

CAS SciFinder Discovery Platform™

# BETWEEN IDEAS AND ANSWERS ARE CONNECTIONS THAT MATTER

For Academics

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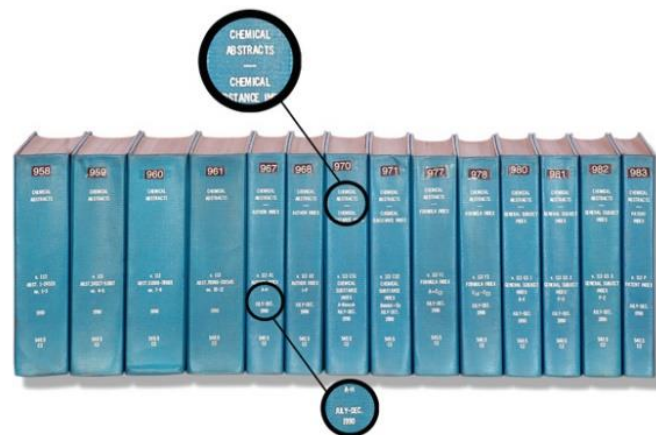
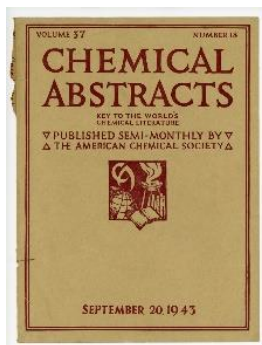
# CAS accelerates breakthroughs

At CAS, our passion is advancing scientific progress. As a leader in scientific information solutions, we curate, connect, and analyze the world's published science to accelerate discovery.

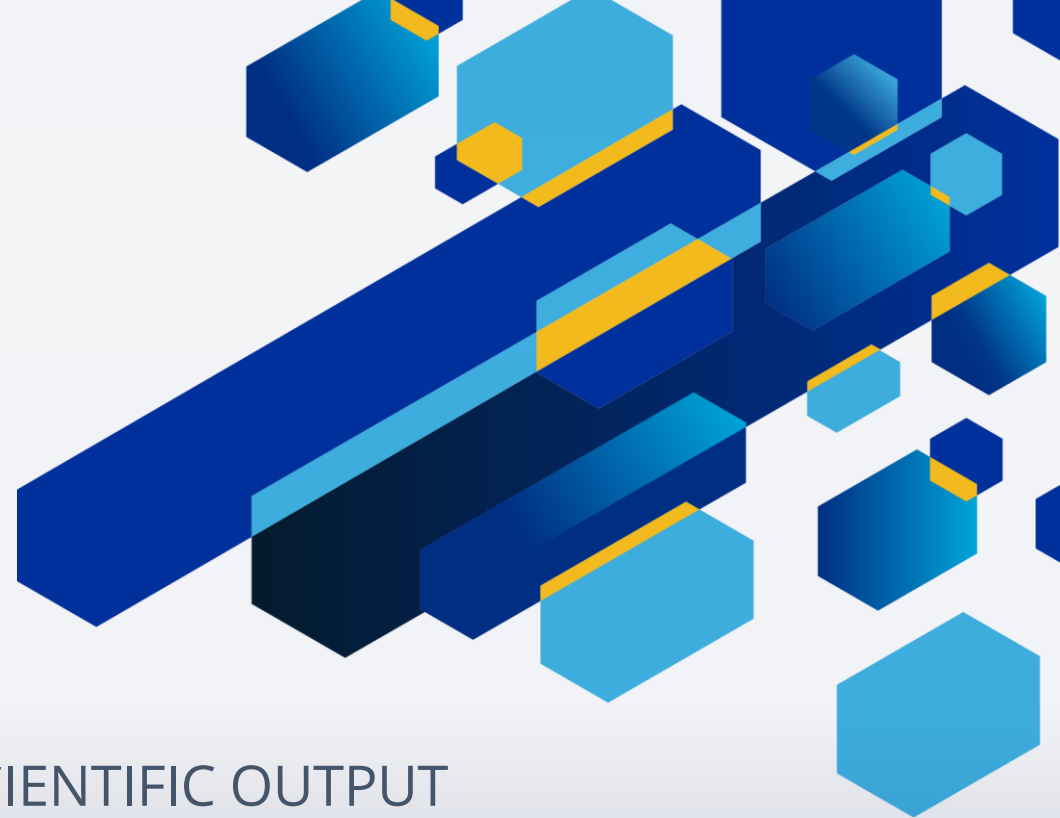
We are proud to partner with innovators and educators across academia, providing the hindsight, insight, and foresight they need to build upon the past and discover a better future.

**BETWEEN IDEAS AND ANSWERS  
ARE CONNECTIONS THAT MATTER**

# CAS is the Authority for Chemistry



Authoritative source for  
chemical names, structures and  
CAS Registry Numbers<sup>®</sup>

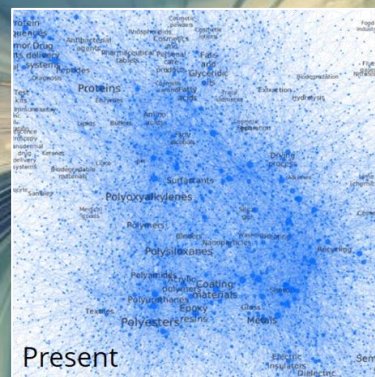
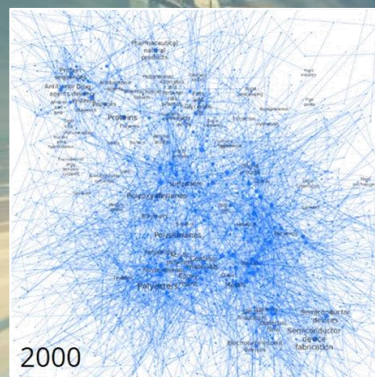
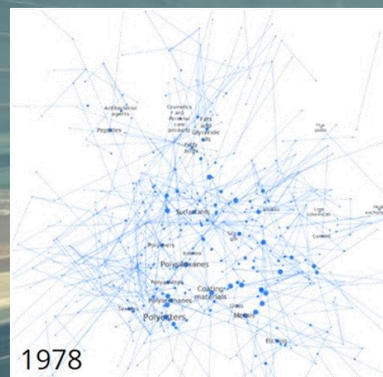


GLOBAL SCIENTIFIC OUTPUT  
**DOUBLES EVERY  
9 YEARS**

# IMPORTANCE OF MANAGING SCIENTIFIC INFORMATION CONTINUES TO ESCALATE



## Scientific Information Trends

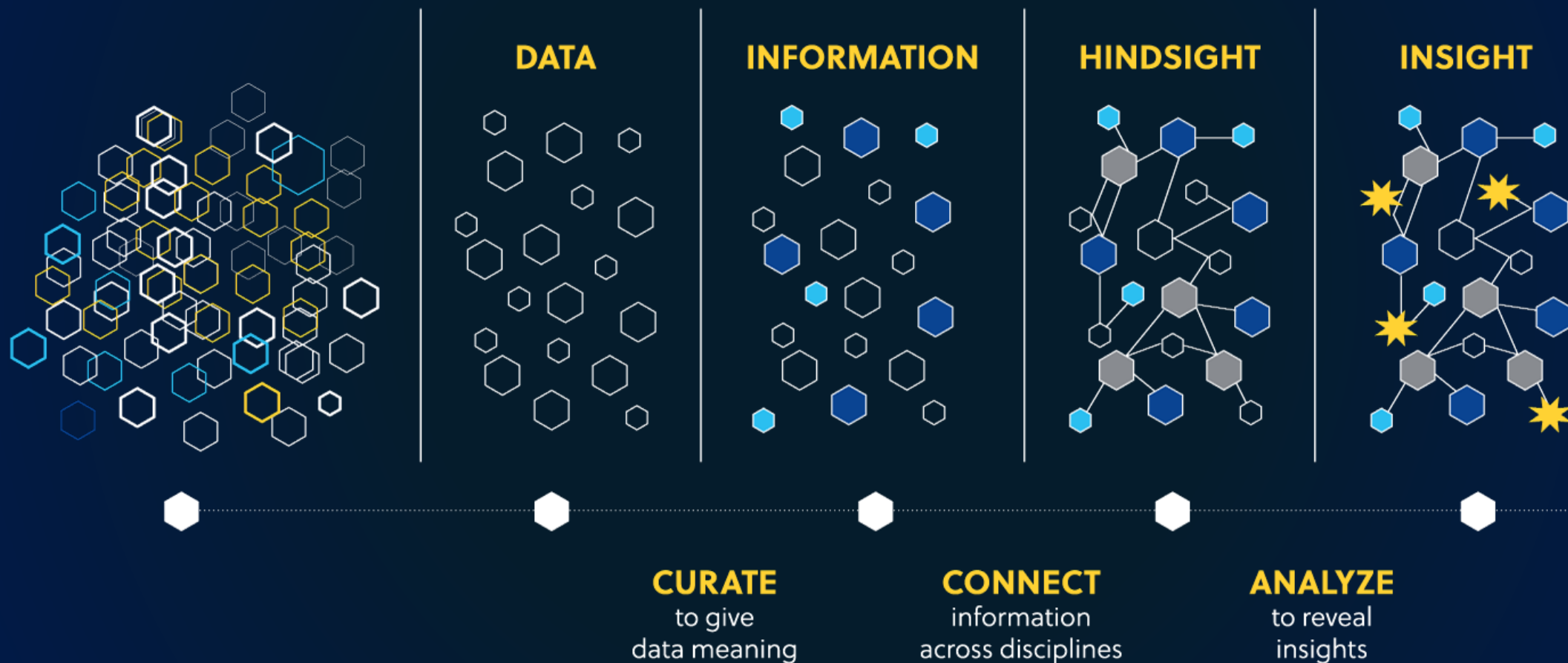


- Volume
- Complexity
- Interconnectedness

1. CAS Proprietary data, CAS Analytics & Insights

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# CAS scientists curate, connect, and analyze scientific knowledge

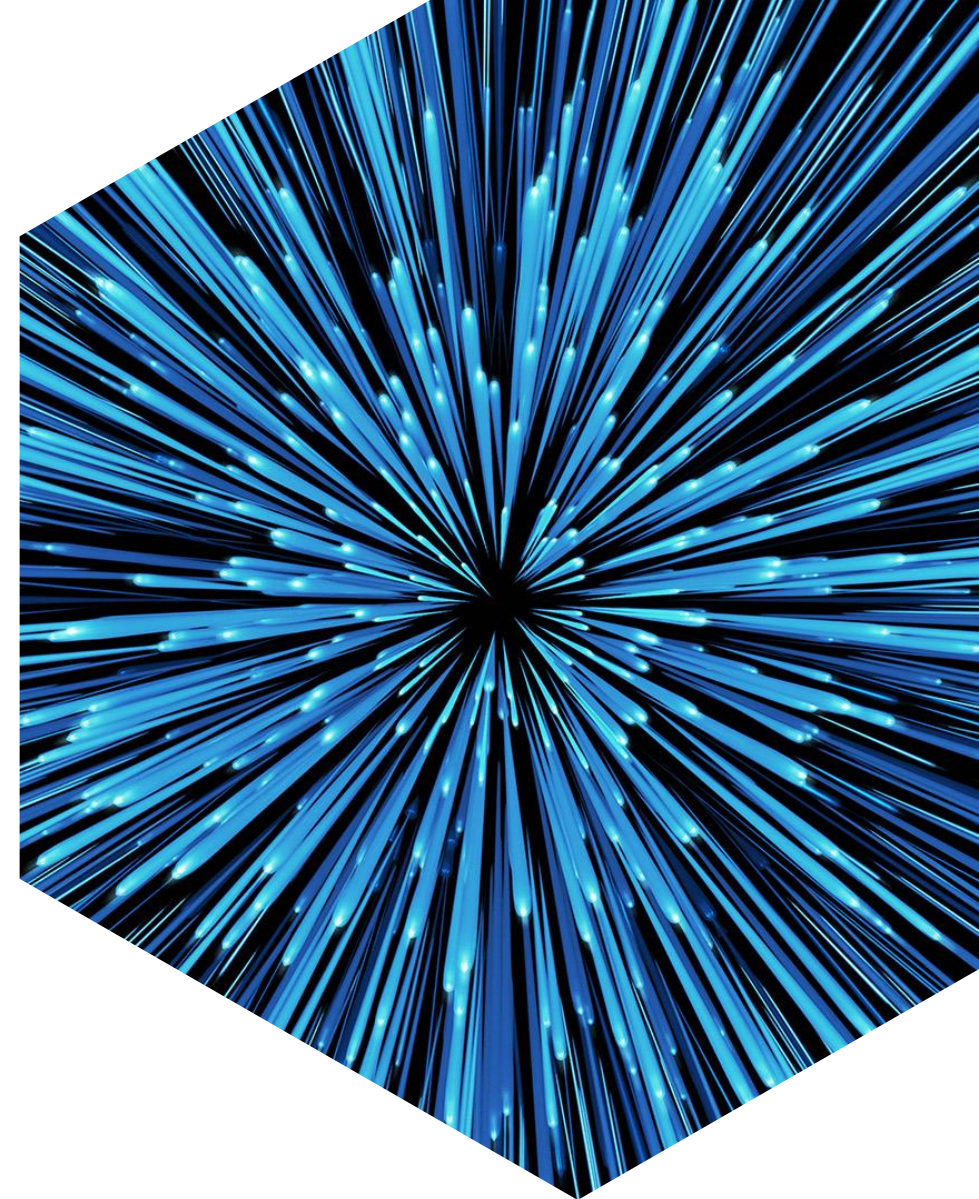


# CAS SciFinder Discovery Platform

As the volume of scientific information continues to grow, finding exactly what you need – the connections amid the chaos – can be challenging.

Researchers need best-in-class scientific information solutions to help them bring new ideas to life faster.

Whether you're reviewing the literature for funding applications and manuscripts, developing experimental plans for new projects, or searching for collaborators to help you advance the research in your field, CAS SciFinder Discovery Platform speeds your connection to relevant insights.





## Navigation Tool for Scientists

# CAS SciFinder Discovery Platform



# CAS is a trusted partner

to innovation leaders across industries

**PHARMA**  
 **49** of the  
**TOP 50**  
pharma companies<sup>1</sup>

**ACADEMIC**  
 **100** of the  
**TOP 100**  
universities<sup>2</sup>

**GOVERNMENT**  
 **10** of the  
**TOP 10**  
global patent offices<sup>3</sup>

**BIOTECH**  
 **10** of the  
**TOP 10**  
biotech companies<sup>4</sup>

**CHEMICAL**  
 **46** of the  
**TOP 50**  
chemical companies<sup>5</sup>

1. <https://www.pharmexec.com/view/2021-pharma-50>.

2. <https://www.shanghairanking.com/rankings/gras/2021/RS0103>

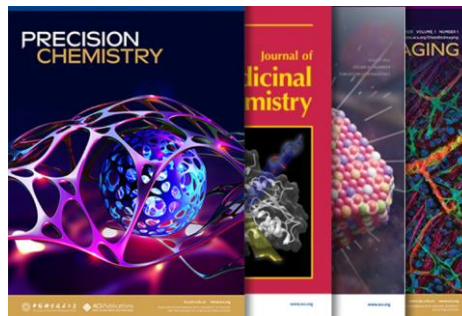
3. [https://www.wipo.int/edocs/pubdocs/en/wipo\\_pub\\_943\\_2020.pdf](https://www.wipo.int/edocs/pubdocs/en/wipo_pub_943_2020.pdf)

4. <https://www.investopedia.com/articles/markets/122215/worlds-top-10-biotechnology-companies-jnj-rogvx.asp>

5. <https://cen.acs.org/business/finance/CENs-Global-Top-50-2021/99/i27>

# CAS SciFinder Discovery Platform for Academics

Informing and enhancing the foundational scientific pursuits in Academia



**CAS SciFinder Discovery Platform** is designed to support multiple stages and types of scientific research and combines task-specific information solutions, including **CAS SciFinder<sup>n</sup>**, **CAS Formulus<sup>®</sup>**, and **CAS Analytical Methods<sup>™</sup>** with **ChemZent<sup>®</sup>** and the **CAS Content Collection<sup>™</sup>**, the most complete source of scientific information in the world.

# CAS SciFinder Discovery Platform for Academics

Speed up your science and learning with the leader in scientific intelligence

## Unmatched content

Directly access to the most comprehensive collection of chemical reactions, substances, patents, and scientific literature.

## Specialized technology

Tap into the smartest, most powerful science-aware search engine.

## Human expertise

Our scientists work in tandem with technology to identify concepts and relationships beyond keywords.

The screenshot displays the CAS SciFinder web interface. At the top, the navigation bar includes the CAS SciFinder logo, a 'Saved and Alerts' notification bell, a 'History' clock icon, and an 'Account' user profile icon. Below the navigation bar is a light blue banner with a left-pointing arrow, a message: 'You can now use [BLAST search](#) to mine our newly enhanced collection of more than 500M proteins and nucleotides from 60+ patent authorities dating back to 1957. Plus [visually review sequence similarity and frequency](#) across your patent search results.', and a right-pointing arrow. The main content area is divided into two columns. The left column, titled 'Searching for...', contains a vertical list of search categories: 'All', 'Substances' (highlighted with a blue bar), 'Reactions', 'References', 'Suppliers', 'Biosequences', and 'Retrosynthesis'. The right column, titled 'Substances', features a search instruction: 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)'. Below this is a search input field with the placeholder text 'Enter a query...'. To the right of the input field are a 'Draw' icon and a search button. Below the input field is a dropdown menu currently set to 'Molecular Formula'. To the right of the dropdown is a close button (X). Below the dropdown is a '+ Add Advanced Search Field' button. At the bottom right of the search area, there are 'Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N' and a link: '[Learn more about SciFinder<sup>®</sup> Advanced Search.](#)'

# CAS SciFinder Discovery Platform for Academics

Anticipating your information needs to accelerate your research.

The screenshot displays the CAS SciFinder interface. At the top, the search bar contains the query "novel coronavirus nonpeptide inhibitors". Below the search bar, the results page shows 3,512 results. A specific result is highlighted: "Structure-Based Drug Design and Structural Biology Study of Novel Nonpeptide Inhibitors of Severe Acute Respiratory Syndrome". The authors listed are Lu, I-Lin; Mahindroo, Neeraj; Liang, Po-Hsiung; Wu, Su-Ying. The journal is "Journal of Medicinal Chemistry" (2006), 49(17). The abstract snippet reads: "The core structures of these two hits, defined by their ability to bind to the viral protein, were derived from these two hits exhibited IC<sub>50</sub> values of 0.1 and 0.2 μM, respectively." A "Full Text" button is visible below the abstract. A "Save Results and Create Alert" dialog box is overlaid on the page, allowing the user to save the search and create an alert. The dialog includes a "Name" field, "Save Options" (Query Only, Selected Answers, All Answers), "Alert Frequency" (No Alerts, As Available, Weekly, Monthly), and a "New Tag" field with a "Tag Color" dropdown (Dark Red).

## Search faster and smarter

Quickly retrieve relevant and timely information from the critical scientific literature.

## Stay connected

Easily set up alerts to stay abreast of the latest journal publications and patents in your field of research.

# CAS SciFinder Discovery Platform for Academics

Unlocking research productivity with the most advanced retrosynthetic planning solution

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Overview Steps Predicted Results ON View Excluded Options Save

Plan Information

Estimated Yield: 33%  
Overall Price: \$16.98  
(USD per 100 grams)

Commercially Available: A, B, D, E

Plan Options

Synthetic Depth: 3  
Predicted Rules: Common  
Break & Protect Bonds: No  
Starting Material Cost Limit: \$500.00/mol  
Edit Plan Options

Scoring Profiles

Complexity Reduction

Convergence

Evidence

Max Yield 97%

Avg. Yield 66%

Max Yield -

Retrosynthesis Step Key

Researchers can clearly understand the diversity of alternatives and evidence for the planned synthetic route

## Synthesize

Access target molecules through published and predicted transformations.

## Explore

Address synthetic challenges for known or novel compounds.

## Identify

Explore new breakthroughs in methods development.

# CAS SciFinder Discovery Platform for Academics

Comprehensive bioactivity data to study how molecules interact with biological systems



## Extensive collection

More than 45 million bioactivity measurements and 90,000 defined targets across more than 10 million unique substances relevant to Medicinal Chemists



## Critical information

The data required for running analyses of SAR, ADME, and toxicology to understand the effect of a molecule on a target



## Intuitive search

Extensive filtering options and a tabular display with overview of ligand structure, pharmacological parameters, and assay details

# CAS SciFinder Discovery Platform for Academics

Improved information to accelerate drug discovery research with CAS Scifinder<sup>n</sup>

The screenshot displays the CAS SciFinder Discovery Platform interface. At the top, there is a navigation bar with the CAS SciFinder logo, a 'Saved' button, a 'History' button, and an 'Account' button. Below this is a light blue banner with a left arrow, a paragraph of text about COVID-19 research, and a right arrow. The main content area is divided into two columns. The left column, titled 'Searching for...', contains a vertical list of search categories: 'All', 'Substances', 'Reactions', 'References' (which is highlighted in blue), 'Suppliers', 'Biosequences', and 'Retrosynthesis'. The right column, titled 'References', has a search bar with the placeholder text 'Enter a query...'. To the right of the search bar are 'Draw' and 'Search' icons. Below the search bar is a dropdown menu with the text 'Select an Option'. A red hand cursor is pointing to the 'Structure Activity Relationships' option in this dropdown. To the right of the dropdown menu is a 'Learn more about SciFinder<sup>n</sup> Advanced Search.' link. At the bottom left, there is a 'Recent Search History' section with a text input field containing 'January 26, 2020'.

## Searching for SAR Data

Content that specifically targets a ligand, target, and/or disease can be searched through advanced search.

Content answers can be highlighted in detail records.

# CAS SciFinder Discovery Platform for Academics

Enhancing biological research with new biosequence search in CAS SciFinder<sup>®</sup>

## Unmatched content

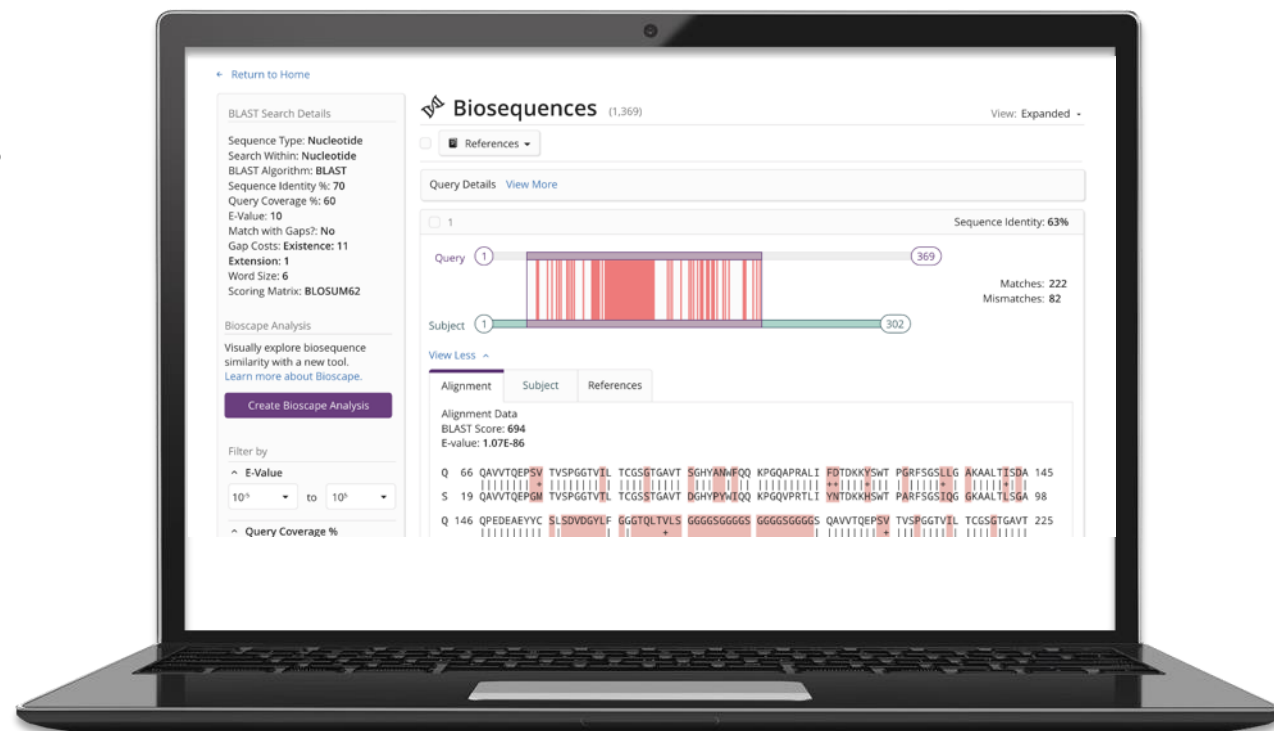
Newly enhanced collection of more than 500 million proteins and nucleotides from 60+ patent authorities dating back to 1957

## Specialized technology

Multiple search options to support your sequence search needs, including BLAST, CDR, and Motif search

## Human expertise

Both human and machine-curated biosequence collection including curated sequences not found in electronic sequence listing and other databases





# CAS SciFinder Discovery Platform for Academics

A single-source discovery platform for in-depth, multi-disciplinary scientific methods

The screenshot displays the CAS SciFinder interface. On the left is a navigation sidebar with sections for 'Analyte', 'Matrix', 'Method Category', 'Technique', and 'Year'. The main area is titled 'Results (11278)' and shows a search result for 'Analysis of Dehydroepiandrosterone in Blood plasma by Solid phase extraction' (CAS MN: 2-111-CAS-270275). The result details include:

- Analyte:** Estradiol; 7 $\alpha$ -Hydroxy-DHEA; Dehydroepiandrosterone; Dihydrotestosterone; Testosterone; Androstenediol; Estrone; Dehydroepiandrosterone sulfate; Androstenedione
- Matrix:** Blood plasma
- Other Materials:** Reagent: Dithioerythritol; Ethyl acetate; Ammonium iodide; Methanol; N-Methyl-N-(trimethylsilyl)trifluoroacetamide; Buffers  
Material: C18 sorbent: HP-ULTRA1 capillary column (17 m  $\times$  0.2 mm i.d., 0.11  $\mu$ m film  
[View All](#)
- Method Category:** [Biomarker](#) [Medicine Assay](#)
- Technique:** Electron ionization mass spectrometry; Quadrupole tandem mass spectrometry; Gas chromatography; Solid phase extraction
- Equipment Used:** Microwave oven; GC system; Triple quadrupole mass spectrometer
- Source:** Profiling of steroid metabolic pathways in human plasma by GC-MS/MS combined with microwave-assisted derivatization for diagnosis of gastric disorders  
Lee, Wonwoong; Lee, Hyunjung; Kim, You Lee; Lee, Yong Chan; Chung, Bong Chul; Hong, Jongki  
International Journal of Molecular Sciences (2021), 22 (4), -. MDPI AG  
[Full Text](#)

## Integrated

Seamlessly integrated into CAS SciFinder<sup>n</sup>

## Comprehensive

Hundreds of thousands of methods across multiple fields of study, including organic compound, bioassay, and water analysis

## Focused

Designed with analytical chemistry processes in mind as a single source for searching and comparing published scientific methods and techniques

# CAS SciFinder Discovery Platform for Academics

Learn how industry develops safe and effective products with the world's leading collection of formulations

**Pharmaceutical Solutions for Delivering Drug to Lung: Drug Delivery Systems or Respiratory System Agents, Etc.**

Location: Example 2, Table 2

Purpose: Antiasthmatics, Drug delivery systems, Respiratory system agents

Target: Asthma, Drugs, Homo sapiens, Respiratory system disease

Delivery Route: Inhalation drug delivery systems

Physical Form: Solutions

[Add to Compare](#)

Component	Function	Amount Reported
Salbutamol	hygroscopic agents	0.1 %
Sodium chloride	pharmaceutical excipients	0.1 %
Group: ethanol/water		
Ethanol	cosolvents	50 % v/v
Water	-	50 % v/v


**PATENT**

Delivery of submicrometer and nanometer aerosols to the lungs using hygroscopic excipients or dual stream nasal delivery

Assignee : Virginia Commonwealth University  
US20120251594  
Language: English

[Patent PDF](#) [View in CAS SciFinder®](#)

[View Formulation Detail](#)

[8 Similar Formulations - View All](#) (opens in a new window) 

## Chemistry beyond synthesis

Understand a formulation's origin and effectiveness with access to the best information for active ingredients and excipients.

## Discover industry insights

Get insights beyond literature and interact with formulations data curated from patents, journals, and product inserts.

## Comprehensive information

Evaluate ingredients and manufacturing processes while exploring regulatory requirements in one easy interface.

# CAS SciFinder Discovery Platform for Academics

Access essential historical chemistry insights with ChemZent®

References search for "Pasteur, L." Author Name

Substances Reactions Citing Save and Alert

Filter Behavior: Filter by Exclude

Document Type: Journal (38), Patent (5), Review (1), Biography (3), Book (2), View All

Language: Undetermined (21), German (17), English (5), French (3)

46 Results | Sort: Publication Date: Oldest | View: Partial Abstract

1

**On grape acid**  
By: PASTEUR, L.  
Chemisches Zentralblatt (1849), 20(46), 731-732 | Language: German, Database: CHEMZENT

Machine Translated: The harvested grapes acid has been of KESTNEK detected after the discovery but never again. The process has in one quantity of this acid, received from the detector itself bekam with envelope of polarization appa Rates proved, that it consists of two different acid ", of which one to the right, the other to the left deflects. This capacity corresponding to designates the same said first Dextroracemsaure, the second Laevoracemsaure (Acide dextrora-cemique et Uvoracemique). The right ahlenkende acid liess is in no property of the wine acid different. The Laevoracemsaure and their salts have now ...

View More

ChemZent Full Text

Substances (2) Reactions (0) Citing (0) Citation Map

2

**On the aspartic acid and malic acid**  
By: PASTEUR, L.  
Chemisches Zentralblatt (1851), 22(49), 769-772 | Language: German, Database: CHEMZENT

Machine Translated: In its final form of embodiment of malic acid and asparagine acid has Pasteur already indicated, that both the capacity have Delbricalionschene deflecting and that this property by all compounds of these acids through fortallanz. At the same

## Comprehensive foundational chemistry

English language translations of German abstracted publications from 1830-1969 with >800K documents and 3+ million abstracts

## Exclusive online access

Only online source of Chemisches Zentralblatt with machine translated English abstracts and access to original German versions.

## Completely Integrated

Indexed to fit seamlessly into CAS SciFinder<sup>®</sup> workflows with CAS-controlled vocabulary

# BETWEEN IDEAS AND ANSWERS ARE CONNECTIONS THAT MATTER



**Görkem Mergen, PhD**  
CSM & BD Specialist  
[gmergen@acs-i.org](mailto:gmergen@acs-i.org)