

## IK-Cape File Supply System

For 5+ Million Chemical Compounds

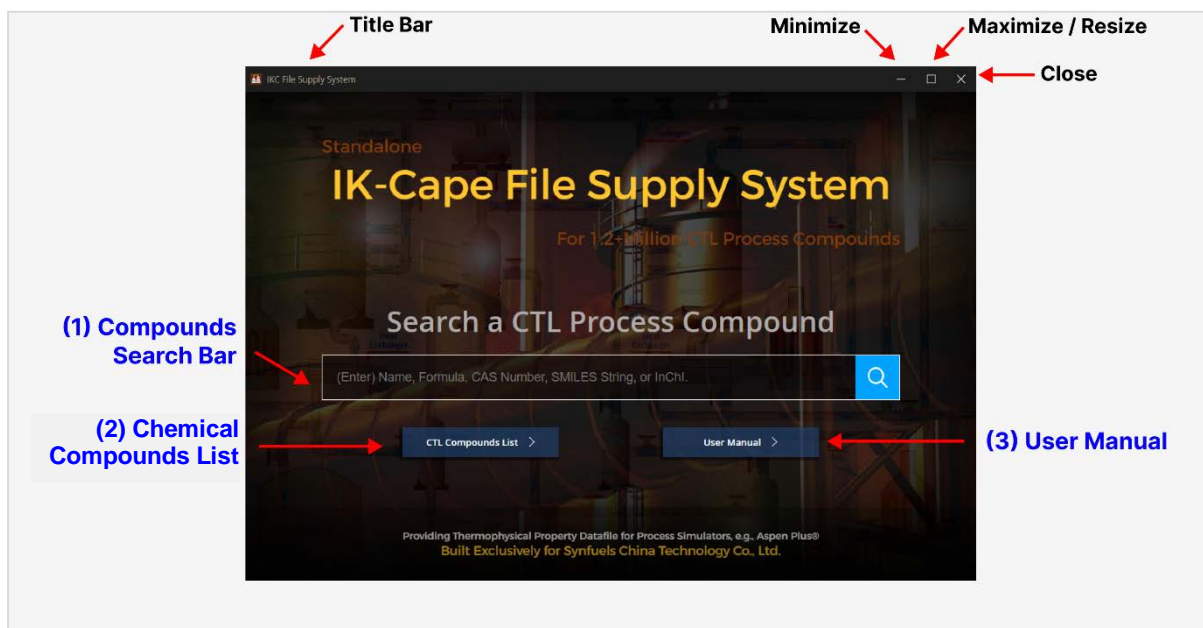
### User Manual

#### 1. How to Use the IK-Cape File Supply System

This chapter explains how to run and use the IK-Cape File Supply System.

##### 1-1. Main Window User Interface

The user interface of the main window of the IK-Cape File Supply System is as shown in the below image.



##### (1) Compounds Search Bar

Use the Compounds Search Bar to conveniently search for the compound of your choice or a similar compound among 5 million+ compounds. Refer to **1-2. Compounds Search** for detailed directions.

##### (2) Chemical Compounds List

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Click on the CHEMICAL Compounds List Button to go to the window where you can search for all lists of the 5 million+ compounds in order. Refer to **1-3. Compounds List Search** for detailed directions.

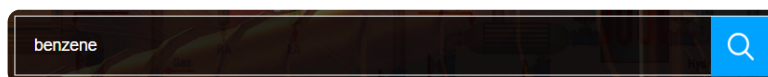
### (3) User Manual

Click on the User Manual Button to open the user manual, which is this document.

## 1-2. Search Compounds

Use the Compounds Search Bar to search for a specific compound or a similar compound among 5 million+ compounds. You may use the Name, Formula, CAS Registry Number, SMILES String, InChI, InChIKey, and MOLINSTINCTS ID as a chemical identifier for the search.

Enter benzene in the Compounds Search Bar as shown in the below image and press the Enter Key on the keyboard or mouse click the magnifier button on the right side of the image to go to the search result window.



The interface of the search result window is shown below.

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The screenshot displays the 'IKC File Supply System' window. At the top, a 'Search Results' section (1) indicates '1000+ compound(s) found' and provides a search bar with 'benzene' entered. Below this are buttons for 'CTL Compounds List' and 'User Manual'. The main area shows 'Compound Cards' (2). The first card (3) for benzene includes its chemical structure, a right-click menu with 'Copy Image' and 'Save as Image', and a table of identifiers: MOLINSTINCTS ID (0001-5nm9), Formula (C6H6), Molecular Weight (78.11184 g/mol), IUPAC Name (benzene), SMILES (c1ccccc1), InChI (InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H), InChIKey (UHOVQNZJYSORNB-UHFFFAOYSA-N), and Matched String (benzene). Below the table are buttons (4) 'Extract IKC File' and (5) 'View IKC File'. A second card for allylbenzene is shown below. At the bottom, a pagination bar (6) shows '1' selected out of 10 items.

### (1) Search Results

You may check the number of searched compounds at the top of the search result window. The Compound Search Bar, CHEMICAL Compounds List, and User Manual buttons enable re-using functions of the main window.

### (2) Compound Card

The bottom of the search result window lists Compounds Cards searched in the order of highest similarity. 10 Compound Cards are listed per page and each Compound Card contains the compound image and information on chemical identifiers such as MOLINSTINCTS ID, Formula, Molecular Weight, IUPAC Name, SMILES, and InChI. Mouse right-click over the image and a menu will appear for copying or saving the image. Below the Chemical Identifier are the Extract IKC File and View IKC File buttons.

### (3) Copy Image, Save as Image

Mouse right-click over the image and a menu will appear for using image-related functions. Click on Copy Image to copy the image to the clipboard, which can be pasted (shortcut Ctrl+v) into another document program right away. Click on Save as Image and a window will open for saving the image. Go to the folder where you want to save and click on the Save button to save the image in png format.

### (4) Extract IKC File

Click the Extract IKC File button and a window will open for saving the IK-Cape File of the relevant compound. Go to the folder where you want to save and click on the Save button to save the IK-Cape File.

### (5) View IKC File

Click on the View IKC File button and a window will open for immediately checking the contents of the IK-Cape File of the relevant compound.

### (6) Page Navigation

Use the Scroll Bar of the search result window or the Scroll Wheel of the mouse to reach the bottom of the page and find Page Navigation. Using this function, you will be able to check more search results.

#### Tip! Shortcuts of the Search Result Window

The Home, End, PageUp and PageDown buttons on the keyboard can be used to explore search results.

- Home: Go to the top of research results
- End: Go to the bottom of research results
- PageUp: Scroll up search results
- PageDown: Scroll down search results

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#### Tip! Stop Search

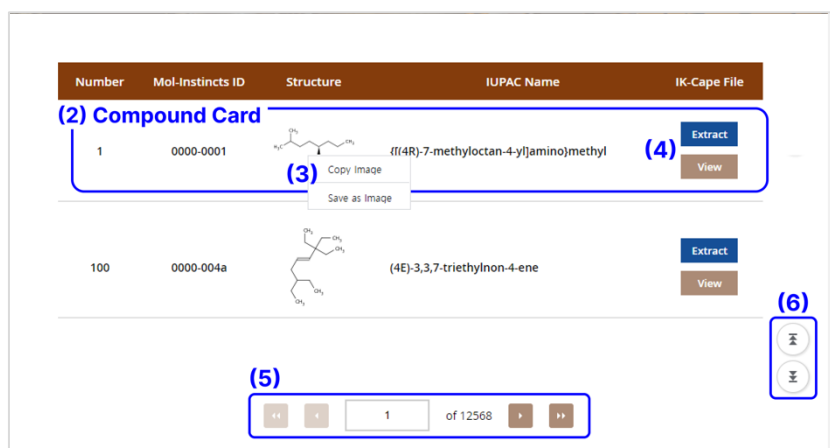
When the user uses a specific chemical identifier to attempt a search, compounds that are highly similar to the entered search word are found among the 5 million+ compounds. Therefore, in the case of specific searches, the search may take a long time. The IKC File Supply System provides the user with a feature to stop the search if it takes too long. When a search is attempted, a window will be created to show that the search is in progress as shown in the below image. The search can be stopped by pressing the Stop Searching button at the bottom of the window.





### 1-3. Explore Compounds List

Click on the Chemical Compounds List button on the main window or the search result window to go to the window where all lists of the 5 million+ compounds can be explored in order.

The interface of the Compounds List Exploration Window is as below.



Number	Mol-Instincts ID	Structure	IUPAC Name	IK-Cape File
1	0000-0001		(4R)-7-methyloctan-4-yl[amino]methyl	<div>Extract View</div>
100	0000-004a		(4E)-3,3,7-triethylnon-4-ene	<div>Extract View</div>

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Navigation buttons

#### (1) Full List of CHEMICAL Process Compounds

The top of the Compounds List Exploration Window shows that the number of explorable compounds is 5 million+. Then there are the Compound Search Bar and User Manual buttons that enable re-using of the functions on the main window.

#### (2) Compound Card

Below the Compound List Exploration Window is the Compound List in the order of ChemEssen

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Mol-Instincts ID with 100 Compounds per page. Each Compound information displays the Mol-Instincts ID, 2D Structure, and IUPAC Name. Mouse right-click over the image and a menu will appear for copying or saving the image. On the right are IK-Cape File-related Extract and View buttons.


### (3) Copy Image, Save as Image

Menus such as Copy Image and Save as Image appear in the same way as in the Compounds Search Result Window. Save the image to the clipboard or save it to the disk as a png file.



### (4) Extract or View

This option offers the same functions as the Extract IKC File and View IKC File buttons of the Compounds Search Result Window. Save the IKC File of the compound to the disk by clicking on the Extract button or use the View button to immediately check the contents of the IKC File.

### (5) Page Navigation

Use the Scroll Bar or the Scroll Wheel of the mouse to reach the bottom of the page and find Page Navigation. Use this to check more list exploration results. Click on the  button of Page Navigation to go to the last page and check the total number of compounds built into the program (more than 5 million).

### (6) Top or Bottom

Since 100 Compounds List Exploration Results are listed per page, the Top and Bottom buttons are provided to immediately move to the top and bottom of the page. As shown in the image, click on the  button at the bottom right of the page to go to the bottom of the page, and click on the  button to go to the top of the page. These buttons each correspond to the Home key and End key on the keyboard. Use the PageUp and PageDown buttons on the keyboard to scroll up or down five list exploration results at a time and explore the page.