

CAS SCIFINDER®

FOR ACADEMIA

# QUICK REFERENCE GUIDE

**CAS**



A division of the  
American Chemical Society

# Contents

3	<u>Solution Interface</u>
3-4	<u>References Search</u>
5-6	<u>Substances Search</u>
7	<u>Advanced Search</u>
8	<u>CAS Roles</u>
9	<u>CAS Lexicon</u>
10-11	<u>Search CAS Sequences</u>
12	<u>Bioactivity Data</u>
13-14	<u>Reactions Search</u>
15-18	<u>Retrosynthesis Planner</u>
19	<u>Markush</u>
19	<u>CAS PatentPak<sup>®</sup></u>
20	<u>Suppliers Search</u>
20	<u>ChemDoodle<sup>®</sup></u>
21	<u>Prior Art Analysis</u>
21	<u>Login, Feedback, Training, Support</u>

# Solution interface and References search

## Main interface

The options below are found on the main interface in CAS SciFinder.

Callouts for the main interface:

- Access CAS Formulus® and CAS Analytical Methods™
- Click the CAS logo to return to the main search page
- Access alerts
- Access account settings
- Combine saved sets
- Download
- Save answers, create alerts, add to project, and share results
- Save and Alert
- Add to Project
- Share Results
- Copy Search to Clipboard

## Search interface

CAS SciFinder features a streamlined search interface.

Callouts for the search interface:

- Enter the query
- Access user-specific content recommendations
- Access projects, saved items, history, downloads, and submit feedback
- Execute the search or press ENTER
- Access fielded search, available for substances and references
- Launch the structure editor

## References search results

Performing a References search provides you with access to a full result set in an easy-to-use interface where:

- References are default sorted by relevance with customizable sorting options.
- You can focus your answer set further using filters.
- You can save searches, send a link, set up alerts, or add results to a project list.
- You can quickly access full details for any of the references displayed.

Callouts for the references search results page:

- View indexed substances
- View indexed reactions
- Combine current with saved set
- Download answers
- Deselect applied filters
- Clear All Filters
- Sort answers
- Clear all filters
- Click title to open reference detail
- Change how answers are displayed
- Save or add to project
- Select Filter by or Exclude, then select filter categories
- Access full-text options
- Retrieve substance, reaction, or citation data for this reference
- Select filters to refine answers

# Reference detail and search operators

## Reference detail

Access full details for each reference found in CAS SciFinder.

### Fruit juice-containing **food** products with refreshing and cooling flavors

46 0 6 Citation Map View forward and backward citations Save

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder<sup>®</sup> users. [View content from CAS Formulus®](#) in this document. [Learn more about Formulus®](#).

In this Reference

By: Shimizu, Toru; Shigeta, Yoshinari; Kunieda, Satomi

- [IPC Data](#)
- [CAS Concepts](#)
- [Substances](#)
- [Formulations](#)
- [Cited Documents](#)

A fruit juice-containing **food** product contains, in addition to a fruit component and a sweet base, (a) one or more refreshing substances selected from the group consisting of **menthol**, menthone, camphor, pulegol, isopulegol, pulegone, cineol, mint oil, peppermint oil, spearmint oil, eucalyptus oil, and fractions thereof, and (b) one or more cool-tasting substances selected from the group consisting of 3-(l-menthoxy)propane-1,2-diol, N-ethyl-p-menthane-3-carboxamide, 3-(l-menthoxy)-2-methylpropane-1,2-diol, p-menthane-3,8-diol, 2-(l-menthoxy)ethan-1-ol, 3-(l-menthoxy)propan-1-ol, 4-(l-menthoxy)butan-1-ol, cyclic carboxamides, acyclic carboxamides, N,2,3-trimethyl-2-iso-Pr butanamide, a menthoxy alkanol (alkyl group having 2-6 carbons), a menthoxy alkyl ether (alkyl group having 1-6 carbons), and a menthoxy alkanediol (alkyl group having 3-6 carbons). Thus, an orange juice beverage may contain **menthol** as the refreshing component and 3-(1-menthoxy)-1,2-propanediol as the cool-tasting component.

Table of contents provides a quick overview and navigation to content

Keywords: fruit juice flavor **food** beverage **menthol**

PatentPak Viewer Get Prior Art Analysis Full Text

View bibliographic details

Patent Number	Publication Date	Application Number	Application Date	Kind Code
WO2005048743	2005-06-02	WO2004-JP17524	2004-11-18	A1

Assignee	Source	Database Information	Language
Takasago International Corporation, Japan	World Intellectual Property Organization	AN: 2005:470226 CAN: 143:25602	English

#### Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2005048743	English	A1	<a href="#">PDF</a>   <a href="#">PDF+</a>   <a href="#">Viewer</a>	2005-06-02	WO2004-JP17524	2004-11-18
JP2005143461	Undetermined	A				2003-11-19

PDF displays original patent PDF  
PDF+ displays the full text with a table of marked-up substances  
Viewer displays the interactive version of annotated full text

## Boolean operators

You can use logical operators to create precise text queries.

Use parentheses to group logical expressions, such as related terms using "OR", ex:

References (flavor **or** odor) **and** menthol **not** cigarette Draw

**AND** Requires both terms to be present within the document

**OR** Requires either one or both terms to be present (connect synonyms with OR)

**NOT** Excludes documents from an answer set containing the word(s) after NOT



Wildcards allow for more comprehensive results in reference, substance, and filter searches. Internal and right-hand truncation is possible.

\* Replaces 0 to any number of characters

ex: polymorph\* | immunoglobulin\*conjugate\*

? Replaces 0 or 1 character in reference searching

ex: benzonorbornen?

Phrases containing double quotes will be searched as a precise phrase.

Ex: a search for "Programmed cell death protein" only finds results that exactly match: "Programmed cell death protein".

# Substance name and structure search

## Substances search

You can search substances by placing one or more substance names or identifiers into the query box. You can also draw or edit a structure. Below are name search option examples.

**Streptomycin**

Finds Streptomycin record

**57-92-1**

Finds Streptomycin record, uses CAS Registry Number® as identifier

**Streptomycin sulfate**

Finds three records: Streptomycin, Streptomycin sulfate, and Sulfate

**"Streptomycin sulfate" Streptomycin**

Finds two records: Streptomycin sulfate and Streptomycin

**Sulfoximin\***

Finds all names that start with the stem Sulfoximin

**WO2019234160**

Finds all indexed substances for this patent

The screenshot shows the top navigation bar with tabs for All, Substances, Reactions, References, and Suppliers. The search bar contains the text "Enter chemical name query". Below the search bar are several search options: "Add Advanced Search Field", "Add advanced search fields" (with a sub-option for "Retrosynthetic Analysis"), "Search CAS Lexicon", "Search CAS Sequences", and "Search Patent Markush". A "Click to draw new structure" button is located in the top right corner. A "Click query structure to edit" button is positioned above a simple sulfur atom structure. A "Check to perform Markush search" checkbox is at the bottom right.

## Substances search results

Substances search results are displayed in an intuitive interface where you will see the most relevant results for your search, including critical property information and high-resolution structure images.

The screenshot displays the search results interface. On the left, there are filters for "Structure Match" (As Drawn, Substructure, Similarity), "Analyze Structure Precision", "Chemscape Analysis", and "Filter Behavior". The main results area shows a list of substances with their CAS numbers and chemical structures. A detailed view of a substance is shown on the right, including its CAS number (149104-88-1), name ([4-(Methylsulfonyl)phenyl]boronic acid), and a list of related data (Substance Details, Bioactivity Data, Reactions, Synthesize, Retrosynthetic Analysis, References, Suppliers). A "Retrieve data related to substance" dropdown menu is visible. A "Search a (sub)structure within this set of substances" button is also present. The detailed view includes a chemical structure and buttons for "Open editor with this structure" and "Download .sdf or .mol. Copy Smiles to Clipboard".

# Substance detail and structure editor

## Substance details

When you click a CAS Registry Number for one of your Substances search results, substance details including structure, molecular formula, properties, and further data are displayed.

CAS Registry Number: 90357-06-5

4,364 233 116

**Molecular formula in hill order**: C<sub>18</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>4</sub>S

**Systematic name**: Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI, ACI)

**GHS Hazard pictograms**, full list in tab at bottom of page

Key Physical Properties	Value	Condition
Molecular Weight	430.38	-
Melting Point (Experimental)	190-195 °C (decomp)	-
Boiling Point (Predicted)	650.3±55.0 °C	Press: 760 Torr
Density (Predicted)		

**Other Names**

- Experimental Properties
- Experimental Spectra

**Key properties**

**Chemical identifier list** contains SMILES, InChI, systematic, trivial, and trade names. Names are extracted from analyzed publications

Properties and spectra are either listed or available in linked source publications

Canonical SMILES: N#CC1=CC=C(C=C1C(F)(F)F)NC(=O)C(O)C(C)S(=O)(=O)C2=CC=C(F)C=C2

InChI: InChI=1S/C18H14F4N2O4S/c1-17(26,10-29(27,28)14-6-3-12(19)4-7-14)16(25)24-13-5-2-11(9-23)15(8-13)18(20,21)22/h2-8,26H,10H2,1H3,(H,24,25)

InChI Key: LKJYPSCBVHEWU-UHFFFAOYSA-N

9 Other Names for this Substance

- M-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide (ACI)
- Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-, (±) (ZCI)
- (±)-4'-Cyano-α,α-trifluoro-3-[(p-fluorophenyl)sulfonyl]-2-methyl-m-lactotoluidide
- Bicalutamide

## CAS Draw editor

You can define structure and reaction queries using the CAS Draw structure editor.

CAS Draw

Import and export structure files

Enter CAS Registry Number, SMILES, or InChI to create structure

Enter a CAS Registry Number, SMILES, or InChI...

Lasso | Marquee tool: Selects. Ctrl-click to select or deselect individual objects.

Learn about keyboard shortcuts (e.g., drawing hetero atoms easily)

Hetero atom and H isotope selection

Draw atoms and bonds | Eraser

Pick element symbol from periodic table | Shortcuts

Variable selection | Define own variables (R Groups)

Add attachment point to fragment | Select from templates

Add positive charge | Add negative charge

Repeating groups | Carbon chain tool

Define variable point of attachment at ring | Lock rings

Lock atoms | Rotate/Flip fragment

Reaction role | Atom mapping

Bond mapping | Draw reaction arrow

Draw bonds. ▲ indicate further options are available

Draw rings

Resize window

Type element symbol to draw

Zoom: 90%

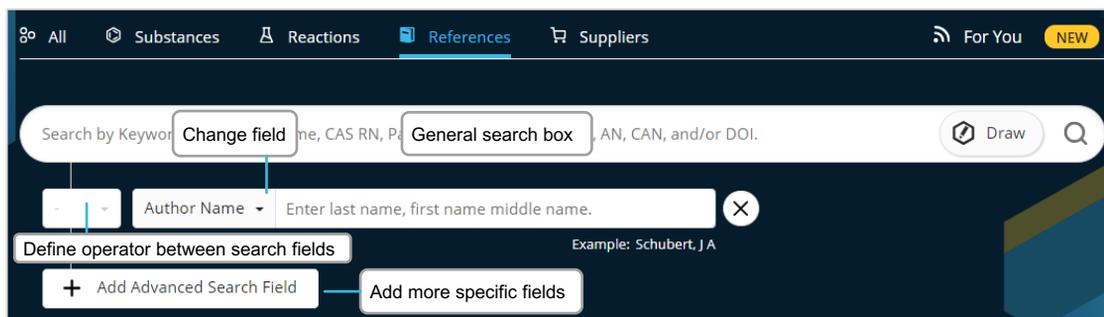
OK Cancel

# Advanced Search

## Performing an Advanced Search

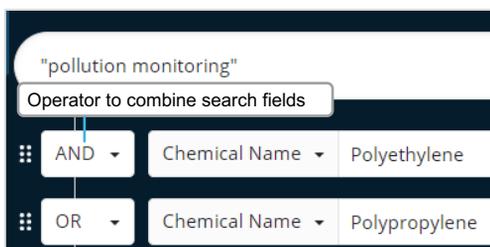
You can perform specific References and Substances searches using fields found on the main search page in CAS SciFinder.

- Operators are processed in this order: **OR, AND, NOT**
- Operators are not available for a search using a single advanced search field
- Wildcards are allowed, e.g., peek\*
- Use up to 50 Advanced Search fields (49 if also using the main search field)



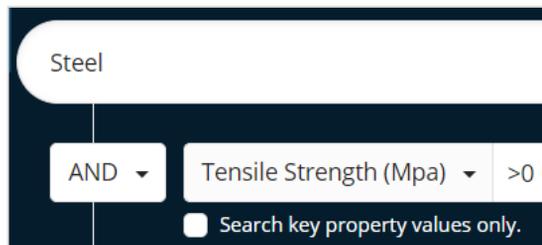
## Advanced Search examples

### Advanced References Search



Query interpretation:  
"pollution monitoring" and (polyethylene or polypropylene)

### Advanced Substances Search



Query interpretation:  
Steel with tensile strength property information



## Available Advanced Search fields

You can utilize many search fields and categories as part of an Advanced Search query, including:

### References Search

- Authors
- Publication Name
- Organization
- Title
- Abstract/Keywords
- Concept
- Substances
- Bioactivity Data
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

### Substances Search

- Molecular Formula
- CAS Registry Number
- Chemical Identifier
- Document Identifier
- Patent Identifier
- Experimental Spectra
- Bioactivity Data
- Biological
- Chemical Properties
- Density
- Electrical
- Lipinski
- Magnetic
- Mechanical
- Optical and Scattering
- Structure Related
- Thermal

# CAS Roles

## CAS Roles overview

Roles are linked to substances, allowing you to find focused publications connecting a substance of interest to its specific role within the scope of the publication.

- Super roles are broad categories and comprise all related specific roles. Examples are Analytical Study, Preparation, or Occurrence.
- Specific roles are more precise, relating to aspects such as the use of the substance in an analytical study as an analyte (Analyte) or the occurrence of a compound in an organism (Natural Product Occurrence).

## Roles in substance results

From a search on substance(s), the roles filter will indicate the types of roles that are connected to the substance(s) in the publications.

Reference Role

By Count | Alphanumeric

Example of 'reference roles' appearing in a substance answer set

Number of substance(s) in the answer set with that role

0 Selected

- Adverse Effect (15)
- Agricultural Use (29)
- Analyte (17)
- Diagnostic Use (3)
- Food or Feed Use (120)
- Formation, Non-preparative
- Pharmacological Activity (10)
- Physical, Engineering, or Chemical Process (888)

## Roles in reference results

Roles will appear as a filter in reference results whenever you have retrieved hits in the substance indexing segment of the records, i.e., by retrieving substance names or performing a crossover after substance-based searches.

**Example:** I am interested in the subject of (marine) pollution. How can I find publications where polypropylene is specifically described as a pollutant?

The search for polypropylene retrieves many references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 3,661 publications that describe polypropylene as a pollutant. The Search Within function or concepts can be used to restrict results to marine pollution.

Substances Polypropylene

9003-07-0

(C3H6)x  
Polypropylene

321K References | 7,909 Reactions | 27 Suppliers

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Substance Role

- Uses (268K)
- Properties (61K)
- Process (52K)
- Biological Study (23K)
- Preparation (19K)
- Pollutant (3,661)

View All

Language

456,514 Results

Sort: Relevance View: Full Abstract

1

Microstructure of polypropylene

By: Busico, Vincenzo; Cipullo, Roberto

Progress in Polymer Science (2001), 26(3), 443-533 | Language: English, Database: CPlus

A review, with 175 references, on catalyst technologies for manufacture of polypropylene with well-controlled microstructure and properties for advanced applications. The development of transition metal catalysts with tunable structure and selectivity is discussed. Polypropylene products with novel and well-controlled microstructure are described. The use of high-field <sup>13</sup>C NMR methods to study the stereochem. of polypropylene is also discussed.

Full Text

Substance (1) Reactions (0) Citing (385) Citation Map

After clicking "View All", more specific roles can be selected

Substance Role

By Count | Alphanumeric

1 Selected

- Uses (268K)
- Technical or Engineered Material Use (191K)
- Polymer in Formulation (81K)
- Properties (61K)
- Process (52K)
- Biological Use, Unclassified (3,793)
- Pollutant (3,661)
- Biological Study, Unclassified (2,558)
- Miscellaneous (2,444)

View All

Language

Publication Year

1974 to 2023

Microplastics in marine environment review of methods for identification and quantification

By: Hidalgo-Ruz, Valeria; Gutwirth, Lars; Thompson, Richard C.; The, Martin

Environmental Science & Technology (2012), 46(6), 3060-3075 | Language: English, Database: CPlus and MEDLINE

This review of 68 studies compares the methodologies used for the identification and quantification of microplastics from the marine environment. Three main sampling strategies were identified: selective, volume-reduced, and bulk sampling. Most sediment samples came from sandy beaches at the high tide line, and most seawater samples were taken at the sea surface using neuston nets. Four steps were distinguished during sample processing: separation, filtration, sieving, and visual sorting of microplastics. Visual sorting was one of the most commonly used methods for the identification of microplastics (using type, shape, degradation stage, and color as criteria). Chem. and phys. characteristics (e.g. specific  $\lambda$ ) were also used. The most reliable method to identify the chem. composition of microplastics is by IR spectroscopy. Most studies reported that plastic fragments were polyethylene and polypropylene polymers. Units commonly used for abundance estimates are "items per m<sup>3</sup>" for sediment and sea surface studies and "items per m<sup>3</sup>" for water column studies. Mesh size of sieves and filters used during sampling or sample processing influence abundance estimates. Most studies reported two main size ranges of microplastics: (i) 500  $\mu$ m - 5 mm, which are retained by a 500  $\mu$ m sieve/net, and (ii) 1-500  $\mu$ m, or fractions thereof that are retained on filters. We recommend that future programs of monitoring continue to distinguish these size fractions, but we suggest standardized sampling procedures which allow the spatiotemporal comparison of microplastic abundance across marine environments.

Full Text

Substances (3) Reactions (0) Citing (2,289) Citation Map

9003-53-6

Substances

Substances (3)

CAS RN Chemical Name Role

9003-53-6 Polypropylene

Every publication in this set of 3,661 references discusses polypropylene in the context of a pollutant

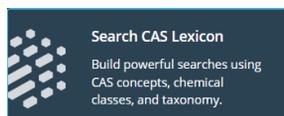
# CAS Lexicon

## CAS Lexicon overview

The CAS Lexicon is an ideal tool to understand CAS concept hierarchies, identify scientific expressions, gather relevant keyword synonyms for query building, or perform narrow and focused Lexicon searches.

The CAS Lexicon is an ontology of CAS Concepts. CAS Concepts are controlled terms describing the focus of a publication. They are added manually by CAS scientists, based on full-text analysis. The CAS Lexicon contains subject, chemical class, and taxonomic indexing terms in a hierarchy with broader and narrower terms. Concept indexing will be done on the highest level of detail possible, given the information present in the source document. Broader terms do not include more detailed concepts.

## Access and navigation



Start by clicking on 'CAS Lexicon' on the landing page, enter a concept or synonym and navigate through the hierarchy of broader and narrower terms. Only one hierarchy level is shown at a time.

Users can build highly specific CAS Lexicon search queries by selecting concepts and adding them to the query window on the right. Only the selected CAS Concepts will be searched.

Operators can be used to combine different concepts

Click 'Add to Query' to populate the pane on the right with selected terms

# Search CAS Sequences

## Search options

You can search sequences using three different modalities:

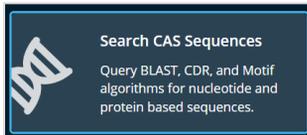
- BLAST: Search similar sequences
- CDR: Search antibodies and t-cell receptors via CDRs
- Motif: Search using variability symbols

## BLAST similarity search

BLAST allows you to search for similar nucleotide and amino acid sequences. Alignment results are shown in an intuitive graphical layout with easy-to-use precision filtering for identity and coverage percentages. Reference results are linked to the sequence hits.

To perform a BLAST search:

- Open the CAS Sequences module from the main CAS SciFinder search page.
- Load a sequence from a file or paste a sequence.
- Take advantage of supported formats: Sequences containing residues represented by single-letter codes (e.g., in the FASTA format). Leading numbers are not allowed.
- Note that sequence input may contain a header line (starting with >). Sequences can be separated by (multiple) headers, thus allowing for batch processing.
- Adjust BLAST parameters as desired and start the sequence search.



The screenshot shows the BLAST search interface with the following components and callouts:

- Sequence Search options:** A callout box pointing to the tabs for BLAST, CDR, and Motif.
- Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane:** A callout box pointing to the "Upload Sequence (.fasta or .txt)" button.
- Paste sequence into this window:** A callout box pointing to the text input area containing the sequence: `> human insulin sequence  
fvnqhlcghslveaylvcgerrgffytptktgiveqcctsicslyqlenycn`
- Include NCBI sequences:** A callout box pointing to the "Include NCBI Sequences" checkbox, which is checked.
- Advanced BLAST parameters:** A callout box pointing to the "Advanced Sequence Search" section, which includes:
  - Alignment Identity %: 100%
  - Match with Gaps?: No
  - Gap Costs: Existence 11 Extension 1
  - Query Coverage %: 90
  - Word Size: 3
  - Scoring Matrix: BLOSUM62
  - BLAST Algorithm: BLASTp
  - E-Value: 10
  - Exclude Low Complexity Regions: No

# BLAST results analysis

## Access results

Sequence search results appear in the Recent Search History and general Search History. Click 'View Results' to view sequence answers.

Sequences  
1:34 PM

Sequence Type: Protein  
Search Within: Proteins  
NCBI Included: Yes  
BLAST Algorithm: BLASTp  
Alignment Identity: -  
Query Coverage: 90%

> human insulin sequence  
fvnqhlcgshlveaylvcgergffytptktgiveqcctsiclslyqlenycn

View Results

Edit Search

Complete

Results will expire on  
Oct 31, 2023.

## View results

When viewing BLAST sequence similarity results:

- Alignments are sorted by Sequence Identity.
- Simplified graphical overview shows alignment quality.
- Mismatches are indicated by red lines.
- Detailed alignments can be viewed in the 'Alignment' tab.
- Subject details and patent previews are available in separate tabs.
- Click to retrieve related references.
- XLSX result download is available.

Sequences search for your query

References [Get references for all sequences](#)

92 Alignment Identity: 89.09%

Query 1 50 Query Length

Subject 1 55 Subject Length

Matches: 49  
Mismatches: 6

Alignment Length: 49+6=55 (includes a gap of 5 residues)

Alignment Details | Subject and links to NCBI and substance information in CAS SciFinder | Reference previews

Alignment | Subject | References

Alignment Data  
BLAST Score: 231  
E-Value: 5.12823e-26

Match

+ Mismatch: Query aa aligned to functionally equivalent subject aa

Get References for this sequence

Start residue of alignment in query and subject sequences

Gap in the query sequence

```
Q 1 FVNQHLCGSH LVEA-YLVCG ERGFFYTPKT ----GIVEQC CTSICSLYQL ENYCN 55
S 1 FVNQHLCGSH LVEALYLVCG ERGFFYTPK S DDARGIVEQC CTSICSLYQL ENYCN 55
```

## Filter results

Filtering dynamically changes your results.

E-Value: 0 to 10<sup>6</sup>

Query Coverage %: 0 to 100

Subject Coverage %: 0 to 100

Alignment Identity %: 0 to 100

Sequence Length: 26 to 9521

Organisms:  
 Homo sapiens (25)  
 Mus musculus (25)

# Bioactivity data

## Searching for targets, ligands, and diseases

The advanced search fields in Substances and References search allow you to find targets, ligands, and diseases with the according bioactivity data. This will search for substance and/or literature within the CAS Life Sciences accordion.

The first screenshot shows the 'Substances' search interface with a callout: 'Substances with bioactivity data are searched'. The second screenshot shows the 'References' search interface with a callout: 'Literature with bioactivity data is searched'. The third screenshot shows a search for 'Renin receptor ATP6IP2' with a callout: 'Enter a target'. A common callout across the screenshots states: 'Select target, ligand, or disease (further bioactivity search field can be added and combined)'. The 'Bioactivity Data' filter is expanded in all three, showing options for Target, Ligand, and Disease.

## Bioactivity data filter in reference and substance search

Two screenshots showing search results with bioactivity filters. The left screenshot shows a list of filters: Structure Activity Relationships (527), Absorption, Distribution, Metabolism, Excretion (110), and Toxicity (5). A callout says: 'Filter to refine by the availability of SAR, ADME, and Toxicity data'. The right screenshot shows a similar list of filters: Structure Activity Relationships (18K), Toxicity (1,566), and Absorption, Distribution, Metabolism, Excretion (1,259). A callout says: 'Filter to refine by the availability of SAR, ADME, and Toxicity data'. A chemical structure of a chiral amine is shown at the bottom right.

## Bioactivity data in Substance details

The screenshot shows the 'Structure Activity Relationships' section of a substance details page. It includes a table with columns: Target, Function, Parameter, Value, Disease, Organism, Assay, and Source. The first row shows: Target: 17-beta-hydroxysteroid dehydrogenase type 2, Function: Inhibitor, Parameter: Activity, Value: 111 %, Disease: -, Organism: HOMO SAPIENS, Assay: (1) CAS. A callout 'Filter functionality' points to the 'Filter' icon. A callout 'Visualization of target, ligand, and disease' points to the 'Knowledge Graph' icon. A callout 'Shows full assay details' points to a pop-up window showing assay information for Chloroquine (Ligand 54-05-7) targeting 17-beta-hydroxysteroid dehydrogenase type 2. The assay procedure is: 'Percent remaining activity of human 17-beta-hydroxysteroid dehydrogenase type 2 expressed in HEK 293 cells in presence of 50 nCi [2,4,6,7-3H]-ESTRADIOL and 500 uM NAD+ upon incubation with 20 uM compound in 20 mM Tris-HCl, pH 7.4 for 10 min at 37 degree C'. Other assay details include Condition: Temperature: 37 °C, Parameter: Activity, Value: 111 %, and Biological System: in vitro; HOMO SAPIENS; HEK 293; Human.

## Bioactivity data in Reference details

The screenshot shows the 'Structure Activity Relationships' section of a reference details page. It includes a table with columns: Ligand, Target, Function, Parameter, Value, Disease, Organism, and Assay. The first row shows: Ligand: 2460481-54-1, Target: Transforming growth factor-beta-induced protein ig-h3, Function: Binder, Parameter: Ka, Value: No interaction, Disease: Neoplasm, Organism: -, Assay: View Detail.

# Reactions search

## Performing a Reactions search

Reaction queries can be set up using CAS Reaction Numbers, substance names, CAS Registry Numbers, document identifiers, a chemical structure, or text-based reaction searching.

## Reactions search results

By default, reaction search results are grouped into schemes with identical reactants and products. A panel of filters, including yield and steps, allows for further refinement.

For single-step, single-stem reactions, you may view similar reactions based on the similarity of adjacent atoms to the specific reaction center.

- **Broad:** Retrieve reactions that share a reaction center with the selected reaction.
- **Medium:** Retrieve reactions that share a reaction center as well as adjacent atoms.
- **Narrow:** Retrieve reactions with a shared reaction center and extended atoms and bonds.

# Reaction details

## Reviewing Reaction details

The details of a reaction provide you with access to information including solvents, catalysts, reagents, conditions, and experimental protocols extracted from the publication and its supplement.

Get Similar Reactions [Search for similar reactions](#)

**Reaction Overview**  
Steps: 1 Yield: 85%

**Reaction reference**  
JOURNAL  
[Development of a Scalable Synthesis of an Azaindole-Pyrimidine Inhibitor of Influenza Virus Replication](#)  
By: Liang, Jiang [View all authors](#)  
View All [Organic Process Development](#) (2016), 20(5), 965-969  
[View Source](#) [Full Text](#)

Company/Organization  
Vertex Pharmaceuticals Incorporated  
Boston, Massachusetts 02210  
United States

**Step 1**

**Stage**    **Reagents**    **Catalysts**    **Solvents**    **Conditions**

1	<a href="#">Triethylamine</a> <a href="#">Diphenylphosphoryl azide</a>	-	<a href="#">Toluene</a>	2 h, reflux; reflux → 60 °C
2	-	-	-	overnight, 60 °C → 80 °C

[View alternatives](#) [Alternative Steps \(5\)](#)

**Experimental Protocols**  
[View detailed procedures](#)

**Products** [Ethyl \(1\*R\*,3\*S\*\)-3-\[\(benzyloxycarbonyl\)amino\]cyclohexanecarboxylate](#), Yield: 85%

**Reactants** [1-Ethyl \(1\*R\*,3\*S\*\)-1,3-cyclohexanedicarboxylate](#)  
[Benzyl alcohol](#)

**Reagents** [Triethylamine](#)  
[Diphenylphosphoryl azide](#)

**Solvents** [Toluene](#)

**Procedure** 1. Add diphenylphosphoryl azide (DPPA) (166 mL, 769 mmol) and triethylamine (107 mL, 769 mmol) to (1*S*, 3*R*)-3-ethoxycarbonylcyclohexanecarboxylic acid (140 g, 700 mmol) in toluene (1.4 L).

**Characterization Data** [View characterization data](#)

^ **Ethyl (1*R*,3*S*)-3-[(benzyloxycarbonyl)amino]cyclohexanecarboxylate**

<b>Proton NMR Spectrum</b>	(300 MHz, CDCl <sub>3</sub> ) δ 7.48-7.30 (m, 5H), 5.11 (s, 2H), 4.67 (s, 1H), 4.13 (q, J = 7.1 Hz, 2H), 3.55 (s, 1H), 2.42 (t, J = 11.8 Hz, 1H), 2.28 (d, J = 12.6 Hz, 1H), 2.10-1.79 (m, 3H), 1.50-1.19 (m, 6H), 1.19-1.00 (m, 1H).
<b>Optical Rotatory Power</b>	−33.3° (c = 1 in DCM).
<b>HRMS</b>	(ESI) [M + H] <sup>+</sup> calculated for C <sub>17</sub> H <sub>24</sub> NO <sub>4</sub> 306.1700, found 306.1700
<b>State</b>	sticky solid

CAS Method Number 3-451-CAS-15598720

**Transformations** [Overview of transformations](#)  
1. Schmidt Reaction

**Reaction Notes** [Further important notes](#)  
scalable

# Retrosynthesis planner

## Launching the tool

There are two primary ways to launch the 'Retrosynthetic Analysis' in CAS SciFinder:

1. Draw or import a structure into the retrosynthesis draw window accessed by clicking on the 'Retrosynthetic Analysis' option on the landing page. The drawn substance can be novel.
2. Click on the 'Start Retrosynthetic Analysis' option found on the substance flyout window.

The screenshot displays the CAS SciFinder interface. At the top, a navigation bar includes 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. A search bar prompts users to search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Below the search bar are three main action buttons: 'Retrosynthetic Analysis', 'Search CAS Lexicon', and 'Search CAS Sequences'. The 'Retrosynthetic Analysis' button is highlighted with a blue '1' and a red arrow. Below this, the 'Retrosynthetic Analysis' window is open, showing a chemical structure of a complex molecule. The window includes a toolbar, a text input field for CAS Registry Number, SMILES, or InChI, and a 'Start Retrosynthetic Analysis' button. The molecular formula is given as  $C_{15}H_{12}F_3N_3O_2S$  (355.34). To the right, a substance flyout window is open for CAS RN 2408121-76-4, displaying the CAS Name: 2-[Methoxy[5-[(trifluoromethyl)-1,2,4-oxadiazol-3-yl]-2-thienyl]methyl]-5-meth... and a list of actions: 'Get Substance Details', 'Get Bioactivity Data', 'Get Reactions (1)', 'Synthesize (1)', 'Start Retrosynthetic Analysis', 'Get References (1)', and 'Get Suppliers (0)'. The 'Synthesize (1)' option is highlighted with a blue '2'. A chemical structure of the target molecule is shown on the right, with a trifluoromethyl group highlighted in green. At the bottom of the flyout window are 'Edit Structure', 'Reset', and download icons.

# Retrosynthesis planner

## Selecting plan options

You can edit plan options to:

- Increase the synthetic depth.
- Protect bonds through the entire synthetic route.
- Define bonds to be broken in the first disconnection.
- Change the starting material cost limit.
- Create a predictive plan with more meaningful alternatives, e.g., poly or heterocyclic molecules.

Once you have selected the desired options, click the 'Create Retrosynthesis Plan' button.

**Retrosynthesis Plan Options for drawn structure** Powered by ChemPlanner®

**Select Synthetic Depth** [Learn more.](#)

1  
 2  
 3  
 4

**Break and Protect Bonds** [Learn more.](#)

Break Bond  Protect Bond [Clear All Bond Selections](#)

**Set Rules Supporting Predicted Reactions** [Learn more.](#)

Common  
 Uncommon (includes Common Rules)  
 Rare (includes Common and Uncommon Rules)

**Set Starting Materials Cost Limit** [Learn more.](#)

1000 USD/mol

Email me when my plan is complete

[Create Retrosynthesis Plan](#)

**Chemical Structure:** COC(=C1C=CC=C1)C2=CC=CC=C2C3=CC=CS3C4=CC=CC=C4C5=CC=CC=C5C6=CC=CC=C6C7=CC=CC=C7C8=CC=CC=C8C9=CC=CC=C9C10=CC=CC=C10C11=CC=CC=C11C12=CC=CC=C12C13=CC=CC=C13C14=CC=CC=C14C15=CC=CC=C15C16=CC=CC=C16C17=CC=CC=C17C18=CC=CC=C18C19=CC=CC=C19C20=CC=CC=C20C21=CC=CC=C21C22=CC=CC=C22C23=CC=CC=C23C24=CC=CC=C24C25=CC=CC=C25C26=CC=CC=C26C27=CC=CC=C27C28=CC=CC=C28C29=CC=CC=C29C30=CC=CC=C30C31=CC=CC=C31C32=CC=CC=C32C33=CC=CC=C33C34=CC=CC=C34C35=CC=CC=C35C36=CC=CC=C36C37=CC=CC=C37C38=CC=CC=C38C39=CC=CC=C39C40=CC=CC=C40C41=CC=CC=C41C42=CC=CC=C42C43=CC=CC=C43C44=CC=CC=C44C45=CC=CC=C45C46=CC=CC=C46C47=CC=CC=C47C48=CC=CC=C48C49=CC=CC=C49C50=CC=CC=C50C51=CC=CC=C51C52=CC=CC=C52C53=CC=CC=C53C54=CC=CC=C54C55=CC=CC=C55C56=CC=CC=C56C57=CC=CC=C57C58=CC=CC=C58C59=CC=CC=C59C60=CC=CC=C60C61=CC=CC=C61C62=CC=CC=C62C63=CC=CC=C63C64=CC=CC=C64C65=CC=CC=C65C66=CC=CC=C66C67=CC=CC=C67C68=CC=CC=C68C69=CC=CC=C69C70=CC=CC=C70C71=CC=CC=C71C72=CC=CC=C72C73=CC=CC=C73C74=CC=CC=C74C75=CC=CC=C75C76=CC=CC=C76C77=CC=CC=C77C78=CC=CC=C78C79=CC=CC=C79C80=CC=CC=C80C81=CC=CC=C81C82=CC=CC=C82C83=CC=CC=C83C84=CC=CC=C84C85=CC=CC=C85C86=CC=CC=C86C87=CC=CC=C87C88=CC=CC=C88C89=CC=CC=C89C90=CC=CC=C90C91=CC=CC=C91C92=CC=CC=C92C93=CC=CC=C93C94=CC=CC=C94C95=CC=CC=C95C96=CC=CC=C96C97=CC=CC=C97C98=CC=CC=C98C99=CC=CC=C99C100=CC=CC=C100

**Callouts:**

- Change the number of disconnections in the plan
- Break bond in first disconnection
- Protect bond(s) in entire plan
- Clear selections
- Select uncommon or rare rules supported by fewer literature examples
- Change upper cost limit for starting materials (USD/mol or USD/g)
- First bond to be broken
- Protected bonds
- Generate plan

# Retrosynthesis plan and alternative steps

## Open the plan

An Experimental plan is typically available within a few seconds. The calculation of a Predictive Retrosynthesis Plan can take longer.

Retrosynthesis Plan for drawn structure

View plan information

Plan Information

Estimated Yield: 22%  
Overall Price: \$48.62  
(USD per 100 grams)

Scoring Profiles

Complexity Reduction ●  
Convergence ●  
Evidence ●  
Cost ●  
Yield ●  
Atom Efficiency ●

Apply Reset Scoring

Experimental Steps Predicted Steps

Edit Plan Options

Exclude steps or substances

Download, Share, and Save your plan

Powered by ChemPlanner\*

View Excluded Options

Save

View plan steps

Show experimental steps

Switch predicted steps on/off

Blue lines mark experimental steps

Green dotted lines indicate predicted steps

Adjust scoring options

Review and select alternative disconnections

Max Yield 79%

Avg. Yield 59%

Max Yield 83%

Avg. Yield 47%

Avg. Yield 50%

Reset

Feedback

## Alternative steps

Get an overview of all experimental and predicted disconnections along with the evidence reactions displayed as a reaction answer set. You can access these evidence reactions from either the (1) link in the steps overview or (2) alternative reaction scheme.

Step Evidence

A → B + C 1.1 Reagents: Butyllithium  
Average Yield: 47%  
Evidence (16)  
Alternative Steps

B → D + E 1.1 Reagents: Potassium *tert*-butoxide  
Solvents: Tetrahydrofuran  
View All  
Average Yield: 59%  
Evidence (23)  
Alternative Steps (34)  
[Experimental Protocols](#) 1

C → F + G 1.1 Reagents: Diisopropylethylamine  
Ammonium chloride  
O-(7-Azabenzotriazol-1-yl)-N,N,N,N-tetramethyluronium hexafluoro phosphate  
Solvents: Dimethylformamide; 2 d, rt  
View All  
Average Yield: 50%  
Evidence (38)  
Alternative Steps (48)  
[Experimental Protocols](#)

D → H + I Predicted Step Only  
No reaction summary  
View All  
Maximum Yield: 79%  
Evidence (1)  
Alternative Steps (11)

E → J 1.1 Solvents: Carbon tetrachloride  
Maximum Yield: 83%  
Evidence (1)  
Alternative Steps (14)

Filter by

Alternative Step Type  
 Predicted (48)

Stereochemistry  
 Non-Selective (48)

5 of 15

Predicted Step

Select View 8 similar Alternatives 2 View Evidence Average Yield: 63%

Grouped similar reactions

Reactions from Retrosynthesis Plan Evidence

References

Filter Behavior Filter by Exclude

Search Within Results

Yield  
 90-100% (2)  
 80-89% (3)  
 70-79% (10)  
 50-69% (15)  
 30-49% (2)  
View All

Number of Steps  
 1 (55)

Non-Participating Functional Groups

55 Results Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction) Steps: 1

Suppliers (49) Suppliers (51) Suppliers (61)

31-614-CAS-29434160 Steps: 1

Preparation of piperidine-containing compounds for treating and preventing metabolic and cerebrovascular diseases

By: Rodriguez, Martha E.; et al  
World Intellectual Property Organization,  
WO2010080864 A1 2010-07-15

PatentPak Full Text

Evidence reactions for (predicted) disconnection of precursor C

# Retrosynthesis scoring options

## Scoring options

For plans with predicted steps, you may increase or decrease the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

- Each scoring profile may be set to Off (extreme left), Low, Medium, or High (extreme right).
- The default setting for each profile is 'Medium' as shown below.

## Scoring profiles

For plans with predicted steps, you may increase or reduce the score assigned to steps and alternatives by each profile, which determines what is displayed in the plan/alternative steps.

Each scoring profile may be set to **Off** (extreme left), **Low**, **Medium**, or **High** (extreme right); the default setting for each profile is "Medium," as shown below. Moving the slider all the way to the left turns that profile's scoring "Off," and it will not be a factor step selection or alternative ranking.

The screenshot shows a control panel for retrosynthesis scoring. It includes a 'Plan Information' section with 'Estimated Yield: 76%' and 'Overall Price: \$599.28 (USD per 100 grams)'. Below this is a 'Scoring Profiles' section with six sliders: Complexity Reduction, Convergence (set to Medium), Evidence, Cost, Yield, and Atom Efficiency. At the bottom of the sliders are two buttons: 'Apply' (highlighted with a green border) and 'Reset Scoring'.

### Complexity Reduction

Reduces the complexity of a step's reactants compared to its product.

**In retrosynthesis plans, you typically want high complexity reduction.**

### Convergence

Determines how "branched" the plan is; **you typically want the plan to be as branched as possible (high convergence)**, rather than linear.

For a given step, the more precursors there are, and the closer their relative sizes are, the more it's considered convergent.

**Increasing Convergence displays steps/alternatives with more reactants.**

### Evidence

Ranks plan steps/alternatives based on the number of evidence examples supporting the particular reaction type.

**More evidence examples for a step means that the reaction type has more applications and is more versatile in terms of conditions and substrates**, and hence predictions made based on it are probably more reliable.

**Increasing Evidence displays steps/alternatives with more supporting examples.**

### Cost

Weighs the expenses of the reactions by ranking starting materials based on the lowest price found amongst catalogs.

### Yield

Applies to the yield of each step in the plan, which contributes to the yield of the target molecule.

**Increasing the Yield displays a higher yield target molecule and steps/alternatives.**

### Atom Efficiency

Reduces reactant parts not included in a plan step's product.

**Increasing Atom Efficiency displays steps/alternatives with the least amount of reactant atoms that do not map to the product.**

Clicking the **Apply** button redraws the retrosynthesis plan with the revised scoring profiles; clicking **Reset Scoring** restores the "Medium" default.

A close-up view of the two buttons at the bottom of the scoring interface: a blue 'Apply' button with a white border and a light blue 'Reset Scoring' button.

# Markush search and CAS PatentPak

## Markush search

Markush structure searches can be performed using the 'Search Patent Markush' option while in Substances search mode.

The screenshot shows the CAS SciFinder interface for a Markush search. The search bar contains 'Enter a query...'. The main area displays a chemical structure with Markush symbols (G1-G4) and a search type of 'Markush structure search type'. The results panel shows 96 results, with 'As Drawn (96)' selected. A callout points to the 'Search Patent Markush' checkbox. Another callout points to the 'Markush location' dropdown menu. A third callout points to the 'Link to a specific patent reference' link. A fourth callout points to the 'Link to CAS PatentPak Viewer' link. A fifth callout points to the 'Assembled Markush hit structure' section. A sixth callout points to the 'Filter by patent authority' section.

## CAS PatentPak

There are three CAS PatentPak options for viewing a patent PDF:

- **PDF:** Full-text patent PDF only; text-searchable PDF
- **PDF+:** Full-text patent PDF with marked-up Key Substances; text-searchable PDF
- **Viewer:** Patent PDF with linked markups of Key Substances (see below)

The screenshot shows the CAS PatentPak interface for viewing a patent PDF. The interface includes a search bar, a drawing tool, and a results panel. Callouts highlight the 'Download PDF including list of marked-up substances and annotations' link. A callout points to the 'Marks key substance curated by CAS scientists' link. A callout points to the 'Link to related information' link. A callout points to the 'Highlighted key substance is marked' link. A callout points to the 'Link to location of substance in patent' link. The main area displays a chemical structure of a lithium secondary battery electrolyte with marked-up substances. The results panel shows a list of substances with their CAS RN and names. A callout points to the 'Li' substance in the list. A callout points to the 'Li+' substance in the list. A callout points to the 'Li+' substance in the list.

# Suppliers search and ChemDoodle

## Suppliers search

The Suppliers search allows you to directly access chemical catalog information based on chemical structure, names, or other identifiers.

The screenshot shows a search results page for the CAS number "7664-93-9". The interface includes a filter sidebar on the left, a main results table, and a detailed product view for the first result.

**Suppliers search for "7664-93-9"**

Filter Behavior: Filter by (selected), Exclude

490 Results

Sort options: Sort: Relevance

Supplier	Substance	Purity	Purchasing Det
1 Oakwood Chemical Product List United States Last Updated: 1 Mar 2024	7664-93-9 Sulfuric Acid, ACS Grade	95-98%	Order From Sup 100 ml, USD 25 1 L, USD 40.00 2.5 L, USD 80.00
2 Link to detail			
3			

**Oakwood Chemical Product List**

Preferred Supplier

Web: <https://www.oakwoodchemical.com>

Email: [sales@oakwoodchemical.com](mailto:sales@oakwoodchemical.com)

Phone: 1-800-467-3386

Item Details

Chemical Name: Sulfuric Acid, ACS Grade

Order Number: 25494

Purity: 98%

Quantity, Price: 100 ml, USD 25.00; 1 L, USD 40.00; 2.5 L, USD 80.00

Bulk Available

Stock Status: Maintained in stock

Pricing Information: 1 Mar 2024

Last Updated: 1 Mar 2024

Order From Supplier

Substance Information

CAS Registry Number: 7664-93-9

CAS Name: Sulfuric acid

O=S(=O)(O)O

## ChemDoodle

The ChemDoodle structure editor is available in addition to the standard CAS Draw editor. ChemDoodle is useful for mobile devices such as tablets.

The screenshot shows the ChemDoodle chemical structure editor interface. It features a toolbar with various drawing and editing tools, a central workspace with a chemical structure, and a sidebar with additional tools.

ChemDoodle

Model with CAS Registry Number

Clear | Eraser

Labeling

Undo | Redo

Templates

Draw bonds

Draw rings

Add charges

Chain tool

Repeating groups

Variable point of attachment

Lock atoms/chains/rings

Add attachment point to fragment

Make reaction

Reaction mapping

Break/form bonds

Zoom

Open | Save

Cc1ccc(cc1)C(=O)Nc2ccc(F)c(F)c2

# Prior Art Analysis

## Reviewing Prior Art

When viewing a patent reference detail page, an option to 'Get Prior Art Analysis' is available. Results will also appear in the search history. This is how it works:

- Provides an AI-based relevance prediction.
- Is based on a single patent document as the starting point.
- Includes analysis of CAS concepts, indexed substances, IPC codes, and additional full-text.
- Generates a list of relevance-ranked previously known documents, comprising patent and non-patent literature.

The screenshot displays the SciFinder interface for a patent reference. The title is "Aqueous dendritic amine coatings containing dendritic poly(amido)amine (PAMAM)". Below the title, there are icons for citation count (13), user count (0), likes (1), and a citation map. A "Get Prior Art Analysis" button is highlighted with a callout box that says "Initiate the analysis from the detailed record view". Below the reference details, there is a "References" section showing "Prior Art Analysis (195)" and a "View Results" button. A "View Results from the search history" button is also visible at the bottom right of the screenshot.

## Login, feedback, training, and support

### Login details

Log in at [scifinder-n.cas.org](https://scifinder-n.cas.org)

Use your existing CAS SciFinder username and password.

### Feedback button

Provide direct feedback to CAS from within the CAS SciFinder solution.

### Training

Upcoming events and webinars:

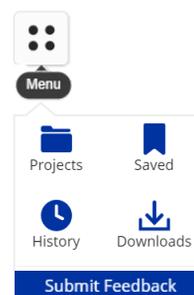
[www.cas.org/cas-webinars](https://www.cas.org/cas-webinars)

Recorded events and webinars:

[www.cas.org/cas-past-webinars](https://www.cas.org/cas-past-webinars)

CAS SciFinder training topics:

[www.cas.org/support/training/scifinder-n](https://www.cas.org/support/training/scifinder-n)



### Support contact

Email [help@cas.org](mailto:help@cas.org) to reach a CAS Customer Center representative in North America.

If you are outside of North America, see this website for regional contacts: <https://www.cas.org/contact>

CAS connects the world's scientific knowledge to accelerate breakthroughs that improve lives. We empower global innovators to efficiently navigate today's complex data landscape and make confident decisions in each phase of the innovation journey. As a specialist in scientific knowledge management, our team builds the largest authoritative collection of human-curated scientific data in the world and provides essential information solutions, services, and expertise. Scientists, patent professionals, and business leaders across industries rely on CAS to help them uncover opportunities, mitigate risks, and unlock shared knowledge so they can get from inspiration to innovation faster. CAS is a division of the American Chemical Society.

**Connect with us at [cas.org](https://cas.org)**

Solution images are included for illustrative purposes only. Your experience may vary based on recent enhancements or product license.

© 2024 American Chemical Society. All rights reserved.

SCIACDENGRF101245240414 - A4

