



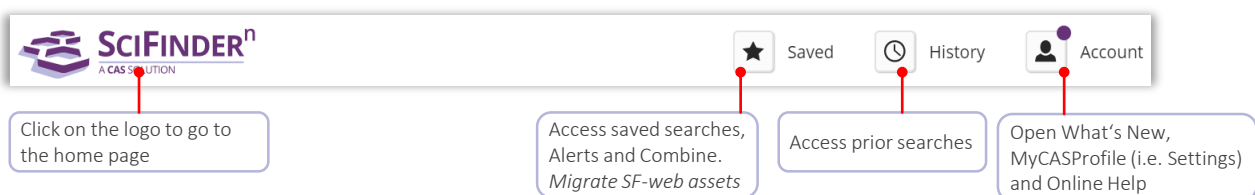
# SCIFINDER<sup>n</sup>

A CAS SOLUTION

## Quick Reference Guide

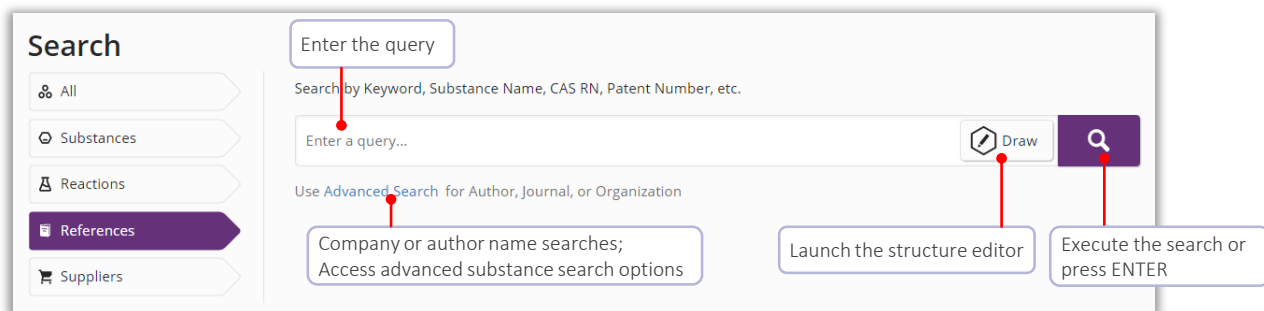
- 1-2 Interface and Reference search
- 3-4 Substance search and structure editor
- 5-6 Reaction search
- 7-8 Retrosynthesis Planner
- 9 Markush search and PatentPak
- 10 Suppliers search and ChemDoodle<sup>®</sup>
- 11 Login and Support

# Interface and Reference Search



## Search Interface

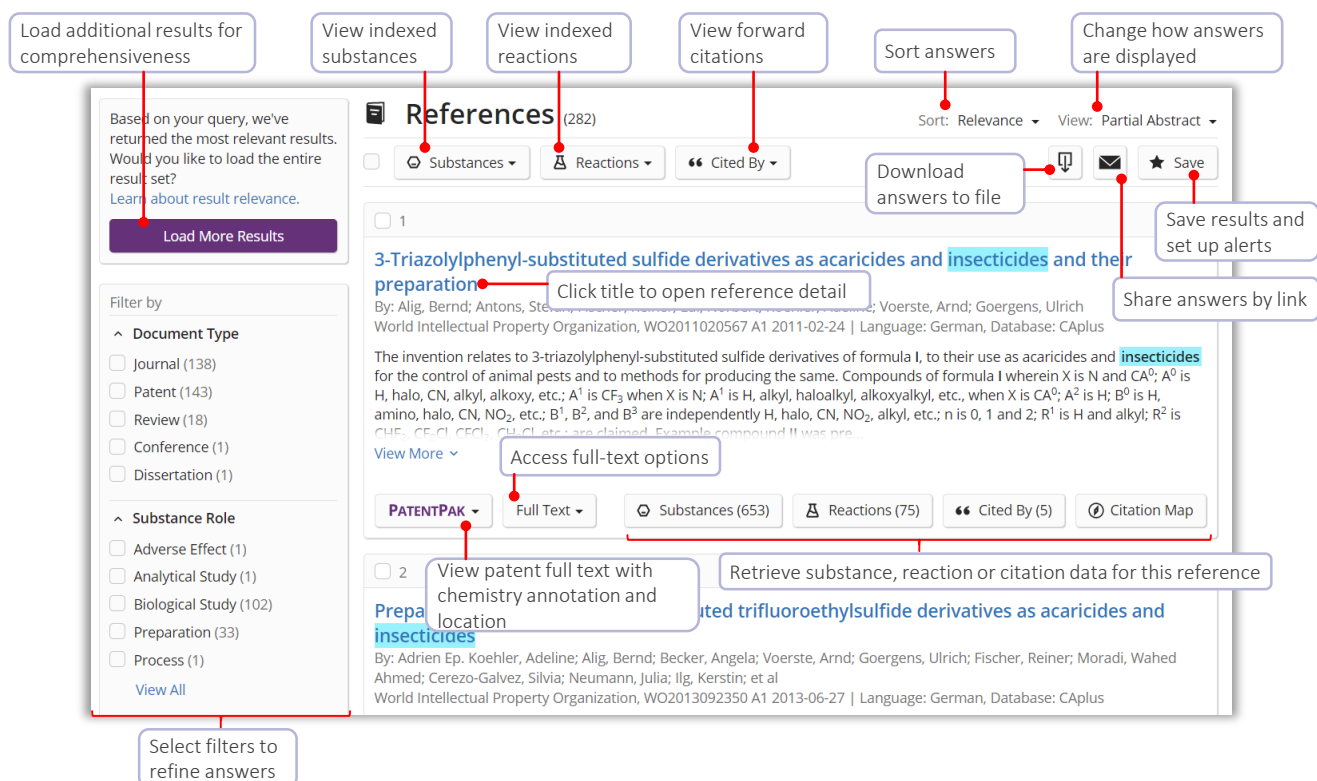
SciFinder<sup>n</sup> features a streamlined search interface.



## 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



# 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

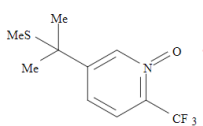
**Source**  
United States

**Database Information**  
AN: 2014:3851  
CAN: 160-144592  
CAplus

**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 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
CA2876184	English					2012-06-30
WO2014004086	English					2013-06-12
						2013-06-12
						2013-06-12

Subject matter and substance indexing is added by CAS scientists

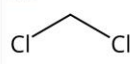
- Concepts
- Substances
- Citations

View reference list of this document

**Substances**

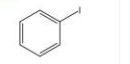
Substances (31)

75-09-2



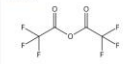
CH<sub>2</sub>Cl<sub>2</sub>  
Dichloromethane  
**PatentPak:**  
Role: Reactant, Reactant or Reagent

591-50-4




C<sub>6</sub>H<sub>5</sub>I  
Iodobenzene  
**PatentPak:**  
Role: Reagent, Reactant or Reagent

407-25-0



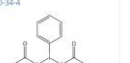
C<sub>6</sub>H<sub>5</sub>O<sub>2</sub>  
Trifluoroacetic anhydride  
**PatentPak:**  
Role: Reagent, Reactant or Reagent

429-04-2



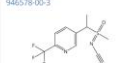
N≡C-NH<sub>2</sub>  
Cyanamide  
**PatentPak:**  
Role: Reagent, Reactant or Reagent

3240-34-4



C<sub>10</sub>H<sub>11</sub>O<sub>4</sub>  
Iodobenzene diacetate  
**PatentPak:**  
Role: Reagent, Reactant or Reagent

946578-00-3



C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>O<sub>5</sub>  
Sulfoxalor  
**PatentPak:**  
Role: Reagent, 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"

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

# Substance Name and Structure Searching

## Name searches

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

Vanillin

Finds Vanillin record

57-92-1

Finds Vanillin record, uses CAS Registry number as identifier

Vanillin stearate

Finds 3 records: Vanillin, Vanillin stearate and Stearate

"Vanillin stearate" Vanillin

Finds 2 records: Vanillin stearate and Vanillin

Vanillin\*

Finds all names that start with the term Vanillin

WO2019020773

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, the 'Click query structure to edit' button, and the 'Search Patent Markush' checkbox. Below the search bar, the '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 results list shows three entries: 90357-06-5 (Bicalutamide), 149104-88-1 (4-(Methylsulfonyl)phenylboronic acid), and 373384-18-0 (3-Methylsulfonylphenylboronic acid). Callouts highlight the 'Click Registry Number to open details' button, the 'Retrieve data related to substance' dropdown menu (showing Substance Detail, Reactions, Synthesize, etc.), the 'Open editor with this structure' button, and the 'Download .sdf, .mol, .cxf, .png' options. A detailed view of Dapsone (CAS RN 80-08-0) is shown, with callouts for 'Click on structure to open flyout window' and 'Reference Roles (also called substance roles) encode the new information reported about a substance'.

**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)phenylboronic acid

Click Registry Number to open details

373384-18-0

C7H9BO4S

(3-Methylsulfonyl)phenylboronic acid

Expands the answer to full view for that specific result

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

80-08-0

C12H12N2O

Dapsone

Click on structure to open flyout window

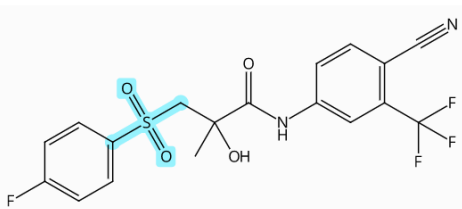
14K References 3,151 Reactions 107 Suppliers

# 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 <sup>3</sup>	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

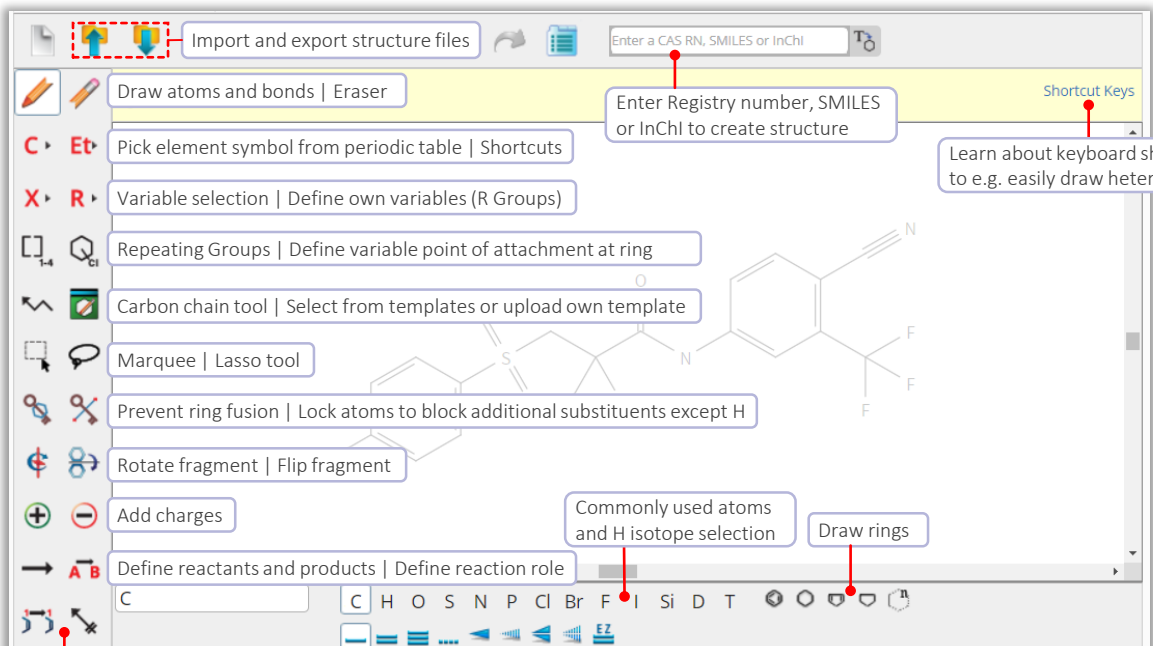
Experimental Properties

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

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

Enter a query...

Edit

Click on reaction query to edit

Edit DrawingRemove

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)

View Expanded

References

View substance information

Yield range for displayed reactions

Scheme 1 (30 Reactions)

View substance information

View substance information

View reaction detail

View reaction reference

Suppliers (93)

Suppliers (131)

Reaction Summary

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

Reaction Summary

Steps: 1 Yield: 88%

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

et al  
China, CNT06957879 A 2017-07-18

PATENTPAK

Full Text

Reaction Summary

Steps: 1 Yield: 81%

Process for producing vanillin from immobilized microor ganisms by surface culture

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

PATENTPAK

Full Text


View All Reaction Summaries

Collapse Scheme






Filter reaction results

# Reaction Details

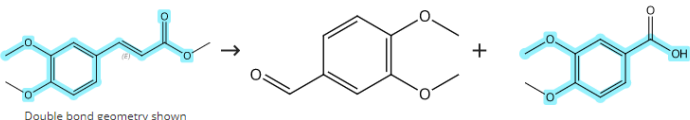
Detailed information includes solvents, catalysts, reagents, conditions and experimental protocols extracted from the publication and its supplemental information.




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(TAmL) 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 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
- 3 Structured based reaction query without any results (not pictured)

The screenshot shows the SciFinder interface with the 'Reactions' tab selected. A callout box points to the 'Create Retrosynthesis Plan' icon, stating: 'Make sure *Reactions* is selected to view the Create Retrosynthesis Plan icon'. Another callout box points to the 'Create Retrosynthesis Plan' button, stating: 'Access plan options before launching the retrosynthesis tool'. The flyout window shows a chemical structure of Olaparib with a 'Create Retrosynthesis Plan' button (labeled 1) and a 'Set Plan Options' button (labeled 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. The 'Retrosynthesis' tab is selected, and the 'Steps' sub-tab is active. A callout box points to the 'Edit Plan Options' button, stating: 'Access plan options from the top bar'. Another callout box points to the 'Experimental' step key, stating: 'Red lines mark experimental steps, i.e. those reported in the literature'. A third callout box points to the 'Predicted' step key, stating: 'Review alternative disconnections'. A fourth callout box points to the 'ON' toggle for predicted steps, stating: 'Switch predicted steps on/off'. The reaction plan shows a sequence of steps (A, B, C, D, E, F, G, H, I, J) with chemical structures and suppliers. Step A is marked as experimental (red line), while steps B through J are marked as predicted (green dotted lines). The plan information shows an estimated yield of 28% and an overall price of \$1,217.28 (USD per 100 grams). The plan is commercially available for steps B, D, E, F, G, H, I, and J.



# 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 points to step 1, stating 'Select alternative - the plan will be reorganized'. Another callout box points to step 2, stating 'Evidence reactions for predicted disconnection'. The right side shows a detailed view of a reaction scheme (Scheme 1) with reagents, solvents, and conditions. A callout box points to the 'Evidence' link, stating 'Evidence reactions for predicted disconnection'.

## 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' (with a callout 'Change number of disconnections in the plan'), 'Set Rules Supporting Predicted Reactions' (with a callout 'Select uncommon or rare rules supported by fewer literature examples'), and 'Break and Protect Bonds' (with a callout 'Break bond in first disconnection'). A callout box at the top right states 'Maintains connectivity of bonds through the entire synthetic route'. A callout box at the bottom right says 'Let us know if you have any questions or comments' with a feedback icon. The interface is powered by ChemPlanner®.

# 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

Link to a specific patent reference

Markush search option

Markush definition location

Link to PatentPak viewer

Link to 3<sup>rd</sup> party full text options

## PatentPak Viewer

Display controls

Download PDF

Download PDF including chemistry annotations

Link to location of substance in patent

Key substances identified in the patent are annotated

Link to related information

Highlighted key substance is marked

Marks key substance curated by CAS scientists

# 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 shows 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 like TCI Research Chemicals (SGD) and Alfa Aesar. A "Supplier Detail" pop-up window is shown for TCI Research Chemicals (SGD), displaying contact information, catalog details, and an order link. Annotations highlight key features:

- Preferred/non-preferred supplier tagging:** Indicated by a red dot and a label pointing to the supplier status in the results table.
- Link to detail:** A red line connects the supplier name in the table to the "Supplier Detail" pop-up window.
- Sort options:** A dropdown menu showing options like Relevance, Supplier: A to Z, Supplier: Z to A, Ships Within, and Purity.
- Contact information:** A label pointing to the contact details in the "Supplier Detail" window.
- Catalog details:** A label pointing to the chemical name, order number, and pricing in the "Supplier Detail" window.
- Order link:** A label pointing to the "Order From Supplier" link in the "Supplier Detail" window.

## 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 toolbar includes various drawing tools and functions. Annotations highlight key features:

- Center:** A button for centering the structure.
- Flip fragment:** A button for flipping a fragment.
- Cut | Copy | Paste:** Buttons for editing the structure.
- Model with CAS Registry Number:** A button for loading a structure from a CAS Registry Number.
- Clear | Eraser:** Buttons for clearing or erasing parts of the structure.
- Labeling:** A button for labeling atoms or groups.
- Undo | Redo:** Buttons for undoing or redoing actions.
- Templates:** A button for applying templates.
- Open | Save:** Buttons for opening or saving the structure.
- Zoom:** A button for zooming in or out.
- Draw bonds:** A button for drawing bonds.
- Draw rings:** A button for drawing rings.
- Add charges:** A button for adding charges.
- Chain tool:** A button for drawing chains.
- Repeating groups:** A button for drawing repeating groups.
- Variable point of attachment:** A button for drawing variable points of attachment.
- Lock atoms/chains/rings:** A button for locking parts of the structure.
- Make reaction:** A button for making reactions.
- Reaction mapping:** A button for mapping reactions.
- Break/form bonds:** A button for breaking or forming bonds.

# Login and Support

## Login Details

- Login at <https://scifinder-n.cas.org>
- Use your existing SciFinder username and password
- Create a new SciFinder<sup>n</sup> 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](mailto:amanson@acs-i.org) to organize your on-site or online session, or to ask questions

## Contact Customer Support

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