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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	SPEED	CONFIDENCE
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of researchers agree CAS SciFinder[n] allows them to be more innovative than other research solutions.[1]	of researchers agree CAS SciFinder[n] allows them to work more quickly than other research solutions.[1]	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.
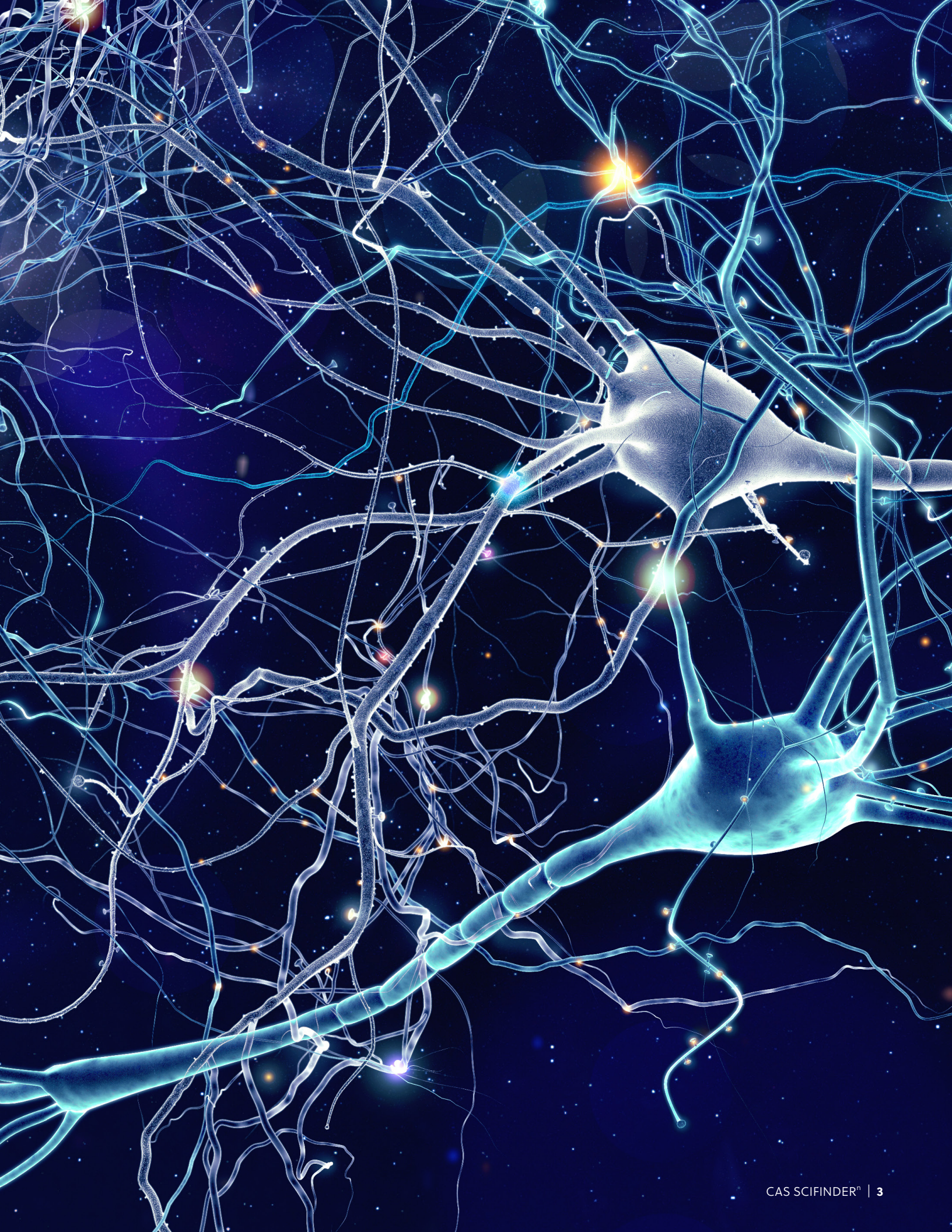
Perform literature reviews

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?
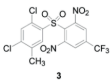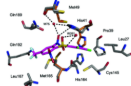Learn about result relevance.

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📖 **References** (3,640)

Sort: Relevance ▾ | View: Partial Abstract ▾

☐ 🔧 Substances ▾ | ⚗ Reactions ▾ | 66 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 IC₅₀ va...

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Full Text ▾ | 🔧 Substances (25) | ⚗ Reactions (0) | 66 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

Filter Behavior
[Filter by] [Exclude]

⌃ Document Type
☐ Journal (3,251)
☐ Patent (165)
☐ Review (755)
☐ Clinical Trial (61)
☐ Commentary (3)
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⌃ Language
☐ English (3,483)
☐ Chinese (67)
☐ Japanese (37)
☐ Russian (20)

Feedback

⊘ **Citation Map**

Filter By | Cited By | Citing

Filter Behavior
[Filter by] [Exclude]

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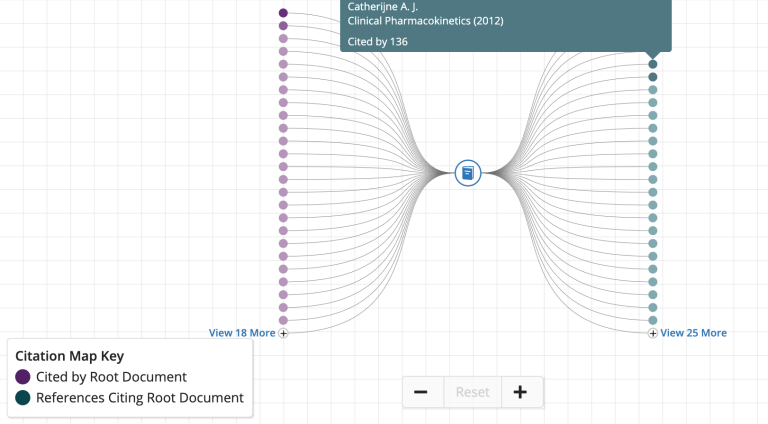☐ Commentary (1)
☐ Conference (5)
View All

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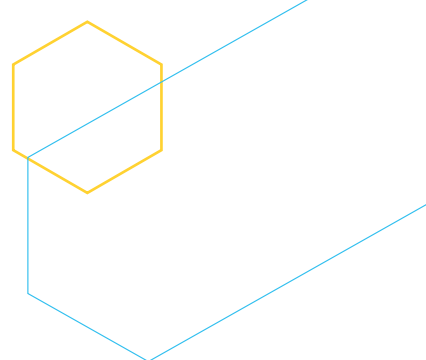Drugs (1998), 55(4), 563-584 | Language: English,

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

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

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Mine substances and reactions

CAS SciFinder[n] provides access to the world's most trusted substance resource, the CAS Registry

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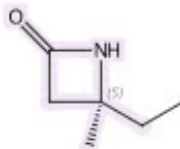
Substances (3,884)

Sort: Relevance ▾   View Partial ▾

☐   📓 References ▾   ⚗ Reactions ▾   🛒 Suppliers ▾   🗗   ✉   ★ Save

☐ **1821732-51-7**
View Detail
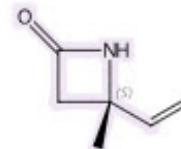
Absolute stereochemistry shown

$C_6H_{11}NO$
2-Azetidinone, 4-ethyl-4-methyl-, (4S)-

📓 0 References	⚗ 0 Reactions	🛒 1 Supplier

☐ **39155-99-2**
View Detail
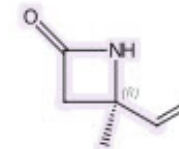
Absolute stereochemistry shown

C_6H_9NO
2-Azetidinone, 4-ethenyl-4-methyl-, (S)-

📓 1 Reference	⚗ 0 Reactions	🛒 1 Supplier

☐ **39155-98-1**
View Detail

Absolute stereochemistry shown

C_6H_9NO
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				Chromophores for photochromic compositions useful for three dimensional display applications
Reagents	Potassium *tert*-butoxide	Steps:	1	View Reference Detail
Catalysts	-	Yield:	100%	By: Gu, Tao; et al
Solvents	Dimethylformamide			World Intellectual Property Organization, WO2015164390 A1 2015-10-29
Conditions	overnight, rt			

PATENTPAK ▾   Full Text ▾
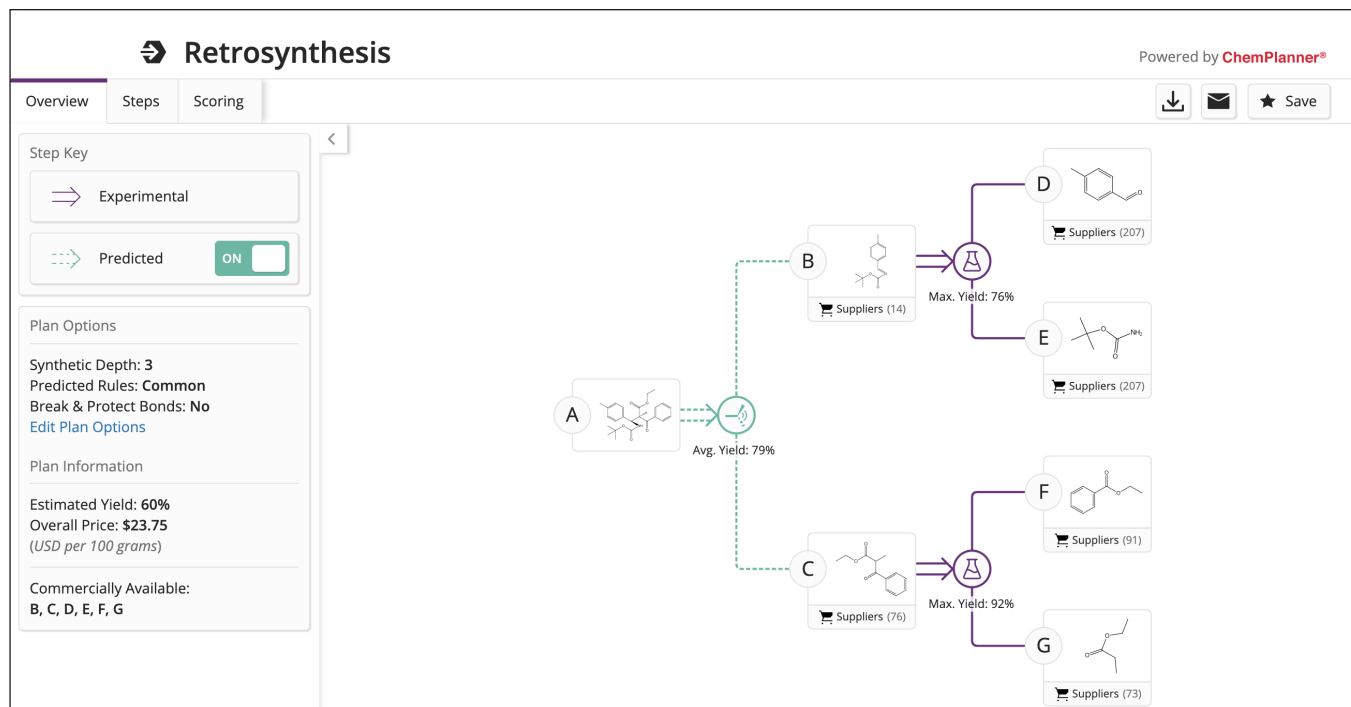
Devise
synthetic plans

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.

⮑ Retrosynthesis

Overview | Steps | Scoring

⬇ | ✉ | ★ Save

Step Key

⟹ Experimental

⇢ Predicted | ON

Plan Options

Synthetic Depth: **3**
Predicted Rules: **Common**
Break & Protect Bonds: **No**
Edit Plan Options

Plan Information

Estimated Yield: **60%**
Overall Price: **$23.75**
(*USD per 100 grams*)

Commercially Available:
B, C, D, E, F, G

B 🛒 Suppliers (14)
A Avg. Yield: 79%
C 🛒 Suppliers (76) — Max. Yield: 92%

Max. Yield: 76%

D 🛒 Suppliers (207)
E 🛒 Suppliers (207)
F 🛒 Suppliers (91)
G 🛒 Suppliers (73)

Experimental Protocols

Synthetic Methods

Products	Ruthenium, carbonylchloro[2-[1-(hydroxy-κO)-2-naphthalenyl]-1-diazenecarbothioamidato-$\kappa N^2,\kappa S$] (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$_2$Cl$_2$. 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

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- 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
CATAGCTACGACTAGATCGATCGATCAGCUATCGATCCGUACT
```

Advanced Biosequence Search ⌃   Adjust Parameters for Short Sequences | Reset All

Sequence Identity % ❓	Match with Gaps?	Gap Costs ❓
100	● Yes ○ No	Linear

Query Coverage % ❓	Word Size ❓	Reward for Match, Penalty for Mismatch ❓
100	28	-2

BLAST Algorithm	E-Value ❓	Exclude Low Complexity Regions ❓
MegaBlast	10	No

Sequence Type:
Nucleotide | Protein

Search Within:
● Nucleotides   ○ Proteins

Search Databases:
☐ CAS Biosequences
☐ NCBI Public Database

Limit Total Sequence Results to:
100

🔍 Start Biosequence Search

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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.
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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 1 ─────────────────── 369

Subject ① 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
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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.

Patent Markush (6)

As Drawn (6)
Substructure (151)

Patent Markush Match

Filter by
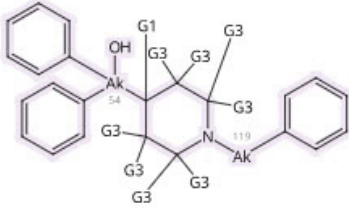
Patent Office
- [ ] World Intellectual Property Organization (5)
- [ ] Korea, Republic of (1)

□ References ▾

□ **KR2010125109**
View Reference Detail
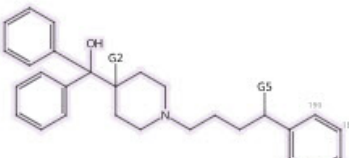

Patent claim 1

PATENTPAK ▾   Full Text ▾

54: alkyl <containing 1-10 C> (opt. substd. by G2)
119: alkyl <containing 1-10 C> (opt. substd. by G2)
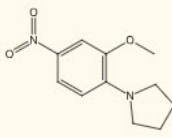
□ **WO2014052836**
View Reference Detail

Patent claim 1

PATENTPAK ▾   Full Text ▾

184,185,187,188,190: opt. substd. by 1 or more G11
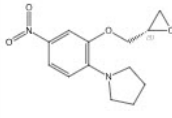
Key Substances in Patent

CAS RN
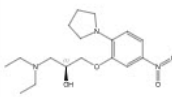67828-57-3

Analyst Markup Locations (1)
📍 Page 21

CAS RN
501007-24-5

Analyst Markup Locations (1)
📍 Page 21

CAS RN
501007-25-6

Step-2:

5   [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,

10   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:

15   [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

20   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 %.

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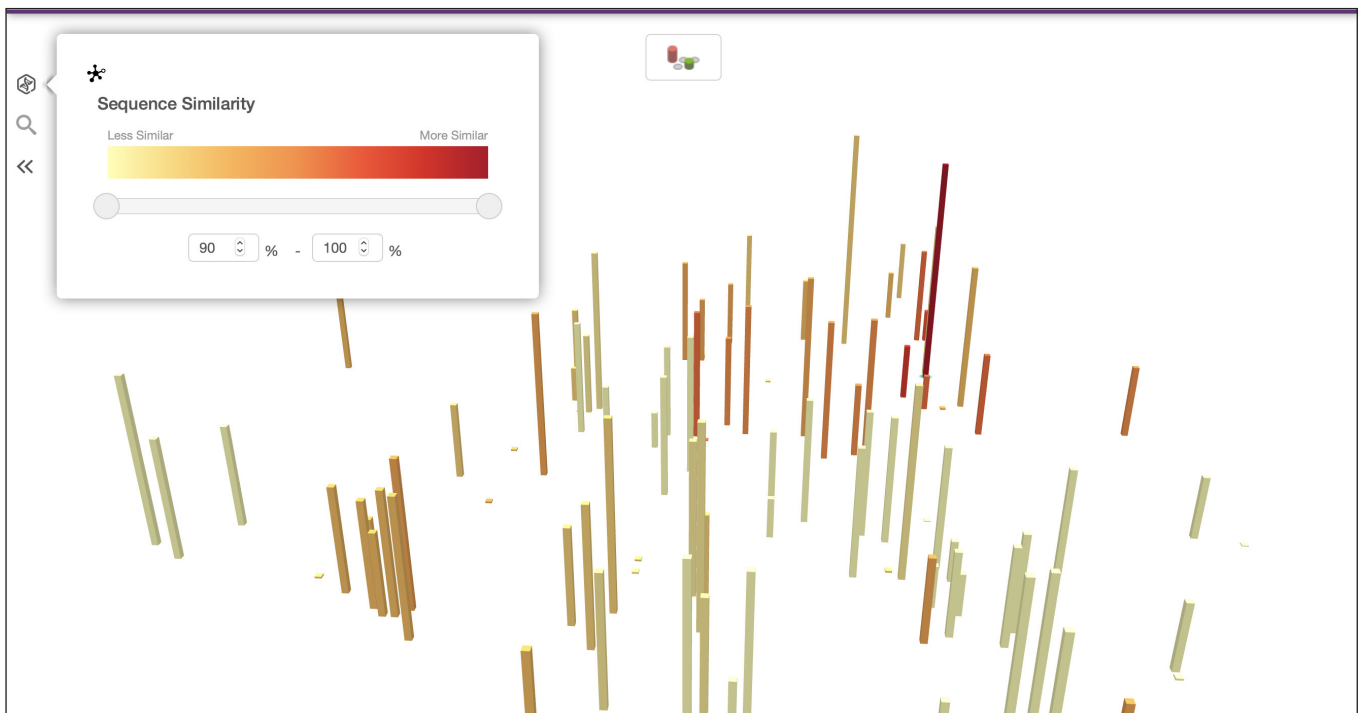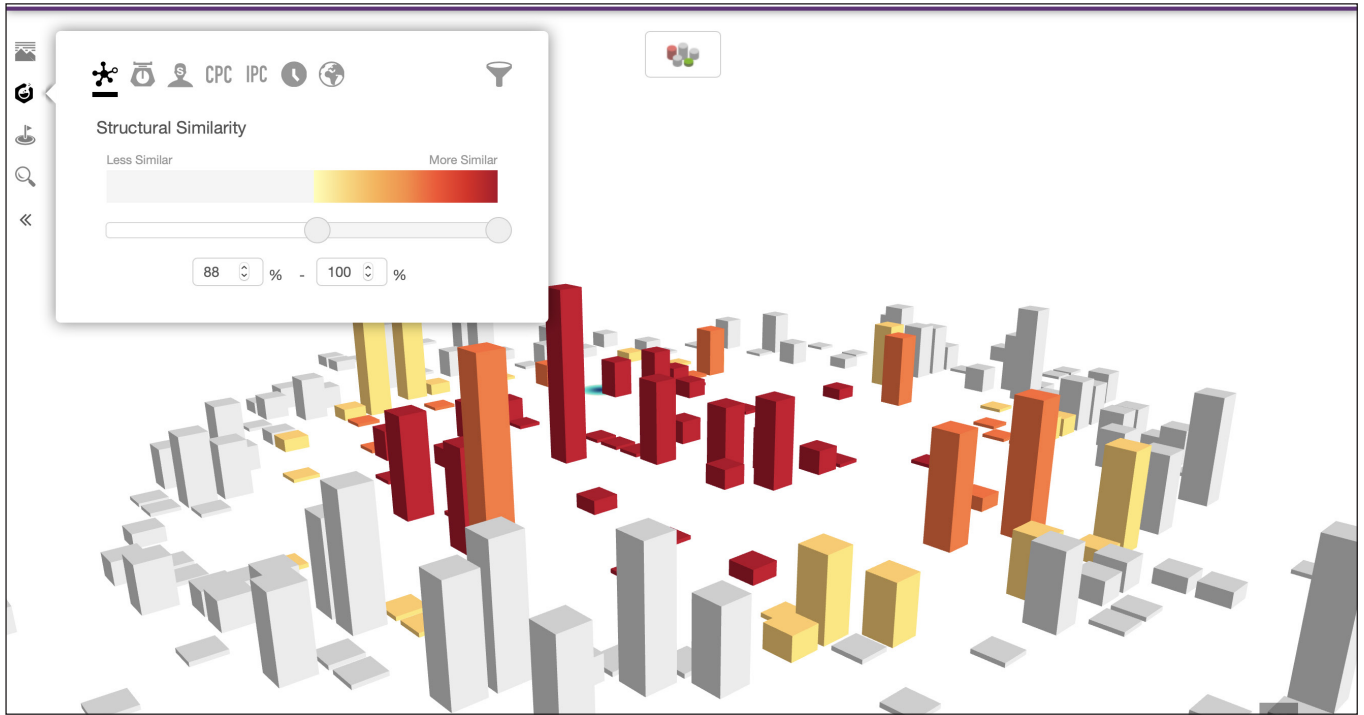
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Before heading to the lab, scientists from leading commercial, academic and government organizations worldwide turn to CAS SciFinder^n to develop their research plan. Integrated throughout CAS SciFinder^n, CAS Commercial Sources help those scientists 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.

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🛒 **Suppliers** (85)

Sort: Ships Within ▾

☐

⬇ ✉

Supplier	Substance	Details		Availability
1				
1PlusChem ⬡	1125-88-8	Purity		USD 40
1Pluschem Product List	Benzaldehyde Dimethyl Acetal	**95-98%**		Maintained in stock
United States		Quantity		Ships within 1 week
Updated Mar 31, 2021	Order Number: 1P0034Y6	100g ▾		**View Detail**
👁 👁				Order from Supplier ⬈
2				
A2B	1125-88-8	Purity		USD 14
A2B Chem Product List	Benzaldehyde dimethyl acetal	**95-98%**		Maintained in stock
United States		Quantity		Ships within 1 week
Updated Mar 22, 2021	Order Number: AB45582	100g ▾		**View Detail**
👁 👁				Order from Supplier ⬈
3				
aablocks	1125-88-8	Purity		USD 16
AA BLOCKS LLC Product List	Benzaldehyde dimethyl acetal	**95-98%**		Maintained in stock
	Order Number: AA0034FO	Quantity		Ships within 1 week

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)
☐ Kilograms or greater (27)

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🛒 **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
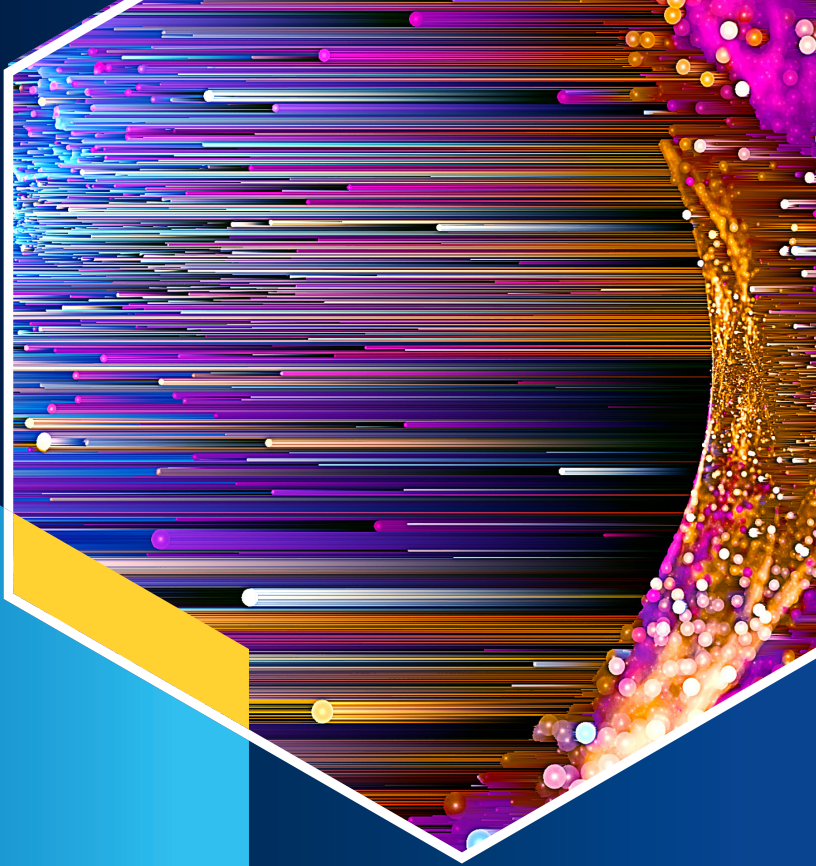
CAS Registry Number	1125-88-8
CAS Name	**Benzaldehyde dimethyl acetal**

Additional Contact Information

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💬 Feedback

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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.

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