

CAS SCIFINDER DISCOVERY PLATFORM™

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

Bring your research ideas to life faster
with the CAS SciFinder Discovery Platform.

CAS

A division of the
American Chemical Society



Experience everything the CAS SciFinder Discovery Platform has to offer

As the volume of scientific information continues to grow, finding exactly what you need—the connections amid the chaos—can be challenging. Whether you are 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, the CAS SciFinder Discovery Platform speeds your connection to relevant insights.

"CAS SciFinder" makes the whole process of research and writing more efficient. To do great, you need to be up-to-date!"

Ibrahim Alfurayj
Graduate Student / Post Doc,
Case Western Reserve
TechValidate, TVID: A89-6FB-4ED

"I wouldn't be able to do my job without it."

Chip Nataro
Faculty, Lafayette College
TechValidate, TVID: 5A5-CE3-9C7

"CAS SciFinder" is like air for my research... you don't know how good it is until you don't have it."

Marcelo D Preite
Faculty, uc.cl
TechValidate, TVID: 910-7F8-D86

"CAS SciFinder" helps me design my synthetic plans and keep up-to-date on my research field. I haven't found any other product able to do this."

Laura Morelli
Scientist, University of Milan
TechValidate, TVID: FA9-363-5C8

The CAS SciFinder Discovery Platform is designed to support multiple stages and types of scientific research. It combines task-specific information solutions and tools, including CAS SciFinderⁿ, retrosynthetic planning, sequences, bioactivity, visualizations, CAS Formulus[®], CAS Analytical MethodsTM, and ChemZent[®], making it the most complete source of scientific information in the world.

The CAS SciFinder Discovery Platform supports the foundational scientific needs of your research community.

- Leverage the most advanced relevance engine in the industry and discover more relevant and timely information faster.
- Access one source for all substance-related information and plan experiments with confidence.
- Identify and optimize synthetic routes through a full retrosynthetic analysis of known and undisclosed substances.
- Find the best research protocols by searching and comparing hundreds of thousands of published scientific methods.
- Uncover information about active ingredients and excipients that guide the design of new formulations.
- Explore the pharmacology of drug-target-toxicity interactions with SAR and ADMET analysis.
- Search and analyze protein and nucleic acid sequences and related references that assist in life science research.
- Review historical insights from Chemisches Zentralblatt for comprehensiveness in chemistry literature reviews.

Connect to relevant and timely information

The challenge to retrieve relevant and timely information from an ever-increasing, vast collection of complex scientific literature can seem insurmountable. With the most advanced relevance engine in the industry, CAS SciFinder[®] helps you search faster and smarter, anticipating your information needs to accelerate your research.

Our global network of scientists extracts key information from the world's published scientific literature daily, making connections only possible with the combined power of expert human analysis and advanced data technology. Worried about missing the latest journal publications or patents in your field of research? With CAS SciFinder[®], you won't miss a thing.

"CAS SciFinder[®] makes finding relevant publications much faster, giving more time for in-lab experimentation."

Graduate Student / Post Doc, Educational Institution
TechValidate, TVID: F88-FA8-815

"The Alerts that I have set up to keep me up-to-date with the publications in my field is one of CAS SciFinder[®]'s greatest tools."

Graduate Student / Post Doc,
Educational Institution
TechValidate, TVID: C12-8A1-8B8

The screenshot shows the CAS SciFinder interface with a search for "novel coronavirus peptide". The search results page includes a "References search for 'novel coronavirus peptide'" section with filters for Substances, Reactions, Citing, and Knowledge Graph. A "Publication Year" bar chart is visible on the left, showing a significant increase in publications starting around 2018. A "Save Results and Create Alert" dialog box is open in the top right, allowing users to save their search and set up alerts. The dialog includes options for "Save Options" (Query Only, Selected Answers, All Answers) and "Alert Frequency" (No Alerts, As Available, Weekly, Monthly). It also allows for adding existing tags (e.g., "Coronavirus") and creating new tags.

Use advanced filters to narrow your results by document type, author, organization, publication year, and more. Set up Alerts to be notified when new research is published in your field.

The screenshot displays the "Citation Map" for the article "Structure-Based Drug Design and Structural Biology Study of Novel Nonpeptide Inhibitors of Severe Acute Respiratory Syndrome Coronavirus Main Protease". The map shows a central node with lines radiating outwards to other nodes, representing citations and citing works. A tooltip is visible over one of the nodes, providing details about the cited work: "A novel coronavirus associated with severe acute respiratory syndrome" by Ksiazek, Thomas G.; Erdman, Dean; Goldsmith, Cynthia S.; Zaki, Sherif R.; Peret, Teresa; Emery, Shannon; Tong, Suxiang; Urbani, Carlo; Comer, James A.; Lim, Wilina; et al. (2003), New England Journal of Medicine. The tooltip also includes buttons for "Expand Citations" and "Create Map".

Extend your exploration of relevant scientific literature with a Citation Map of research cited by (backward) and citing (forward) a publication of interest.

Plan your experiments with confidence

Your cutting-edge research requires authoritative, high-quality information on substances and chemical reactions. With data on more than 250 million organic and inorganic substances and 130 million single and multi-step reactions, CAS SciFinder[®] is your one true source to identify a substance and its related chemical structure, names, regulatory information, and properties, as well as reaction schemes, step-by-step experimental procedures, detailed reaction conditions, and yields.

Your successful chemical synthesis starts with a detailed synthetic plan, but uncovering, comparing, and piecing together reaction pathways can be challenging. For known substances and those not previously reported in the literature, CAS SciFinder[®] will perform a full retrosynthetic analysis to help you identify synthetic routes to fit your needs. Determine price, chemical suppliers, step-by-step methods, product yields, and more— all before you head to the lab.

"I find the retrosynthesis capability of CAS SciFinder[®] really unique and extremely helpful to design my synthesis routes."

Graduate Student / Post Doc, Educational Institution
TechValidate, TVID: 7AA-C7C-71D



"Being able to search for journal articles, reactions, and substances all on one platform is very useful. I also like being able to search using a chemical structure, which isn't something you can do with just Google."

Graduate Student / Post Doc, Educational Institution
TechValidate, TVID: 790-B0F-A51

The image shows two overlapping windows from the CAS SciFinder interface. The background window is titled "Substances search for drawn structure" and displays a grid of search results. Each result includes a chemical structure, a CAS Registry Number (e.g., 1234638-45-9), and a molecular formula (e.g., C₁₄H₇Cl₂F₃N₂O₄). The results are filtered by similarity (3 Selected) and number of components (1). The foreground window is titled "CAS Draw" and shows a chemical structure editor with a toolbar and a canvas containing a complex organic molecule. The molecular formula for the drawn structure is C₁₄H₇Cl₂F₃N₂O₄ (441.13).

Find detailed substance information by searching with a chemical name, CAS Registry Number®, or draw exactly the structure you want to find with built-in, easy-to-use structure editors.

The image shows the "Retrosynthesis Plan for drawn structure" interface in CAS SciFinder. The plan is powered by ChemPlanner and displays a multi-step synthesis route starting from a target molecule (A) and breaking it down into precursors (B, C, D, E, F, G, H). Each step is represented by a chemical structure and a yield percentage. For example, step A to B has a Max Yield of 96%, and step E to F has a Max Yield of 85%. The interface includes a sidebar with various filters and options, such as "Predicted Results" (ON), "View Excluded Options", and "Save". The bottom of the screen displays copyright information: "Copyright © 2022 American Chemical Society. All Rights Reserved. | 京ICP备13047075号-3" and links for "Help", "Contact Us", and "Legal".

Plan your synthesis of a novel or known substance with a retrosynthetic analysis powered by computer-aided synthesis design.

Seamlessly investigate sequences and bioactivity data

Integrated with the world's most comprehensive collection of chemical reactions, substances, and indexed scientific literature, you'll find one of the largest, most comprehensive sources of sequence and bioactivity data. This information helps ensure you're aware of the most recent research to inspire new ideas.

The extensive collection of bioactivity data consists of more than 10 million truly unique substances with more than 45 million bioactivity measurements and 90,000 defined targets, including all human targets. Explore the pharmacology of drug-target-toxicity interactions with SAR and ADMET analysis to uncover novel targets for therapeutic intervention and gauge the safety of unique compounds. The sequence functionality within CAS SciFinder[®] enables a simultaneous query of journals, public databases, patents, and more, saving time and ensuring thoroughness in your literature searches. Perform BLAST, CDR, and Motif searches across more than 700 million protein and nucleic acid sequences in the database, helping you identify the most critical information for your research.



Structure Activity Relationships CAS LIFE SCIENCES

Absorption, Distribution, Metabolism, and Excretion Data CAS LIFE SCIENCES

Toxicity CAS LIFE SCIENCES

Ligand Target Function Parameter Value Disease Organism Clear All Filters

Ligand	Target	Function	Parameter	Value	Disease	Organism	Assay Information
2460476-35-9	GLP-1R	Inhibition	IC50	0.54 nM	Malaria	-	View Detail
2460476-35-9	GLP-1R	Inhibition	IC50	0.75 nM	Malaria	-	View Detail
2460476-35-9	GLP-1R	Inhibition	IC50	21 nM	Malaria	-	View Detail
2460476-35-9	GLP-1R	Inhibition	IC50	>25,556 nM	Malaria	-	View Detail
2460476-35-9	GLP-1R	Inhibition	Selectivity	>47,326	Malaria	-	View Detail
2460476-35-9	GLP-1R	Inhibition	ED50	10 mg/kg	Malaria	Mouse	View Detail
2460476-35-9	GLP-1R	Inhibition	ED90	30 mg/kg	Malaria	Mouse	View Detail
2460476-35-9	GLP-1R	Inhibition	IC50	84 nM	Malaria	Human	View Detail

Prev 1 2 3 4 5 ... 325288 Next Go to Page: ###

Review structure-activity relationship data to identify content and access details specific to a ligand, target, or disease.

CAS SciFinder[®] Substances Enter a query... Draw

Sequences search for your query

References

BLAST Search Details

Sequence Type: **Protein**
 Search Within: **Proteins**
 BLAST Algorithm: **BLASTp**
 NCBI Included: **No**
 Alignment Identity: -
 Query Coverage: **90%**
 E-Value: **10**
 Match with Gaps?: **No**
 Gap Costs: **Existence 11**
 Extension **1**
 Word Size: **3**

Bioscape Analysis

Visually explore sequence similarity with a new tool. [Learn more about Bioscape.](#)

[Create Bioscape Analysis](#)

Query Details GGTYSCHFGLTWCKPQGG [View More](#)

1,196 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 100%

Matches: 20
Mismatches: 0

[View Less](#)

Alignment Subject References

Alignment Data
 BLAST Score: 126
 E-Value: 2.46639e-9

Q 1 GGTYSCHFGLTWCKPQGG 20

Easily find regions of local similarity between protein and nucleotide sequences using the BLAST search capability within CAS SciFinder[®].

Learn from the experience of other scientists

Whether you are researching an established process to follow, seeking to understand how to produce safe and effective products, or searching for historical chemistry insights, the CAS SciFinder Discovery Platform provides the integrated solutions you need.

The screenshot displays the CAS Analytical Methods web interface. At the top, the search bar contains 'Browse: Biomarker Medicine Assay'. The left sidebar features a navigation menu with categories: Analyte (680), Matrix (4488), Method Category, Technique, and Year. The main content area shows search results for 'Biomarker Medicine Assay' (11278 results). The top result is 'Analysis of Dehydroepiandrosterone in Blood plasma by Solid phase extraction' (CAS MN: 2-111-CAS-270275). The details for this method include: Analyte (Testosterone, Dehydroepiandrosterone sulfate, etc.), Matrix (Blood plasma), Other Materials (Reagent: Methanol; Ethyl acetate; N-Methyl-N-(trimethylsilyl)trifluoroacetamide; Dithioerythritol; Ammonium iodide; Buffers), 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), and 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).

A single-source discovery platform for in-depth scientific methods, CAS Analytical Methods™ will help you discover the best scientific process to follow. Search hundreds of thousands of methods across multiple fields of study, giving you a comprehensive tool for comparing published scientific methods and techniques.

"The first thing I do when researching synthetic routes is to check existing ones on CAS Analytical Methods."

Undergrad Student, Educational Institution
TechValidate. TVID: 7FB-98D-CC7

The screenshot displays the CAS Formulus interface. On the left, there is a filter sidebar with categories like Industry, Purpose, Information Included, Document Type, Organization, and Publication Year. The main content area shows a search result for 'Laundry Detergent Composition' with a table of components and their functions.

Component	Function	Amount Reported
Group: Laundry detergents	laundry detergent	1.5 g/L
Water vapor	-	-
Sodium silicate	filler, coating agent	6.0 wt %
Cosmetic fragrance products	perfume	0.3 wt %
Zeolites, synthetic	-	2.5 wt %
Additional group components reported		
Water	solvent	800 mL

The right-hand window shows a 'Formulation Detail' for 'Liquid Laundry Detergent Composition: Laundry Detergents'. It includes a 'JOURNAL' section with a snippet about the improvement of washing properties and a table of 'Formulation Ingredients'.

Component	Function	Amount Reported	Optionality
Fatty alcohols, ethoxylated	-	5-15 %	Mandatory
Polycosyethylene lauryl ether sodium sulfate	-	5-15 %	Mandatory
Soaps	-	5-15 %	Mandatory
Phosphates	-	<5 %	Mandatory
Enzymes	-	-	Mandatory
Group: Cosmetic fragrance products	fragrances	-	Mandatory
Group: Preservatives	preservatives	-	Mandatory

With CAS Formulus® you have access to the world's leading collection of formulations, leading you to insights that go beyond literature. Understand a formulation's origin and effectiveness with access to the best information for active ingredients and excipients. Evaluate ingredients and manufacturing processes; and explore regulatory requirements in one easy interface.

The screenshot shows the CAS SciFinder interface. The search query is 'References search for "Pasteur, L." Author Name'. The results are filtered by 'Substances' and show 46 results. The first result is 'On grape acid' by PASTEUR, L., with a machine-translated English abstract.

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 lies is in no property of the wine acid different. The Laevoracemsaure and their salts have now ...

The second result is 'On the aspartic acid and malic acid' by PASTEUR, L., also with a machine-translated English abstract.

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 Polarisationebene deflecting and that this property by all compounds of these acids through fortplanze. At the same time bemerkle the same, that the natural fumaric acid, such as by distillation of malic acid obtained is not this property theilen. At that time was DESSAIGNES, that said acidic fumaric acid ammonia in aspartic acid uiuwundellii remove. Connecting the mutual

ChemZent® is the only online source of Chemisches Zentralblatt, with machine-translated English abstracts and the original German versions. Indexed to fit seamlessly into CAS SciFinder® workflows, this comprehensive source features more than 800,000 documents and over 3 million abstracts.



CAS is a leader in scientific information solutions, partnering with innovators around the world to accelerate scientific breakthroughs. CAS employs over 1,400 experts who curate, connect, and analyze scientific knowledge to reveal unseen connections. For over 100 years, scientists, patent professionals, and business leaders have relied on CAS solutions and expertise to provide the hindsight, insight, and foresight they need so they can build upon the learnings of the past to discover a better future. CAS is a division of the American Chemical Society.

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