

SciFINDER

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How to... Create a Reference Answer Set

Find references quickly and easily

In SciFinder®, you search bibliographic content from two of the world's largest sources of publicly available references for chemistry and related sciences: CAPLUSSM from CAS and MEDLINE® (PubMed) from the National Library of Medicine®. Select from various reference search options, based on the information at hand and your research needs. This guide explains how to conduct each type of reference search. When you have your answer set, refer to "How to ... Work with Reference Answer Sets" for ways to evaluate the results and target the most relevant answers. For more detailed information about SciFinder, consult the online help or visit www.cas.org/training/scifinder.

Types of Reference Searches

1 On the **Explore** tab, under **REFERENCES**, you can search by any of the seven options.

2 Click **Advanced Search** to see criteria for narrowing a search:

Tip

- For most keyword searches, it is often best to start with a broad search and narrow the results later.
- To find specific references, add **Advanced Search** criteria.

1 On the **Explore** tab, under **REFERENCES**, you can search by any of the seven options.

2 Click **Advanced Search** to see criteria for narrowing a search:

Advanced Search ☒ Always Show

Publication Years
Examples: 1995, 1995-1999, 1995-, -1995

Document Types

<input type="checkbox"/> Biography	<input type="checkbox"/> Historical
<input type="checkbox"/> Book	<input type="checkbox"/> Journal
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Letter
<input type="checkbox"/> Commentary	<input type="checkbox"/> Patent
<input type="checkbox"/> Conference	<input type="checkbox"/> Preprint
<input type="checkbox"/> Dissertation	<input type="checkbox"/> Report
<input type="checkbox"/> Editorial	<input type="checkbox"/> Review

Languages

<input type="checkbox"/> Chinese	<input type="checkbox"/> Japanese
<input type="checkbox"/> English	<input type="checkbox"/> Polish
<input type="checkbox"/> French	<input type="checkbox"/> Russian
<input type="checkbox"/> German	<input type="checkbox"/> Spanish
<input type="checkbox"/> Italian	

Author Last Name First Middle

Company

- These search limiters are available as part of the **Refine** and **Analyze** functions, so you can also apply them later in your search process.

Search by Research Topic

The screenshot shows the SciFinder web interface. At the top are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar contains two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there is a list of search criteria: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. The 'Research Topic' option is highlighted with a blue bar and a purple diamond icon with the number 1. Below this, the 'SUBSTANCES' section has 'Chemical Structure' listed. The main content area is titled 'REFERENCES: RESEARCH TOPIC ?'. It features a large text input box containing the example query 'clean up of oil spill in ocean'. Below the input box, there are 'Examples:' listed: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the main area, there is a link for 'Advanced Search' (marked with a purple diamond icon and the number 3) and a checked checkbox labeled 'Always Show'.

1 To begin, click **Research Topic**.

2 Enter your search concept(s) in the text box.

- A search concept, or keyword, is a term or phrase relevant to your topic of interest.
- Enter up to seven concepts, separated by prepositions, in English.
 - Recommendation: enter two or three concepts, separating each concept with a preposition. Use additional concepts to refine your answer set later.
- Use "not" or "except" to exclude a term.

3 Click **Search**.

Tip

You can include up to three synonyms or acronyms for a concept. Place them in parentheses immediately following the concept and separate them with commas. E.g., cat (kitten, feline, felis catus)

Continued

4

Select All Deselect All

1 of 11 Research Topic Candidates Selected

		References
<input type="checkbox"/>	193 references were found containing all of the concepts "clean", "oil spill" and "ocean" closely associated with one another.	193
<input checked="" type="checkbox"/>	670 references were found where all of the concepts "clean", "oil spill" and "ocean" were present anywhere in the reference.	670
<input type="checkbox"/>	1578 references were found containing the two concepts "clean" and "oil spill" closely associated with one another.	1578
<input type="checkbox"/>	2403 references were found where the two concepts "clean" and "oil spill" were present anywhere in the reference.	2403
<input type="checkbox"/>	3306 references were found containing the two concepts "clean" and "ocean" closely associated with one another.	3306
<input type="checkbox"/>	8579 references were found where the two concepts "clean" and "ocean" were present anywhere in the reference.	8579
<input type="checkbox"/>	3685 references were found containing the two concepts "oil spill" and "ocean" closely associated with one another.	3685
<input type="checkbox"/>	5291 references were found where the two concepts "oil spill" and "ocean" were present anywhere in the reference.	5291
<input type="checkbox"/>	645013 references were found containing the concept "clean".	645013
<input type="checkbox"/>	15717 references were found containing the concept "oil spill".	15717
<input type="checkbox"/>	562745 references were found containing the concept "ocean".	562745

5 Get References

SciFinder returns a set of **Topic Candidates**.

- 4
- Select the answer set that you want to use.
- Click the box to select an option.
 - A checkmark indicates it has been selected.

- 5
- Click **Get References**.

SciFinder Considers Terms to be...	When the Terms Are Found...
"As entered"	Exactly as you have entered them
"Closely associated with one another"	Within the same sentence or title
"Present anywhere within a reference"	Anywhere (perhaps widely separated) within a record's title, abstract, or indexing
"Containing the concept"	Somewhere in the record

Now what?

After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to... Work with Reference Answer Sets."

Tip

All concepts "present anywhere in the reference" is often a good starting point if comprehensiveness is important. If the number of references is too large or you only need a few good answers, consider selecting the narrower option in which all of the concepts are "closely associated with one another."

Search by Author Name

The screenshot shows the SciFinder interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar contains a 'REFERENCES' section with a list of search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. The 'Author Name' option is selected. Below this is a 'SUBSTANCES' section. The main area is titled 'REFERENCES: AUTHOR NAME'. It contains three input fields: 'Last Name *' (with 'Kobilka' entered), 'First' (with 'Brian' entered), and 'Middle' (empty). Below these fields is a checkbox labeled 'Look for alternate spellings of the last name' which is checked. A blue 'Search' button is located below the checkbox. To the right of the 'Search' button is a 'Tips' box. Below the search area is a table showing the results of the search. The table has two columns: 'References' and 'References'. The first column lists four author name candidates, all of which are selected (indicated by a checkmark in a box). The second column shows the number of references for each candidate. At the bottom of the table is a 'Get References' button.

1 To begin, click **Author Name**.

2 Enter as much of the name as you know.

- Only the **Last** name is required. Include the **First** and **Middle** names or initials to improve the search results.
- Enter punctuation (spaces, hyphens, etc.) as if you were writing the name.
- Replace special characters with equivalent character(s), e.g., ae replaces ä.
- For optimal retrieval, "Look for alternative spellings of the last name" is selected by default.

3 Click **Search**.

4 SciFinder returns a list of authors. The number of references associated with each name appears on the right.

- Click the box next to any name(s) you want to select and a checkmark appears.

5 Click **Get References**.

Tips

- For complicated names, try multiple searches and determine which search gives the best results.
- Under the Tools drop down, you can also combine answer sets.

	References
<input checked="" type="checkbox"/> KOBILKA B	17
<input checked="" type="checkbox"/> KOBILKA B K	111
<input checked="" type="checkbox"/> KOBILKA BRIAN	110
<input checked="" type="checkbox"/> KOBILKA BRIAN K	284

Now what?

After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to... Work with Reference Answer Sets."

Tip

Create a Keep Me Posted (KMP) automatic alert if you want to know when new records for this author become available. See "How to Create a Keep Me Posted (KMP) Alert" for more information.

Search by Company Name

The screenshot shows the SciFinder web interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar under the 'REFERENCES' heading lists search criteria: 'Research Topic', 'Author Name', 'Company Name' (which is highlighted with a blue bar and a purple diamond labeled '1'), 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Below this is a 'SUBSTANCES' section. The main area is titled 'REFERENCES: COMPANY NAME' with a help icon. It contains a text input box with 'Owens Corning Fiberglas' (labeled with a purple diamond '2') and examples '3M' and 'DuPont' below it. A blue 'Search' button (labeled with a purple diamond '3') is at the bottom of the main area.

1 To begin, click **Company Name**.

2 Enter the name of one organization into the query entry text box.

3 Click **Search**.

Tip

Create a Keep Me Posted (KMP) automatic alert if you want to know when new records for this author become available. See the "Create and Manage Alerts (KMPs)" guide for more information.

Company Name Searching Guidelines

- SciFinder considers various spellings, acronyms, abbreviations, and related terms when retrieving results. It does not consider mergers and acquisitions.
- SciFinder automatically searches common synonyms and abbreviations. For example, entering "Company" or "Co." returns the same results.

Now what?

After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to... Work with Reference Answer Sets."

Search by Document Identifier

1 To begin, click **Document Identifier**.

2 Enter up to 25 identifiers, one per line, in the query entry text box.

3 Click **Search**.

Tip

SciFinder ignores punctuation and accepts both two-digit and four-digit formats for years. Therefore, the search term 1983:4296 will retrieve both the PubMed ID 834296 and the CAlus Accession Number 1983:4296. Select the document of interest when you review the answers.

Searchable Document Identifiers

Type of Identifier	Example
Accession number: A unique number applied to a record when it is created. It begins with the year followed by sequential numbering.	CAplus: 2012:1527010 MEDLINE: 1998010009
Digital object identifier (DOI): an alphanumeric character string that uniquely identifies an electronic document over the course of its lifetime.	10.1021/jp204843r

Now what?

After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to... Work with Reference Answer Sets."

Search by Journal

1 To begin, click **Journal**.

2 Enter a **Journal Name** (required).
 ■ Enter data in additional fields to retrieve more specific answers.

3 Click **Search**.

Tip

Create a broad search and then narrow search results by using refine and analyze options.

Field	Data Accepted
Journal Name	<ul style="list-style-type: none"> Full name, abbreviation, or acronym Abbreviations or acronyms must not contain spaces or punctuation Maximum of 30 characters
Volume	Number (38) or alphanumeric string (45a) <ul style="list-style-type: none"> A Journal Name must be specified before a Volume, Issue, or Starting Page can be recognized
Issue	Number (16) or month (June)
Starting Page	Number (46), letters (iii), or alphanumeric string (m287)
Title Word(s)	Key words, a partial title or a full title

Now what?

After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to... Work with Reference Answer Sets."

Search by Patent

Explore **Saved Searches** **SciPlanner**

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent**
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

REFERENCES: PATENT

2 Patent Number
US 6448377
Examples: WO 2001011365

Assignee Name
Examples: Cancer Research Technology Limited

Inventor Last Name * First Middle

Publication Year
Examples: 1995, 1995-1999, 1995-, -1995

3 **Search**

Tip
One number can retrieve both a granted patent and an unrelated patent application. You can easily select the record of interest while reviewing the search results.

1 To begin, click **Patent**.

2 Enter a **Patent Number**.

- Acceptable patent numbers include any number that identifies a patent, such as patent application numbers, priority application numbers, and patent numbers.

Type of Identifier	Example
Patent Application Number	WO 2012-US29090
Priority Application Number	US 1996-15450P
Patent Number	JP 2001519650

Alternatively, you can enter an **Assignee Name** or **Inventor Name**.

- Enter data in several fields to create a narrower search.

3 Click **Search**.

Now what?

After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to... Work with Reference Answer Sets."

Search by Tags

A tag is a user-defined keyword that you can apply to references in one or more answer sets. When you save an answer set, the tag is saved with the associated reference. Search a tag to retrieve any references to which the tag was applied.

1 To begin, click **Tags**.

2 From the displayed list, select the tag that you want to search.

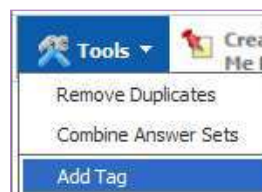
SciFinder retrieves all of the records to which that tag has been applied. This feature allows you to pull references from several different answer sets and place them all into a new answer set.

Now what?

After you click **Get References**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to... Work with Reference Answer Sets."

Tip

When reviewing your search, you can apply tags to records by selecting Add Tag from the Tools menu. In the dialog box, enter the key word(s) that you want to apply as a tag. After they are created, tags become searchable.



How to...Create a Substance Answer Set

Select among five search techniques to find substances

Substances can be described by multiple names or other characteristics, so SciFinder® gives you the flexibility to approach a substance search from different starting points, depending on your research needs. No matter how you begin, your results are from the CAS REGISTRYSM, the most trusted and comprehensive collection of publicly available chemical substances in the world. Refer to “How to ... Work with Substance Answer Sets” for ways to evaluate the results and find the most relevant answers. To learn more about using SciFinder, consult the online Help or visit www.cas.org/training/scifinder.

Types of Substance Searches

1 On the **Explore** tab, under **SUBSTANCES**, you can search by any of the five options.

2 Click **Advanced Search** to see criteria that you can add to a search to make it more specific.

TIP
CXF is the file extension for saved structures and reactions in SciFinder.

Advanced Search	
Characteristics	<input type="checkbox"/> Single component
	<input type="checkbox"/> Commercially available
	<input type="checkbox"/> Included in references
Classes	<input type="checkbox"/> Alloys
	<input type="checkbox"/> Coordination compounds
	<input type="checkbox"/> Incompletely defined
	<input type="checkbox"/> Mixtures
	<input type="checkbox"/> Polymers
	<input type="checkbox"/> Organics, and others not listed
Studies	<input type="checkbox"/> Analytical
	<input type="checkbox"/> Biological
	<input type="checkbox"/> Preparation
	<input type="checkbox"/> Reactant or reagent

▪ These options are available in **Refine** and **Analyze**, so you can also apply them later in your search process.

Search by Chemical Structure

1 Select **Chemical Structure**.

2 Click either the **Java** or **Non-Java** tab to select the type of **Structure Editor** that you want to use. Then click the picture of the structure drawing window to launch the **Structure Editor**.

Tip
To learn about structure drawing, refer to the online Help or the "Introduction to the SciFinder Drawing Editor" tutorial on cas.org.

3 Draw your structure.

4 Specify the type of structure search.

5 Click **OK** to transfer the structure and type of search to the search page.

Continued

SELECT...	IF YOU WANT TO RETRIEVE...
Exact Search	The specific structure as drawn in the query, including: <ul style="list-style-type: none"> Stereoisomers Salts and mixtures Polymers with one exactly matching monomer Isotopes Tautomers
Substructure Search	The structure as drawn or as part of a larger molecule in which there is: <ul style="list-style-type: none"> Substitution at open positions Additional ring fusion
Similarity Search (Queries cannot include variable groups, repeating groups or variable attachment positions)	Similar chemical structures containing: <ul style="list-style-type: none"> Positional isomers Different or fewer substituents Different ring systems

3 Draw your structure.

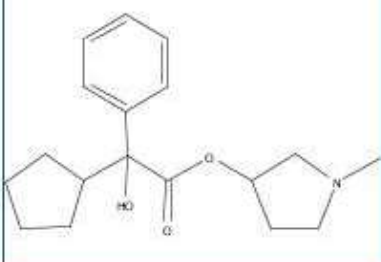
4 Specify the type of structure search.

5 Click **OK** to transfer the structure and type of search to the search page.

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



Search Type:

☐ Exact Structure

☒ Substructure

☐ Similarity

☐ Show precision analysis

Click image to change structure view detail.

Import CXF

6 **Search**

Advanced Search

Tip

Optional: Select Show precision analysis to include additional structure criteria in your search, as shown below:

SUBSTANCES	
Select All Deselect All	
0 of 3 Precision Candidates Selected	
<input type="checkbox"/> Conventional Substructure	84370
<input type="checkbox"/> Closely Associated Tautomers and Zwitterions	31
<input type="checkbox"/> Loosely Associated Tautomers and Zwitterions	3
<input type="checkbox"/> Other	0
Get Substances	

Precision Analysis Window (Unrelated Example)

6 Click **Search** to retrieve the answers that meet your query requirements.

7 For **Similarity** searches, after you click **Search**, you will see a **Similarity Candidates** window. To select the degree(s) of similarity for your answers, check the box(es) of interest. Then, click **Get Substances**.

SUBSTANCES	
Select All Deselect All	
3 of 9 Similarity Candidates Selected	
<input checked="" type="checkbox"/> ≥ 99 (most similar)	18
<input checked="" type="checkbox"/> 95-98	168
<input checked="" type="checkbox"/> 90-94	74
<input type="checkbox"/> 85-89	213
<input type="checkbox"/> 80-84	686
<input type="checkbox"/> 75-79	1436
<input type="checkbox"/> 70-74	3324
<input type="checkbox"/> 65-69	5915
<input type="checkbox"/> 0-64 (least similar)	19313
Get Substances	

Now what?

After you click Search, SciFinder will retrieve the answers that meet your query requirements. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Substance Answer Set."

Search by Markush Structure

The screenshot illustrates the SciFinder interface for searching by Markush structure. It shows the navigation menu on the left, the 'SUBSTANCES: MARKUSH' window, and the 'Structure Editor' with a chemical structure being drawn. The 'Drawing Editor' on the right shows the 'Markush' search type selected.

Search by **Markush** to find patents that contain Markush structures which meet your structure query requirements.

- 1 To begin, click **Markush**.
- 2 Click the picture of the structure drawing window to launch the **Structure Editor**.
- 3 Draw your structure.
- 4 Specify the type of structure search and then click **OK** to transfer the structure and type of search to the search page.

SELECT...	IF YOU WANT TO RETRIEVE...
Variable only at the specified positions	Structures in which substitution is only allowed where it is specifically indicated by R-groups or other variable atom or bond features
Substructure of more complex structures	Structures in which substitution is allowed on all positions where it is not explicitly blocked

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure substructure > substances (535)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

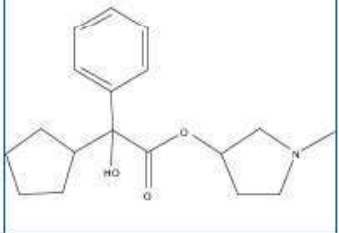
REACTIONS

- Reaction Structure

SUBSTANCES: MARKUSH ?

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF

Search Type:

- ☐ Allow variability only as specified
- ☒ Substructure

5 Search

5 Click **Search** to find the answers that meet your query requirements.

SciFinder is useful for a preliminary patentability or freedom to operate search. For a thorough patentability search, consult a patent attorney, information professional or Science IP at CAS.

Tip

A Markush search is a great way to extend a structure search, especially if you did not find any substances with a structure search and are interested in patentability.

Now what?

After you click Search, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Reference Answer Set."

Search by Molecular Formula


The screenshot shows the SciFinder web interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar contains two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'SUBSTANCES', several options are listed: 'Chemical Structure', 'Markush', 'Molecular Formula' (which is highlighted with a blue bar and a callout '1'), 'Property', and 'Substance Identifier'. The main content area is titled 'SUBSTANCES: MOLECULAR FORMULA' and contains a search box with the text 'C18 H25 N O3' (callout '2'). Below the search box, there are 'Examples:' listed as 'H4SiO4' and '(C3H6O.C2H4O)x'. A blue 'Search' button is located below the examples (callout '3').

1 To begin, click **Molecular Formula**.

2 Enter the molecular formula into the query box.

3 Click **Search**.

Tip

Click a  to access context-specific online help. Click it next to Molecular Formula to see the help messages that provide many examples about how to search Molecular Formulas for polymers, salts and structure repeating units.

Molecular Formula Query Guidelines

- Specify the full molecular formula; include the total number of hydrogens (Hill Order not required).
- For best results, it is useful to separate each element symbol and its count with a space.
- Capitalize the first character for multi-character symbols, and use lower case for the second letter (i.e., Si, Cl, Fe).
- You can search two isotopes: D = deuterium and T= tritium.

Now what?

Molecular Formula searches often retrieve many isomeric substances and it is necessary to narrow answers. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Substance Answer Set."

Search by Property

The screenshot shows the SciFinder 'Search by Property' interface. On the left, a sidebar contains two sections: 'REFERENCES' and 'SUBSTANCES'. The 'SUBSTANCES' section is active, showing a list of search criteria: Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. A blue diamond with the number '1' points to the 'Property' option. The main area is titled 'SUBSTANCES: PROPERTY'. It features two radio buttons: 'Experimental' (selected) and 'Predicted'. A blue diamond with the number '2' points to the 'Experimental' radio button. Below the 'Experimental' radio button is a dropdown menu showing 'Density (g/cm³)' and a text input field containing '>10'. A blue diamond with the number '3' points to the input field. Below the input field, examples are listed: 'Examples: 44, 25-35, >125'. Below the 'Predicted' radio button is a dropdown menu showing 'Select Property...' and an empty text input field. Below the input field, examples are listed: 'Examples: 44, 25-35, >125'. At the bottom of the main area is a large blue 'Search' button, with a blue diamond and the number '4' pointing to it.

1 To begin, click **Property**.

2 Click the appropriate radio button to select either **Experimental** or **Predicted** property. Next, click the drop-down menu and select the specific type of property you want to search.

3 Enter the value or range.

4 Click **Search** to retrieve the answers that meet your query requirements.

Tip

If your property search results in a large answer set, you can narrow it by specifying additional criteria using **Refine** or **Analyze**.

Now what?

After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Substance Answer Set."

Search by Substance Identifier

Explore ▼ Saved Searches ▼ SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier**

SUBSTANCES: SUBSTANCE IDENTIFIER ?

103-90-2
Endoxane
PVC

Enter one per line.
Examples:
50-00-0
999815
Acetaminophen

Search

1 To begin, click **Substance Identifier**.

2 Enter up to 25 substance identifiers, one per line, in the query box.

- A substance identifier can be a CAS Registry Number® or a chemical name.
- Simple chemical names, trade names, abbreviations and common names often result in relevant answers.

3 Click **Search** to retrieve the answers which meet your query requirements.

Tip

For complex, systematic names such as some IUPAC names, consider searching by the chemical structure. It is often easier to match a structure rather than it is to match all of the chemical symbols and punctuation exactly as it is entered into the database.

Now what?

After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion PDF document titled, "How to... Work with a Substance Answer Set."

How to...Create a Reaction Answer Set

Find all relevant reactions based on criteria you specify

Search the world's largest, publicly available source of reactions and quickly find highly relevant results, no matter the size of your answer set. This How to Guide explains a variety of ways to design your reaction search. Refer to "How to... Work with a Reaction Answer Set" to learn about tools and techniques to easily sort, organize and narrow your results and find the most relevant answers. For more training resources, consult the online Help or visit www.cas.org/training/scifinder.


Begin a Reaction Search

The screenshot displays the SciFinder web interface. On the left, the navigation pane shows categories: REFERENCES, SUBSTANCES, and REACTIONS. Under REACTIONS, 'Reaction Structure' is selected and highlighted with a blue bar and a callout '1'. The main content area is titled 'REACTIONS: REACTION STRUCTURE'. It features a 'Structure Editor' section with 'Java' and 'Non-Java' tabs, a 'Click to Edit' button, and a 'Search Type' section with radio buttons for 'Allow variability only as specified' and 'Substructure'. Below this is an 'Import CXF' button and a large blue 'Search' button. At the bottom, there are links for 'Advanced Search' and a checked 'Always Show' checkbox. A 'ChemDraw' integration box is also present, encouraging users to launch searches directly from ChemBioDraw Ultra 14. A callout '2' points to the 'Click to Edit' button in the Structure Editor.

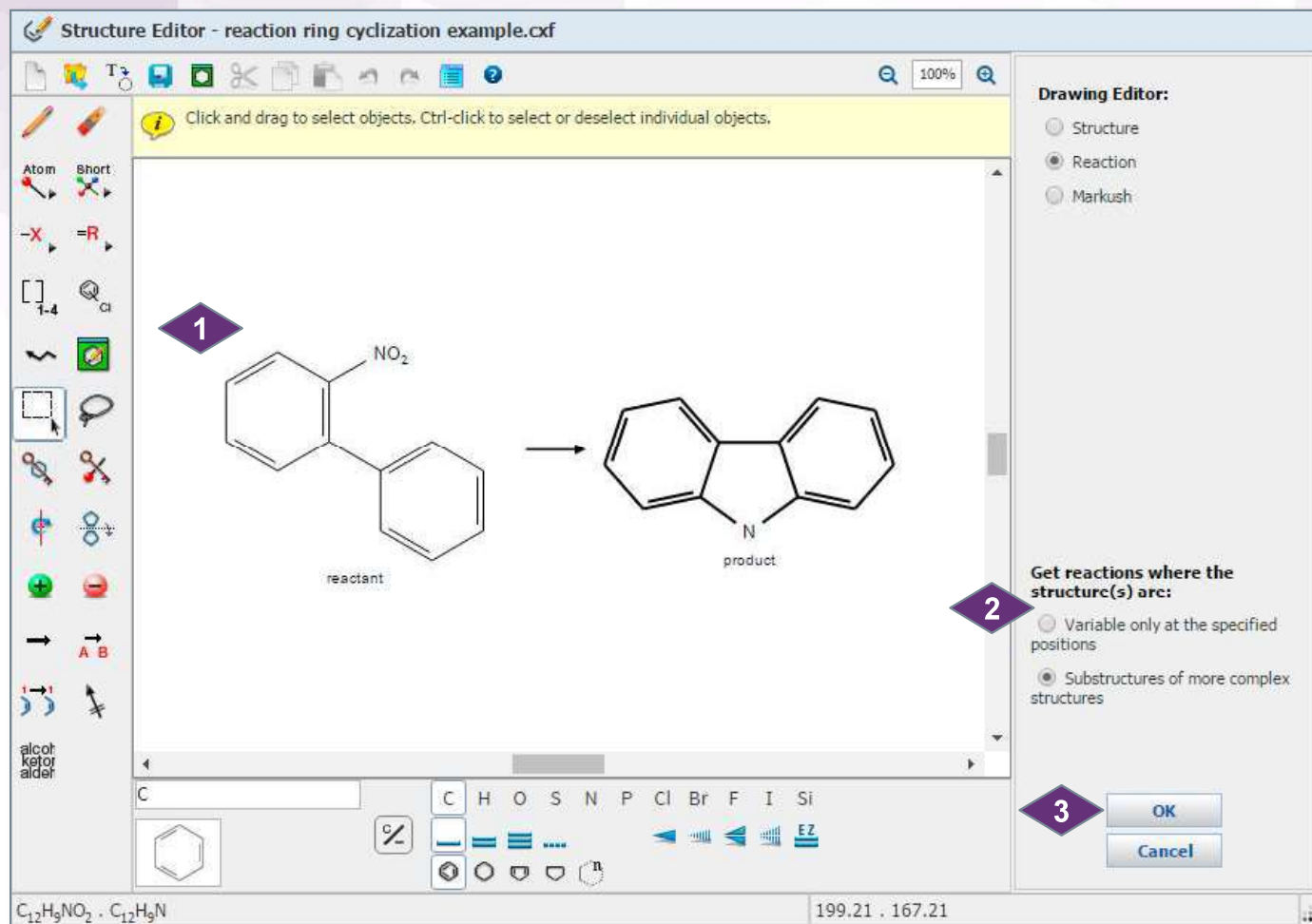
1 To begin, go to the left navigation pane and click **Reaction Structure**.

2 Click either the **Java** or **Non-Java** tab to select the type of **Reaction Editor** that you want to use. Then click the picture of the reaction drawing window to launch the **Reaction Editor**.

Tip

Click  to access context-specific online help.

Draw the Reaction



1 Draw your reaction.

Learn how to draw in the **Reaction Editor** with the following tutorials, available in the online **SciFinder Help**:

- “Draw Structures”
- “Draw Reactions”

2 Select the type of reaction search that you want to conduct.

Select...	If You Want To...
Variable only at the specified positions	Prohibit substitution at all atoms (except variables and R-groups) and prohibit additional ring fusion.
Substructure of more complex structures	Allow additional substitution and ring fusion.

3 Click **OK** to transfer the reaction and type of search to the search page.

Tip on Stereo Searching

CAS scientists report structure data as it appears in the original document. If no stereo is identified, then the molecule is listed as a “flat” (2-dimensional) structure. If you search stereo bonds, you can miss relevant data that was listed in the literature only in a 2-dimensional format, whereas searching the flat structure will retrieve both 2-dimensional and 3-dimensional (stereo) structures.

Search the Reaction

Explore ▾ Saved Searches ▾ SciPlanner

REACTIONS: REACTION STRUCTURE ?

Structure Editor:

Java Non-Java

Search Type:

☐ Allow variability only as specified

☒ Substructure

Click image to change structure or view detail.

Import CXF

ChemDraw

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

Search

1 Advanced Search ☒ Always Show

2

Solvents [Select Solvents](#)

Non-participating Functional Groups [Select Groups](#)

Number of Steps

Examples: 1, 1-3, 1-, -3

Classifications

☐ Biotransformation ☐ Non-catalyzed

☐ Catalyzed ☐ Photochemical

☐ Chemoselective ☐ Radiochemical

☐ Combinatorial ☐ Regioselective

☐ Electrochemical ☐ Stereoselective

☐ Gas-phase

Sources

☒ Any source

☐ Patents only

☐ Sources other than patents

Publication Years

Examples: 1995, 1995-1999, 1995-, -1995

3

When you click **OK** in the **Reaction Editor**, your reaction and **Search type** are transferred to the reaction search page.

1 (optional) Click **Advanced Search** to see additional search options.

2 (optional) Select limiters, such as **Number of Steps**, to further restrict your search.

3 Click **Search**.

Tip

The limiters are available as part of the **Refine** and **Analyze** functions, so it is often advantageous to start with a broad search and narrow the answer set later.

Now what?

After you click **Search**, SciFinder will retrieve the answers which meet your query requirements. To learn about working with the answers, please see the companion document titled, "How to... Work with a Reaction Answer Set."

Other Ways to Create a Reaction Answer Set

You can also create a reaction answer set after you get either reference or substance answers.



1 After you get a reference or substance answer set, click **Get Reactions** on the toolbar.

2

2 After you get a substance answer set, mouse over a substance until a blue box appears around it. Click the double blue arrows in the upper right, and then select either **Synthesize this...** or **Get Reactions where Substance is a >** and select the reaction role for the substance.

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