

# HOW TO

## Explore by Molecular Formula

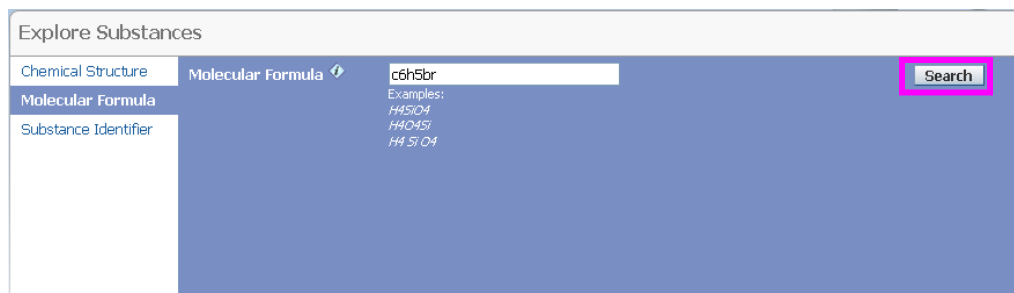


SciFinder<sup>®</sup> offers a variety of ways to find chemical substances. Use Explore by Molecular Formula to find substances by using a molecular formula.


This feature is useful for:

- Finding and verifying chemical names, CAS Registry Numbers, molecular formulas, and other substance information
- Obtaining predicted and experimental property data
- Identifying commercial sources
- Retrieving regulatory compliance information
- Obtaining articles and patents that discuss the substance

1. Type a molecular formula.  
Click **Search**.



Explore Substances

Chemical Structure	Molecular Formula 	<input type="text" value="c6h5br"/>	<input type="button" value="Search"/>
Molecular Formula		Examples: H4SiO4 H4O4Si H4 Si O4	
Substance Identifier			

**Tips:**

- Arrange the atoms in any order that is logical to you. If SciFinder cannot interpret the formula, you will get a message asking you to add capitalization and/or spaces.
- To search multicomponent substances, separate each component with a period.

**Note:** Only one molecular formula may be searched at a time.

## 2. Review your answers.

To locate supplier information for a substance, click **Commercial Sources**.

The screenshot shows the 'Substances' interface with three substance detail panels. The first panel, '1. Substance Detail 108-86-1', shows the chemical structure of bromobenzene (C<sub>6</sub>H<sub>5</sub>Br) and lists various links: '~14,519 References', 'Reactions', 'Commercial Sources' (highlighted in pink), 'Regulatory Information', and 'Link'. The second panel, '2. Substance Detail 4165-57-5', shows the chemical structure of 1,2,3,4,5-d5, 6-bromobenzene (C<sub>6</sub>BrD<sub>5</sub>) and lists: '~155 References', 'Reactions', 'Commercial Sources', 'Regulatory Information', and 'Link'. The third panel, '3. Substance Detail 55450-33-4', shows the chemical structure of bromobenzene radical ion (C<sub>6</sub>H<sub>5</sub>Br) and lists: '~63 References', 'Reactions', 'Commercial Sources', 'Regulatory Information', and 'Link'.

## 3. Click the company's name for full details, such as contact information.

The screenshot shows the 'Commercial Sources' interface with a list of product lists. The third entry, '3. Absolute Standards Product List', is highlighted in pink. Below it is the 'Commercial Source Detail' for this entry, showing contact information for Absolute Standards, Inc. and a chemical structure of bromobenzene.

**Commercial Sources**

109 Commercial Sources 0 Selected | Keep Selected | Remove Selected | Print | Export

Select All | Deselect All | Sort by: Catalog Name | Answers per Page [20] | 1 2 3 4 5 6

1. ABCR Product List  
Company Name: ABCR GmbH KG, Publication Date: 11 Apr 2007  
Order Number: AB109479, Quantity: 500 g, 10 kg, 2  
108-86-1 Bromobenzene  
[Link](#)
2. Absolute Standards Product List  
Company Name: Absolute Standards, Inc., Publication Date: 4 May 2009  
Order Number: 32011, Quantity: N/A  
108-86-1 Bromobenzene  
[Link](#)
3. Absolute Standards Product List  
Company Name: Absolute Standards, Inc., Publication Date: 4 May 2009  
Order Number: 70044, Quantity: N/A  
108-86-1 Bromobenzene  
[Link](#)

**Commercial Source Detail**

3. Absolute Standards Product List

4 May 2009

Order Number: 70044  
Quantity: N/A  
Price: contact supplier

CAS Registry Number: 108-86-1  
Bromobenzene

**Absolute Standards, Inc.**  
P O Box 5585  
Hamden, CT, 06518  
USA  
Phone: 800-368-1131  
Fax: 800-410-2577  
Email: customerserv@absolutestandards.com  
Web: http://www.absolutestandards.com

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4. Work with substances...

SciFinder allows you to work with substance answer sets in a variety of ways. For hints and tips, see the How To Guides for:

- Working with Substance Answer Sets: Overview
  - Analyze Substance Answer Sets
  - Refine Substance Answer Sets
  - View Properties
  - Combine Answer Sets
  - Print, Save, and Export Results
- 



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