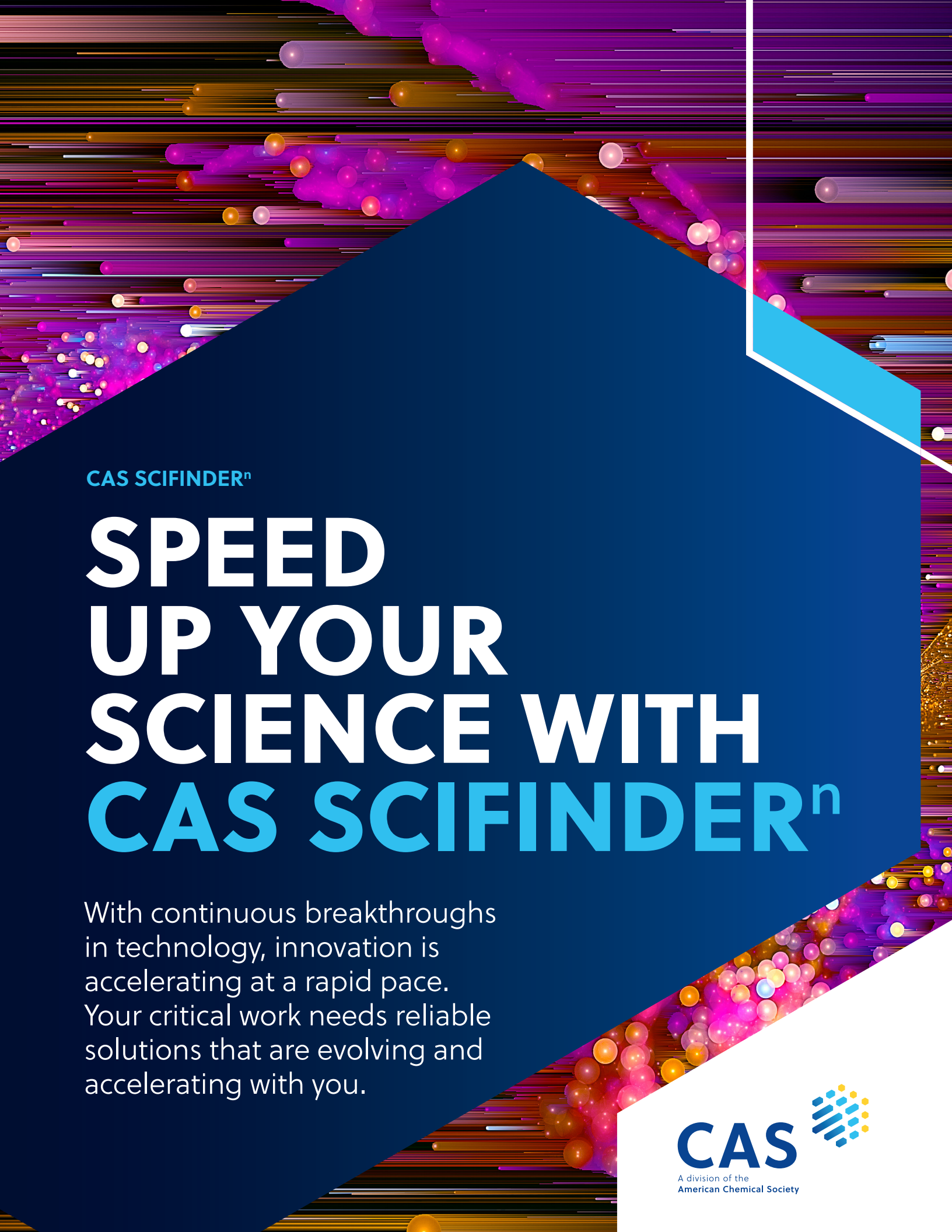

CAS SCIFINDERn
SPEED UP YOUR SCIENCE WITH CAS SCIFINDERn
With continuous breakthroughs in technology, innovation is accelerating at a rapid pace. Your critical work needs reliable solutions that are evolving and accelerating with you.
CAS
A division of the American Chemical Society

Whether you need to expand your innovation pipeline to fulfill investor expectations, keep up to date with the industry landscape and your competitors, or identify new business opportunities, CAS SciFinder^{n} speeds the process of finding relevant, actionable insights.

Featuring the renown CAS Content Collection relied upon by the scientific community and the most advanced relevance engine in the industry, CAS SciFinder^{n} produces better research in less time.

INNOVATION

84%

of researchers agree CAS SciFinder^{n} allows them to be more innovative than other research solutions.[1]

SPEED

77%

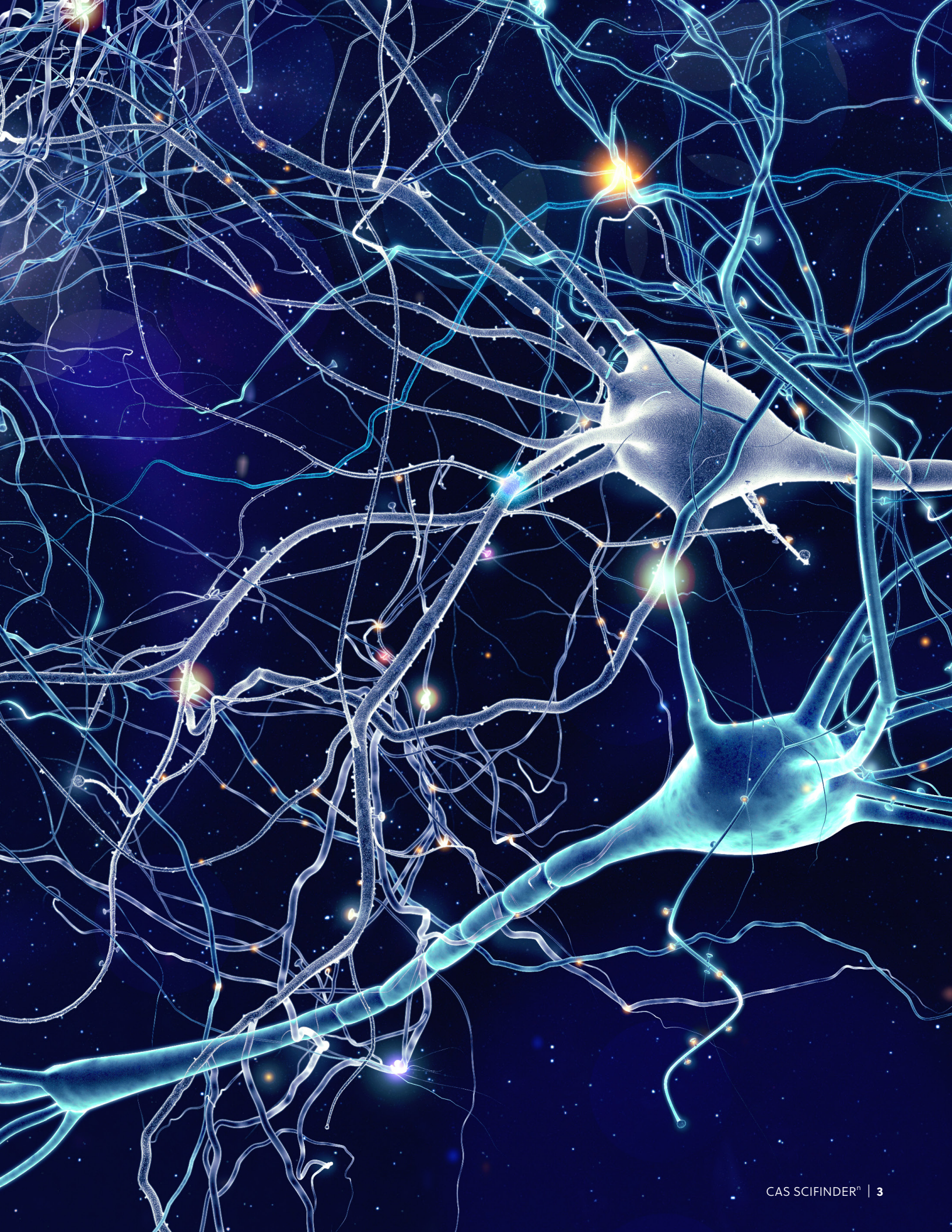
of researchers agree CAS SciFinder^{n} allows them to work more quickly than other research solutions.[1]

CONFIDENCE

84%

of researchers agree CAS SciFinder^{n} allows them to work more confidently compared to other research solutions.[1]

1. CAS SciFinder^{n} Productivity Survey 2020.



Perform literature reviews

CAS SciFinder^{n} halves the time needed to perform literature reviews[1]

In today's competitive landscape, your research team needs to quickly gain knowledge and insights. You can't afford to spend hours sifting through irrelevant patent and journal content. That's why we designed CAS SciFinder^{n} with the most chemistry-aware relevance engine in the industry. It doesn't just search faster, it helps you search smarter, anticipates your information needs and accelerates your work. Details from global scientific references are added to the CAS Content Collection every day to keep you up to date on the world's published scientific patent and journal literature across multiple disciplines. CAS scientific analysts extract and verify a multitude of data and key insights from each publication, making connections and uncovering trends only possible with the combined power of expert human analysis and advanced data technology.

1. CAS SciFinder^{n} Productivity Survey 2020.

References | novel coronavirus nonpeptide inhibitors | Draw

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
Learn about result relevance.
Load More Results

Filter Behavior
Filter by | Exclude

Document Type
- Journal (3,251)
- Patent (165)
- Review (755)
- Clinical Trial (61)
- Commentary (3)
View All

Language
- English (3,483)
- Chinese (67)
- Japanese (37)
- Russian (20)

References (3,640)

Sort: Relevance | View: Partial Abstract

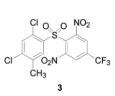
Substances | Reactions | Cited By | Save

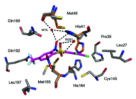
1

Structure-Based Drug Design and Structural Biology Study of Novel Nonpeptide Inhibitors of Severe Acute Respiratory Syndrome Coronavirus Main Protease

By: Lu, I-Lin; Mahindroo, Neeraj; Liang, Po-Huang; Peng, Yi-Hui; Kuo, Chih-Jung; Tsai, Keng-Chang; Hsieh, Hsing-Pang; Chao, Yu-Sheng; Wu, Su-Ying

Journal of Medicinal Chemistry (2006), 49(17), 5154-5161 | Language: English, Database: CAplus and MEDLINE





Severe acute respiratory syndrome coronavirus (SARS-CoV) main protease (M^{pro}), a protein required for the maturation of SARS-CoV, is vital for its life cycle, making it an attractive target for structure-based drug design of anti-SARS drugs. The structure-based virtual screening of a chem. database containing 58 855 compounds followed by the testing of potential compounds for SARS-CoV M^{pro} inhibition leads to two hit compounds The core structures of these two hits, defined by the docking study, are used for further analog search. Twenty-one analogs derived from these two hits exhibited IC_{50} va...

View More

Full Text | Substances (25) | Reactions (0) | Cited By (86) | Citation Map

2

Structure-Based Design, Synthesis, and Biological Evaluation of a Series of Novel and Reversible Inhibitors for the Severe Acute Respiratory Syndrome-Coronavirus Papain-Like

Feedback

Citation Map

Filter By | Cited By | Citing

Filter Behavior
Filter by | Exclude

Document Type
- Journal (150)
- Review (54)
- Clinical Trial (28)
- Commentary (1)
- Conference (5)
View All

Author
- Mueller, Guenter (6)
- Malerczyk, V. (5)
- Neuvonen, Pertti J. (5)
- Niemi, Mikko (5)
- Backman, Janne T. (4)
View All

Concept

Glimepiride: a review of its use in the management of type 2 diabetes mellitus

By: Langtry, Heather D.; Balfour, Julia A.

Drugs (1998), 55(4), 563-584 | Language: English,

Full Text

Impact of obesity on drug metabolism and elimination in adults and children
By: Brill, Margreke J. E.; Diepstraten, Jeroen; van Rongen, Anne; van Kralingen, Simone; van den Anker, John N.; Knibbe, Catherijne A. J.
Clinical Pharmacokinetics (2012)
Cited by 136

View 18 More | View 25 More

Citation Map Key
- Cited by Root Document
- References Citing Root Document

Reset

Feedback

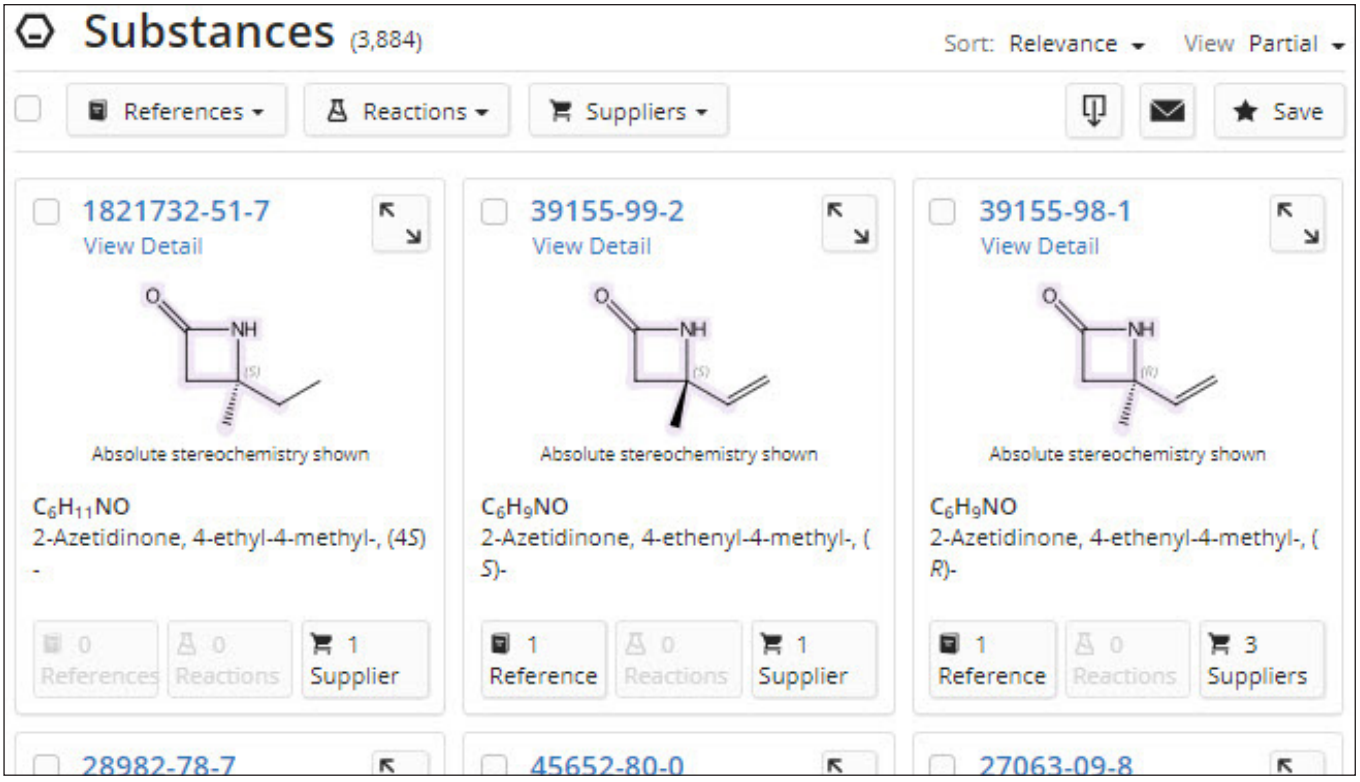
Copyright © 2021 American Chemical Society. All Rights Reserved. | 京ICP备13047075号-3

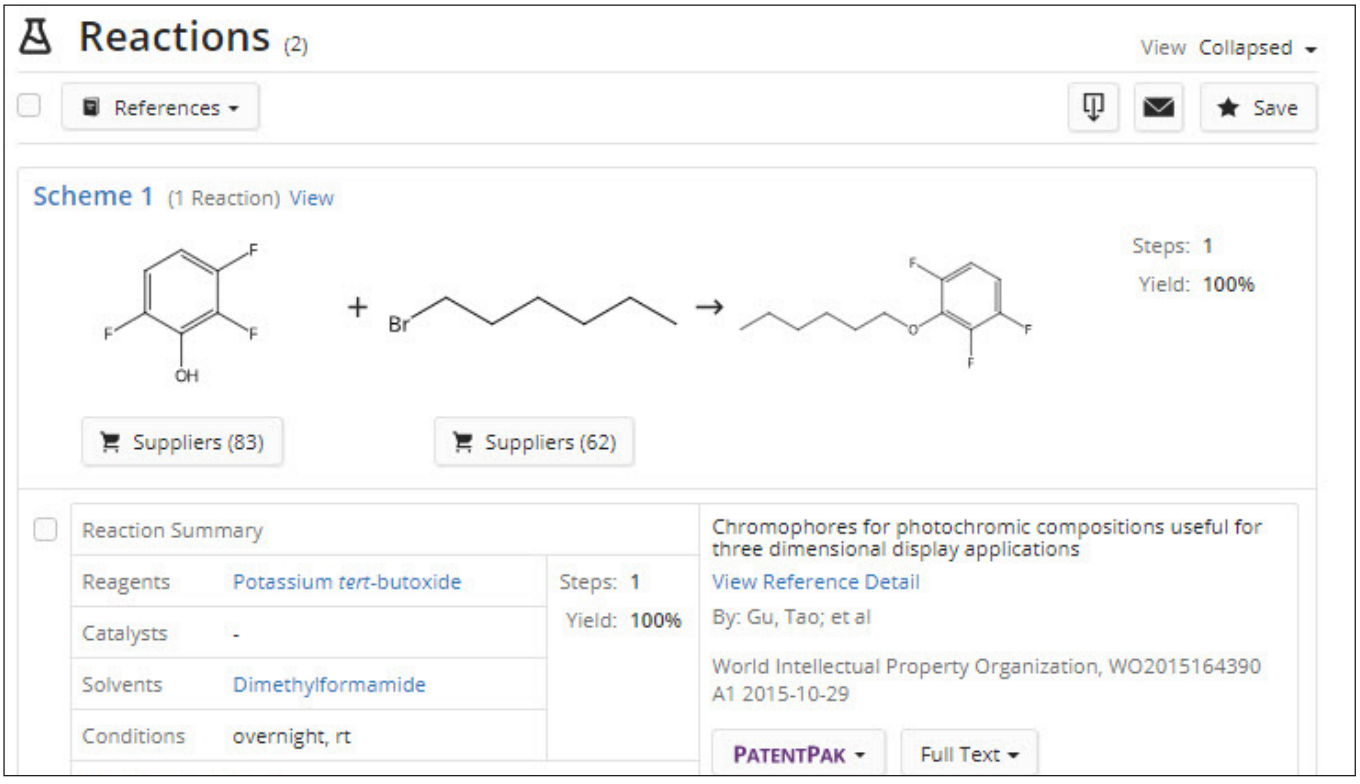
Help | Contact Us | Legal

Mine substances and reactions

CAS SciFinder^{n} provides access to the world's most trusted substance resource, the CAS Registry

You need the most current and accurate substance and reaction information available to quickly and confidently inform your critical research activities with key insights. A global network of expert scientists curate and aggregate the world's scientific scholarly journals, patents, dissertations and seminal reference works daily and make them fully discoverable through the advanced technology of CAS SciFinder^{n}. That makes it your one true source for authoritatively identifying a chemical substance and its related chemical structures, chemical names, regulatory information and properties, including the CAS Registry Number®, as well as reaction schemes, step-by-step experimental procedures, detailed conditions and product yields.


Substances (3,884)
Sort: Relevance
View Partial
References
Reactions
Suppliers
Save
1821732-51-7
View Detail
Absolute stereochemistry shown
C6H11NO
2-Azetidinone, 4-ethyl-4-methyl-, (4S)-
0 References
0 Reactions
1 Supplier
39155-99-2
View Detail
Absolute stereochemistry shown
C6H9NO
2-Azetidinone, 4-ethenyl-4-methyl-, (S)-
1 Reference
0 Reactions
1 Supplier
39155-98-1
View Detail
Absolute stereochemistry shown
C6H9NO
2-Azetidinone, 4-ethenyl-4-methyl-, (R)-
1 Reference
0 Reactions
3 Suppliers
28982-78-7
45652-80-0
27063-09-8

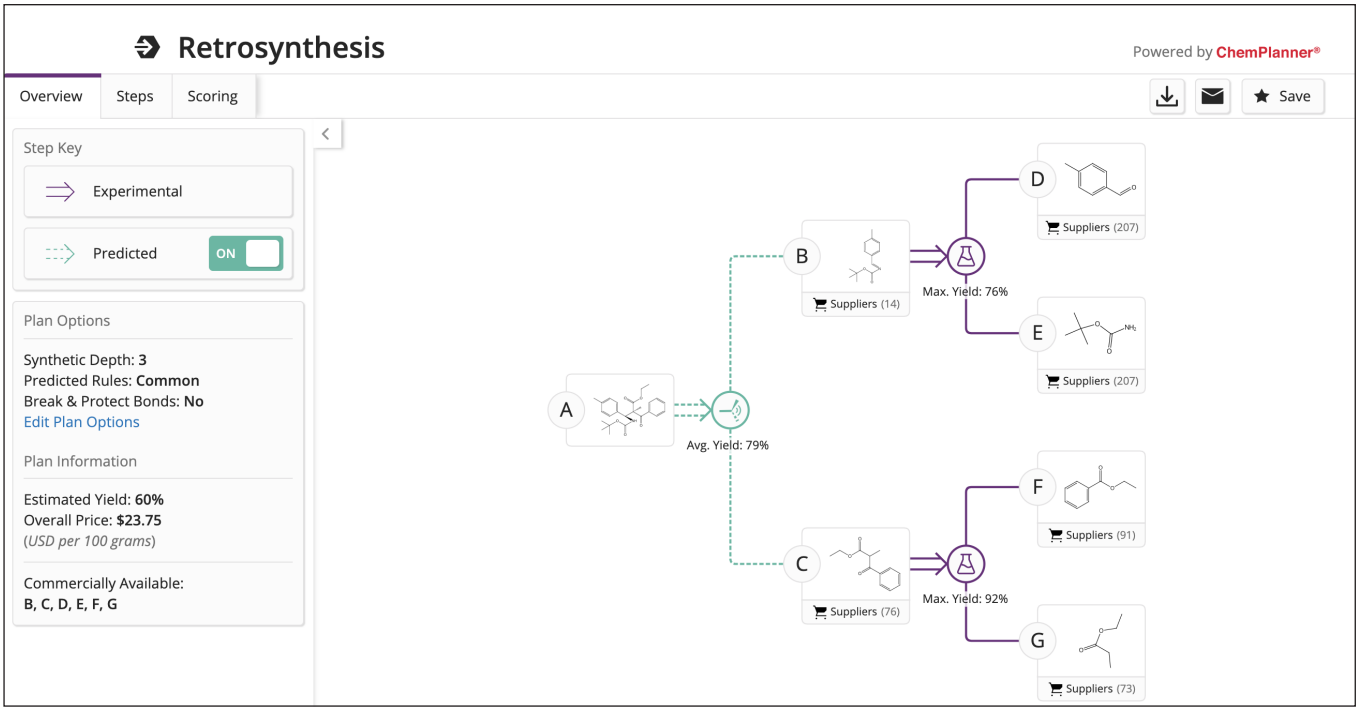

Reactions (2)
View Collapsed
References
Save
Scheme 1 (1 Reaction) View
Steps: 1
Yield: 100%
Suppliers (83)
Suppliers (62)
Reaction Summary
Reagents Potassium tert-butoxide
Catalysts -
Solvents Dimethylformamide
Conditions overnight, rt
Steps: 1
Yield: 100%
Chromophores for photochromic compositions useful for three dimensional display applications
View Reference Detail
By: Gu, Tao; et al
World Intellectual Property Organization, WO2015164390 A1 2015-10-29
PATENTPAK
Full Text

Devise synthetic plans

CAS SciFinder^{n} halves the time required for synthetic planning[1]

Being successful in the lab requires a great synthetic plan. Your chemists are juggling many variables, especially when devising routes to novel compounds with no literature-based precedent. For both known and unknown molecules, CAS SciFinder^{n} will perform a full retrosynthetic analysis fueled by the renowned CAS collection of reactions. The best potential synthetic routes are determined based on steps from both the literature and predicted steps generated by our synthetic chemistry engine. The algorithm can be customized to fit specific requirements of the synthesis and the plan is easily navigated to evaluate alternative routes. Each plan also offers quick access to information on material suppliers, step-by-step methods curated by experts, product yields, and more.

1. CAS SciFinder^{n} Productivity Survey 2020.



Experimental Protocols

Synthetic Methods

Products	Ruthenium, carbonylchloro[2-[1-(hydroxy-κ*O*)-2-naphthalenyl]-1-diazenecarbothioamidato-κN^2,κ*S*](triphenylphosphine)-, Yield: 80%
Reactants	Carbonylchlorohydrotris(triphenylphosphine)ruthenium 2-(1-Oxo-2(1*H*)-naphthalenylidene)hydrazinecarbothioamide
Solvents	Benzene
Procedure	1. Add the appropriate ligand (0.023-0.029 g, 0.1 mmol) in 1:1 M ratio to a solution of Ruthenium(II) complex (0.1 g, 0.1 mmol) in benzene (20 cm^3). 2. Heat the mixture under reflux for 5 h on water bath. 3. Concentrate the resulting solution to 3 cm^3. 4. Precipitate the product by the addition of petroleum ether (60-80 °C). 5. Recrystallize the mixture using CH_2Cl_2. 6. Dry the residue under vacuum to obtain the product.
Transformation	Aromatization of Six-Membered Rings Coordination of a Metal to Carbon and Heteroatom Ligand Substitution

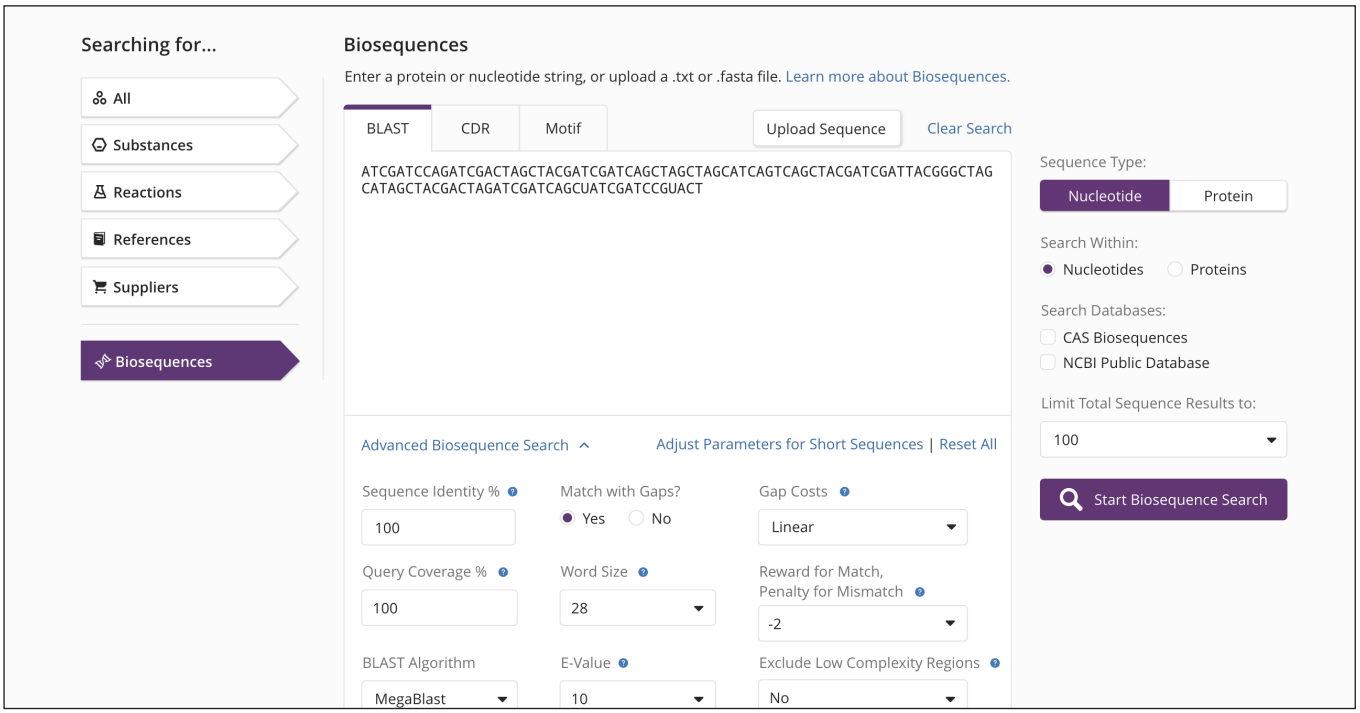
Conduct comprehensive biologics research

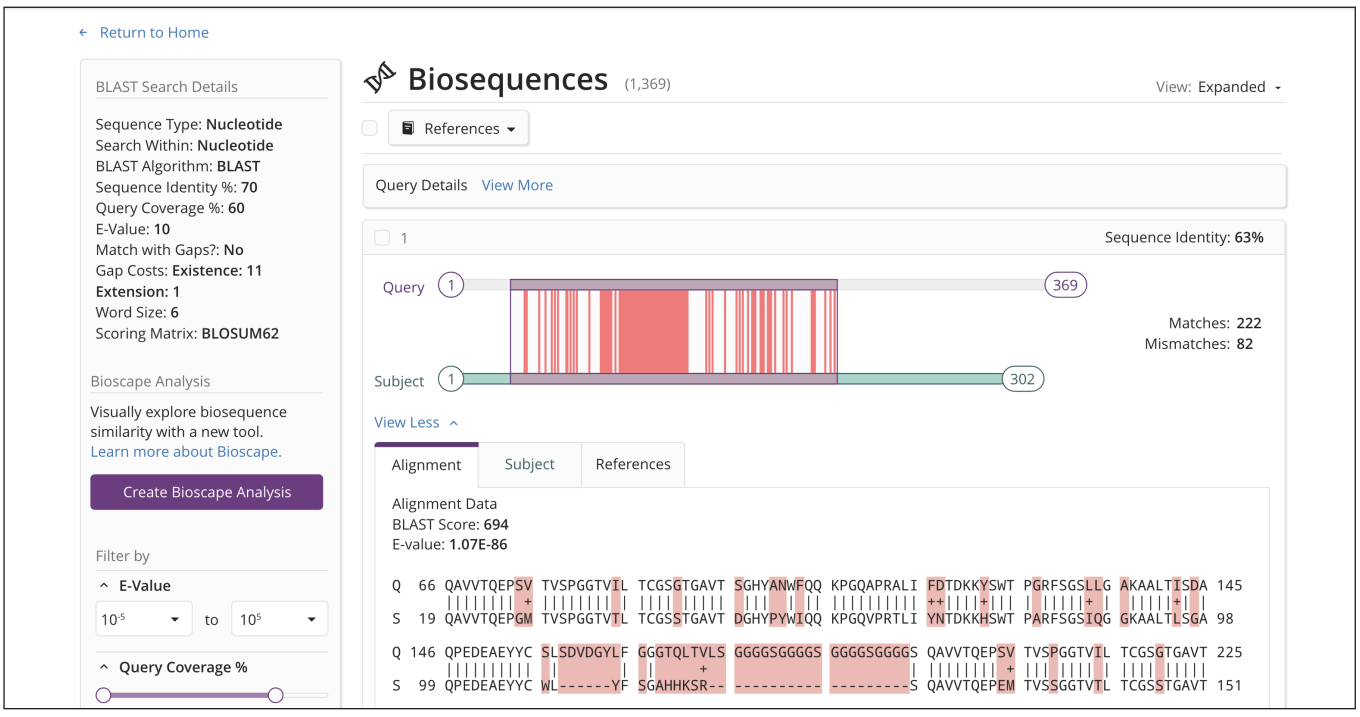
CAS SciFinder^{n} powers your biologics R&D program to new levels

Integrated with the world's most comprehensive collection of chemical reactions, substances, and indexed scientific literature, CAS SciFinder^{n} provides advanced search, visualization, filtering and analysis capabilities for one of the largest, most comprehensive collections of protein and nucleic acid sequences as well as modified peptides and small molecules. In addition to public datasets like those from NCBI* and extensive datasets from global patents, the CAS biosequences collection includes millions of human curated and indexed sequences from non-patent literature, including 12K+ scientific journals, not found in other databases. Many sequences are expertly annotated by CAS scientists to capture information on chemical modifications, sequence origin, function, gene designation, variant and isoform information, with important synonyms such as trivial names, trade names and lab codes also added. You can also search bioactivity and target indicator data for drug-like substances including both small molecules and biologics.

Not only does CAS SciFinder^{n} offer the most comprehensive patent collection related to biologic drug discovery, it has one of the largest collections of scientific journal records, including PubMed's biomedical and life science articles and abstracts. With value-added indexing by CAS scientists including cited and citing references and direct links to full-text publications (where available), you can uncover connections between biosequences and patent and non-patent* literature that you can't see anywhere else.

*Coming soon

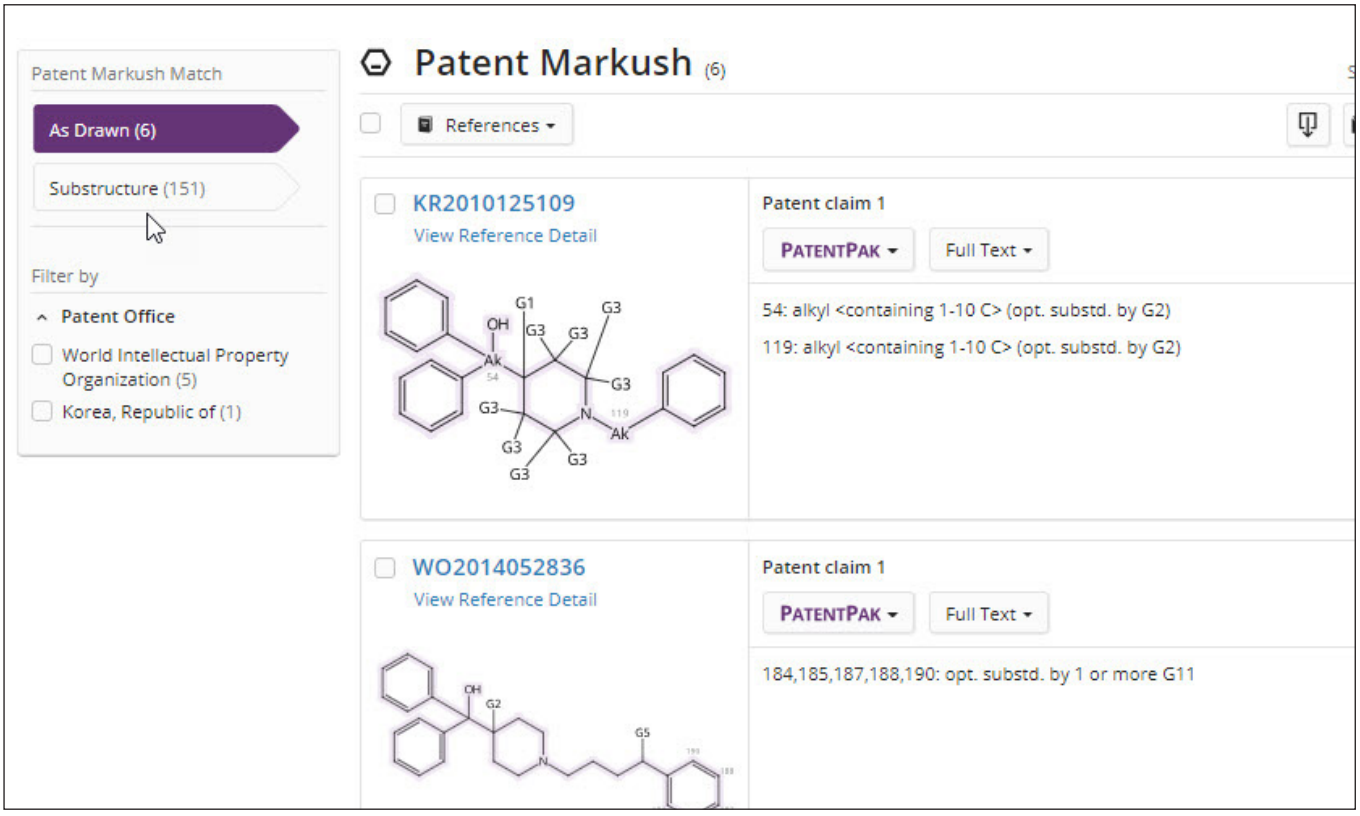

Searching for...
All
Substances
Reactions
References
Suppliers
Biosequences
Biosequences
Enter a protein or nucleotide string, or upload a .txt or .fasta file. Learn more about Biosequences.
BLAST
CDR
Motif
Upload Sequence
Clear Search
ATCGATCCAGATCGACTAGCTACGATCGATCAGCTAGCTAGCATCAGTCAGCTACGATCGATTACGGGCTAG
CATAGCTACGACTAGATCGATCAGCUATCGATCCGUACT
Sequence Type:
Nucleotide
Protein
Search Within:
Nucleotides
Proteins
Search Databases:
CAS Biosequences
NCBI Public Database
Limit Total Sequence Results to:
100
Start Biosequence Search
Advanced Biosequence Search
Adjust Parameters for Short Sequences | Reset All
Sequence Identity %
100
Match with Gaps?
Yes
No
Gap Costs
Linear
Query Coverage %
100
Word Size
28
Reward for Match, Penalty for Mismatch
-2
BLAST Algorithm
MegaBlast
E-Value
10
Exclude Low Complexity Regions
No

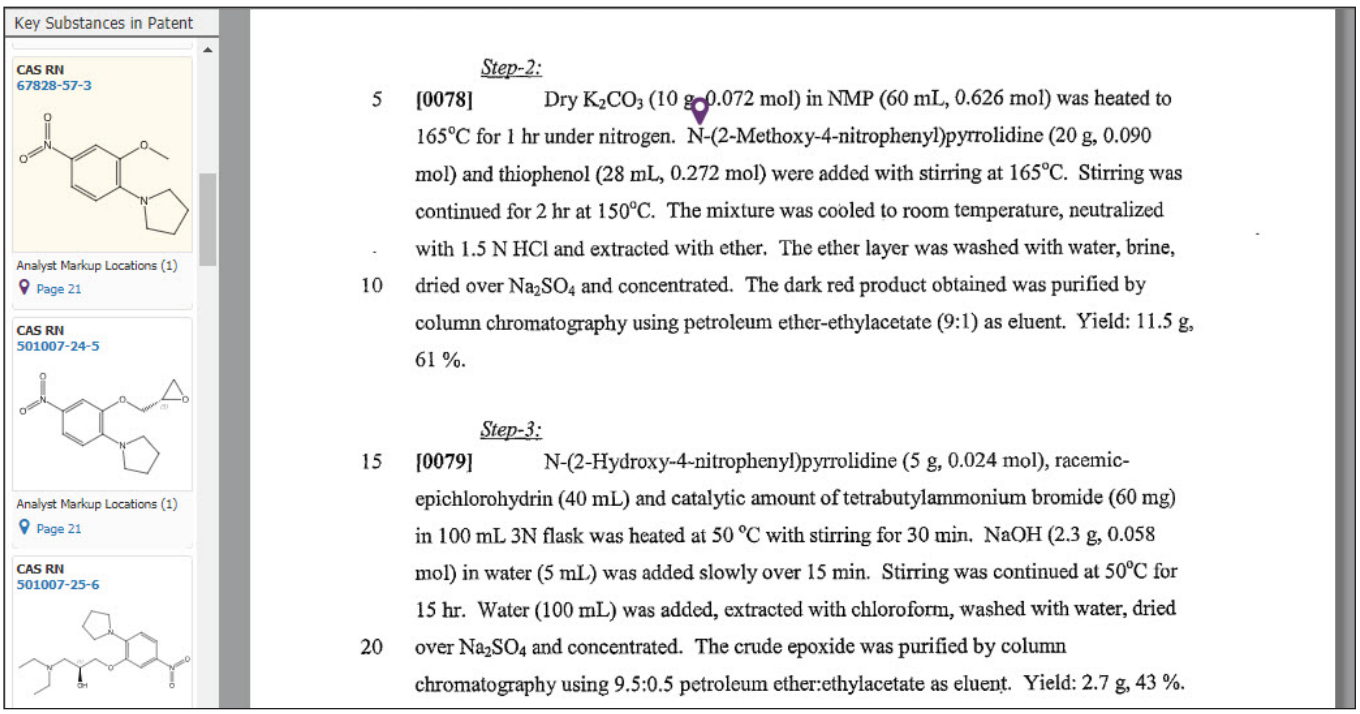

Return to Home
BLAST Search Details
Sequence Type: Nucleotide
Search Within: Nucleotide
BLAST Algorithm: BLAST
Sequence Identity %: 70
Query Coverage %: 60
E-Value: 10
Match with Gaps?: No
Gap Costs: Existence: 11
Extension: 1
Word Size: 6
Scoring Matrix: BLOSUM62
Bioscape Analysis
Visually explore biosequence similarity with a new tool.
Learn more about Bioscape.
Create Bioscape Analysis
Filter by
E-Value
10-5
to
105
Query Coverage %
Biosequences (1,369)
View: Expanded
References
Query Details View More
1
Sequence Identity: 63%
Query
1
369
Subject
1
302
Matches: 222
Mismatches: 82
View Less
Alignment
Subject
References
Alignment Data
BLAST Score: 694
E-value: 1.07E-86
Q 66 QAVVTQEPSV TVSPGGTVIL TCGSGTGAVT SGHYANWFQQ KPGQAPRALI FDTDKKYSWT PGRFSGSLLG AKAALTISDA 145
S 19 QAVVTQEPGM TVSPGGTVTL TCGSSTGAVT DGHYPYWIQQ KPGQVPRTLI YNTDKKHSWT PARFSGSIQG GKAALTLSGA 98
Q 146 QPEDEAEYYC SLSDVDGYLF GGGTQLTVLS GGGGSGGGGS GGGGSGGGGS QAVVTQEPSV TVSPGGTVIL TCGSGTGAVT 225
S 99 QPEDEAEYYC WL------YF SGAHHKSR-- ---------- ---------S QAVVTQEPEM TVSSGGTVTL TCGSSTGAVT 151

Inform IP strategy

CAS SciFinder^{n} reduces the time needed to analyze the IP landscape

In order to successfully manage your research portfolio and bring your innovation to market, it's essential to first understand the technology landscape. CAS SciFinder^{n} can help answer a host of IP-related questions such as: Where are the opportunities for innovation? Are there infringement risks? Who else is working in this space? CAS SciFinder^{n} gives you access to industry-leading capabilities like patent Markush searching and content such as patents that have been chemically annotated by our expert scientists, so you can stay on top of the technological landscape.





Step-2:

[0078] Dry K_2CO_3 (10 g, 0.072 mol) in NMP (60 mL, 0.626 mol) was heated to 165°C for 1 hr under nitrogen. N-(2-Methoxy-4-nitrophenyl)pyrrolidine (20 g, 0.090 mol) and thiophenol (28 mL, 0.272 mol) were added with stirring at 165°C. Stirring was continued for 2 hr at 150°C. The mixture was cooled to room temperature, neutralized with 1.5 N HCl and extracted with ether. The ether layer was washed with water, brine, dried over Na_2SO_4 and concentrated. The dark red product obtained was purified by column chromatography using petroleum ether-ethylacetate (9:1) as eluent. Yield: 11.5 g, 61 %.

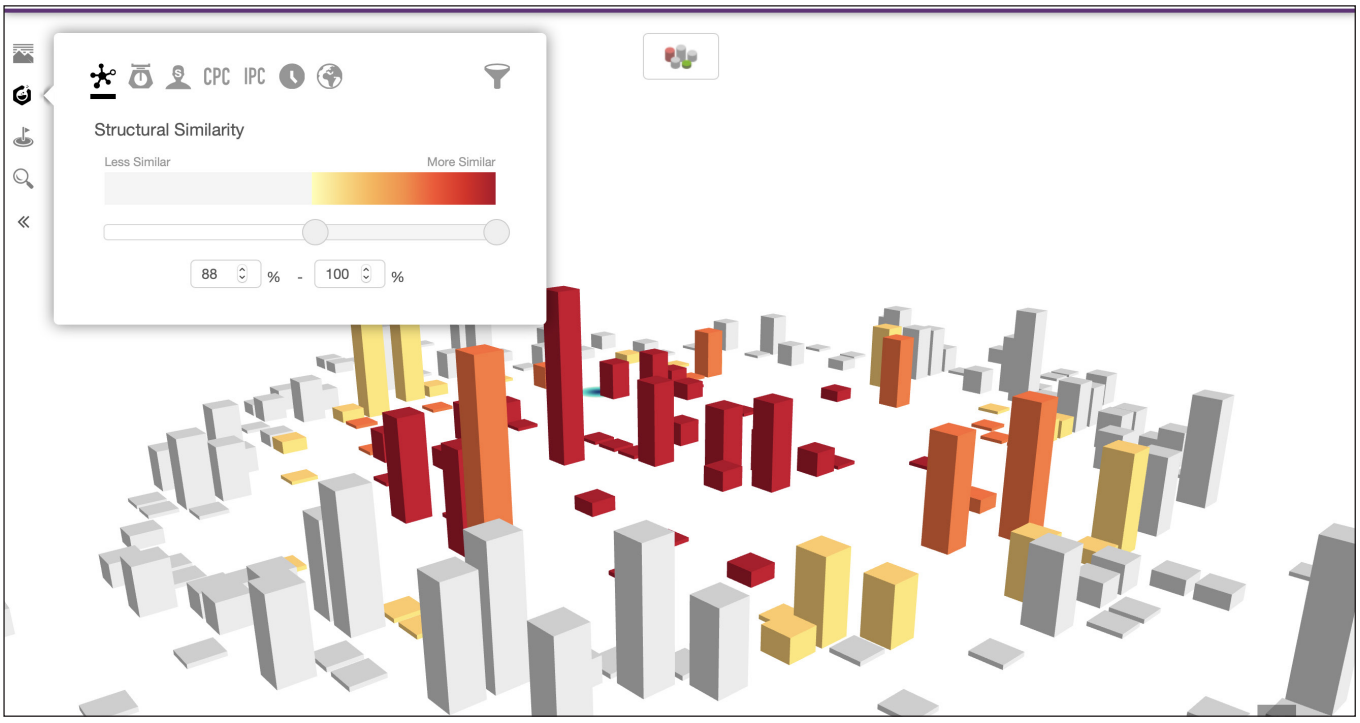
Step-3:

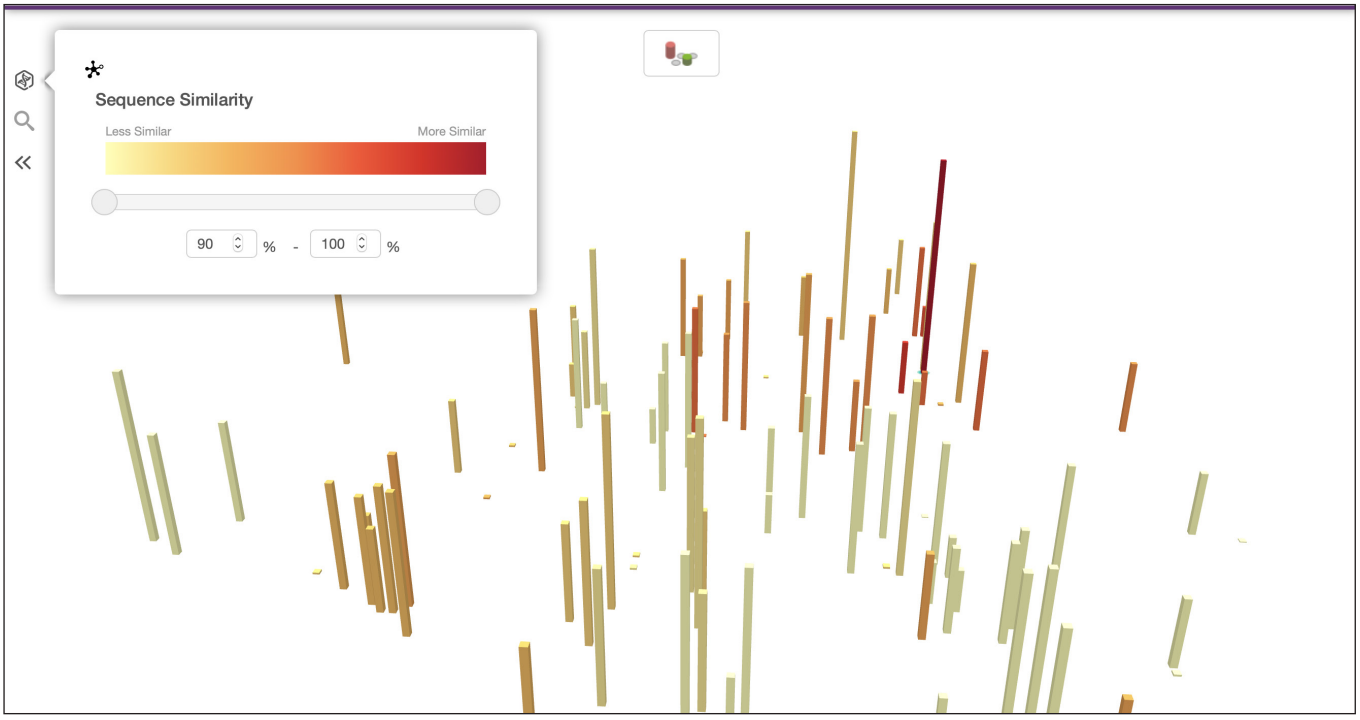
[0079] N-(2-Hydroxy-4-nitrophenyl)pyrrolidine (5 g, 0.024 mol), racemic-epichlorohydrin (40 mL) and catalytic amount of tetrabutylammonium bromide (60 mg) in 100 mL 3N flask was heated at 50 °C with stirring for 30 min. NaOH (2.3 g, 0.058 mol) in water (5 mL) was added slowly over 15 min. Stirring was continued at 50°C for 15 hr. Water (100 mL) was added, extracted with chloroform, washed with water, dried over Na_2SO_4 and concentrated. The crude epoxide was purified by column chromatography using 9.5:0.5 petroleum ether:ethylacetate as eluent. Yield: 2.7 g, 43 %.

Visualize search results

CAS SciFinder^{n} offers visual context for substance and biosequence result sets

With the overwhelming volume of scientific data today, it can be challenging to pinpoint trends, patterns and outliers to gain understanding and make better decisions faster. Now CAS SciFinder^{n} provides user-friendly visualization tools to help you turn information into insights. Graphically explore the structural similarity of chemicals compared to one another and the patents associated with them. Review your biosequence search results visually and evaluate sequence space from an IP perspective. You can change how the results bars are displayed, group and refine your results to highlight key information, and even save for later viewing.

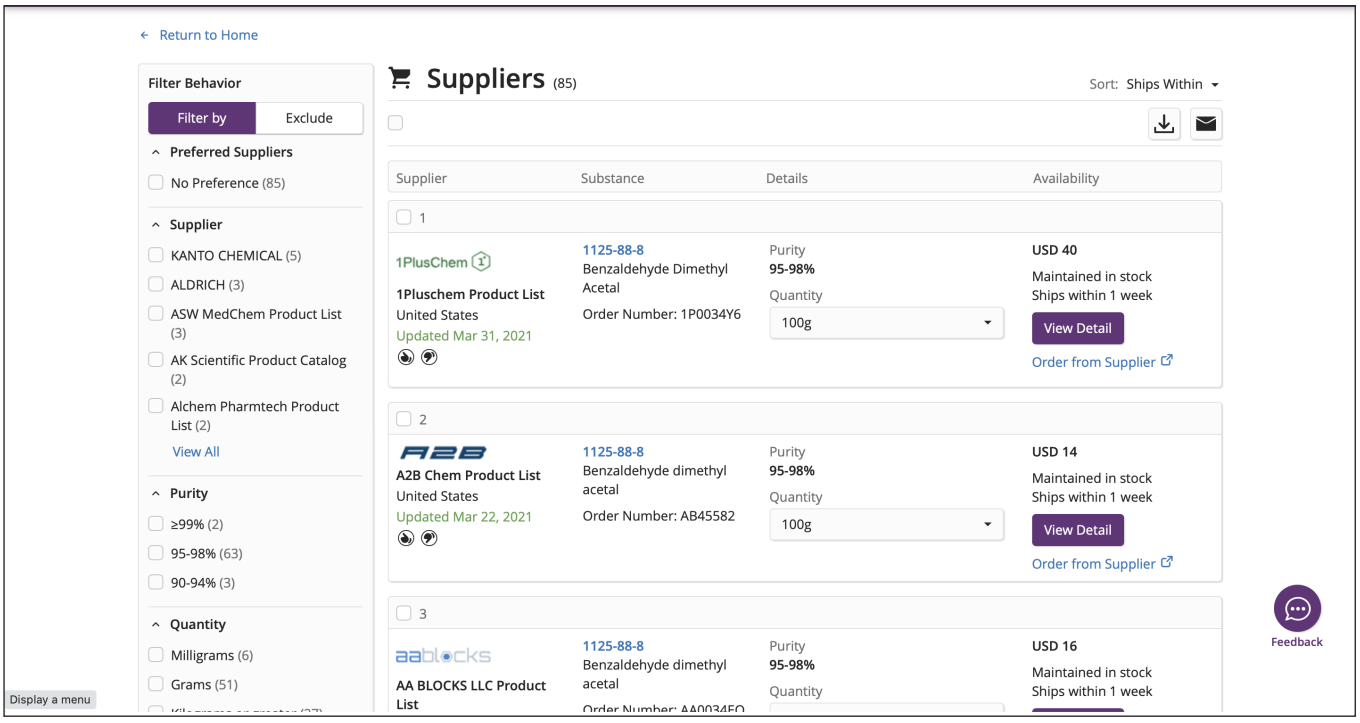

CPC
IPC
Structural Similarity
Less Similar
More Similar
88
%
-
100
%

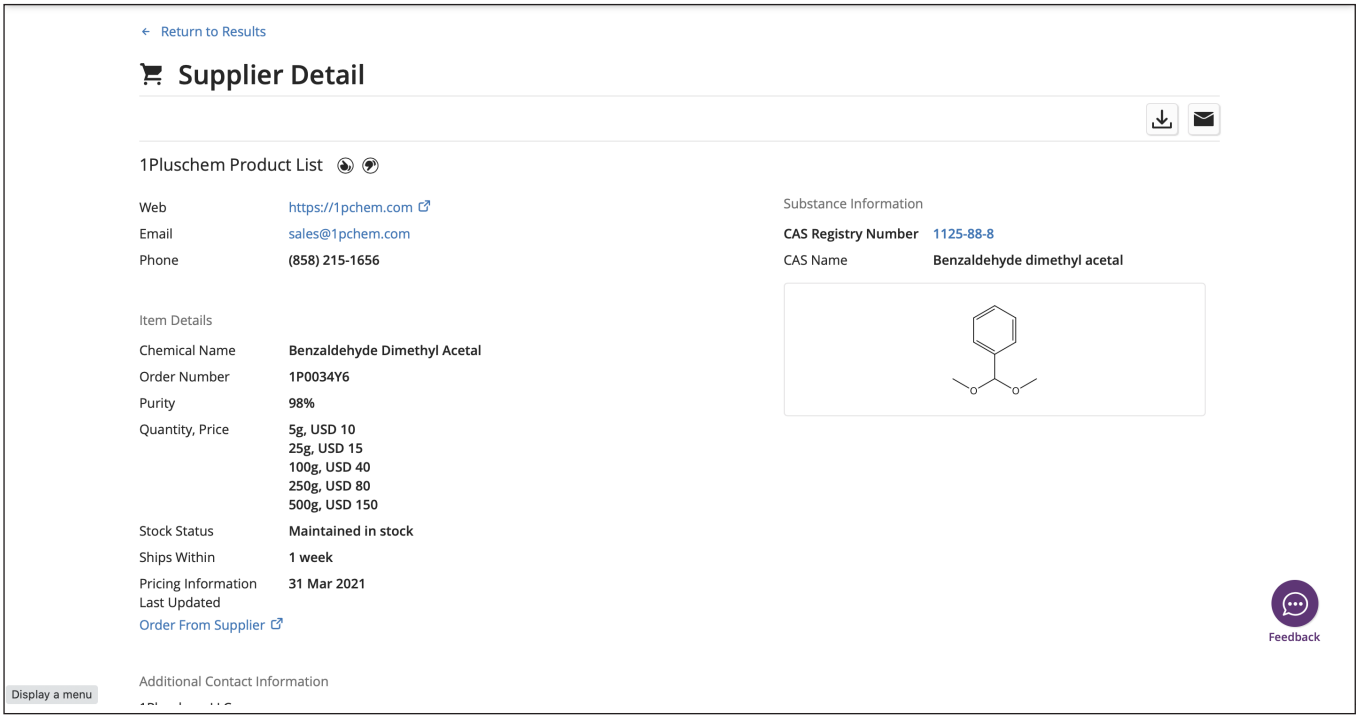

Sequence Similarity
Less Similar
More Similar
90
%
-
100
%

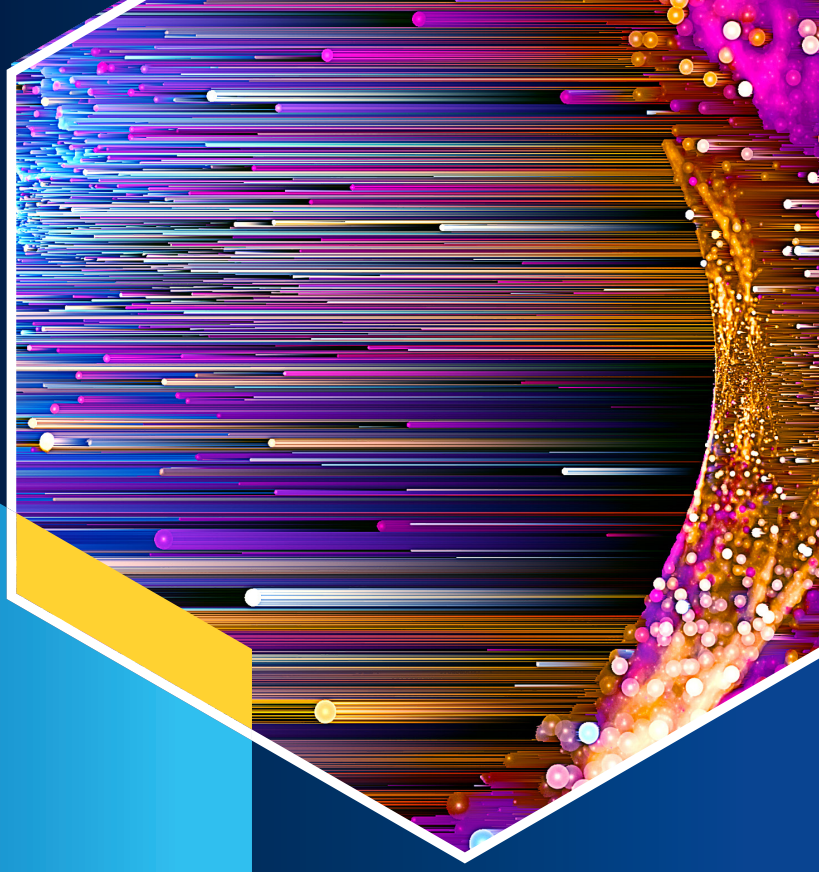
Find commercially available chemicals

CAS SciFinder^{n} contains the market-leading index of chemicals from worldwide suppliers

Before heading to the lab, scientists from leading commercial, academic and government organizations worldwide turn to CAS SciFinder^{n} to develop their research plan. Integrated throughout CAS SciFinder^{n}, CAS Commercial Sources help those scientists quickly and easily find and compare commercial supplier sources for needed materials. This up-to-date resource contains millions of commercially available chemical products from the verified catalogs of hundreds of suppliers. Listings include available quantities, prices, and supplier contact information, many with direct order links to purchase the material on the supplier's web site.


Return to Home
Filter Behavior
Filter by
Exclude
Preferred Suppliers
No Preference (85)
Supplier
KANTO CHEMICAL (5)
ALDRICH (3)
ASW MedChem Product List (3)
AK Scientific Product Catalog (2)
Alchem Pharmtech Product List (2)
View All
Purity
≥99% (2)
95-98% (63)
90-94% (3)
Quantity
Milligrams (6)
Grams (51)
Suppliers (85)
Sort: Ships Within
Supplier
Substance
Details
Availability
1
1PlusChem
1Pluschem Product List
United States
Updated Mar 31, 2021
1125-88-8
Benzaldehyde Dimethyl Acetal
Order Number: 1P0034Y6
Purity
95-98%
Quantity
100g
USD 40
Maintained in stock
Ships within 1 week
View Detail
Order from Supplier
2
A2B Chem Product List
United States
Updated Mar 22, 2021
1125-88-8
Benzaldehyde dimethyl acetal
Order Number: AB45582
Purity
95-98%
Quantity
100g
USD 14
Maintained in stock
Ships within 1 week
View Detail
Order from Supplier
3
AA BLOCKS LLC Product List
1125-88-8
Benzaldehyde dimethyl acetal
Purity
95-98%
Quantity
USD 16
Maintained in stock
Ships within 1 week
Feedback
Display a menu


Return to Results
Supplier Detail
1Pluschem Product List
Web
https://1pchem.com
Email
sales@1pchem.com
Phone
(858) 215-1656
Item Details
Chemical Name
Benzaldehyde Dimethyl Acetal
Order Number
1P0034Y6
Purity
98%
Quantity, Price
5g, USD 10
25g, USD 15
100g, USD 40
250g, USD 80
500g, USD 150
Stock Status
Maintained in stock
Ships Within
1 week
Pricing Information Last Updated
31 Mar 2021
Order From Supplier
Substance Information
CAS Registry Number
1125-88-8
CAS Name
Benzaldehyde dimethyl acetal
Additional Contact Information
Feedback
Display a menu



CAS SciFinder^{n} is a solution within the CAS SciFinder Discovery Platform, an enterprise solution created to help get discoveries to market faster and optimize profitability. CAS SciFinder Discovery Platform provides researchers with the information they need to avoid surprises and make smart investments with insight into the latest discoveries and competitive intelligence.

CAS is a leader in scientific information solutions, partnering with global innovators to accelerate breakthroughs by curating, connecting, and analyzing the world's scientific knowledge.

Connect with us at cas.org.

CAS
A division of the
American Chemical Society

© Copyright 2021 American Chemical Society. All rights reserved

SCIGENENGBRO100034210524