



SciFinder<sup>n</sup>

## Quick Reference Guide

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# Interface and Reference Search

**CAS SciFinder<sup>n</sup>**

- Saved**: Access saved searches, Alerts and Combine. Migrate SF-web assets
- History**: Open prior searches
- Account**: Open What's New, Settings Online Help or Log Out

Links to further CAS solutions, e.g. Analytical Methods, Formulus, or the STN IP Protection Suite

Click on the logo to go to the search landing page

## Search Interface SciFinder<sup>n</sup> features a streamlined search interface.

**Searching for...**

- All
- Substances**
- Reactions
- References
- Suppliers
- Biosequences

**Substances**

Enter the query

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

**Draw** **Q**

+ Add Advanced Search Field

Learn more about SciFinder<sup>n</sup> Advanced Search.

Access fielded search, available for substances and references

Launch the structure editor

Execute the search or press ENTER

## Reference Search The References display features visualizations, dynamic facets and an easy-to-use layout

- References are ranked and sorted by relevance
- You may save your searches, send a link or set-up alerts
- Filters allow you to focus the answers
- PatentPak shows the location of the indexed substances in the patent full-text

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 (116)
  - Patent (241)
  - Review (9)
- Substance Role
  - Biological Study (289)
  - Uses (206)
  - Process (39)
  - Analytical Study (33)
  - Properties (5)

**View indexed substances**

**View indexed reactions**

**View forward citations**

**Sort answers**

**Change how answers are displayed**

**Save results, set up alerts**

**Save**

**Download answers to file**

**Share answers**

**Clear All Filters**

**Clear all filters**

**Deselect applied filters**

**Click title to open reference detail**

**Check location of substances in patent full text**

**Access full-text options**

**Retrieve substance, reaction or citation data for this reference**

**Select filters to refine answers**

**Load further potentially relevant results for better comprehensiveness**

**First select Filter by or Exclude, then select filter categories**

**References** (360)

Sort: Relevance View: Partial Abstract

Filtering: Concept: Flavor X

Excluding: Concept: Antibacterial agents X

1

**Volatile release from**

By: Linforth, Rob; Taylor, Andrew  
Perfumer & Flavorist (1998), 23(3), 47-48, 50, 52-53 | Language: English, Database: CAplus

Instrumental anal. was used to monitor menthol and menthone in the breath of individuals eating a range of mint-flavored candies (including chewing gum). The data demonstrate the reproducibility of breath volatile anal. for assessing aroma release from mint-flavored products.

Full Text

Substances (2) Reactions (0) Cited By (19) Citation Map

2

**Confectionery composition including an elastomeric component, a cooked saccharide component, and a sensate**

By: Gebreselassie, Petros; Luo, Shih; John, Kabse; Kishor

2006-11-30 | Language: English, Database: CAplus

The present invention relates to a confectionery composition including cooked saccharide portion and an elastomeric material

PATENTPAK Full Text

Substances (48) Reactions (0) Cited By (6) Citation Map

# Reference detail and search

**Publication source information**

Patent

**Patent Information**

Patent Number  
US20140005234

Publication Date  
2014-01-02

Application Number  
US2013-13919035

Application Date  
2013-06-17

Kind Code  
A1

Assignee  
Unknown

Source  
United States

**Database Information**

AN: 2014:3851  
CAN: 160:144583  
Capius

Insecticidal N-substituted sulfilimine and **sulfoximine** pyridine N-oxides

By: Bland, Douglas C.; Ross, Ronald, Jr.; Johnson, Peter L.; Johnson, Timothy C.

**Abstract:** N-substituted sulfilimine and **sulfoximine** pyridine N-oxides were prepared according to the invention and their use in controlling insects and other invertebrates are provided. Further embodiments, forms, objects, features, advantages, aspects, and benefits shall become apparent from the description.

**Display of representative graphic**

**Access other full-text options**

PATENTPAK Viewer Full Text

**PDF displays original patent PDF  
PDF+ displays full-text with table of indexed substances  
Viewer displays interactive version of annotated full-text**

**Patent Family**

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
US20140005234	English	A1	PDF   PDF+   Viewer	2014-01-02	US2013-13919035	2013-06-17
		P			US2012-61666814P	2012-06-30
CA2876184	English	A1		2014-01-03	CA2013-2876184	2013-06-12
WO2014004086	English					

**Subject matter and substance indexing is added by CAS scientists**

Concepts

Substances

Citations

**View reference list of this document**

**Second line with priority details for initial provisional application**

**Substances**

Substances (31)

75-09-2 CH <sub>2</sub> Cl <sub>2</sub> Dichloromethane PatentPak: Role: Reactant, Reactant or Reagent	591-50-4 C <sub>6</sub> H <sub>5</sub> I Iodobenzene PatentPak: Role: Byproduct, Preparation	407-25-0 C <sub>6</sub> F <sub>5</sub> O <sub>2</sub> Trifluoroacetic anhydride PatentPak: Role: Reactant, Reactant or Reagent
420-04-2 CH <sub>3</sub> N <sub>2</sub> Cyanamide PatentPak: Role: Reagent, Reactant or Reagent	3240-34-4 C <sub>10</sub> H <sub>11</sub> O <sub>4</sub> Iodobenzene diacetate PatentPak: Role: Reactant, Reactant or Reagent	946578-00-3 C <sub>10</sub> H <sub>10</sub> F <sub>10</sub> N <sub>2</sub> O <sub>5</sub> Sulfonaflor PatentPak: Role: Reactant, Reactant or Reagent

## Boolean Operators Logical operators define precise text queries

Use parentheses to group logical expressions such as OR'ed synonyms, e.g.: (flavor or odor) and menthol

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

**OR** Requires either one or both concepts to be present  
Connect synonyms with OR

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



## Wildcards Wildcards allow for more comprehensive retrieval and more precision Use in reference and substance name searches

Internal and right-hand truncation is available

**\*** Replaces 0 to any number of characters E.g.: polymorph\* | immunoglobulin\*conjugate\*

**?** Replaces 0 or 1 character E.g.: benzonorbornen?

Terms masked with double quotes will be searched as a phrase, e.g.: "Programmed cell death protein"

# Substance name and structure

## Name searches

Search with one or more substance names or identifiers

Streptomycin

57-92-1

Streptomycin sulfate

"Streptomycin sulfate" Streptomycin

Sulfoximin\*

WO2019234160

Finds Streptomycin record

Finds Streptomycin record, uses CAS Registry number as identifier

Finds 3 records: Streptomycin, Streptomycin sulfate and Sulfate

Finds 2 records: Streptomycin sulfate and Streptomycin

Finds all names with the stem Sulfoximin

Finds all indexed substances for this patent

## Structure searches

Substance searches returns results in an intuitive layout. The display highlights most relevant hits, critical property information and high-resolution images

The screenshot displays the CAS SciFinder search results page. The top section shows the search criteria and options. Below, a list of substances is presented, each with a card containing its name, CAS number, chemical structure, and associated data (References, Reactions, Suppliers). Callouts provide instructions on how to interact with the interface, such as clicking on a structure to open details or using the ChemScape Analysis tool.

**Search Interface:**

- Searching for... Substances
- Enter a query...
- Click to draw new structure
- Click query structure to edit
- Checkmark to perform Markush search

**Structure Match Filters:**

- As Drawn (103)
- Substructure (5.2M)
- Similarity (529)
- Analyze Structure Precision

**Substance Cards:**

- 90357-06-5: Bicalutamide (C<sub>18</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>4</sub>S)
- 149104-88-1: Dapsone (C<sub>7</sub>H<sub>9</sub>BO<sub>4</sub>S)
- 80-08-0: Dapsone (C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>S)
- 73231-34-2: Florfenicol (C<sub>12</sub>H<sub>14</sub>Cl<sub>2</sub>FNO<sub>4</sub>S)

**ChemScape Analysis:**

- Visually explore structure similarity with a powerful new tool.
- Learn more about ChemScape.
- Create ChemScape Analysis
- Start ChemScape Analysis

**Filter Behavior:**

- Filter by Exclude
- Commercial Availability
- Reaction Role
- Reference Role
- Preparation (2.7M)
- Synthetic Preparation (2.6M)
- Uses (2.4M)
- Prophetic Synthesis or Use (2.4M)
- Biological Study (2.3M)

**Substance Details (Dapsone):**

- Retrieve data related to substance
- Substance Detail
- Reactions (3,877)
- Synthesize (102)
- Create Retrosynthesis Plan
- References (15K)
- Suppliers (112)
- Open editor with this structure
- Download .sdf or .mol. Copy Smiles to Clipboard

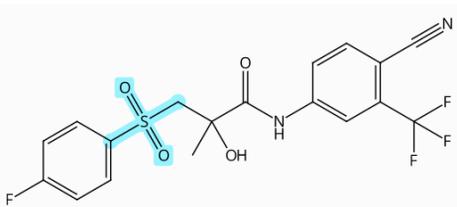
**Reference Roles (also called substance roles) encode the new information reported about a substance**

# Substance detail and structure editor

## Substance detail

Click on the CAS Registry number to show substance details with structure, molecular formula, properties and further data

CAS Registry Number  
90357-06-5



Molecular formula in hill order  
 $C_{18}H_{14}F_4N_2O_4S$

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

Key Physical Properties	Value	Condition
Molecular Weight	430.37	-
Melting Point (Experimental)	190-195 °C (decomp)	-
Boiling Point (Predicted)	650.3±55.0 °C	Press: 760 Torr
Density (Predicted)	1.52±0.1 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.49±0.29	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Other Names and Identifiers

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

9 Other Names for this Substance

- (±)-4'-Cyano- $\alpha,\alpha,\alpha$ -trifluoro-3-[p-fluorophenyl]propanamide
- Bicalutamid
- Casode
- Casodex

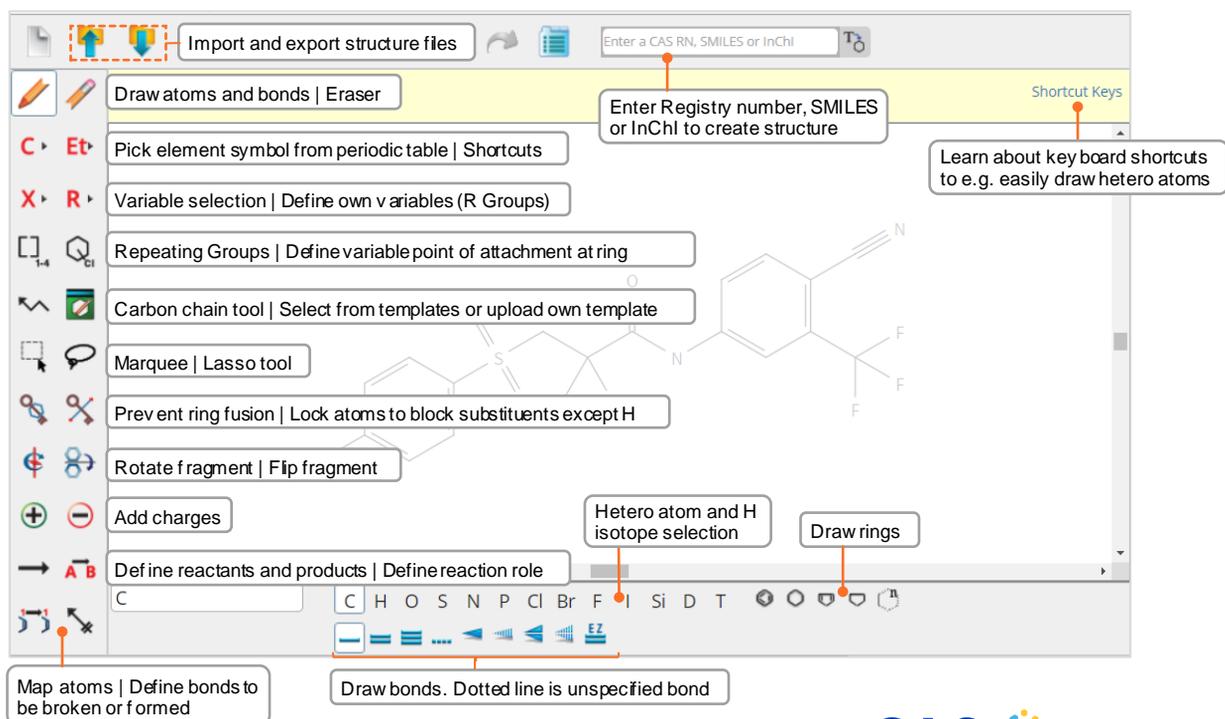
Properties are either listed or available in linked source publications

Chemical names listed comprise systematic, trivial and tradenames, as well as development codes. Names are extracted from analyzed publications.

Key properties

## CAS Draw editor

Define structure and reaction queries with the structure editor



Import and export structure files

Enter a CAS RN, SMILES or InChI

Shortcut Keys

Draw atoms and bonds | Eraser

Enter Registry number, SMILES or InChI to create structure

Pick element symbol from periodic table | Shortcuts

Learn about key board shortcuts to e.g. easily draw hetero atoms

Variable selection | Define own variables (R Groups)

Repeating Groups | Define variable point of attachment at ring

Carbon chain tool | Select from templates or upload own template

Marquee | Lasso tool

Prevent ring fusion | Lock atoms to block substituents except H

Rotate fragment | Flip fragment

Add charges

Define reactants and products | Define reaction role

Hetero atom and H isotope selection

Draw rings

Map atoms | Define bonds to be broken or formed

Draw bonds. Dotted line is unspecified bond

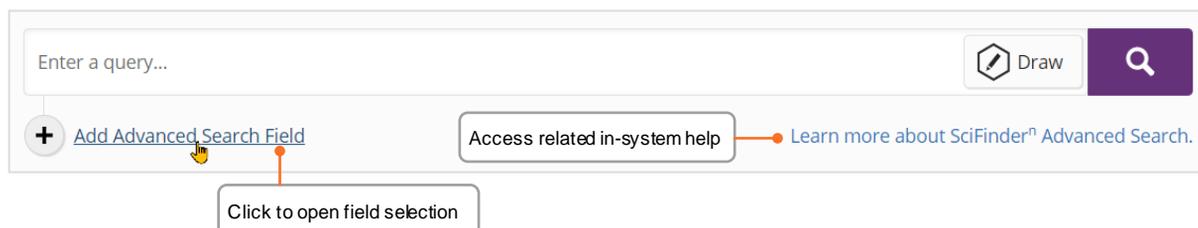
C H O S N P Cl Br F I Si D T

# Advanced search query builder

## Advanced Search Query Builder

Provides specific reference and substance search fields from SciFinder<sup>n</sup>'s landing page

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



## Examples

### Reference Search

Operator to combine search fields

"pollution monitoring"

AND Chemical Name polyethylene

OR Chemical Name polypropylene

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

### Substance Search

steel\*

AND Tensile Strength (Mpa) >0

Experimental values only.

Query interpretation:  
Steel with tensile strength property information

## Advanced Search Fields

The below advanced search fields are available

### Reference

- Author Name
- Journal Name
- Organization Name
- Title
- Concepts
- Substances
- Publication Year
- Document Identifier
- Patent Identifier

### Substance

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

# CAS Roles

## CAS Roles

Roles are linked to the substances and allow you to find focused publications connecting the 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. They relate to aspects such as the use of the substance in an analytical study as an analyte (Analyte) or the occurrence of a compound in a plant (Natural Product Occurrence)

## Roles in substance results

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

## Roles in reference results

Roles will appear as a filter in reference result sets whenever you have retrieved hits in the substance indexing segment of the records, i.e. by retrieving substance names or performing a crossover after structure-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 a large number of references. The substance role window shows all roles that apply to Polypropylene in this answer set. The **Pollutant** role indicates there are 1648 publications that describe polypropylene as a pollutant.

# Biosequence searching

## Development

Sequence searching is developed in stages. June 2021 status:

- BLAST: Search similar sequences **Implemented**
- CDR: Search antibodies via antigen binding sites **Implemented**
- Motif: Search conserved shorter sequence patterns **Implemented**
- Global crossover from sequences to patents **Implemented**

- Crossover from sequences to scientific literature In development

## BLAST similarity search

BLAST allows 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.

### Perform a BLAST search

- Open the Biosequences module from the main SciFinder<sup>®</sup> search page
- Load sequence from file or paste sequence
- Supported formats: Sequences containing residues represented by single-letter codes, e.g. in the FASTA format. Leading numbers are not allowed.
- Sequence input may contain header line (starting with >). Sequences can be separated by (multiple) headers, thus allowing for batch processing
- Adjust BLAST parameters as desired and start biosequence search

The screenshot displays the Biosequences search interface. On the left, a sidebar titled 'Searching for...' contains navigation buttons for 'All', 'Substances', 'Reactions', 'References', 'Suppliers', and 'Biosequences'. The main area is titled 'Biosequences' and includes a text input field for a protein or nucleotide string, with an 'Upload Sequence' button and a 'Clear Search' link. Below the input field, a sample sequence is shown: '> Human Insulin Sequence' followed by 'FVNQHLGSHLVEALYLVCGERGFFYTPKTKGIVEQCCTSIICSLYQLNENYCN'. Two callout boxes provide instructions: 'Paste sequence into this window' and 'Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane'. To the right, search options are set: 'Sequence Type' is 'Protein', 'Search Within' is 'Proteins', and 'Limit Total Sequence Results to:' is '20000'. A 'Start Biosequence Search' button is at the bottom right. Below the search form, the 'Advanced Biosequence Search' section is expanded, showing parameters: 'Sequence Identity %' is '-', 'Match with Gaps?' is 'No', 'Gap Costs' is 'Existence 11 Extension 1', 'Query Coverage %' is '90', 'Word Size' is '3', 'Scoring Matrix' is 'BLOSUM62', 'BLAST Algorithm' is 'BLASTp', 'E-Value' is '10', and 'Exclude Low Complexity Regions' is 'No'. A callout box on the left points to this section, labeled 'Advanced BLAST parameters'.



# Reaction searching

**Reaction searches** Reactions queries can be substance names, CAS Registry Numbers, document identifiers, or a chemical structure

- Reactions are grouped into schemes with identical reactants and products
- Reactions are sorted by yield within a scheme
- Find reactions by substance name, registry number, document identifier or chemical structure

**Searching for...**

- All
- Substances
- Reactions**
- References
- Suppliers
- Biosequences

**Reactions**

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query... Edit Q

Select reactions

Click on reaction query to edit

Edit Drawing Remove

Create Retrosynthesis Plan

**View by structure match**

Structure Match

- As Drawn (0)
- Substructure (198)**
- Similarity (1,758)

**Filter Behavior**

- Filter by
- Exclude

**Yield**

- 90-100% (13)
- 80-89% (16)
- 70-79% (29)
- 50-69% (23)
- 30-49% (12)

[View All](#)

**Number of Steps**

- 1 (198)

**Non-Participating Functional Groups**

- Carbamate (55)
- Ketone (47)
- Cyclic ketone (46)
- Halide (45)
- Carboxylic ester (25)

[View All](#)

**Reaction Mapping**

- Mapping Data Available (177)

**Filter reaction results**

**View all reaction summaries of the scheme**

**View substance information**

**View reaction reference**

**View suppliers**

**View reaction detail**

**Yield for displayed reactions**

**Scheme 10 (4 Reactions)**

Relative stereochemistry shown

Suppliers (94)

Suppliers (86)

Steps: 1  
Yield: 67%

Reaction Summary	Reagents	Steps	Yield	Reference
<input type="checkbox"/>	Triethylamine Diphenylphosphoryl azide Water	1	67%	<b>Preparation of quinoline-3-carboxamides as H-PGDS inhibitors</b> By: Cadilla, Rodolfo; et al World Intellectual Property Organization, WO2017103851 A1 2017-06-22 <a href="#">PATENTPAK</a> <a href="#">Full Text</a>
<input type="checkbox"/>	Triethylamine Diphenylphosphoryl azide Water	1	67%	<b>Preparation of 1,3-disubstituted cyclobutane or azetidine derivatives as hematopoietic prostaglandin D synthase (H-PGDS) inhibitors</b> By: Deaton, David Norman; et al World Intellectual Property Organization, WO2018069863 A1 2018-04-19 <a href="#">PATENTPAK</a> <a href="#">Full Text</a>

[View Reaction Detail](#)

[View All 4 Reactions](#)

[Collapse Scheme](#)

# Reaction details

## Reaction details

Details incl. solvents, catalysts, reagents, conditions and experimental protocols extracted from the publication and its supplement

Absolute stereochemistry shown. Rotation (+)

[Stage 2]

Absolute stereochemistry shown. Rotation (-)

85%

Suppliers (38)

Suppliers (126)

Supplier (1)

Steps: 1

Yield: 85%

**Reaction reference**

Reference

Development of a Scalable Synthesis of an Azaindoly-Pyrimidine Inhibitor of Influenza Virus Replication

By: Liang, Jianglin; et al  
View All

Organic Process Research & Development (2016), 20(5), 965-969

**View all authors**

Full Text

**Step 1**

[View alternative steps](#) Alternative Steps (5)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Triethylamine Diphenylphosphoryl azide	-	Toluene	2 h, reflux; reflux → 60 °C
2	-	-	-	overnight, 60 °C → 80 °C

CAS Reaction Number: 31-451-CAS-15598720

## Experimental Protocols

### MethodsNow™

View experimental protocols, including detailed procedures

Products	Ethyl (1R,3S)-3-[(benzyloxycarbonyl)amino]cyclohexanecarboxylate, Yield: 85%
Reactants	1,3-Cyclohexanedicarboxylic acid, 1-ethyl ester, (1R,3S)- Benzyl alcohol
Reagents	Triethylamine Diphenylphosphoryl azide
Solvents	Toluene
Procedure	<ol style="list-style-type: none"><li>1. Add diphenylphosphoryl azide (DPPA) (166 mL, 769 mmol) and triethylamine (107 mL, 769 mmol) to (1S, 3R) -3-ethoxycarbonylcyclohexanecarboxylic acid (140 g, 700 mmol) in toluene (1.4 L).</li><li>2. Reflux the mixture for 2 h under N<sub>2</sub>.</li><li>3. Cool the reaction mixture to 60°C and add benzyl alcohol (87 mL, 839 mmol) in one portion.</li><li>4. Heat the mixture to 80°C overnight.</li><li>5. Stir the mixture and separate the layers.</li></ol>

### Characterization Data

View characterization data

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

Proton NMR Spectrum	(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).
Optical Rotatory Power	=-33.3° (c = 1 in DCM).
HRMS	(ESI) [M + H] <sup>+</sup> calculated for C <sub>17</sub> H <sub>24</sub> NO <sub>4</sub> 306.1700, found 306.1700
State	sticky solid

# Retrosynthesis planner

## Launch plan generation

There are two options to launch SciFinder<sup>n</sup>'s Retrosynthesis Planner

- 1 Draw reaction structure and create plan from Edit icon
- 2 Open structure flyout window and start plan generation

Make sure *Reactions* is selected

Click "Create Retrosynthesis Plan" to open plan options and generate the plan

1 Create Retrosynthesis Plan

CAS RN  
2408121-76-4  
CAS Name  
Pyridine, 2-[methoxy[5-(5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl)-2-thienyl]meth...

Substance Detail

Reactions (1)

Synthesize (1)

2 Create Retrosynthesis Plan

References (1)

Suppliers (0)

Edit Structure - Reset +

## Plan options

Edit plan options to...

- increase the synthetic depth
- protect bonds through the entire synthetic route
- define bonds to be broken in the first disconnection
- create a plan with more meaningful alternatives, e.g. for poly- or heterocyclic molecules

Change number of disconnections in the plan

Plan Options

Powered by ChemPlanner<sup>®</sup>

Select Synthetic Depth

Synthetic depth restricts the number of steps generated in the plan. [Learn More.](#)

1  
 2  
 3  
 4

1 2 3

Break and Protect Bonds

You may select one bond to break in the first step of the plan. Any bonds you protect will not break, though their order may change. [Learn More.](#)

Break Bond  Protect Bond Clear All Bond Selections

Break bond in first disconnection

Protect bond in entire plan

Clear selections

Set Rules Supporting Predicted Reactions

Common rules are supported by many literature examples. Uncommon and Rare rules are supported by fewer examples, but may expose novel approaches. [Learn More.](#)

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

Select uncommon or rare rules supported by fewer literature examples

1st bond to be broken

Protected bonds

Create Retrosynthesis Plan  Email me when my Retrosynthesis Plan is Complete

Generate plan

# Retrosynthesis plan and alternative steps

## Open plan

The Experimental Plan is available within a few seconds, the calculation of the Predictive Retrosynthesis Plan will take a bit longer

**Retrosynthesis** Powered by ChemPlanner®

Overview Steps Predicted Results **ON** Switch predicted steps on/off Download, Save and Share your plan

Plan Information  
Estimated Yield: 16%  
Overall Price: \$161.72 (USD per 100 grams)  
Commercially Available: E, F, G, H, I

Plan Options  
Synthetic Depth: 3  
Predicted Rules: Common  
Break & Protect Bonds: Yes  
Edit Plan Options

Scoring Profiles  
Adjust Scoring Options  
Complexity Reduction  
Convergence  
Evidence  
Cost  
Yield

Retrosynthesis Step Key  
Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.  
Experimental Steps  
Predicted Steps

View Plan Steps  
View plan information  
Green dotted lines indicate predicted steps  
Purple lines mark experimental steps, i.e. those reported in the literature  
Review alternative disconnections

## Alternative steps

Provide an overview of all experimental and predicted disconnections  
Evidence reactions are displayed as a reaction answer set

- Access Evidence Reactions from the 1 link in the steps overview or 2 the alternative reaction scheme

Overview Steps Predicted

View step specific evidence and alternate steps below or select the node between steps on the plan.

**A → B + C**  
Average Yield: 47%  
Evidence (14)  
Alternative Steps

**B → D + E**  
Average Yield: 53%  
Evidence (77)  
Alternative Steps (39)

**C → F + G**  
Average Yield: 66%  
Evidence (2,347)  
Alternative Steps (45)

Alternative Steps (45)  
Filter by  
Alternative Step Type  
Predicted (45)  
Stereochemistry  
Non-Selective (45)  
Number of Steps  
Non-Participating Functional Groups  
Experimental Protocols  
Synthetic Methods (1,344)  
Experimental Procedure (513)

**Reactions (1,663)**  
Evidence reactions for (predicted) disconnection of C  
Filtering: Experimental Protocols: 2 Selected  
Scheme 1 (1 Reaction) Steps: 1 Yield: 92%  
Scheme 2 (1 Reaction) Steps: 1 Yield: 89%

Select alternative - the plan will be reorganized  
Select  
Predicted Step  
Evidence (46)  
Average Yield: 67%

# Scoring Options

## Scoring Options

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

Overview Steps Scoring

Scoring Profiles

Complexity Reduction

Convergence  Medium

Evidence

Yield

Atom Efficiency

Apply 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.**

**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.

Apply Reset Scoring

# Markush Searching and PatentPak

## Markush searching

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

The screenshot shows the CAS SciFinder interface with the following annotations:

- Markush search type:** Points to the 'Patent Markush Match' section, specifically the 'As Drawn (96)' and 'Substructure (119)' buttons.
- Filter by first patent authority:** Points to the 'Filter Behavior' section, specifically the 'Filter by' button and the 'Patent Office' list (World Intellectual Property Organization, United States, European Patent Organization, China, United Kingdom).
- Markush search option:** Points to the 'Search Patent Markush' checkbox in the 'References' section.
- Markush location:** Points to the 'Patent claim 2' dropdown menu.
- Link to PatentPak Viewer:** Points to the 'PATENTPAK' dropdown menu.
- Link to a specific patent reference:** Points to the patent number 'WO2002017896'.

## PatentPak

Up to three 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 PatentPak Viewer interface with the following annotations:

- Display controls:** Points to the 'PAGE 12 / 15', 'ZOOM', and 'DOWNLOAD PDF' buttons.
- Download PDF including chemistry annotations:** Points to the 'PDF+' button.
- Link to location of substance in patent:** Points to the 'Analyst Markup Locations (1)' link.
- Key substances identified in the patent are annotated:** Points to the 'Key Substances in Patent' section.
- Link to related information:** Points to the 'Substance Detail' sidebar.
- Highlighted key substance is marked:** Points to the highlighted chemical structure of Lithium trifluoromethanesulfonate.
- Marks key substance curated by CAS scientists:** Points to the 'Li' marker in the chemical structure.

# Supplier Searching and ChemDoodle®

## Suppliers searching

Suppliers searching allows for direct access to chemical catalog information based on chemical structure, names or other identifiers

The screenshot displays the 'Suppliers' search results page. On the left, a 'Filter Behavior' panel allows filtering by 'Preferred Suppliers' and 'Purity'. The main table lists suppliers with columns for 'Supplier', 'Substance', 'Purity', and 'Purchasing Details'. A callout box labeled 'Preferred/non-preferred supplier tagging' points to a supplier icon. A 'Link to detail' callout points to a supplier entry. A 'Supplier Detail' pop-up window shows information for 'TCI Europe Research Chemicals', including contact details, item details for 'Hydrogen Peroxide (35% in Water)', and a chemical structure HO-OH. Callouts in the pop-up identify 'Preferred/non-preferred supplier tagging', 'Contact information', 'Catalog details', and 'Order link'.

## ChemDoodle®

ChemDoodle structure editor is available in addition to the standard CASdraw editor. ChemDoodle is useful for tablets and mobile devices.

The screenshot shows the ChemDoodle structure editor interface. A toolbar at the top includes 'Center', 'Flip fragment', and 'Cut | Copy | Paste'. A 'ChemDoodle' menu is open, listing tools such as 'Clear | Eraser', 'Labeling', 'Draw bonds', 'Draw rings', 'Add charges', 'Chain tool', 'Repeating groups', 'Variable point of attachment', 'Lock atoms/chains/rings', 'Make reaction', 'Reaction mapping', and 'Break/form bonds'. Other callouts point to 'Undo | Redo', 'Templates', 'Open | Save', and 'Zoom'. A chemical structure is visible in the background.

# Login, Feedback and Support

## Login Details

- Login at <http://scifinder-n.cas.org>
- Use your existing SciFinder username and password

## Feedback Button

Provide direct feedback to CAS



Feedback

## Learn More

SciFinder<sup>n</sup> Training Topics:

<https://www.cas.org/support/training/scifinder-n>

Upcoming and recorded SciFinder<sup>n</sup> webinars:

<https://www.cas.org/about/events/scifinder-webinars>

## Contact Customer Support

Email [help@cas.org](mailto:help@cas.org) to speak with a CAS Customer Center representative

## CAS Contacts

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[help@cas.org](mailto:help@cas.org)