



SciFinderⁿ

Quick Reference Guide

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- 3-4 Substance Search and Structure Editor
- 5 Advanced Search Query Builder
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- 7-8 Biosequence Search
- 9-10 Reaction Search
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- 14 Markush Search and PatentPak
- 15 Supplier Search and ChemDoodle
- 16 Login, Feedback and Support

Interface and Reference Search

CAS SciFinder[®] Saved History Account

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

Search Interface SciFinder[®] 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](#) [Search](#)

+ Add Advanced Search Field [Learn more about SciFinder[®] 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](#)

References (360)

Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Download answers to file Save results, set up alerts

Filtering: Concept: Flavor X Deselect applied filters Share answers Clear All Filters

Excluding: Concept: Antibacterial agents X Clear all filters

View indexed substances View indexed reactions View forward citations Sort answers Change how answers are displayed

1 **Volatile release from** Click title to open reference detail

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

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: Gabrzelasica, Petros; Luo, Shih-John; Kabse, Kishor
2006-11-30 | Language: English, Database: CAPIus

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

Retrieve substance, reaction or citation data for this reference

Check location of substances in patent full text Access full-text options

Load further potentially relevant results for better comprehensiveness

First select Filter by or Exclude, then select filter categories

Select filters to refine answers

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: 160-144582
CAplus

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

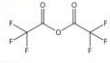
View reference list of this document


Substances


Substances (31)

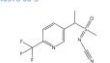
75-09-2
Cl-CH2-CH2-Cl
Dichloromethane
Reagent

991-59-4

Iodobenzene
Reagent

407-25-0

Trifluoroacetic anhydride
Reagent

420-04-2

Cyanamide
Reagent

3240-34-4

Iodobenzene diacetate
Reagent

946578-00-3

Sulfosulfur
Reagent

Second line with priority details for initial provisional application

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.: benzonorboren?

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

Searching for...

- All
- Substances**
- Reactions
- Biosequences

Substances

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

Enter a query... [Add Advanced Search Field](#)

Click to draw new structure

Click query structure to edit

Checkmark to perform Markush search

Structure Match

- As Drawn (103)
- Substructure (5.2M)**
- Similarity (529)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. [Learn more about Chemscape.](#)

Create 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)

Start Chemscape Analysis

Substances (5,267,645)

Change sort criterion Sort: Number of Suppliers View: Partial

References Reactions Suppliers Save

1 **90357-06-5**

149104-88-1

Click Registry Number to open details

Change amount of details displayed

Click on structure to open flyout window

Retrieve data related to substance

Open editor with this structure

Download .sdf or .mol. Copy Smiles to Clipboard

2 **80-08-0**

C₁₈H₁₄F₄N₂O₄S
Bicalutamide

3,624 References 214 Reactions 129 Suppliers

C₇H₉BO₄S
CAS RN 80-08-0
CAS Name Dapsone

2 Suppliers

4 **73231-34-2**

1,227 References **2,321** Reactions **103** Suppliers

C₁₂H₁₄Cl₂FNO₄S
Florfenicol

3,736 References 721 Reactions 112 Suppliers

576 References 1,217 Reactions 108 Suppliers

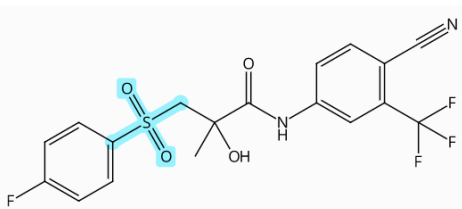
Reference Roles (also called substance roles) encode the new information reported about a substance

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
 $C_{18}H_{14}F_4N_2O_4S$

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

| 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 ³ | Temp: 20 °C; Press: 760 Torr |
| pKa (Predicted) | 11.49±0.29 | Most Acidic Temp: 25 °C |

Experimental Properties | Spectra

Key properties

Other Names

Experimental Properties

Properties are either listed or available in linked source publications

Other Names and Identifiers

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

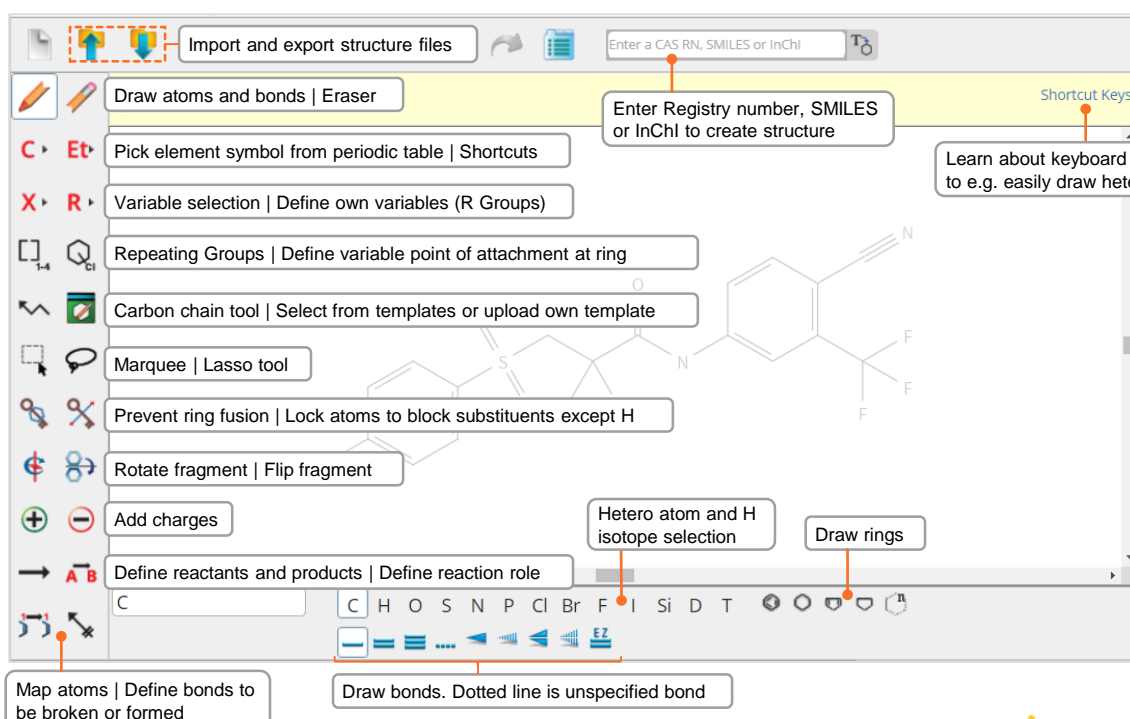
9 Other Names for this Substance

(±)-4'-Cyano- α,α,α -trifluoro-3-[(p-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide
Bicalutamide
Casode
Casodex

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

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 keyboard 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

Hetero atom and H isotope selection

Draw rings

Define reactants and products | Define reaction role

Map atoms | Define bonds to be broken or formed

Draw bonds. Dotted line is unspecified bond

Advanced search query builder

Advanced Search Query Builder

Provides specific reference and substance search fields from SciFinderⁿ'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)

Enter a query... Draw

+ Add Advanced Search Field Access related in-system help Learn more about SciFinderⁿ Advanced Search.

Click to open field selection

Examples

Reference Search

"pollution monitoring"

AND Chemical Name polyethylene

OR Chemical Name polypropylene

Operator to combine search fields

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

References Edit Search "pollution monitoring"

Click 'Edit Search' to modify the Advanced Search

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.

Reference Role

By Count **Alphanumeric**

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

Substance(s) in the answer set with that role.

- Analytical matrix (1)
- Analytical Reagent Use (1)
- Analytical Role, Unclassified (1)
- Formation, Unclassified (1)
- Geological or Astronomical Occurrence (1)

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.

Substances polypropylene

9003-07-0

CC(C)C

(C₃H₆)
Polypropylene

278K References | 6,321 Reactions | 20 Suppliers

Filter by

- Document Type
- Substance Role
 - Uses (231K)
 - Properties (55K)
 - Process (43K)
 - Biological Study (19K)
 - Preparation (17K)
 - Pollutant (1,657)

View All

References (278,226)

Sort: Publication Date: Newest | View: F

Substances Reactions Cited By

1

Water recovery by treatment of food industry wastewater using membrane processes

By: Hernandez, Karina; Muro, Claudia; Ortega, Rosa Elena; Velazquez, Sarai; Riera, Francisco

Environmental Technology (2021), 42(5), 775-788 | Language: English, Database: CAPlus and MEDLINE

View Abstract

Full Text

Substances (6) Reactions (0) Cited By (0)

Substance Role

By Count **Alphanumeric**

1 Selected

- Uses (231K)
- Technical or Engineered Material Use (161K)
- Polymer in Formulation (68K)
- Properties (55K)
- Process (43K)
- Biological Use, Unclassified (3,100)
- Miscellaneous (2,377)
- Occurrence (2,053)
- Biological Study, Unclassified (1,909)
- Pollutant (1,657)

After clicking 'View All', specific roles can be selected

References (1,657)

Substances Reactions Cited By

1

Wastewater treatment alters microbial colonization

By: Kelly, John J.; London, Maxwell G.; McCormick, Amanda R.; Rojas, M

PLoS One (2021), 16(1), e0244443 | Language: English, Database: CAPlus

View Abstract

Full Text

Substances (3)

Every publication in this set of 1,657 references discusses polypropylene in the context of 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 SciFinderⁿ 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...' lists various search categories, with 'Biosequences' selected. The main area is titled 'Biosequences' and contains a search form. The form includes a text input field for the sequence, an 'Upload Sequence' button, and a 'Clear Search' button. Below the input field, there are two callout boxes: one for 'Paste sequence into this window' and another for 'Upload FASTA sequence from file w/o preceding numbers or paste into the BLAST pane'. The search form also includes a 'Sequence Type' dropdown (set to 'Protein') and a 'Search Within' dropdown (set to 'Proteins'). A 'Limit Total Sequence Results to:' dropdown is set to '20000'. A 'Start Biosequence Search' button is located at the bottom right of the search form. Below the search form, there is an 'Advanced Biosequence Search' section with various parameters: 'Sequence Identity %' (set to '-'), 'Match with Gaps?' (set to 'No'), 'Gap Costs' (set to 'Existence 11 Extension 1'), 'Query Coverage %' (set to '90'), 'Word Size' (set to '3'), 'Scoring Matrix' (set to 'BLOSUM62'), 'BLAST Algorithm' (set to 'BLASTp'), 'E-Value' (set to '10'), and 'Exclude Low Complexity Regions' (set to 'No'). A callout box labeled 'Advanced BLAST parameters' points to this section.

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

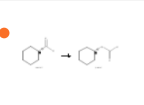
Reactions

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)

View all reaction summaries of the scheme

View substance information

View suppliers

View reaction reference

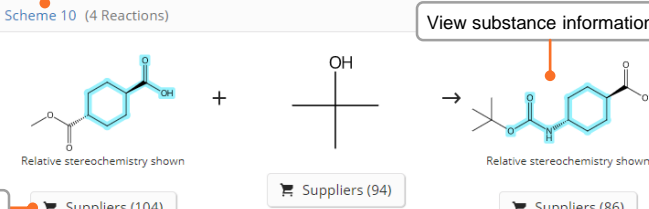
View reaction detail

View substance information

Yield for displayed reactions

Filter reaction results

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

[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%

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

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](#)

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

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).
2. Reflux the mixture for 2 h under N₂.
3. Cool the reaction mixture to 60°C and add benzyl alcohol (87 mL, 839 mmol) in one portion.
4. Heat the mixture to 80°C overnight.

6. Stir the mixture and separate the layers.

Characterization Data [View characterization data](#)

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

Proton NMR Spectrum (300 MHz, CDCl₃) 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]⁺ calculated for C₁₇H₂₄NO₄ 306.1700, found 306.1700

State sticky solid

Retrosynthesis planner

Launch plan generation

There are two options to launch SciFinderⁿ'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

2 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[®]

Select Synthetic Depth

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

1
2
3
4

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

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 View Plan Steps View 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

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) ①
Alternative Steps (45)

Alternative Steps (45)

Filter by

- Alternative Step Type
 - Predicted (45)
- Stereochemistry
 - Non-Selective (45)

Filter Behavior Filter by Exclude

Yield

- 90-100% (266)
- 80-89% (271)
- 70-79% (291)
- 50-69% (456)
- 30-49% (228)

Number of Steps

- 1 (1,663)

Non-Participating Functional Groups

- Alkene (609)
- Cyclic alkene (603)
- Diene (335)
- Ether (324)
- Halide (286)

Experimental Protocols

- Synthetic Methods (1,344)
- Experimental Procedure (513)

Reactions (1,663)

Filtering: Experimental Protocols: 2 Selected

Evidence reactions for (predicted) disconnection of C

Scheme 1 (1 Reaction) Steps: 1 Yield: 92%

Decarboxylative Cross-Coupling of Azoyl Carboxylic Acids with Aryl Halides

1.1 Reagents: Silver carbonate
Catalysts: Triphenylphosphine, Palladium chloride
Solvents: Toluene, Dimethylacetamide; 16 h, 135 °C

By: Zhang, Fengzhi; et al
Organic Letters (2010), 12(21), 4745-4747

View Reaction Detail Experimental Protocols Full Text

Scheme 2 (1 Reaction) Steps: 1 Yield: 89%

Select alternative - the plan will be reorganized

Select Predicted Step Evidence (46) Average Yield: 67%

3 of 45

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

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 in Substances search mode. On the left, there are filters for 'Markush search type' (As Drawn (96), Substructure (119)) and 'Filter by first patent authority' (World Intellectual Property Organization (55), United States (25), European Patent Organization (8), China (3), United Kingdom (2)). The main area displays 'Patent Markush (96)' results. A callout box highlights the 'Search Patent Markush' checkbox and the 'Markush search option' label. Another callout points to the 'PATENTPAK' dropdown menu, labeled 'Markush location'. A third callout points to a specific patent entry, labeled 'Link to a specific patent reference'. A fourth callout points to the 'PATENTPAK Viewer' link, labeled 'Link to PatentPak Viewer'.

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. At the top, there are controls for 'Display controls', 'Download PDF', and 'Download PDF including chemistry annotations'. The main content area displays patent text with chemical structures and annotations. A callout box points to a chemical structure, labeled 'Link to location of substance in patent'. Another callout points to a highlighted key substance, labeled 'Highlighted key substance is marked'. A third callout points to a key substance, labeled 'Marks key substance curated by CAS scientists'. A fourth callout points to a list of key substances, labeled 'Key substances identified in the patent are annotated'. The interface also shows a sidebar with 'Key Substances in Patent' and a 'Substance Detail' panel with various options like 'Reactions (1,784)', 'Synthesize (94)', 'Create Retrosynthesis Plan', 'References (7,297)', and 'Suppliers (82)'. A 'Link to related information' callout points to the 'Li' key substance.

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, there is a 'Filter Behavior' panel with options to 'Filter by' or 'Exclude'. Below this, there are sections for 'Preferred Suppliers' (with a 'No Preference (12)' option), 'Supplier' (listing various catalogs like Hayashi Pure Chemical, abcr GmbH, etc.), 'Purity' (95-98% (2), <90% (1)), and 'Quantity' (Grams (8), Kilograms or greater (2)). The main area shows a list of 12 suppliers, with the first one being TCI Europe Research Chemicals. A callout box labeled 'Preferred/non-preferred supplier tagging' points to a radio button next to the supplier name. A 'Link to detail' callout points to the supplier's name. A 'Sort options' dropdown menu is open, showing options like 'Relevance', 'Supplier: A to Z', 'Supplier: Z to A', 'Ships Within', and 'Purity'. The 'Supplier Detail' view for TCI Europe Research Chemicals is shown, featuring 'Preferred/non-preferred supplier tagging' and 'Contact information' (web, email, phone). It also includes 'Catalog details' (chemical name, order number, quantity, price, stock status, ships within) and an '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. At the top, there are menu options: 'Center', 'Flip fragment', and 'Cut | Copy | Paste'. Below these is a toolbar with various drawing tools. A callout box labeled 'ChemDoodle' points to the toolbar. Other callouts include 'Lasso', 'Clear | Eraser', 'Labeling', 'Undo | Redo', 'Templates', 'Open | Save', 'Zoom', and 'Model with CAS Registry Number'. The main area displays a chemical structure of a complex organic molecule. At the bottom, there are 'OK' and 'Cancel' buttons.

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



Learn More

SciFinderⁿ Training Topics:

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

Upcoming and recorded SciFinderⁿ webinars:

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

Contact Customer Support

Email help@cas.org to speak with a CAS Customer Center representative