

# How to...Work with a Substance Answer Set

## Easily identify and isolate substances of interest

Quickly retrieve relevant information from the world's largest, publicly available source of substances and references. This guide provides an overview of some of the sort, refine and analyze tools for confidently evaluating and narrowing even a large answer set. From there, two clicks retrieve references or reactions associated with your substance of interest. For more detailed information and additional training resources, consult the online Help or visit [www.cas.org/training/scifinder](http://www.cas.org/training/scifinder).

## Substance Search Results

**SUBSTANCES** Get References Get Reactions Get Commercial Sources Tools Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine **1** Sort by: Relevance **2** Display Options

0 of 535 Substances Selected Page: 1 of 27

Analyze by: Substance Role

Biological Study 352  
Preparation 326  
Uses 237  
Reactant or Reagent 58  
Properties 43  
Prophetic in Patents 20  
Process 14  
Analytical Study 9  
Formation, Nonpreparative 3  
Occurrence 2

**1. 13118-11-1**  
~21 ~16   
  
**C<sub>18</sub> H<sub>25</sub> N O<sub>3</sub>**  
Benzeneacetic acid, alpha-cyclopentyl-alpha-hydroxy-, 1-methyl-3-pyrrolidinyl ester  
▶ **Key Physical Properties**  
Regulatory Information  
Experimental Properties

**2. 616866-21-8**  
~7   
  
**C<sub>18</sub> H<sub>25</sub> N O<sub>3</sub>**  
Benzeneacetic acid, alpha-cyclopentyl-alpha-hydroxy-, (3R)-1-methyl-3-pyrrolidinyl ester, (alphaR)-  
▶ **Key Physical Properties**

**3. 207856-83-5**  
~5   
  
**C<sub>18</sub> H<sub>25</sub> N O<sub>3</sub>**  
Benzeneacetic acid, alpha-cyclopentyl-alpha-hydroxy-, (3S)-1-methyl-3-pyrrolidinyl ester, (alphaS)-  
▶ **Key Physical Properties**

**4. 207856-85-7**  
~5

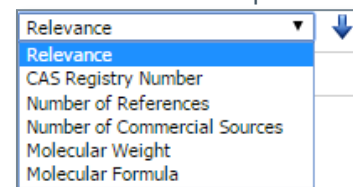
**5. 937179-78-7**  
~4

**6. 873912-87-9**  
~3

**Tip**  
Default sort options vary depending on the type of search conducted.

- Molecular formula, property and substance identification searches are sorted by CAS Registry Number®.
- Similarity search results are sorted by similarity score.
- Markush patent results are sorted from the newest to oldest reference.

**1** Exact and substructure answer sets are sorted by relevance. Click the drop-down arrow to select another sort option.



- The blue arrow indicates that the results are sorted from most to least relevant. Click the arrow to reverse the sort order.

**2** The number of retrieved substances and the number selected are displayed.

- To select an answer, click the box to the left of the answer number.
- Click the drop-down arrow for options related to selected answers.

The screenshot shows the SciFinder search results page. At the top, there are navigation buttons: 'Get References', 'Get Reactions', 'Get Commercial Sources', 'Tools', 'Create Keep Me Posted Alert', and 'Send to SciPlanner'. Below these is a 'Sort by: Relevance' dropdown and a 'Display Options' button. A status bar indicates '0 of 535 Substances Selected' and 'Page: 1 of 27'. The main content area displays three search results. The first result, with CAS number 13118-11-1, is highlighted. A context menu is open over it, showing options: 'View Substance Detail', 'Explore by Structure', 'Synthesize this...', 'Get Reactions where Substance is a' (with a sub-menu for Product, Reactant, Reagent, Reactant/Reagent, Catalyst, Solvent, Any Role), 'Get Commercial Sources', 'Get Regulatory Information', 'Get References', 'Export as Image', 'Export as molfile', and 'Send to SciPlanner'. The chemical structure of Benzeneacetic acid,  $\alpha$ -cyclopentyl- $\alpha$ -hydroxy-, 1-methyl-3-pyrrolidinyl ester is shown in red. Below the structure, the molecular formula  $C_{18}H_{25}NO_3$  and the name are listed, along with links for 'Key Physical Properties', 'Regulatory Information', and 'Experimental Properties'.

3 Click **Display Options** to specify the number of answers displayed per page (15, 20, 25 or 50) and to select the number of columns to display.

4 Use the page controls to navigate through your answer set.

5 Mouse over a substance to access additional substance information and tools.

- Click the double blue arrow to access the additional search and export options shown here.
- Click the magnifying glass icon to launch the **Quick View**, a separate window that summarizes data about the substance (not shown)
- Close the **Quick View** window to return to the active session.

#### Each answer includes:

- The CAS Registry Number; it is a link to the **Substance Detail** page
- Active icons indicate the availability of:
  - References for the substance
  - Reaction data
  - Chemical supplier information
- The chemical structure; the part that matches your query is red
- The molecular formula
- The CA Index Name (useful for government documents)
- Links to **Regulatory information**, **Spectra** and **Experimental Properties**, when available

# Substance Detail

**SUBSTANCE DETAIL** [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

[Return](#) [Previous](#) | [Next](#)

**1** 1. CAS Registry Number 13118-11-1

~21 ~16

**C<sub>18</sub> H<sub>25</sub> N O<sub>3</sub>**  
Benzoic acid,  $\alpha$ -cyclopentyl- $\alpha$ -hydroxy-, 1-methyl-3-pyrrolidinyl ester

**Molecular Weight**  
303.40

**Boiling Point (Predicted)**  
Value: 434.6 $\pm$ 45.0 °C | Condition: Press: 760 Torr

**Density (Predicted)**  
Value: 1.17 $\pm$ 0.1 g/cm<sup>3</sup> | Condition: Temp: 20 °C Press: 760 Torr

**pKa (Predicted)**  
Value: 12.19 $\pm$ 0.29 | Condition: Most Acidic Temp: 25 °C

**2** **Other Names**  
Mandelic acid,  $\alpha$ -cyclopentyl-, 1-methyl-3-pyrrolidinyl ester (6CI,7CI)  
N-Methyl-3-pyrrolidinyl cyclopentylmandelate

[Expand All](#) | [Collapse All](#)

**3** **EXPERIMENTAL PROPERTIES**

**EXPERIMENTAL SPECTRA**

**PREDICTED PROPERTIES**

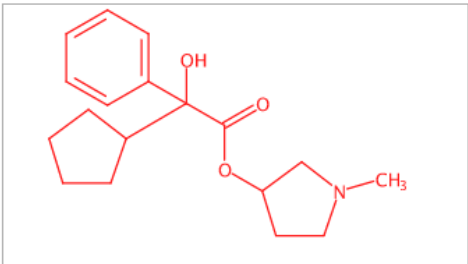
**PREDICTED SPECTRA**

**REGULATORY INFORMATION**

**CAS REFERENCE ROLES**

**ADDITIONAL DETAILS**

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The chemical structure shows a central carbon atom bonded to a phenyl ring, a hydroxyl group (OH), a cyclopentyl ring, and an ester group. The ester group consists of a carbonyl group (C=O) bonded to an oxygen atom, which is further bonded to a 1-methyl-3-pyrrolidinyl ring system.

Click a CAS Registry Number on the answer page to open the **Substance Detail** page. It summarizes the available information for a substance.

**1** The display at the top of the page includes the **CAS Registry Number**, molecular formula, CA Index Name, Molecular Weight and some common properties for this substance.

**2** **Other Names** lists up to five chemical name synonyms.

- When more names are available, a **Show More** link is at the bottom of the list

**3** To explore details about a substance, expand a menu by clicking the arrow next to a content area.

- At the top of these menus are **Expand All** and **Collapse All** links

4

#### EXPERIMENTAL PROPERTIES

##### Optical and Scattering Thermal

Optical and Scattering Properties	Value	Condition	Note
Refractive Index	1.5256	Wavlen: 589.3 nm; Temp: 23 °C	(1)CAS

##### Notes

(1) Lunsford, Carl D.; US 2956062 1960 CAPLUS 🔍

#### EXPERIMENTAL SPECTRA

##### <sup>1</sup>H NMR

<sup>1</sup> H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See full text		(2)CAS

##### Notes

(2) Ji, F.; Journal of Pharmacy and Pharmacology 2005, V57(11), P1427-1435 CAPLUS 🔍

#### PREDICTED PROPERTIES

##### Biological Chemical Density Lipinski Structure Related Thermal

Biological Properties	Value	Condition	Note
Bioconcentration Factor	1.0	pH 7 Temp: 25 °C	(3)
Concentration Factor	1.0	pH 7 Temp: 25 °C	(3)

### Tip

**CAS Reference Roles** indicate the function of a substance in the document. CAS Analysts have applied roles as part of the indexing process since 1967. The **Preparation** role goes back to 1907.

4

You can expand the menus to see more information about a content area, as shown here. In many cases, tabs provide convenient access to additional information.

#### PREDICTED SPECTRA

##### <sup>1</sup>H NMR <sup>13</sup>C NMR

<sup>1</sup> H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See spectrum		(4)

##### Notes

(4) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V11.01 (© 1994-2016 ACD/Labs)

#### REGULATORY INFORMATION

##### Regulatory Synonyms

##### Regulatory Overview by Country

##### Confidentiality Status

Public

##### European Union

##### File Segment

#### CAS REFERENCE ROLES

Roles	Patents	Nonpatents
Analytical Study		✓
Occurrence		✓
Preparation	✓	✓
Prophetic in Patents	✓	
Reactant or Reagent	✓	✓

# Evaluate Answers with Analysis Options

**1** Analyze by: **2**

**3** Show More

**Analyze - Substance Role**

10 Items 0 Selected Export

Sort by: Frequency

Select bars to view only those substances within the current answer set.

Analysis Option	Count
<input type="checkbox"/> Biological Study	352
<input type="checkbox"/> Preparation	326
<input type="checkbox"/> Uses	237
<input type="checkbox"/> Reactant or Reagent	58
<input type="checkbox"/> Properties	43
<input type="checkbox"/> Prophetic in Patents	20
<input type="checkbox"/> Process	14
<input type="checkbox"/> Analytical Study	9
<input type="checkbox"/> Formation, Nonpreparative	3
<input type="checkbox"/> Occurrence	2

Apply Cancel

**1** By default, the answer set is analyzed by **Substance Role**.

**2** Click the drop-down arrow to see the available **Analyze by:** options.

**3** Click **Show More** to see additional data, when available, or to select more than one analysis subset.

- Click the box to the left of a subset to select it.
- Sort by** either **Frequency** (the default) or **Natural Order** (alphanumeric order).

Sort by: Frequency

Frequency

Natural Order

# Narrow an Answer Set after Analysis

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

⚠ 115 substances with the Bioactivity Indicator **Respiratory system agents (all)** are displayed **2** Keep Analysis Clear Analysis

Chemical Structure substructure > substances (535) > 13118-11-1

SUBSTANCES ⓘ Get References Get Reactions Get Commercial Sources Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Sort by: Relevance Display Options

0 of 535 Substances Selected Page: 1 of 6

Analyze by: Bioactivity Indicators

Receptor antagonists (all) 136

Nervous system agents (all) 131

**Respiratory system agents (all) 115**

Anti-inflammatory agents (all) 35

Ophthalmic agents (all) 35

Receptor agonists (all) 33

Immune agents (pharmaceutical) 31

Cardiovascular agents (all) 23

Antifibrotic agents 17

Gastrointestinal agents (all) 17

Show More

31. **475468-09-8** (Component: 202185-74-8) ~23 ~3  
  
Absolute stereochemistry.

51. **873295-30-8** (Component: 13283-82-4) ~3

52. **873295-35-3** ~3  
  
16053-58-0  
C<sub>3</sub>H<sub>3</sub>O<sub>3</sub>S  
  
13283-82-4  
C<sub>19</sub>H<sub>28</sub>N O<sub>3</sub>

**C<sub>19</sub>H<sub>28</sub>N O<sub>3</sub> · Br**  
Pyrrolidinium, 3-[[[(2*R*)-2-cyclopentyl-2-hydroxy-2-phenylacetyl]oxy]-1,1-dimethyl-, bromide (1:1), (3*R*)-

**C<sub>19</sub>H<sub>28</sub>N O<sub>3</sub> · F**  
Pyrrolidinium, 3-[[[2-cyclopentyl-2-hydroxy-2-phenylacetyl]oxy]-1,1-dimethyl-, fluoride (1:1)

**Tip**

- **Bioactivity Indicators** are a predefined set of bioactivity terms for which relationships have been identified between substances and documents in the content.
- **Target Indicators** are a predefined set of protein, enzyme and other target terms for which relationships have been identified between substances and documents in the content.

**1** Click an **Analyze** bar to display that subset of answers. In this example, the answer set is analyzed by **Bioactivity Indicators** and **Respiratory system agents (all)**.

- The analysis bar turns yellow.
- Other bars can also turn completely or partly yellow to indicate that substances from the selected bar are also present in other subsets.
- Click **Substance Detail** to see a summary of bioactivity and target indicator data, when available.

**2** The yellow status bar indicates the answers that are currently displayed.

- Click **Keep Analysis** to make these answers your new answer set.
- Click **Clear Analysis** to return to your original answer set.



# Narrow an Answer Set with Refine Options

**1** Refine

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Sort by: Relevance

0 of 115 Substances Selected

Page: 1 of 6

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

Java Non-Java

Click image to change structure or view detail.  
Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

**2** Refine

**1. 475468-09-8**  
(Component: 202185-74-8)  
~23 ~3  
  
• Br -  
Absolute stereochemistry.  
**C<sub>19</sub> H<sub>28</sub> N O<sub>3</sub> · Br**  
Pyrrolidinium, 3-[[[(2R)-2-cyclopentyl-2-hydroxy-2-phenylacetyl]oxy]-1,1-dimethyl-, bromide (1:1), (3R)-

**2. 873295-30-8**  
(Component: 13283-82-4)  
~3  
  
• F -  
**C<sub>19</sub> H<sub>28</sub> N O<sub>3</sub> · F**  
Pyrrolidinium, 3-[[[(2-cyclopentyl-2-hydroxy-2-phenylacetyl)oxy]-1,1-dimethyl-, fluoride (1:1)

**3. 873295-35-3**  
~3  
16053-58-0  
C H<sub>3</sub> O<sub>3</sub> S  
  
**C<sub>19</sub> H<sub>28</sub> N O<sub>3</sub> · C H<sub>3</sub> O<sub>3</sub> S**  
Pyrrolidinium, 3-[[[(2-cyclopentyl-2-hydroxy-2-phenylacetyl)oxy]-1,1-dimethyl-, methanesulfonate

**4. 1262431-94-6**  
~16 ~2  
312753-06-3  
C<sub>24</sub> H<sub>28</sub> N<sub>2</sub> O<sub>3</sub>  
  
**C<sub>19</sub> H<sub>28</sub> N O<sub>3</sub> · C H<sub>3</sub> O<sub>3</sub> S**  
Pyrrolidinium, 3-[[[(2-cyclopentyl-2-hydroxy-2-phenylacetyl)oxy]-1,1-dimethyl-, methanesulfonate

**5. 1613757-92-8**  
~2  
13283-82-4  
C<sub>19</sub> H<sub>28</sub> N O<sub>3</sub>  
  
**C<sub>19</sub> H<sub>28</sub> N O<sub>3</sub> · C H<sub>3</sub> O<sub>3</sub> S**  
Pyrrolidinium, 3-[[[(2-cyclopentyl-2-hydroxy-2-phenylacetyl)oxy]-1,1-dimethyl-, methanesulfonate

**6. 1613758-02-3**  
~2  
13283-82-4  
C<sub>19</sub> H<sub>28</sub> N O<sub>3</sub>  
  
**C<sub>19</sub> H<sub>28</sub> N O<sub>3</sub> · C H<sub>3</sub> O<sub>3</sub> S**  
Pyrrolidinium, 3-[[[(2-cyclopentyl-2-hydroxy-2-phenylacetyl)oxy]-1,1-dimethyl-, methanesulfonate

**1** Click the **Refine** tab and click a radio button to select a **Refine by:** option.

**2** Specify additional criteria below the refine options.

**3** Click **Refine**.

## Tip

To **Refine by Chemical Structure**, click the thumbnail to re-open the **Structure Editor**.

Structure Editor

Draw or change atoms or bonds.

Get substances that match your query using:

- Exact search
- Substructure search

OK Cancel

Modify the structure and click **OK**. The modified structure is then displayed in the thumbnail on the **Refine** tab. Click **Refine** and the answer set is narrowed based on the new criteria.

# Manage Your Searching

The screenshot shows the SciFinder web interface. At the top, there is a navigation bar with 'CAS Solutions' on the left, 'Preferences | SciFinder Help' in the center, and 'Sign Out' on the right. Below this is a main menu with 'Explore', 'Saved Searches', and 'SciPlanner'. To the right of the menu are 'Save', 'Print', and 'Export' buttons. The main content area shows a breadcrumb trail: 'Chemical Structure substructure > substances (535)'. Below the breadcrumb are several action buttons: 'SUBSTANCES', 'Get References', 'Get Reactions', 'Get Commercial Sources', 'Tools', 'Create Keep Me Posted Alert', and 'Send to SciPlanner'. Twelve purple diamond-shaped callouts with numbers 1 through 12 are overlaid on the interface, pointing to specific features.

1 Access **Preferences** and **SciFinder Help** options: **Help**, **Training**, **What's New** and **Contact Us**.

2 Click the **Explore** drop-down arrow to start a new references, substances or reactions search.

3 Click the **Saved Searches** drop-down arrow to access **Saved Answer Sets**, **Keep Me Posted** answer sets and your search **History**.

4 Click **SciPlanner** to open the SciPlanner workspace.

- It is an interactive window where you can store and organize reference, substance and reaction search results.

5 Click **Save**, **Print** or **Export** to open a dialog window and initiate each of these processes.

- See "How to... Print, Save and Export" for more information.

6 The breadcrumb trail shows each step in your current search history. Mouse over a step to see more information about it. Click a step to return to that part of the search.

7 Click **Get References** to retrieve references for part or all of your answer set.

8 Click **Get Reactions** to retrieve reactions for part or all of your answer set.

9 Click **Get Commercial Sources** to retrieve suppliers for part or all of your substances.

10 Click the **Tools** drop-down arrow to combine this answer set with a previously saved answer set (**Combine Answer Sets**).

11 **Create Keep Me Posted Alert**, when active, allows you to create an automated alert based on the current search strategy.

12 Click **Send to SciPlanner** to send selected answers to the SciPlanner workspace.

- Use it to gather information for a project, create a report or export research to share with colleagues.



## CAS Customer Center

E-mail: [help@cas.org](mailto:help@cas.org)

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