



SCIFINDERⁿ

A CAS SOLUTION

Quick Reference Guide

- 1-2 Interface and Reference search
- 3-4 Substance search and structure editor
- 5-6 Reaction search
- 7-8 Retrosynthesis Planner
- 9 Markush search and PatentPak
- 10 Suppliers search and ChemDoodle[®]
- 11 Login and Support

Interface and Reference Search

Click on the logo to go to the home page

Access saved searches, Alerts and Combine. *Migrate SF-web assets*

Access prior searches

Open What's New, MyCASProfile (i.e. Settings) and Online Help

Search Interface

SciFinderⁿ features a streamlined search interface.

Search

Enter the query

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use [Advanced Search](#) for Author, Journal, or Organization

Company or author name searches; Access advanced substance search options

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 by default
- 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

Load additional results for comprehensiveness

View indexed substances

View indexed reactions

View forward citations

Sort answers

Change how answers are displayed

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 by

Document Type

- ☐ Journal (138)
- ☐ Patent (143)
- ☐ Review (18)
- ☐ Conference (1)
- ☐ Dissertation (1)

Substance Role

- ☐ Adverse Effect (1)
- ☐ Analytical Study (1)
- ☐ Biological Study (102)
- ☐ Preparation (33)
- ☐ Process (1)

[View All](#)

Select filters to refine answers

References (282)

Sort: Relevance View: Partial Abstract

Substances Reactions Cited By

Download answers to file

Save results and set up alerts

Share answers by link

Click title to open reference detail

Access full-text options

View patent full text with chemistry annotation and location

Retrieve substance, reaction or citation data for this reference

3-Triazolyphenyl-substituted sulfide derivatives as acaricides and insecticides and their preparation

By: Alig, Bernd; Antons, Steffen; Voerste, Arnd; Goergens, Ulrich
World Intellectual Property Organization, WO2011020567 A1 2011-02-24 | Language: German, Database: CPlus

The invention relates to 3-triazolyphenyl-substituted sulfide derivatives of formula I, to their use as acaricides and insecticides for the control of animal pests and to methods for producing the same. Compounds of formula I wherein X is N and CA⁰ is H, halo, CN, alkyl, alkoxy, etc.; A¹ is CF₃ when X is N; A¹ is H, alkyl, haloalkyl, alkoxyalkyl, etc., when X is CA⁰; A² is H; B⁰ is H, amino, halo, CN, NO₂, etc.; B¹, B², and B³ are independently H, halo, CN, NO₂, alkyl, etc.; n is 0, 1 and 2; R¹ is H and alkyl; R² is CHF₂, CF₂Cl, CF₂Br, CH₂Cl etc.; are claimed. Example compound II was prepared...

View More

PATENTPAK Full Text Substances (653) Reactions (75) Cited By (5) Citation Map

Reference Detail and Search Operators

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: 160-144592

CAPLUS

Subject matter and substance indexing is added by CAS scientists

☒ Concepts
☒ Substances
☒ Citations

View reference list of this document

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.

Chemical structure of a pyridine N-oxide derivative, showing a pyridine ring with an N-oxide group (=O) and a trifluoromethyl group (CF₃) at the 3-position, and a sulfoximine group (-N(SMe)₂) at the 4-position.

Access 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

Substances

Substances (31)

75-09-2

CH₂Cl₂
Dichloromethane
PatentPak:
Role: Reactant, Reactant or Reagent

591-50-4

C₆H₅I
Iodobenzene
PatentPak:
Role: Reagent, Preparation

407-25-0

C₆F₁₂O₄
Trifluoroacetic anhydride
PatentPak:
Role: Reactant, Reactant or Reagent

420-54-2

CH₂N₂
Cyanamide
PatentPak:
Role: Reagent, Reactant or Reagent

3240-34-4

C₁₀H₉IO₄
Iodobenzene diacetate
PatentPak:
Role: Reactant, Reactant or Reagent

946578-00-3

C₁₀H₁₀F₂N₂O₅
Sulfaxalor
PatentPak:
Role: Reactant, Reactant or Reagent

Boolean Operators

Logical operators are available to define precise text queries

Use parentheses to group logical expressions such as OR'ed synonyms, e.g.:
(fungicide OR pesticide) AND strobilurin

AND Requires both words, phrases, or concepts to be present within the document



OR Requires either one or both words, phrases, or concepts to be present
Connect synonyms with OR



NOT Excludes documents from an answer set. Be careful when using the NOT operator, you cannot always assess the context of document texts



Wildcards, Masking Wildcards and masking allow for more comprehensive retrieval and more precision respectively | 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.: 1,?-hexanediol

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

Substance Name and Structure Searching

Name searches

Search with one or more substance names, identifiers, and document ID

Vanillin
57-92-1
Vanillin stearate
"Vanillin stearate" Vanillin
Vanillin*
WO2019020773

Finds Vanillin record
Finds Vanillin record, uses CAS Registry number as identifier
Finds 3 records: Vanillin, Vanillin stearate and Stearate
Finds 2 records: Vanillin stearate and Vanillin
Finds all names that start with the term Vanillin
Finds all indexed substances for this patent

Structure searches

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

The screenshot illustrates the SciFinder search workflow. At the top, the 'Search' bar allows users to enter a query by substance name, CAS RN, or patent number. Callouts highlight the 'Enter query' field, the 'Advanced Search' link for molecular formulas and properties, and the 'Click to draw new structure' button. Below the search bar, a 'Substances' results page is shown, sorted by 'Number of Suppliers'. Callouts point to the 'Structure Match' filter (with options like 'As Drawn', 'Substructure', and 'Similarity'), the 'Identify tautomers or specific bond configurations' link, and the 'Commercial Availability' and 'Reaction Role' filters. The main results area displays three substance cards. Callouts indicate how to 'Click Registry Number to open details', 'Click on structure to open flyout window', and 'Retrieve data related to substance'. A detailed flyout window for Dapsone (CAS 80-08-0) is shown, listing substance details, reactions, synthesis, references, and suppliers. Callouts also point to the 'Open editor with this structure' button and the 'Download .sdf, .mol, .cxf, .png' options.

Search

Search by Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use [Advanced Search](#) for Molecular Formula, Substance Property, or Experimental Spectra

Click to draw new structure

Click query structure to edit

Access advanced substance search options: molecular formulas, properties and spectra line values

Checkmark to perform Markush search

Select type of structure match

Change sort criterion

Change amount of details displayed

Substances (4,303,959)

Sort: Number of Suppliers View Partial

Structure Match

As Drawn (102)

Substructure (4.3M)

Similarity (519)

Analyze Structure Precision

Identify tautomers or specific bond configurations

Commercial Availability

Available (1.5M)

Not Available (2.7M)

Reaction Role

Product (588K)

Reactant (140K)

Reagent (394)

Catalyst (396)

Solvent (46)

Reference Role

Adverse Effect (4,438)

Analytical Study (8,123)

Biological Study (1.6M)

Combinatorial Study (2,775)

Formation (2,623)

View All

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

90357-06-5

C18H14F4N2O4S

Bicalutamide

3,844 References 202 Reactions 125 Suppliers

149104-88-1

C7H9BO4S

[4-(Methylsulfonyl)phenyl]boronic acid

Click Registry Number to open details

373384-18-0

C7H9BO4S

(3-Methylsulfonylphenyl)boronic acid

Expands the answer to full view for that specific result

80-08-0

C12H12N2

Dapsone

Click on structure to open flyout window

Retrieve data related to substance

Substance Detail

Reactions (3,151)

Synthesize (87)

Create Retrosynthesis Plan

References (14K)

Suppliers (107)

Open editor with this structure

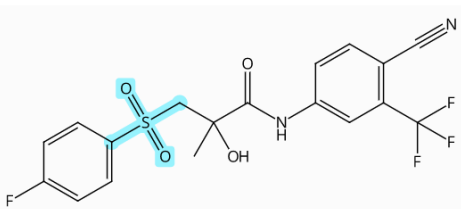
Download .sdf, .mol, .cxf, .png

Substance Detail and Structure editor

Substance detail

Click on the image 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

9 Other Names for this Substance

- (±)-4'-Cyano-α,α,α-trifluoro-3-[(p-fluorophenyl)sulfonyl]-2-methyl-m-lactotulidide
- Bicalutamide
- Casode
- Casodex
- Cosudex
- ICI 176334

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

Other Names

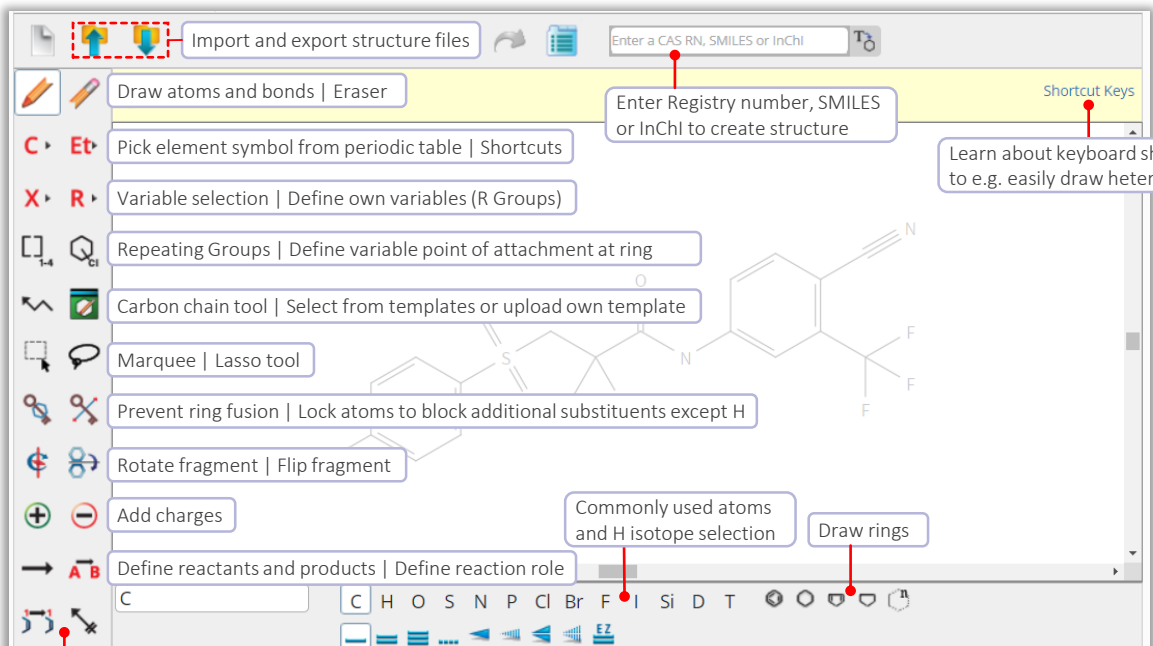
Experimental Properties

Properties are either listed or available in linked source 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

Pick element symbol from periodic table | Shortcuts

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 additional substituents except H

Rotate fragment | Flip fragment

Add charges

Define reactants and products | Define reaction role

Commonly used atoms and H isotope selection

Draw rings

Map atoms | Define bonds to be broken or formed

Draw bonds. Dotted line is unspecified bond

Reaction Searching

Reaction searches

Reactions queries can be substance names, CAS Registry Numbers, document identifiers, or chemical structures

- 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, chemical structure or reaction scheme

Search

All
Substances
Reactions
References
Suppliers

Select reactions

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Edit

Click on reaction query to edit

Edit Drawing Remove

Create Retrosynthesis Plan

Set Plan Options

Recent Search History

Structure Match

As Drawn (61)
Substructure (6,410)
Similarity (27K)

View by structure match

Filter by

Yield
Number of Steps
Non-Participating Functional Groups
Experimental Protocols
Reaction Type
Stereochemistry
Reagent
Catalyst
Solvent
Commercial Availability
Reaction Notes
Stereoselective (1,191)
Regioselective (380)
Prophetic Reaction (267)
Chemoselective (209)
Biotransformation (87)
View All

Search Within Results

Source Reference

Document Type

Reactions (6,410)

References

Scheme 1 (30 Reactions)

View substance information

Steps: 1 Yield: 81-98%

Yield range for displayed reactions

View suppliers

Suppliers (93)

Suppliers (131)

View substance information

Reaction Summary

1.1 Reagents: Hydrogen peroxide
Catalysts: Triaquea[μ-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO¹]](μ₃-[1,3,5-benzenetricarbox...
Solvents: Ethanol, Acetonitrile; 1 h, rt → 100 °C

Steps: 1 Yield: 98%

Catalytic activity of HKUST-1 in the oxidation of trans-ferulic acid to vanillin

By: Yepez, Rebeca; et al
New Journal of Chemistry (2015), 39(7), 5112-5115

Full Text

View Reaction Detail Experimental Protocols

View reaction detail

Steps: 1 Yield: 88%

1.1 Solvents: Water; 24 h, 40 °C
1.2 pH 5

View reaction reference

Biotransformation of ferulic acid to vanillin by Bacillus D LF-15161

et al
China, CNT06957879 A 2017-07-18

PATENTPAK Full Text

View Reaction Detail

Reaction Summary

1.1 Solvents: Water; 24 h, 37 °C

Steps: 1 Yield: 81%

Process for producing vanillin from immobilized microorganisms by surface culture

By: Asaff Torres, Ali; et al
World Intellectual Property Organization, WO2008130210 A1 2008-10-30

PATENTPAK Full Text

View Reaction Detail

View All Reaction Summaries

Collapse Scheme

Filter reaction results

Reaction Details

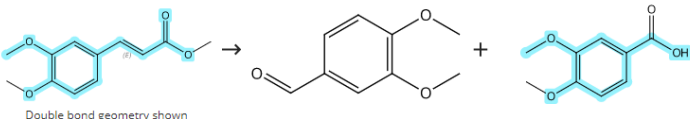
Detailed information includes solvents, catalysts, reagents, conditions and experimental protocols extracted from the publication and its supplemental information.



Reactions



Reaction Detail (Scheme 10, Reaction 1 of 1)



Double bond geometry shown

 Suppliers (25)

 Suppliers (117)

 Suppliers (112)

Download reaction detail incl. experimental protocol 

  Save

Steps: 1
Yield: 42%

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Iodobenzene diacetate	Fe-TAML (complexes with lithium)	Acetone Diphenyl ether Water	1 h, 25 °C
2	Sodium sulfite	-	Water	-

CAS Reaction Number: 31-486-CAS-7572332

Notes

green chemistry-solvent, alternative preparation shown, other products also formed with 14% yield, selective oxidation

Experimental Protocols

MethodsNow™

Products

Veratric acid, Yield: 7%

3,4-Dimethoxybenzaldehyde, Yield: 42%

Diphenyl ether

Water

Procedure

1. Charge a dry, inert Radleys tube with the substrate (1 mmol), diphenyl ether (0.1-0.25 equivalent), Fe(TAmI) Li (1 mol-%), and anhydrous acetone (5 ml), under argon atmosphere.
2. Add the solution on a Radleys carousel and thermostated at 25 °C.
3. Add iodobenzene diacetate (2 mmol) to the mixture.
4. Stir the tube for 1 hour.
5. Add saturated aqueous sodium sulfite (5 ml) to the mixture.
6. Extract the mixture with ethyl acetate (3×5 ml).
7. Dry the obtained solution on 3Å molecular sieves.

Transformation

Ozonolysis

Scale

milligram

Characterization Data

3,4-Dimethoxybenzaldehyde

State colorless oil.

View experimental protocols, including detailed procedures (abbreviated display)

View characterization data, like 1H NMR, 13C NMR, IR and other information as reported

Reference

Fe(TAML)Li/(diacetoxyiodo) benzene-Mediated Oxidation of Alcohols: Evidence for Mild and Selective C-O and C-C Oxidative Cleavage in Lignin Model Transformations

By: Napoly, Francois; et al
[View All](#)

European Journal of Organic Chemistry (2014), 2014(4), 781-787

Full Text 

Company/Organization

UMR CNRS 5246, Institut de Chimie et Biochimie Moléculaire et Supramoléculaire
Université Claude Bernard Lyon 1
Villeurbanne 69622
France

Retrosynthesis Planner

Launch plan generation

There are three 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
- 3 Structured based reaction query without any results (not pictured)

The screenshot shows the SciFinder interface with a chemical structure of Olaparib. Annotations include:

- A callout box pointing to the 'Reactions' dropdown menu: "Make sure *Reactions* is selected to view the Create Retrosynthesis Plan icon".
- A callout box pointing to the 'Create Retrosynthesis Plan' button: "Access plan options before launching the retrosynthesis tool".
- A callout box pointing to the 'Edit Drawing' button: "1 Create Retrosynthesis Plan".
- A callout box pointing to the 'Set Plan Options' button: "2".

Open plan

The Experimental Plan is available within a few seconds. As soon as the calculation of the Predictive Retrosynthesis Plan is finished, a notification will pop up in that retrosynthetic plan. You will also be informed via email.

The screenshot shows the SciFinder Retrosynthesis interface with a reaction plan. Annotations include:

- A callout box pointing to the 'Edit Plan Options' button: "Access plan options from the top bar".
- A callout box pointing to the 'Experimental' step key: "Red lines mark experimental steps, i.e. those reported in the literature".
- A callout box pointing to the 'Predicted' step key: "Review alternative disconnections".
- A callout box pointing to the 'ON' switch for predicted steps: "Switch predicted steps on/off".
- A callout box pointing to the 'Avg. Yield: 72%' label: "Green dotted lines indicate predicted steps".

Alternative Steps and Plan Options

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

The screenshot displays the 'Alternative Steps' section of the ChemPlanner interface. On the left, a list of steps is shown, with step 1 highlighted. The main area shows a list of alternative steps (48 total) with filters for Yield and Number of Steps. A callout box labeled '1' points to the 'Evidence' link for step 1. Another callout box labeled '2' points to the 'Evidence' link for step 2. A third callout box labeled 'Select alternative - the plan will be reorganized' points to the 'Select' button. The right side shows a detailed view of a reaction scheme, including reagents, solvents, and a reaction summary.

Overview Steps

Alternative Steps (48)

Filter by

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Summary

1.1 Reagents: Butyllithium
Solvents: Tetrahydrofuran, Hexane; -78 °C; 2 h, -78 °C
1.2 Solvents: Tetrahydrofuran; -78 °C; 1 h, -78 °C; 18 h, rt
1.3 Reagents: Water; rt

View Reaction Detail Experimental Protocols

7 of 48

8 of 48

Select alternative - the plan will be reorganized

Evidence reactions for predicted disconnection

Combination of two pharmacophoric systems: Synthesis and pharmacological evaluation of spirocyclic pyranopyrazoles with high α_1 receptor affinity

By: Schlager, Torsten; et al
Journal of Medicinal Chemistry (2011), 54(19), 6704-6713

Full Text

Plan options

Edit plan options to...

- Change the synthetic depth
- Maintains connectivity of bonds through the entire synthetic route
- Define bonds to be broken in the first disconnection
- Create a plan with potentially more alternatives, e.g. for poly- or heterocyclic molecules

The screenshot shows the 'Plan Options' dialog box in ChemPlanner. It includes sections for 'Select Synthetic Depth', 'Set Rules Supporting Predicted Reactions', and 'Break and Protect Bonds'. A callout box labeled 'Change number of disconnections in the plan' points to the 'Synthetic depth' options. Another callout box labeled 'Maintains connectivity of bonds through the entire synthetic route' points to the 'Break and Protect Bonds' section. A third callout box labeled 'Break bond in first disconnection' points to the 'Break Bond' button. A fourth callout box labeled 'Select uncommon or rare rules supported by fewer literature examples' points to the 'Uncommon' and 'Rare' rule options. A fifth callout box labeled 'Clear selections' points to the 'Clear All Bond Selections' button. The bottom right corner features a 'Feedback' button.

Plan Options

Select Synthetic Depth

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

1 2 3 4

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)

Create Retrosynthesis Plan

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 Clear selections

Break bond in first disconnection

Select uncommon or rare rules supported by fewer literature examples

Maintains connectivity of bonds through the entire synthetic route

Let us know if you have any questions or comments

Feedback

Markush Searching and PatentPak

Markush searching

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

Markush search type

Filter by patent authority

Markush search option

Markush definition location

Link to PatentPak viewer

Link to 3rd party full text options

PatentPak Viewer

Display controls

Download PDF

Download PDF including chemistry annotations

Link to related information

Highlighted key substance is marked

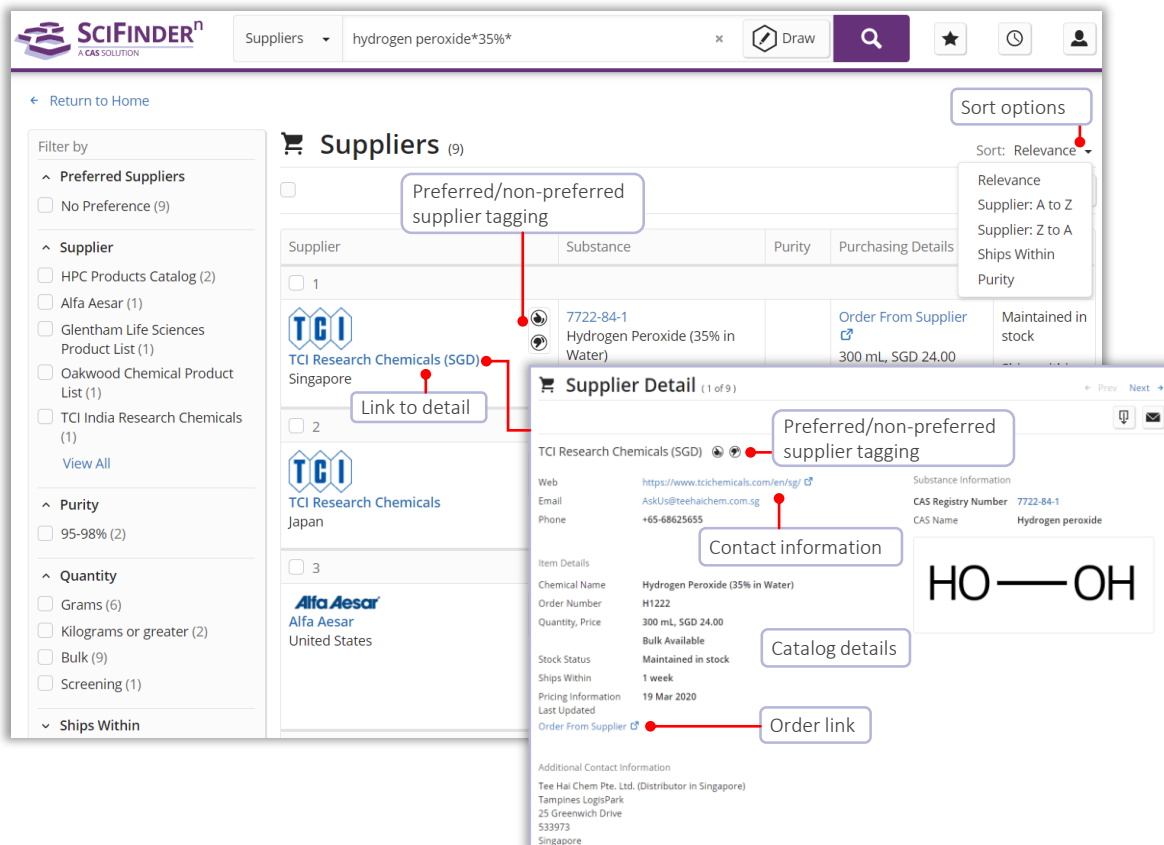
Link to location of substance in patent

Key substances identified in the patent are annotated

Suppliers Searching and ChemDoodle®

Suppliers searching

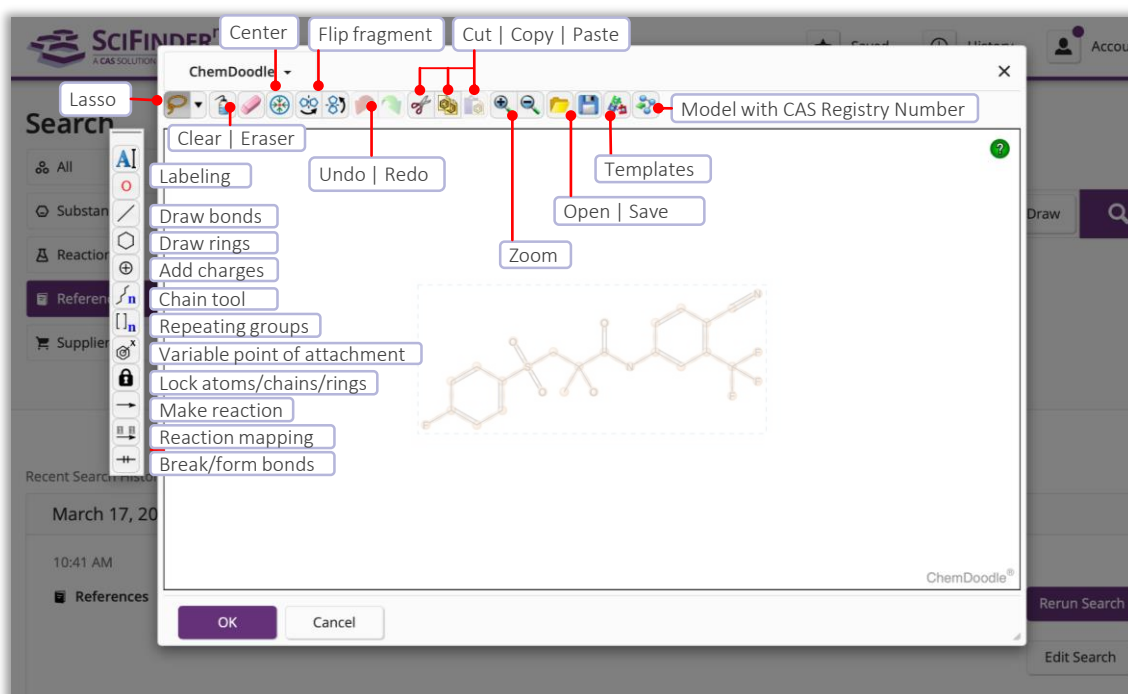
Suppliers searching allows for direct access to chemical catalog information based on chemical structure, names or other identifiers



The screenshot displays the SciFinder Suppliers search results for "hydrogen peroxide*35%". The interface includes a sidebar with filters for Preferred Suppliers, Supplier, Purity, and Quantity. The main results table lists suppliers such as TCI Research Chemicals (SGD) and Alfa Aesar. A callout box labeled "Preferred/non-preferred supplier tagging" points to the supplier status. Another callout labeled "Link to detail" points to the supplier name. A detailed view of TCI Research Chemicals (SGD) is shown, including contact information, catalog details, and an order link. The chemical structure of hydrogen peroxide is displayed as HO-OH.

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. The top toolbar includes options like Center, Flip fragment, Cut | Copy | Paste, Lasso, and Model with CAS Registry Number. The left sidebar lists drawing 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. The main workspace displays a chemical structure of a complex organic molecule. The interface is designed for ease of use on tablets and mobile devices.

Login and Support

Login Details

- Login at <https://scifinder-n.cas.org>
- Use your existing SciFinder username and password
- Create a new SciFinderⁿ account for a new user:
Use the intranet SciFinder Registration URL of your institution

Learn More

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

Ask for a training Ask questions

Contact amanson@acs-i.org to organize your on-site or online session, or to ask questions

Contact Customer Support

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