



# SciFinder<sup>®</sup>

The choice for chemistry research.<sup>™</sup>



# Chemical Abstract Service

- » É uma divisão da American Chemical Society (ACS)
- » Fundada em 1907 para monitorar, resumir e indexar a literatura relacionada com a química e torná-la disponível para a comunidade científica
- » Sua equipe conta com cerca de 1.300 membros - incluindo cientistas, cobrindo mais de 50 idiomas



*A Division of the American Chemical Society*



# SciFinder

» Ferramenta de pesquisa do CAS que permite recuperar e analisar, a partir de uma única plataforma, as informações dos diferentes bancos de dados do CAS.

» Cobertura:

- |               |                        |
|---------------|------------------------|
| ✓ Química     | ✓ Materiais            |
| ✓ Física      | ✓ Microbiologia        |
| ✓ Biologia    | ✓ Farmácia             |
| ✓ Engenharia  | ✓ Têxtil               |
| ✓ Medicina    | ✓ Tecnologia Nuclear   |
| ✓ Agricultura | ✓ Geologia             |
| ✓ Alimentos   | ✓ ... e outras tantas. |



# Bases de dados

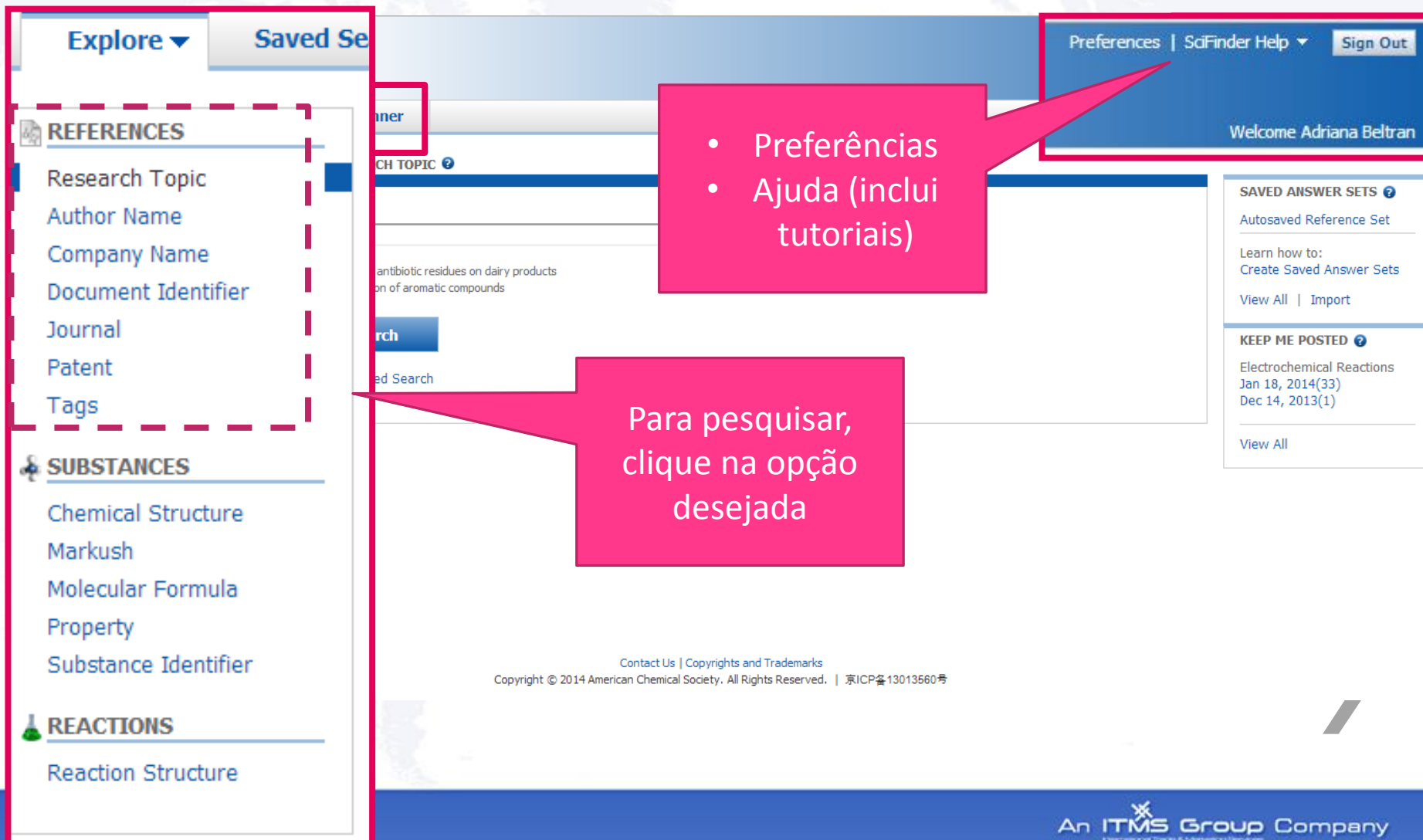




# SciFinder



# SciFinder- Página Inicial



The screenshot shows the SciFinder homepage. A red dashed box highlights the left sidebar menu, which includes sections for REFERENCES, SUBSTANCES, and REACTIONS. A red box highlights the top navigation bar with links for Explore, Saved Sets, Preferences, SciFinder Help, and Sign Out. A red box highlights the main search area with a search bar and a search button. A red box highlights the right sidebar with sections for Saved Answer Sets and Keep Me Posted. A pink callout box points to the search bar with the text 'Para pesquisar, clique na opção desejada'. Another pink callout box points to the Preferences and SciFinder Help links with the text 'Preferências' and 'Ajuda (inclui tutoriais)'.

**Explore ▼** **Saved Se**

**REFERENCES**

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

**SUBSTANCES**

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

**REACTIONS**

- Reaction Structure

**Preferences** | **SciFinder Help ▼** **Sign Out**

Welcome Adriana Beltran

**SAVED ANSWER SETS**

Autosaved Reference Set

Learn how to:  
Create Saved Answer Sets

View All | Import

**KEEP ME POSTED**

Electrochemical Reactions  
Jan 18, 2014(33)  
Dec 14, 2013(1)

View All

Para pesquisar, clique na opção desejada

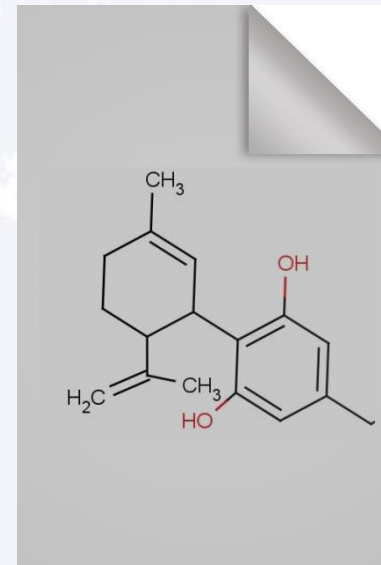
Preferências  
Ajuda (inclui tutoriais)

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International Trade & Technology Services

# Explorar Referências

- » Tema
- » Autor
- » Companhia
- » Identificador de Documento
- » Periódico
- » Patente
- » Etiquetas (pessoal)



# Explorar Referências

- » A interface de busca permite a utilização de frases (limite de complexidade até 5 palavras)
- » Pode-se utilizar parentêses para indicar sinônimos de um conceito particular
- » Pode-se utilizar “aspas” para encontrar conceitos exatamente como digitados.
- » Pode-se utilizar operadores Booleanos: OR, AND, WITH, NOT
- » Pode-se utilizar CAS RN na busca por tema
- » SciFinder tem um “Thesaurus” e um dicionário de sinônimos.





# Explorar Referências

## » SciFinder Smarts

Termo de Busca	Termos Associados
Sinônimos incluindo termos controlados	- Acetaminofen, Paracetamol
Formas alternativas	- Freeze, froze, frozen, freezing - Waste water, wastewater - Antibacteriano, anti-bacteriano
Formas de plural irregular	- Woman, women - Ox, oxen - Mice, mouse, mousse - Half life, half-life, halflife, halflives, half live, half lives, halflive, halflives
Abreviações Padrões do CAS	- Oxidation, Oxidn
Grafia Americana e Britânica	- Synthesize, synthesise
Regras de trucagem para recuperar palavras começando com palavras de tronco comum	- Palavras terminadas em <b>-tion</b> com uma raiz de pelo menos 5 letras são truncadas (depletion – deple?) - Palavras contendo <b>-able</b> , <b>-ed</b> , <b>-ing</b> como sufixos são truncadas (solvable – solv?) - Palavras contendo <b>-e</b> no final (disease – diseases?)


## Explorar Referências – Pesquisa

- » Pesquisa simples por tema: escrever a palavra chave ou frase (não é necessário o uso de booleanos ou truncagem)

**REFERENCES: RESEARCH TOPIC** ?

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

**Search**

 Advanced Search



# Explorar Referências – Pesquisa avançada

## 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

» Somente disponível na pesquisa por tema

➤ Delimitar por:

- Ano(s)
- Tipo de documento
- Idioma
- Autor
- Companhia



## Explorar Referências – Resultados

» Aparecem várias opções (depende do tema pesquisado):

- > Frase exata
- > Com ambos conceitos relacionados
- > Com ambos conceitos em qualquer parte da referência
- > Somente o primeiro conceito
- > Somente o segundo conceito

Select All Deselect All

0 of 5 Research Topic Candidates Selected

- ☐ 5 references were found containing **"adverse effects of quinine"** as entered.
- ☐ 107 references were found containing the two concepts **"adverse"** and **"quinine"** closely associated with one another.
- ☐ 1255 references were found where the two concepts **"adverse"** and **"quinine"** were present anywhere in the reference.
- ☐ 1733855 references were found containing the concept **"adverse"**.
- ☐ 27906 references were found containing the concept **"quinine"**.

Get References

Seleciono a minha preferência e clico em "Get References"

# Explorar Referências – Página de Resultados

**SciFinder®**

Preferences | SciFinder Help | Sign Out

Welcome Adriano Balleza

Save | Print | Export

22 duplicates were automatically removed.

Research Topic "adverse effects of quinine" > references

**REFERENCES**

Analyze | Refine | Categorize

Analyze by: Author Name

Avery Simon V	3
Bunnag D	3
Harinasuta T	3
Karbwang J	3
Pleass Richard J	3
Anonymous	2
Arguin Paul M	2
Du Jie	2
Esamai F	2
Goad Jeffery A	2

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

Sort by: Accession Number

0 of 85 References selected

1. **Early safety assessment of human oculotoxic drugs using the zebrafish visualmotor response**

By Deeti, Sudhakari; O'Farrell, Breandan N.  
From Journal of Pharmacology and Therapeutics Methods (2014), 69(1), 1-8. | Language: English, Database: CAPLUS

Many prescribers... predict drug-induced... After 48 h... behavioral... assessed... response... study confirmed...

2. **Artesunate... of adverse events focussing on delayed haemolysis**

By Rolling, Thie... From Malaria Jo... Background... efficacy and... malaria in... retrospective...

ite compared to **quinine** is superior in antiparasitic... and haemolysis after parenteral artesunate for severe... the use of parenteral **quinine**. Methods: In this... between 2006 and 2012. The primary endpoint was...

**Annotations:**

- Links para visualização rápida e opções de texto completo
- Título do documento. Para ver os detalhes, clicar no
- Posso salvar a minha pesquisa ou exportar em formato :
  - Pdf
  - Txt
  - Rtf
- Classificar os resultados por :
  - Como foram indexados
  - Nome do Autor
  - Data de publicação
  - Quantas vezes foi citado
  - Título
- Resumo do documento sempre em inglês)



## Explorar Referências – Resultados

### » Ferramentas

- > Analizar
- > Categorizar
- > Refinar
- > Guardar respostas (completa ou parcial)
- > Keep me Posted (completo ou parcial)
- > Enviar a SciPlanner
- > Obter Referências, Substâncias, Reações, Referências relacionadas.
- > Combinar varias pesquisas



# Explorar Referências – Detalhes do documento

## REFERENCE DETAIL

Get Substances

Return

### 2. Artesunate versus quinine in the haemolysis

By: Rolling, Thierry; Wichmann, Dominic; Schmied

Background: Severe malaria is a potentially life-threatening disease. Lowering mortality showing a better short-term survival has been published recently. So far, delayed haemolysis at the University Medical Center Hamburg-Eppendorf those who received artesunate. As secondary endpoint, 16 patients contributed sufficient data to assess artesunate as an adjunct treatment - and five patients were treated with quinine.

Ind

Pha

## Concepts

Antimalarials  
Combination chemotherapy  
Human  
Plasmodium falciparum

comparative anal. of adverse events in patients treated with severe imported malaria with special focus on the

Hemoglobins

## Citations

Anon; Centralized information system for infectious diseases (CISID), <http://data.euro.who.int/cisid>  
Anon; Infektionsepidemiologisches Jahrbuch meldepflichtiger Krankheiten für 2011/2012  
Askling, H; Malar J 2012, 11, 328  
Dondorp, A; Lancet 2005, 366, 717  
Dondorp, A; Lancet 2010, 376, 1647  
Sinclair, D; Cochrane Database Syst Rev 2012, 6, CD005967  
Eder, M; Pathog Glob Health 2012, 106, 181  
Anon; Leitlinie: Diagnostik und Therapie der Malaria, [http://www.awmf.org/uploads/tx\\_szleitlinien/015-001 Leitlinie Diagnostik und Therapie der Malaria.pdf](http://www.awmf.org/uploads/tx_szleitlinien/015-001 Leitlinie Diagnostik und Therapie der Malaria.pdf)  
WHO, World Health Organization; Guidelines for the treatment of malaria, 2nd edition 2010  
Cramer, J; Malar J 2011, 10, 256  
Wolf, L; J Emerg Med 1992, 10, 295  
Alkadi, H; Chemotherapy 2007, 53, 385  
Caramello, P; J Antimicrob Chemother 2012, 67, 2053  
Kreftmeijer-Vegter, A; Malar J 2012, 11, 102  
Rolling, T; Malar J 2012, 11, 169  
Zoller, T; Emerg Infect Dis 2011, 17, 771  
Anon; Rare disease (orphan) designations, [http://www.ema.europa.eu/docs/en\\_GB/document\\_library/Brochure/2011/03/WC500104234.pdf](http://www.ema.europa.eu/docs/en_GB/document_library/Brochure/2011/03/WC500104234.pdf)  
Anon; ATU nominative, protocole d'utilisation thérapeutique et de recueil d'informations, MalacefW (artesunate) 60mg, poudre et solvant pour solution injectable  
Centres for Disease C, Prevention; MMWR Morb Mortal Wkly Rep 2013, 62, 5  
Angus, B; Blood 1997, 90, 2037  
Chotivanich, K; J Infect Dis 2000, 182, 629  
Das, B; J Vector Borne Dis 2008, 45, 83  
Campos, S; Kidney Int 2001, 59, 1044  
Seguro, A; Am J Trop Med Hyg 2002, 67, 473  
White, N; Lancet Infect Dis 2007, 7, 549  
Sterns, R; Evaluation of the patient with hyponatremia 2013  
Ellison, D; N Engl J Med 2007, 356, 2064  
Hoorn, E; Malar J 2012, 11, 26  
Holst, F; Am J Trop Med Hyg 1994, 50, 602  
Akuthota, P; Clin Microbiol Rev 2012, 25, 649  
Solomon, J; Semin Respir Crit Care Med 2006, 27, 192  
Kohno, S; Jpn J Med 1990, 29, 248  
Anon; Pneumotox v2.0, [www.pneumotox.com](http://www.pneumotox.com)

## Tags

0 Tags | Edit Tags

## Comments

0 Comments Sort by: Newest First | Older First

No comments

Informação do documento

Referências. Em azul as que estão no SciFinder

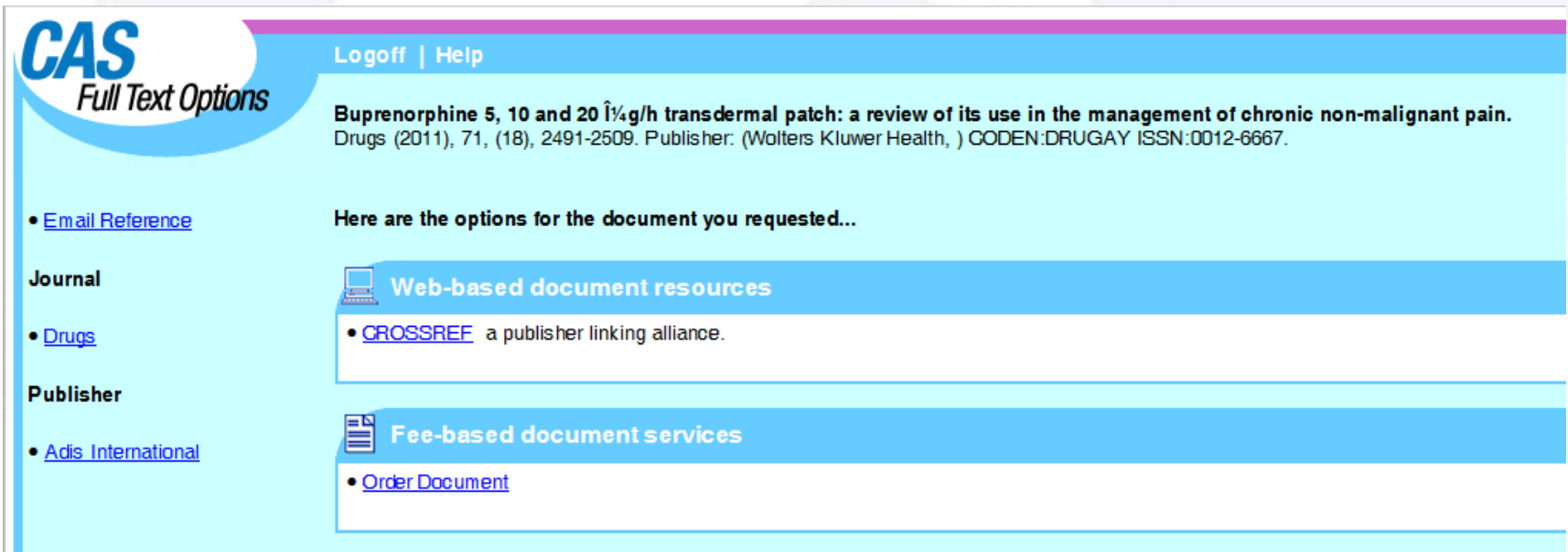
Conceitos para novas pesquisas

Marcadores e comentários

# CAS Full Text Options®

## » Opções de ir direto a:

- > Página do editor
- > Página do periódico
- > Página do documento de texto completo (tarifas podem ser aplicadas para download)



The screenshot shows the CAS Full Text Options web interface. On the left is a navigation menu with links for Email Reference, Journal, Drugs, Publisher, and Adis International. The main content area displays a document title: 'Buprenorphine 5, 10 and 20 1/4g/h transdermal patch: a review of its use in the management of chronic non-malignant pain.' Below the title, it says 'Here are the options for the document you requested...'. There are two sections: 'Web-based document resources' containing a link to CROSSREF, and 'Fee-based document services' containing a link to Order Document.

**CAS**  
*Full Text Options*

Logoff | Help

**Buprenorphine 5, 10 and 20 1/4g/h transdermal patch: a review of its use in the management of chronic non-malignant pain.**  
Drugs (2011), 71, (18), 2491-2509. Publisher: (Wolters Kluwer Health, ) CODEN:DRUGAY ISSN:0012-6667.

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

**Web-based document resources**

- [CROSSREF](#) a publisher linking alliance.

**Fee-based document services**

- [Order Document](#)

**Journal**

- [Drugs](#)

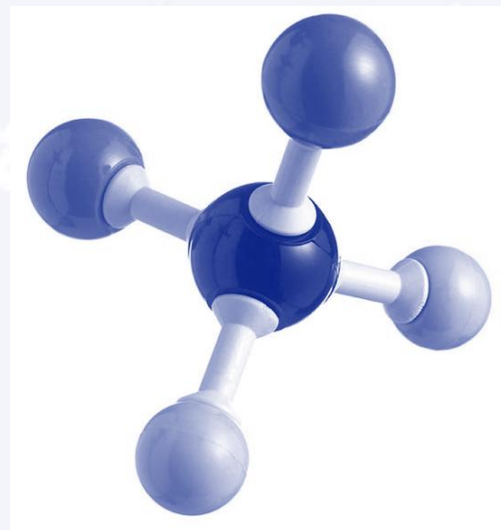
**Publisher**

- [Adis International](#)

• [Email Reference](#)

# Explorar Substâncias

- » Estrutura química (editor)
- » Markush (editor)
- » Fórmula molecular
- » Propriedades
- » Identificador de substâncias

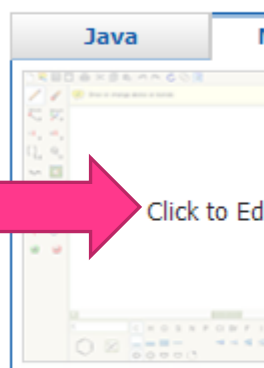


# Explorar Substâncias - Editor de estruturas

- » Pesquisa por estrutura química
- » É possível importar estruturas desenhadas em outros editores de estrutura (ChemDraw)

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:



Import CXF

Search

Advanced Search

Advanced Search

☐ Always Show

Characteristics

- ☐ Single component
- ☐ Commercially available
- ☐ Included in references

Classes

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

Studies

- ☐ Analytical
- ☐ Biological
- ☐ Preparation
- ☐ Reactant or reagent

but having to resolve Java issues.  
above the structure editor box.



# Explorar Substâncias - Editor de estruturas

The screenshot shows the 'Structure Editor' window. It features a top toolbar with icons for file operations and editing. On the left is a vertical toolbar with icons for drawing atoms, bonds, and rings. On the right is a 'Drawing Editor' panel with radio buttons for 'Structure', 'Reaction', and 'Markush'. Below that is a search panel titled 'Get substances that match your query using:' with radio buttons for 'Exact search', 'Substructure search', and 'Similarity search'. At the bottom is a 'Properties' panel with a 'Scale' dropdown set to 100. The main workspace is currently empty. The status bar at the bottom displays 'C8 H10 N4 O2 (query)' and '194.19'.

**Menu:**

- Importar
- Salvar
- Imprimir
- Cortar
- Copiar
- Colar
- Desfazer

**Ferramentas de desenho**

**Lápis e borracha**

**Átomos e estruturas**

**Ligação variável**

**Modelos e**

**Selecionar**

**Bloquear átomo**

**Virar e girar**

**Adicionar carga**

**Drawing Editor:**

- ☒ Structure
- ☐ Reaction
- ☐ Markush

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

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

**Aceptar**

**Cancelar**

**Scale** 100

**C8 H10 N4 O2 (query)**

**194.19**



## Explorar Substâncias - Pesquisa

- » Pesquisar por identificador de substância (substance identifier)

**SUBSTANCES: SUBSTANCE IDENTIFIER ?**

58-08-2  
capsaicin  
dichlorodiphenyltrichloroethane

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

**Search**



# Explorar Substâncias - Resultados

Substance Identifier "58-08-2; capsaicin; dichlorodi..." > substances (3)

**SUBSTANCES** ?

Get References Get Reactions Get Commercial Sources Tools

Analyze Refine

Analyze by: Substance Role

Analytical Study 3

Biological Study 3

Formation, Nonpreparative 3

Miscellaneous 3

Occurrence 3

Preparation 3

Process 3

Properties 3

Prophetic in Patents 3

Reactant or Reagent 3

Show More

Sort by: CAS Registry Number

1. 404-8

2. **58-08-2**

~8071

~20

Classificar os resultados por :

- CAS RN
- Núm. de referências
- Peso Molecular
- Fórmula molecular

Clique para ver detalhes da substância

Opções de Menu

CAS Registry Number: 58-08-2

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

Export as molfile

Send to SciPlanner

**C<sub>8</sub> H<sub>10</sub> N<sub>4</sub> O<sub>2</sub>**

1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-

Regulatory Information

Spectra

Experimental Properties

# Explorar Substâncias - Resultados

## » Ferramentas

- > Analisar
- > Refinar
- > Guardar respostas
- > Enviar ao SciPlanner
- > Obter Referências, Reações, Fornecedores, Informação regulamentaria



# Explorar Substâncias - Detalhes da substância

**SUBSTANCE DETAIL** ?

Return

**CAS Registry Number:** 58-08-2

C<sub>8</sub> H<sub>10</sub> N<sub>4</sub> O<sub>2</sub>

1H-Purine-2,6-dione, 3,7-dimethylxanthine; 3,7-Dihydro-1-methyl-2,6-dioxo-1,2,3,4-tetrahydropyrimidin-4-yl methylcarbamate; Caffeine (8CI); 1,3,7-Trimethylxanthine; 3,7-Dihydro-1-methyl-2,6-dioxo-1,2,3,4-tetrahydropyrimidin-4-yl methylcarbamate; Cafeina; Caffedrine; Caffeine; Durvitan; Guaranine; Koffein; Midron extra; Miudol; NSC 62700; Palergot-C; Phensal; Refregal; Synalgos; Thein; Theine; Theophylline

**Deleted CAS Registry Number:**

**Source of Registration:**

~31,615 References

~201 Commercial Sources

**Document Types:** Book, Journal Article, Review, etc.

**CAS Indexing:**

Analytical Study

Biological Study

Combustion Study

Formulation Nonpreparative

Miscellaneous

Occurrence

Preparation

Process

Properties

Get References

Get Reactions

Get Commercial Sources

Get Regulatory Information

**CAS Registry Number:** 58-08-2

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a Reactant

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Export as molfile

Send to SciPlanner

- Referências
- Fornecedores
- Tipos de documentos que mencionam a substância
- Propriedades experimentais e previstas
  - Biológicas
  - Químicas
  - Densidade
  - Lipinsky
  - Espectros
  - Relacionadas com a estrutura
  - Termais

Opções de Menu



# Explorar Reações- Editor de estruturas

» Igual ao de substâncias, com mais opções

Reaction Editor

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

Atom Short

-X =R

1-4 Cl

Definir o papel

Rastrear átomos

Formar ou quebrar ligações

Grupos funcionais

Drawing Editor:

☐ Structure

☒ Reaction

☐ Markush

Get reactions where the structure(s) are:

☐ Variable only at the specified positions

☒ Substructures of more complex structures

Acceptar

Cancelar

C H O S N P Cl Br F I Si

Scale 100

C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub> (reaction query) 194.19



# Explorar Reações - Página de resultados

The screenshot shows the 'REACTIONS' results page. On the left, the 'Analyze' tab is active, displaying a list of reagents with their counts: HCl (13), H2SO4 (11), KOH (11), H2O (8), HCO2H (7), HNO3 (7), NaH (6), AcOH (5), EtOH (5), and Fe (5). A 'Show More' button is at the bottom. The main area shows a reaction step with a chemical structure of a pyridine derivative. Annotations in pink and blue boxes highlight key features: 'Número de pasos' (Number of steps) points to the 'Single Step' label; 'Classificar os resultados por : Como foram indexados, Procedimento experimental, Número de pasos, % de produto, Ano de Publicação' (Classify results by: How they were indexed, Experimental procedure, Number of steps, % of product, Year of Publication) points to the 'Steps/Stages' section; 'Enviar ao SciPlanner' (Send to SciPlanner) points to the top right button; 'Etapas' (Steps) points to the 'Steps/Stages' section; and 'Link para a referência' (Link to the reference) points to the 'References' section.

**REACTIONS** ?

Analyze Refine

Analyze by: ?  
Reagent (New) ▼

HCl	13
H2SO4	11
KOH	11
H2O	8
HCO2H	7
HNO3	7
NaH	6
AcOH	5
EtOH	5
Fe	5

Show More

1. View in Detail [Link](#)

Single Step Hover over any structure for more info.

Me  
N  
C  
N  
Me  
~201

Overview

**Steps/Stages**

1.1 S:EtOH, 14 h,  
1.2 C:15244-77-6,

References

rhine-rhodium halide catalyst system for synthesis of acetic acid and acetic anhydride and its application

Quick View Full Text

By Lu, Yunjiang et al

From Faming Zhuanli Shenqing, 101143339, 19 Mar 2008

Send to SciPlanner

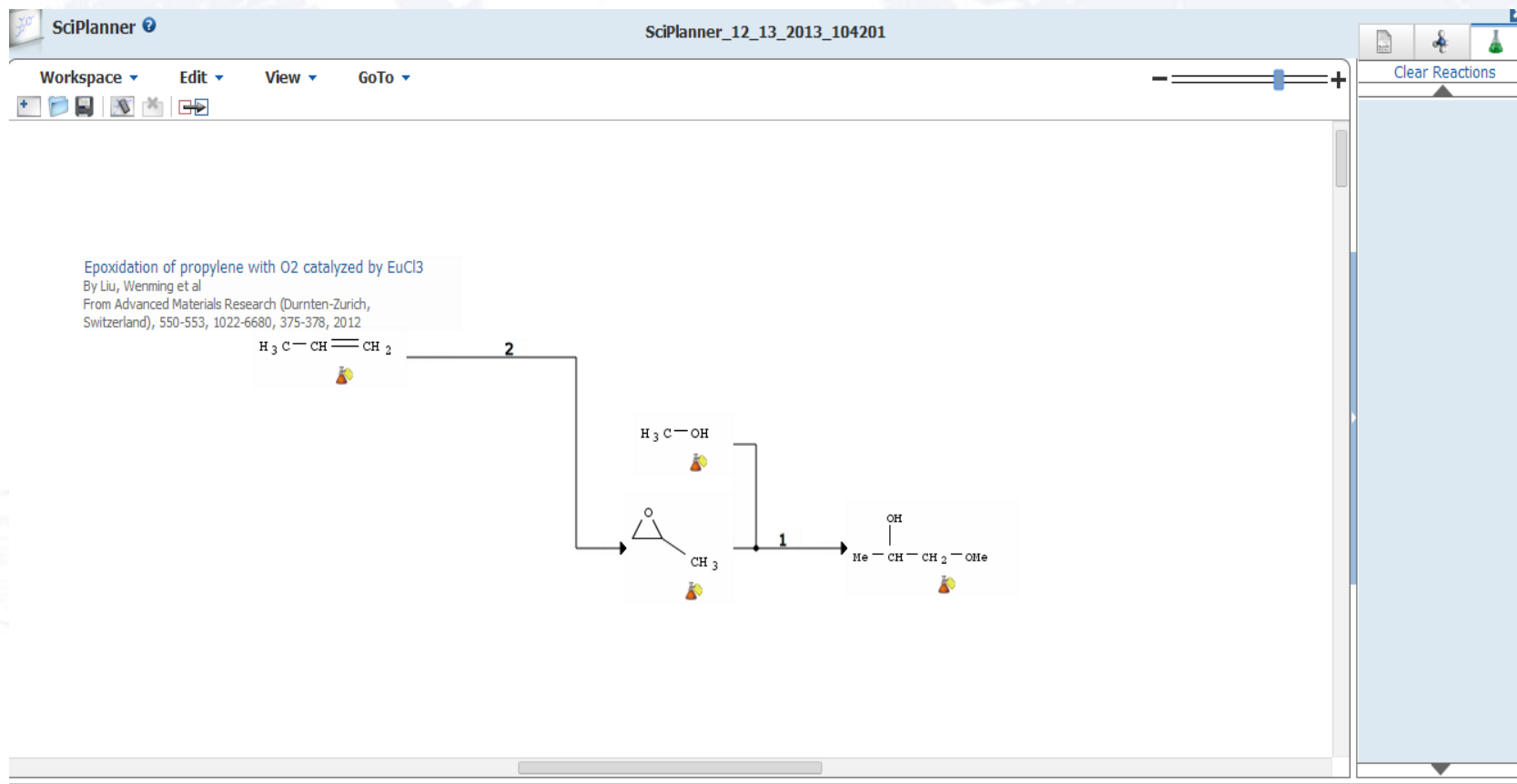
Page: 1 of 4

Etapas

Link para a referência

# Sci Planner

- » Tutorial: <http://www.cas.org/etrain/scifinder/sciplanner.html>
- » Mostra da área de trabalho :



# Contato

- » ITMS Group
- » (11) 5051-0975
- » [help@itmsgroup.net](mailto:help@itmsgroup.net)

