

# Product Manual



**Labwise**

**AI-assisted Retrosynthesis System**

**February 26, 2024**

**C12.ai**

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# I. Introduction

Labwise is a cutting-edge application designed to offer AI-assisted retrosynthesis services for scientists, leveraging the most recent generative AI technologies. From their computers, users can utilize Labwise to explore AI-crafted synthesis routes and experiments.

This manual aims to guide users through the main functionalities of Labwise. It includes detailed, step-by-step instructions for performing retrosynthesis designs using generative AI models, and the relevant prior reactions for references for each reaction in the synthesis routes.

## II. Getting Started

This section presents the basic workflow of conducting a retrosynthesis design, aiming to familiarize you with the product's capabilities and interface. This overview provides an understanding of the essential functionalities, facilitating a quick start with Labwise. Subsequent sections will explore more sophisticated features of our product and improving your proficiency with the system.

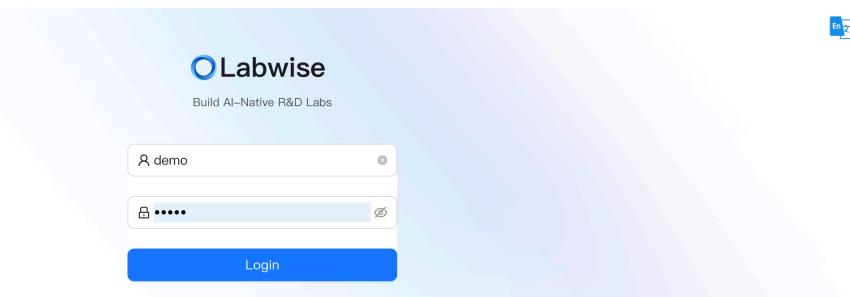
### 1. Login and layout

Should you already have an account, you can proceed to Step 2 for the login process. In case you do not yet have an account, we would recommend reaching out to your Labwise administrator for setting up your account.

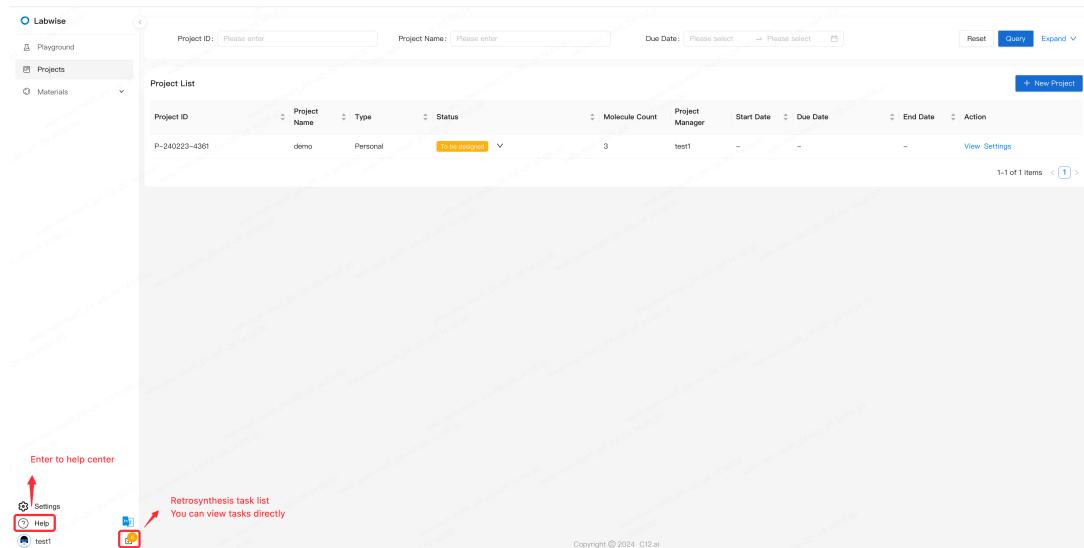
Labwise administrators are advised to visit <http://labwise.domain.com:1337/admin> and login using the credentials "admin@localhost" (password provided separately). For further details, administrators are welcome to refer to Admin Operations Guide.

Assume the hostname of the machine running Labwise is labwise.domain.com.

- 1) Launch your web browser and navigate to <https://labwise.domain.com>. On the following page, enter your account credentials (username and password) to log in to the system.**



- 2) The left column serves as the primary navigation bar.** Within the "Project" module, you will have the ability to add projects, molecules, and initiate retrosynthesis design tasks. Alternatively, the "Playground" module allows for directly inputting molecule structures and immediately starting the design process. This setup is designed to streamline your workflow, whether you're managing comprehensive projects or experimenting with individual molecules.



Project ID: Please enter Project Name: Please enter Due Date: Please select Start Date: Please select End Date: Please select

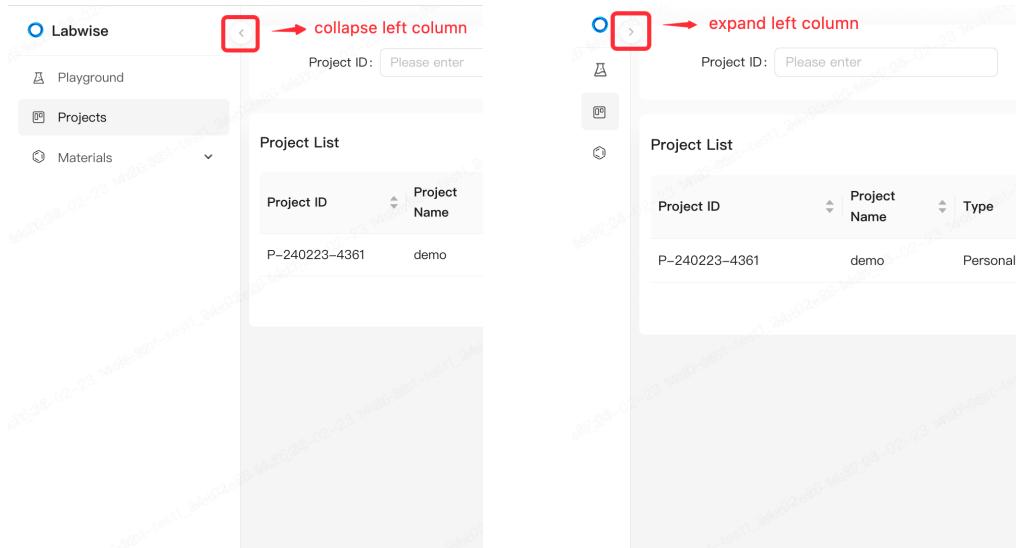
**Project List**

Project ID	Project Name	Type	Status	Molecule Count	Project Manager	Start Date	Due Date	End Date	Action
P-240223-4361	demo	Personal	To be designed	3	test1	-	-	-	<a href="#">View Settings</a>

1-1 of 1 items < (1) >

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- 3) Click the collapse/expand button to fold/unfold the navigation panel on the left.



Project ID: Please enter

**Project List**

Project ID	Project Name
P-240223-4361	demo

Project ID: Please enter

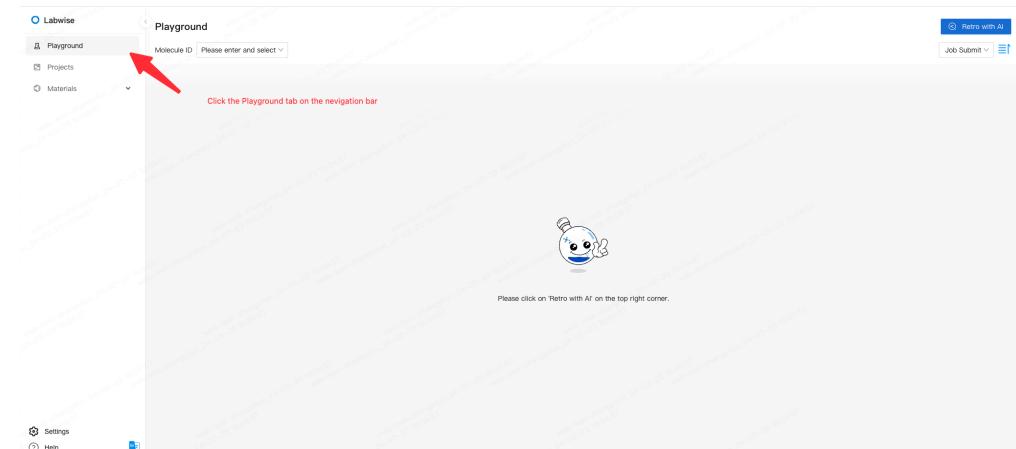
**Project List**

Project ID	Project Name	Type
P-240223-4361	demo	Personal

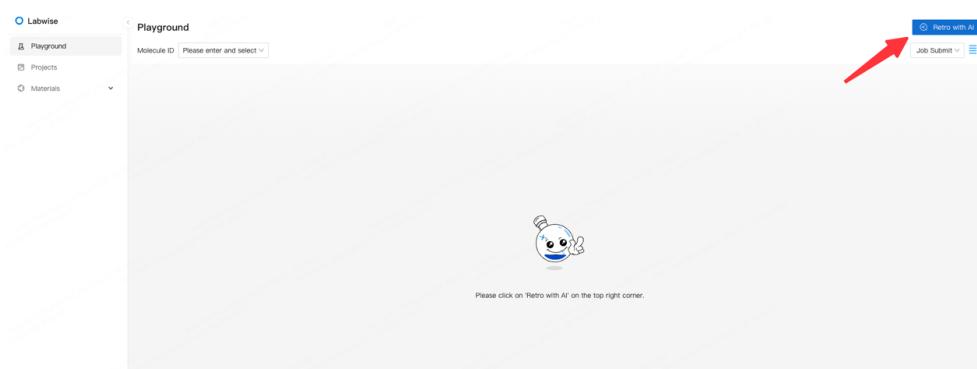
## 2. Playground

Playground is designed for first-time users to get familiar with our system quickly.

- 1) Enter Playground



## 2) Start a retrosynthesis design



**Note:** The initial visit to this page may require several seconds to load the frontend assets. Subsequent page visits should be fast.

## 3) Input a target compound

- Give the molecule an ID

Molecule ID: Please enter

Structural Formula Recognition (Supports jpg/png Image Size Not Exceeding 1MB)

Fast Mode Optimal Mode Recommended

Max RXN steps: 20

Max Design Time(min): Please enter

Price Threshold (¥ / g): ¥ 1,000

\* Material Supplier:

- leyan (2023-09-02) ×
- bidepharm (2024-01-05) ×
- aladdin (2023-10-09) ×
- + 2 Raw material source...

Advanced settings: Starting Materials to Avoid:

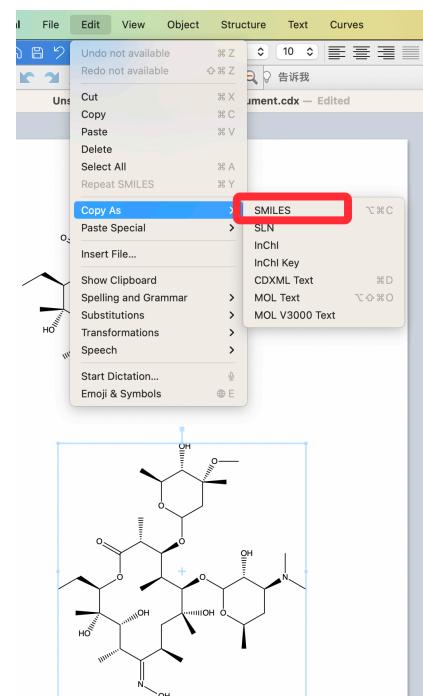
Preferred Starting Material:

Cancel Submit

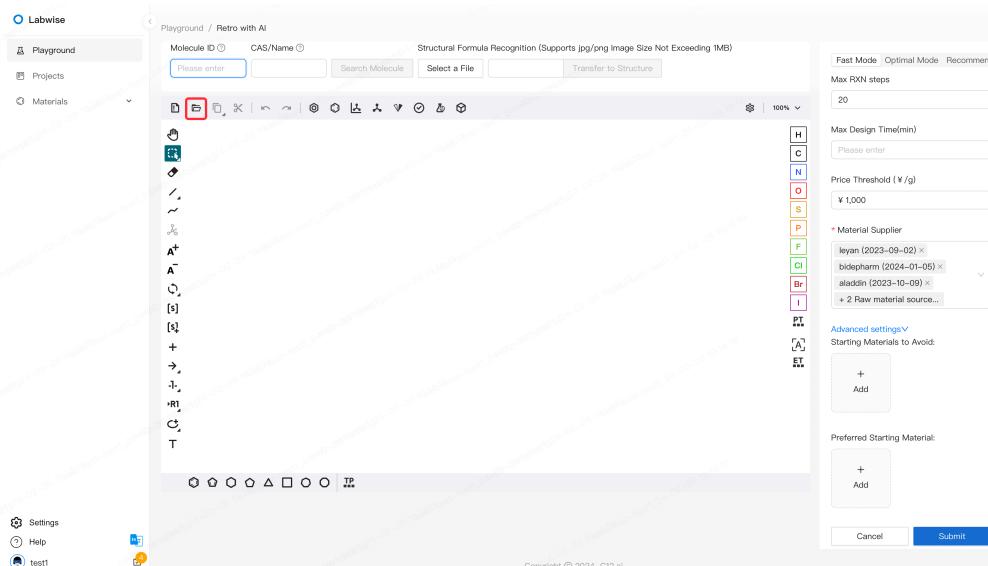
- Input the molecule structure by one of the following methods:

a) Copy the smiles from ChemDraw or from other sources

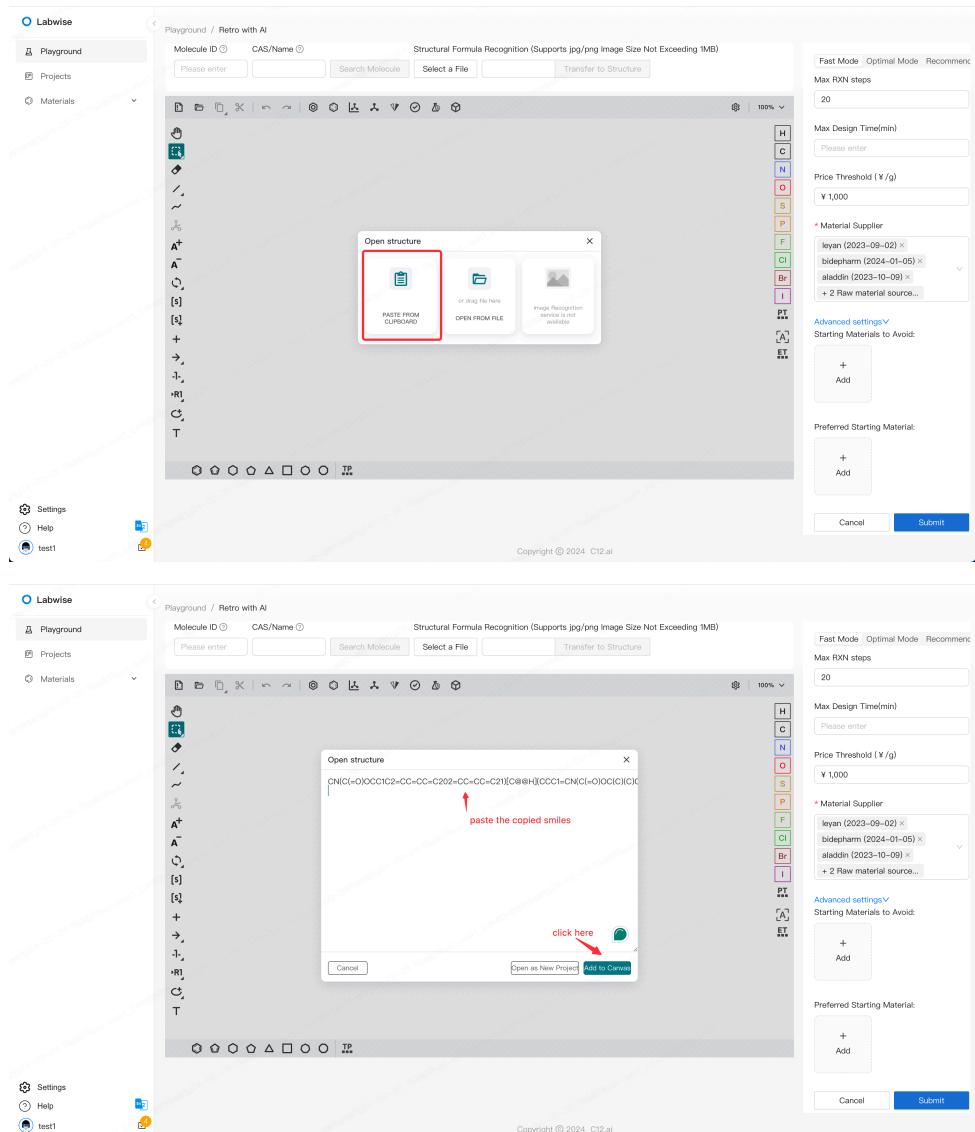
In ChemDraw:



In Labwise, click the folder icon, then click "paste from clipboard" to paste the smiles copied just now.



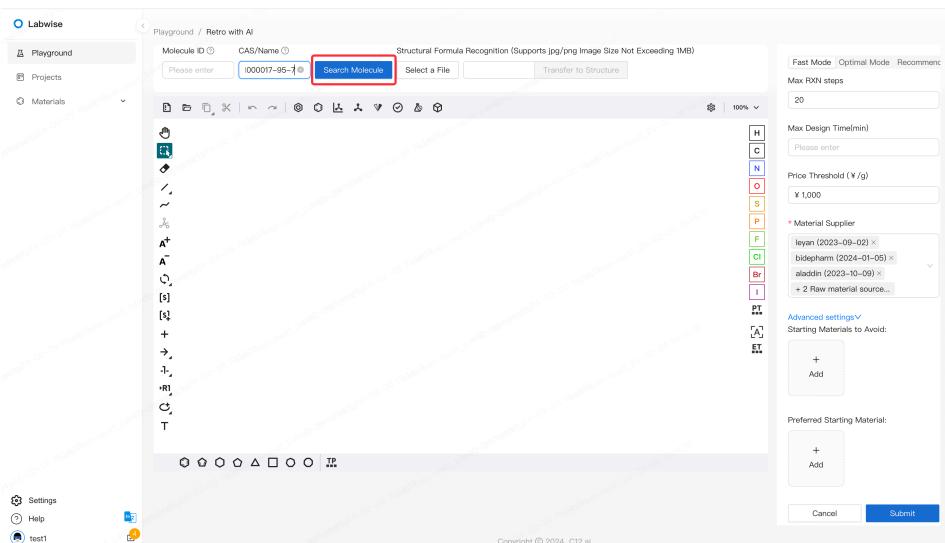
The screenshot shows the Labwise interface with the 'Playground / Retro with AI' tab selected. On the left, there's a sidebar with 'Playground', 'Projects', and 'Materials'. The 'Materials' section has a folder icon highlighted with a red box. The main area shows search fields for 'Molecule ID' and 'CAS/Name', and a 'Structural Formula Recognition' section. On the right, there are settings for 'Max RXN steps' (set to 20), 'Max Design Time(min)', 'Price Threshold (¥ /g)' (set to ¥1,000), and a 'Material Supplier' dropdown containing 'leyan (2023-09-02)', 'lidepharm (2024-01-05)', and 'aladdin (2023-10-09)'. There are also sections for 'Advanced settings', 'Starting Materials to Avoid', and 'Preferred Starting Material'.



The screenshot shows the C12.ai interface with the 'Playground / Retro with AI' tab selected. In the center, there's a canvas with a toolbar on the left containing various chemical drawing tools. A modal window titled 'Open structure' is open, showing three options: 'PASTE FROM CLIPBOARD' (highlighted with a red box), 'OPEN FROM FILE', and 'Image Recognition service is not available'. The input field in the modal contains the SMILES string: CN(C(=O)OCC1C2=CC=CC=C2O1)C@H)(CC1=CN(C(=O)C(C)C)C1. Red arrows point to the 'paste the copied smiles' text and the 'Add to Canvas' button.

Now the structure should be displayed in the canvas.

## b) Enter the molecule's name or CAS number



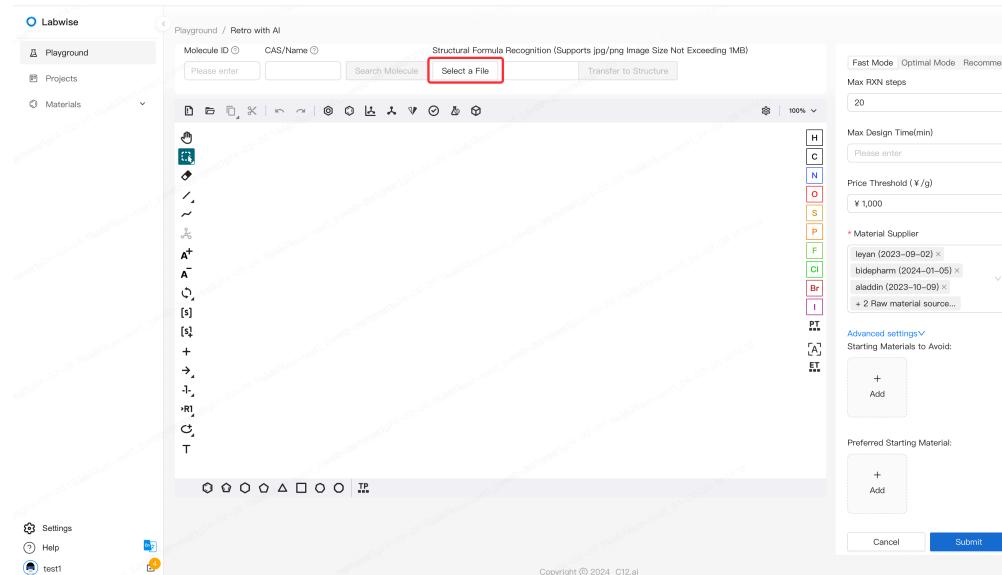
The screenshot shows the C12.ai interface with the 'Playground / Retro with AI' tab selected. In the top navigation bar, the 'Search Molecule' input field contains the value '1000017-95-1'. This input field is highlighted with a red box. Next to it is the 'Search Molecule' button, which is also highlighted with a red box. The rest of the interface includes a toolbar on the left, a canvas area, and various settings and search bars on the right.

Click “Search Molecule” after entering the molecule’s CAS number or name.

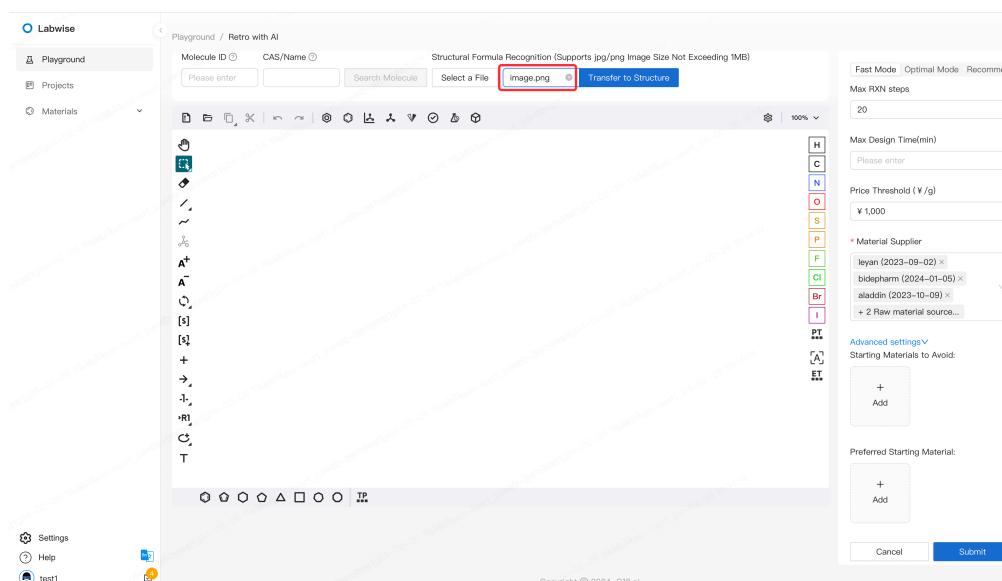
Note: this method is only applicable for common molecules. If the corresponding molecule cannot be found, please use other methods.

c) Use a molecule image

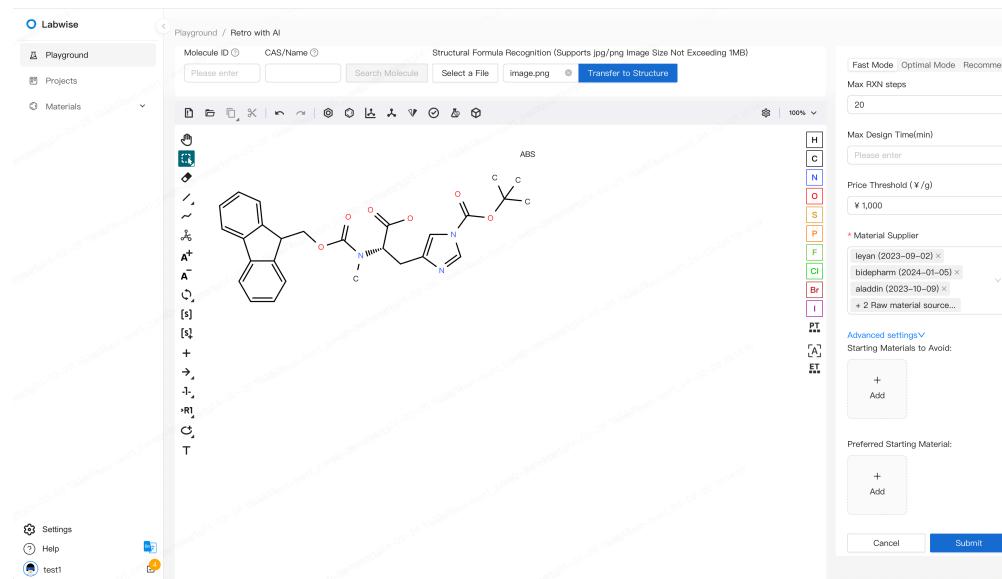
You can click “select a file” to brows the saved jpg/png files in your local disk.



It takes a few seconds for Labwise to recognize the structure.

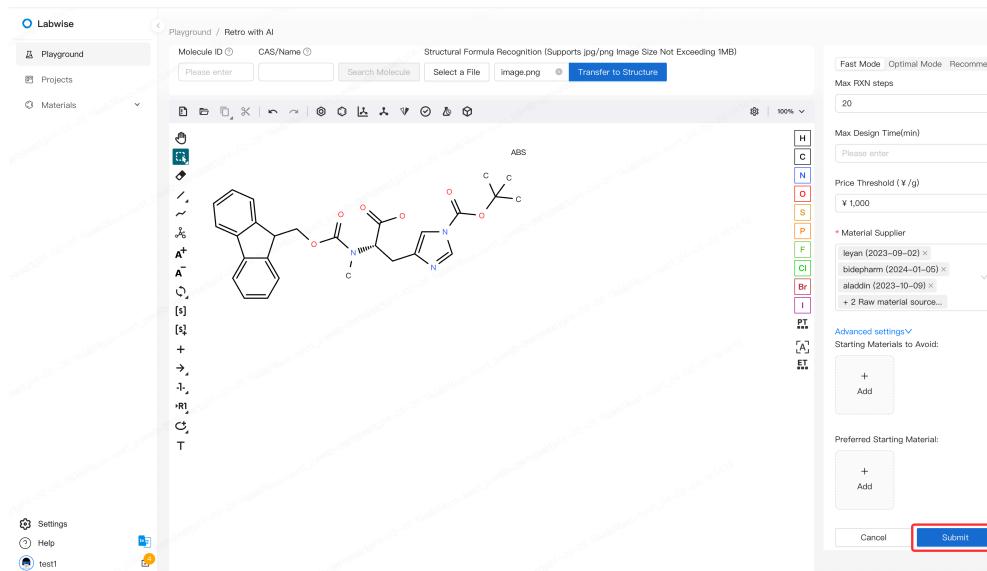


Now, you should see the structure of the molecule displayed in the canvas.



#### 4) Start a retrosynthesis run

- Click “Submit” to start a retrosynthesis run. You can choose to customize the following parameters on the right part of the screen for individual run, if needed.

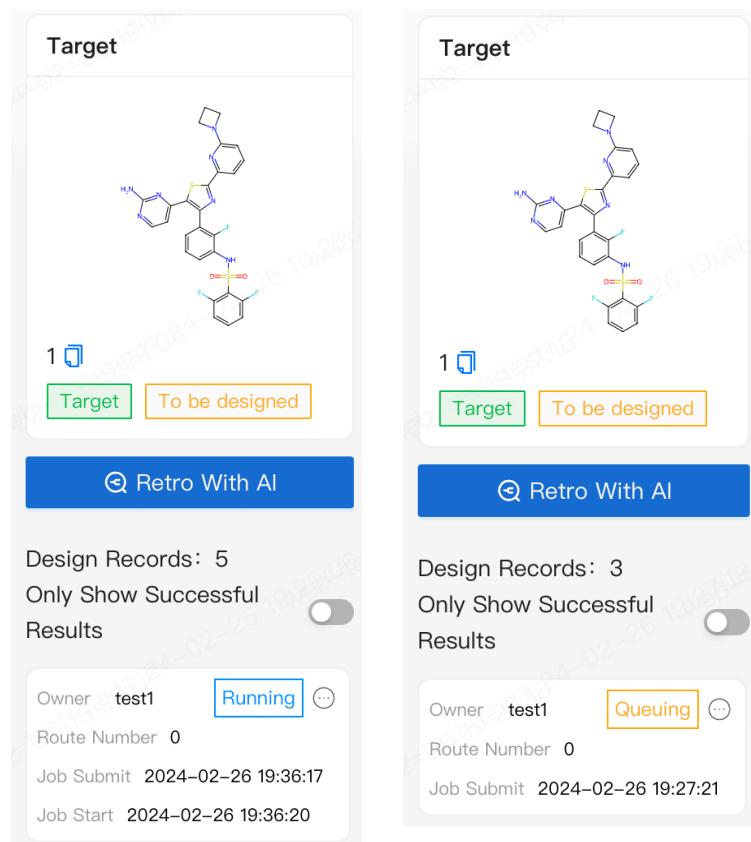


- Max RXN Steps:** specifies the maximum steps of reaction in all routes that AI would design. Set a higher value if the molecule is complicated.
- Price Threshold:** specifies the maximum unit price of the starting materials used in the AI-designed route.
- Material Supplier:** only use the starting materials from these suppliers.
- Preferred Starting Materials:** specify more starting materials in addition to the material library from the specified suppliers.
- Starting Materials to Avoid:** specify materials that AI cannot use.

- Advanced Settings: collapsed by default, is meant for internal debugging, and should generally be ignored by users.

## 5) Review ongoing retrosynthesis runs

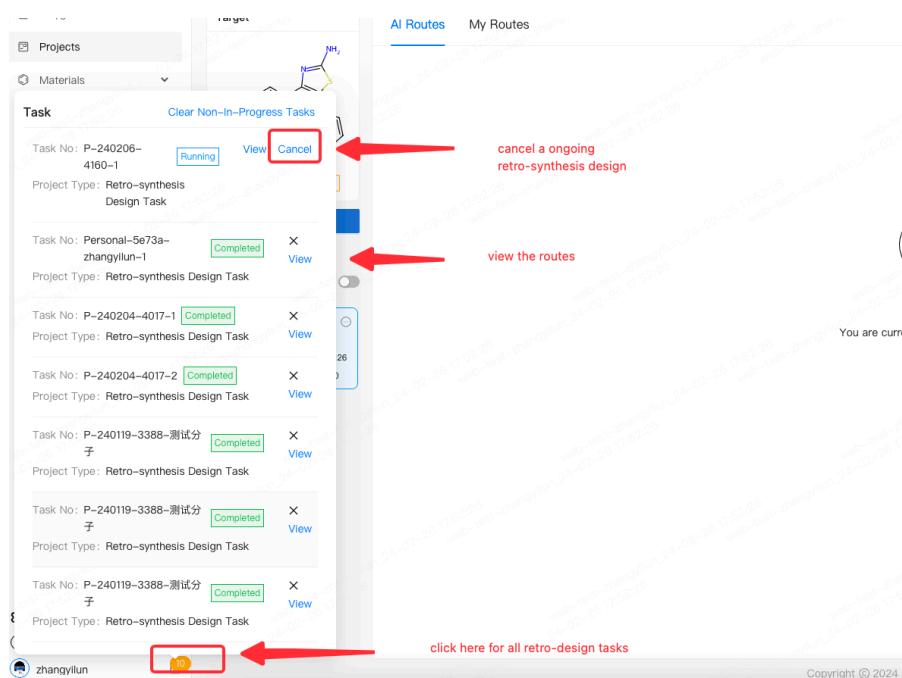
- After starting a retrosynthesis run, you should see a new card marked "in progress", indicating that the run is actively being processed.
- If multiple molecule retrosynthesis runs are submitted, the later runs are queued with the status "Queuing".



- For in progress runs, if the AI finds a new routes, there is a red number prompt on the card showing the number of newly designed routes, and the user can click the card to review them.



- Once a retrosynthesis run is started, you can safely leave this page and work on other molecules. You can review all your retrosynthesis runs in the action sheet in the lower left corner.
- After a run is completed, a notification is popped up. Click the “View” button to review routes designed by AI. Before the retrosynthesis run is done, you can click "Cancel" to cancel the run, and no route will be saved.



Projects Materials

**Task**

Clear Non-in-Progress Tasks

Task No: P-240206-4160-1 Running View Cancel

Project Type: Retro-synthesis Design Task

Task No: Personal-5e73a-zhangylun-1 Completed X View

Project Type: Retro-synthesis Design Task

Task No: P-240204-4017-1 Completed X View

Project Type: Retro-synthesis Design Task

Task No: P-240119-3388-测试分子 Completed X View

Project Type: Retro-synthesis Design Task

Task No: P-240119-3388-测试分子 Completed X View

Project Type: Retro-synthesis Design Task

Task No: P-240119-3388-测试分子 Completed X View

Project Type: Retro-synthesis Design Task

**AI Routes** **My Routes**

cancel a ongoing retrosynthesis design

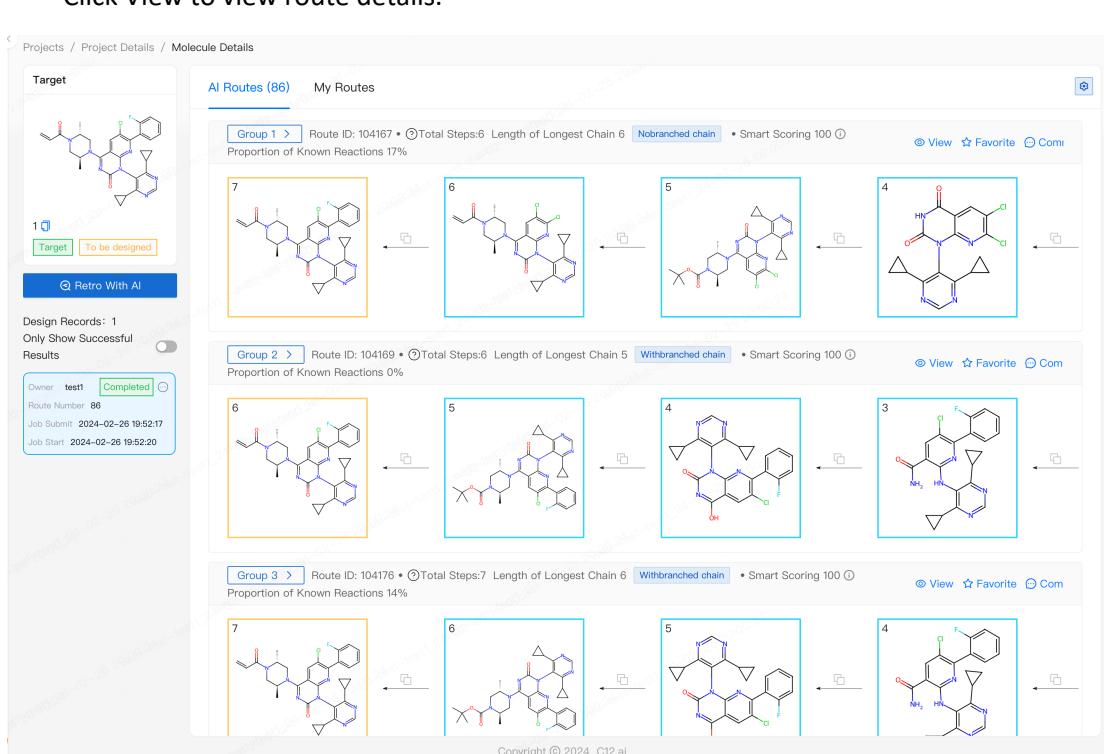
view the routes

click here for all retro-design tasks

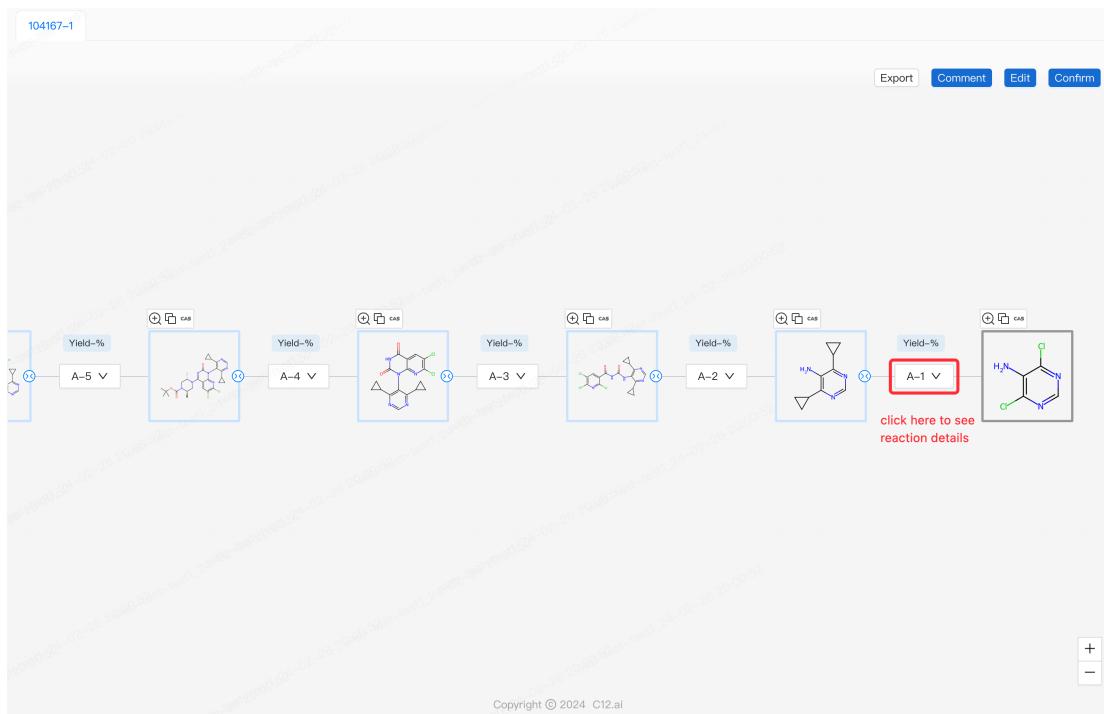
Copyright © 2024

## 6) Review routes designed by AI

- AI-generated synthesis routes are displayed as the main paths with the target product in a yellow box, intermediates in blue, and key starting materials in a black dashed box. You can slide horizontally to view the entire path. Each of the molecules and the reactions is clickable, allowing you to copy their SMILES for detailed analysis.
  - Route length: If there are multiple branching schemes under the same longest chain, it represents the total number of steps of the branching scheme with the shortest total number of steps.
  - Total steps: the total number of steps in the route.
  - Length of Longest Chain: If the synthesis route does not have branches, then this number is equivalent to the “Total steps” mentioned above. If the synthesis route has multiple branches, then this number represents the length of the longest branch.
  - Path branch flag: Indicates "no branched chain", "branched chain", or "multiple branched chains".
  - Smart scoring: algorithm designated score of each route ranging between 0 and 100.
  - Proportion of Known Reactions: the proportion of reactions reported in literature/patents in the route to the total number of steps in the route.
- Click View to view route details.



- If there are multiple branch chain schemes, the user will be prompted that the longest chain has multiple branch chains and can switch to view multiple branch chain schemes.



- Click the reaction to see the reaction details.

Projects / Project Details / Molecule Details / Routes Review

104167-1

**Reaction A-1**

Previous Step Next Step

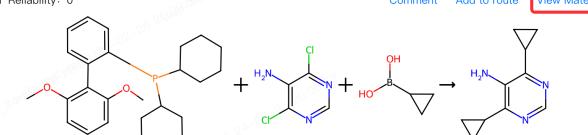
**Reaction Records**

AI-designed Reactions

from this task  
Reaction1 Reliability: 0

click here to see materials

Comment Add to route View Materials



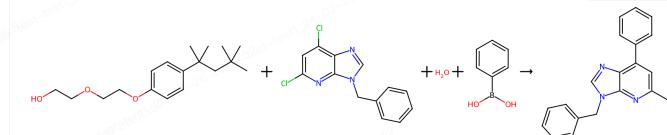
**Reaction Library**

reference reactions from literature and patents

Only show reactions with procedure

Similarity: 0.944 Yield: 79.00%

Reference for Reaction



Procedure

Reference Journal

Bioorganic and Medicinal Chemistry Letters; vol. 21, 21; (2011); p. 6398 – 6403

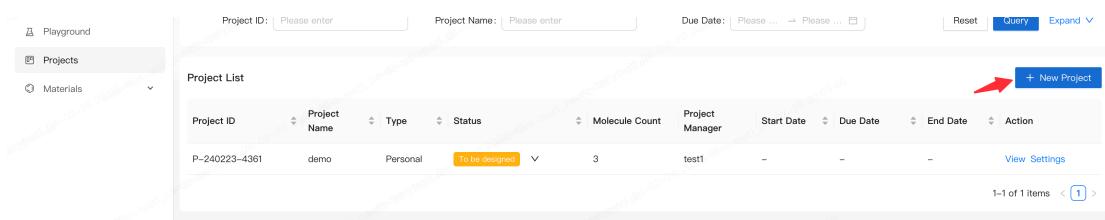
## III. Advanced Usage

### 1. Project management

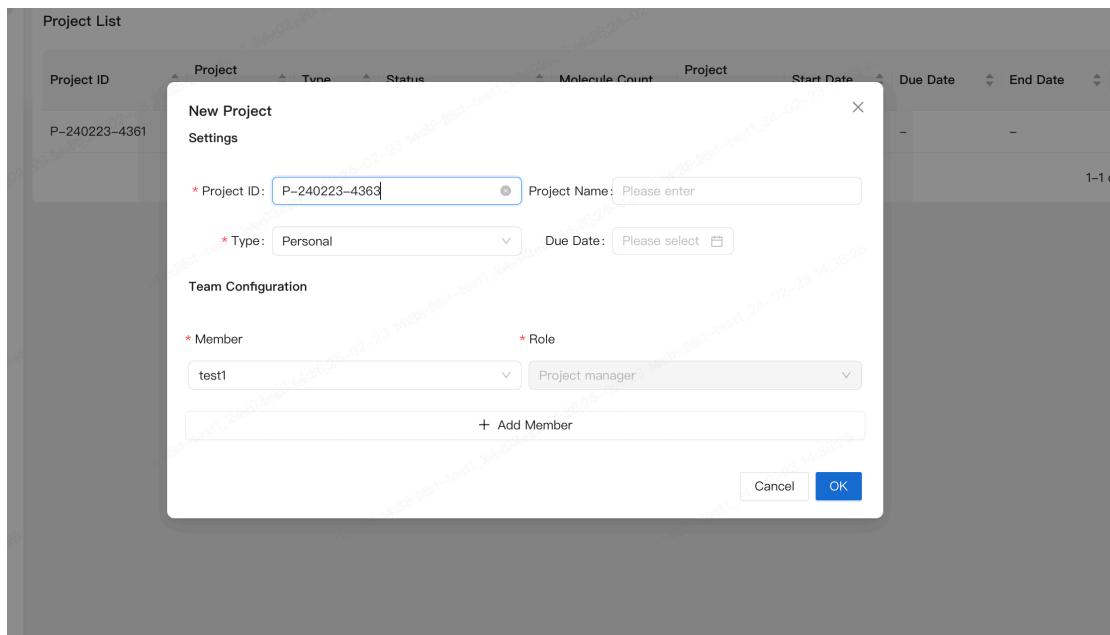
A project creates a virtual team space for sharing knowledge and information. The creator of the project is automatically designated as the owner. Only the owner and invited collaborators have the rights to view and manage the project's content, including molecular structures and synthesis routes. Other users are not allowed to access any project information. Within the project, members can add molecules, execute retrosynthesis runs, and review and comment on routes, facilitating team collaborations.

#### 1) Create a project

- Click the “New Project” button shown in the figure below.



- The pop-up box after clicking the button is shown in the following figure: the upper part lists the basic information of the project. The lower part is the personnel configuration. By default, the user who creates the project is the project manager.
  - Click “Add Member” and enter new account information to add other account users to this project.
  - The trial version only provides two roles, project manager and project member. The licensed version can customize roles and their permissions according to organizational relations.
  - Project managers can add, delete, and modify members in this project. Project members have no permissions to make any modification on the project members.



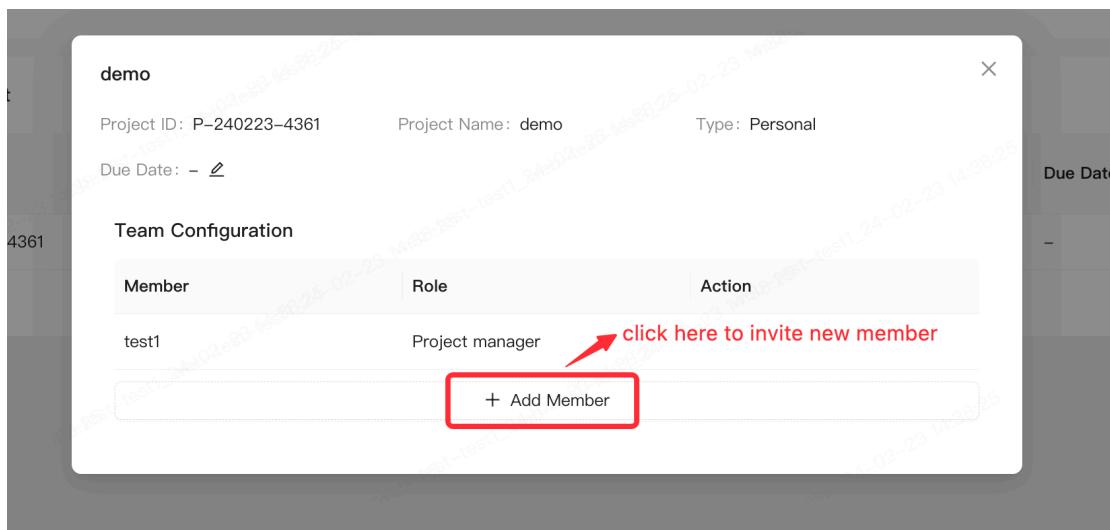
## 2) Edit a project

- For a project, click “Settings” in the operation column to the right of the project record to update the project delivery date and change the project member.

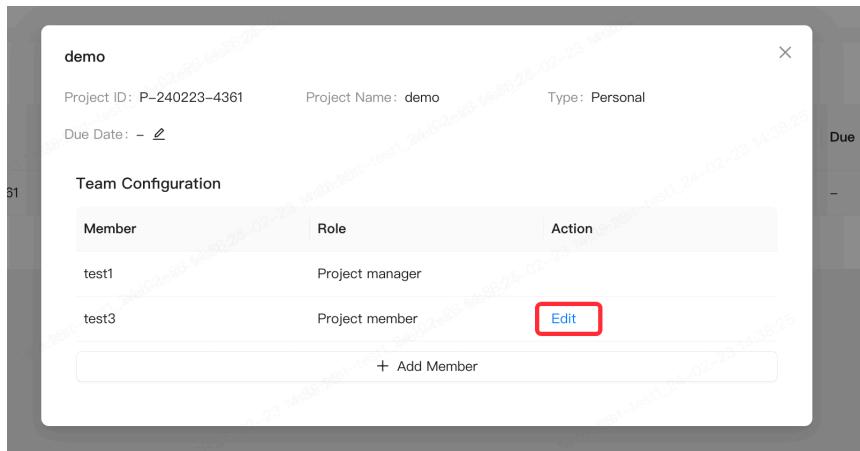
Project List											+ New Project
Project ID	Project Name	Type	Status	Molecule Count	Project Manager	Start Date	Due Date	End Date	Action		
P-240223-4361	demo	Personal	To be designed	0	test1	-	-	-	<a href="#">View</a> <a href="#">Settings</a>		

1-1 of 1 items < 1 >

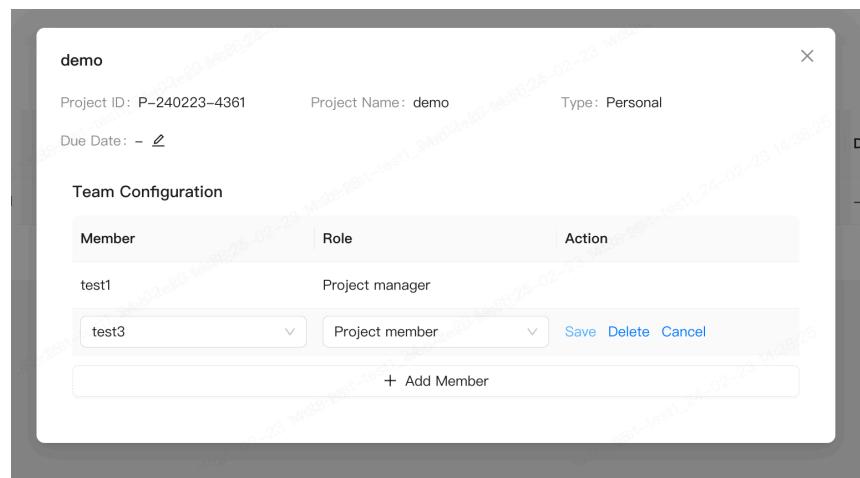
- Click “Add Member” in the image below to invite new members.



- The project manager can click this “Edit” button to edit the permissions of the members who have joined the project or click "Delete" to move the member out of the project.

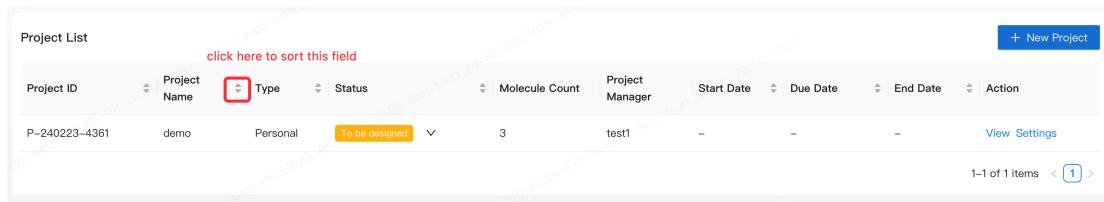


->

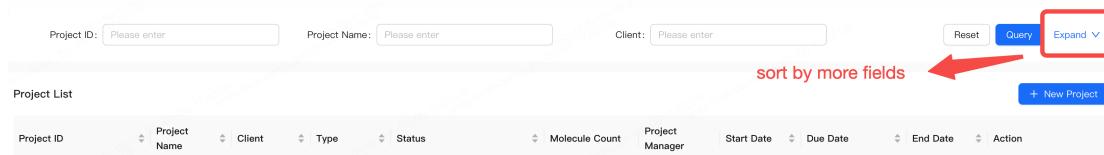


### 3) Sort and filter

- In the project list, we can sort the project accordingly in ascending and descending order by clicking the up and down triangle buttons next to each field.

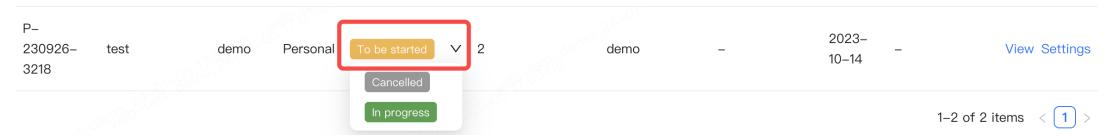


- Click the "Expand" to add filters to the projects. Click the "Reset" button to reset the filters and click the "Query" button to confirm the filter and query.

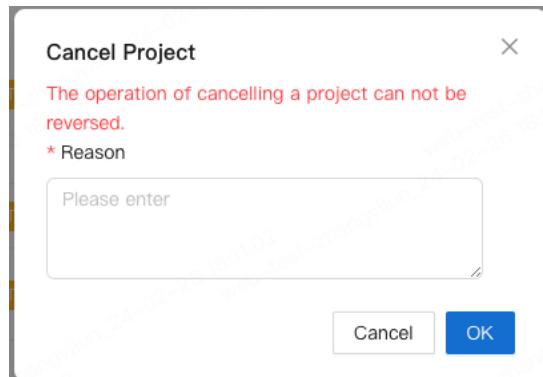


### 4) Cancel a project

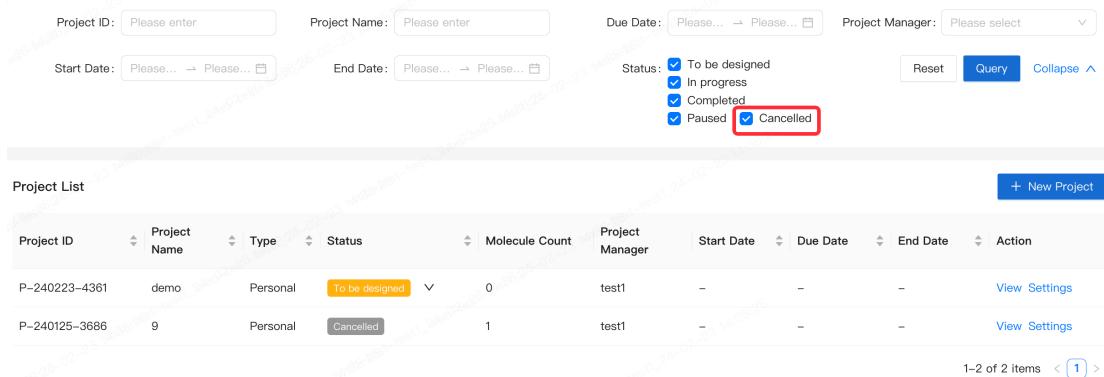
- Click on the status icon of the project in the figure below to change the status of the project to cancelled, enter the reason for cancellation, and click Confirm.



P-  
230926- test demo Personal To be started 2 demo - 2023-  
10-14 View Settings  
Cancelled In progress  
1-2 of 2 items < 1 >



- Cancelled projects are not displayed in the list by default. Check the "Cancelled" status in the filter and click "Query" to see the previously cancelled items.

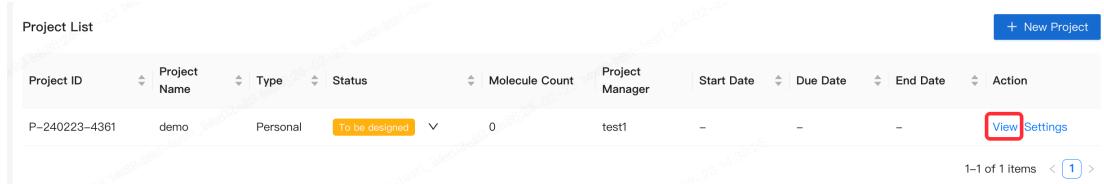


Project ID: Please enter Project Name: Please enter Due Date: Please... → Please... Project Manager: Please select  
Start Date: Please... → Please... End Date: Please... → Please... Status:  To be designed  In progress  Completed  Paused  Cancelled  
Reset Query Collapse ▲  
1-2 of 2 items < 1 >

Project List											+ New Project
Project ID	Project Name	Type	Status	Molecule Count	Project Manager	Start Date	Due Date	End Date	Action		
P-240223-4361	demo	Personal	To be designed	0	test1	-	-	-	<a href="#">View</a>	<a href="#">Settings</a>	
P-240125-3686	9	Personal	Cancelled	1	test1	-	-	-	<a href="#">View</a>	<a href="#">Settings</a>	

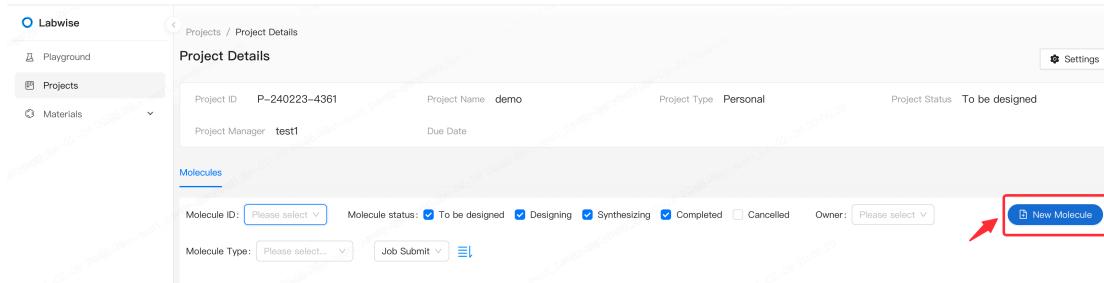
## 5) Add molecules and start retrosynthesis runs

- Click the "View" button in the operation column to the right of the project record to enter the project details.



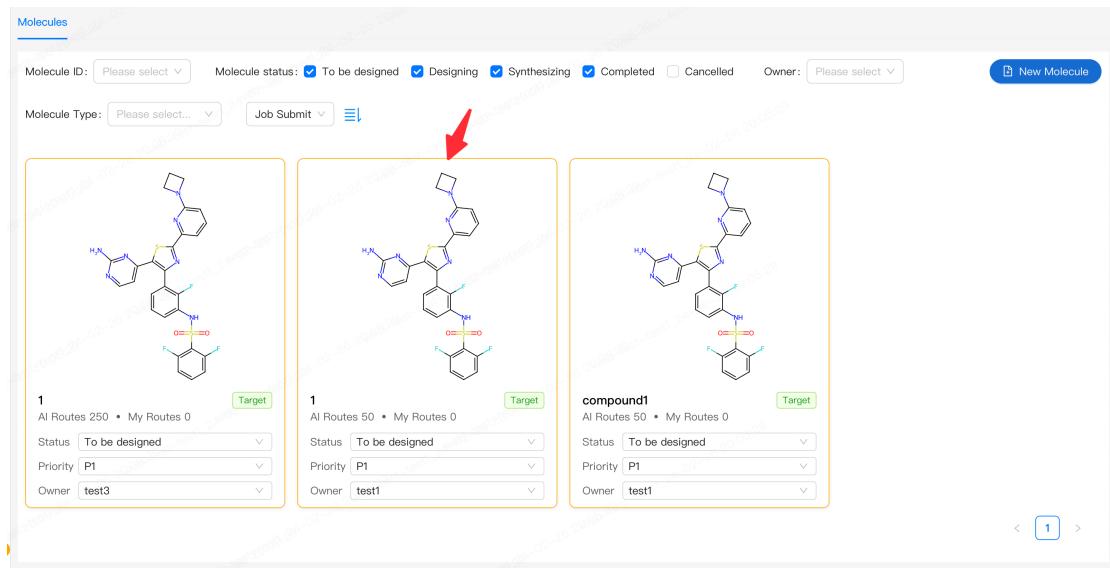
Project List + New Project  
Project ID Project Name Type Status Molecule Count Project Manager Start Date Due Date End Date Action  
P-240223-4361 demo Personal To be designed 0 test1 - - - [View](#) [Settings](#)  
1-1 of 1 items < 1 >

- Click the "Add Molecule" button in the upper right corner.



Labwise Projects / Project Details Project Details  
Project ID P-240223-4361 Project Name demo Project Type Personal Project Status To be designed  
Project Manager test1 Due Date  
Molecules  
Molecule ID: Please select... Molecule status:  To be designed  Designing  Synthesizing  Completed  Cancelled Owner: Please select...  
Molecule Type: Please select... Job Submit

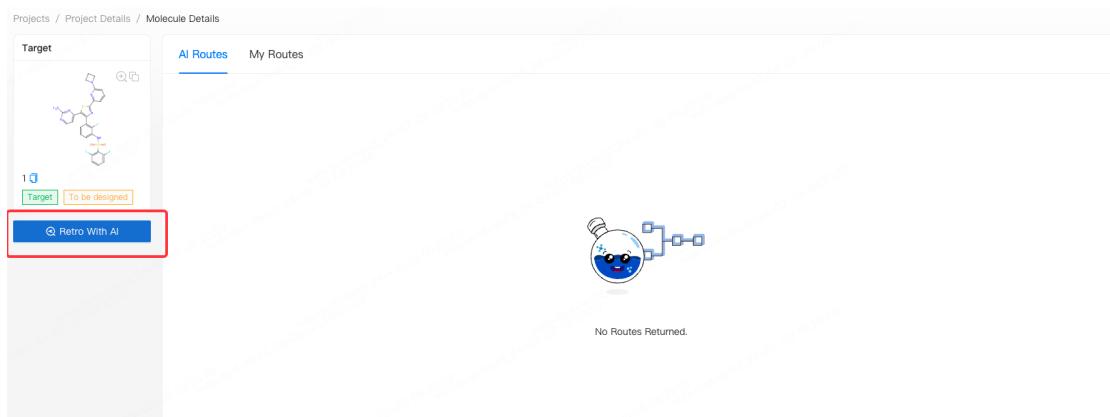
- Then you can follow the instruction mentioned in the previous [section II.2](#) to input the molecule information and its structure.
- Click on the molecular card to enter the molecular details.



The screenshot shows the 'Molecules' section of the C12.ai platform. There are three molecular cards displayed:

- Card 1:** Shows a complex organic molecule structure. Below it, the ID is '1', status is 'To be designed', priority is 'P1', and owner is 'test3'. A green 'Target' button is present.
- Card 2:** Shows the same complex organic molecule structure. Below it, the ID is '1', status is 'To be designed', priority is 'P1', and owner is 'test1'. A green 'Target' button is present. This card is highlighted with a red arrow.
- Card 3:** Shows a complex organic molecule structure. Below it, the ID is 'compound1', status is 'To be designed', priority is 'P1', and owner is 'test1'. A green 'Target' button is present.

- Click "Retro with AI", fill in the design requirements as needed in the pop-up window, and click "submit" to initiate the retrosynthesis task.



The screenshot shows the 'Project Details / Molecule Details' page for molecule '1'. The 'Target' section displays the molecule structure. The 'AI Routes' section shows the following details:

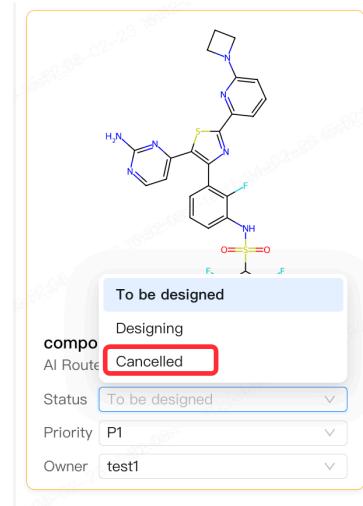
- Molecule ID: 1
- Status: To be designed
- Priority: P1
- Owner: test3

A red box highlights the blue 'Retro With AI' button. Below the button, there is a message: 'No Routes Returned.' and a cartoon character icon.

- The next steps are same as introduced in the previous [section II.2](#).

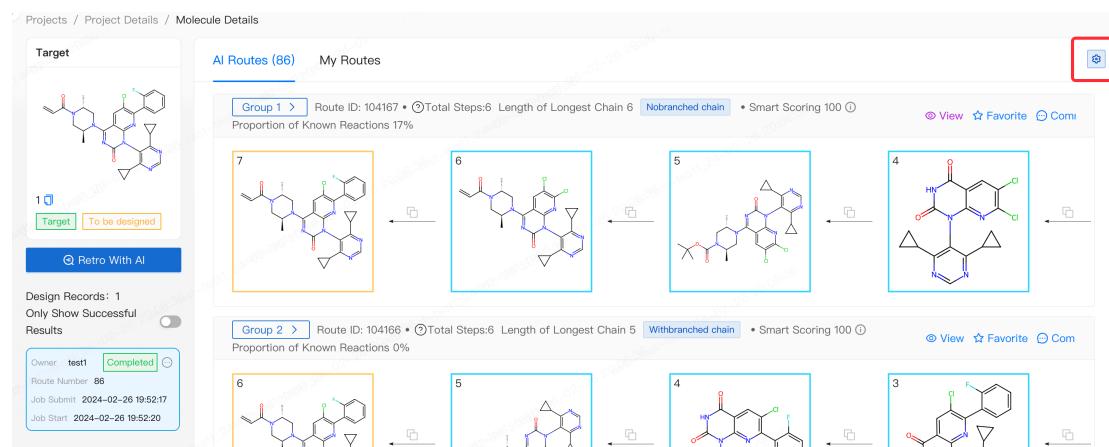
## 6) Cancel a molecule

- You can change the molecule's state to "Cancelled" at the molecular state of the molecule card.



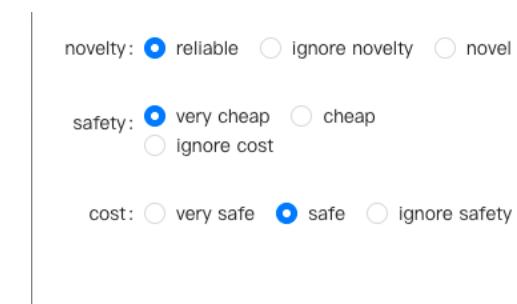
## 2. Route preferences

- After you entered the AI route list page, there's a preference setting in the right-up corner of the page



The screenshot shows the AI Routes (86) section. On the right, there is a small icon with a gear and a wrench, which is the preference settings icon. The routes are grouped into two sections: Group 1 and Group 2. Each group shows a sequence of reaction steps with numbered boxes (1 through 7). The first route in Group 1 is highlighted with an orange border.

- Click the icon, you can set the preference as needed

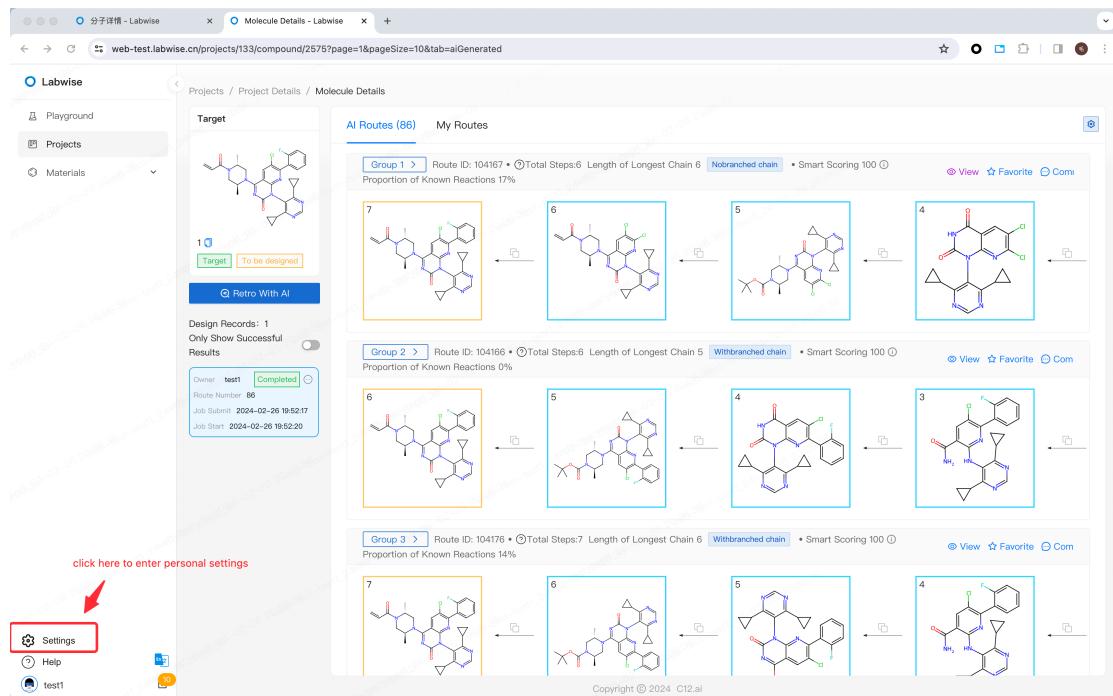


The dialog box contains three sections of preferences:

- novelty:**  reliable  ignore novelty  novel
- safety:**  very cheap  cheap  ignore cost
- cost:**  very safe  safe  ignore safety

## 3. Personalized settings

- Click the setting button located at the lower left of the navigation bar



click here to enter personal settings

Settings

Help

test1

Owner: test1 | Completed | Route Number: 86 | Job Submit: 2024-02-26 19:52:17 | Job Start: 2024-02-26 19:52:20

AI Routes (86) My Routes

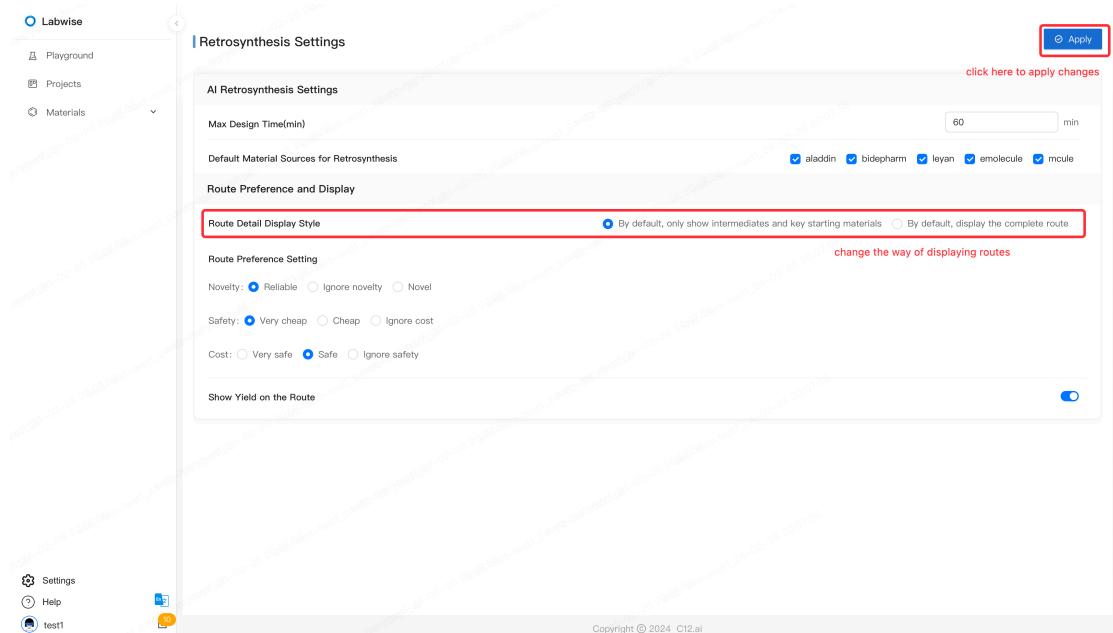
Group 1 > Route ID: 104167 • Total Steps: 6 Length of Longest Chain 6 Nobranched chain • Smart Scoring 100 0% Proportion of Known Reactions 17%

Group 2 > Route ID: 104168 • Total Steps: 6 Length of Longest Chain 5 Withbranched chain • Smart Scoring 100 0% Proportion of Known Reactions 0%

Group 3 > Route ID: 104176 • Total Steps: 7 Length of Longest Chain 6 Withbranched chain • Smart Scoring 100 14% Proportion of Known Reactions 14%

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**2) Once you changed your preference (shown below), click the “Apply” button. The setting in this page will be the default setting when you use these functions afterwards**



click here to apply changes

Apply

click here to enter personal settings

Settings

Help

test1

Max Design Time[min]

60 min

Default Material Sources for Retrosynthesis

aladdin bidepharm leyan emolecule mcule

Route Preference and Display

Route Detail Display Style

By default, only show intermediates and key starting materials  By default, display the complete route

change the way of displaying routes

Route Preference Setting

Novelty:  Reliable  Ignore novelty  Novel

Safety:  Very cheap  Cheap  Ignore safety

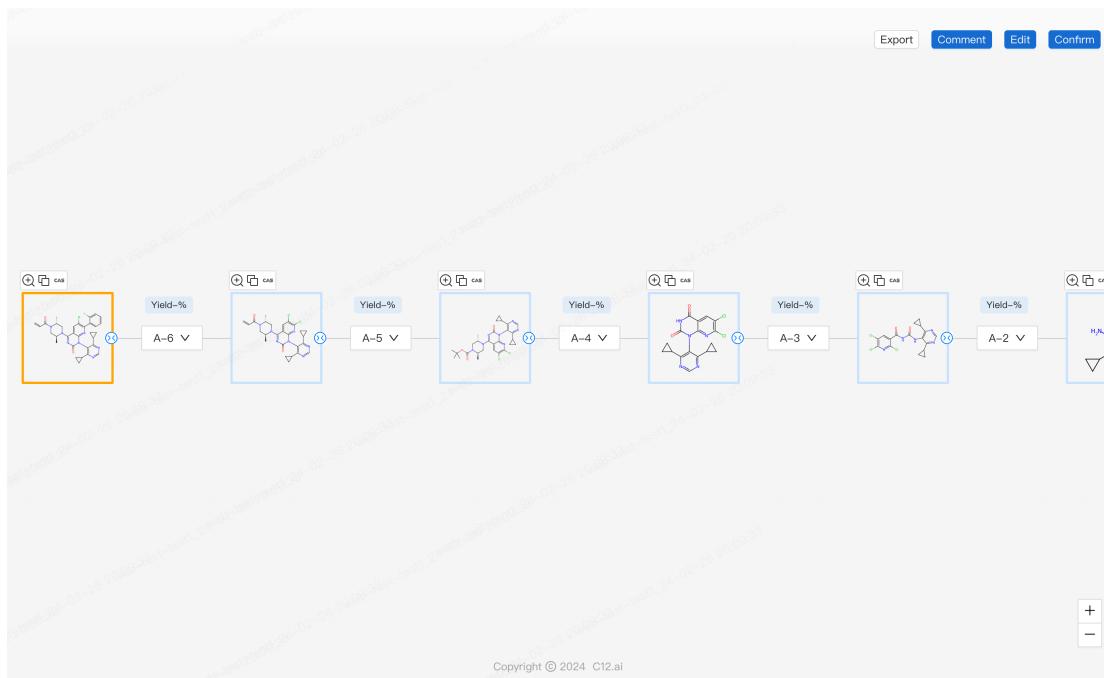
Cost:  Very safe  Safe  Ignore cost

Show Yield on the Route

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**Note:** Here you can change the way routes are displayed: showing only intermediates and key starting materials, or the complete route. The two pictures below show the difference:

**a) Only the intermediates and key starting materials:**

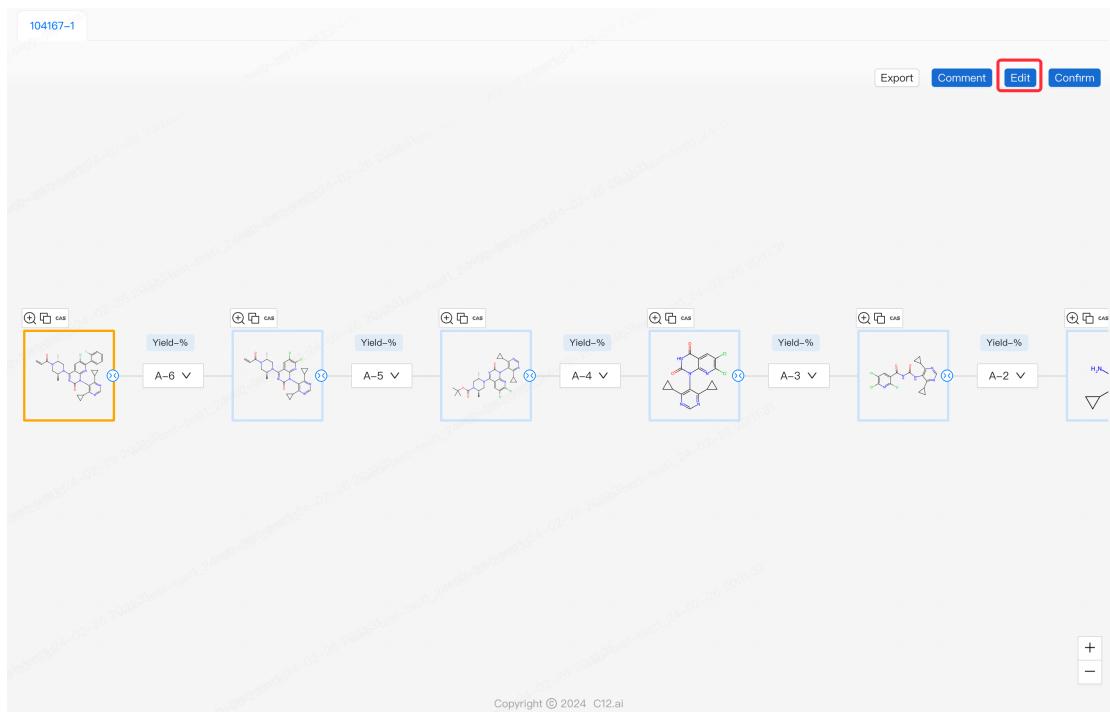


b) The full route



#### 4. Retrosynthesis from an intermediate compound or a starting material

- 1) After you entered the route detail page (shown below), click the “edit” button to make changes to the routes



**2) Click the retro icon on the molecule for which you want to explore new routes**



**3) In the popped-up page follow the same steps in [Section II.2](#) to start a retrosynthesis run.**

Projects / Project Details / Molecule Details

**Target**



223ddd2c-d... ⓘ  
show all materials ⌂ To be design

**AI Routes**

Q Retro With AI



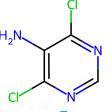
No Routes Returned.

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- 4) Once a proper route is generated, click the “View” button and then “choose”, the new route will be appended to the original route

Projects / Project Details / Molecule Details

**Target**



223ddd2c-d... ⓘ  
show all materials ⌂ To be design

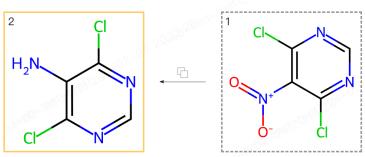
**AI Routes (2)**

Q Retro With AI

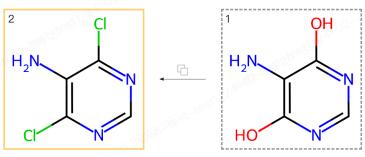
Design Records: 1  
Only Show Successful Results

Owner: test1 [Completed] ⓘ  
Route Number: 2  
Job Submit: 2024-02-26 20:13:28  
Job Start: 2024-02-26 20:13:30  
Job End: 2024-02-26 20:13:50

**Group 1 >** Route ID: 104253 • Total Steps: 1 Length of Longest Chain 1 Nobranch chain • Smart Scoring 60 ⓘ  
Proportion of Known Reactions 100% ⌂ View ⌂ Favorite ⌂ Com:



**Group 2 >** Route ID: 104252 • Total Steps: 1 Length of Longest Chain 1 Nobranch chain • Smart Scoring 60 ⓘ  
Proportion of Known Reactions 100% ⌂ View ⌂ Favorite ⌂ Com:



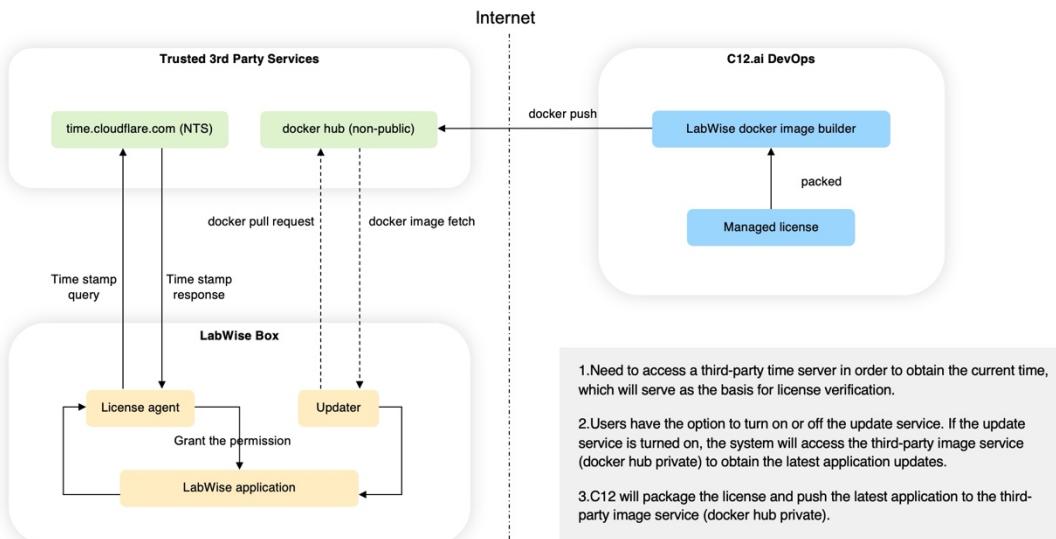
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## IV. Security and Privacy

As illustrated in the following figure, Labwise only connects to two trusted third-party services, one for checking the timestamps for license validation, and the other for checking for product updates. Other than these two services, the system makes NO external network connections.

All your data is stored on your local server with strong encryption and security measures, ensuring your exclusive access any of your data.



## V. Support

Please contact [c12\\_support@c12.ai](mailto:c12_support@c12.ai) for any questions or suggestions.