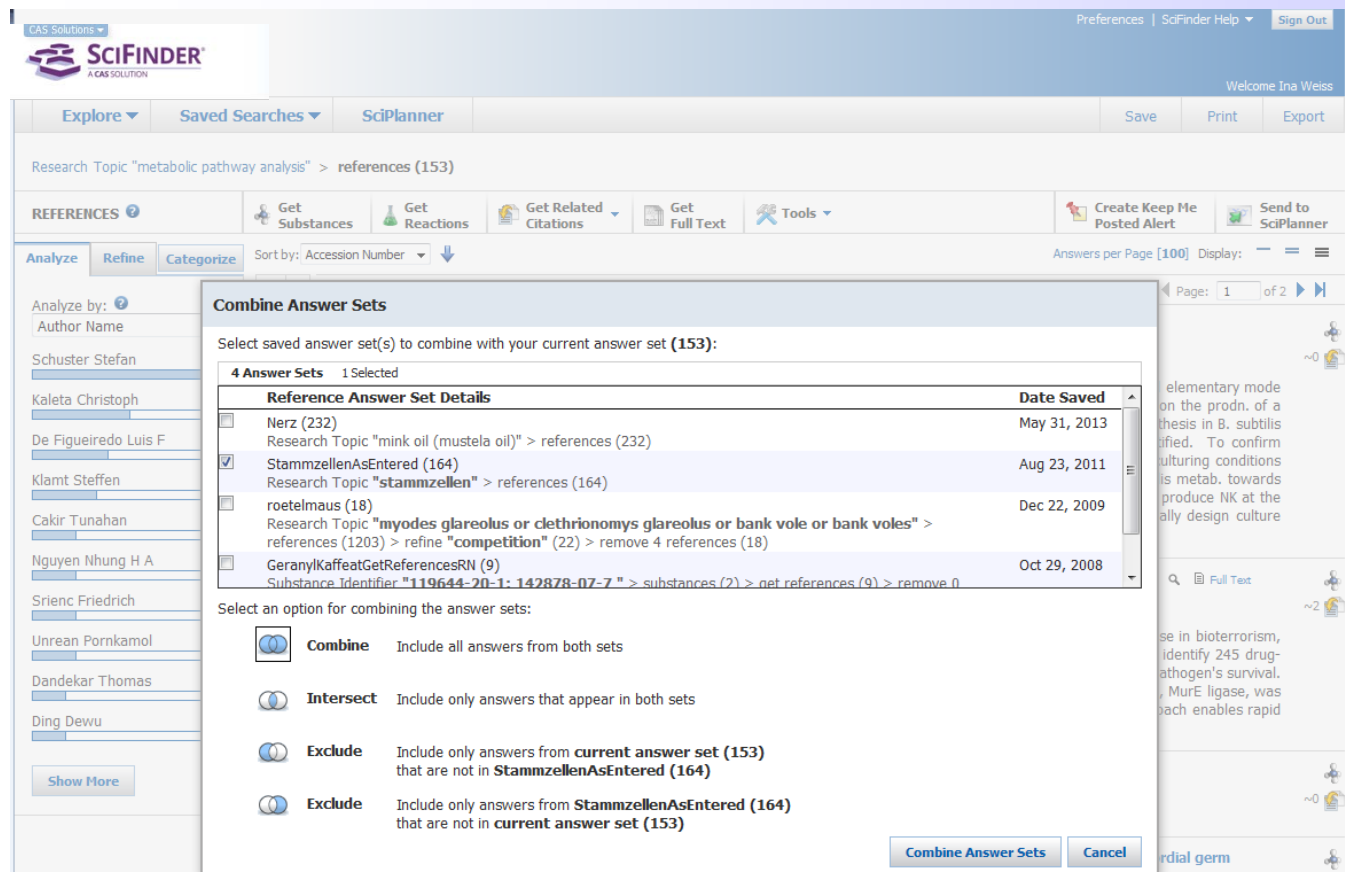
**Full Analysis:** erfolgt automatisch bei bis zu 20.000 Antworten. Bei **Show More** können mehr als 10 Analyse-Ergebnisse angesehen werden.

# Combine



Ein **Combine** ist seit Ende März 2010 auch aus einer aktuellen Recherche heraus möglich.

Beim Klick auf **Tools/ Combine Answer Sets** kommt man zu den gespeicherten Antwortsätzen und kann 1 bis mehrere Antwortsätze für ein **Combine** mit dem bisherigen Rechercheergebnis auswählen.



## Combine (2)

CAS Solutions

**SCIFINDER**  
A CAS SOLUTION

Explore Saved Searches SciPlanner

Research Topic "competition" > references (155932)

SAVED ANSWER SETS ? **Combine Answer Sets** Delete Selected

SAVED SEARCHES

Saved Answer Sets  
Keep Me Posted  
History

2 of 6 Reference Answer Sets Selected

References (6) Substances (2) Reactions (1)

- competition (20000)  
Research Topic "competition" > references (155932)
- bank voles (1219)  
Research Topic "myodes glareolus (clethrionomys glareolus, bank vole or bank voles)" > references (1483) > remove 264 references (1219)

Ein **Combine** ist auch mit bei CAS gespeicherten Antwortsätzen möglich.  
Akademische Nutzer können maximal 50 Antwortsätze speichern.

# Combine bei mehr als 2 Antwortsätzen

Research Topic "food" > references (1054987)

SAVED ANSWER SETS

Combine Answer Sets Delete Selected

SAVED SEARCHES

3 of 9 Reference Answer Sets Selected

References (9) Substances (2) Reactions (1)

Food (20000)  
Research Topic "food" > references (1054987) Edit

Tomato paste (3316)  
Research Topic "tomato paste" > references (3316) Edit

Autor O.I.Kvasenkov (20000)  
Author Name "Kvasenkov, O I" > references (25155) Edit

**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

Combine Answer Sets Cancel

Verknüpfung mehrerer Suchschritte mit „or“ bzw. „and“ ist möglich.

Combine Reference Answer Sets "Food AND Tomato paste AND Auto..." (481)

REFERENCES

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

Answers per Page [100] Display: [ ]

0 of 481 References Selected

1. **Method for production of preserves "chopped hazel grouse cutlets with garnish and red main sauce"** Quick View Other Sources  
By Kvasenkov, O. I.  
From Russ. (2013), RU 2482743 C1 20130527. | Language: Russian, Database: CAPLUS

FIELD: food industry.SUBSTANCE: invention relates to the technology of preserved second-course lunches production. The method envisages recipe components preparation, wheat bread soaking in milk and chopping, hazel grouse flesh and raw tallow chopping, the listed components mixing with part of salt and part of black hot pepper to produce mince, the mince moulding, mealing in wheat crumbs and frying in melted butter to produce cutlets, carrots, parsley roots and bulb onions cutting, sauteing in melted butter and straining, sugar peas and green cutting and freezing, sunflower flour pouring with bone broth and maintenance for swelling, mixing carrots, parsley roots, bulb onions, sugar peas, green and sunflower flour with tomato paste, sugar, the remaining salt, the remaining black hot pepper and laurel leaf, the cutlets, the produced mixture and bone broth packing, sealing and sterilisation.EFFECT: method allows to reduce the manufactured target product adhesion to container walls.

2. **Method for production of preserves "moscow cutlets with onion sauce"** Quick View Other Sources  
By Kvasenkov, O. I.  
From Russ. (2013), RU 2482742 C1 20130527. | Language: Russian, Database: CAPLUS

FIELD: food industry.SUBSTANCE: invention relates to the technology of preserved second-course lunches production. The method envisages recipe components preparation, wheat bread soaking in drinking water and chopping, chopping beef, raw beef tallow and part of bulb onions, the listed components mixing with part of salt and part of black hot pepper to produce mince, the mince moulding, mealing in wheat crumbs and frying in melted fat to produce cutlets, carrots, parsley roots and the remaining bulb onions cutting, sauteing in melted fat and straining, French beans and green cutting and freezing, sunflower flour pouring with bone broth and maintenance for swelling, mixing carrots, parsley roots, sauteed part of bulb onions, French beans, green and sunflower flour with tomato paste, acetic acid, sugar, the remaining salt, the remaining black hot pepper and laurel leaf, the cutlets, the produced mixture and bone broth packing, sealing and sterilisation.EFFECT: method allows to reduce the manufactured target product adhesion to container walls.

3. **Method for production of preserves "moscow cutlets with cabbages and sour cream sauce with tomato paste"** Quick View Other Sources  
By Kvasenkov, O. I.  
From Russ. (2013), RU 2482741 C1 20130527. | Language: Russian, Database: CAPLUS

Analyze by:	Count
Author Name	
Kvasenkov O I	481
Kas Yanov G I	18
Lyallina A P	6
Vasil'eva T A	6
Belozherov G A	4
Petrov A N	3
Borisovets E I	2
Nikonova T I	2
Bulavintseva E N	1
Kovalevskaya I F	1

Show More

# Combine von 2 und mehr Keep Me Posted Results

**metabolic pathway analysis** Edit Enabled

Search Strategy:

Select All Deselect All

Results Selected Results **Combine** Delete

<input checked="" type="checkbox"/>	Jun 1, 2013 (24)	<a href="#">Link</a>
<input checked="" type="checkbox"/>	May 25, 2013 (21)	<a href="#">Link</a>
<input type="checkbox"/>	May 18, 2013 (25)	<a href="#">Link</a>

**Dynamic optimization** Edit Enabled

Search Strategy:

Select All Deselect All

Results Selected Results **Combine** Delete

<input checked="" type="checkbox"/>	May 25, 2013 (1)	<a href="#">Link</a>
<input checked="" type="checkbox"/>	May 18, 2013 (1)	<a href="#">Link</a>
<input checked="" type="checkbox"/>	Apr 27, 2013 (3)	<a href="#">Link</a>
<input type="checkbox"/>	Apr 20, 2013 (4)	<a href="#">Link</a>

**Combine Keep Me Posted Results**

Select an option for combining 2 results from profile metabolic pathway analysis

**Combine** Include all answers from both result sets

**Intersect** Include only answers that appear in both result sets

**Exclude** Include only answers from Jun 01, 2013 that are not in May 25, 2013

**Exclude** Include only answers from May 25, 2013 that are not in Jun 01, 2013

**Combine Results** **Cancel**

**Combine Keep Me Posted Results**

Select an option for combining 3 results from profile Dynamic optimization

**Combine** Include all answers from all selected results sets

**Intersect** Include only answers that appear in all selected results sets

**Combine Results** **Cancel**

Combine Keep Me Posted "metabolic pathway analysis" [5 Results Combined] (129) > remove 7 references (122)

Nach einem Combine von mehreren KMP Ergebnissen kann man eventuelle doppelte Einträge entfernen. Bei Voreinstellung von **Remove Duplicate References** erfolgt dies automatisch!

# Categorize

CAS Solutions | SCIFINDER | A CAS SOLUTION | Preferences | SciFinder Help | Sign Out | Welcome Ina Weiss

Explore | Saved Searches | SciPlanner | Save | Print | Export

Research Topic "cinnabaric acid in human" > references (17)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools

Analyze | Refine | **Categorize** | Sort by: Accession Number | 0 of 17 References Selected | Answers per Page [100] Display: [ ] [ ] [ ]

Analyze by: Author Name

- Duke G A 3
- Choisy Patrick 2
- Lagrange Alain 2
- Lalleman Boris 2
- Nishimura R 2
- Pipkin George E 2
- Schlegel J U 2
- Shirasawa Eiichi 2
- Acher F 1
- Battaglia G 1

Show More

1. **Aminophenoxazinones as Inhibitors of Indoleamine 2,3-Dioxygenase (IDO). Synthesis of Exfoliazone and Chandrananimycin A**

By Pascale Daffreloy-Siegel, David Dore, David Meady, Christopher J...

**Categorize**

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

Category Heading	Category	Index Terms	Selected Terms
All	Reactants & reagents (25)	<b>Select All</b> <b>Deselect All</b>	Click 'X' to remove the category from 'Selected Terms' Synthetic chemistry > Reactants & reagents (3 Terms)
General chemistry	Prepared substances (23)	<input type="checkbox"/> 1429632-39-2 1	
Biotechnology	Reactions (5)	<input type="checkbox"/> 1429632-40-5 1	
Biology	Purified substances (1)	<input type="checkbox"/> 1429632-43-8 1	
Genetics & protein chemistry		<input type="checkbox"/> 1429632-44-9 1	
<b>Synthetic chemistry</b>		<input type="checkbox"/> 1429632-45-0 1	
Technology		<input type="checkbox"/> 2-Amino-3-methylphenol 1	
Analytical chemistry		<input type="checkbox"/> 2-Aminophenol 1	
Physical chemistry		<input type="checkbox"/> 2-Aminoresorcinol 1	
Polymer chemistry		<input type="checkbox"/> 2-Nitroresorcinol 1	
Environmental chemistry		<input type="checkbox"/> 3,4-Dihydro-2H-pyran 1	
		<input type="checkbox"/> 3-Hydroxy-2-nitrobenzoic acid 1	
		<input checked="" type="checkbox"/> 4-(Hydroxymethyl)-2-nitrophenol 1	
		<input checked="" type="checkbox"/> 4-Hydroxy-3-nitrobenzaldehyde 1	

Synthetic chemistry > Reactants & reagents > 3 Index Term(s) Selected

OK   Cancel

2. The u...  
By Mold, ...  
From PCT...

The invention provides a method of treating an autoimmune disorder, the method comprising administering to a subject in need thereof, a therapeutically effective amt. of a compds. I [R<sup>1</sup>, R<sup>2</sup> = H, NH<sub>2</sub>, C<sub>1-6</sub> alkylamine, CO<sub>2</sub>H etc.; m = 1-3, n = 1-4], and salts and isomers thereof. The compds. of the invention include e.g. **cinnabaric acid**. Immune disorder is an autoimmune disorder selected from the group consisting of multiple sclerosis, myasthenia gravis, Guillan-Barre syndrome (antiphospholipid syndrome), systemic lupus erythematosus, Behcet's syndrome, Sjogren's syndrome, rheumatoid arthritis, Hashimoto's disease/hypothyroiditis, primary biliary cirrhosis, mixed connective tissue disease, chronic active hepatitis, Graves' disease/hyperthyroiditis, scleroderma, chronic idiopathic thrombocytopenic purpura, diabetic neuropathy and septic shock.

I



# Comments

CAS Solutions | Preferences | SciFinder Help | Sign Out

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Explore | Saved Searches | **SciPlanner** | Link | Save | Print | Export

Research Topic "biological robustness" > references (57) > **Biological robustness**

REFERENCE DETAIL | Get Related Citations | Link to Other Sources | Send to SciPlanner

Return | Previous | Next

## 18. Biological robustness

By: Kitano, Hiroaki

A review. **Robustness** is a ubiquitously obsd. property of biol. systems. It is considered to be a fundamental feature of complex evolvable systems. It is attained by several underlying principles that are universal to both biol. organisms and sophisticated engineering systems. **Robustness** facilitates evolvability and robust traits are often selected by evolution. Such a mutually beneficial process is made possible by specific architectural features obsd. in robust systems. But there are trade-offs between **robustness**, fragility, performance and resource demands, which explain system behavior, including the patterns of failure. Insights into inherent properties of robust systems will provide the authors with a better understanding of complex diseases and a guiding principle for therapy design.

### Indexing

General Biochemistry (Section6-0)

### Concepts

#### QUICK LINKS

0 Tags, 1 Comment

#### SOURCE

*Nature Reviews Genetics*  
Volume5  
Issue11  
Pages826-837  
Journal; General Review  
2004  
CODEN:NRGAAM  
ISSN:1471-0056  
DOI:10.1038/nrg1471

## Comments

1 Comment | Sort by: Newer First | Older First

Zum Thema "biological robustness" gibt es in SciFinder weitere Arbeiten: Link: [https://scifinder-preview.cas.org/scifinder/view/link\\_v1/answerset.html?l=0TvlBlcjQgy3Ien0QixE5ZNcazwjq5U8CFgXU7VwvnEd2RevA7P6ZsG40rUINYduSFFZ7AifPnzXEMmoentSvQ](https://scifinder-preview.cas.org/scifinder/view/link_v1/answerset.html?l=0TvlBlcjQgy3Ien0QixE5ZNcazwjq5U8CFgXU7VwvnEd2RevA7P6ZsG40rUINYduSFFZ7AifPnzXEMmoentSvQ)

Posted September 16, 2009 7:15 AM | Edit | Delete  
Last Modified June 04, 2013 3:15 AM

⚠ Your changes have been saved.

Add Comment: Maximum of 1024 characters per comment; 50 comments per reference.

Zu jeder Literaturstelle kann man bis zu **50 Kommentare** verfassen, die jeweils maximal **1024 Zeichen** haben dürfen.

Die jeweils noch **verfügbaren Zeichen** werden beim Schreiben des Kommentars angezeigt.

Characters Remaining: **1024**

# Tags

CAS Solutions  
**SCIFINDER**  
A CAS SOLUTION

Explore Saved Searches SciPlanner

Research Topic "biological robustness" > references (57) > Biological robustness

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

REFERENCES: TAGS

Click a tag to retrieve references associated with that tag.

A	autorensuche scriba 17 september 2009
C	cholesterol regulation as entered
M	modeling of host-pathogen-interaction
T	testmethode für mikroorganismen
W	westerhoff 2009 1987

CAS Solutions  
**SCIFINDER**  
A CAS SOLUTION

Explore Saved Searches SciPlanner

Research Topic "robustness" > references (38862) > refine "human" (9609)

REFERENCES

Get Substances Get Reactions Get Related Citations

Analyze Refine Categorize

Sort by: Accession Number

0 of 9609 References Selected

Tools

- Remove Duplicates
- Combine Answer Sets
- Add Tag

1. Development of structure-activity relationship for metal oxide nanoparticles...  
By Liu, Rong; Zhang, Hai Yuan; Ji, Zhao Xia; Rallo, Robert; Xia, Tian; Chang, Dong; Hwang, Inse; Andrej, Corbin; Yoram...  
From Nanoscale (2013), 5(12), 5644-5653. | Language: English, Database: CAPLUS

2. Use of the Cultex Radial Flow System as an in vitro exposure method to assess acute pulmonary toxicity of fine dusts and nanoparticles with special focus on the intra- and inter-laboratory reproducibility...  
By Strenzitz, Dirk; Mehle, Niklas; Pohl, Christine; Papritz, Mirko; Stenger, Bernhard; Schmidt, Annette; Kikipatrick, Charles James; Thermann, Horst; Vogel, Richard; Hoffmann, Sebastian; et al  
From Chemo-Biological Interactions, Ahead of Print. | Language: English, Database: CAPLUS

## Add Tags

ⓘ Only 500 answers can be tagged at one time.

Add tags to:

- All answers (9609)
- Only selected answers (9609)

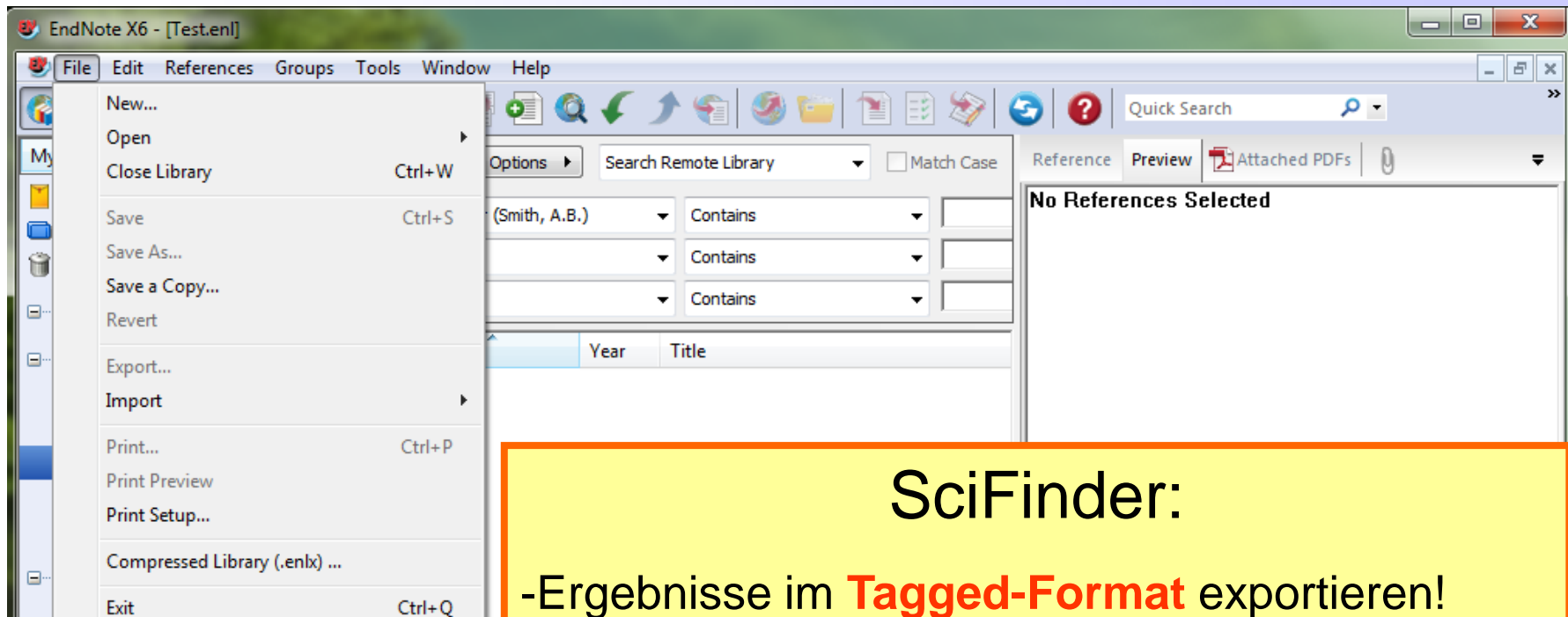
Add Tags: Separate multiple tags with semicolons, 100 characters per tag, 50 tags per reference

Save

Cancel

# Import von Daten aus SciFinder

- Treffer in SciFinder speichern
- In EndNote File / Import anklicken

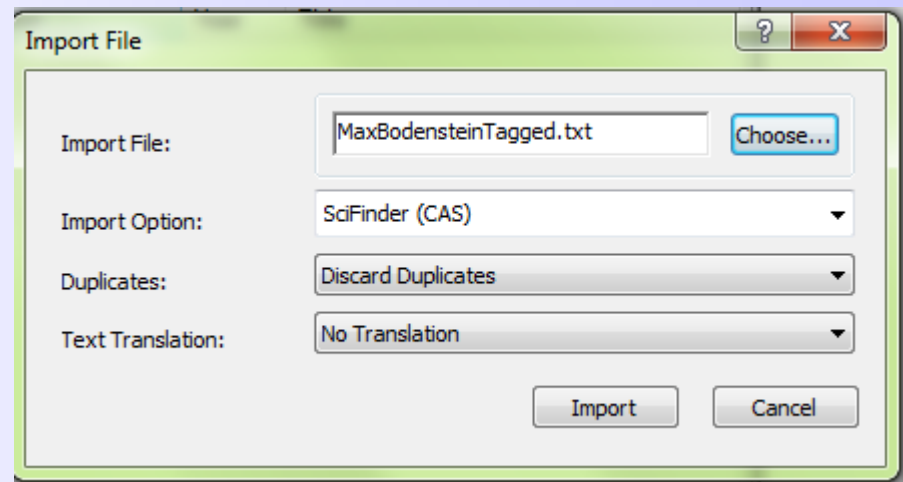
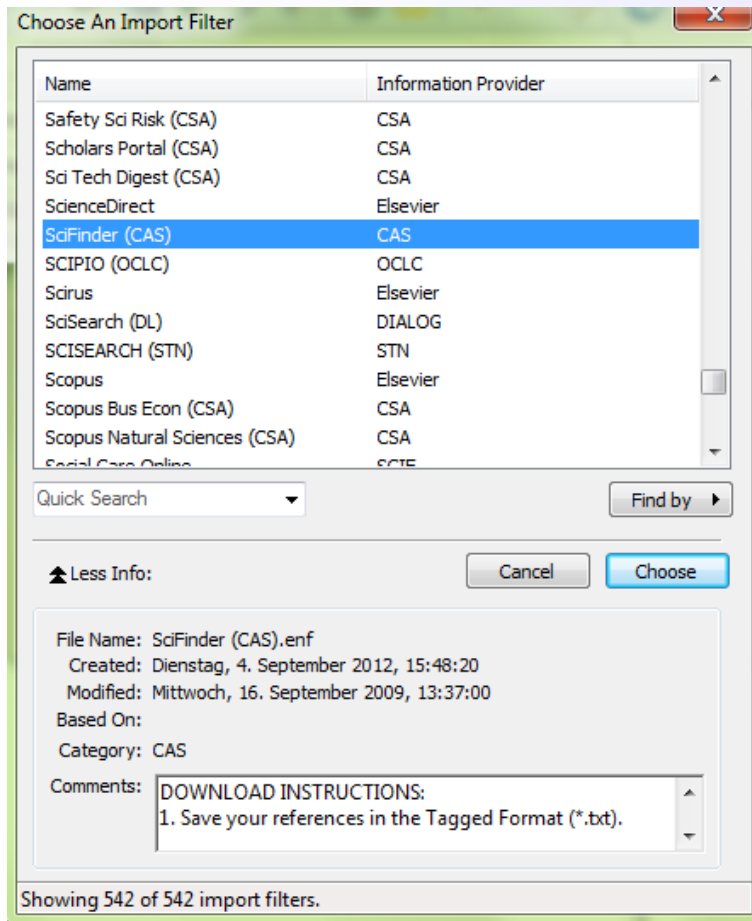


## SciFinder:

- Ergebnisse im **Tagged-Format** exportieren!
- Ergebnisse in diesem Format können in alle gängigen Literaturverwaltungsprogramme importiert werden!!

## Import aus SciFinder (2)

- Bei **Other Filters** wählt man **SciFinder** aus und bei Import Data File die Datei mit den Ergebnissen aus SciFinder



# Import von Daten aus SciFinder in EndnoteWeb

ENDNOTE®

## Anmelden oder ein Konto erstellen

E-Mail:

Kennwort:

Anmelden

Angemeldet bleiben

[Haben Sie Ihr Kennwort vergessen?](#)

**Institutionell/Shibboleth:** Melden Sie sich über die [institutionelle Anmeldung](#)

**Probieren Sie EndNote desktop 30 Tage lang.** Sie werden es mögen.  
Zugriff von überall – am Rechner und online.

Herunterladen



## Suchen

Durchsuchen Sie Online-Datenbanken nach Referenzen oder importieren Sie Ihre eigenen.



## Speichern

Organisieren und gruppieren Sie Referenzen nach Ihren Wünschen.



## Erstellen

Verwenden Sie Cite While You Write, um Lebensläufe und Literaturverzeichnisse zu erstellen und zu formatieren.



## Teilen

Teilen Sie Ihre Forschung und Referenzen mit Kollegen.

Willkommen, Ina

Web of Science™ | ResearcherID | Abmelden | Hilfe

## ENDNOTE® basic

Meine Referenzen | Erfassen | Organisieren | Format | Optionen | Verbinden<sup>Beta</sup>

[Schnelleinstieg ausblenden](#)

Bereich ausbl.

### Schnellsuche

Suchen nach

in Alle Referenzen

Suchen

### Meine Referenzen

Alle Referenzen (19)

[Nicht zugeordnet] (3)

Merkliste (0)

Papierkorb (0)

▼ Eigene Gruppen

Test (16)

## Erste Schritte mit



### Suchen

**Sammeln Sie** Referenzen, indem Sie Online-Datenbanken durchsuchen oder Ihre eigene Sammlung importieren.

- Online-Datenbank durchsuchen
- Referenz manuell erstellen
- Referenzen importieren



### Speichern Und Teilen

**Organisieren** und gruppieren Sie Referenzen nach Ihren Wünschen. Teilen Sie Ihre Gruppen dann mit Ihren Kollegen.

- Neue Gruppe erstellen
- Eine Gruppe freigeben
- Doppelte Referenzen suchen



### Erstellen

Verwenden Sie unser Plugin, um beim Schreiben Literaturverzeichnisse **zu formatieren** und Referenzen zu zitieren.

- Cite While You Write™-Plug-in
- Formatierte Bibliografie erstellen
- Dokument formatieren



### Verbinden<sup>Beta</sup>

Verbinden Sie sich mit Forschern aus aller Welt und **tauschen** Sie sich mit ihnen aus.

- Jetzt verbinden

# Import von Daten aus SciFinder in EndnoteWeb (2)

Willkommen, Ina

## ENDNOTE® basic

Meine Referenzen | Erfassen | Organisieren | Format

Onlinesuche | Neue Referenz | Referenzen importieren

### Referenzen importieren

Aus EndNote importieren?

Datei:  Keine Datei ausgewählt.

Importoption:  Favoriten auswählen

Nach:

Willkommen, Ina | Web of Science™ | ResearcherID | Abmelden | Hilfe

## ENDNOTE® basic

Meine Referenzen | Erfassen | Organisieren | Format | Optionen | Verbinden

### Schnellsuche

Suchen nach  
in: Alle Referenzen

### Meine Referenzen

Alle Referenzen (23)  
[Nicht zugeordnet] (3)  
Merkliste (0)  
Papierkorb (0)  
Eigene Gruppen  
Test (20)

### Test

10 pro Seite anzeigen | Seite 1 von 2 |  |  |

Alle | Seite | Zu Gruppe hinzufügen... | Sortieren nach: Erster Autor - A bis Z

Autor	Jahr	Titel
		Screening lactic acid bacteria capable of ameliorating lactose intolerance, by selecting bacterium having enhanced enteroadherence property and lactose degrading activity, from lactic acid bacteria belonging to genus Lactobacillus; ameliorating lactose...
Arah Onyebuchi, A.	2005	Health system outcomes and determinants amenable to public health in industrialized countries: a pooled, cross-sectional time series analysis BMC public health
Arah, Onyebuchi A.	2005	Health system outcomes and determinants amenable to public health in industrialized countries: A pooled, cross-sectional time series analysis BMC Public Health

Willkommen, Ina

## ENDNOTE® basic

Meine Referenzen | Erfassen | Organisieren | Format | Optionen | Verbinden

### Schnellsuche

Suchen nach  
in: Alle Referenzen

### Meine Referenzen

Alle Referenzen (23)  
[Nicht zugeordnet] (3)  
Merkliste (0)  
Papierkorb (0)  
Eigene Gruppen  
Test (20)

### Referenz in 'Alle Referenzen' anzeigen

◀ Datensatz 1 von 1 ▶

### Bibliografische Felder:

Dokumenttyp: Journal Article

Author: Gueguen, L.

Title: Milk calcium: functions, benefits, requirements and bioavailability Le calcium du lait: fonctions, interets, besoins, biodisponibilite

Year: 2005

Journal: Cahiers de Nutrition et de Dietetique

Volume: 40

Issue: 1

Pages: 0007-9960

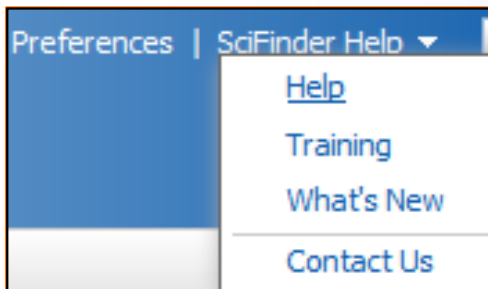
► Anhänge:

Optionale Felder:

Abstract: More than 99% of body calcium are localized in bones, and it is mainly known as a dietary factor in the prevention of osteoporosis. However, its role is not limited to bone health. Recent studies suggest its role in the prevention of arterial hypertension, cardiovascular diseases, renal calculi, colorectal cancer, overweight and obesity. The recommended calcium intake in France varied from 800 to 1200 mg/day based on age and physiological status. This recommendation is justified by the net requirements for

# SciFinder: Hilfeseiten

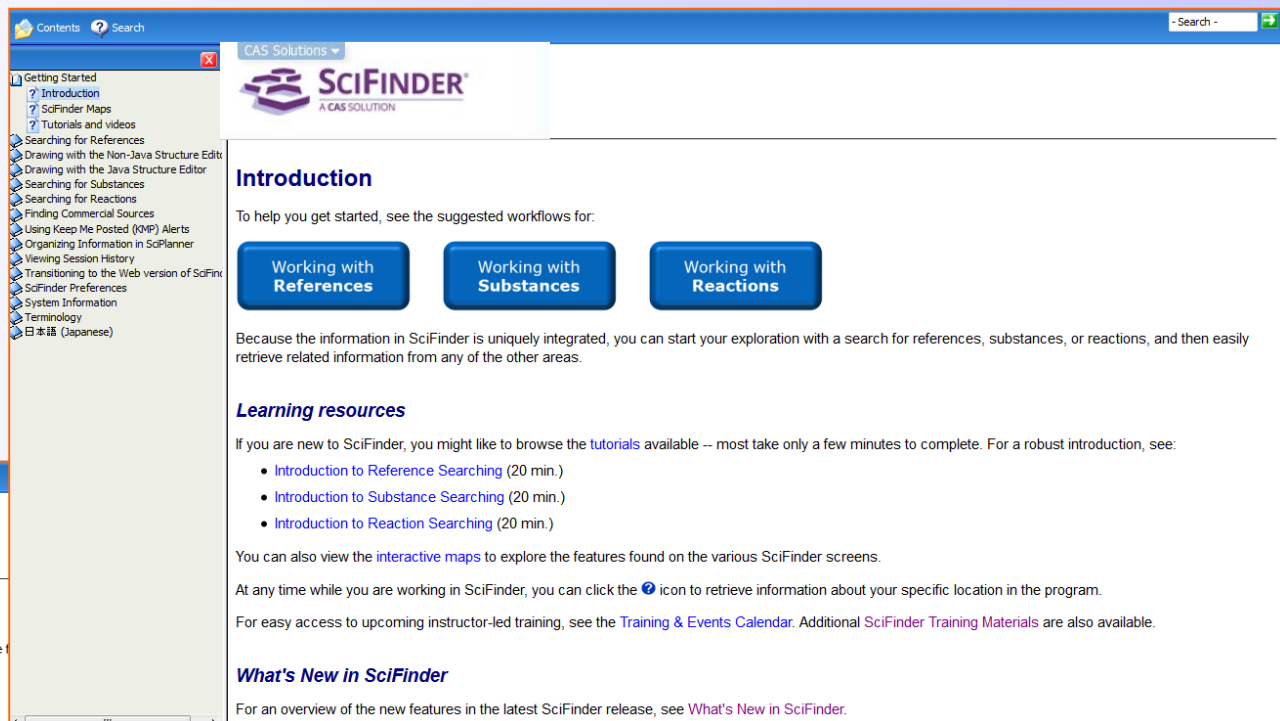
<https://scifinder.cas.org/help/scifinder/R32/index.htm>



Preferences | SciFinder Help ▾

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- Contact Us

**Zugriff online, während der Recherche**



Contents Search CAS Solutions

## Introduction

To help you get started, see the suggested workflows for:

- Working with References
- Working with Substances
- Working with Reactions

Because the information in SciFinder is uniquely integrated, you can start your exploration with a search for references, substances, or reactions, and then easily retrieve related information from any of the other areas.

### Learning resources

If you are new to SciFinder, you might like to browse the [tutorials](#) available -- most take only a few minutes to complete. For a robust introduction, see:

- Introduction to Reference Searching (20 min.)
- Introduction to Substance Searching (20 min.)
- Introduction to Reaction Searching (20 min.)

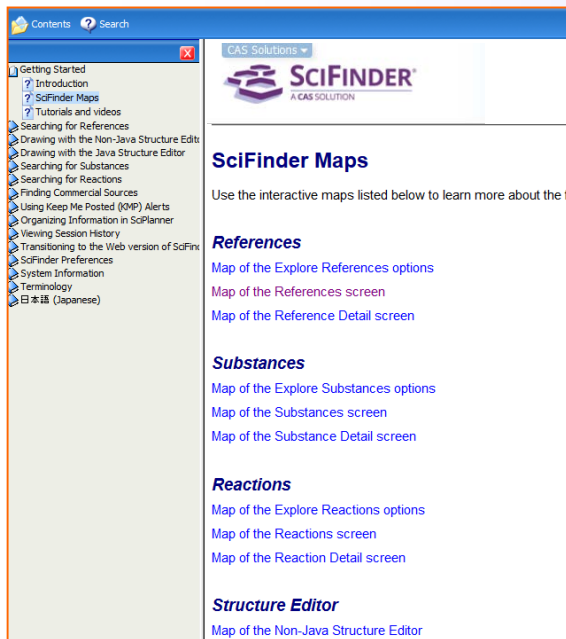
You can also view the [interactive maps](#) to explore the features found on the various SciFinder screens.

At any time while you are working in SciFinder, you can click the [i](#) icon to retrieve information about your specific location in the program.

For easy access to upcoming instructor-led training, see the [Training & Events Calendar](#). Additional [SciFinder Training Materials](#) are also available.

### What's New in SciFinder

For an overview of the new features in the latest SciFinder release, see [What's New in SciFinder](#).



Contents Search CAS Solutions

## SciFinder Maps

Use the interactive maps listed below to learn more about the

### References

- Map of the Explore References options
- Map of the References screen
- Map of the Reference Detail screen

### Substances

- Map of the Explore Substances options
- Map of the Substances screen
- Map of the Substance Detail screen

### Reactions

- Map of the Explore Reactions options
- Map of the Reactions screen
- Map of the Reaction Detail screen

### Structure Editor

- Map of the Non-Java Structure Editor

Über die o.g. Adresse kann man die Hilfeseiten auch unabhängig von der SciFinder-Nutzung aufrufen.

# CAS-Hilfen für SciFinder

<http://www.cas.org/training/scifinder>

## SciFinder Training Materials

CAS Solutions ▾



On-demand SciFinder® training resources are short, targeted materials, organized by search type. Titles marked with an asterisk (\*) are designed to help you get you started quickly with searching in SciFinder. [Special topics](#) for more advanced users are also available.

New and occasional users may also find the [Recorded Virtual Classes](#) materials helpful. Download the materials and listen to the recordings at your convenience.

### Need-to-Know Videos

Three minutes of practical, real-world applications of SciFinder features and capabilities. *(Special thanks to Dr. Michael Christiansen of Utah State University for his contributions to these videos.)*

#### Structure Searching

- [Input Structures Using the Drawing Editor](#)
- [Search for Chemical Compounds Using a Structure Search](#)
- [Find Property Data, Regulatory Information, Commercial Availability, Synthesis Information](#)

#### Reaction Searching

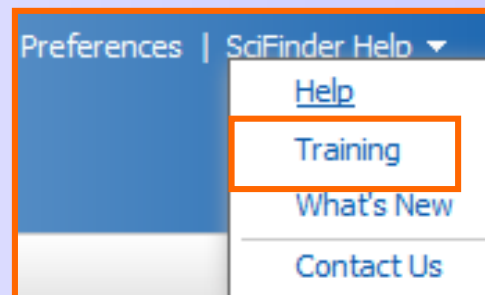
- [Search for Specific Reactions or Reaction Type](#)
- [Use SciPlanner to Plan a Synthesis Project](#)

#### Reference Searching

- [Search for a Specific Topic](#)
- [Search by Author Name](#)

#### General Topics

- [SciFinder PatentPak™ - A Patent Workflow Solution](#)
- [Save and Combine Search Results](#)
- [Find Competitive Intelligence Information and Stay Up to Date on New Developments](#)



Zugriff online, während der Recherche

## Tutorials

### Overview Materials

- [SciFinder Overview Presentation \(PDF\)](#)
- [Introduction to SciFinder](#)

### Reference Searching

- [Introduction to Reference Searching \(tutorial\)\\*](#)
- [文献检索简介 \(tutorial\)\\*](#)
- [Introducción a la búsqueda de Referencias \(tutorial\)\\*](#)
- [Introdução à Pesquisa por Referência \(tutorial\)\\*](#)
- [How to Create a Reference Answer Set - Search by Research Topic, Author Name, Company Name, and Document Identifier. \(PDF\)\\*](#)
- [How to Work with a Reference Answer Set - Analyze, Refine, and Categorize search results. \(PDF\)\\*](#)
- [Effective Keyword Searching Tips \(PDF\)\\*](#)
- [Search by Research Topic and Set Up Alerts to Keep Current - \(7 minutes\)](#)



# Was gibt es Neues bei SciFinder?

<http://www.cas.org/products/scifinder/whats-new-in-scifinder>

## What's New in SciFinder

CAS Solutions



**SCIFINDER**  
A CAS SOLUTION

## Preserve Your Most Valuable Resource - Time - With PatentPak™ (February 2015)

PatentPak is a robust, new patent workflow solution designed to radically reduce the time spent acquiring and searching through multiple patents to find vital chemistry. PatentPak is available as an add-on to SciFinder and features:

- Full text PDFs from 11 major patent offices
- Patent Family PDFs in multiple languages
- Patent page numbers for key indexed substances

SciFinder interface showing search results for patent WO 2012007375. The interface includes a search bar, navigation tabs (Explore, Saved Searches, SciPlanner), and a list of references. The selected reference is titled "1. Pyrazolo[1,5-a]pyrimidine and thieno[3,2-b]pyrimidine derivatives as IRAK4 modulators and their preparation". A red arrow points to the "PatentPak" label next to the patent title. A table below the title lists patent details:

Patent No.	Kind	Language
WO 2012007375	A1	English
CN 102985426	A	Chinese
JP 2013511018	T	Japanese
KR 2013132396	A	Korean
US 20120015992	A1	English
US 20140303149	A1	English

Navigation menu with the following items: Preferences, SciFinder Help, Help, Training, What's New (highlighted), Contact Us.

Zugriff online, während der Recherche

# SciFinder-Portal in Jena



 IVS Chemisch-Geowiss. Fakultät  
Wiss. Informationsstelle BPFakultät

FSU Jena

CAS Solutions  
**SCIFINDER**  
A CAS SOLUTION

## Aktuelle Informationen zu SciFinder

Aktuelle Informationen zu SciFinder

SciFinder Übersicht

SciFinder Registrierung

SciFinder Anleitungen (ppt/pdf)

SciFinder Anleitung (Browser)

SciFinder unter Linux

SciFinder: Sign In

SciFinder Recherchestrategien

SciFinder auf der Homepage von CAS

Seit Februar 2008 steht an der Uni Jena der SciFinder mit einer neuen Oberfläche zur Verfügung. Die Nutzung erfolgt über einen Browser, eine Softwareinstallation ist nicht mehr nötig.

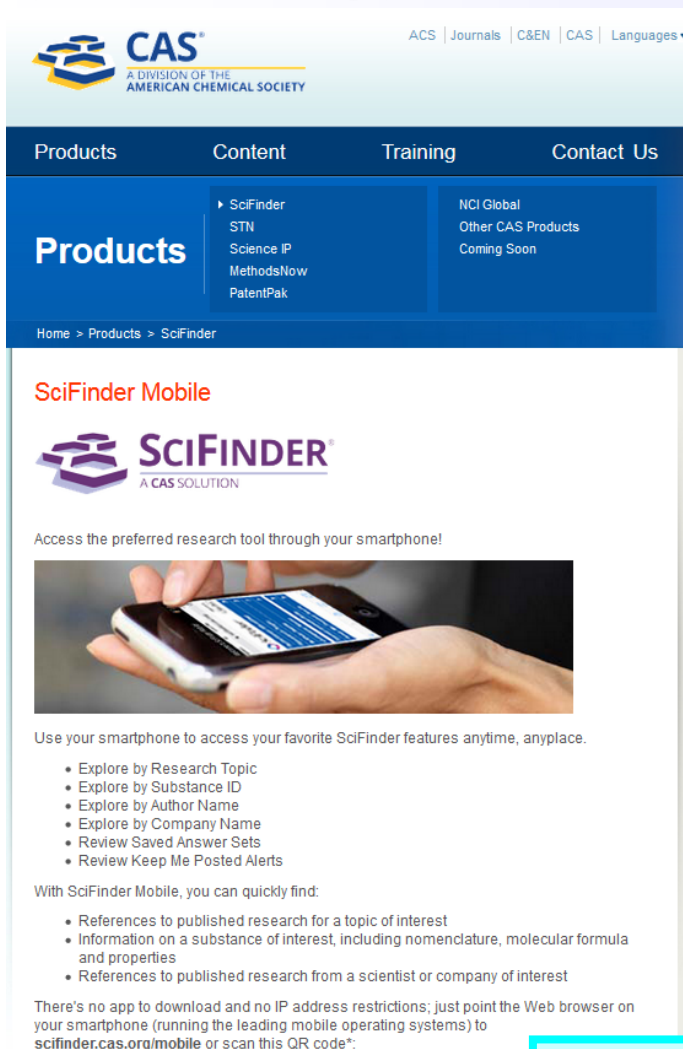
Vor der allerersten Nutzung des neuen SciFinders müssen Sie sich bei CAS [als Nutzer registrieren](#).

**Viel Spaß bei der Arbeit mit dem neuen SciFinder!**

<http://pinguin.biologie.uni-jena.de/SFHomepage/index.html>

# SciFinder auf dem Smartphone

<http://www.cas.org/products/scifinder/sf-mobile>



The screenshot shows the CAS website interface. At the top, there is the CAS logo and navigation links for ACS, Journals, C&EN, CAS, and Languages. Below this is a main navigation bar with 'Products', 'Content', 'Training', and 'Contact Us'. The 'Products' section is expanded, showing 'SciFinder' as a primary option, along with 'STN', 'Science IP', 'MethodsNow', and 'PatentPak'. To the right, there are links for 'NCI Global', 'Other CAS Products', and 'Coming Soon'. Below the navigation, a breadcrumb trail reads 'Home > Products > SciFinder'. The main content area is titled 'SciFinder Mobile' and features the SciFinder logo with the tagline 'A CAS SOLUTION'. A sub-header reads 'Access the preferred research tool through your smartphone!' followed by an image of a hand holding a smartphone displaying the SciFinder mobile interface. Below the image, text states 'Use your smartphone to access your favorite SciFinder features anytime, anywhere.' and lists several features: 'Explore by Research Topic', 'Explore by Substance ID', 'Explore by Author Name', 'Explore by Company Name', 'Review Saved Answer Sets', and 'Review Keep Me Posted Alerts'. Further down, it says 'With SciFinder Mobile, you can quickly find:' and lists 'References to published research for a topic of interest', 'Information on a substance of interest, including nomenclature, molecular formula and properties', and 'References to published research from a scientist or company of interest'. At the bottom, it notes 'There's no app to download and no IP address restrictions; just point the Web browser on your smartphone (running the leading mobile operating systems) to [scifinder.cas.org/mobile](http://scifinder.cas.org/mobile) or scan this QR code\*:'.

- Einfache Recherchen in SciFinder kann man seit April 2011 auch mit dem Smartphone machen.
- Die Nutzung erfolgt über eine spezielle Internetadresse und mit dem eigenen Benutzernamen und Passwort für SciFinder!

Einfach den QR-Code mit dem Smartphone fotografieren und die mobile SciFinder- Nutzung kann beginnen.

(Einen kostenlosen QR-Code Reader für Ihr Smartphone erhalten Sie unter <http://get.neoreader.com>)



Zugang zum mobilen SciFinder:  
<http://scifinder.cas.org/mobile>





## Teil 3: Suche von Strukturen und Reaktionen

- Suche nach chemischen Substanzen über den Namen oder mit der Registry - Nummer
- Suche nach chemischen Substanzen mit einer Strukturrecherche
- Substruktursuche, Strukturähnlichkeitssuche
- Reaktionssuche
- Struktursuche - ohne Zeichnen der Verbindung
- Nach der Reaktionssuche - weiter ohne Zeichnen der Verbindung
- SciPlanner: interaktive Syntheseplanung

# Suche nach chemischen Substanzen über den Namen oder mit der Registry-Nummer

**Gesucht:  
Biosynthese von Ochratoxin A oder D  
mit Aspergillus-Spezies**

CAS Solutions

SCIFINDER<sup>®</sup>  
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags
- SUBSTANCES**
- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier**
- REACTIONS
- Reaction Structure

SUBSTANCES: SUBSTANCE IDENTIFIER ?

ochratoxin A  
ochratoxin D

Enter one per line.  
Examples:  
50-00-0  
999815  
Acetaminophen

Search

Maximal **20 Substanzen** können bei **Substance Identifier** untereinander geschrieben werden.

# Liste der gefundenen Substanzen

CAS Solutions

SCIFINDER  
A CAS SOLUTION

Explore | Saved Searches | SciPlanner

Substance Identifier "ochratoxin a; ochratoxin d" > substances (2)

Get References | Get Reactions | Get Commercial Sources | Tools

Sort by: CAS Registry Number

0 of 2 Substances Selected

1. 911450-31-3

2. 393-17-9

Analyze by: Substance Role

- Analytical Study: 2
- Biological Study: 2
- Preparation: 2
- Combinatorial Study: 1
- Formation, Nonpreparative: 1
- Occurrence: 1
- Process: 1
- Properties: 1
- Reactant or Reagent: 1
- Uses: 1

Unspecified  
Ochratoxin A

Send to SciPlanner

Display Options

Answers per Page: 15, 20, 25, 50

Layout Options: 2 columns, 3 columns, 4 columns

Namen, Summenformel, Eigenschaften dieses Treffers ansehen

Zugang zu den Abstracts, zu den Reaktionen bzw. zu den Anbietern der Substanz

Answers pro Seite von 15-50 und Spalten von 1-4 sind wählbar.

Cc1oc(=O)c2c(O)c(Cl)ccc2c1C(=O)N[C@@H](C(=O)O)Cc3ccccc3

Absolute stereochemistry, Rotation (-).

C<sub>20</sub>H<sub>18</sub>ClN<sub>1</sub>O<sub>6</sub>  
L-Phenylalanine, N-[[[(3R)-5-chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1H-2-benzopyran-7-yl]carbonyl]-

Regulatory Information  
Experimental Properties

# Relevanzranking bei den Treffern der Substanzsuche

CAS Solutions

**SCIFINDER**  
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "ochratoxin A" > **substances (1)** > 303-47-9 > get reactions (22)

**SUBSTANCES** ?

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

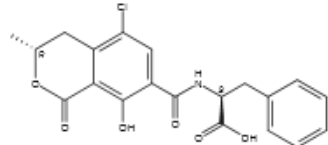
Analyze by: ?  
Substance Role ▾

Analytical Study 1  
Biological Study 1  
Combinatorial Study 1  
Formation, Nonpreparative 1  
Occurrence 1  
Preparation 1  
Process 1  
Properties 1  
Reactant or Reagent 1  
Uses 1

Sort by: CAS Registry Number ▾

- CAS Registry Number
- Number of References
- Number of Commercial Sources (New)
- Molecular Weight
- Molecular Formula

1. ~4936 ~62



Rotation (-), Absolute stereochemistry.

**C<sub>20</sub>H<sub>18</sub>ClNO<sub>6</sub>**  
L-Phenylalanine, *N*[[[(3*R*)-5-chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1*H*-2-benzopyran-7-yl]carbonyl]-

Regulatory Information  
Experimental Properties

Die Ergebnisse einer Substanzsuche über den Namen bzw. die RN - Nummer kann man mit „Sort by“

- nach der CAS-RN
- der Substanznummer
- dem Molekulargewicht
- und der Summenformel sortieren.

# Einzelansicht der Substanz (1)

SUBSTANCE DETAIL ?

Get References

Get Reactions

Get Commercial Sources

Return

## 2. CAS Registry Number 303-47-9

~4,959   ~64 

**C<sub>20</sub> H<sub>18</sub> Cl N O<sub>6</sub>**

L-Phenylalanine, *N*-[[[(3*R*)-5-chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1*H*-2-benzopyran-7-yl]carbonyl]-

### Molecular Weight

403.81

### pKa (Predicted)

Value: 3.29±0.10 | Condition: Most Acidic Temp: 25 °C

### Melting Point (Experimental)

Value: 169 °C

### Boiling Point (Predicted)

Value: 632.4±55.0 °C | Condition: Press: 760 Torr

### Density (Predicted)

Value: 1.425±0.06 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr

### Other Names

Alanine, *N*-[(5-chloro-8-hydroxy-3-methyl-1-oxo-7-isochromanyl)carbonyl]-3-phenyl-, (-)- (8CI)

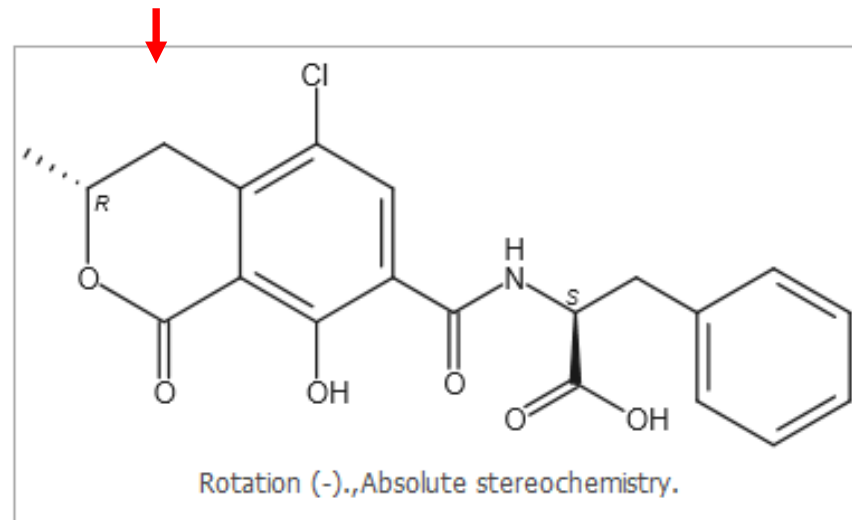
L-Phenylalanine, *N*-[(5-chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1*H*-2-benzopyran-7-yl)carbonyl]-, (*R*)-

Ochratoxin A (7CI)

(*R*)-*N*-[(5-Chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1*H*-benzo[*c*]pyran-7-yl)carbonyl]-3-phenylalanine

3*R*.14*S*-Ochratoxin A

## Strukturformel



## Wichtige Stoffeigenschaften

Oben: Systematischer Name

Unten: Weitere Namen, (Handels- und Trivialnamen)



# Einzelansicht der Substanz (2) - Eigenschaften

Expand All | Collapse All

- ▶ EXPERIMENTAL PROPERTIES
- ▶ EXPERIMENTAL SPECTRA
- ▶ PREDICTED PROPERTIES
- ▶ PREDICTED SPECTRA
- ▶ REGULATORY INFORMATION
- ▶ CAS REFERENCE ROLES
- ▶ ADDITIONAL DETAILS

▼ EXPERIMENTAL PROPERTIES

Biological | Chemical | **Optical and Scattering** | Thermal

Optical and Scattering Properties	Value	Condition
Optical Rotatory Power	+68 °	Conc: 0.041 g/100mL; Solv: methanol
Optical Rotatory Power	-31.5 °	Conc: 0.5 g/100mL; Solv: chloroform
Optical Rotatory Power	-118 °	Solv: chloroform (67-66-3)

Notes

- (6) Gabriele, Bartolo; Synthesis 2009, (11), P1815-1820 CAPLUS 🔍
- (8) Cramer, Benedikt; Bioorganic & Medicinal Chemistry 2010, V18(1), P343-347 CAPLUS 🔍
- (37) "Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)

▼ EXPERIMENTAL SPECTRA

**<sup>1</sup>H NMR** | <sup>13</sup>C NMR | IR | Mass | UV and Visible

<sup>1</sup> H NMR Properties	Value	Condition
Proton NMR Spectrum	See full text	
Proton NMR Spectrum	See full text	
Proton NMR Spectrum	See full text	

Notes

- (6) Gabriele, Bartolo; Synthesis 2009, (11), P1815-1820 CAPLUS 🔍
- (7) Dais, Photis; Journal of Physical Chemistry B 2005, V109(35), P16926-16936 CAPLUS 🔍
- (8) Cramer, Benedikt; Bioorganic & Medicinal Chemistry 2010, V18(1), P343-347 CAPLUS 🔍

Links zu den verfügbaren Eigenschaften

# Bioactivity Indicators und Target Indicators

Substance Identifier "valproic acid" > substances (1) > 99-66-1

SUBSTANCE DETAIL

Get References

Get Reactions

Get Commercial Sources

Return

CAS Registry Number 99-66-1

~9,345 ~106

$C_8H_{16}O_2$

Pentanoic acid, 2-propyl-

Molecular Weight

144.21

pKa (Predicted)

Value: 4.82±0.20 | Condition:

Melting Point (Experimental)

Value: 25 °C

Boiling Point (Experimental)

Value: 221-222 °C | Condition:

Density (Experimental)

Value: 0.904 g/cm<sup>3</sup> | Condition:

Other Names

Valeric acid, 2-propyl- (6CI, 7C)

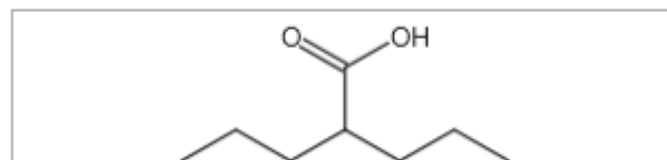
2,2-Di-*n*-propylacetic acid

2-Propylpentanoic acid

2-Propylvaleric acid

4-Heptanecarboxylic acid

View more...



- ▶ EXPERIMENTAL SPECTRA
- ▶ PREDICTED PROPERTIES
- ▶ PREDICTED SPECTRA
- ▶ REGULATORY INFORMATION
- ▶ BIOACTIVITY INDICATORS
- ▶ TARGET INDICATORS
- ▶ CAS REFERENCE ROLES
- ▶ ADDITIONAL DETAILS

## BIOACTIVITY INDICATORS

### Indicators

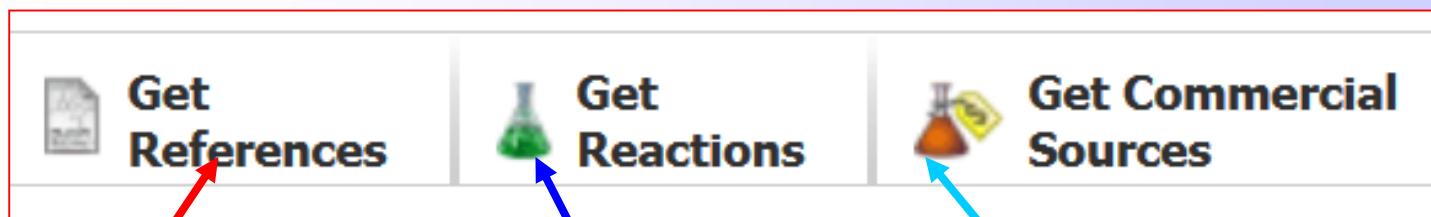
Indicators	References
Anti-infective agents (all) >> Antibiotics	77
Anti-infective agents (all) >>> Anti-HIV agents	57
Anti-infective agents (all) >>> Antiviral agents	63
Anti-inflammatory agents (all) > Anti-inflammatory agents	119
Anti-inflammatory agents (all) > Nonsteroidal anti-inflammatory drugs	76
Antitumor agents (all) > Antiangiogenic agents	54
Antitumor agents (all) > Antitumor agents	803
Cytoprotective agents (all) > Cytoprotective agents	61
Cytoprotective agents (all) > Neuroprotective agents	284
Enzyme inhibitors (all) > Histone deacetylase inhibitors	205
Ion channel blockers (all) > Calcium channel blockers	57
Nervous system agents (all) >>> Analgesics	113
Nervous system agents (all) >> Anti-Alzheimer agents	61
Nervous system agents (all) >> Anticonvulsants	2087
Nervous system agents (all) >>> Anticonvulsants	2087
Nervous system agents (all) >>> Antidepressants	363

## TARGET INDICATORS

### Indicators

Indicators	References
Apoptosis-regulating proteins (all) > Bax proteins	37
Apoptosis-regulating proteins (all) > Bcl-2 proteins	82
Apoptosis-regulating proteins (all) > Bcl-x proteins	17
Calcium-binding proteins (all) > Osteocalcins	13
Caspase recruitment domain-containing proteins (all) >> Caspase-9	27
Cell cycle regulatory proteins (all) >>> Cyclin-dependent kinase 4	10
Cell cycle regulatory proteins (all) >> Cyclin-dependent kinase inhibitor proteins	81
Cell cycle regulatory proteins (all) >>> Cyclins	51
Cytokines (all) > Cytokines	21
Cytokines (all) >> Interferons	26
Cytokines (all) >>> Interleukin 1β	33
Cytokines (all) >>> Interleukin 1β	33
Cytokines (all) >>> Interleukin 6	34

# Weitere Ansichtsmöglichkeiten bei den Substanztreffern



**Textstellen dieser Verbindung in CAPIus und Medline**

**Reaktionen aus der Datenbank CASREACT**

**Lieferanten dieser Verbindung**



# Textstellen zur Herstellung von „Ochratoxin A“ mit

## „Get References“

CAS Solutions

SCIFINDER  
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "ochratoxin A" > substances (1) > get references (0)

SUBSTANCES ?

Analyze Refine

Analyze by: ?

Substance Role ▾

Analytical Study 1

Biological Study 1

Combinatorial Study 1

Formation, Nonpreparative 1

Occurrence 1

Preparation 1

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. 303-47-9

~4936

~62

a)

Rotation (-), Absolute stereochem

$C_{20}H_{18}ClNO_6$   
L-Phenylalanine, *N*-[[[(3*R*)-5-chloro-3,4-dihydroxy-3-methyl-1-oxo-1*H*-2-benzopyr-5-ylidene]amino]propanoic acid

Get References

Get Reactions

Limit results to:

- 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 Cancel


**Hinweis:** Bei der Auswahl von **References associated with** recherchiert man (ausser bei Preparation) **nicht** im gesamten Bestand von CAPlus!!! Siehe Informationen zu CAS Roles (Seite 4):


<http://www.cas.org/ASSETS/EB85B919049C4E448DCF8D391788F0DD/casroles.pdf>

# Trefferliste im Standard - Format

Substance Identifier "ochratoxin a; ochratoxin d" > substances (2) > **get references (642)** > refine "aspergillus" (394)


REFERENCES ?

 Get Substances

 Get Reactions

 Get Related Citations

 Tools ▾

 Create Keep Me Posted Alert

Analyze

**Refine**

Categorize

Sort by: Accession Number ▾ ↓

0 of 642 References Selected

Page: <<

Refine by: ?

Research Topic

Author

Company Name

Document Type

Publication Year

Language

Database

Research Topic

aspergillus


Examples:

*The effect of antibiotic residues on dairy products*

*Photocyanation of aromatic compounds*

Refine

1. **Method for preparing and purifying ochratoxin A and ochratoxin B**

 Quick View  Other Sources

By Wu, Aibo; Zhao, Zhiyong; Song, Suquan; Wang, Jianhua; Liu, Na; Nie, Dongxia; Yang, Xianli; Lin, Shanhai  
From Faming Zhuanli Shenqing (2014), CN 104178535 A 20141203. | Language: Chinese, Database: CAPLUS

2. **Comparison of five different C18 HPLC analytical columns for the analysis of ochratoxin A in different matrices**

 Quick View  Other Sources

By Sultan, Y.; Magan, N.; Medina, A.  
From Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2014), 971, 89-93.  
| Language: English, Database: CAPLUS

3. **Improved method for the simultaneous determination of aflatoxins, ochratoxin A and Fusarium toxins in cereals and cereal derived products by liquid chromatography-tandem mass spectrometry after multi-toxin immunoaffinity clean-up**

 Quick View  Other Sources

By Lattanzio, Veronica Maria Teresa; Ciasca, Biancamaria; Powers, Stephen; Visconti, Angelo  
From Journal of Chromatography A (2014), 1354, 139-143. | Language: English, Database: CAPLUS

4. **Evaluation by means of HPLC-MS of aflatoxins and OTA production by 20 strains of Aspergillus and Penicillium isolated from compost**

Herstellung von „Ochratoxin A“ mit **Get References** nach Einschränken mit **aspergillus** über **Refine by Research Topic**

# Nachweise zur Herstellung von „Ochratoxin A“ mit „Get Reactions“

CAS Solutions  
**SCIFINDER**  
A CAS SOLUTION

Explore Saved Searches SciPlanner

Substance Identifier "ochratoxin A" > substances (1) > 303-47-9

Get References Get Reactions Get Commercial Sources

Return

CAS Registry Number 303-47-9

~4,936 ~62

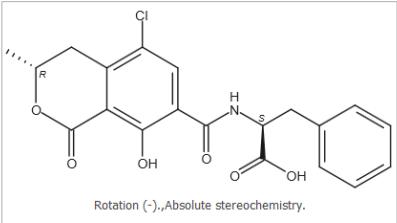
**C<sub>20</sub> H<sub>18</sub> Cl N O<sub>6</sub>**  
L-Phenylalanine, N-[[[(3R)-5-chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1H-2-benzopyran-7-yl]carbonyl]-

**Molecular Weight**  
403.81

**pKa (Predicted)**  
Value: 3.29±0.10 | Condition: Most Acidic Temp: 25 °C

**Melting Point (Experimental)**  
Value: 169 °C

**Boiling Point (Predicted)**



Rotation (-), Absolute stereochemistry.

### Get Reactions

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

- Product
- Reactant
- Reagent
- Reactant or reagent

Get Cancel

CAS Solutions Preferences | SciFinder Help | Sign Out

Access provided by FSU Jena  
Welcome Ina Weiss

Explore Saved Searches SciPlanner Save Print Export

Substance Identifier "ochratoxin A" > substances (1) > 303-47-9 > **get reactions (22)**

REACTIONS Get References Tools

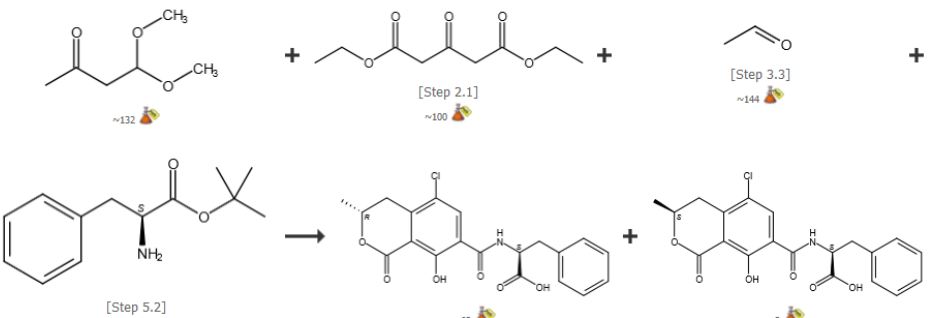
Analyze Refine Group by: No Grouping Sort by: Accession Number Display Options

Analyze by: Catalyst DMF 5 KOH 1 Show More

0 of 22 Reactions Selected

1. View Reaction Detail Link

5 Steps Hover over any structure for more options.



[Step 2.1] [Step 3.3] [Step 5.2]

# Alle Schritte einer Reaktion auf einen Blick

Anklicken: **View Reaction Detail**

REACTION DETAIL ⓘ

[Get Reference Detail](#) [Get Full Text](#) [Get Similar Reactions](#) [Send to SciPlanner](#)

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

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

OCCO + COCC → C=C

Stages	Notes	Yield
1.1 R:H <sub>2</sub> O, C:12027-38-2, 250°C, 30 bar	thermal, microreactor used, high pressure, flow system, gas phase, other products also detected, solid-supported catalyst, silicotungstic acid on silica support, Reactants: 2, Reagents: 1, Catalysts: 1, Steps: 1, Stages: 1 <b>Transformation:</b> Uncategorized	

[Experimental Procedure](#)

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

### SOURCE

Process for preparing alkenes from oxygenates with supported heteropoly acid catalysts 🔍  
Partington, Stephen Roy  
Assignee BP P.L.C., UK  
2011

### PATENT INFORMATION

Sep 1, 2011  
WO 2011104494  
A1

### NUMBER OF STEPS

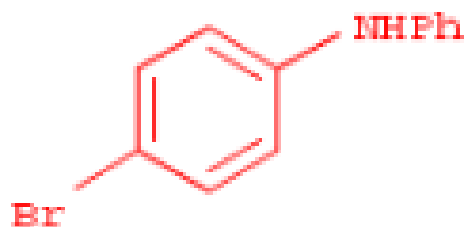
1

Einzelne Reaktionsschritte sind sichtbar.

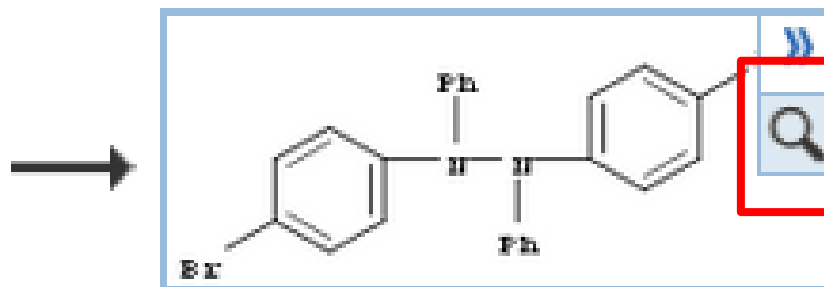
Ausgangsstoffe und Produkte für Substanzinformationen sind anklickbar.

# Interaktive Anzeigen bei Reaktionen (1)

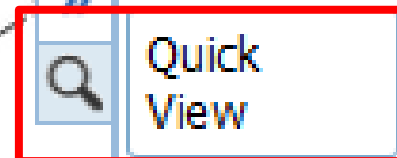
Single Step *Hover over any structure for more options.*



~65



71%



Mit dem *Quick View* kann man sich den Namen der Verbindung anzeigen lassen und welche Informationen über sie vorhanden sind.

## Quick View

**CAS Registry Number:** 38131-83-8

**Formula:** C<sub>24</sub>H<sub>18</sub>Br<sub>2</sub>N<sub>2</sub>

**CA Index Name:** Hydrazine, 1,2-bis(4-bromophenyl)-1,2-diphenyl-

### Other Names

1,2-Bis(*p*-bromophenyl)-1,2-diphenylhydrazine

### Number of References

~3

### Document Types

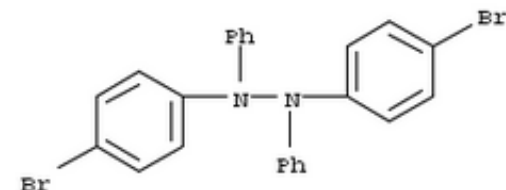
Journal

### Properties

Predicted

### Commercial Sources

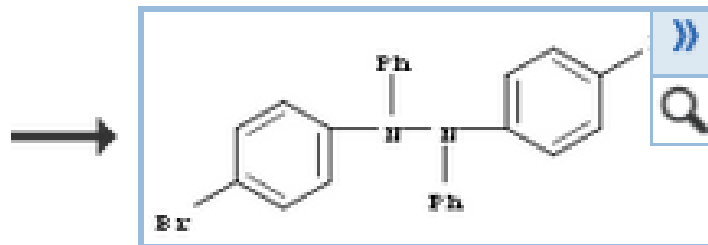
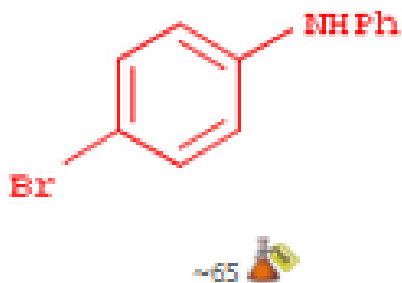
Not Available





## Interaktive Anzeigen bei Reaktionen (2)

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



Click for more options

71%

CAS Registry Number: 60-29-7

View Substance Detail

Explore by Structure ▶

Synthesize this...

Get Reactions where Substance is a ▶

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Send to SciPlanner

Product

Reactant

Reagent

Reactant/Reagent

Catalyst

Solvent

Any Role

Hervorragende  
Möglichkeit zur Suche  
nach mehrstufigen  
Synthesen (Retrospektive  
Syntheseplanung)

Klicken auf die für Sie  
interessante  
Verbindung und  
wählen dann die  
gewünschte  
weiterführende  
Information aus.

# Sortiermöglichkeiten bei den Reaktionstreffern

Group by: No Grouping

- No Grouping
- Document
- Transformation

Group by: No Grouping

Sort by: Experimental Procedure

- Experimental Procedure
- Accession Number
- Number of Steps
- Product Yield
- Publication Year

0 of 22 Reactions Selected

1. View Reaction Detail [Link](#)

5 Steps *Hover over any structure for more options.*

Group by: Transformation

Sort by: Frequency

- Frequency
- Title

0 of 22 Reactions Selected

1. Hydrolysis or Hydrogenolysis of Carboxylic Esters or Thioesters  
4 Reactions

Y = O, S

2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids  
2 Reactions

3. Acylation of Nitrogen Nucleophiles with Carboxylic Esters and Analogs  
1 Reaction

Group by: Document

Sort by: Accession Number

- Accession Number
- Experimental Procedure
- Number of Steps
- Product Yield
- Publication Year

0 of 22 Reactions Selected

1. First Synthesis of a Stable Isotope of Ochratoxin A Metabolite for a Reliable De

5 Reactions

5 Steps *Hover over any structure for more options.*

Group by Document:

Aus jeder Publikation wird nur eine Reaktion angezeigt.

Group by Transformation:

Sortierung nach Reaktionstyp

# Anzeige ausführlicher Synthesevorschriften schon im SciFinder

REACTIONS ⓘ

Analyze

Refine

Analyze by: ⓘ

Experimental Procedure ▾

Experimental Procedures

Available

87

Experimental Procedures Not Available

62

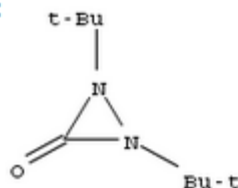
Führen Sie eine Analyse nach „*Experimental Procedure*“ durch und wählen dann, die Antworten aus, die diese Angaben enthalten.

Overview

Steps/Stages

1.1 C:CuBr, S:MeCN, 3 min, rt

1.2 R:



2 h, rt

Notes

scalable, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Facile Cu(I)-Catalyzed Oxidative Coupling of Anilines to Azo Compounds and Hydrazines with Diaziridinone under Mild Conditions

[Quick View](#) [Full Text](#)

By Zhu, Yingguang and Shi, Yian

From Organic Letters, 15(8), 1942-1945; 2013

Experimental Procedure

**LETTERS**

General/Typical Procedure: **Representative procedure for oxidative coupling of secondary anilines (Scheme 4):** To a 50 mL single-necked flask equipped with a stir bar were added bis(4-bromophenyl)amine (**4f**) (2.616 g, 8.0 mmol), CuBr (0.0574 g, 0.40 mmol) and CH<sub>3</sub>CN (16 mL). After the mixture was stirred at rt for 3 min, di-*tert*-butyldiaziridinone (**1**) (1.498 g, 8.8 mmol) was added in one portion. The reaction mixture was vigorously stirred at rt for 2 h, concentrated and purified by flash chromatography (silica gel, hexanes:dichloromethane = 4:1) to give hydrazine **5f** (Scheme 4, **5f** **1,1,2,2-Tetrakis(4-bromophenyl)hydrazine** Scheme 4, **5e** **1,2-Bis(4-bromophenyl)-1,2-diphenylhydrazine** White solid; yield 71%. mp 86-88 °C; IR (film) 1584, 1487 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.39-7.07 (m, 16H), 7.05-6.86 (m, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 142.8, 142.6, 132.3, 129.5, 123.1, 119.6, 118.5, 114.4; Anal. Calcd for C<sub>24</sub>H<sub>18</sub>Br<sub>2</sub>N<sub>2</sub>: C, 58.33; H, 3.67; N, 5.67. Found: C, 58.11; H, 3.89; N, 5.62

„*Experimental Procedure*“ wird nach Anklicken ausgeklappt.

# Ansichtmöglichkeit „Experimental Procedure“ auch über die Sortier- bzw. Gruppierungsfunktion

Group by:  Sort by:

Group by:  Sort by:

▼ Overview

**Steps/Stages**

- 1.1 R:BuLi, R:*i*Pr<sub>2</sub>NH, S:THF, S:Me(CH<sub>2</sub>)<sub>4</sub>
- 1.2 S:THF, -78°C; 30 min, -78°C
- 1.3 10 min, -78°C; 45 min, 0°C
- 1.4 R:AcOH
- 2.1 R:SO<sub>2</sub>Cl<sub>2</sub>, S:CH<sub>2</sub>Cl<sub>2</sub>, 18 h, rt
- 2.2 R:LiOH, S:H<sub>2</sub>O, S:EtOH, 1 h, reflux;
- 2.3 R:HCl, S:H<sub>2</sub>O, 1 h, rt
- 3.1 R:Cl(O=)CC(=O)Cl, C:DMF, S:CH<sub>2</sub>Cl<sub>2</sub>
- 3.2 R:Et<sub>3</sub>N, S:CH<sub>2</sub>Cl<sub>2</sub>, S:DMF, rt; 15 min,
- 3.3 R:Et<sub>3</sub>CCO<sub>2</sub>H, S:CH<sub>2</sub>Cl<sub>2</sub>, rt; 1 h, rt

Experimental Procedure

▼ Experimental Procedure

**SYNTHESIS** **Sequence 1**

**Step 1**

***tert*-Butyl L-Phenylalaninate (7)** Concd HClO<sub>4</sub> (70%; 1.5 mL, 2.5 g, 17.4 mmol) was slowly added to a suspension of L-phenylalanine (1.8 g, 10.9 mmol) in *t*-BuOAc (27.0 mL, 23.3 g, 200 mmol) under N<sub>2</sub> at 0 °C. After stirring of the mixture at 25 °C for 12 h, H<sub>2</sub>O (55 mL) followed by 1 N HCl (30 mL) were added. The mixture was basified to pH 9 by the addition of 10% aq K<sub>2</sub>CO<sub>3</sub> soln, and then extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 × 25 mL). The combined organic layers were dried (Na<sub>2</sub>SO<sub>4</sub>). After filtration, the solvent was removed by rotary evaporation, and the crude product

▼ Experimental Procedure

**Organic LETTERS** **Step 1**

Preparation of 5-chloro-8-hydroxy-3-methyl-1-oxoisochroman-7-carboxylic acid **7** called OTo Sulfuryl chloride (0.69 mL, 8.6 mmol, 5 eq) was added to a stirred solution of **6** (429 mg, 1.71 mmol, 1 eq) in anhydrous dichloromethane (8.5 mL) under argon. The resulting mixture was stirred for 18 h at room temperature and then concentrated under reduced pressure to give ethyl 5-chloro-8-hydroxy-3-methyl-1-oxoisochroman-7-carboxylate as an orange sticky oil (490mg), which was suspended in ethanol (12 mL). 4 M LiOH<sub>aq</sub> (4.3 mL) was added and the mixture was allowed to reflux for 1 h. At this point, both ester and lactone were

# Suche nach chemischen Substanzen mit einer Strukturrecherche

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'CAS Solutions' and 'SciFINDER A CAS SOLUTION'. Below this, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows a breadcrumb trail: 'Substance Identifier "ochratoxin A" > substances (1) > get references (673)'. On the left, a sidebar lists various search criteria under 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags) and 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier). Under 'REACTIONS', 'Reaction Structure' is listed. The main panel is titled 'SUBSTANCES: CHEMICAL STRUCTURE' and features a 'Structure Editor' section with 'Java' and 'Non-Java' tabs, a 'Click to Edit' button, and an 'Import CXF' button. To the right, the 'Search Type' options are 'Exact Structure', 'Substructure' (selected), and 'Similarity'. There is also a checkbox for 'Show precision analysis'. A 'Search' button is located at the bottom of the main panel. A 'ChemDraw' logo is visible, with a link to 'Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. Learn More'. At the bottom left, there is a link for 'Advanced Search'.

**Findet konkrete chemische Verbindungen, aber auch deren Derivate**

**Verschiedene Struktureditoren verfügbar**

**CXF (Chemical eXchange Format) (.cxf)**

# Java-basierter Struktureditor für Struktur- und Reaktionssuchen

- Voraussetzung: Java Runtime Environment (JRE) und das zugehörige Java Plug-in, um JRE mit dem jeweiligen Browser zu verbinden
- [http://www.java.com/de/download/windows\\_xpi.jsp?locale=de](http://www.java.com/de/download/windows_xpi.jsp?locale=de)
- für 64-bit-Browser ist die Java-64-bit-Version nötig
- **Windows:** Java 1.6.0\_35 oder höher, 1.7.0\_65 oder höher
- **Mac OS X:** 10.6 bis 10.7.3 nutzen Java-Version 1.6.0\_65, neuere Mac-Versionen: Java 1.7.0\_65 oder höher
- **Einfacher:** Verwenden des **Non-Java-Struktureditors**



The screenshot shows the Java website's download page for Windows. At the top, there is a search bar and navigation links for 'Java in Aktion', 'Downloads', and 'Hilfe'. The main heading is 'Download von Java für Windows', with the recommended version being 'Empfohlen Version 7 Update 13 (Dateigröße: 856 KB)'. A prominent red button says 'Einverstanden und mit kostenlosem Download beginnen'. Below this, a message states: 'Durch das Herunterladen von Java bestätigen Sie, dass Sie die Bedingungen der Endbenutzerlizenzvereinbarung gelesen und akzeptiert haben.' A blue icon with a checkmark indicates that after installation, the browser must be restarted. There are links for 'Installationsanweisungen' and 'Systemvoraussetzungen'. A footer note mentions that Java software is also referred to as Java Runtime, Runtime Environment, Runtime, JRE, Java Virtual Machine, Virtual Machine, Java VM, JVM, VM, or Java-Download. The Oracle logo is in the bottom right corner.

# Generieren einer Strukturformel

The screenshot shows the 'Structure Editor' window. A red box highlights the 'T' icon in the top toolbar, with a red arrow pointing to a text box. The text box contains the following information:

**Eingabe von**

- **CAS-Registry-Nummern**
- **SMILES** (Simplified Molecular Input Line Entry Specification)
- **InChI-Codes** (International Chemical Identifier)

Strukturen aus ISIS/Draw kann man einfach mit Copy/Paste in den Struktureditor von SciFinder übertragen.

On the right side, another red box highlights the 'Drawing Editor' panel, which includes the following options:

**Get substances that match your query using:**

- Exact search
- Substructure search
- Similarity search

Buttons for 'OK' and 'Abbrechen' are also visible in this panel.

The bottom of the interface shows a search bar with '(query)', a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a 'Scale' set to 100.

# Hilfen beim Zeichnen von Strukturen (1)

The screenshot shows the Structure Editor interface with several key components highlighted by red boxes and arrows:

- Top toolbar:** A red box highlights the 'Structure Drawing' icon (a document with a pencil), with an arrow pointing to a blue text box.
- Options panel:** A red box highlights the 'Structure Drawing' section, which includes settings for 'Clipboard', 'Colors', 'Locations', 'Structure Drawing', and 'Toolbars'. A blue text box is positioned over this area.
- Templates panel:** A red box highlights the 'Rings' category in the left sidebar, with a dashed red arrow pointing to a blue text box. The right side of this panel shows four ring templates: benzene, cyclohexane, cyclopentane, and cyclopentadiene.
- Bottom toolbar:** A red box highlights the benzene ring template icon, with a dashed red arrow pointing to the same blue text box.

**Voreinstellungen für das Zeichnen von Strukturen vornehmen**

**Auswählen und Einfügen von vorgefertigten Strukturfragmenten**

**Options**

- Valency checking
- Use fixed drawing length
- Standard bond length (mm):
- Use fixed drawing angles
- Drawing angle (degrees):
- Display tooltips
- Keep selection windows open
- Node Display:
- Position number:
- Font Scaling:
- Zoom Level:

**Get substances that match your query using:**

- Exact search
- Substructure search
- Similarity search

Buttons: OK, Abbrechen

Scale: 100

(query)



# Hilfen beim Zeichnen von Strukturen (2)

- Zeichenstift
- Atome auswählen
- Variable Atome
- Structure Repeating Unit
- Zeichnet Ketten
- Verschiebt Atome
- Verhindert Ringbildung
- Dreht die Struktur
- Positive Ladung

Radiergummi

Shortcuts (OMe, i-Bu, Ph ...)

Definiert R-Gruppen (erlaubte Substituenten)

Variable Point of Attachment

Vorgefertigte Strukturfragmente (Templates)

Lasso zum Auswählen

Verhindert Substitution am Atom

Spiegelt die Struktur

Negative Ladung

Vorauswahl einiger Atome

Bindungsauswahl

Stereobindungen

Zeichnet 3-15-gliedrige Ringe

Zeichnet 3-15-gliedrige Ringe



# Suche nach der exakten Struktur

The screenshot shows the SciFinder interface. On the left, the 'SUBSTANCES' category is selected in the navigation menu. The main area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. A chemical structure editor shows a benzene ring with a bromine atom at the para position and a nitrogen atom at the other para position, which is connected to another benzene ring. The 'Search Type' is set to 'Exact Structure', and the 'Show precision analysis' checkbox is checked. A 'Search' button is located below the structure editor.

Präzisionsanalyse sollte bei der Suche nach Stereo-Verbindungen, Komplexen bzw. Tautomeren aktiviert sein.

## Begrenzung der Suche auf Stoffklassen (Advanced Search)

The screenshot shows the 'Advanced Search' filters. Under 'Characteristics', 'Single component', 'Commercially available', and 'Included in references' are unchecked. Under 'Classes', 'Organics, and others not listed' is checked. Under 'Studies', 'Analytical', 'Biological', 'Preparation', and 'Reactant or reagent' are unchecked.

## Trefferliste

The screenshot shows the search results page for 'Chemical Structure exact with limiters > substances (4)'. The results are sorted by 'Relevance'. Four results are displayed:

- 1. Substance Detail 54446-36-5**  
C<sub>12</sub> H<sub>10</sub> Br N  
Benzenamine, 4-bromo-*N*-phenyl-  
~86
- 2. Substance Detail 77181-34-1**  
C<sub>12</sub> H<sub>10</sub> Br N  
Benzenamine, 4-bromo-*N*-phenyl-, radical ion(1+) (9CI)  
~1
- 3. Substance Detail 81587-90-8**  
C<sub>12</sub> H<sub>9</sub> Br N  
Amidogen, (4-bromophenyl)phenyl-  
~1
- 4. Substance Detail 113336-81-5 (Component: 54446-36-5)**  
C<sub>12</sub> H<sub>10</sub> Br N . Na  
Benzenamine, 4-bromo-*N*-phenyl-, sodium salt (9CI)  
~1

# Substruktursuche – Suche nach Substitutionen

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK  
Abbrechen

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure substructure with limiters > substances (12379)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

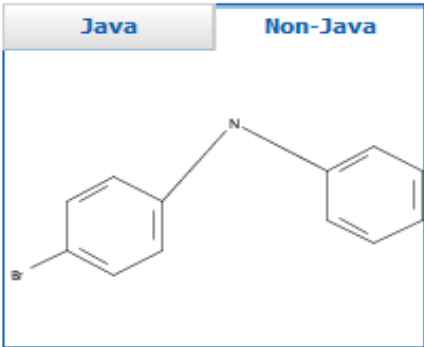
SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



Search Type:

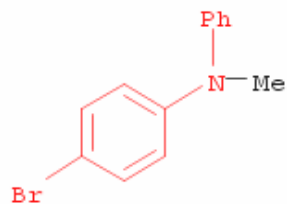
- Exact Structure
- Substructure
- Similarity

Show precision analysis

Click image to change structure or view detail.

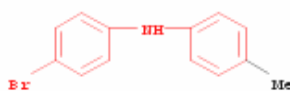
Search

4. Substance Detail  
336190-16-0



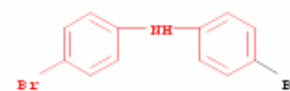
**C<sub>13</sub> H<sub>12</sub> Br N**  
Benzenamine, 4-bromo-*N*-methyl-*N*-phenyl-

5. Substance Detail  
858516-23-1



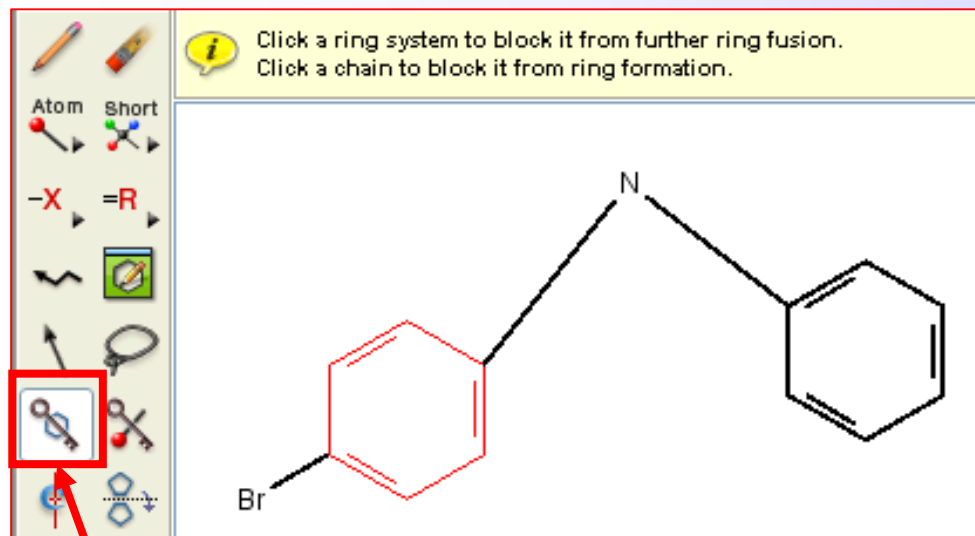
**C<sub>13</sub> H<sub>12</sub> Br N**  
Benzenamine, 4-bromo-*N*-(4-methylphenyl)-

6. Substance Detail  
16292-17-4



**C<sub>12</sub> H<sub>9</sub> Br<sub>2</sub> N**  
Benzenamine, 4-bromo-*N*-(4-bromophenyl)-

# Substruktursuche ohne Bildung neuer Ringe

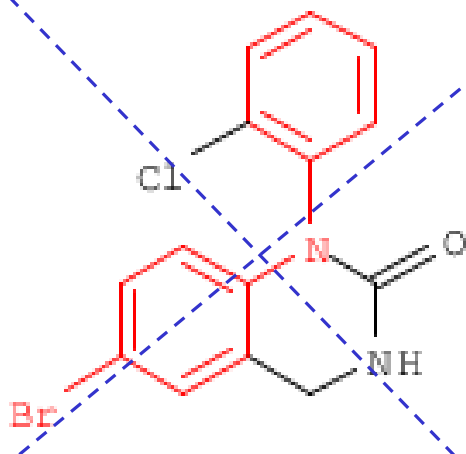


Get substances that match your query using:

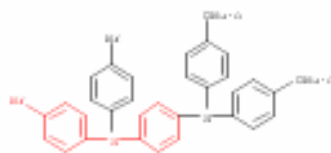
- Exact search
- Substructure search
- Similarity search

OK

Abbrechen



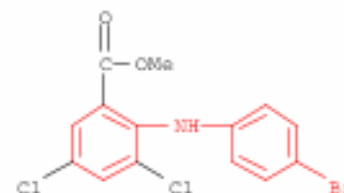
2. 1001618-54-7



**C<sub>38</sub> H<sub>38</sub> Br<sub>2</sub> N<sub>2</sub> O<sub>2</sub>**

1,4-Benzenediamine, N1,N1-bis(4-bromophenyl)-N4,N4-bis(4-butoxyphenyl)-

3. 1001254-82-5



**C<sub>14</sub> H<sub>10</sub> Br Cl<sub>2</sub> N O<sub>2</sub>**

Benzoic acid, 2-[(4-bromophenyl)amino]-3,5-dichloro-, methyl ester

# Strukturähnlichkeitssuche

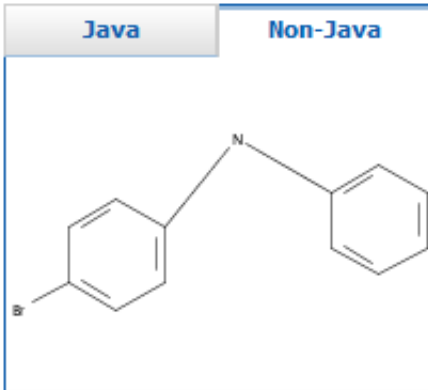
Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

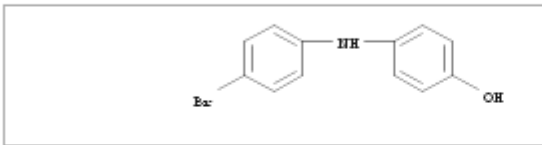
Click image to change structure or

Chemical Structure similarity

SUBSTANCES	
Select All Deselect All	
0 of 9 Similarity Candidates Selected	
Substances	
<input type="checkbox"/> ≥ 99 (most similar)	5
<input type="checkbox"/> 95-98	2
<input type="checkbox"/> 90-94	27
<input checked="" type="checkbox"/> 85-89	43
<input type="checkbox"/> 80-84	77
<input type="checkbox"/> 75-79	12696
<input type="checkbox"/> 70-74	1031
<input type="checkbox"/> 65-69	4044
<input type="checkbox"/> 0-64 (least similar)	16945

Score: 87

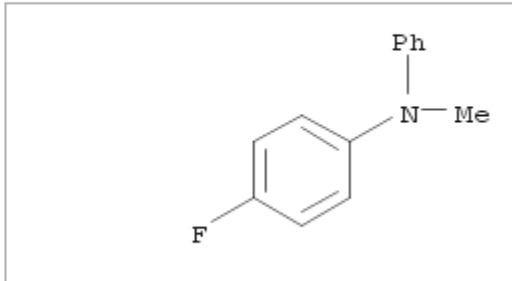
10. 237877-07-9



**C<sub>12</sub> H<sub>10</sub> Br N O**  
Phenol, 4-[(4-bromophenyl)amino]-

Score: 87

11. 902781-07-1



**C<sub>13</sub> H<sub>12</sub> F N**  
Benzenamine, 4-fluoro-N-methyl-N-phenyl-

# Reaktionssuche über die Struktur

CAS Solutions



Explore

Saved Searches

SciPlanner

Substance Identifier "ochratoxin A" > substances (1) > get references (673)

## REFERENCES

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

## SUBSTANCES

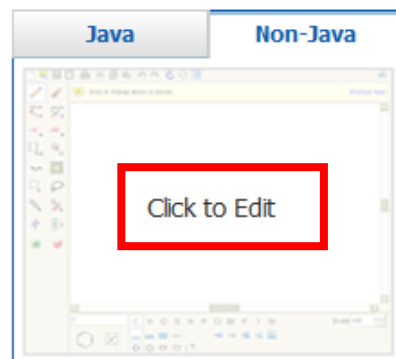
Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

## REACTIONS

Reaction Structure

## REACTIONS: REACTION STRUCTURE

Structure Editor:



Search Type:

- Allow variability only as specified
- Substructure

Import CXF

Search

Advanced Search



Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

# Hilfen beim Zeichnen von Reaktionen

Die Strukturen für Reaktionssuche-Anfragen werden mit den schon beschriebenen Hilfsmitteln generiert. Zusätzlich stehen diese Tools zur Verfügung:



**Reaction Arrow** - Zum **automatischen Erteilen der Rollen** in einer Reaktion klicken Sie auf den Reaktionspfeil und positionieren Sie ihn auf dem Zeichenbrett rechts neben den Ausgangsstoff, klicken und ziehen Sie bei gedrückter linker Maustaste bis vor das Reaktionsprodukt. Die „Etiketten“ Reactant or Reagent/ Material/ Product erscheinen.

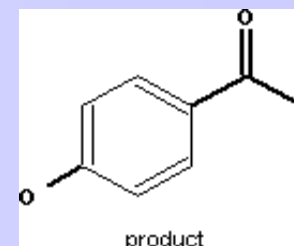


**Reaction Role** - Klicken Sie diesen Button an und **weisen** Sie damit den gezeichneten Strukturen ihre **Rolle bei der Reaktion zu**.

Tippen Sie eine Teilstruktur an, im sich öffnenden Fenster, wählen Sie die entsprechende Rolle aus und gehen auf „OK“. Die (Teil)struktur hat nun ein „Etikett“.

Select a role for the structure fragment:

- product
- reactant
- reagent
- reactant/reagent
- any role



alch  
keton  
aldehyd

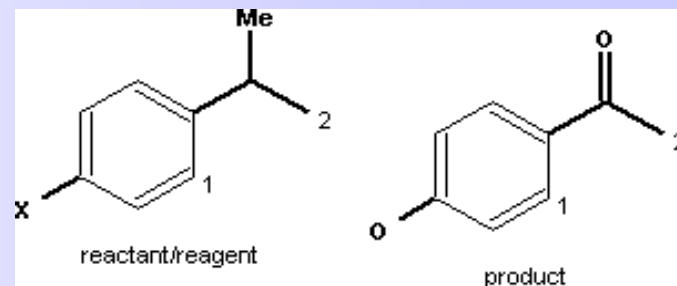
**Funktional Groups** (**Geht im Moment bei der Non-Java-Version noch nicht!**)

Über diesen Button kann man ohne Zeichnen von Strukturen Reaktionen von Substanzklassen suchen.

1 → 1

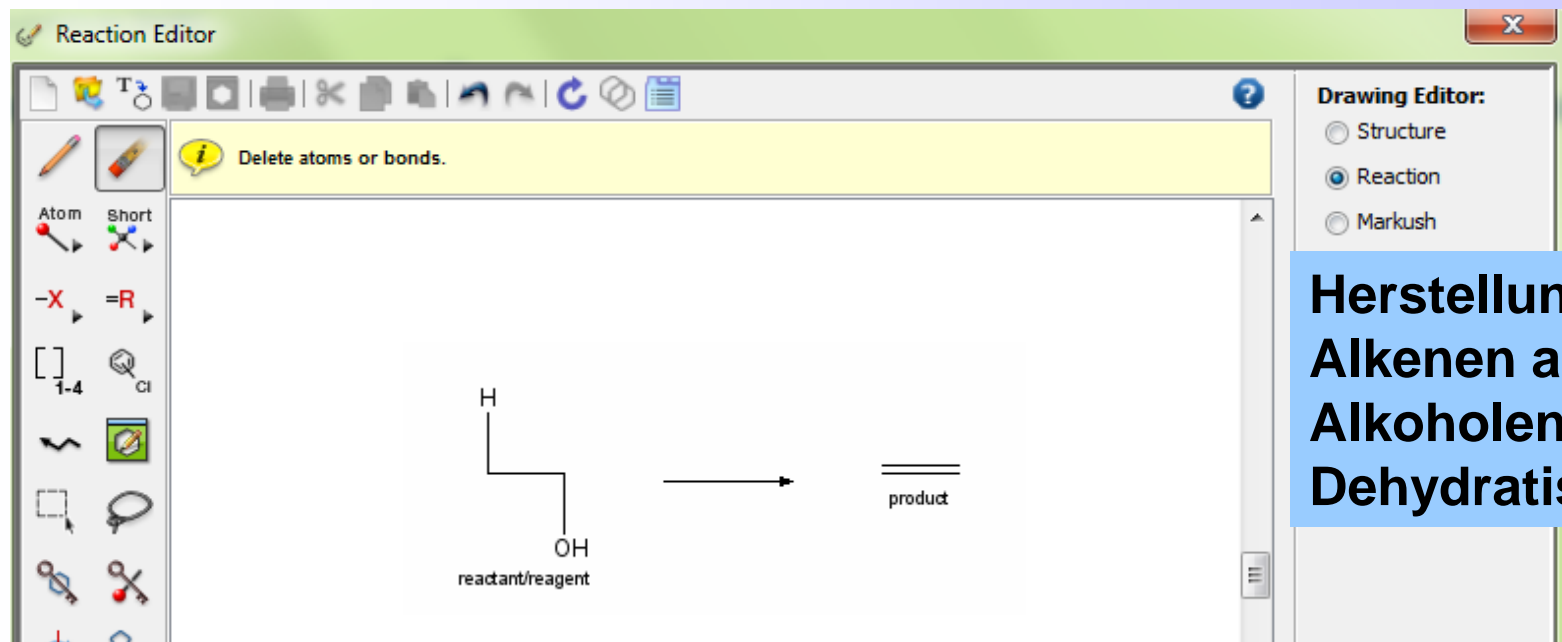


**Reaction Mapping** - Nachdem Sie Ausgangsstoff und Produkt gezeichnet und mit ihrer „Rolle“ in der Reaktion versehen haben, können Sie mit diesem Button zusammengehörende Atumpaare aus Edukt und Produkt definieren (Atom 1 im Edukt entspricht Atom 1 im Produkt). Klicken Sie dazu nacheinander die entsprechenden Atome an. Beide Atome erhalten die selbe Nummer.



**Reaction Site Marking** - Markieren Sie damit eine oder mehrere Bindungen im Ausgangsstoff, die bei der Reaktion geändert/gebrochen werden bzw. Bindungen im Produkt, die sich ändern/entstehen (eine Doppellinie kennzeichnet nun diese Bindungen).

# Beispiel einer Reaktionssuche



Herstellung von Alkenen aus Alkoholen durch Dehydratisierung

Explore ▾ Saved Searches ▾ SciPlanner

❗ Search could not be performed. Correct the error(s) indicated below.

Chemical Structure substructure > substances (8488)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS: REACTION STRUCTURE ?

Click image to change structure

Search Type:

- Allow variability only as specified
- Substructure

Reaction is too general. Select limiter(s) below, add more details to drawing, or [lock out rings and chains](#)

Search

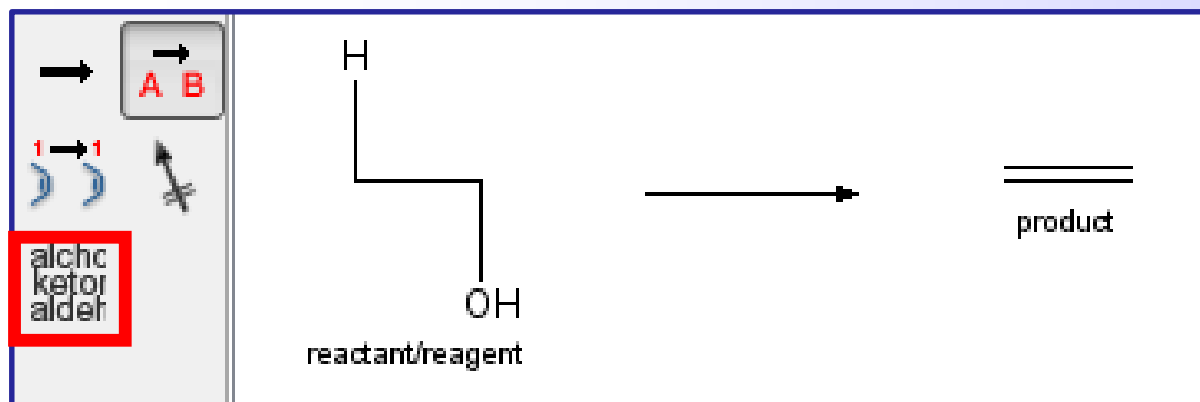
Get reactions where the structure(s) are:

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

OK  
Abbrechen



# Ausweg: Suche mit Funktionellen Gruppen



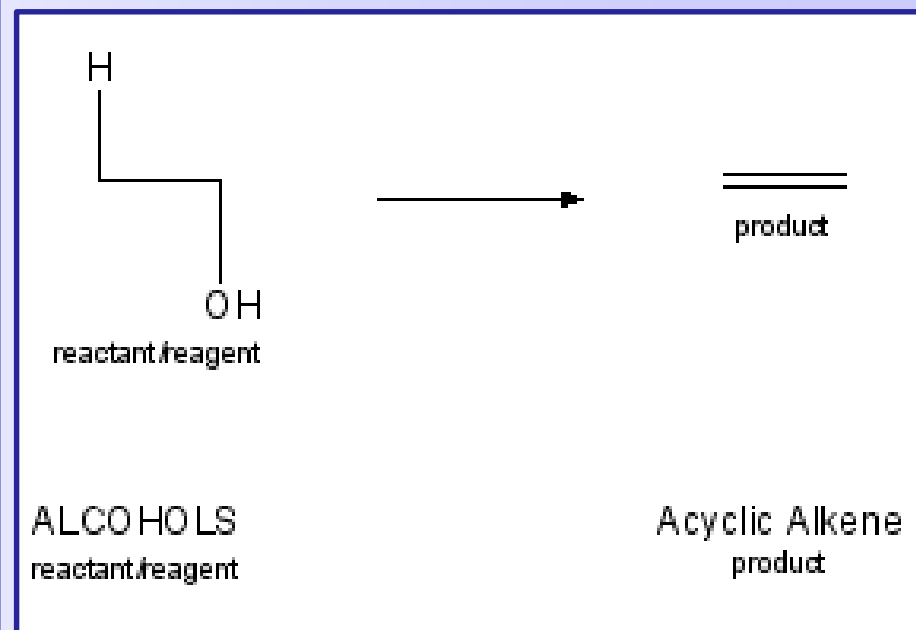
Functional Groups

Select a term below. Then click in the structure drawing window to draw the term.

ALKENES	ALKENES is a class that includes:
ALCOHOLS	<b>Acyclic Alkene</b>
<b>ALKENES</b>	Alkene
ALKYNES	Allyl Alcohol
AMINES	Allyl Halide
CARBONATE DERIVATIVES	Cyclic Alkene
CARBOXY DERIVATIVES	Diene
HALIDES	Enamine
HETEROCYCLES	Ketene
KETONES	Ketenimine

Terms displayed

All  Class Terms  Rings  Non-rings



# Zu viele Treffer? → Refine by Reaction Structure

CAS Solutions | Preferences | SciFinder Help | Sign Out

WELCOME Ina Weiss

Explore | Saved Searches | SciPlanner | Save | Print | Export

Reaction Structure substructure > reactions (522530)

REACTIONS | Get References | Tools

Group by: No Grouping | Sort by: Relevance

0 of 522530 Reactions Selected

1. View Reaction Detail | Link | Similar Reactions

Single Step | Hover over any structure for more options.

HO-CH2-CH2-Hg-Br → H2C=CH2

100%

2. View Reaction Detail | Link | Similar Reactions

Single Step | Hover over any structure for more options.

Sample Analysis: Catalyst

4-DMAP

Pd

Pd(PPh3)4

p-MeC6H4SO3H

Py • p-MePhSO3H

n-Pr4N+ • RuO4-

CuI

246047-72-3

D-Camphorsulfonic acid

PdCl2(PPh3)2

Show More

Analyze | Refine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Reaction Structure:

Click image to change structure or view detail

Search type: **Substructure**

Refine

Page [50] Display: [ ] [ ]

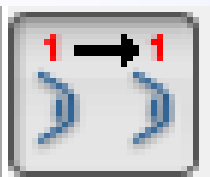
Page: 1 of 10451

Classification: # Conditions: CH2N2, stages in any one step: 1

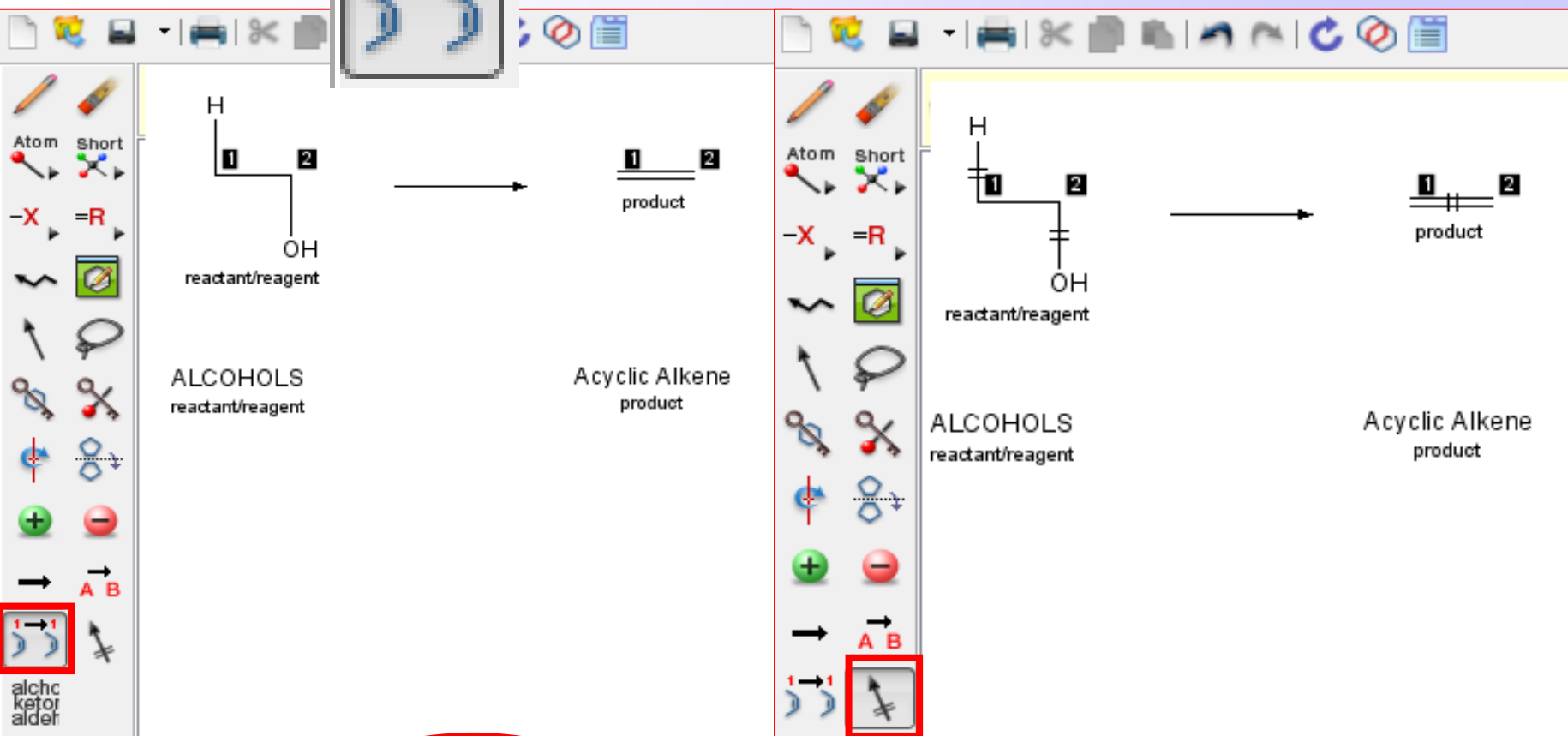
Reference: The addition of N2 to alkenes by Chatt, J. From Chemical Reviews 1951

# Refine by Chemical Structure:

## Mapping



## Reaction Site




The image displays two side-by-side chemical reaction editors. Both editors show a reaction where ethanol (reactant/reagent) is converted to ethene (product). The reactant is labeled 'ALCOHOLS reactant/reagent' and the product is labeled 'Acyclic Alkene product'. The atoms in the reactant are numbered 1 and 2. In the left editor, the 'Mapping' tool (represented by two blue curved arrows) is selected in the toolbar. In the right editor, the 'Reaction Site' tool (represented by a black arrow pointing to a grey square) is selected. Both editors have a toolbar with various icons for editing, including 'Atom', 'Short', '-X', '=R', and 'A B'.

0 of 41470 Reactions Selected

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

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

$$\text{HO}-\text{CH}_2-\text{CH}_2-\text{H} + \text{H}_3\text{C}-\text{CH}_2-\text{O}-\text{CH}_2-\text{CH}_3 \longrightarrow \text{H}_2\text{C}=\text{CH}_2$$


# Einschränken über Ausbeute, Ein-/Mehrstufenreaktion, Reaktionsklassifizierung

**REACTIONS** ?

Analyze Refine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Product Yield:  %

Upper Limit Example: 80

%

Lower Limit Example: 20

Include answers that have no product yield

Refine

**REACTIONS** ?

Analyze Refine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Number of Steps:

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

**REACTIONS** ?

Analyze Refine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Reaction Classification(s):

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

**REACTIONS** ?

Analyze Refine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Excluding Reaction Classification(s):

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

**REACTIONS** ?

Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 188 Reactions Selected

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

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

CC(C)(O)C#C >> CC(C)=C#C

91%



# Exportieren von Reaktionen

Explore ▾ Saved Searches ▾ SciPlanner Save answers to your computer. Export

Reaction Structure structure variable only at spe... > reactions (196) > refine "90 - % yield" (9)

## Export

### Export:

- All
- Selected
- Range

### For:

#### Offline review

- Portable Document Format (\*.pdf)
- Rich Text Format (\*.rtf)

### Details:

#### File Name: \*

Reaction\_03\_14\_2014\_204720

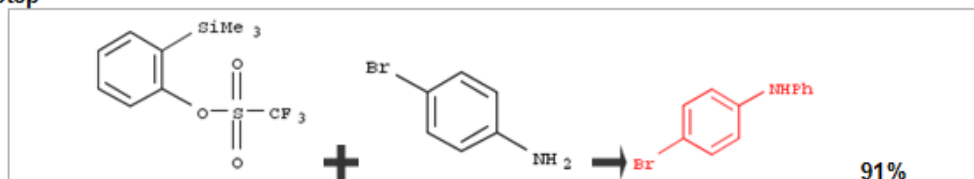
#### Format:

- Summary
- Detail

#### Include:

- Experimental Procedure (if available)
- Overview
- Task History

## 5. Single Step



### Overview

Steps/Stages	Notes
1.1R:CsF, S:MeCN, 10 h, rt	Reactants: 2, Reagents: 1, Solvent: 1, Steps: 1, Stages: 1, Most stages in any one step: 1
	<b>References</b> <a href="#">Facile N-Arylation of Amines and Sulfonamides and O-Arylation of Phenols and Arenecarboxylic Acids</a> By Liu, Zhijian and Larock, Richard C. From Journal of Organic Chemistry, 71(8), 3198-3209; 2006

### Experimental Procedure

	General/Typical Procedure: General Procedure for the Mono-N-arylation of Aromatic Amines
--	--

# Speichern der zu den Reaktionen gehörenden Quellen mit der entsprechenden Zusammenfassung

# Wechsel zwischen Struktur-, Reaktions- und Markush-Editor

The image displays three overlapping windows of the software interface, illustrating the transition between different editing modes:

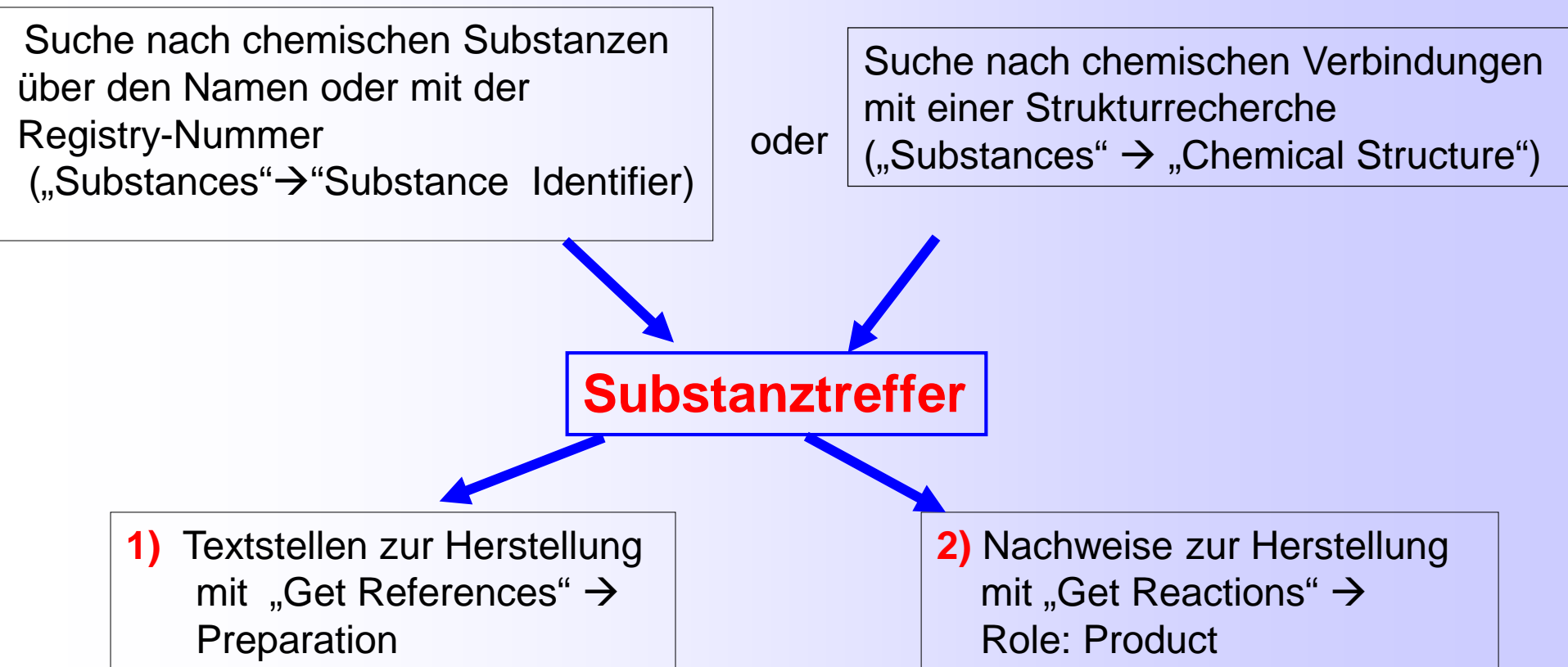
- Top-left window (Structure Editor):** The "Drawing Editor" panel on the right has the "Structure" radio button selected and highlighted with a red box.
- Middle window (Reaction Editor):** The "Drawing Editor" panel on the right has the "Reaction" radio button selected and highlighted with a red box.
- Bottom-right window (Structure Editor):** The "Drawing Editor" panel on the right has the "Markush" radio button selected and highlighted with a red box.

Each window features a toolbar on the left with various drawing tools (atoms, bonds, rings) and a central workspace for drawing. The bottom-right window also includes a bottom panel with element selection buttons (C, H, O, S, N, P, Cl, Br, F, I, Si) and a "Scale" control.

Durch Ziehen an der unteren rechten Ecke kann die Größe des Zeichenfensters verändert werden.

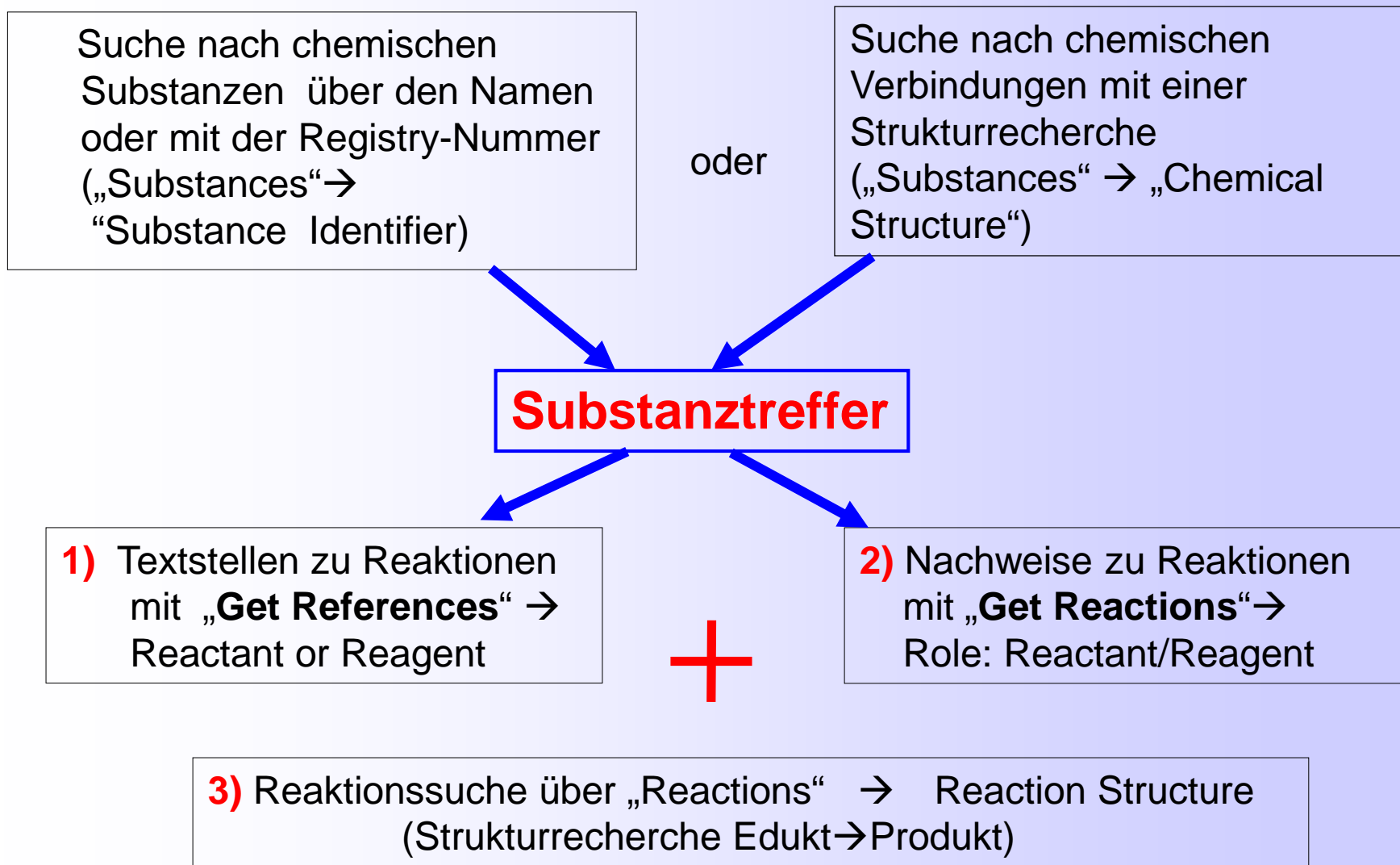


# Suche nach allen Herstellungsvorschriften einer Substanz





# Suche nach allen Reaktionen einer Substanz



**Vollständige Suche: 1+2+3 Zur Ergänzung auch in Reaxys und Science of Synthesis suchen!**

# Struktursuche - ohne Zeichnen der Verbindung!

CAS Solutions  
**SCIFINDER**  
A CAS SOLUTION

Explore ▾ Saved Searches ▾ SciPlanner

Opened saved answer set "Autosaved Reference Set" (48) > get substances (74) > keep 4 substances (4) > keep 2 substances (2) > keep 1 substance (1)

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

Sort by: CAS Registry Number ▾

0 of 1 Substance Selected

1. Substance Detail  
29883-15-6

CAS Registry Number: 29883-15-6

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Send to SciPlanner

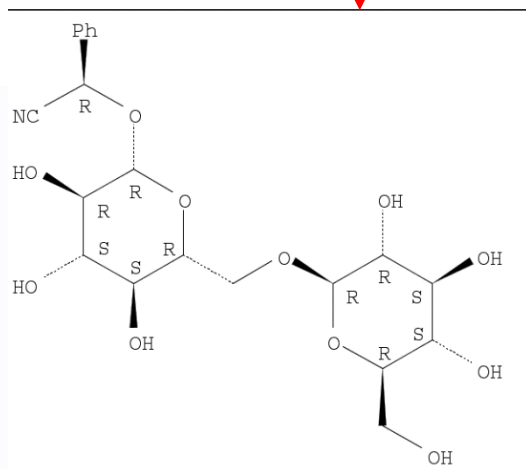
Chemical Structure

Markush Patents by Structure

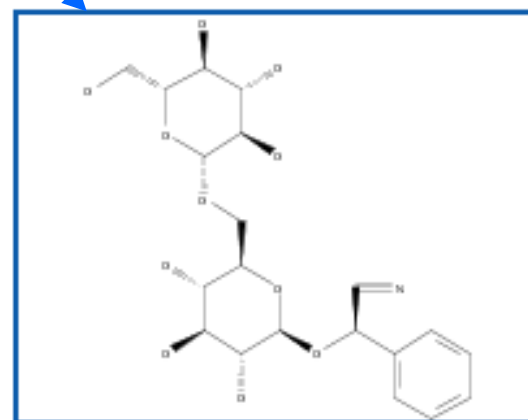
Reactions

**C<sub>20</sub> H<sub>27</sub> N O<sub>11</sub>**  
Benzeneacetonitrile, α-[[6-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-, (αR)-

Show More



1. Klicken Sie - z.B. nach einer Namens- bzw. Registry-Nummernsuche auf den Doppelpfeil rechts oben im Feld mit der Strukturformel.
2. Wählen Sie „Explore by Structure“ aus.
3. Die Struktur erscheint im Suchfeld.
4. Einzelheiten der Struktur ändern oder Suche beginnen.

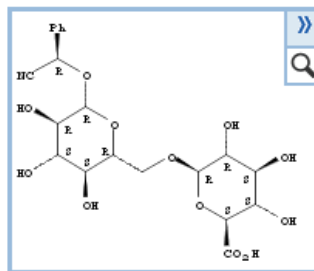
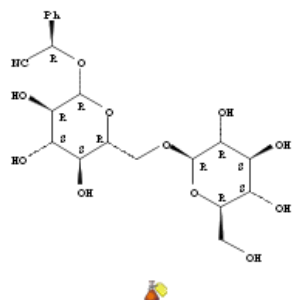


Click image to change structure or view detail.

# Nach der Reaktionssuche – Weiter ohne Zeichnen der Verbindung!

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

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



45%

CAS Registry Number: 876395-75-4

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Send to SciPlanner

Chemical Structure

Markush Patents by Structure

Reactions

Overview

Steps/Stages

1. Klicken Sie nach einer Reaktionssuche auf die Doppelpfeile im Bild der Verbindung, für die nähere Informationen gebraucht werden:
  - Herstellungen, Reaktionen usw.
  - Textstellen zu allen Aspekten (References)
  - Eigenschaften (Substance Details)
  - Zulassungsinformationen (Regulatory Information)
2. Für eine Substruktursuche:

Wählen Sie „Explore by Structure“ und dann „Chemical Structure“ bzw. „Reactions“ aus, die Struktur erscheint im Suchfeld. Einzelheiten der Struktur können geändert werden oder mit der Substruktursuche/Reaktionssuche kann sofort begonnen werden.

# Hilfe bei Struktur- und Reaktionssuchen

<http://www.cas.org/training/scifinder>

## Substance Searching

- [Introduction to Substance Searching \(tutorial\)\\*](#)
- [Introducción a la búsqueda de Sustancias \(tutorial\)\\*](#)
- [How to Create a Substance Answer Set - Search by chemical structure, molecular formula, and substance identifier. \(PDF\)\\*](#)
- [How to Work with a Substance Answer Set - Analyze and refine search results. \(PDF\)\\*](#)
- [Introduction to the SciFinder Drawing Editor - Use templates and shortcuts. Enter structures with CAS Registry Numbers<sup>®</sup>. \(tutorial\)\\*](#)
- [Customize the SciFinder Drawing Editor - Set drawing preferences, customize common atoms palette, and create templates. \(tutorial\)](#)
- [Which Drawing Tools Control Variability? \(~10 minutes\)](#)
- [Which Type of Structure Search Should you Choose? \(~10 minutes\)](#)
- [Use SciFinder to Check for Substance Novelty and Properties - \(~10 minutes\)](#)
- [What is a Markush Search? Why is it Important? \(~10 minutes\)](#)
- [How to Find Commercial Sources \(PDF\)](#)

## SciFinder Training Materials



## Reaction Searching

- [Introduction to Reaction Searching \(tutorial\)\\*](#)
- [Introducción a la búsqueda de Reacciones \(tutorial\)\\*](#)
- [How to Create a Reaction Answer Set - Draw and search reactions. Get Reactions tool. \(PDF\)\\*](#)
- [How to Work with a Reaction Answer Set - Analyze and Refine search results. Group by Document or Transformation. \(PDF\)\\*](#)
- [Draw Reactions - Apply variables and shortcuts. Assign reaction sites and map atoms. \(tutorial\)\\*](#)
- [Plan a Synthesis Project - Send data to SciPlanner™ and merge reactions into a synthesis plan. \(tutorial\)](#)
- [How Can Drawing Tools Effect Reaction Search Results? \(~11 minutes\)](#)
- [Find Experimental Procedures to Synthesize Substances \(~10 minutes\)](#)
- [Organize Your Data. Plan and Share a Project. \(~6 minutes\)](#)
- [Virtual Class Resources](#)

## Außerdem: Dreiminütige “Need-to-Know Videos”

- Structure Searching
- Reaction Searching
- Reference Searching
- General Topics

# Weitere Hilfen - SciFinder Virtual Classes

## Substance Searching: Search for Substance Data

- [Part 1](#) (Search by Substance Identifier. Find property data and commercial suppliers.)
- [Part 2](#) (Conduct an Exact search. Refine. Find preparation information. Create an alert.)
- [Part 3](#) (Conduct a Substructure search. Analyze and Refine search results.)
- [Workbook for Parts 1-3 \(PDF\)](#)
- [Exercises for Parts 1-3 \(PDF\)](#)
- [Download structure file for exercises](#)
- [Slides only \(PDF\)](#)

<http://www.cas.org/training/scifinder/virtual-classes>

## Reaction Searching: Search For Reactions Using Substructures

- [Part 1](#) (Reaction substructure search. Group results.)
- [Part 2](#) (Analyze and refine reaction answer sets. Get experimental procedures. Group by transformation type.)
- [Part 3](#) (Use SciPlanner™. Find commercial sources for substances.)
- [Workbook for Parts 1-3 \(PDF\)](#)
- [Exercises for Parts 1-3 \(PDF\)](#)
- [Download reaction file for exercises](#)
- [Download SciPlanner file for exercises](#)
- [Slides only \(PDF\)](#)

## Reference Searching: Search For References by Research Topic

- [Part 1](#) (Formulate a query and remove duplicate answers. Use Refine to narrow an answer set.)
- [Part 2](#) (Create a Keep Me Posted (KMP) alert. Sort by cited references. Analyze an answer set, and access full text.)
- [Part 3](#) (Use Categorize. Export and save answer sets. Retrieve associated substances.)
- [Workbook for Parts 1-3 \(PDF\)](#)
- [Exercises for Parts 1-3 \(PDF\)](#)
- [Slides only \(PDF\)](#)

## SciPlanner - neue Wege der Forschungsplanung

- SciPlanner - interaktiver Arbeitsplatz, der es Nutzern ermöglicht, angepasste Reaktionswege zu entwickeln sowie SciFinder-Ergebnisse zu organisieren und zu verwalten
- Reaktionen, Experimentmethoden, Substanzen und Referenzen aus verschiedenen Dokumenten können integriert werden
- <http://www.youtube.com/watch?v=FsOvKsALKb4&feature=related>
- Senden von Daten zum SciPlanner:  
[http://www.cas.org/etrain/scifinder/planner\\_intro.html](http://www.cas.org/etrain/scifinder/planner_intro.html)
- Arbeiten mit den Objekten im "Workspace":  
[http://www.cas.org/etrain/scifinder/planner\\_workspace.html](http://www.cas.org/etrain/scifinder/planner_workspace.html)
- **Erstellung eines Syntheseplanes**  
(Send data to SciPlanner™ and merge reactions into a synthesis plan. - tutorial)  
<http://www.cas.org/etrain/scifinder/sciplanner.html>

# SciPlanner

CAS Solutions



Preferences | SciFinder Help | Sign Out

Welcome Ina Weiss

Explore

Saved Searches

SciPlanner

Link

Save

Print

Export

Substance Identifier "Progesterone" > substances (1) > 57-83-0

SUBSTANCE DETAIL

Get References

Get Reactions

Get Commercial Sources

Get Regulatory Information

Send to SciPlanner

Return

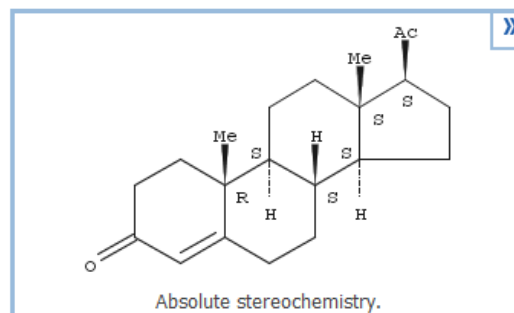
CAS Registry Number: 57-83-0

C<sub>21</sub> H<sub>30</sub> O<sub>2</sub>

Pregn-4-ene-3,20-dione

Progesterone (8CI); 4-Pregnene-3,20-dione; Agolutin; Bio-luton; CIDR; Corlutin; Corlutina; Corluvite; Corporin; Corpus luteum hormone; Crinone; Cyclogest; Duraprogen; EAZI-BREED CIDR; Endometrin; Estima; Flavolutan; Fologenon; Gesterol; Gestiron; Gestone; Gestormone; Gestron; Glanducorpin; Gynlutin; Gynolutone; Hormoflaveine; Hormoluton; Lipo-Lutin; Lucorteam Sol; Lugesteron; Lugesterone; Luteal Hormone; Luteinique; Luteocrin normale; Luteodyn; Luteogan; Luteohormone; Luteol; Luteopur; Luteosan; Luteostab; Luteosterone; Luteovis; Luteum; Lutex; Lutidon; Lutin; Lutinus; Lutociclina; Lutocyclin M; Lutocyclin; Lutocyclin M; Lutocyclin; Lutoform; Lutogyl; Lutren; Lutromone; Microgest; Minagest; NSC 64377; NSC 9704; Nalutron; P4; Percutacrine Luteinique; Piaponon; Primolut; Prochieve; Progeffik; Progekan; Progestan; Progestasert; Progesterol; Progestin; Progestogel; Progestol; Progeston; Progesterone; Progestron; Prolets; Prolidon; Proluton; Prometrium; Prontogest; Protormone; Sincrogest; Syngesterone; Syngestrets; Syntolutan; U 3672; Utrogest; Utrogestan; Vitarrine;  $\Delta^4$ -Pregnene-3,20-dione

Deleted CAS Registry Numbers: 8012-32-6, 8023-13-0, 257630-50-5, 753497-20-0



Explore

Saved Searches

SciPlanner



Substance sent to SciPlanner

SciPlanner™ ist eine Möglichkeit, um mit Ergebnissen aus SciFinder zu arbeiten.

# SciPlanner (2)

The screenshot shows the SciPlanner software interface. The title bar reads "SciPlanner" and "SciPlanner\_04\_12\_2011\_HRT\_Progesteron". The workspace contains two text blocks and a chemical structure. The first text block is titled "Bioidentical hormones for menopausal hormone therapy: variation on a theme" and is attributed to Fugh-Berman Adriane and Bythrow Jenna. The second text block is titled "Combinations for hormone replacement therapy containing a natural estrogen, a natural progestogen and a natural androgen" and is attributed to PCT Int. Appl., 9806404, Feb 19, 1998. A chemical structure of a steroid hormone is displayed in the center. On the right side, there is a panel titled "Clear Substances" containing a list of chemical structures. A tooltip with the text "Click and drag to move. Ctrl-click to move a copy." is positioned over the list, with a green arrow pointing from a text box at the bottom of the slide to the tooltip.

Details aus der eigenen Liste in SciPlanner kann man sich mit „**Click to magnify image**“ ansehen.

Ergebnisse aus der Liste auf der rechten Seite übernimmt man mit „**Click and drag to move**“ oder „**Ctrl-click to move a copy**“.



# SciPlanner: Export

SciPlanner\_04\_12\_2011\_HRT\_Progesteron

Workspace Edit View GoTo

Bioidentical hormones for menopausal hormone therapy: variation on a theme  
By Fugh-Berman Adriane and Bythrow Jenna  
From Journal of general internal medicine, 22, 7, 1030-4, 2007

Combinations for hormone replacement therapy containing a natural estrogen, a natural progesterone and a natural androgen  
From PCT Int. Appl., 9806404, Feb 19, 1998

Export \* Required

**For:**

**Offline Review**

- Portable Document Format (\*.pdf)
- Citations (\*.ris)
- Image (\*.png)

**Saving Locally**

- SciPlanner eXchange (\*.plx)

**Details:**

**File Name: \***  
SciPlanner\_04\_12\_2011\_HRT\_Proge:

**Title**  
\_\_\_\_\_

**Include:**

- SciPlanner Image
- Reaction Details
- Substance Details
- Reference Details

Export Cancel

Clear Substances

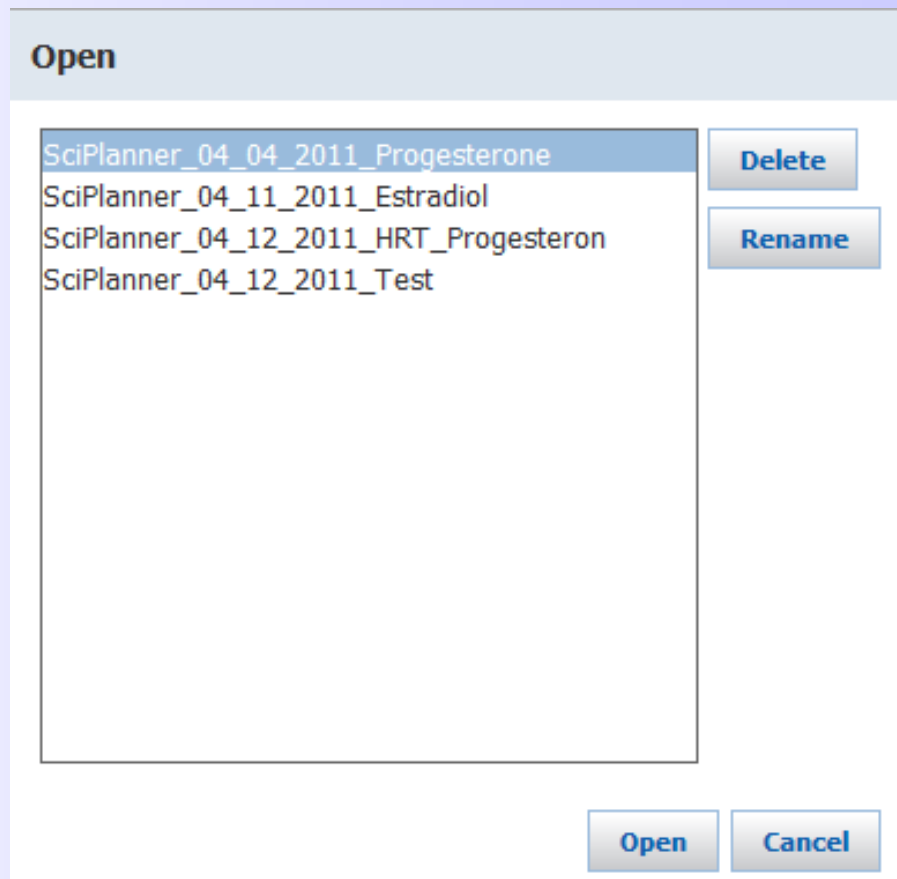
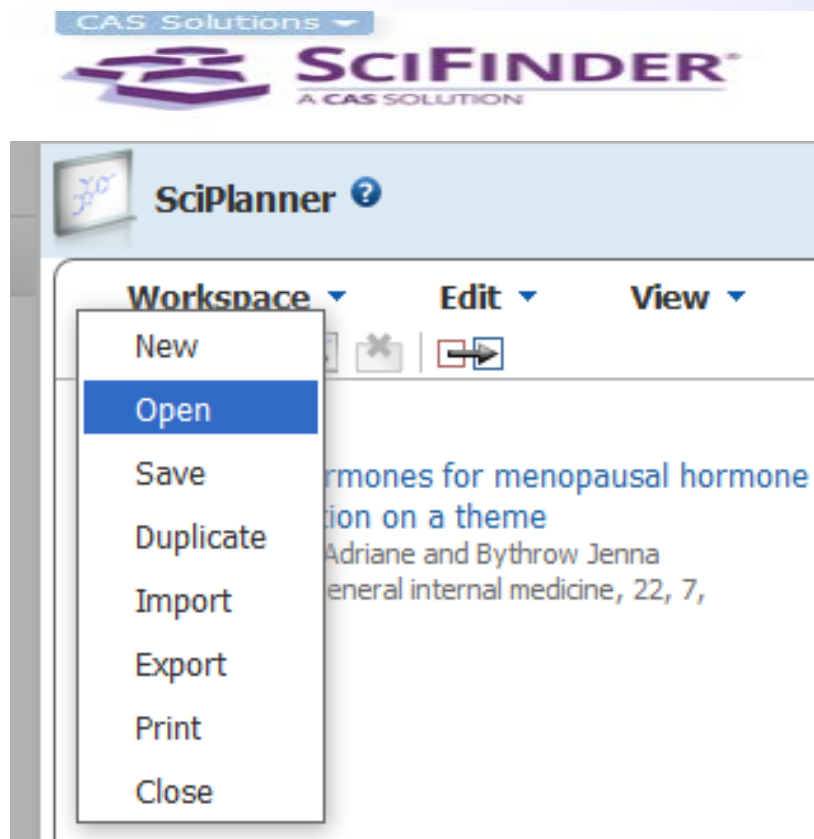
SciFinder® Page 1

Bioidentical hormones for menopausal hormone therapy: variation on a theme  
By Fugh-Berman Adriane and Bythrow Jenna  
From Journal of general internal medicine, 22, 7, 1030-4, 2007

Combinations for hormone replacement therapy containing a natural estrogen, a natural progesterone and a natural androgen  
From PCT Int. Appl., 9806404, Feb 19, 1998

Jeder Nutzer kann maximal **20 Pläne** mit bis zu 200 einzelnen Substanzen in SciPlanner speichern und insgesamt maximal 100 Einträge (combined references, Reaktionen oder Substanzen).

# SciPlanner: Öffnen von gespeicherten Vorlagen



# Patente im SciFinder

Patentrecherchen einschließlich  
(Markush-) Struktursuchen



# Übersicht

- Patente im SciFinder/ Patentarten in der Chemie/ Informationen aus Patenten
- Patentrecherchearten/ Erfinderrecherche/Anmelder-, Inhaberrecherche
- Stand der Technik-Recherchemöglichkeiten (Bsp. Thalidomid-Derivate)
  - Suche nach Thalidomid-Abkömmlingen über „Research Topic „(Wortsuche)
  - Tipp: „Research Topic“ mit RN- Nummer
  - Struktursuche ohne Zeichnen
  - Substanz“arten“ in Patenten
  - Markush-Struktursuchen
- Patentangaben im Einzeltreffer/ Zugang zu den Patentvolltexten
- Patentstatistiken im SciFinder mit „Analysis“
- Zusammenfassung



## Patente im SciFinder

- Mehr als 10 Mio. Patente von 63 Patentämtern, ab 1878
- Patente indexiert aus mehr als 35.000 Klassen der IPC (International Patent Classification) und 99 Klassen der U.S. National Patent Classification: alle Patente mit chemierelevantem Inhalt (Chemie, Biochemie, Pharmazie, Materialwissenschaften u.a.) ausgewählt
- Patente der neun wichtigsten Patentämter weltweit mit ihren bibliographischen Daten schon innerhalb von zwei Tagen aufgenommen



# Patentarten in der Chemie

- Stoffpatente
- Verfahrenspatente
- Anwendungspatente
  - Allgemeine Anwendungen
  - Diagnostika, PharmazeutikaErste und zweite Indikation

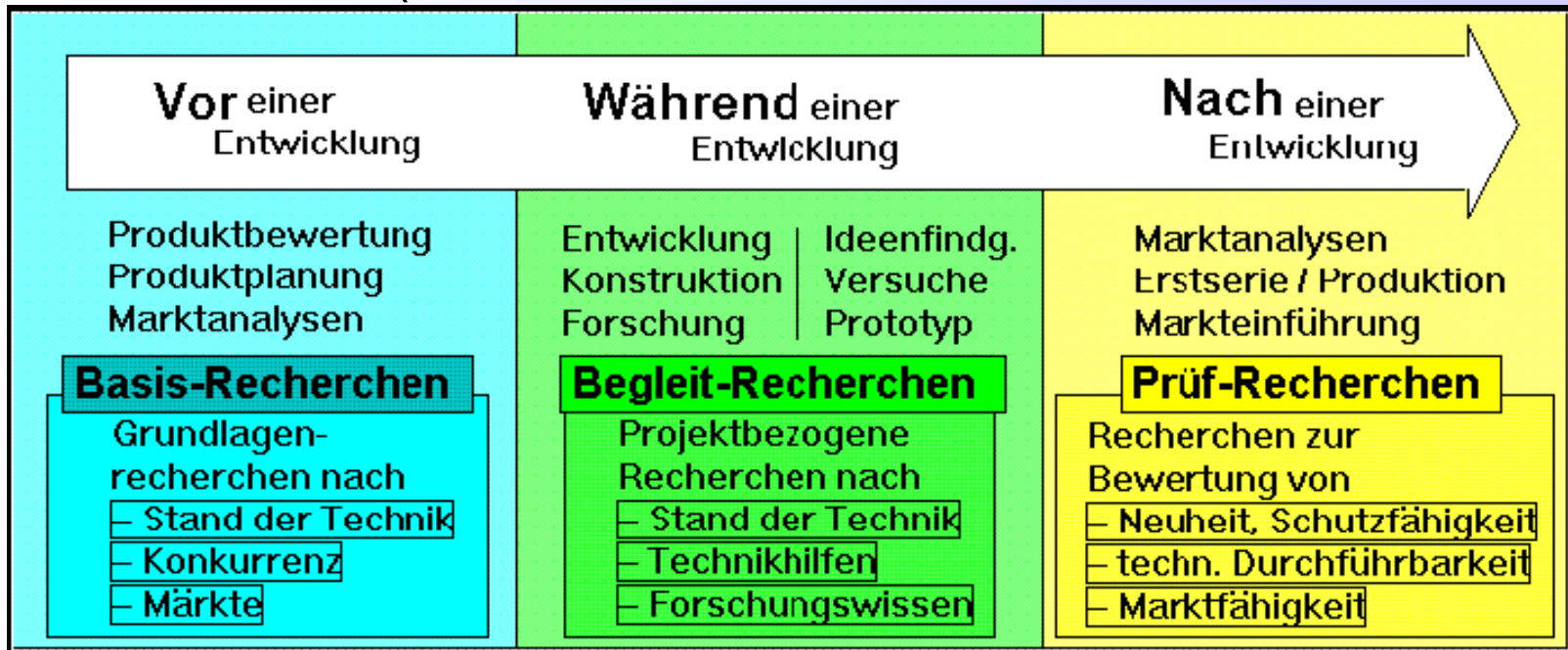


Chemierelevante Patente nicht nur in Sektion C der IPC, sondern auch in Sektion A



## Informationen aus Patenten

- **Technisches Wissen:** Gebiet der Erfindung mit bisherigem Stand der Technik, technisches Problem und seine Lösung durch die Erfindung, mindestens ein Ausführungsbeispiel, Vorteile der Erfindung, Darstellung der Patentansprüche
- Bibliographische Daten: Angaben zum Erfinder, Anmelder, Priorität, Patentklasse(n), Datum der Patentanmeldung/ Offenlegung/ Patenterteilung
- Rechtsstand (Zurücknahme, Erlöschen, Inhaberwechsel)





# Patentrecherchearten im SciFinder

<b>Rechercheart</b>	<b>Ziel</b>
<b>Anmelderrecherche</b>	Anmeldungen und Schutzrechte eines bestimmten Unternehmens oder einer Person
<b>Stand der Technik</b>	Überblick zu bestimmten wissenschaftlichen Gebieten oder Technologien
<b>Neuigkeitsrecherche</b>	Für eine konkrete Erfindungsidee wird die Chance einer erfolgreichen Patentanmeldung geprüft
<b>Freedom to operate</b>	Sicherstellung der freien Benutzbarkeit einer Technologie oder Substanz durch freien Stand der Technik
<b>Verletzungsrecherche</b>	Gibt es gültige Schutzrechte Dritter, die durch ein Produkt oder Verfahren verletzt werden können?
<b>Einspruchsrecherche</b>	Stand der Technik vor Priorität einer anzugreifenden Anmeldung
<b>Marktrecherche</b>	Überblick über ein spezifisches Marktsegment mittels der getätigten Patentanmeldungen



# Erfinderrecherche

The screenshot shows the SciFinder interface. On the left, there is a navigation menu with sections: REFERENCES, SUBSTANCES, and REACTIONS. Under REFERENCES, the following options are listed: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent (highlighted with a red box), and Tags. Under SUBSTANCES, the options are: Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. Under REACTIONS, there is a single option: Reactions. The main area is titled 'REFERENCES: PATENT'. It contains a search form with the following fields: Patent Number (with examples: WO 2001011365), Assignee Name (with examples: Cancer Research Technology Limited), Inventor Last Name \* (with First and Middle columns), and Publication Year (with examples: 1995, 1995-1999, 1995-, -1995). A red box highlights the Inventor Last Name, First, and Middle fields. A red arrow points from the 'Patent' option in the left menu to the search form. A blue 'Search' button is located at the bottom of the form.

Suche nach Erfindern - so findet man Mitbewerber und Konkurrenten.

Hier kann der Suchzeitraum schon vorab auf bestimmte Jahrgänge eingeschränkt werden.

Ausschnitt aus der Trefferliste

1. [Method for generation of ionic conducting surface structures and use](#) 🔍 📄 Full Text  
By Delaney, Joseph T.; Schubert, Ulrich S.  
From PCT Int. Appl. (2011), WO 2011012225 A1 20110203. | Language: English, Database: CAPLUS
2. [Method for generating photonically treated printed structures on surfaces, apparatus, and use thereof](#) 🔍 📄 Full Text  
By Delaney, Joseph T.; Schubert, Ulrich S.  
From PCT Int. Appl. (2011), WO 2011006641 A1 20110120. | Language: English, Database: CAPLUS

# Inhaber-/Anmelderrecherche

The screenshot shows the SciFinder interface with the following elements:

- Top navigation: CAS Solutions, SCIFINDER, A CAS SOLUTION, Pref
- Secondary navigation: Explore, Saved Searches, SciPlanner
- Breadcrumb: Patent "Schubert, Ulrich S" > references (18)
- Left sidebar: REFERENCES (highlighted), Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent (highlighted), Tags, SUBSTANCES (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), REACTIONS
- Main search area: REFERENCES: PATENT, Patent Number (Examples: WO 2001011365), Assignee Name (Jenapharm highlighted, Examples: Cancer Research Technology Limited), Inventor Last Name \* (First, Middle), Publication Year (Example: 1994)
- Search result snippet: 94. Multiphase hormonal system for contraception, By: Moore, Claudia; Oettel, Michael, Assignee: Jenapharm GmbH, Germany

Suche nach Firmen/Einrichtungen - so findet man Mitbewerber, Konkurrenten, Lizenznehmer bzw. – geber

Hier kann der Suchzeitraum schon vorab auf bestimmte Jahrgänge eingeschränkt werden.

Beispieltreffer

## 94. Multiphase hormonal system for contraception

By: Moore, Claudia; Oettel, Michael  
Assignee: Jenapharm GmbH, Germany

The title system comprises combinations of estrogens and a gestagen to be administered during the 1st 3 phases of the ovarian cycle and an estrogen prepn. to be applied in the 4th phase. Thus, film tablets were provided for administration on the following days of the ovarian cycle contg., in addn. to std. excipients, the following active agents (in mg): days 1-7, ethynylestradiol (I) 0.050, levonorgestrel (II) 0.010, estradiol valerate (III) 1.000; days 8-14, I 0.075, II 0.050, III 1.000; days 15-21, I 0.005, II 0.075, III 1.000; days 22-28, III 1.000.

### Patent Information

Patent No.	Kind	Date	Application No.	Date
DE 4313926	A1	Nov 3, 1994	DE 1993-4313926	Apr 28, 1993

### Priority Application

DE 1993-4313926	Apr 28, 1993
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# Suche mit Company Name + Refine/Document Type/Patent

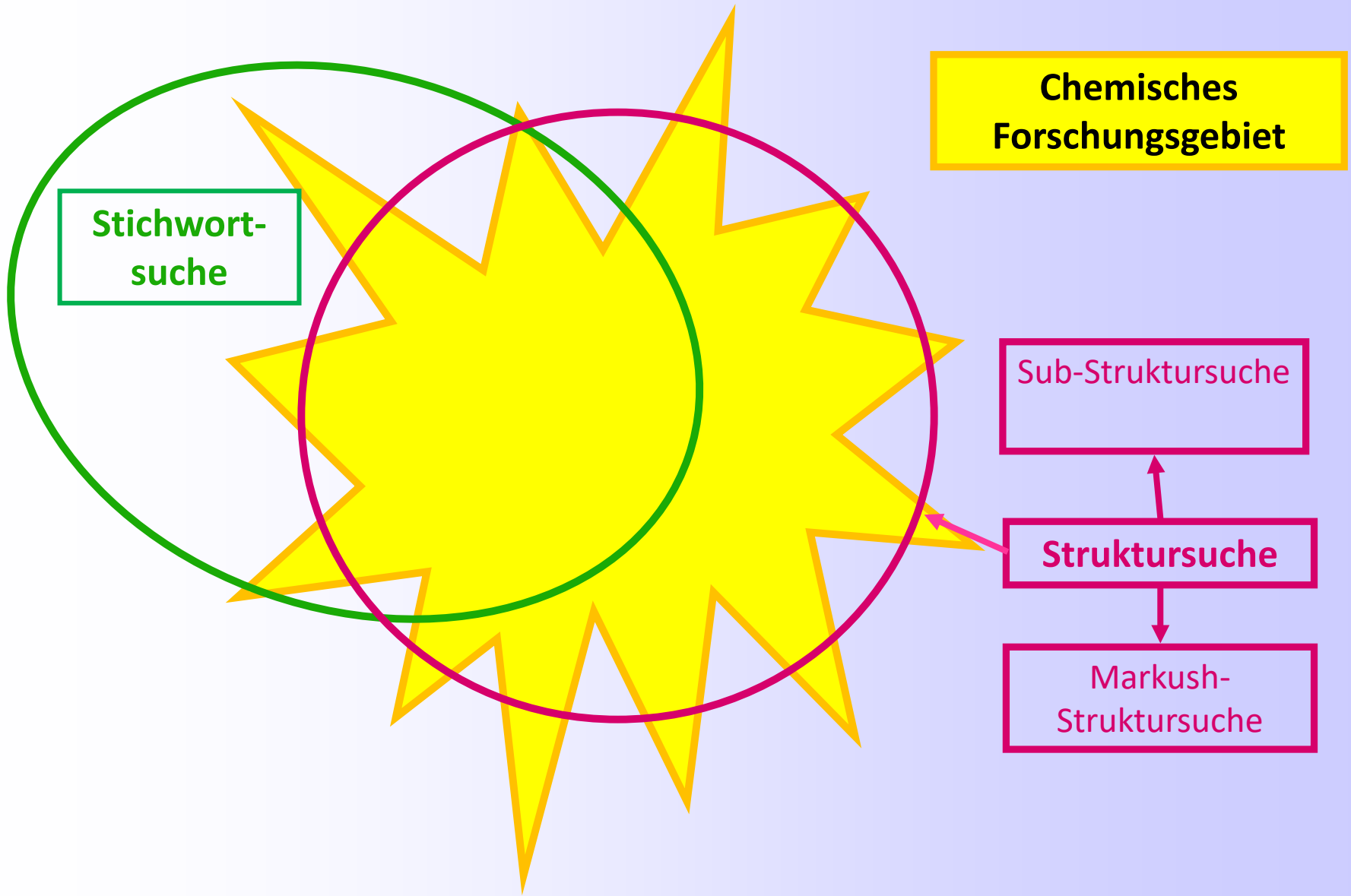
The screenshot shows the SciFinder interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, the search path is 'Patent "Jenapharm" > references (413) > Multiphase hormonal system for...'. A sidebar on the left contains a list of filters: 'REFERENCES', 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. The 'Company Name' filter is selected, and the search term 'Jenapharm' is entered in the search box. Below the search box, there are examples: '3M' and 'DuPont'. A 'Search' button is located at the bottom of the search area.

The screenshot shows the 'REFERENCES' sidebar on the right side of the SciFinder interface. It has three tabs: 'Analyze', 'Refine', and 'Categorize'. Under the 'Refine by:' section, there are several radio button options: 'Research Topic', 'Author', 'Company Name', 'Document Type', 'Publication Year', 'Language', and 'Database'. The 'Document Type' option is selected and highlighted with a red box. Below this, there is a section titled 'Document Type(s)' with a list of document types: 'Biography', 'Book', 'Clinical Trial', 'Commentary', 'Conference', 'Dissertation', 'Editorial', 'Historical', 'Journal', 'Letter', 'Patent', 'Preprint', 'Report', and 'Review'. The 'Patent' option is checked and highlighted with a red box. At the bottom of the sidebar, there is a 'Refine' button.

- Nutrient composition for women intending to become pregnant, in pregnancy, and in lactation** [Quick View](#) [Other Sources](#)  
No Inventor data available  
From Ger. Gebrauchsmusterschrift (2010), DE 202009016672 U1 20100506. | Language: German, Database: CAPLUS  
A nutritional supplement in capsular form for use by women comprises: (a) folic acid/folates, vitamin B1, vitamin B2, vitamin B6, vitamin B12, niacin, vitamin D3, vitamin E; (b) iodine, calcium, magnesium; and (c) docosahexaenoic acid; the wt. of components being (by wt. of the total formulation): (a) 2-10%; (b) 15-50%; and (c) 20-70%.
- Inorganic flow aid for feeds [Machine Translation].** [Quick View](#) [Other Sources](#)  
By Linde, Hellmut; Anger, Immo; Roessler, Norbert  
From Ger. Offen. (1992), DE 4105856 A1 19920827. | Language: German, Database: CAPLUS
- Fourrages medicinals** [Quick View](#) [Other Sources](#)  
By Kramer, Axel Dd; Wanffen, Wolfgang Dd; Ehlert, Dieter Dd; Kruligk, Frank Dd; Grubel, Gerhard Dd  
From Rom. (1986), RO 88515 A2 19860130. | Language: Romanian, Database: CAPLUS



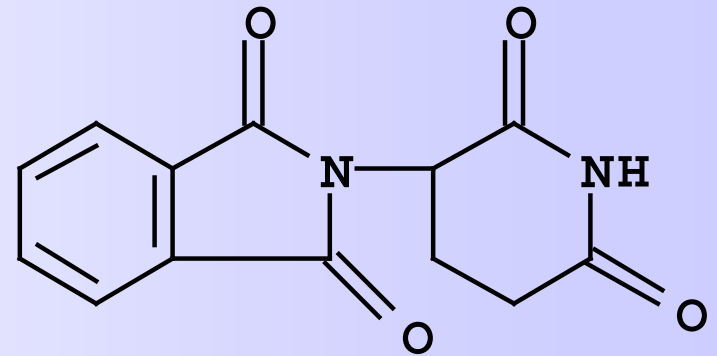
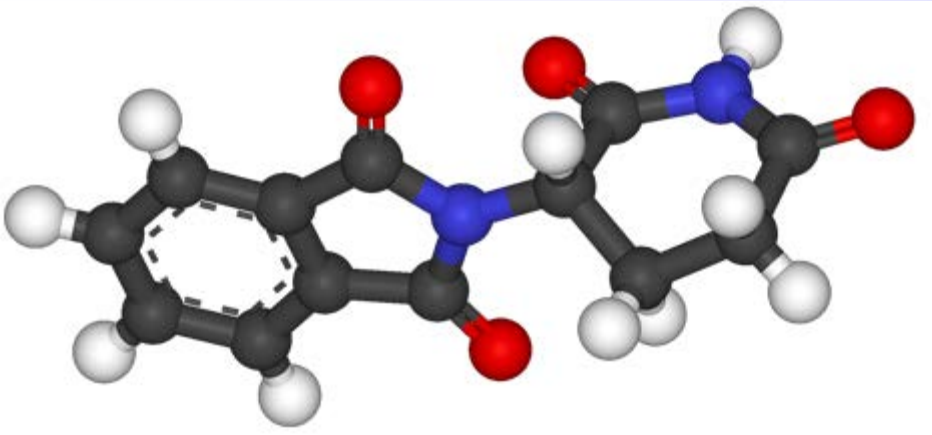
# Stand der Technik - Recherchemöglichkeiten





## Beispiel: Thalidomidähnliche Substanzen und ihre Wirkungen/Anwendungen

Thalidomid = Wirkstoff des Schlaf- und Beruhigungsmittels, das unter dem Markennamen Contergan® verkauft wurde





## Neue Indikationen für Thalidomid

- **Eigenschaften**
    - entzündungshemmend
    - tumorhemmend
    - vermindert Gefäßneubildung
  - **therapeutische Effekte** bei verschiedenen Krankheiten
    - Lepra u.a. Hauterkrankungen, multiple Myelome
    - Autoimmunerkrankungen, Krebs, AIDS, Rheuma, MS
  - **großes Marktpotential**
  - Patentschutz für Thalidomid seit Jahren ausgelaufen
- **Suche nach Derivaten, Hoffnung:**  
**Ähnliche Strukturaufbau → ähnliche Wirkung**

# Einige Namen für Thalidomid

- 1H-Isoindole-1,3(2H)-dione, 2-(2,6-dioxo 3-piperidiny)-
- Phthalimide, N-(2,6-dioxo-3-piperidyl)-
- ( $\pm$ )-Thalidomide
- $\alpha$ -(N-Phthalimido)glutarimide
- $\alpha$ -N-Phthalylglutaramide
- $\alpha$ -Phthalimidoglutaramide
- 1,3-Dioxo-2-(2,6-dioxopiperidin-3-yl) isoindoline
- 3-Phthalimidoglutaramide
- N-Phthaloylglutamimide
- N-(2,6-Dioxo-3-piperidyl) phthalimid
- Thalidomide
- Thalomid
- Celgene
- Contergan
- Distaval
- Kevadon
- Myrin
- Neurosedyn
- Pantosediv
- Quetimid
- Sauramide
- Sedalis
- Sedoval
- Softenil
- Softenon
- Suaramide
- Talimol
- Talinol

**Mögliche Begriffe  
für Freitextsuche  
mit  
Research Topic**

# Suche nach Thalidomid-Abkömmlingen über „Research Topic“

SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "thalidomide analogs (thalidomi..." with limiters

REFERENCES: RESEARCH TOPIC ⓘ

thalidomide analogs (thalidomide derivatives, thalidomide compounds, substituted thalidomides)

Examples:

0 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 421 references were found containing at least one of the concepts "thalidomide analogs", "thalidomide derivatives", "thalidomide compounds" or "substituted thalidomides".	421
<input type="checkbox"/> 87 references were found containing the concept "thalidomide analogs".	87
<input type="checkbox"/> 194 references were found containing the concept "thalidomide derivatives".	194
<input type="checkbox"/> 171 references were found containing the concept "thalidomide compounds".	171
<input type="checkbox"/> 31 references were found containing the concept "substituted thalidomides".	31

Publication Years

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

Document Types

- Biography
- Book
- Clinical Trial
- Commentary
- Historical
- Journal
- Letter
- Patent



# Trefferliste bei Research Topic

Research Topic "thalidomide analogs (thalidomi..." with limiters > **references (419)** > Preparation of pyridine compou...

REFERENCES ?

Get Substances

Get Reactions

Get Related Citations

Tools

Create Keep Me Posted Alert

Send SciPla

Analyze

Refine

Categorize

Sort by: Accession Number

0 of 419 References Selected

Analyze by: ?

Author Name

Xi Ning 12

Zeldis Jerome B 10

Curd John G 9

Fraley Mark E 9

Hartman George D 8

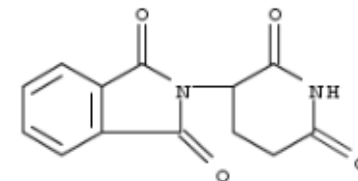
Deng Yongqi 7

Kong Qingzhong 7

401. **Use of neomycin for treating angiogenesis-related diseases**

Quick View Other Sources

By Hu, Guo-Fu; Vallee, Bert L.  
From PCT Int. Appl. (1999), WO 9958126 A1 19991118. | Language: English

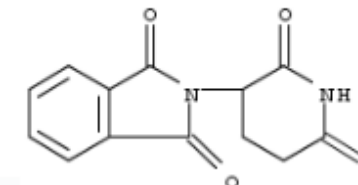


402. **Prevention of adhesions and excessive scar formation using angiogenesis inhibitors**

Quick View Other Sources

By Brem, Harold; Ehrlich, Jason; Folkman, Judah  
From PCT Int. Appl. (1999), WO 9909982 A1 19990304. | Language: English

50-35-1D Thalidomide, analogs



403. **Preparation of thalidomide analogs as immunomodulators.**

Quick View Other Sources

By Zimmer, Oswald; Winter, Werner; Wnendt, Stephan; Zwingenberger, Kai  
From Eur. Pat. Appl. (1998), EP 856513 A2 19980805. | Language: German, Database: CAPLUS

Gegebenenfalls das Suchergebnis über *Categorize/Searched Substances/Thalidomide, Modified* weiter eingrenzen.

Methods and compositions using thalidomide or other angiogenesis-inhibitory compound and anti-inflammatory

Categorize ?

1. Select a heading and category.

2. Select index terms of interest.

Category Heading

Category

Index Terms

Selected Terms

All  
General chemistry  
Biotechnology  
Synthetic chemistry  
Biology

Substances (34423)  
Topics (1741)  
Searched substances (2)

Select All Deselect All  
 Thalidomide 338  
 Thalidomide, Modified 94

Click 'x' to remove the category from 'Selected Terms'  
All > Searched substances (1 Terms)

# Tipp: Research Topic mit RN- Nummer

**SUBSTANCES: SUBSTANCE IDENTIFIER**

Thalidomide

1. 50-35-1

C13H10N2O4  
1H-isoindole-1,3(2H)-dione, 2-(2,6-dioxo-3-piperidinyl)-

**50-35-1D** als Suchterm verwenden  
(D steht für Derivat)

**REFERENCES: RESEARCH TOPIC**

50-35-1D

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

Search

**Substances**

50-06-6D Phenobarbital, 18F-substituted deriv.  
50-35-1D Thalidomide, 18F-substituted deriv.

C13H10N2O4

Es werden 157 Patente mit Thalidomid-Derivaten gefunden.

Publication Years

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

Document Types

- Biography
- Book
- Clinical Trial
- Commentary
- Historical
- Journal
- Letter
- Patent

50-35-1 Thalidomide

50-35-1D Thalidomide, prodrugs, salts, solvates, hydrates or clathrates

C13H10N2O4

# Struktursuche ohne Zeichnen

CAS Solutions  
**SCIFINDER**  
A CAS SOLUTION

Explore Saved Searches SciPlanner

REFERENCES  
Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

SUBSTANCES  
Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

SUBSTANCES: SUBSTANCE IDENTIFIER

thalidomide

Enter one per line.  
Examples:  
50-00-0  
999815  
Acetaminophen

Search

1. Substance Detail  
50-35-1

CAS Registry Number: 50-35-1

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Send to SciPlanner

Chemical Structure

Markush Patents by Structure

Reactions

C13H10N2O4  
1*H*-Isoindole-1,3(2*H*)-dione, 2-(2,6-dioxo-3-piperidinyl)-

SUBSTANCES: CHEMICAL STRUCTURE

Search Type:

Exact Structure

Substructure

Similarity

Show precision analysis

Click image to change structure or view detail.

SUBSTANCES: MARKUSH

Search Type:

Allow variability only as specified

Substructure

Click image to change structure or view detail.

Struktursuche

Markush-Suche

1983 Thalidomid-Abkömmlinge - die in 292 Patenten beschrieben werden - als Treffer

96 Patente mit Thalidomid-Derivaten

# Ergebnis Substruktursuche (1)

Substances search results showing 6 items. The first item is highlighted with a red box. The search results are sorted by Relevance. The first item is 1. Substance Detail 50-35-1, which is Thalidomide. The other items are derivatives of Thalidomide.

Item	Substance Detail	Chemical Formula	Count
1	Substance Detail 50-35-1	C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>	~4871
2	Substance Detail 19171-19-8	C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub>	~251
3	Substance Detail 841-67-8	C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>	~251
4	Substance Detail 2614-06-4	C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>	~133
5	Substance Detail 64567-60-8	C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub>	~32
6	Substance Detail 220460-55-9	C <sub>13</sub> H <sub>9</sub> FN <sub>2</sub> O <sub>4</sub>	~23

Sortieren der Treffer nach der Relevanz, mit „Select All“ alle auswählen, den Haken bei Thalidomid (1. Treffer) wieder entfernen, „Get References“ anklicken.

Ergebnis der Substruktursuche sind 1984 Substanzen: Thalidomid selbst, sowie 1983 Derivate

## Get References

### Retrieve references for:

- All substances
- Selected substances

### Limit results to:

- 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

Cancel

# Ergebnis Substruktursuche (2)

Chemical Structure substructure > substances (1975) > remove 1 substance (1974) > get references (717) > refine "Patents only" (244)

REFERENCES ? Get Substances Get Reactions Get Related Citations Tools

Analyze **Refine** Categorize

Sort by: Accession Number ↓

0 of 292 References selected

Refine by: ?

- Research Topic
- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Review

1. **Preparation of steroidal antiinflammatory prodrugs**  
[Quick View](#) [Other Sources](#)  
By Dos Santos, Jean Leandro; Chin, Chung Man  
From Braz. Pedido PI (2013), BR 2011000318 A2 20130521. | Language: Portuguese, Database: CAPLUS

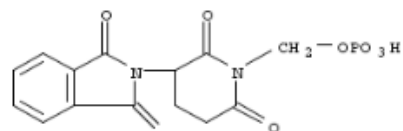
2. **ARRY-520 for use in treating cancer in a patient with low human  $\alpha 1$  acid glycoprotein (AAG) levels**  
[Quick View](#) [Other Sources](#)  
By Brown, Karin; Franklin, Ronald B.; Hingorani, Gary P.; Litwiler, Kevin S.; Tunquist, Brian J.; Walker, Robert J.  
From PCT Int. Appl. (2014), WO 2014028543 A1 20140220. | Language: English, Database: CAPLUS

3. **Cereblon isoforms and their use as biomarkers for therapeutic treatment**  
[Quick View](#) [Other Sources](#)  
By Thakurta, Anjan; Gandhi, Anita; Waldman, Michelle F.; Chopra, Rajesh  
From PCT Int. Appl. (2014), WO 2014028445 A2 20140220. | Language: English, Database: CAPLUS

4. **Methods of treating cancer using 3-(4-((4-(morpholinomethyl)benzyl)oxy)-1-oxoisindolizin-2(1H)-ylidene)benzamide**  
[Quick View](#) [Other Sources](#)  
By Schafer, Peter H.; Gandhi, Anita  
From PCT Int. Appl. (2014), WO 2014025960 A1 20140213. | Language: English, Database: CAPLUS

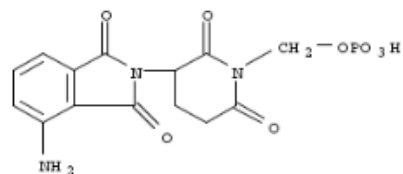
Substances ?

- 1233537-72-8P
- 1233537-73-9P
- 1233537-74-0P
- 1233537-75-1P
- 1233537-76-2P



1233537-77-3P

1233537-78-4P



1233537-79-5P

prepn. of water sol. phosphoric acid monoester derivs. as antitumor agent

Industrial manufacture; Preparation

Für diese 1983 Derivate gibt es 818 Textstellen im SciFinder. Nach dem Einschränken auf den Dokumententyp „Patente“ bleiben 292 Einträge übrig.

# Exkurs: Substanz“arten“ in Patenten

In den Ausführungsbeispielen und Ansprüchen **konkret genannte Substanzen**, die auch **charakterisiert** werden (Struktur, Eigenschaften, Herstellung, Verwendung, Reaktionen)

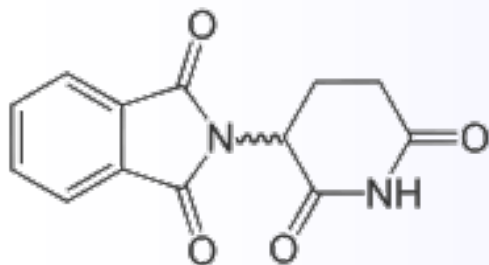
**Patent**

**Markush-Strukturen**  
generische, hypothetische Verbindungen aus den Patentansprüchen

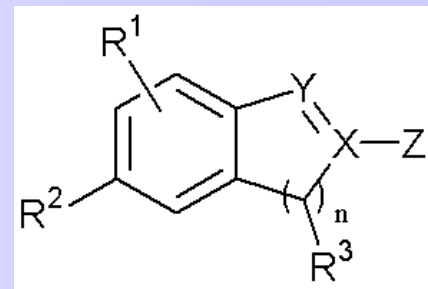
**Prophetische Substanzen**  
In den Ausführungsbeispielen namentlich **genannte Substanzen** bzw. in Tabellen **aufgelistete Verbindungen**, die nicht charakterisiert werden

REGISTRY  
CAPlus

MARPAT



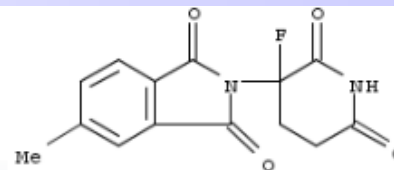
[0032] Analogously are prepared  
3-methyl-4-(3-trifluoromethoxyphenyl)-2-(4-trifluoromethylphenyl)  
5-methyl-4-(3-trifluoromethoxyphenyl)-2-(4-trifluoromethylphenyl)  
4-phenoxy-2-(4-trifluoromethylphenyl)-pyrimidine



# Prophetische Substanzen im SciFinder

- Spezifische chemische Verbindungen (z.B. Reaktanten, isolierte Intermediate, Produkte), die in den Ausführungsbeispielen eines Patentes vorkommen, aber nicht auch in den Ansprüchen
- Werden nicht näher charakterisiert, sondern nur erwähnt
  - als beispielhaft genannte “prophetische Substanzen” → Verbindungen, die nicht mit angeführten Eigenschaften/Reaktionen “unterfüttert” werden (z.B. Schmelzpunkt, Ausbeute), sondern von denen nur ein eindeutiger chemischer Name oder die Struktur angegeben wird oder die in Tabellen angeführt werden
  - mit beispielhaft genannter “prophetischer Verwendung/Herstellung” → Neuartige, aber nicht weiter belegte, spekulative oder theoretisch mögliche Verwendung/Herstellung eines schon bekannten chemischen Stoffes
- Neu identifizierte prophetische Substanzen bekommen Chemical Abstracts Registry Nummern (CAS-RN), werden in REGISTRY aufgenommen und in SciFinder als Ergänzung der Standardindexierung bei Patenten hinzugefügt.
- Prophetische Substanzen werden in den Treffernachweisen bei der Indexierung mit „prophetic“ gekennzeichnet

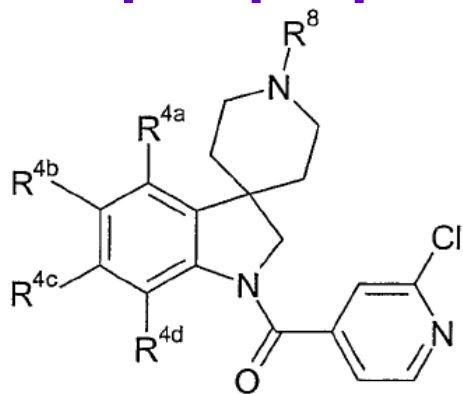
1101879-81-5



Preparation of 2-(2,6-dioxo-3-fluoropiperidin-3-yl)isoindolines for reducing inflammatory cytokine levels.

Prophetic

# Beispiel prophetischer Substanzen in einem Patent



(Ia) Table 1

Prophetische Substanzen werden bei Suchen mit Registry-Nummern oder über normale Struktursuchen **automatisch** gefunden.

Compound	R <sup>8</sup>	R <sup>4a</sup>	R <sup>4b</sup>	R <sup>4c</sup>	R <sup>4d</sup>
I-1	Cinnamyl	H	H	H	H
I-2	4-chlorocinnamyl	H	H	H	H
I-3	4-fluorocinnamyl	H	H	H	H
I-4	4-nitrocinnamyl	H	H	H	H
I-5	4-methoxycinnamyl	H	H	H	H
I-6	4-methylcinnamyl	H	H	H	H
I-7	4-trifluoromethylcinnamyl	H	H	H	H
I-8	4-cyanocinnamyl	H	H	H	H
I-9	2,4-dichlorocinnamyl	H	H	H	H
I-10	2,4-difluorocinnamyl	H	H	H	H
I-11	cinnamyl	Cl	H	H	H
I-12	4-chlorocinnamyl	Cl	H	H	H

Verbindungen ohne charakterisierende MS-Daten  
→ **Prophetische Substanzen**

Table 3	
Compound No	MS data
I-1	444 (95%), 446 (100%)
I-2	478 (100%), 480 (70%), 482 (15%)
I-3	462 (100%), 464 (95%)
I-4	489 (100%), 491 (70%)
I-5	147 (100%), 474 (30%), 476 (80%)
I-12	512 (95%), 514 (100%), 516 (35%), 518 (5%)



# Markush-Strukturen (1)

- Benannt nach Eugene A. Markush, in dessen Patent US1506316 zu Pyrazolon-Farbstoffen sie 1924 erstmals beschrieben wurden.



Patented Aug. 26, 1924.

1,506,316

## UNITED STATES PATENT OFFICE.

EUGENE A. MARKUSH, OF JERSEY CITY, NEW JERSEY, ASSIGNOR TO PHARMA-CHEMICAL CORPORATION, A CORPORATION OF NEW YORK.

PYRAZOLONE DYE AND PROCESS OF MAKING THE SAME.

No Drawing.

Application filed January 9, 1923. Serial No. 611,637.

In den Ansprüchen wurde erstmals nicht nur jeweils eine einzelne chemische Verbindung genannt, sondern eine Auswahl aus verschiedenen Substanzen.

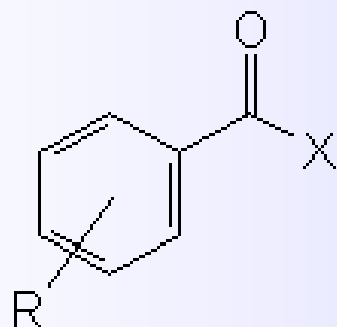
### Claims:

1. The process for the manufacture of dyes which comprises coupling with a halogen-substituted pyrazolone, a diazotized un-  
sulphonated material selected from the group consisting of aniline, homologues of aniline and halogen substitution products of aniline. 95 100

2. The process for the manufacture of dyes which comprises coupling with a halogen-substituted pyrazolone, a diazotized un-  
sulphonated material selected from the group consisting of aniline, homologues of aniline and halogen substitution products of aniline. 105

## Markush-Strukturen (2)

- Strukturformeln mit variablen Symbolen (generisch)
- mit Platzhaltern für bestimmte Substituenten, z.B. **R** für organische Reste (R = Methyl, Isopropyl, Pentyl...) oder **X** für Halogene, Heteroatome (X=N,O,S, Cl,Br...)



R = -CH<sub>3</sub>, -C<sub>2</sub>H<sub>5</sub>

X = H, Cl, Br

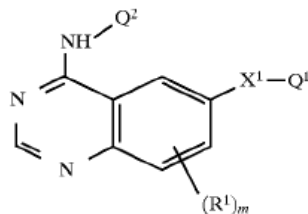
- **eine** Markush-Formel repräsentiert sehr **viele** potentielle chemische Substanzen
- dadurch können in **einer** Patentschrift eine **große Zahl** verschiedener, ähnlicher Verbindungen abgedeckt werden



# Typisches Beispiel für Markush-Strukturen

What we claim is:

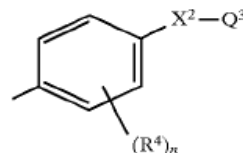
I. A quinazoline derivative of the formula I



wherein X<sup>1</sup> is a direct link;

wherein Q<sup>1</sup> is a 5-membered heteroaryl moiety containing one heteroatom selected from oxygen and sulphur, which heterocyclic moiety is a single ring or is fused to a benzo ring, and Q<sup>1</sup> optionally bears up to 3 substituents selected from halogeno, hydroxy, amino, trifluoromethoxy, trifluoromethyl, cyano, nitro, carboxy, carbamoyl, (1-4C) alkoxy, (1-4C)alkyl, (1-4C)alkoxy, (2-4C) alkenyloxy, (2-4C)alkynyloxy, (1-3C)alkenedioxy, (1-4C) alkylamino, di-[(1-4C)alkyl]amino, pyrrolidin-1-yl, piperidino, morpholino, piperazin-1-yl, 4-(1-4C) alkylpiperazin-1-yl, (2-4C)alkanoylamino, N-(1-4C) alkylcarbamoyl, N,N-di-[(1-4C)alkyl]carbamoyl, amino-(1-4C)alkyl, (1-4C)alkylamino-(1-4C)alkyl, di-[(1-4C) alkyl]amino-(1-4C)alkyl, pyrrolidin-1-yl-(1-4C)alkyl, piperidino-(1-4C)alkyl, morpholino-(1-4C)alkyl, piperazin-1-yl-(1-4C)alkyl, 4-(1-4C)alkylpiperazin-1-yl-(1-4C)alkyl, halogeno-(2-4C)alkoxy, hydroxy-(2-4C) alkoxy, (1-4C)alkoxy-(2-4C)alkoxy, amino-(2-4C)alkoxy, (1-4C)alkylamino-(2-4C)alkoxy, di-[(1-4C)alkyl]amino-(2-4C)alkoxy, pyrrolidin-1-yl-(2-4C)alkoxy, piperidino-(2-4C)alkoxy, morpholino-(2-4C)alkoxy, piperazin-1-yl-(2-4C)alkoxy, 4-(1-4C)alkylpiperazin-1-yl-(2-4C)alkoxy, (1-4C)alkylthio-(2-4C)alkoxy, (1-4C)alkylsulphinyl-(2-4C)alkoxy, (1-4C)alkylsulphonyl-(2-4C)alkoxy, halogeno-(2-4C)alkylamino, hydroxy-(2-4C)alkylamino, (1-4C)alkoxy-(2-4C)alkylamino, amino-(2-4C) alkylamino, (1-4C)alkylamino-(2-4C)alkylamino, di-[(1-4C)alkyl]amino-(2-4C)alkylamino, pyrrolidin-1-yl-(2-4C) alkylamino, piperidino-(2-4C)alkylamino, morpholino-

wherein m is 1 or 2, and each R<sup>1</sup> is independently hydrogen, halogeno, trifluoromethyl, hydroxy, amino, nitro, cyano, carboxy, carbamoyl, (1-4C)alkoxycarbamoyl, (1-4C)alkyl, (1-4C)alkoxy, (1-4C)alkylamino, di-[(1-4C)alkyl]amino, (2-4C)alkanoylamino, N-(1-4C)alkylcarbamoyl or N,N-di-[(1-4C)alkyl]carbamoyl; and wherein Q<sup>2</sup> is phenyl optionally bearing up to 3 substituents selected from halogeno, trifluoromethyl, cyano, hydroxy, amino, nitro, carboxy, carbamoyl, (1-4C) alkoxy, (1-4C)alkyl, (1-4C)alkoxy, (1-4C) alkylamino, di-[(1-4C)alkyl]amino, (2-4C)alkanoylamino, N-(1-4C)alkylcarbamoyl and N,N-di-[(1-4C) alkyl]carbamoyl, or Q<sup>2</sup> is a group of the formula II



wherein X<sup>2</sup> is a group of the formula CO, C(R<sup>3</sup>)<sub>2</sub>, CH(OR<sup>3</sup>), C(R<sup>3</sup>)<sub>2</sub>-C(R<sup>3</sup>)<sub>2</sub>, C(R<sup>3</sup>)=C(R<sup>3</sup>), C≡C, CH(CN), O, S, SO, SO<sub>2</sub>, N(R<sup>3</sup>), CON(R<sup>3</sup>), SO<sub>2</sub>N(R<sup>3</sup>), N(R<sup>3</sup>)CO, N(R<sup>3</sup>)SO<sub>2</sub>, OC(R<sup>3</sup>)<sub>2</sub>, SC(R<sup>3</sup>)<sub>2</sub>, C(R<sup>3</sup>)<sub>2</sub>O or C(R<sup>3</sup>)<sub>2</sub>S wherein each R<sup>3</sup> is independently hydrogen or (1-4C)alkyl, Q<sup>3</sup> is phenyl or naphthyl or a 5- or 6-membered heteroaryl moiety containing up to 3 heteroatoms selected from oxygen, nitrogen and sulphur, which heteroaryl moiety is a single ring or is fused to a benzo ring, and wherein said phenyl or naphthyl group or heteroaryl moiety optionally bears up to 3 substituents selected from halogeno, trifluoromethyl, cyano, hydroxy, amino, nitro, carboxy, carbamoyl, (1-4C)alkoxycarbonyl, (1-4C)alkyl, (1-4C)alkoxy, (1-4C)alkylamino, di-[(1-4C) alkyl]amino, (2-4C)alkanoylamino, N-(1-4C) alkylcarbamoyl and N,N-di-[(1-4C)alkyl]carbamoyl, n is 1, 2 or 3 and each R<sup>4</sup> is independently hydrogen, halogeno, trifluoromethyl, cyano, hydroxy, amino, nitro, (1-4C)alkyl, (1-4C)alkoxy, (1-4C)alkylamino, di-[(1-4C)alkyl]amino or (2-4C)alkanoylamino; or a pharmaceutically-acceptable salt thereof.

# im Patentanspruch

US 5866572  
Quinazoline derivatives



## MARKUSH-Strukturen als Teil von SciFinder

- Generische, hypothetische Substanzen aus den Patentansprüchen
- **Inhalt:**
  - Mehr als 1022000 suchbare Markush-Strukturen aus Patenten des Zeitraums 1961 - heute
  - Mehr als 421000 anzeigbare Patente, die Markush-Strukturen enthalten
  - Anzeigbare Informationen: Bibliographische Angaben, Zusammenfassung, and CAS-Schlagworte (incl. Substanzen)
- **Umfang:**
  - Markush-Strukturen organischer oder organometallischer Moleküle, die in Patenten gefunden werden
  - Nicht enthalten: Legierungen und intermetallische Verbindungen, Metalloxide, anorganische Salze, Polymere
- **Update-Frequenz:**

Täglich mit ca. 60-75 Patenteinträgen und 150-200 Markush-Strukturen

# Ergebnis der Markush-Struktursuche

Markush substructure > **references (96)**

## REFERENCES

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Analyze   Refine   Categorize

Sort by: Accession Number

Analyze by:

Author Name

Muller George W 20

Zeldis Jerome B 14

Chen Roger Shen  
Chu 10

Man Hon Wah 9

0 of 96 References Selected

- 1. **Treatment of brain metastasis from cancer**  
Quick View   Other Sources  
By Quick View   Other Sources   aldomero; Muixi, Laia  
From PCT Int. Appl. (2014), WO 2014147531 A2 20141113. | Language: English, Database: CAPLUS
- 2. **Preparation of isoquinolinamine derivatives useful for the treatment of cancer**  
Quick View   Full Text  
By Kandula, Mahesh  
From PCT Int. Appl. (2014), WO 2014147531 A2 20140925. | Language: English, Database: CAPLUS

Ergebnis der Markush-Suche sind 96 Patente zu Thalidomid-Derivaten. Davon sind 10 Patente nur auf diese Weise gefunden worden.

Tools

- Remove Duplicates
- Combine Answer Sets**
- Add Tag

 **Exclude**

Include only answers from **Markushsuche Thalidomid-Derivate (96)** that are not in **current answer set (676)**

0 of 10 References Selected

- 1. **Preparation of isoquinolinamine derivatives useful for the treatment of cancer**  
Quick View   Other Sources  
By Kandula, Mahesh  
From PCT Int. Appl. (2014), WO 2014147531 A2 20140925. | Language: English, Database: CAPLUS

# Patentangaben im Einzeltreffer

**Erfinder**

**Patentanmelder, -inhaber (Assignee)**

**Veröffentlichungsdatum**  
- Am 31. Mai 2001 wurde das Patent veröffentlicht.

**Patentnummer**

**Anmeldedatum** - Am 29.11.1999 ist das Patent von Grünenthal beim Patentamt eingegangen.

**Prioritätsdatum**

Anmeldetag der ersten Anmeldung eines Schutzrechts, kann für eine Anmeldung bei einem anderen Patentamt in Anspruch genommen werden.

Zur Patentfamilie gehörende **Äquivalenz-Patente**

REFERENCE DETAIL

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**289. Method using a thalidomide compound and an antiinflammatory cytokine for the treatment and/or prophylaxis of interleukin-12-caused diseases**

By: Frosch, Stefanie; Germann, Tieno  
Assignee: Gruenenthal G.m.b.H., Germany

A combination therapy is provided for the treatment of diseases which are caused by the formation of the proinflammatory cytokine interleukin-12 (IL-12), in which a thalidomide compd. [e.g. thalidomide, α-methylthalidomide (EM 978)] and an antiinflammatory cytokine (e.g. IL-10) are applied at the same time.

**Patent Information**

Patent No.	Kind	Date	Application No.	Date
DE 19957342	A1	May 31, 2001	DE 1999-19957342	Nov 29, 1999
WO 2001039758	A2	Jun 7, 2001	WO 2000-EP11179	Nov 11, 2000
WO 2001039758	A3	Mar 28, 2002		
AU 2001013938	A	Jun 12, 2001	AU 2001-13938	Nov 11, 2000
US 20030021763	A1	Jan 30, 2003	US 2002-156771	May 29, 2002

**Priority Application**

DE 1999-19957342	A	Nov 29, 1999
WO 2000-EP11179	W	Nov 11, 2000

**Indexing**

**Substance**

50-35-1

19  
P029-00;  
ER

**QUICK LINKS**  
0 Tags, 0 Comments

**PATENT INFORMATION**  
May 31, 2001  
DE 19957342  
A1

**APPLICATION**  
Nov 29, 1999  
DE 1999-19957342

**PRIORITY**  
Nov 29, 1999  
DE 1999-19957342  
Nov 11, 2000  
WO 2000-EP11179

**SOURCE**  
Ger. Offen.  
8 pp.

synergistic; thalidomide compd. and antiinflammatory cytokine for treatment and/or prophylaxis of interleukin-12-caused diseases

Anti-inflammatory agents | Immunomodulators

# Zugang zu den Patentvolltexten

REFERENCE DETAIL ⓘ

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289. Method using a thalidomide compound and an antiinflammatory cytokine for the treatment and/or prophylaxis of interleukin-12-caused diseases

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Deutsch English Français

Kontakt

Land ändern

Über Espacenet Andere Online-Dienste

Suche Trefferliste Meine Patentliste (0) Abfrageverlauf Nutzereinstellungen Hilfe

Suche → Treffer → DE19957342 (A1)

DE 19957342 (A1)

**Bibliographische Daten**

Beschreibung

Patentansprüche

Originaldokument

**Bibliographische Daten: DE 19957342 (A1)**

★ In "meine Patentliste" übernehmen → Datenfehler melden Drucken

Treatment of interleukin (IL)-12 mediated illnesses comprises simultaneous administration of thalidomide or analogue and antiinflammatory cytokine

Bookmark zur Seite DE 19957342 (A1) - Treatment of interleukin (IL)-12 mediated illnesses comprises simultaneous administration of thalidomide or an...

Veröffentlichungsdatum: 2001-05-31

Erfinder: BOSCH STEFANIE [DE]; GERMAN

Anmelder: GRUENENTHAL GMBH [DE] ±

Klassifikation: - Internationale: A61K38/18; A61K38/19 (IPC1-7): A61K38/19  
- Europäische: A61K38/18E; A61K38/19E

Anmeldenummer: DE19991057342 19991129

Prioritätsnummer(n): DE19991057342 19991129

Auch veröffentlicht als □ US 2003021763 (A1)  
□ WO 0139759 (A2)

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19 BUNDESREPUBLIK DEUTSCHLAND

12 Offenlegungsschrift

10 DE 199 57 342 A 1

5 Int. Cl.<sup>7</sup>: A 61 K 38/19  
A 61 K 31/4025  
A 61 P 29/00  
A 61 P 5/48

21 Aktenzeichen: 199 57 342.5

22 Anmeldetag: 29. 11. 1999

43 Offenlegungstag: 31. 5. 2001

DEUTSCHES PATENT- UND MARKENAMT

DE 199 57 342 A 1



# Das Deckblatt einer Patentschrift

<p>⑩ <b>BUNDESREPUBLIK DEUTSCHLAND</b></p>  <p><b>DEUTSCHES PATENT- UND MARKENAMT</b></p>	<p>⑫ <b>Offenlegungsschrift</b> <b>DE 199 57 342 A 1</b></p> <p>⑳ Aktenzeichen: 199 57 342.5          ㉑ Anmeldetag: 29. 11. 1999          ㉒ Offenlegungstag: 31. 5. 2001</p>	<p>⑨ Int. Cl.<sup>7</sup>: <b>A 61 K 38/19</b> A 61 K 31/4025 A 61 P 29/00 A 61 P 5/48</p> <p style="writing-mode: vertical-rl; transform: rotate(180deg);"><b>DE 199 57 342 A 1</b></p>
<p>㉓ Anmelder: Grünenthal GmbH, 52078 Aachen, DE</p>	<p>㉔ Erfinder: Frosch, Stefanie, Dipl.-Biol. Dr., 52078 Aachen, DE; Germann, Tieno, Dr., 52134 Herzogenrath, DE</p> <p>⑤⑥ Für die Beurteilung der Patentfähigkeit in Betracht zu ziehende Druckschriften:</p> <p>WO 97 41 844 A1          WO 40 269 A2          WO 10 552 A2</p> <p>GALLILY,R.,et.al.: Mycoplasma fermentans - Induced inflammatory response of astrocytes: Selective modulation by aminoguanidine, thalidomide , pentoxifylline and IL-10. Inflammation,1996, 23/6, S.495-505;          PISCITELLI,S.C.: Use of immunomodulation for the treatment of HIV infection. ASHP Annua I Meeting, 1998,Vol.55,June,S.35;</p>	
<p><b>Die folgenden Angaben sind den vom Anmelder eingereichten Unterlagen entnommen</b></p>		
<p>⑤④ Verfahren zur Behandlung und/oder Prophylaxe von IL-12-bedingten Erkrankungen</p> <p>⑤⑤ Es wird eine Kombinationstherapie zur Behandlung von Erkrankungen, die durch die Bildung des entzündungsfördernden Zytokins IL-12 hervorgerufen werden, beschrieben, wobei gleichzeitig eine Thalidomidverbindung und ein antiinflammatorisches Zytokon appliziert werden.</p>		

**Wichtigste bibliographische Daten:**

Titel der Erfindung  
 Dokumentennummer,  
 Dokumentenart  
 Notationen der Internationalen Patentklassifikation (IPC)  
 Erfinder, Anmelder,  
 Patentanwalt/Vertreter  
 Anmeldenummer, Prioritätsangaben, Datumsangaben

**Zusammenfassung:**

Bezeichnung der Erfindung,  
 Kurzfassung des technischen Inhalts der Anmeldung (Problem, Lösung, hauptsächliche Verwendungsmöglichkeit)  
 Häufig: ausgewählte Zeichnung bzw. chemische Strukturformel, die die Erfindung am deutlichsten kennzeichnet.

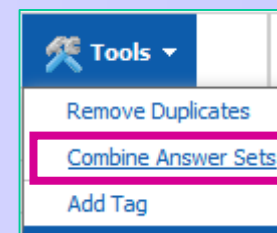




# Vergleich der Suchergebnisse

	Anzahl der gefundenen Patente	Davon nur so gefunden
Research Topic thalidomide analogs (thalidomide derivatives, thalidomide compounds, substituted thalidomides)	419	258 (viele nicht relevant)
50-35-1D	157	49 (alle relevant)
Substruktursuche	292	152 (alle relevant)
Markush-Suche	96	10 (alle relevant)
Summe	686	-

Tipp: Antwortsatz jeder Einzelsuche speichern und mit „Combine Answer Sets“ zusammenfassen.



**Save This Answer Set**

\* Required

**Save:**

All answers

Only selected answers

**Title: \***

Thalidomit-Derivate (Wortsuche)

**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

**Combine Answer Sets** **Cancel**



# Statistische Analyse der Patente (1)

REFERENCES ?

Analyze Refine Categorize

Analyze by: ?

- Author Name
- Author Name
- CAS Registry Number
- CA Section Title
- Company-Organization
- Database
- Document Type
- Index Term
- CA Concept Heading
- Journal Name
- Language
- Publication Year
- Supplementary Terms

REFERENCES ?

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Company-Organization

Merck & Co Inc, USA	21
USA	18
Schering Corporation, USA	17
Celgene Corporation, USA	14
Novacea Inc, USA	9
Board of Regents the University of Texas System, USA	5
Gruenenthal G m b H, Germany	5
Jinan Shuaihua Pharmaceutical Science and Technology Co Ltd, Peop Rep China	5
Peop Rep China	5
Pharmacopeia Inc	5

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Analyze by: ?  
Index Term

Human	245
Antitumor agents	231
Neoplasm	178
Combination chemotherapy	151
Drug delivery systems	143
Interferons	131
Antibodies and Immunoglobulins	123
Mammary gland, neoplasm	115
Lung, neoplasm	105
Carcinoma	102

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Analyze Refine Categorize

Analyze by: ?  
Publication Year

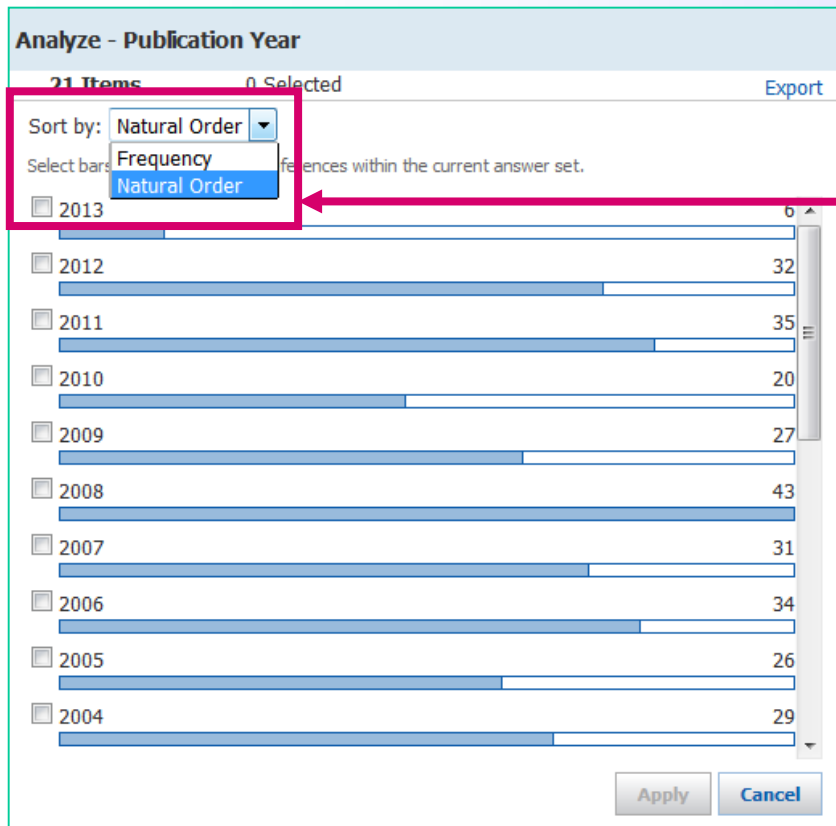
2008	43
2011	35
2006	34
2012	32
2007	31
2004	29
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2003	26
2010	20

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Statistiken zur Analyse der Konkurrenten (Erfinder und Firmen), der möglichen Einsatzgebiete, des zeitlichen Verlaufs (Trend) usw.

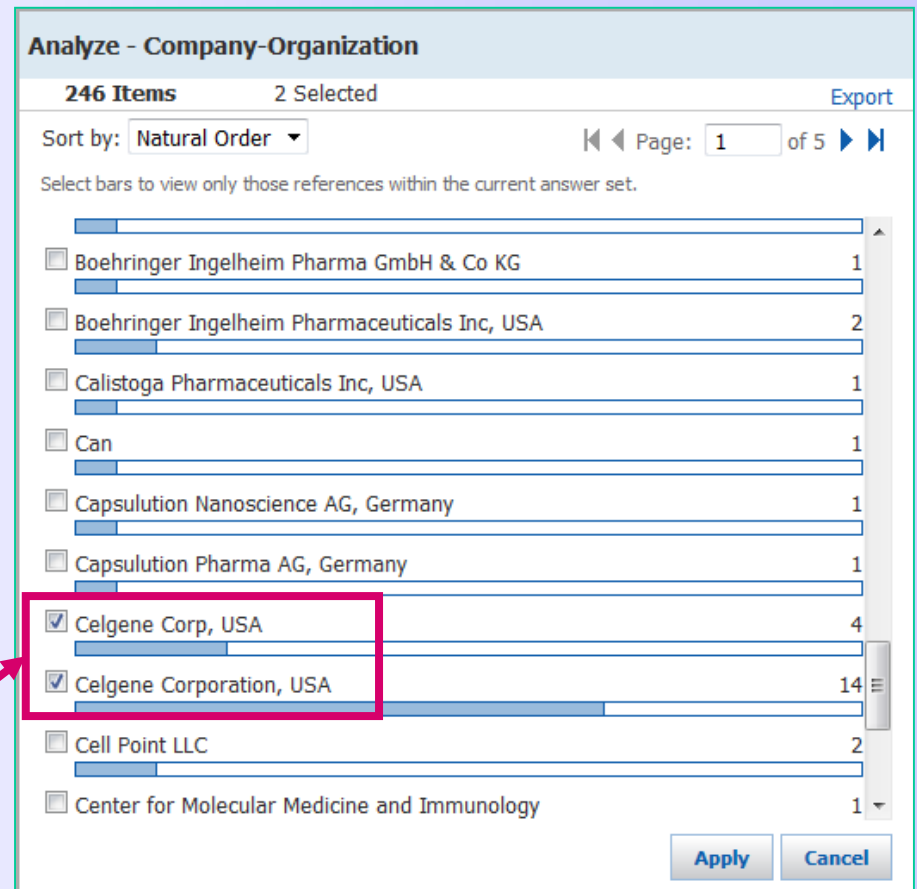


## Statistische Analyse der Patente (2)



Voreingestellt ist die Sortierung nach der Häufigkeit (*Frequency*).  
Das alphabetische Sortieren ist ebenfalls möglich (*Natural Order*)

Firmennamen sind im SciFinder nicht normiert, sondern werden so übernommen, wie sie in den Patenten stehen.



# Export der Patentstatistiken

Export Analysis - Publication Year \* Required

**Export:**

- All
- Selected
- Range

Example: 2-20

**For:**

**Offline review**

- Portable Document Format (\*.pdf)
- Microsoft Excel Worksheet (\*.xls)

**Details:**

**File Name: \***

Analysis\_06\_10\_2013\_Thalidomide\_PY

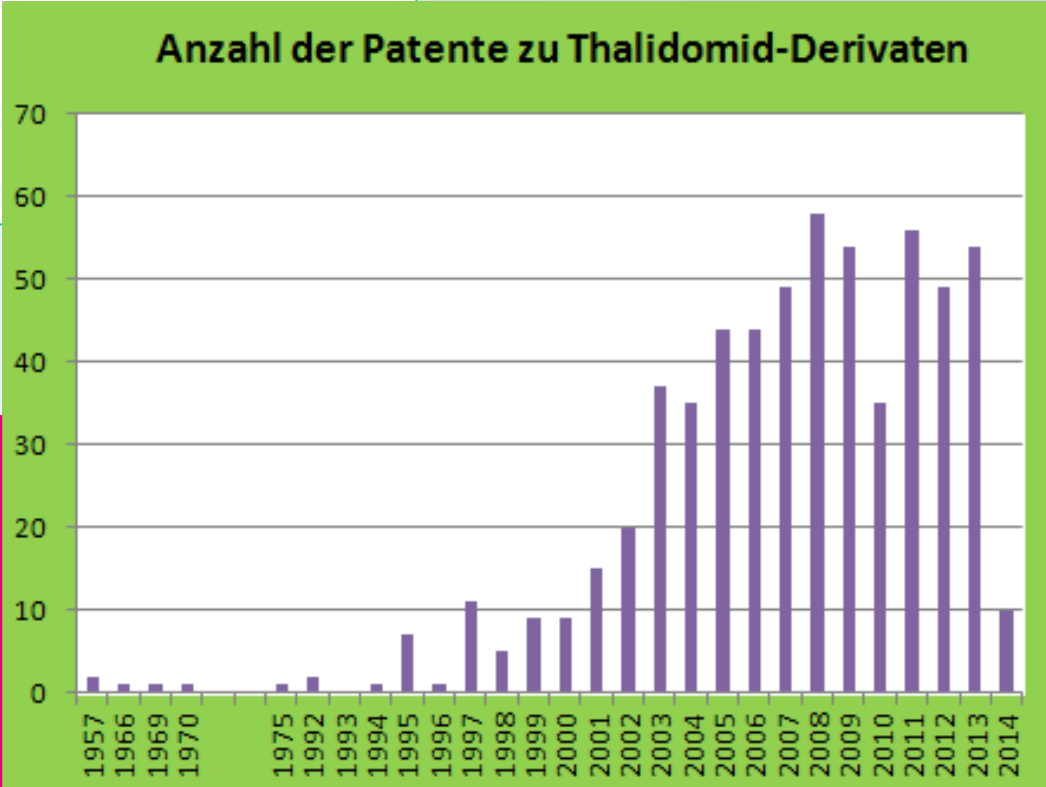
Export der Analysedaten nach Excel

CAS Solutions

**SCIFINDER**  
A CAS SOLUTION

Publication	Mar 17, 2014
0 Selected	Sorted by
Analysis Val	Count
2014	10
2013	54
2012	49
2011	56
2010	35
2009	54
2008	58
2007	49

Ausschnitt der exportierten Ergebnisliste in der Excel-Datei.  
Damit angefertigtes Balkendiagramm zur besseren Veranschaulichung des Trends.





## Resümee

- Vollständige Suche nach Patenten zu chemischen Substanzen nur unter Einbezug von Struktur-Recherchen und Markush-Patenten möglich.
- Eine im SciFinder durchgeführte (Patent)-Recherche findet ausreichend Material, das den Stand der Technik veranschaulicht.
- Um die Neuheit einer Erfindung zu garantieren, ist eine ergänzende professionelle Suche in spezifischen, kommerziellen Patentdatenbanken (INPADOC, World Patent Index) unbedingt nötig.



# Ansprechpartner bei Fragen