PharmaMind

Software User Guide

PharmaMind version: 3.2.0
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Preface

Overview

This document mainly introduces the functions, basic concepts, typical operation procedures and examples of PharmaMind software, so that you can use PharmaMind.

Product Version

The product version corresponding to this document is as follows.

Product name	Product version
PharmaMind	V3.2.0

Audience

- This document is primarily intended for software users using PharmaMind.

Revision history

The revision history accumulates the description of each document update. The latest version of the documentation includes updates from all previous documentation versions.

Revision date	Version	Revision notes
2022-05-19	V3.2.0	Support PharmaMind V3.2.0

Contents

Figure List

Table List

1 Brief Introduction

PharmaMind mainly includes the following modules:

ID	Feature name	Feature description
1	Account login	Basic personal and enterprise account login and registration.
2	Account management	Personal account information display and modification and enterprise sub-accounts management, etc.
3	Structure recognition	Automatic recognition of chemical journals, patents and other documents, as well as editing and downloading of chemical structural formulas, etc.

2 Operating environment and requirements

ID	Environment	Requirements
1	Operating system	Windows10 and Mac operating systems are supported. Both versions of PharmaMind support automatic software updates.
2	Display resolution	The minimum resolution supports 1920*1080, which does not support font enlargement.

3 Instructions

3.1 Account registration

3.1.1 Account registration and login

Click on Register now on Login Page as shown in Figure 1.

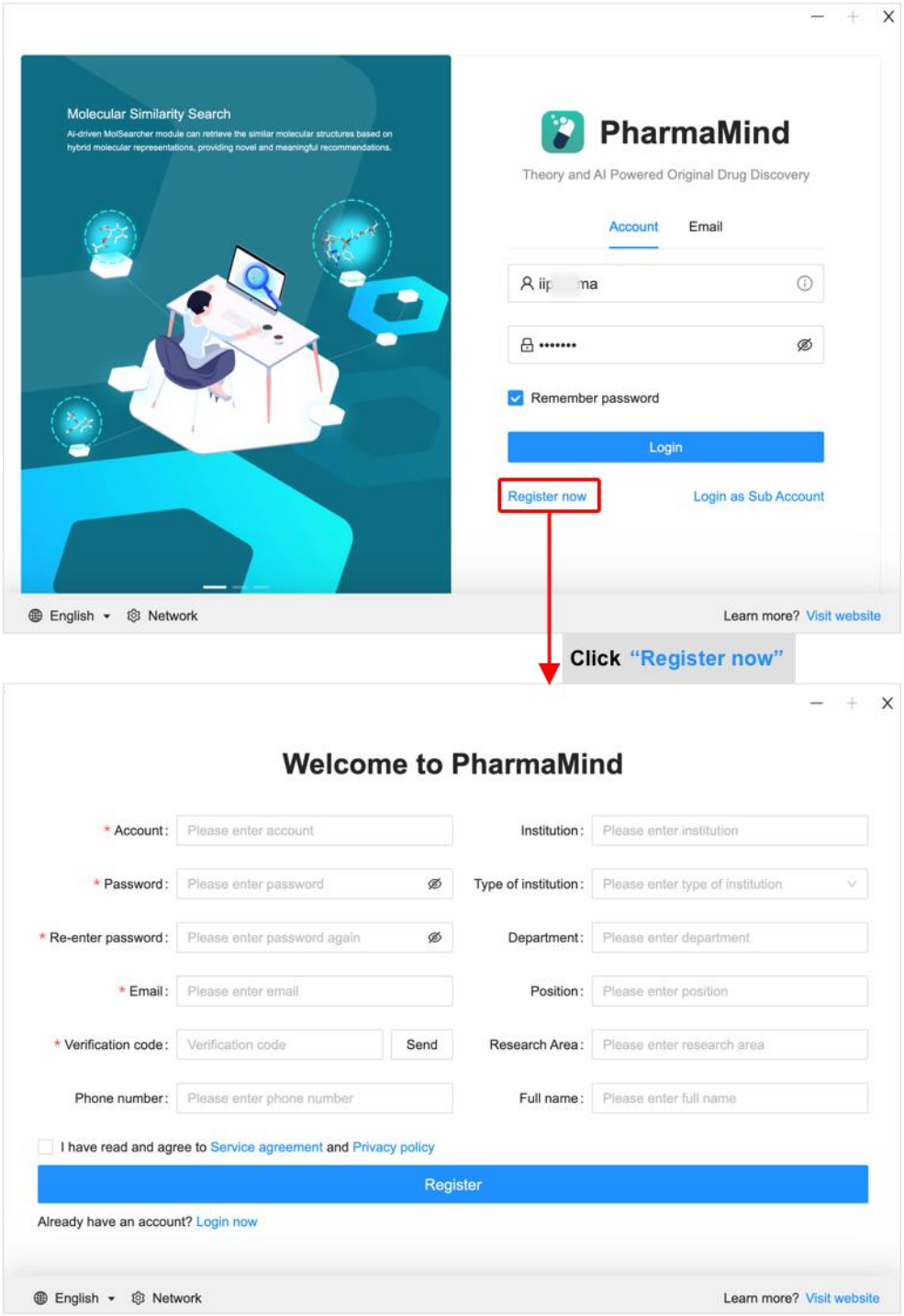

Figure 1 Basic user account registration

Fill out the registration form as shown in Table 1.

编号	表单项	填写要求
1	username	Support Chinese characters, letters, - and _ with a max length of 128
2	password	Your password must contain more than two of the following, numbers letters and special characters with a length of 6-32
3	Re-enter password	Same as above
4	Email address	Enter your email address
5	Verification code	Click to get your verification code and fill in

Table 1 Basic user account registration

Click on “I have read and agree to Service agreement and Privacy policy”.

Click on “Register”.

3.1.2 Enterprise account registration

For enterprise account registration, please contact Infinite Intelligence Pharma：service@iipharma.cn

3.1.3 Basic user account registration

Basic user account can be logged in by password or email address as shown in Figure 2.

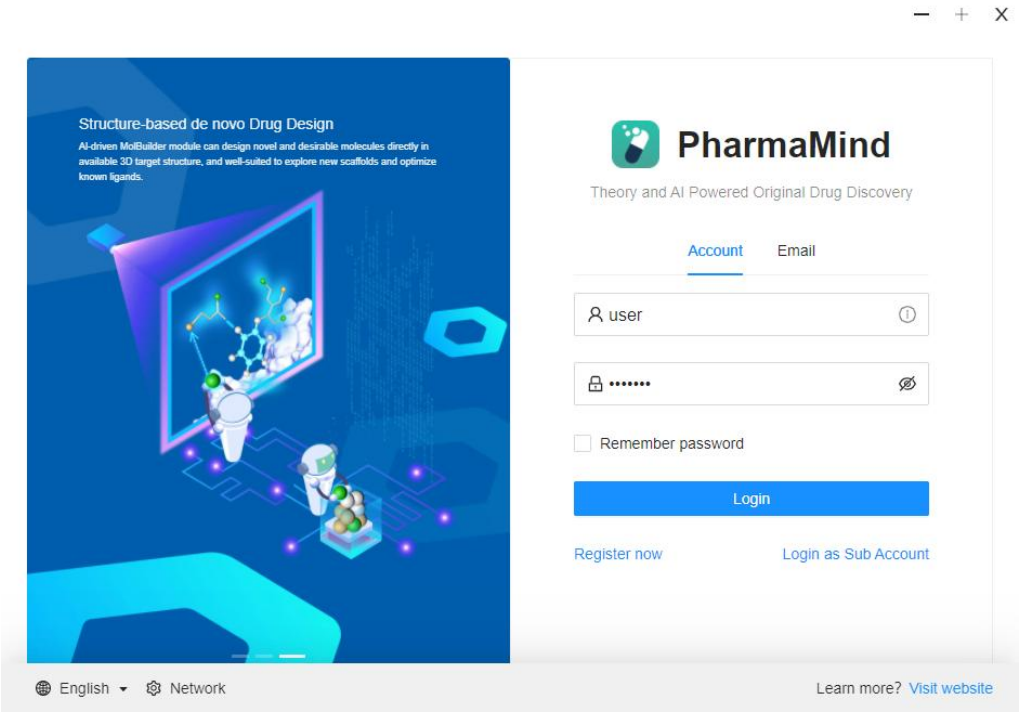

Figure 2 Basic user account login

3.1.4 Enterprise main account login

Enterprise user account login is the same as the basic user account, which can be logged in through the account password or registered email address as shown in Figure 3.

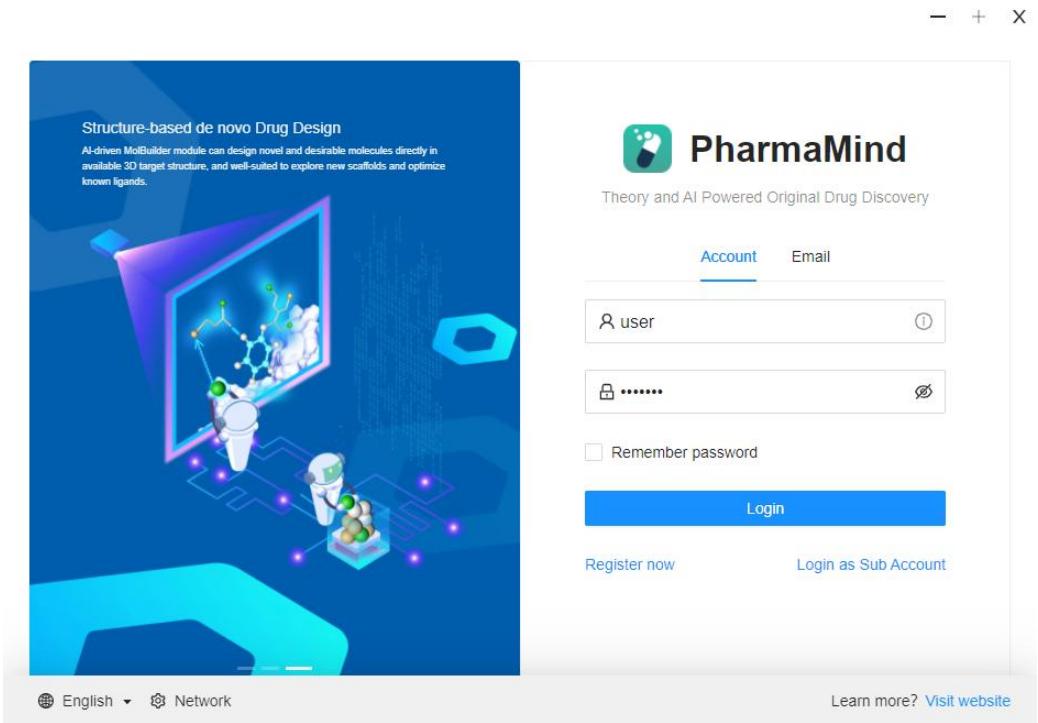

Figure 3 Enterprise main account login

3.1.5 Enterprise sub-account login

For enterprise sub-account login, click on “Sub-account login”, enter your sub-account name, enterprise ID and password, and click on “Login” as shown in Figure 4.

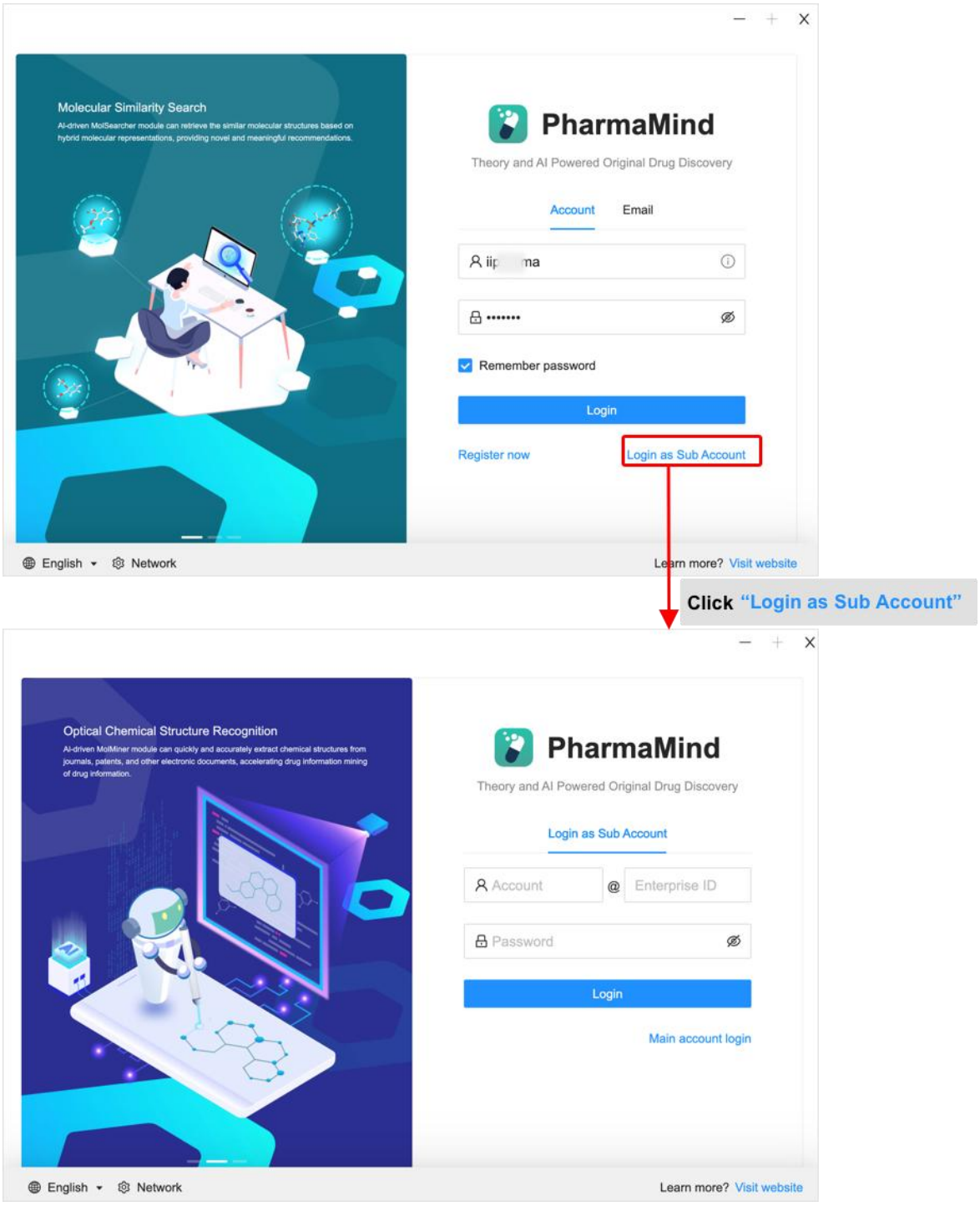

Figure 4 Enterprise sub-account login

3.2 Account management

3.2.1 Account information management and modification

After logging in, click on the account icon in the upper left corner to view and modify your personal account information as shown in Figure 5.

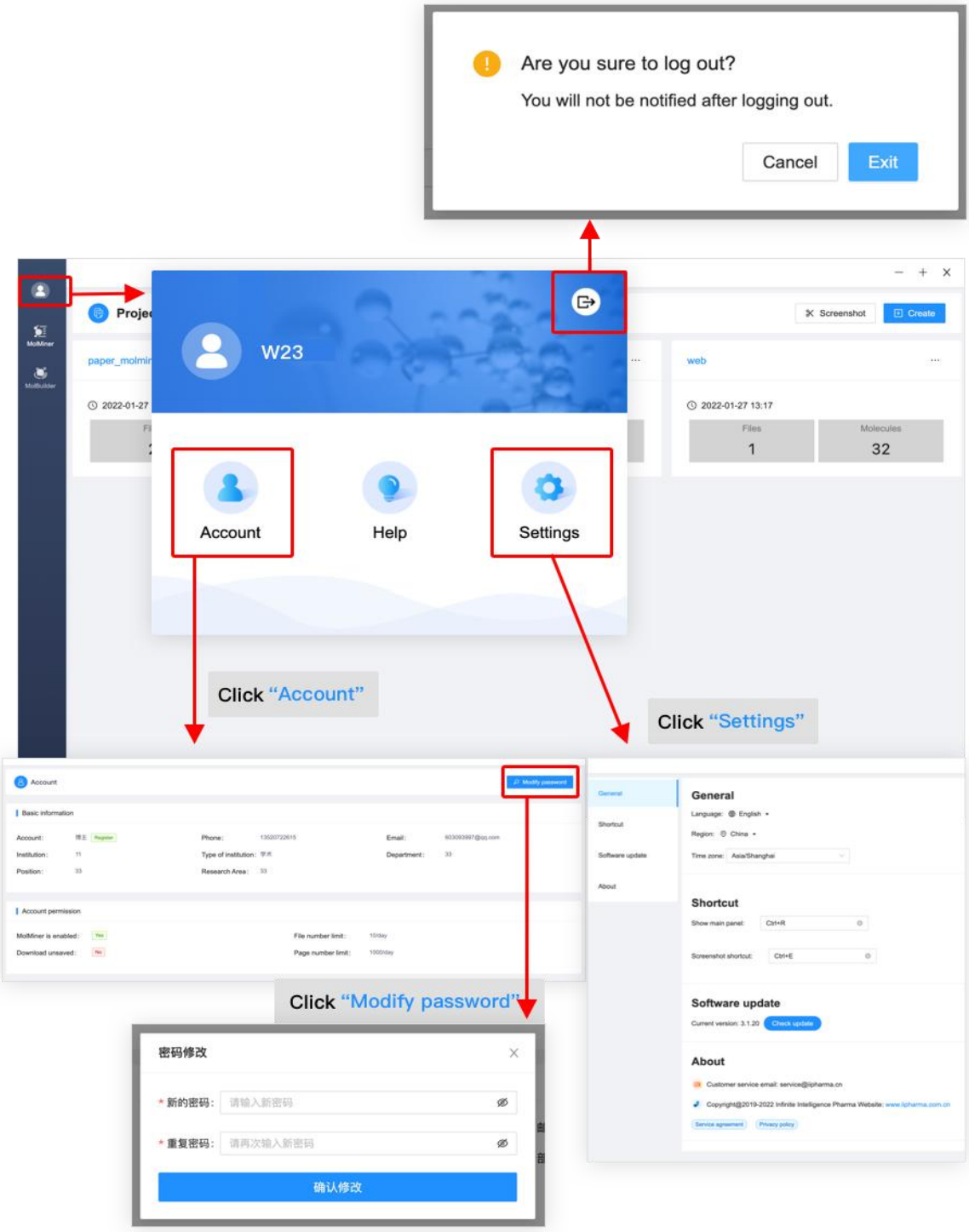

Figure 5 Account information management and modification

3.2.2 Enterprise sub-account management

After enterprise main account login, click on the account icon in the upper left corner to enter your enterprise sub-account management page. Create, remove or modify enterprise sub-accounts as shown in Figure 6 and Figure 7.

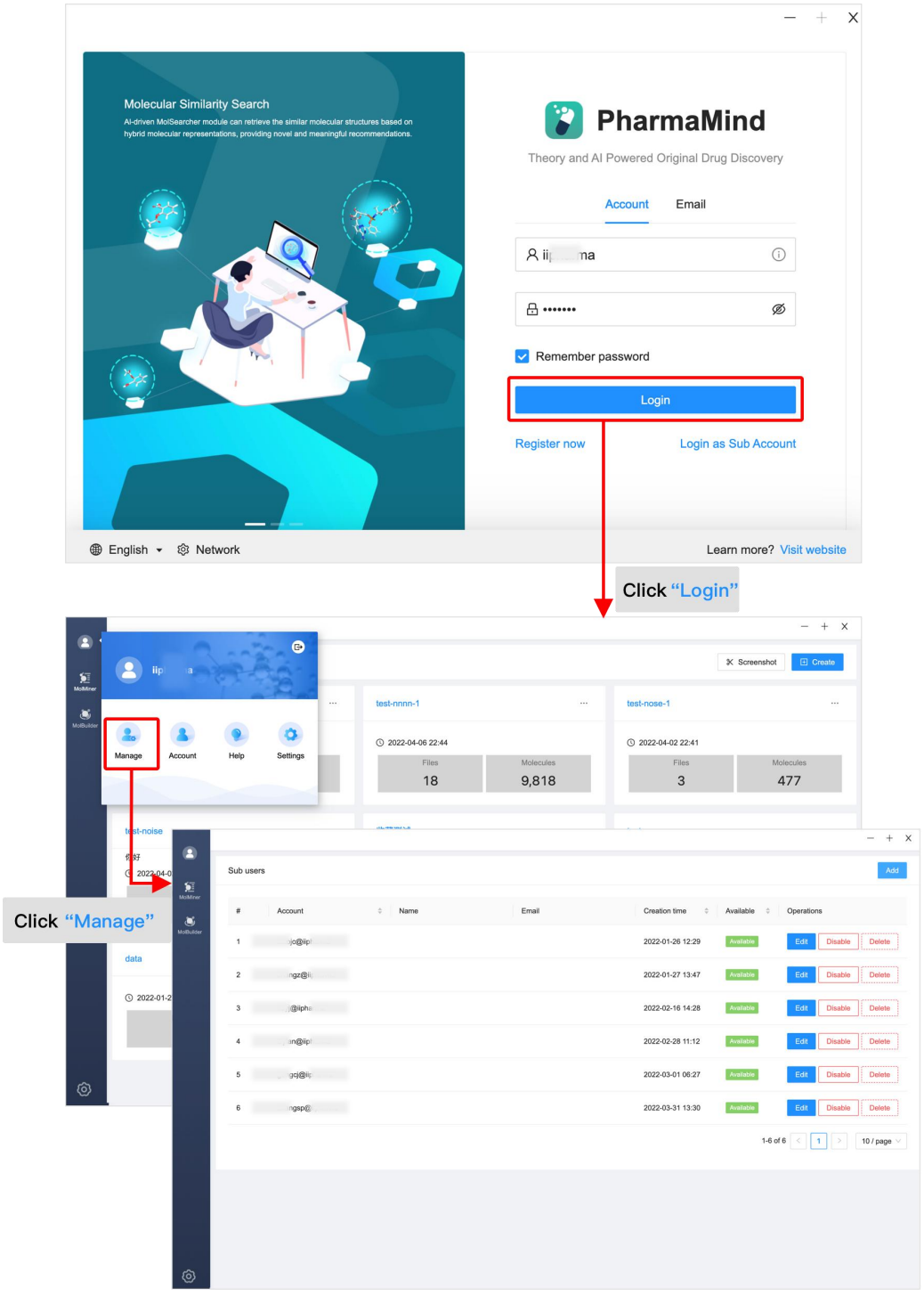

Figure 6 Enterprise sub-account management 1

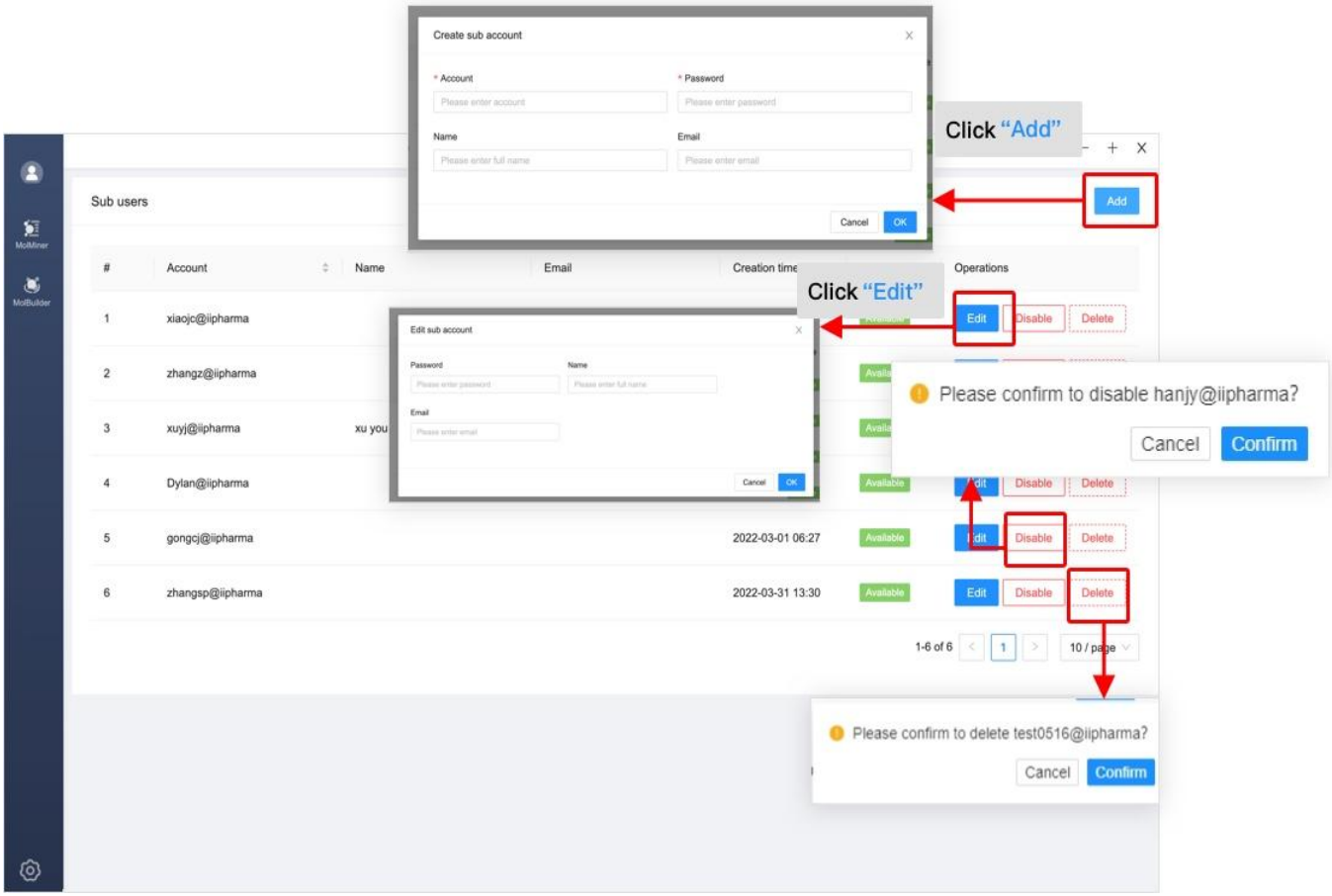

Figure 7 enterprise sub-account management 2

3.3 Structure recognition

3.3.1 Project management

In the project management page, you can create new projects, view, edit and delete existing projects as shown in Figure 8.

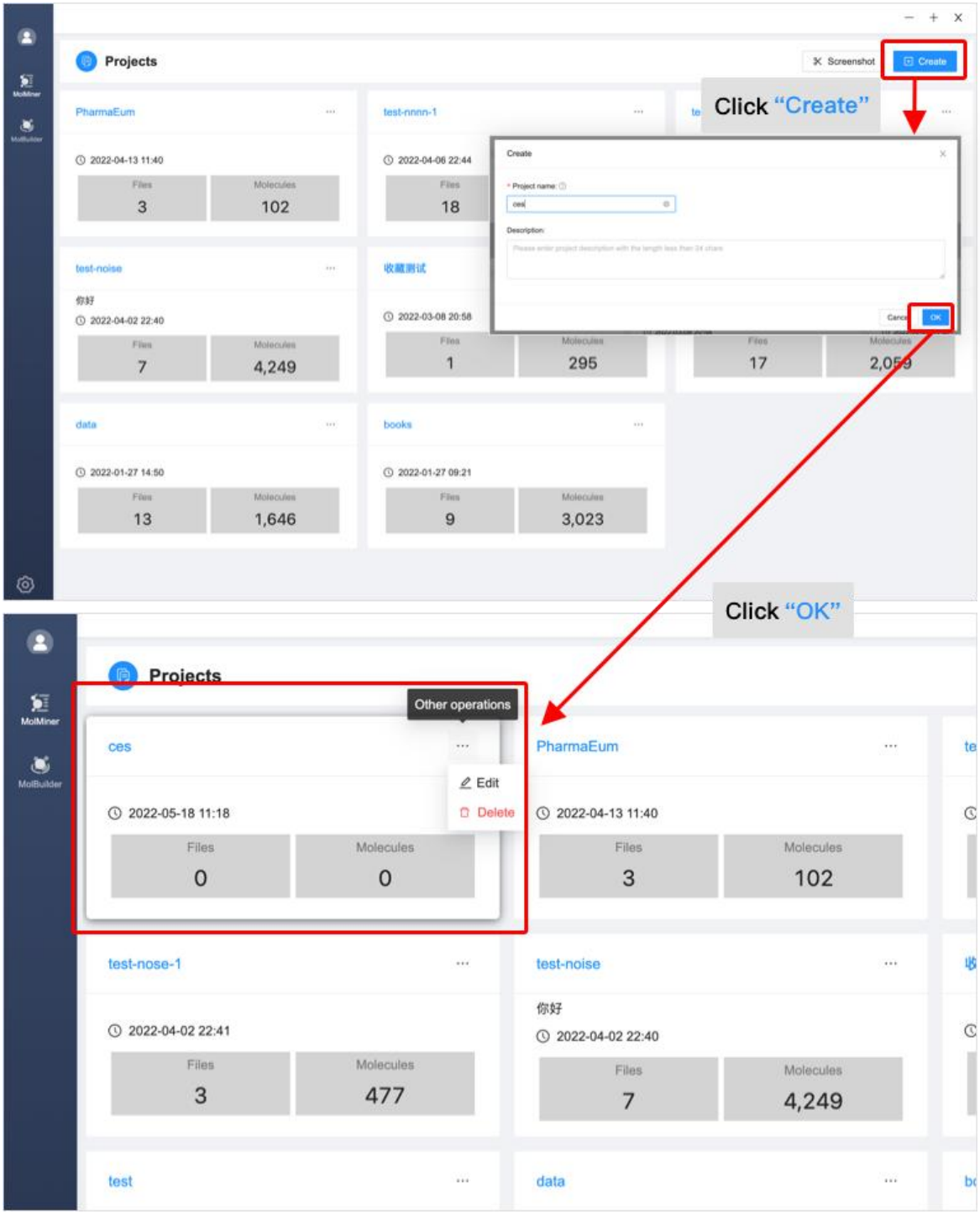

Figure 8 Account management

3.3.2 File management

Click an existing project to enter file management page. On the file management page, click on "Upload file" bottom to upload a PDF file as shown in Figure 9.

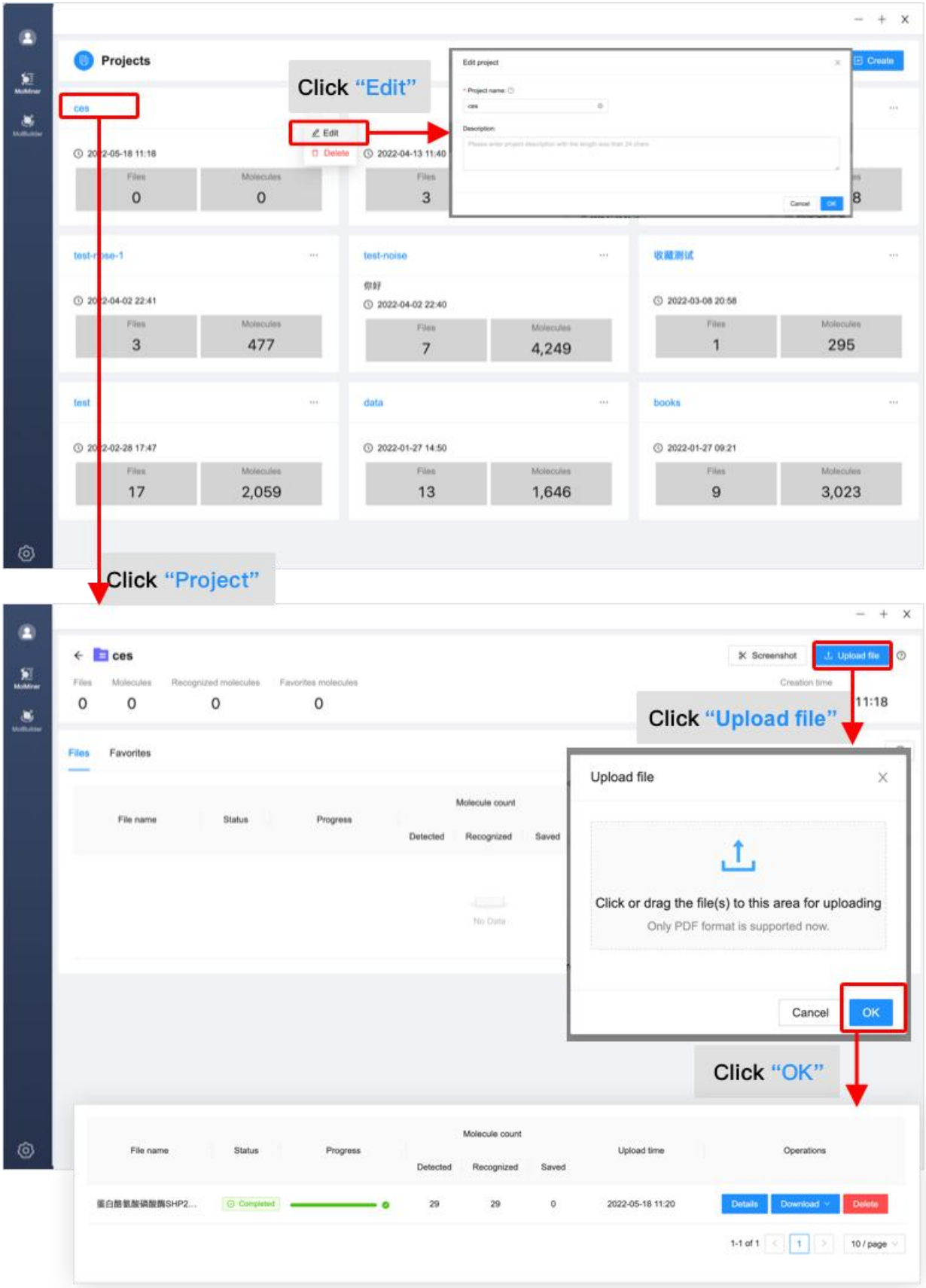

Figure 9 File management

3.3.3 File details

Click on “Details” button to enter the file detail page. On the file detail page, check the status of the current PDF file. You can view the the recognized molecules of the current file on the left and a list of recognized molecules as shown in Figure 10.

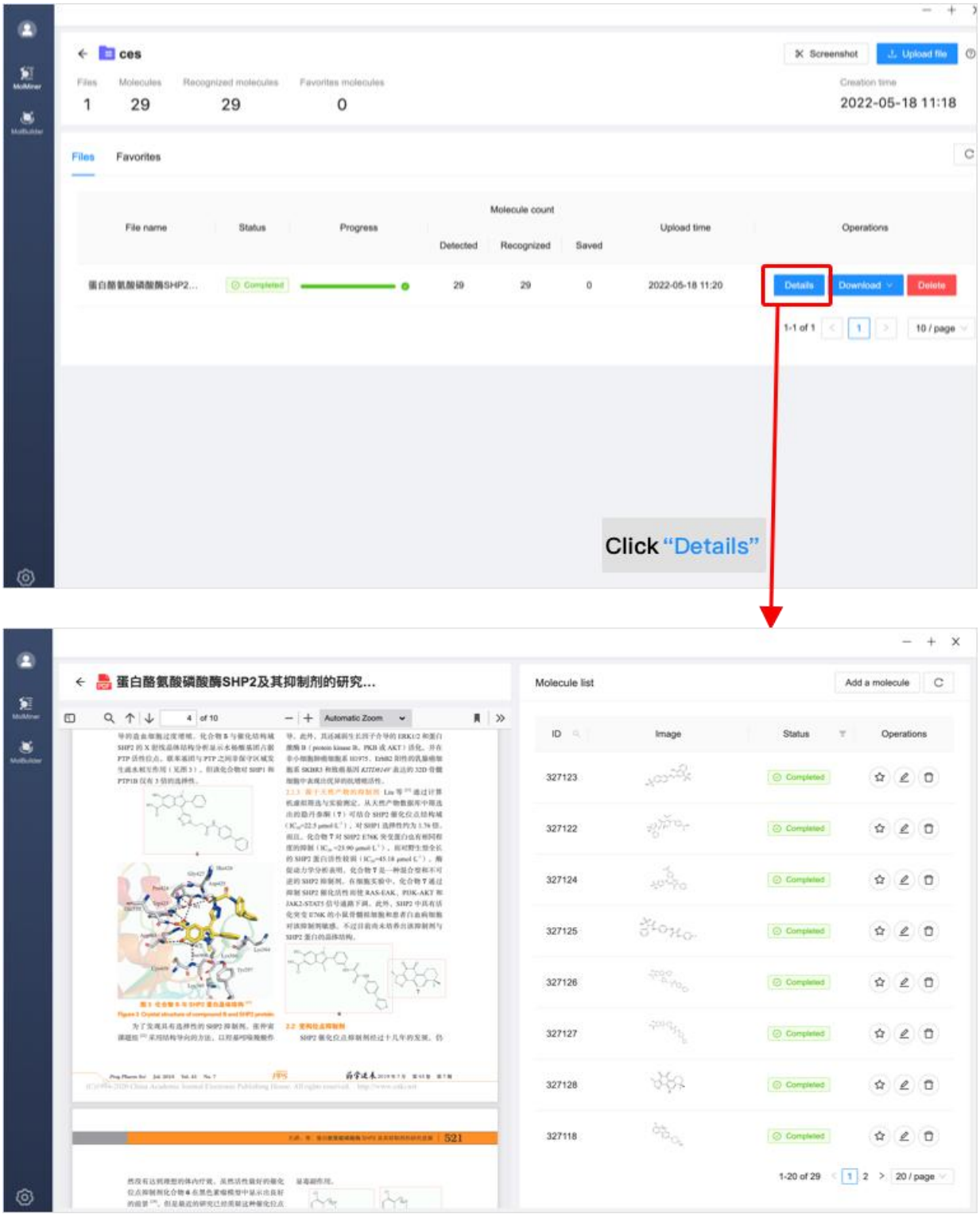

Figure 10 File detail 1

If there are molecules that are not recognized, you can click “Add molecule” in the upper right corner to add a new molecule. After your selection is completed, the molecule will be automatically recognized. If the position of the recognition box is inaccurate, you can re-recognize the molecule structure by editing the box position. You can select other molecules in the molecule list to modify other recognized molecules structures.

See Figure 11 for more details.

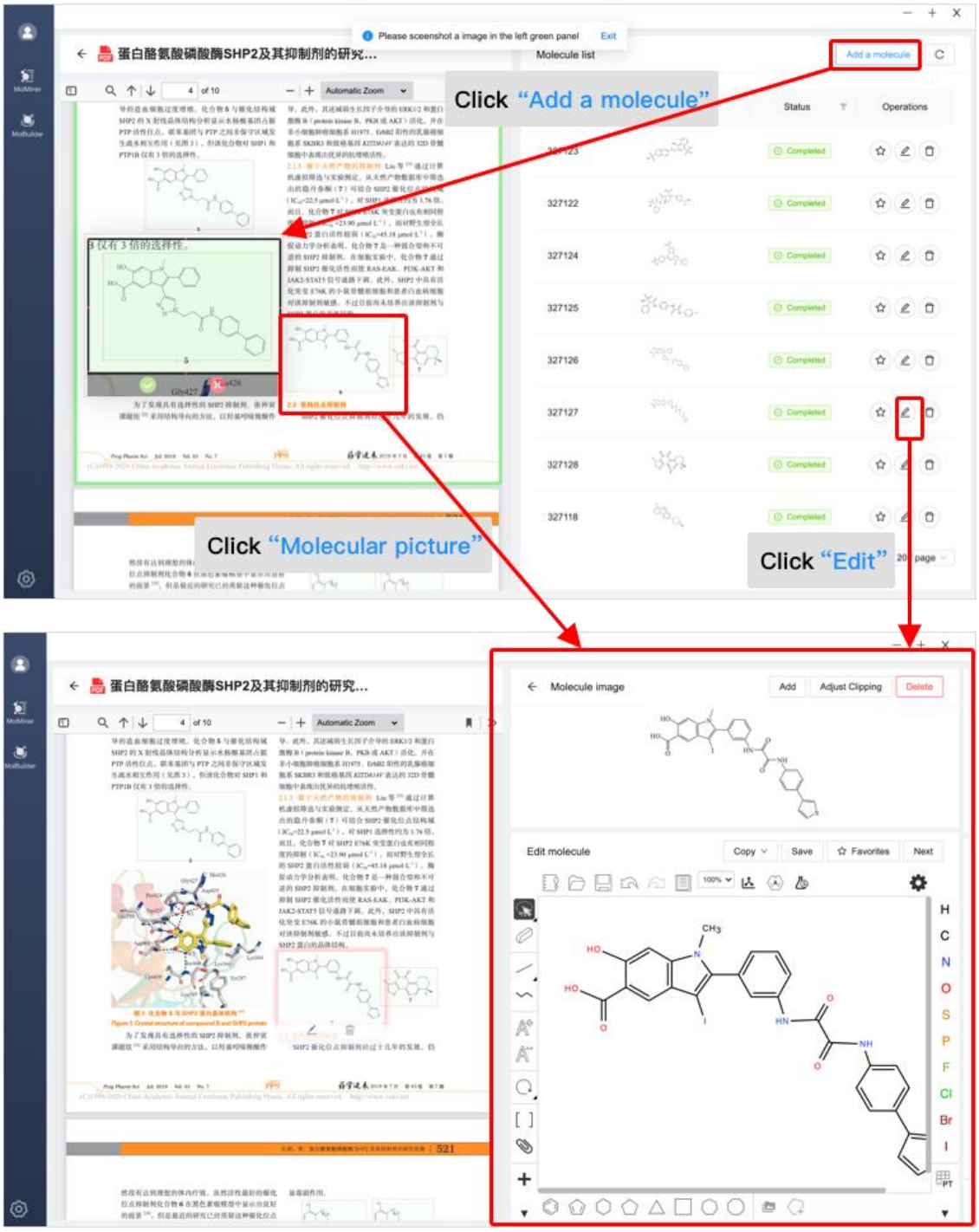

Figure 11 File detail 2

After entering the molecule editor page, you can close the editor by clicking “Edit”.

On the molecule editing page, click “Copy” bottom to copy the molecule in SDF or SMILES format. After editing the molecule, click “Save” button to save the result, and “Next” button to edit the next unsaved molecule.

See Figure 12 for more details.

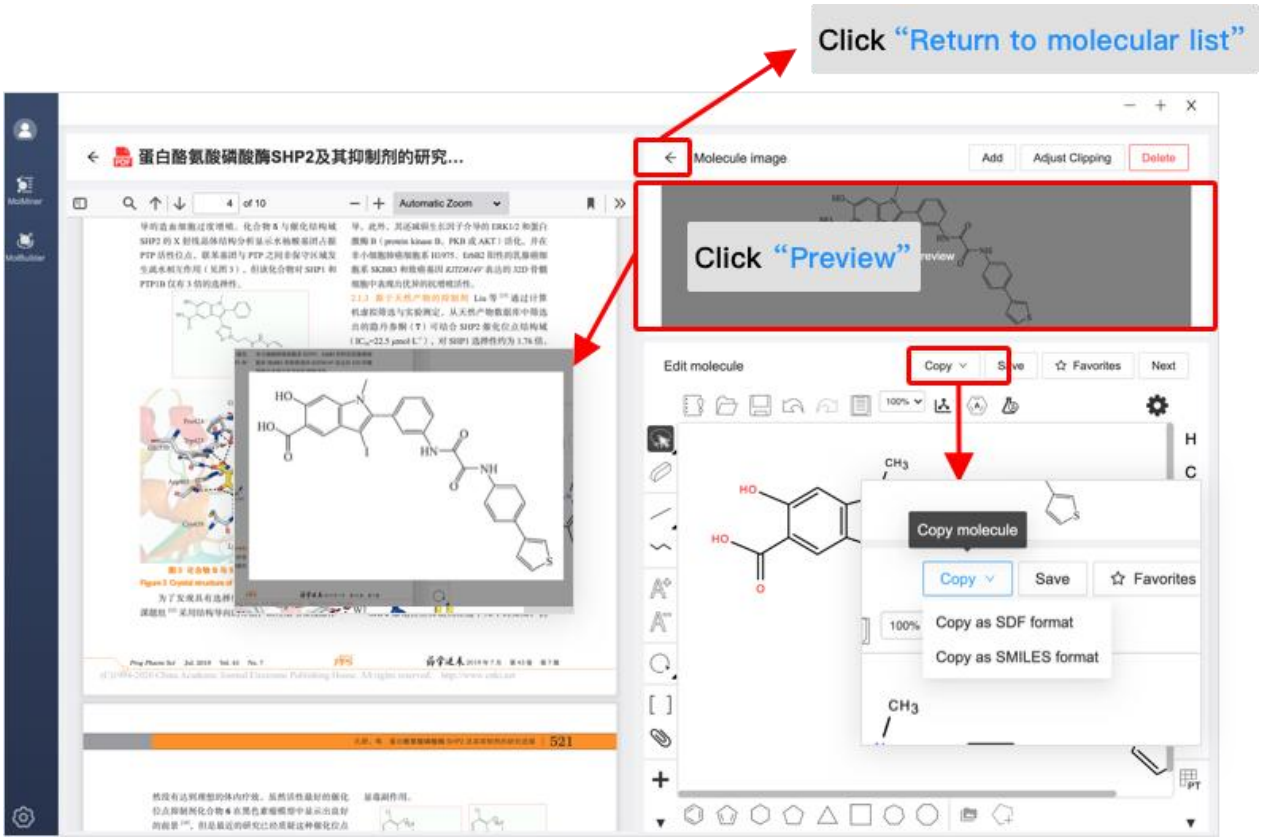

Figure 12 File detail 3

3.3.4 Molecule editing

Molecule editing can be carried out by the molecular editor which is in the lower right corner of the molecule editing page. Molecular editor includes a canvas with several features, the buttons on the top of the canvas consist of the following.

1. **Clear Canvas button** to clear the whole drawing area;
2. **Open and Save buttons** to import a molecule from a molecule file or save it to a supported molecular file format;
3. **Cut, Copy and Paste buttons** to perform corresponding actions;
4. **Scaling button** to change canvas view according to the percentage;
5. **Layout button** to adjust the position of the structure to the best view;

6. **Clean Up button** to improve the appearance of the structure by assigning them uniform bond lenghts and angles;
7. **Aromatize** and **Dearomatize buttons** to convert a structure to the Aromatic or Kekule presentation.
8. **Calculate CIP button** to determine R/S and E/S configuration;
9. **Check Structure button** to check the correctness of molecular properties;
10. **Values Calculation button to display some properties of the structure, such as molecular formula and Molar weight, etc;**

See Figure 13 for more details.

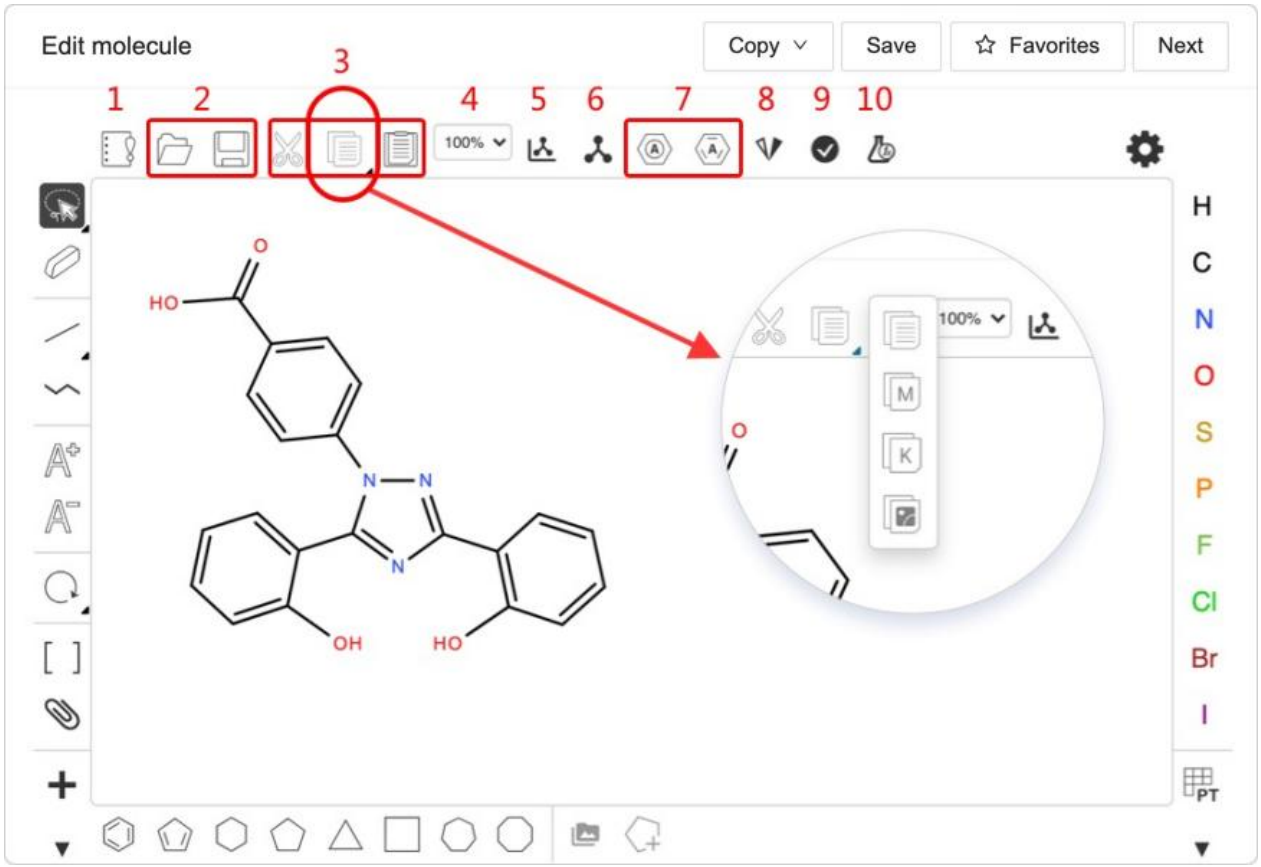

Figure 13 Molecule editing 1

The buttons on the left side of the canvas consist of the following,

1. **Select tools** to select the entire molecule or its fragment in one of the following ways (click on the button to see the list of available options: Lasso tool, Rectangle Selection tool and Fragment Selection tool);
2. **Erase tool** to delete any element of the drawing (atom or bond);
3. **Bond tool** to draw/edit bonds; you can also change the bond type by clicking on it, with these tools, you can draw different bonds;
4. **Chain tool** to draw consecutive single bonds;

5. **Charge button** to change the charge of an atom;
6. **Rotate tool** to rotate the objects you selected; you can also use this tool to flip the objects horizontally or vertically by clicking on it;
7. **S-Group tool**. You can use this tool and the following dialog that appears after selecting a fragment with this tool to abbreviate repetitive structures, polymers or some protective groups;

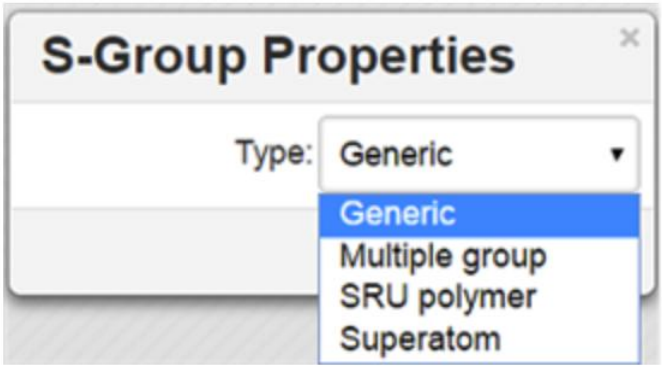

Figure 14 Molecule editing 2

8. **Plus tool** button to draw a reaction;
9. **Reaction Arrow tool** to draw an arrow in the reaction equation; it can be used Plus Tool to edit a reaction;
10. **Mapping tool** to map same atoms in reagents and products;
11. **R-Group tool** to create logic of R-Group member fragment; it can be used to make the Markush structure;
12. **Shape Ellipse tool** to draw graphical objects; such as ellipse, rectangle and line;
13. **Text tool** to add text to the canvas;

See Figure 15 for more details.

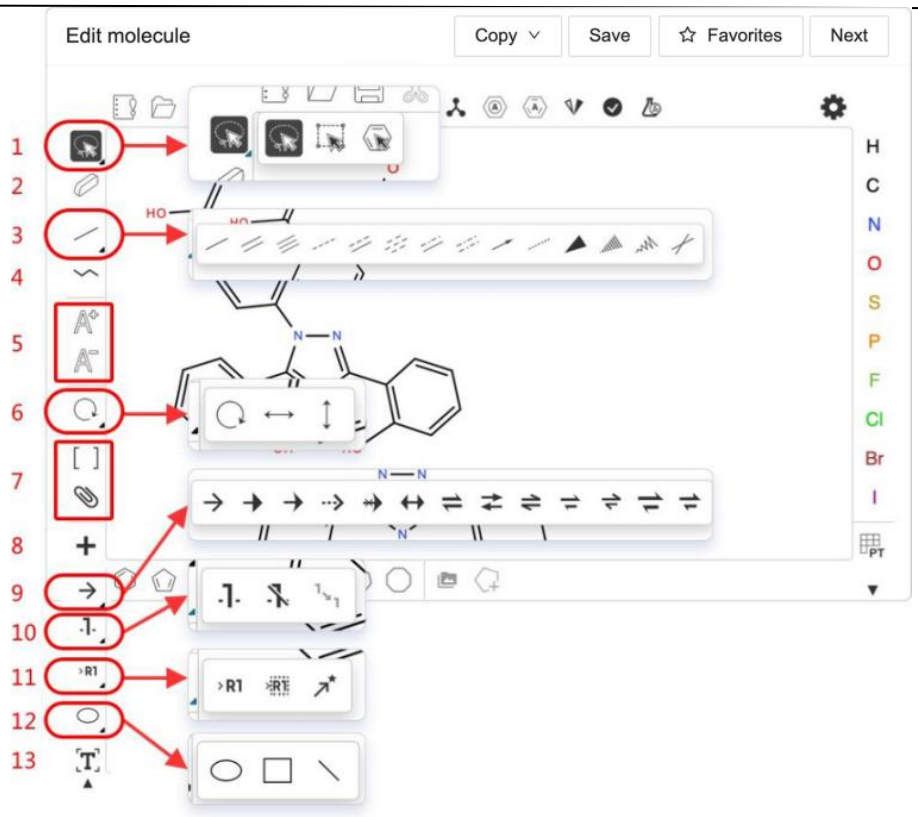

Figure 15 Molecule editing 3

The buttons on the bottom of the canvas are the Templates Toolbar. You can add templates (rings or other predefined structures) to the structure using the Templates Toolbar; The buttons on the right side of the canvas are the Atoms Toolbar, if the desired atom is absent in the toolbar, click on the PT button to invoke the Periodic Table and click on the desired atom.

See Figure 16 for more details.

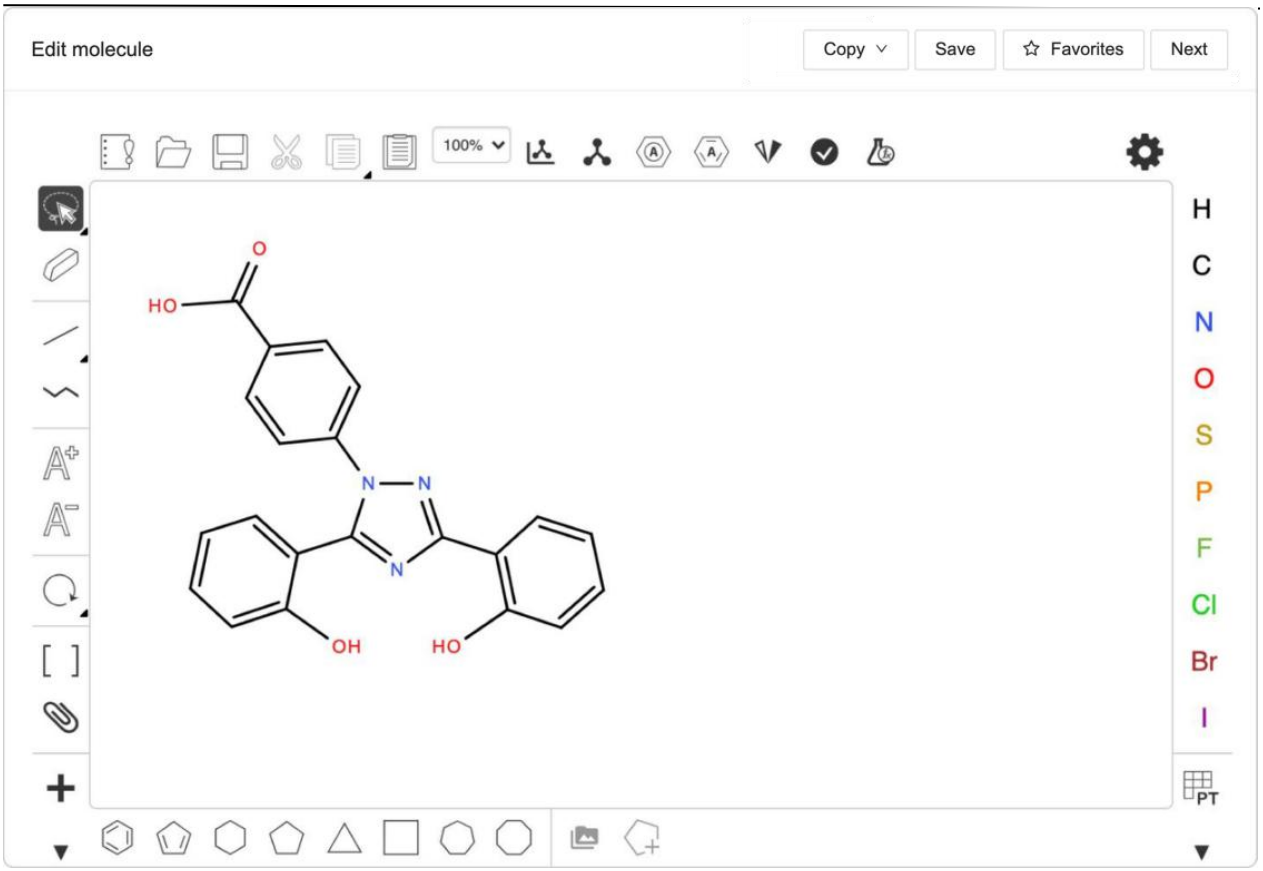

Figure 16 Molecule Editing 4

3.3.5 Recognition by screenshot

You can click on the “Screenshot” button to take a screenshot of the chemical diagram, the structure will be automatically identified and appears on the canvas. Multiple structures will be also able to be identified by one single screenshot. The structure can be copied as SDF format SMILES string, and it can also be added to the favorite folders as well.

See Figure 17 and Figure 18 for more details.

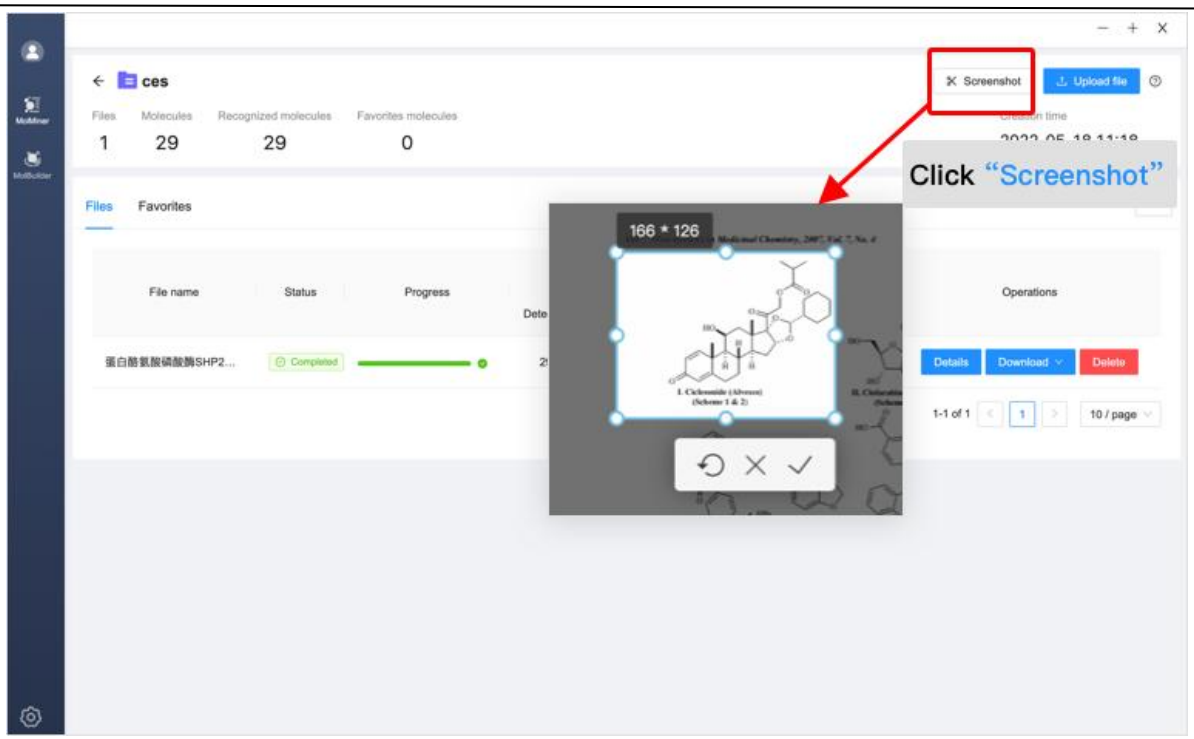

Figure 17 Recognition by Screenshot 1

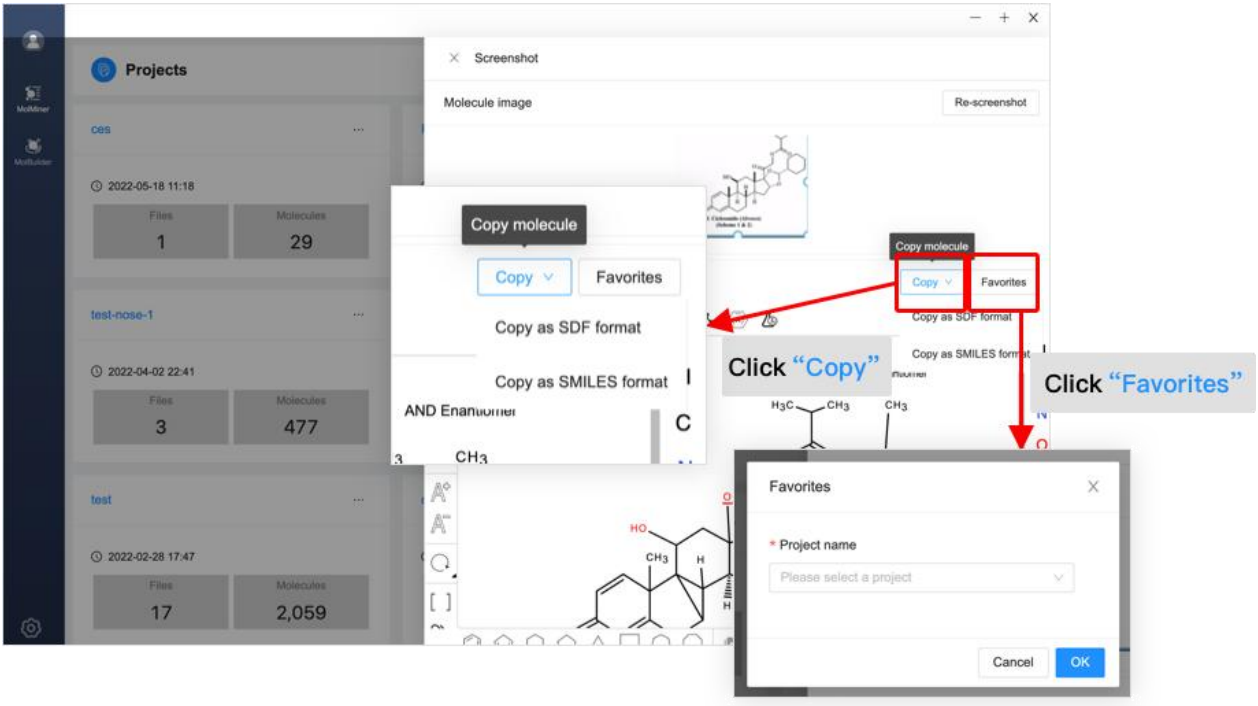

Figure 18 Recognition by Screenshot 2

3.3.6 Favorites

You can add molecules structure from uploaded files or screenshot to Favorites. See Figure 19 for more details.

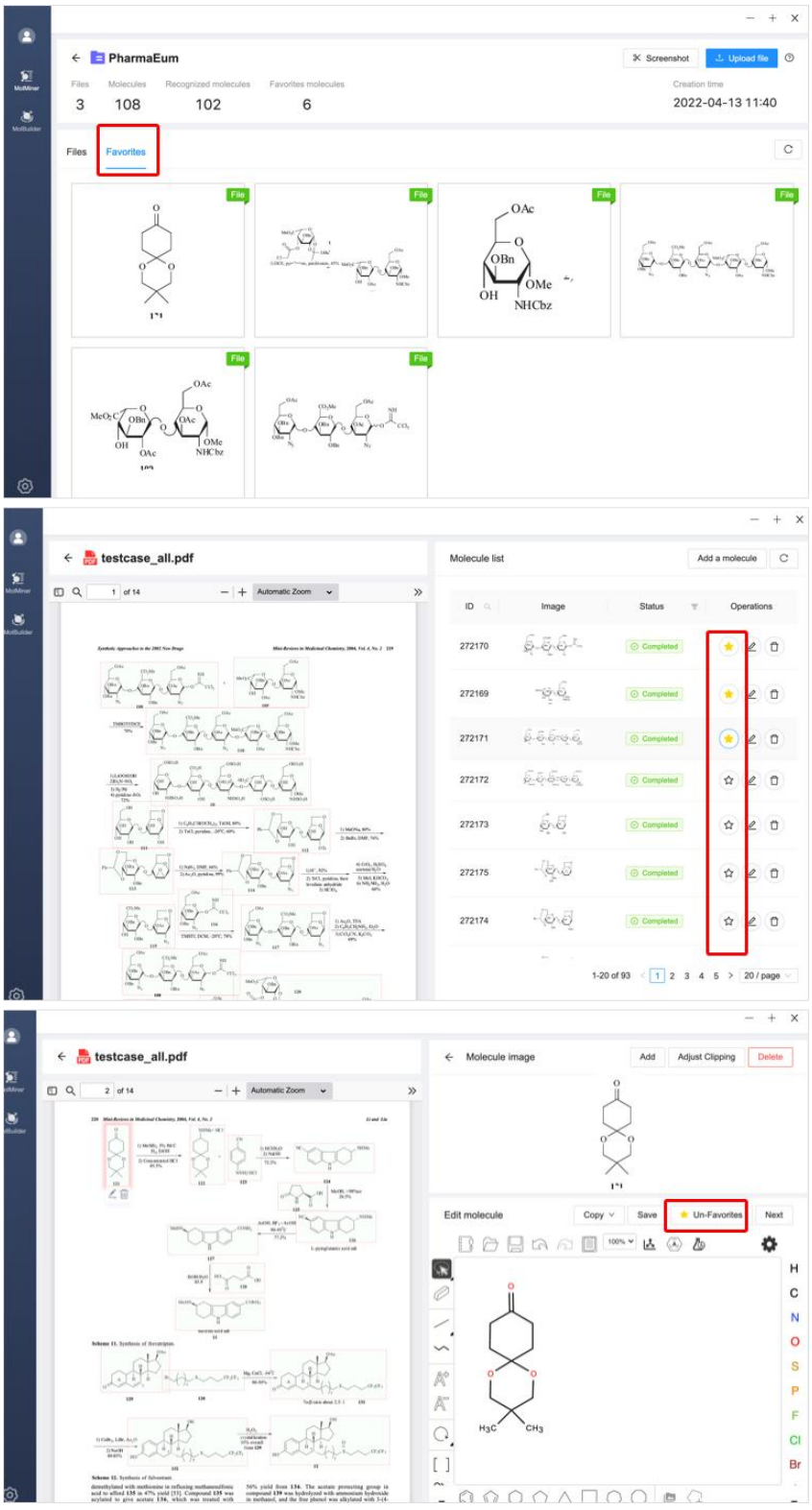

Figure 19 Favorites

3.3.7 Editing with Chemdraw

PharmaMind MolMiner supports interworking with chemdraw, you can use keyboard commands Ctrl-C for copy and Ctrl-V for paste to copy the structure to chemdraw, and PharmaMind MolMiner supports structures from chemraw as well (Ctrl-D and Ctrl-V). These keyboard commands are also available on the Mac (⌘ -C, ⌘ -D, ⌘ -V).

3.4 Settings

Click on the account icon to enter the Settings page to view shortcut keys and others.

See Figure 20 for more details.

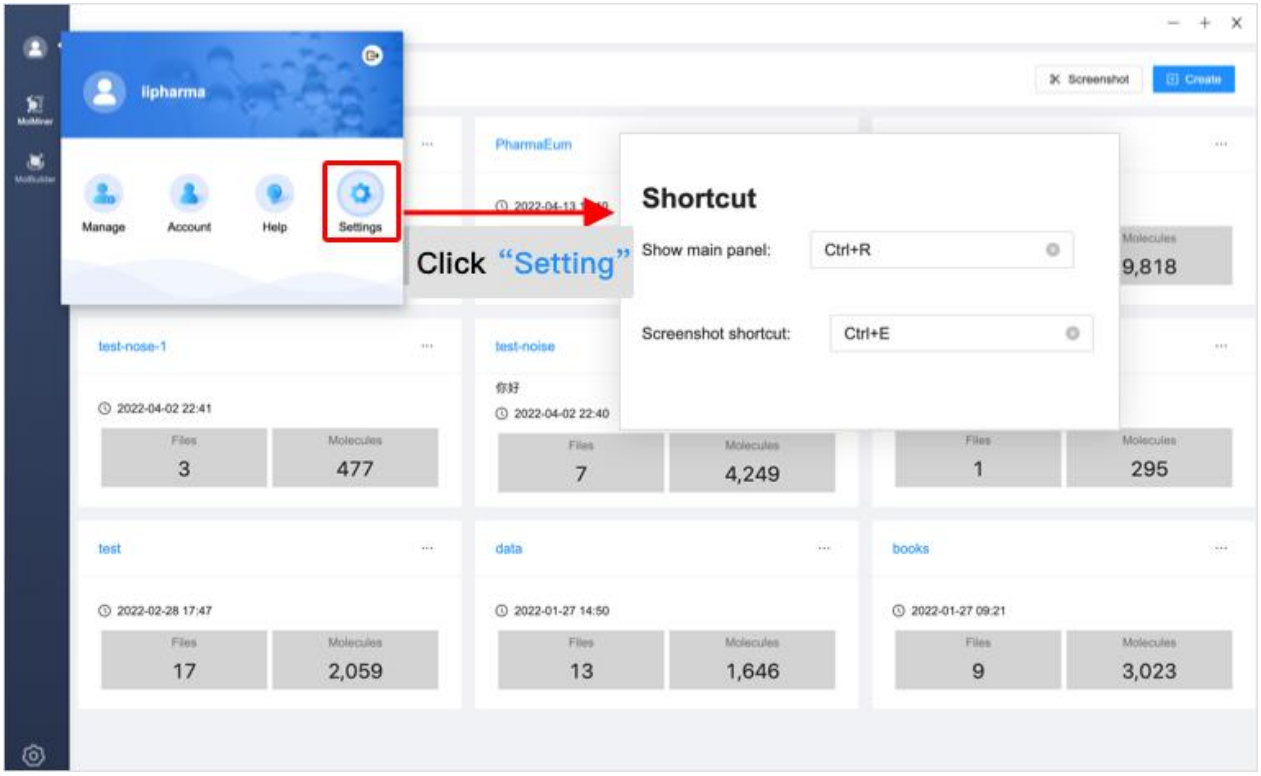

Figure 20 Settings

