CAS

SciFinder Content, Features and Search

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CAS Representative
Today’s discussion

- Introduction of SciFinder

- Reference search
  - Research topics example
  - Author name example

- Substance search
  - Chemical name example
  - Exact structure and substructure example

- Reaction search
  - Drawing reaction tool
  - Reaction example
About CAS

- Chemical Abstracts Service (CAS), a division of the American Chemical Society

- Founded in 1907 to monitor, abstract, and index the world's chemistry-related literature and make it available to the scientific community

- Approximately 1,400 staff members – including CAS scientists, speaking 50 languages among them

- More than 10,000 major scientific journals and patents from 63 patent authorities are reviewed and indexed
CAS provides information to support scientists’ and patent searchers’ workflows

SciFinder provides an innovative interface that streamlines your research process
Rapid accelerated research drives data explosion

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CAS provides comprehensive coverage of science disclosed in a variety of scientific disciplines

- We cover content from >12K Journals, 63 Patent Offices worldwide, Conference proceedings, Dissertations etc.
- Our topics span 80 different sections from Pharmaceutical Science, Materials Science to Waste Water Treatment, Energy Technology and MORE!
How do I use SciFinder?

- Log in with Username and Password

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SciFinder® 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.
How do I use SciFinder?

- Search for References, Substances and Reactions
How do I use SciFinder?

- Innovative interface that allows you to analyze and refine answer sets; save and export results; navigate from reference to substance to reaction search seamlessly.
- Quickly find and analyze information (research topic, structure, reaction).
- Stay current in your field and keep track of competition.
- Share ideas with colleagues and collaborators.
PatentPak™ (optional)

- Instant access to searchable full-text patents from major patent offices around the world
- Patent family coverage in multiple languages
Let’s start the search in SciFinder
Research topics search:

- Enter your topics interest, with 2-3 keywords
- Include prepositions (of, for, etc…) to connect the concepts
- Those synonyms, alternative spellings, plural/singular will be added automatically
- Example: Novel therapy against Malaria (YouYou Tu, The Nobel Prize Winner of Medicine at 2015)
Select candidate references of interest

- As entered: The same as your entry
- Closely associated: Keywords appear on the same unit (like title, abstract or indexing) at the record
- Anywhere in the reference: Keywords appears at the record
Analyze…Refine…Categorize

- **Analyze**: Give your more ideas about the answer set and help to narrow down the answer.

- **Refine**: Narrow down your answer directly by adding more search criteria.

- **Categorize**: Check for the category of index term and narrow down the answer.
Author name search

- Enter as much of the name as you know. The last name is a must.

- Select Look for alternative spellings of the last name to account for name variations and typographical differences.

- YouYou Tu, The Nobel Prize Winner of Medicine at 2015
Check out the possible author names

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Get References
Malaria, caused by Plasmodium falciparum, has been a life-threatening disease for thousands of years. After the failure of international attempts to eradicate malaria in the 1950s, the disease rebounded, largely due to the emergence of parasites resistant to the existing antimalarial drugs of the time, such as chloroquine. This created an urgent need for new antimalarial medicines. In 1997, a national project against malaria was set up in China under the leadership of the Project 523 office. My institute quickly became involved in the project and appointed me to be the head of a malaria research group comprising both phytochemists and pharmacological researchers. Our group of young investigators started working on the isolation, and isolation of compounds with possible antimalarial activities from Chinese herbal materials. During the first stage of our work, we investigated more than 2,000 Chinese herb profiles and identified 846 hits that had possible antimalarial activities. More than 300 hits obtained from ~200 Chinese herbs were evaluated against a mouse model of malaria. However, progress was not smooth, and no significant results emerged easily. The turning point came when an Artemisia annua L. extract showed a promising degree of inhibition against parasite growth. However, this observation was not reproducible in subsequent experiments and appeared to be contradictory to what was recorded in the literature. Seeking an explanation, we carried out an intensive review of the literature. The only reference relevant to use of qinghao (the Chinese name of Artemisia annua L.) for alleviating malaria symptoms appeared in Ge Hong’s A Handbook of Prescriptions for Emergencies: “A handful of qinghao immersed in 2 L of water, wring out the juice and drink it all” (Fig. 1). This sentence gave me the idea that the heating involved in the conventional extraction step used might have destroyed the active components, and that an extract, at a lower temp, might be necessary to preserve antimalarial activity. Indeed, we obtained much better activity after switching to a lower-temp, procedure. Subsequently salvaged the extract into its acidic and neutral portions and, at long last, on 4 Oct. 1971, we obtained a nonionic, neutral ext. that was 100% effective against parasitemia in mice infected with Plasmodium berghei and in monkeys infected with Plasmodium cynomolgi. This finding represented the breakthrough in the discovery of artemisinin.
Substance search- Chemical name

- Enter the substance name, trade name, generic name or the CAS registry number in the **Substance Identifier**

- Get the substance record and find out the below information
  - Experimental and predicted property, Spectra information
  - Related references for the substance
  - Chemical supplier information
  - Related reaction
  - Regulatory information

- Example: Tamiflu
SciFinder Drawing editors

Different structure drawing tools

Commonly used element, bond and ring system
Variable attachment tool

Repeating group tool

Lock rings tool

Lock atoms tool
Chemical structure search

- **Exact structure search**
  - Retrieves substances that contain the exact structure query

- **Substructure search**
  - Retrieves substances that contain the substructure query embedded within their chemical structure.

- **Similarity search**
  - Retrieves substances that are structurally similar to the query.

- **Markush search**
  - Retrieves patent references that contain generic structures that match the Markush structure query.
Exact structure search (4-chlorobenzoic acid)
Analyze/Refine the structure result
Substructure search- add the variable group for the structure

R1: Me, Et
X: any halogen
Reaction drawing editor
Reaction drawing tool

- Reaction arrow tool
- Reaction role tool
- Atom mapping tool
- Reaction site marking tool
- Functional group tool
Reaction Search

- Draw the reactant and product, search from one or both sides of reaction
- Reaction arrow tool to direct the reaction
Check for the reaction and view the experimental procedures

Single Step Hover over any structure for more options.

\[
\text{HO-CH}_2\text{OH} + \text{NH}_2\text{C}_6\text{H}_4 \rightarrow \text{HO-C}_6\text{H}_4\text{N}_2\text{H} \quad 36\%
\]

Overview

Steps/Stages

1.1 CdAl₂O₃, CeCu, CeSiO₂, 240°C

Notes

gas phase, thermal, green chemistry-renewable feedstock, optimized on catalyst; catalyst prepared and used, flow system used, optimization study, fixed bed reactor used. Reactants: 2, Catalysts: 3, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Vapor-phase synthesis of 3-methylindole from glycerol and aniline: the effect of Al₂O₃ promoter and the preparation method on the performance of the Cu-Al₂O₃/SiO₂ catalyst

Q Quick View 0 Other Sources

By Sun, Liding et al.
From Reaction Kinetics, Mechanisms and Catalysts, 109(2), 447-468; 2013

Experimental Procedure

Catalytic activity testing. The catalytic reaction was carried out in a fixed bed continuous flow glass reactor with an inside diameter of 12 mm under atmospheric pressure. The solution of reactants (molar ratio of glycerol/aniline = 1:3) was pumped by flowing H₂ (10 mL/min), steam (12 mL/min) and N₂ (58 mL/min). The reaction was carried out at 240°C. The product obtained from the reaction was analyzed on a SP-6890A gas chromatograph equipped with a SE-54 capillary column. 1-Hexyl alcohol was used as an internal standard. 3-Methylindole. Yield: 36%, Selectivity: 55 (%), Al₂O₃ content: 1.1 (mmol/g). Catalyst: Cu-Al₂O₃/SiO₂, SV = 1700 h⁻¹, LHSV = 0.4 h⁻¹, Glycerol conversion: 66 (%).
Check for the similar reaction
Group the reaction transformation

Reaction Structure structure variable only at spec...  > reactions (25)

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<th>Analyze</th>
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Group by: Transformation

Sort by: Frequency

0 of 25 Reactions Selected

1. Reduction of Alcohols / Dehydroxylation
   19 Reactions
   \[ R-OH \rightarrow R-H \]

2. Deoxygenation of Vicinal Diols
   11 Reactions
   \[
   R^1 R^3 \quad R^1 R^3 \\
   \text{HO} \quad \text{OH} \quad \rightarrow \\
   R^2 R^4 \quad R^2 R^4
   \]

3. Replacement of a Hydroxy/ Alkoxy/ Acyloxy by Nitrogen Nucleophiles
   11 Reactions
   \[
   R^O R^1 + \quad R^2 \quad \rightarrow \\
   R^2 N R^2
   \]

4. Formation of C=C from Alcohols via Dehydration
   8 Reactions
   \[
   R^1 R^3 \quad R^3 R^1 \\
   H \quad \text{OH} \quad \rightarrow \\
   R^2 R^4 \quad R^2 R^4
   \]
SciFinder provides you....

- The most authoritative and comprehensive source for chemical and scientific information
- Intellectually analyzed and value added content by CAS scientists
- Links from references to journal and patent (PatenPak feature option).
  - Enhanced content for properties, spectra, registration, reaction information and etc
  - Personalization features (keep me posted and save as)
Thank You!

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