SciFinder®

SciFinder（Web Version）Structure Diagram
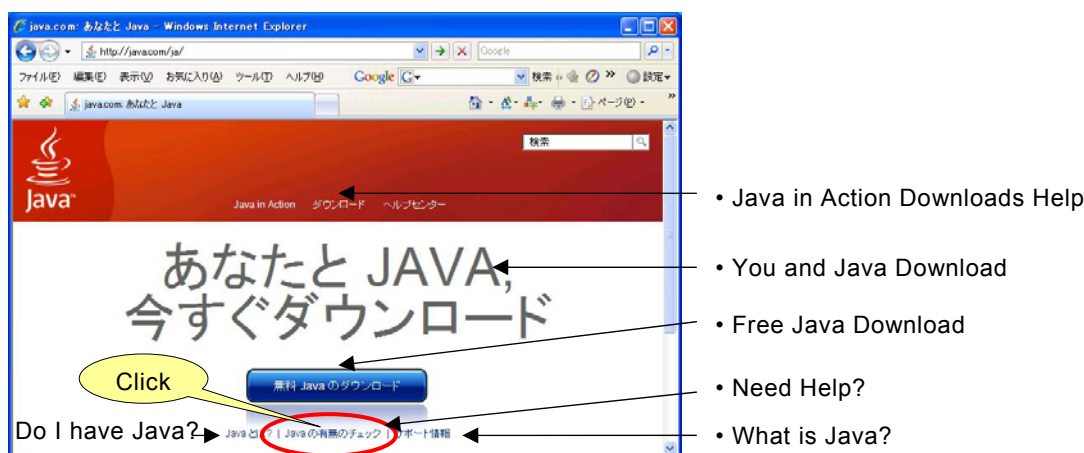
Table of Contents ....

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JAICI

Japan Association for
International Chemical Information
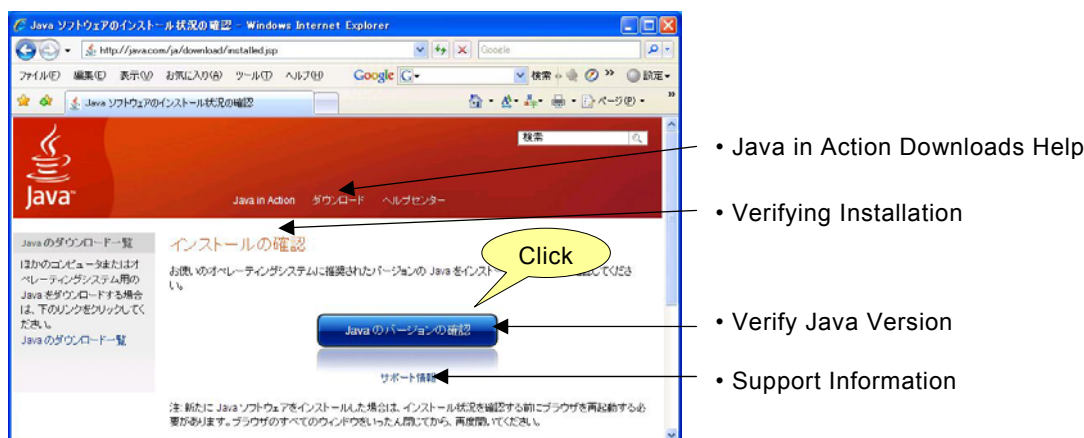
Verify Java version and installation guide

In order to use structure search and reaction search on SciFinder (Web version), you need to have Java plugin (Java Runtime Environment (JRE) 6 Update x) installed. System requirement details can be found on the last page of the "Instruction Manual". Below are version checking and installation process for Windows.

The snap shots below are excerpts from Sun Microsystems, Inc. website. All trademarks and logos associated with Sun, Sun Microsystems, Sun logo, and Java are trademarks and registered trademarks of Sun Microsystems., Inc. America in the United States and other countries.

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① Go to Sun Microsystems, Inc. Java site (http://www.java.com/ja/). Click on the "Do I have Java?" at the bottom part of the screen.

- Java in Action Downloads Help
- You and Java Download
- Free Java Download
- Need Help?
- What is Java?

② In the newly uploaded screen, click the "Verify Java version".

- Java in Action Downloads Help
- Verifying Installation
- Verify Java Version
- Support Information

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※Macintosh Users

Macintosh has verified Java compatibility on Mac OS X 10.4.11 and later, and Mac OS X 10.5 and later.
To get an updated version of Java, use the Software Update from Apple Menu, and it can be automatically setup.
You can also download it from Apple website.

③ If you don't have Version 6 installed, then click the "Download Java now".
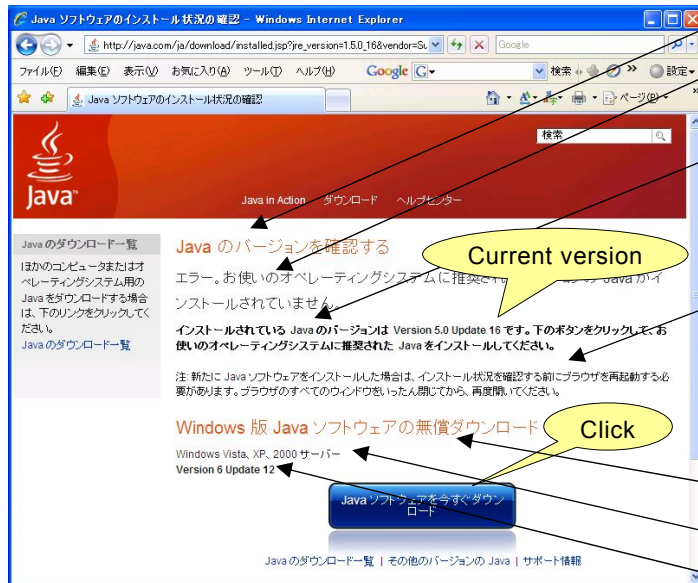
- Verifying Java Version
- Error. You don't have the recommended version installed for your operating system.
- The installed Java version is Version 5.0 Update. Please click the button below to install the recommended Java version for your operating system.
- Note: If you recently completed your Java software installation, you may need to restart your browser (close all browser windows and re-open) before verifying your installation.
- Download Free Java for Windows
- Windows Vista, XP, 2008 server
- Version 6 Update 12

④ If a yellow information bar is displayed at the top of the screen, click the bar and select "Install ActiveX control".
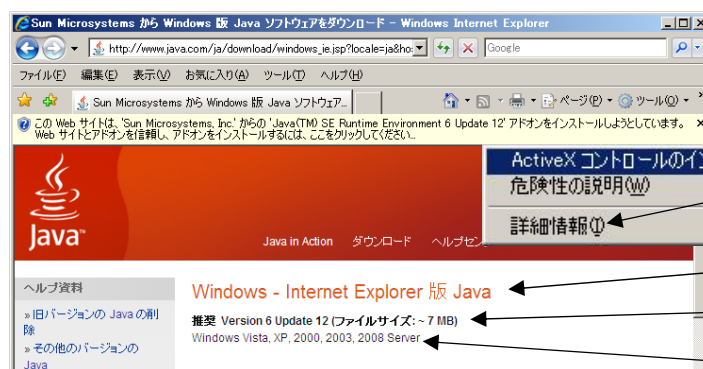

- Install ActiveX control
- Security description
- Detailed information
- Java for Windows – Internet Explorer
- Recommended Version 6 Update 12 (file size: 7 MB)
- Windows Vista, XP, 2000, 2003, 2008 Server

⑤ In the dialog box below, click "Install", and Java will begin to install.
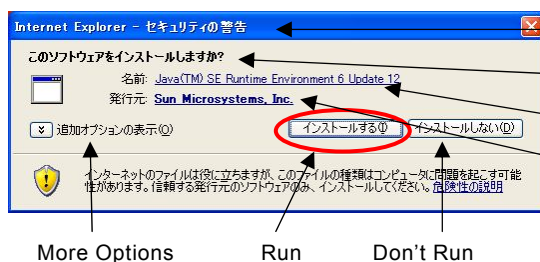
- Internet Explorer – Security warning
- Do you want to run this software?
- Name: Java™ SE Runtime Environment 6 Update 12
- Publisher: Sun Microsystems, Inc.

More Options   Run   Don't Run

⑥ Wait until the download completes.
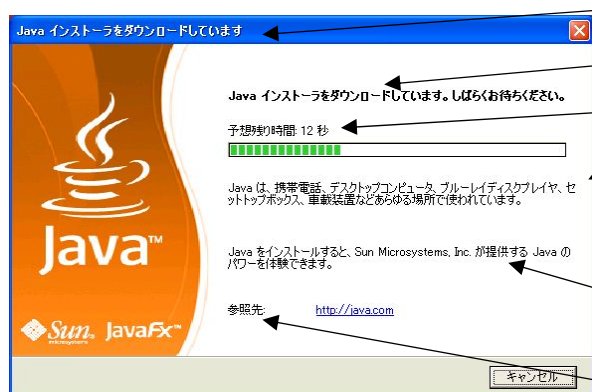
- Downloading Java Installer.
- Downloading Java Installer. Please wait.
- Estimated time left 12 sec
- Java is found everywhere – on mobile phones, desktop computers, Blu-ray Disc players, set top boxes, and even in your car.
- By installing Java, you will be able to experience the power of Java, brought to you by Microsystems, Inc.
- Visit us at java.com
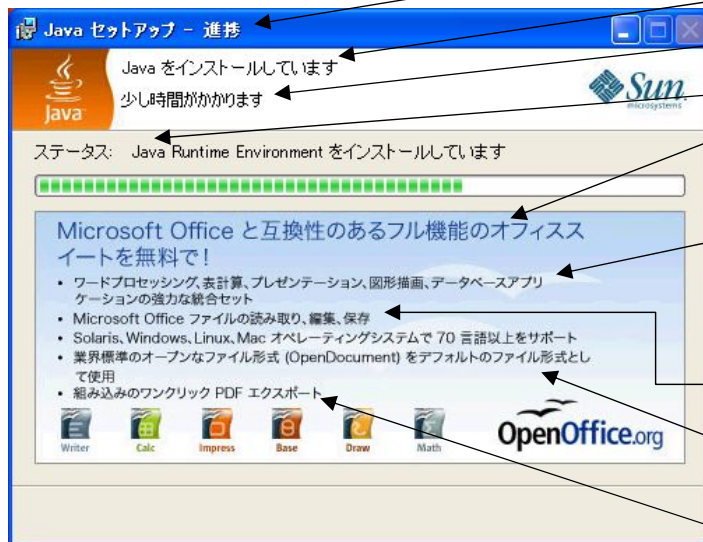
⑦　Read the User Agreement and click "Agree".

Java セットアップ － ようこそ

Java(TM) および JavaFX(TM) へようこそ

Java を使用すると、インターネットの世界をより豊かに体験できます。

JavaFX は、Java を拡張するテクノロジで、あらゆる画面に没入型メディアとコンテンツを配信します。

インストールおよびアップデート処理の一環として、一部の匿名の情報が Sun に送信され、パフォーマンスの向上に役立てられます。この情報送信を無効にする方法を含む詳細については、http://java.com/data を参照してください。

使用許諾契約を表示...

製品をダウンロードするには、「同意」ボタンをクリックして使用許諾契約に同意する必要があります。

□インストール先フォルダの変更　　同意しない(D)　同意する(A) >

Display license agreement　　　　　Do not agree　　Agree

• Java Setup – Welcome

• Welcome to Java™ and JavaFX™

• By using Java, you will have a richer internet experience. JavaFX is a technology that enhances Java and distributes media and contents embedded in every screen.

• As part of installation and update process, a portion of user information will be sent to Sun, and will be used to improve the performance. Please visit http://java.com/data to find out how to disable this data transmission.

• To download the product, click "Agree" button and agree to the license agreement.

⑧　Wait until the installation is complete.

Java セットアップ － 進捗

Java をインストールしています

少し時間がかかります

ステータス：　Java Runtime Environment をインストールしています

Microsoft Office と互換性のあるフル機能のオフィススイートを無料で！

• ワードプロセッシング、表計算、プレゼンテーション、図形描画、データベースアプリケーションの強力な統合セット
• Microsoft Office ファイルの読み取り、編集、保存
• Solaris、Windows、Linux、Mac オペレーティングシステムで 70 言語以上をサポート
• 業界標準のオープンなファイル形式 (OpenDocument) をデフォルトのファイル形式として使用
• 組み込みのワンクリック PDF エクスポート

Writer　Calc　Impress　Base　Draw　Math

OpenOffice.org

• Java Setup – Progress

• Installing Java

• This may take a few minutes

• Status: Installing Java Runtime Environment

• Now you can have a full-featured office suite that's compatible with Microsoft Office for free!

• Powerful, integrated set of word processing, spreadsheet, presentation, drawing and database applications

• Reads, edits and saves Microsoft Office files

• Supports over 70 languages and Solaris, Windows, Links and Mac operating systems

• Uses industry-standard, open fire format (Open Document) as its default file format

⑨　When the screen below is displayed, click "Exit".

Java セットアップ － 完了

Java(TM) のインストールに成功しました。

インターネットで Java のパワーを活用できます。Java を使って何ができるのかについて、詳しくは http://java.com を参照してください。

「完了」をクリックすると、JavaFX ランタイムがダウンロードされます。JavaFX および変更を加える方法については、http://java.com/javafx を参照してください。

Java Update は、お使いのシステムに自動的にダウンロードされます。アップデートがインストール可能になると、そのことが通知されます。この機能を変更する方法については、http://java.com/autoupdate を参照してください。

Check

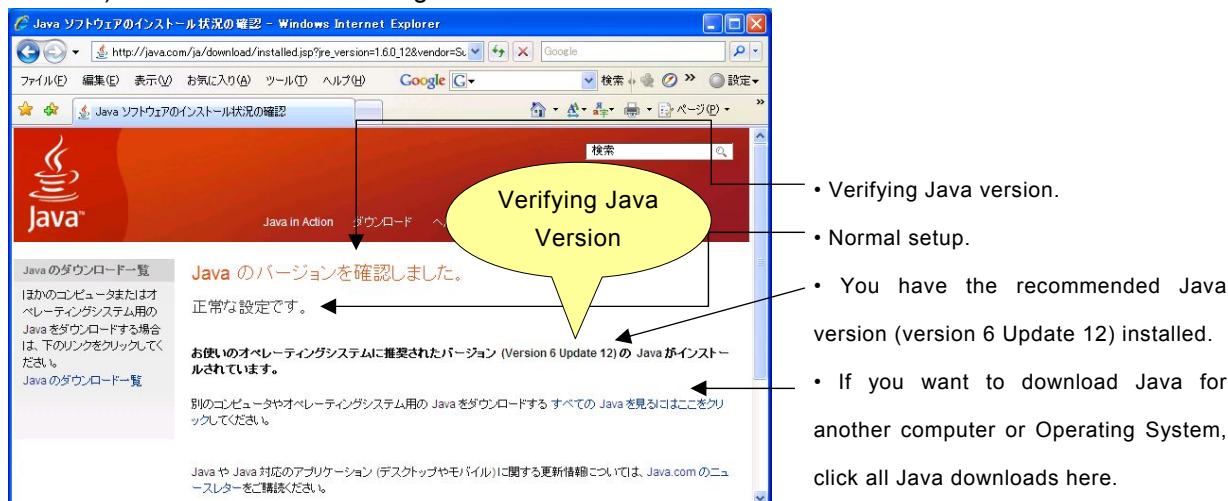☑ インストールを検証するため、ブラウザを再起動します

注：すべてのブラウザウィンドウが閉じられます。「完了」をクリックする前に作業内容を保存してください。

完了

• Java setup – complete

• Java™ installation is successful

• You cannot experience the power of Java on the internet. Go to http://java.com to find out in details what you can do with Java.

• JavaFX will be downloaded once you click close. Please visit http://java.com/javafx for details about JavaFX and on how to add changes to it.

• Java updates will automatically be downloaded. You will be informed of the latest update. To change this, see http://java.com/autoupdate.

• You need to restart your browser to verify the installation.

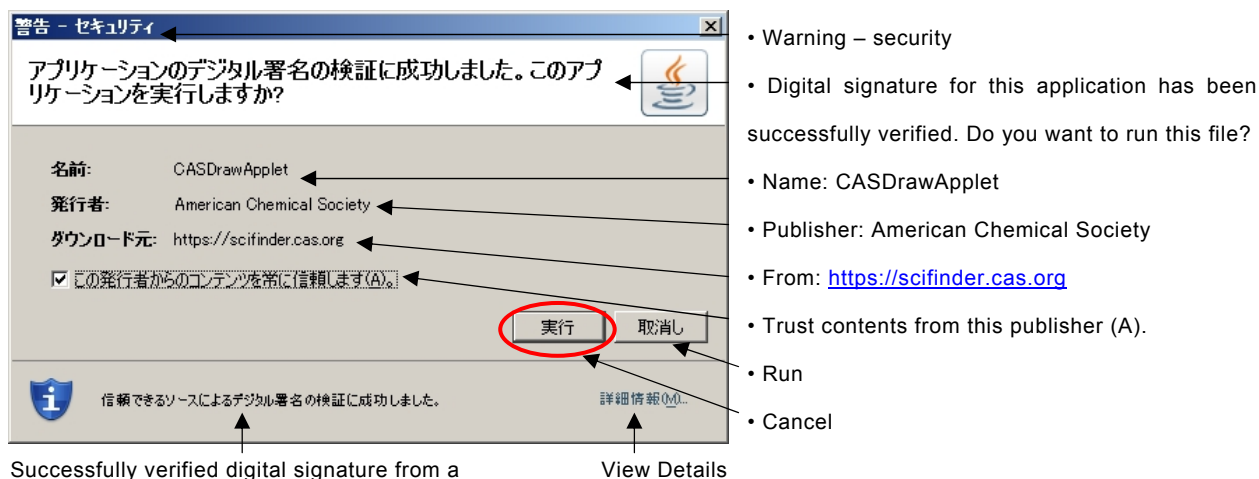• Note: Close all browser windows. Save all your work before clicking "Close"

⑩ You will be automatically directed to an installation verification website. Click the "Verify Java version", and it will verify if the installation was successful.

⑪ When "The setup is normal" is displayed, the Java setup is completed. Login to the SciFinder (Web version) and start the structure diagram screen.

• Verifying Java version.

• Normal setup.

• You have the recommended Java version (version 6 Update 12) installed.

• If you want to download Java for another computer or Operating System, click all Java downloads here.

⑫ When you started the structure diagram screen with SciFinder (Web version) for the first time, Java program execution confirmation screen will be displayed. Click "Execute" and the structure diagram screen will start. If a yellow information bar requesting your permission to execute add-ons appeared at the top of the screen, click the bar and select "Execute ActiveX control".

• Warning – security

• Digital signature for this application has been successfully verified. Do you want to run this file?

• Name: CASDrawApplet

• Publisher: American Chemical Society

• From: https://scifinder.cas.org

• Trust contents from this publisher (A).

• Run

• Cancel

Successfully verified digital signature from a trusted source.

View Details

– 5 –

Structure Diagram Screen

Exact match search

Substructure search

Similar structure Search

Reaction Diagram Screen

Exact match search

Substructure search

Vertical Tools Palette

In the vertical tool palette, you can find various tools to draw or change chemical structures. To use a tool, click on the icon. Then simply move the cursor to the drawing window, and the cursor will change its shape to the icon of the tool you have selected.

| Pencil tool | | Eraser tool |

Atoms menu tool

| Shortcut menu tool |

| X Menu tool | ◎

| R Group tool | ◎

| Repeat Group tool | ◎

| Variable Substituent Position tool | ◎

Chains tool

Templates tool

Selection tool

Lariat tool

| Lock Rings tool | ◎

| Lock Atoms tool | ◎

Rotating tool

Reverse tool

Positive charge tool

Negative charge tool

| Arrows tool | ▲

| Reaction Roles tool | ▲

| Atom Mapping tool | ▲

| Reaction Site tool | ▲

| Functional Group tool | ▲

◎ : Available only for substructure search or reaction search   ▲ : Available only for reaction search

Horizontal Tool Palette

Selected atom box

Frequently used atoms palette

Display scale box

Molecular formula

Bond palette

Rings palette

Stereo bond palette

Molecule mass

Reset atom/bond

Selected ring skeleton

Pencil Tool

Pencil is used for drawing nodes and bond. Atoms and shortcuts will be assigned to nodes.
When you click on the pencil tool icon, the cursor will change into a pencil, and you can link the selected atoms.

You can also change the nodes and the type of bond that are already in the window. First, select the node or bond. Then, move the cursor to the top of the node or bond you want to change. Make sure that the node or bond is highlighted, and then when you click, the node or the type of bond will be changed.

Shortcut Menu Tool

This tool is used for incorporating shortcuts in the structure.

Shortcuts				
CH	Bu-n	o-C_6H_4	CI_3	NH_2
CH_2	Bu-i	m-C_6H_4	CHO	NH_3
Me	Bu-s	p-C_6H_4	CN	NO_2
OMe	Bu-t	CF_2	C(O)CH_3	OH
Et	OBu-n	CF_3	CO_2H	OPO_3H_2
OEt	OBu-i	CCl_2	COOH	OSO_3H
Pr-n	OBu-s	CCl_3	COSH	PO_3H_2
Pr-i	OBu-t	CBr_2	CS_2H	SH
OPr-n	Ph	CBr_3	CSSH	SO_2
OPr-i	OPh	CI_2	NH	SO_3H

Close

When you click the *shortcut menu* icon, the shortcut menu will be displayed.

The shortcut selected on the shortcut menu will be shown in the selected atom box on horizontal tool palette. When you click on the drawing screen or on an existing node with pencil tool, the new shortcut will be displayed.

Terminal group shortcut is not allowed substitution, and its configuration does not include any kind of substituents. Even the Lock Atoms Tool (described below) cannot allow it to make substitution.

X Menu Tool

This menu tool is used to incorporate adjustable atoms in relation to query formulation for sub structure search, or reaction search.

Adjustable atom menu is displayed when you click the **X menu icon**.
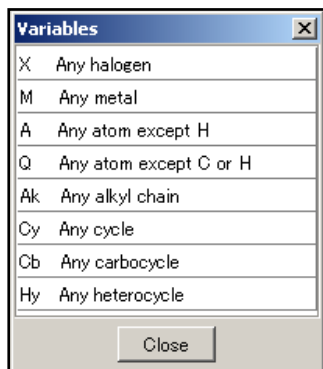
The selected adjustable atom on the X menu will be shown in the selected atom box on the horizontal tool palette. When you move the pencil tool over the drawing window or on top of an existing node and click, a new adjustable atom will be incorporated.

Variables

X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
Ak	Any alkyl chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle

Close

By default, Ak (carbon chain) is surrounded by a square. This means that substitution is not allowed. In this case, there will be no substituents attached to Ak, and the search will be limited to linear chain, branching or unsaturated carbon chain. To allow for Ak substituents, click the Lock Atoms tool and move the cursor on Ak. Once Ak is highlighted, click it and the square will disappear. With Ak allowed for substitution, no matter how the carbon chain is substituted, it can be searched. (For details on substitute prohibition and allowance, see Lock Atoms Tool section.)

R Group Tool
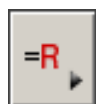
This menu tool is used to incorporate R-group into query formulation for sub structure search, or reaction search. You can define more than 2 substituents for one R-group (Maximum 20 substituents).

When you click the **R Group Tool icon**, the R-group Definitions dialog box will be displayed with R1 highlighted.

R-group Definitions

Atom   Short   −X

R1 =	
R2 =	
R3 =	
R4 =	

Close
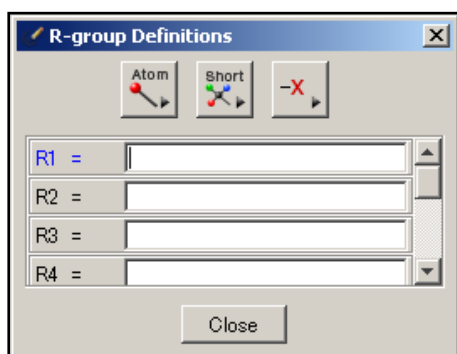
To define R1, click the **Atom, Short, X menu** button in the R-group Definitions dialog box. Select atom, shortcut and adjustable atom respectively. When multiple items are selected, each of them will be separated by comma, and stored in R1.

When you need another R-group, move your cursor to R2, R3, until R10. You can define a maximum of R-group.

To incorporate the R-group in the structure, choose the R-group using R-group Definitions dialog box and use the pencil tool to add it to the structure.

Repeat Group Tool

SSM RXN

This tool is used when drawing a structure that includes repeats (It can also be used to drill-down structures).
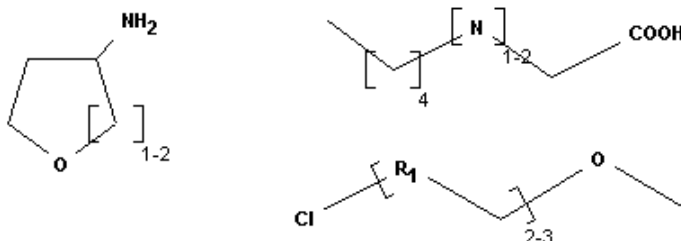
1. After drawing the foundation skeleton that includes the repeating group, click the **Repeat Group tool** icon.
2. Click and drag the cursor over the group to be repeated. The selected group will be highlighted in red.
3. In the From: To: box located at the top of the drawing screen, enter the number of repeats, then click **OK**.
4. The repeated group will be bracketed, and the number of repeats will be shown at the lower right corner of the bracket.

Note: Repeat Group Tool Limitation

- The repeat range is 0 – 20.
- Assigning repeats to Ak only is not possible
- Stereo bond is not possible to assign.
- It is not possible to include the (reaction search only) atomic mapping and reaction site in the repeat range.
- In exact match structure search and similar structure search, only fixed value can be used (entering the same number for both the From: and To: boxes).

Examples

Variable Substituent Position Tool   SSM RXN

This tool is used for assigning variable substitution position of a substituent to a ring or ring system.

1. After drawing the foundation skeleton and substituent separately, click on the **Variable Substituent Position Tool** icon.
2. Click the substituent and drag it to its substitute position. A line will appear between the substituent and substitute position.
3. When you release the drag, the line between the substituent and substitute position will disappear, and a thick line can be seen between the ring and the substituent. You can assign the variable substituent position with this line.
4. To assign multiple substitute position, repeat steps 2 - 3. You will need to assign at least 2 or more substitute positions.
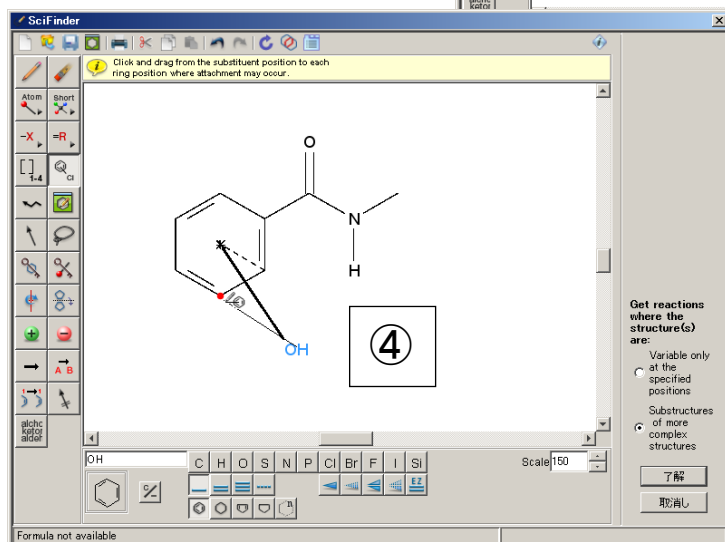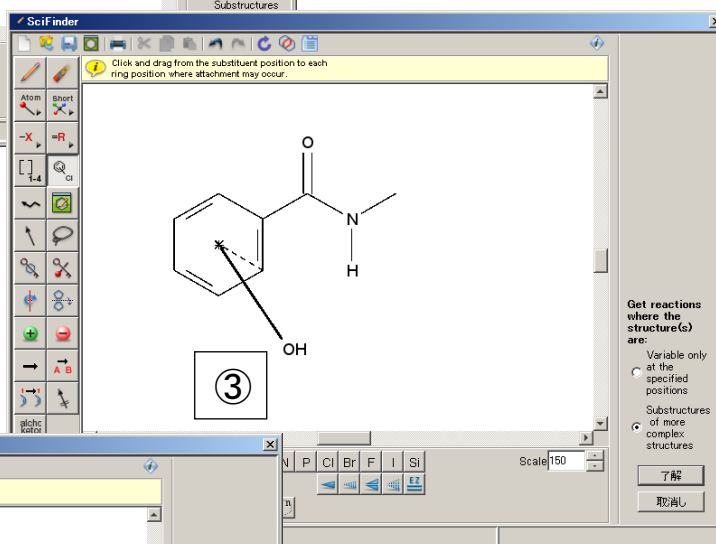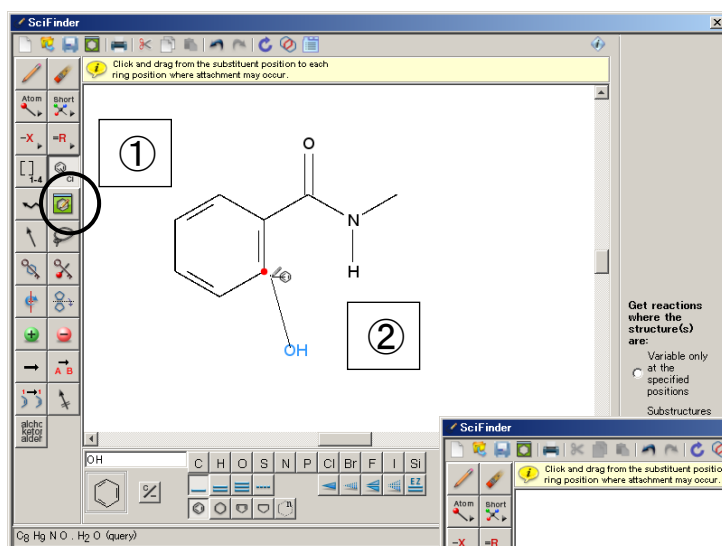
Things to consider when using Variable Substituent Position Tool:

- The maximum number of substituents is 20.
- Only the node of a ring or ring system can be linked to a substituent. It cannot be assigned to a chain node or assigned to multiple ring or ring system simultaneously.
- If you want to assign the presence of multiple substituents, draw as many substituents as you need, then assign each of them the variable substituent position.
- Lock Atoms can be assigned to substituents (prohibiting additional substituents to a specified node).
- You can map the substituent in reaction search.
- Only non-metal atoms, C (Halogen atom), Q (with exception of C and H atoms) and A (except H atom) can be assigned as substitute position.
- Lock Atoms can be assigned to substitute positions.
- The bond between the ring and substituent cannot be assigned as stereo bond. (However, it is possible to assign single bond, double bond, triple bond, and undefined bond.)
- In reaction search, the bond between the ring and substituents can assign the reaction site.

Examples
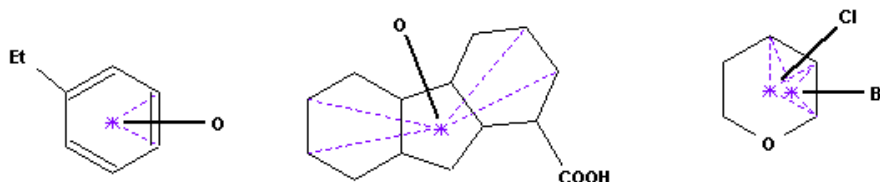
Lock Atoms Tool   SSM   RXN

  Lock Atoms tool is used to prohibit from adding substituents to a specific node in sub structure search and reaction search queries.

To prohibit from adding substituent to a node, click the **Lock Atoms tool icon**. The cursor will assume the shape of this icon.

Bring the end of the key cursor close to the node until the node is highlighted, then click it. A square will surround the node to show that adding substituent is not allowed. This step can be performed for multiple nodes on the screen.

By definition, with the exception of Ak, terminal shortcuts such as Me group are prohibited from subsituent addition. So it is not possible to surround the terminal shortcuts with a square using the above mention step.
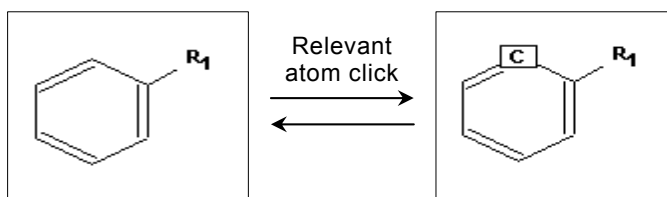
Lock Rings Tool (Lock ring fusion or formation tool)

The Lock Rings tool is used to prohibit the rings from fusing together and to isolate it in sub structure and reaction search queries. It is also used in prohibiting a chain from becoming a part of a ring.

To isolate a ring and chain, click the **Lock Rings tool** icon. The cursor will change its appearance to this icon.

Bring the end of the key cursor close to the ring or a segment of the chain until the ring or chain segment is highlighted, then click it. In order to indicate that the ring is prohibited from fusing, the line will become thick. You can perform this step for multiple rings or chains on the screen.
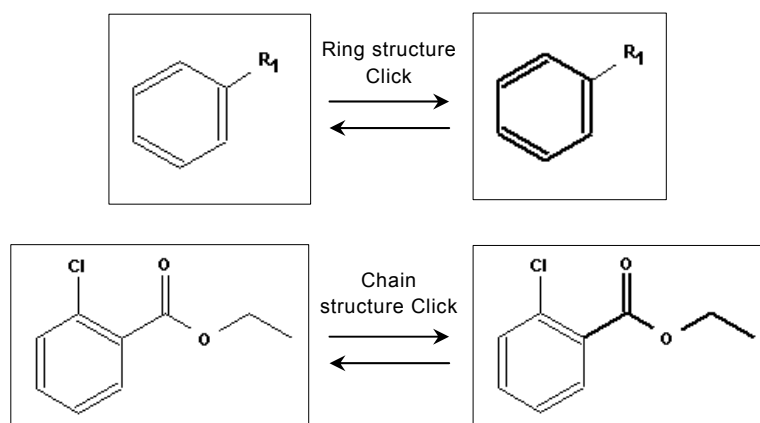
Arrows Tool   RXN
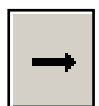
This arrows tool is used in the reaction search query. It automatically assign chemical reaction role to the structure found in the reaction diagram window.

To draw the reaction arrow, click the **Arrows tool** icon. The cursor will change to a horizontal arrow. Click the mouse at an appropriate position and drag the cursor in the direction of the reaction.

If a structure is already in the reaction diagram window, the role will be automatically assigned after taking into consideration the relation of its arrow and position. The previous role will be overwritten. When you want to change the automatically assigned role, use the Reaction Roles tool, which will be discussed next.

Reaction Roles Tool `RXN`
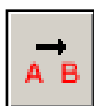
The Reaction Roles tool is used to assign a role such as Reactant/Reagent, Product or Any Role to a chemical structure in the reaction search query.
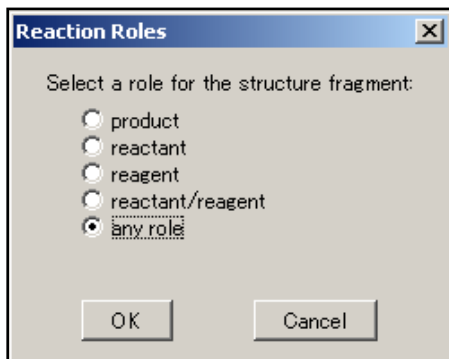
To assign a role, first, click the **Reaction Roles tool** icon, then match the cursor to the structure and click. The Reaction Roles dialog box will appear. Assign the role you want and click **OK**. A label indicating the role will be displayed beneath the assigned structure.

To substitute the role that had been assigned, click the *Reaction Roles tool* again and match the cursor to the structure or label. Click and the Reaction Roles dialog box will appear, select a different role and click **OK**. The previous role will be overwritten and a new label will be displayed beneath the structure.
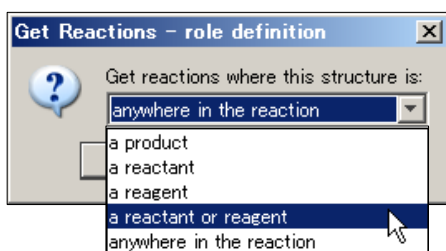
To automatically assign roles, the Arrows tool discussed on the previous page is used. If you are trying to search for reactions that have structures with unassigned roles, the Get Reactions - role definition dialog box will be displayed. If you do not want to assign roles, you either select "anywhere in the reaction" or click **Cancel** to return to reaction diagram window and re-assign the role.

Functional Group Tool (See page 11) can assign non-reacting (functional group that do not react).
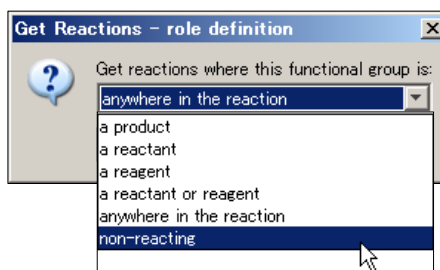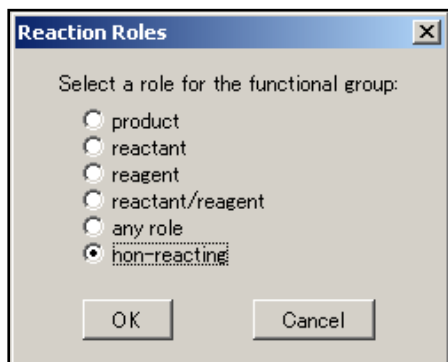
Reaction Site Tool `RXN`

The Reaction Site tool is used for marking the bond whose condition changes along with the reaction in reaction search query. When you click this icon, the cursor will assume the shape of this icon.

To mark the bond, click the **Reaction Site tool** icon. Bring the pointer of the cursor close to the bond you want to mark, and click when the bond is highlighted. To indicate that it is marked, a vertical double line is drawn across the bond.

You can mark the reaction formula as much as you like, but when you mark a bond, your search result will be reduced.

Atom Mapping Tool   RXN
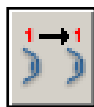
Atomic Mapping tool is used to indicate the relationship of the atoms between reactants and products. The relationship of the reactants and products atom is indicated with a label of a same number starting with 1.

To indicate the atom pair, first draw a reactant and a product. Then, click the **Atom Mapping tool** icon. The cursor will assume its shape when you click the **Atom Mapping tool** Icon. Match the head of the cursor to the reactant you want to indicate, and click it when it is highlighted. A number label will be attached to the node of the reactant. Next, when you click the node of the corresponding product, a label with the same number as the reactants will be attached to the node.

To change or delete the labels, select the Eraser tool and click. Both the reactant and product label will be deleted, and all the number labels that come after the deleted number will go down one value. You can create as many atom pair as you need, but as the atom pair increases, the search result will be reduced.

Functional Group Tool   RXN

When you use the Functional Groups tool, you will be able to draw a reaction that includes functional group name.
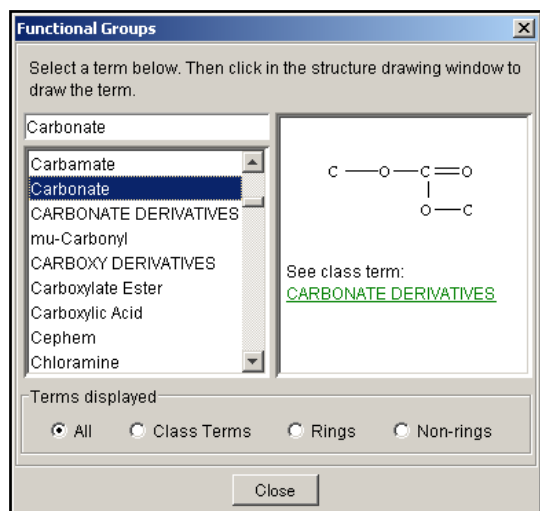
Functional Groups dialog box will be displayed once you click the Functional Groups tool icon, and you can select the functional groups you want to search.

When you select a functional group, the corresponding structure will be displayed on the right.

Roles can be assigned to functional groups using Reaction Roles tool or Arrows tool. The roles assigned to functional groups can also be selected as "non-reacting".
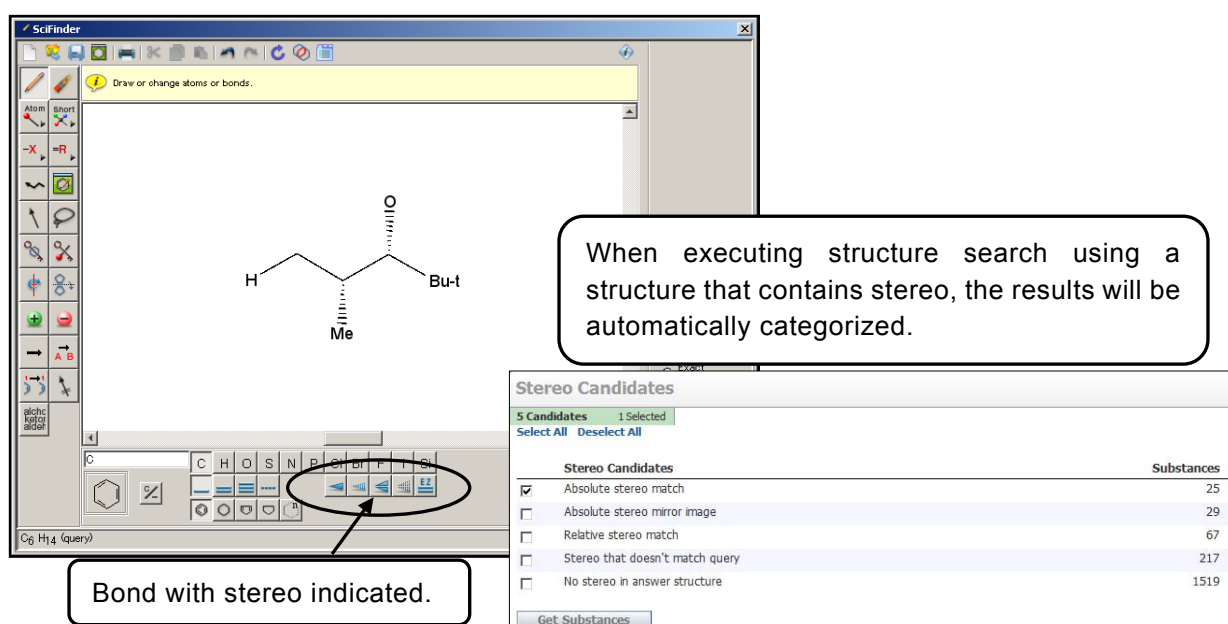
You can also perform a search with a combination of functional group and structure.

Stereo Bond Palette   `SSM`

   This palette is used to indicate single bond and double bond geometric isomerism, asymmetric carbon molecular conformation and the like. From left, there are "single bond that faces this side of the screen", "single bond that faces the back of the screen", "double bond that faces this side of the screen", "double bond that faces the other side of the screen", and "E, Z double bond" types of bond. These bonds will be ignored in reaction search.

   When you click an icon on the palette, that bond will be defaulted and highlighted. When you are searching a structure that has stereo bond, the results are automatically categorized into a structure where the stereochemistry and absolute structure are a match, its enantiomer, a structure where the stereo structure is relatively a match, a structure where the stereochemistry is not a match, a structure without stereo information and the like.

When executing structure search using a structure that contains stereo, the results will be automatically categorized.
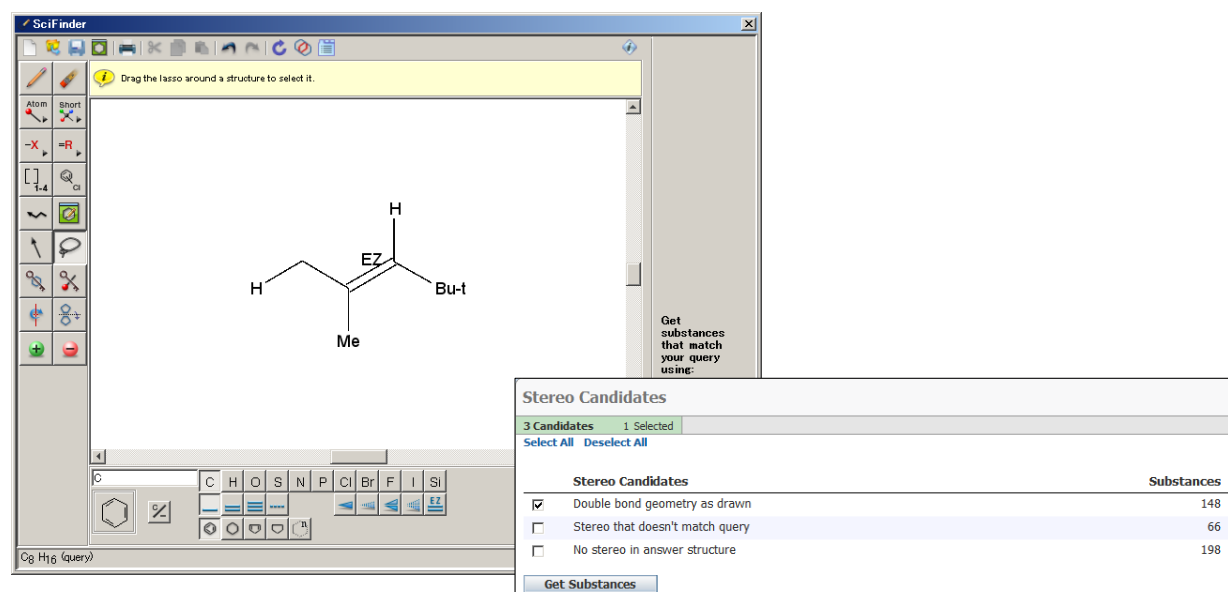
Bond with stereo indicated.

Stereo Candidates	Substances
5 Candidates 1 Selected	
Absolute stereo match	25
Absolute stereo mirror image	29
Relative stereo match	67
Stereo that doesn't match query	217
No stereo in answer structure	1519

   Even for geometric isomers, the search results can be categorized into geometric isometric match, not matching and not indicated.

Stereo Candidates	Substances
3 Candidates 1 Selected	
Double bond geometry as drawn	148
Stereo that doesn't match query	66
No stereo in answer structure	198

Appendix 1. Smartsearch：How the structure search is setup

1. What is Smartsearch?

When a chemical structure is drawn and structure search is performed, a list of substances is displayed. In this process from drawing to displaying the search result, a search function called Smartsearch is working within the SciFinder to maximize the number of results for a structure query.

■ Smartsearch Features

- Read the chemical structure drawn in the structure diagram screen, and considered the drawing various prerequisites.
- Interpreted the structure query created from various aspects, and try to include every substance related to the structure query in the result.

Note: The Smartsearch function is executed with perfect match structure search and substructure search.

2. Specifically, what does Smartsearch do?

■ Smartsearch automatically search for all **substances with the same atomic configuration and bonding** as the query. The results include the following substances.

- ・ Substances that matched perfectly to the structure query
- ・ Stereoisomer's
- ・ Geometric isomers
- ・ Tautomers (Including keto-enol tautomeric pair) and coordinate compounds
- ・ Compounds with electrical charge
- ・ Radicals and radical ion
- ・ Substances containing isotope
- ・ Structure monomer of polymers

■ Specific examples:

・Smartsearch will automatically consider the different position of the single bond or double bond in tautomers such as keno-enol or conjugated system bond, and include them in the result. For example, should a search that was done using one of the following structures, a search that considered other structures will be performed.
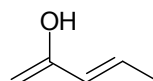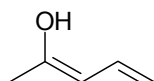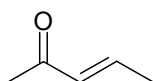
・The tautomers due to different hydrogen bond position within the molecule will also be automatically considered. For example, should a search was done using one of the following structures, a search that considered other structures will be performed.
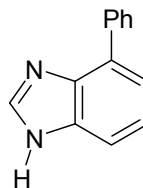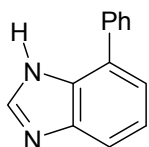
・In structure queries that include metal atoms, Smartsearch will also search for substances with metal atoms that had moved to another position within the molecule. For example, even though the bond with the metal was expressly drawn in the query, it will be searched without the bond. In addition, hydrates are also automatically in the search range. Metal atoms are defined as elements other than these following elements.

> H, B, C, N, O, F, Si, P, S, Cl, As, Se, Br, Te, I, At, He, Ne, Ar, Kr, Xe, Rn.

For example, when searching from the structure on the left (HMg-CH2-CN), the 6 structures on the right will also be included in the result list.
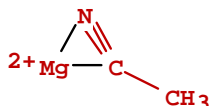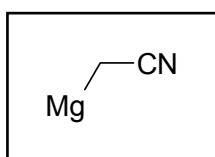
・For fluoresce and phthalein compounds, even if either one, open ring or closed ring form is drawn, the search will automatically be done for both structure. The same goes for glucose and hemiacetal.

For example, when a search was done for the structure on the left, the structure on the right will also be included in the list.
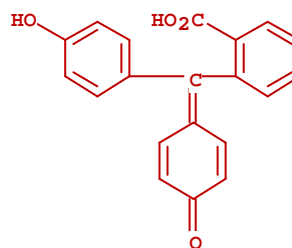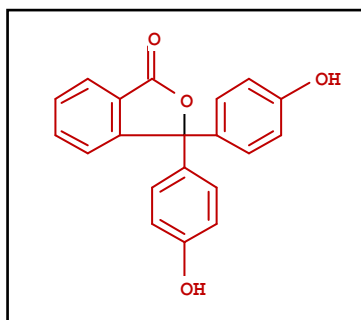
・In the arsenic halide or phosphorus halide structure, Smartsearch will consider cases where halogen atom is ① an ion, ② bonded to arsenic or phosphorus atom, ③ bonded to other halogen atom.

For example, when searching using the structure on the left, the two structures on the right will also be searched.
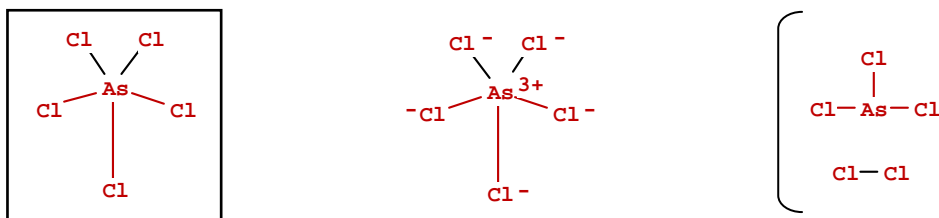
・For structure isomers, if stereo bond is included in the query, the result displayed would have been automatically analyzed for the structure isomer type. If the stereo bond is not included, all substances will be included in the result and displayed.

・As exceptions, special results will not be included to polymers, complex carbohydrates, array, alloys, tabular format inorganic substances, and radical ions. However, if these happened to be a match to the structure of the query, they will be included in the result.

In the structure search, ***rather than the accuracy of the result, the priority is comprehensiveness and ensuring nothing is overlook in the search***. Therefore, it is also possible to find substances that are not intended in the result. However, by using tools such as Keep Selected or Refine Substances, the results can be narrow down. Especially, when using Precision Analysis function during structure search, results with low relevancy can be very well excluded.
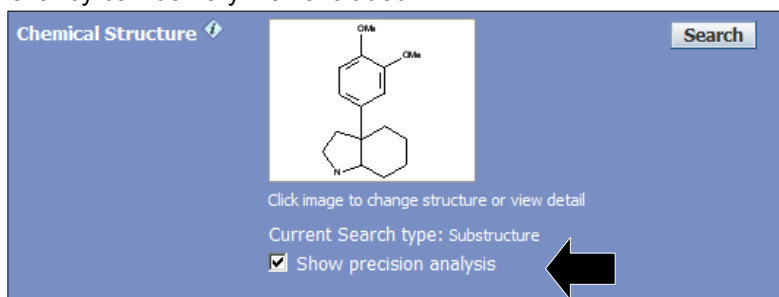
Check the "Show precision analysis" and execute structure search. The result will be automatically categorized.

Results that included narrowed down tautomers and zwitterions.

Results that included narrowed down tautomers and zwitterions.

Results that included tautomers and zwitterions widely.

Other results

When you want to limit to substances that belong to a specific category, check the category and click ***Get Substances***.

At the end, the substances will be narrowed down to almost the same substances to the naked eye. Even in this situation, it does not mean that the exact same substance can be found repeatedly in the result list, but its stereochemical elements maybe different. Click the **CAS registry number** and verify the difference from the substance name.

3. *Perfect Match Structure Search and Substructure Search*

This section explains how Smartsearch work with perfect match and substructure search.

Perfect Match Structure Search

Once the Perfect Match Structure Search is executed, the Smartsearch function will start to work, and substances such as examples given will be included in the result. Polymers, compound, salt and the like will also be automatically covered. To limit the result to specific substances, check the required Characteristic(s), Class(es) in the structure search window.

In Perfect Match search, you are not allowed to add to substituent as you like besides the substituents expressly drawn in the query. In other word, in perfect match search, free atoms do not exist in substitutions, and bonds that have nothing drawn basically will be defaulted to H (hydrogen). Therefore, when performing a perfect match, the result will be the same whether you draw the H or not in the query.

Substructure Search

Once the Substructure Search is executed, the Smartsearch function will start to work, and substances such as examples given will be included in the result. To limit the result to specific substances, check the required Characteristic(s), Class(es) in the structure search window.

In substructure search, substances with additional substituent will also be included in the result. All atoms without bonds will be interpreted as free substituent, and ring fusion is also allowed by default. To prohibit ring fusion, see page 9.

Any kind of substitution is allowed for atoms without bond, but if you use **X menu tool or R Group tool**, you can limit the type of substituents. (See page 5)

4. Troubleshooting Error Messages

There are cases where "Search could not be performed. Correct the error(s) indicated below" error messages are displayed when performing structure search with a wrong structure, or when performing substructure search using simple structure, and search cannot be performed.

When this message is displayed, you have to either search again after re-drawing the structure, or restrict the search options.

By clicking the "lock out rings and chains" in the message displayed beneath the structure formula, you are prohibiting all ring fusions, and limited all chains to chain bond only. This will cause the result to be the same as if you are using Lock Rings tool. After you have done these specifications, execute the search again.

You can also restrict the substances to be searched using filter. The filter displayed here is almost similar with the one shown when you first click the Search button, except for the Formula Weight (molecule mass) filter.

You can restrict the result to substances with molecule mass within the specified range with Formula Weight filter. The number calculated from the structure formula will be automatically entered in the Min box. You can change the Min and Max value to any number you desire. However, the result will also include substances that are within the range of molecule mass specified by one of the component in a multi-component substance.

Appendix 2.   Polymer Search Simplified

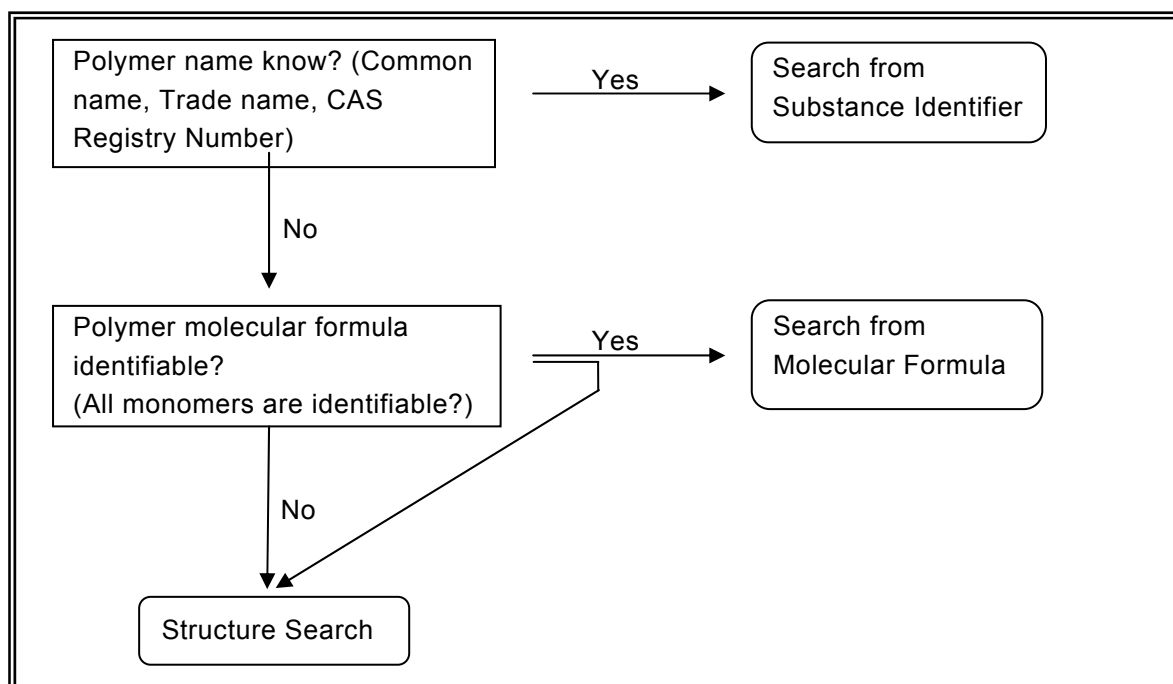## 1. Polymer registration format: Basically by structure monomer

・Homopolymer example

CAS Registry Number: 25188-97-0

$(C_5 H_8 O_2)_x$

2-Propenoic acid, 2-methyl-, methyl ester, homopolymer, syndiotactic

Methacrylic acid methyl ester, polymers, syndiotactic (8CI) ; Acrypet VH 001 ; Co 3D ; PMMA, syndiotactic ; Poly(methyl methacrylate), syndiotactic ; Sumipex AK 150 ; Syndiotactic PMMA ; Syndiotactic methyl methacrylate polymer ; Syndiotactic poly(methyl methacrylate) ; VH 001

Polymer Component

Polymer Class Term: Polyacrylic

Deleted CAS Registry Numbers: 26780-95-0; 104558-77-2

80-62-6
$C_5 H_8 O_2$

・Co-polymer example

CAS Registry Number: 9011-87-4

$(C_5 H_8 O_2 . C_4 H_6 O_2)_x$

2-Propenoic acid, 2-methyl-, methyl ester, polymer with methyl 2-propenoate

Acrylic acid, methyl ester, polymer with Me methacrylate (6CI) ; Methacrylic acid methyl ester, polymer with methyl acrylate (8CI) ; 2-Propenoic acid, methyl ester, polymer with methyl 2-methyl-2-propenoate (9CI) ; 6N ; 80N ; AK 218-44 ; Acrylite H 15-002 ; Acrypet MD ; Acrypet MD 001 ; Acrypet MDK ; Acrypet MF ; Acrypet S ; Acrypet VH ; BR 75 ; Coriplast 3 ; Dakril 2M ; Dakril 4M ; Delaglas A ; Delpet 60N ; Delpet 70H ; Delpet 720V ; Delpet 80N ; Delpet 80NB ; Delpet 80NH ; Delpet LP 1 ; Delpowder 70H ; Delpowder 80NB ; Dianal BR 75 ; G 66 ; G 77 ; HR-L ; Kurapet HR-L ; LP 1 ; Lucryl G 55 ; Lucryl G 66 ; Lucryl G 77 ; Lucryl G 77Q11 ; Lucryl G 88 ; MGC 10 ; Methyl acrylate-methyl methacrylate copolymer ; Methyl acrylate-methyl methacrylate polymer ; Methyl methacrylate-methyl acrylate copolymer ; Methyl methacrylate-methyl acrylate polymer ; Oroglas BS 8 ; Palacos R ; Parabeads ; Parabeads HR-L ; Parapet G 1000 ; Parapet HR 1000LC ; Parapet HR-L ; Plex 8671F ; Plexiglas 6N ; Plexiglas 7H ; Plexiglas 7N ; Plexiglas 8H ; Plexigum M 286 ; Sumipex XX

Polymer Component

Polymer Class Term: Polyacrylic

Deleted CAS Registry Numbers: 66828-12-4; 69071-16-5; 72394-20-8; 84842-62-6; 86904-23-6; 127884-19-9; 142007-95-2; 163546-33-6; 220286-92-0; 320345-13-9

96-33-3
$C_4 H_6 O_2$

80-62-6
$C_5 H_8 O_2$

2. Polymer search

Polymer name know? (Common name, Trade name, CAS Registry Number) ──Yes──► Search from Substance Identifier

│
No
▼

Polymer molecular formula identifiable? (All monomers are identifiable?) ──Yes──► Search from Molecular Formula

│
No
▼

Structure Search

Molecular formula entry reminder (All structure monomers are identifiable)
- ・ Separate each monomer with a period (.)
- ・ Put the whole molecular formula in a bracket, and add an x at its end
- ・ Example (C5 H8 O2 . C4 H6 O2)x
- ・ When there are too many isomers, narrow it down by structure

Structure search reminder

▽When all structure monomers are identifiable
- ・ Draw the structure of known structure monomer
- ・ Restrict to polymers
- ・ Exclude additional component
- ・ Execute perfect match structure search

▽When only a portion of the structure monomer is identifiable
- ・ Draw the structure of known structure monomer
- ・ Restrict to polymers
- ・ Execute perfect match structure search

Explore Substances

Chemical Structure

Chemical Structure

Search

MeO — CH — CH₂

Click image to change structure or view detail
Current Search type: Exact Structure
☐ Show precision analysis

Characteristic(s)
- ☑ Single component ── Presence of additional components
- ☐ Commercially available
- ☐ Included in reference(s)

Class(es)
- ☐ Alloys
- ☐ Coordination compounds
- ☐ Incompletely defined
- ☐ Mixtures
- ☑ Polymers ── Restricted to polymers
- ☐ Organics, and others not listed

Studies
- ☐ Analytical
- ☐ Biological
- ☐ Preparation
- ☐ Reactant or Reagent

3. Polymer Structure Search Examples

200903