ncRNA Network Modeler (NMM)

Fei Liu, Fuwen Luo, Yang Li, Shangshang Mao, Yuhong Li, Jiahui He, Junjie Feng, Junhui Li

School of Software Engineering,

South China University of Technology

April 7, 2020

Contents

1 Introduction

The purpose of this system is to provide users with the construction of non-coding RNA to complete the simulation of non-coding RNA, mainly including two main functions:

(1) non-coding RNA modeling and visualization;

(2) dynamic model management and viewing.

Among them, non-coding RNA modeling and visualization is based on those nodes and lines that users use when drawing and modeling, then generate xml type files.Dynamic model management and viewing refers to saving and managing models throughNinput information in the software.

This software provides biomolecular modeling and simulation functions for researchers in the field of systems biology.

1.1 Non-Coding RNA

A non-coding RNA (ncRNA) is a functional RNA molecule that is transcribed from DNA but not-ntranslated into proteins. Epigenetic related ncRNAs include miRNA,siRNA, piRNA and lncRNA.In general, ncRNAs function to regulate gene expression at thetranscriptional and posttranscriptional level. Those ncRNAs that appear to be involved in epigenetic processes can be divided into two main groups; the short ncRNAs (<30 nts) and the long ncRNAs (>200 nts). The three major classes of short non-coding RNAs are microRNAs (miRNAs),short interfering RNAs (siRNAs), and piwi-interacting RNAs (piRNAs). Both major groups are shown to play a role in heterochromatin formation, histone modification, DNA methylation targeting, and gene silencing.

1.2 NCRV tool

1.2.1 Main functions

This software mainly includes two main functions: (1) non-coding RNA modeling and visualization   (2) dynamic model management and viewing. The following lists all the sub-templates of the two templates:

(1) Non-coding RNA modeling and visualization:

    1) Use the drawing module in the software for biological modeling and drawing

    2) Modify various attributes in the figure

    3) Save and delete the model

    4) Import a new non-coding RNA model

    5) Node external database link

    6) Network analysis function

(2) Dynamic model management and viewing:

    1) Manage model database entries

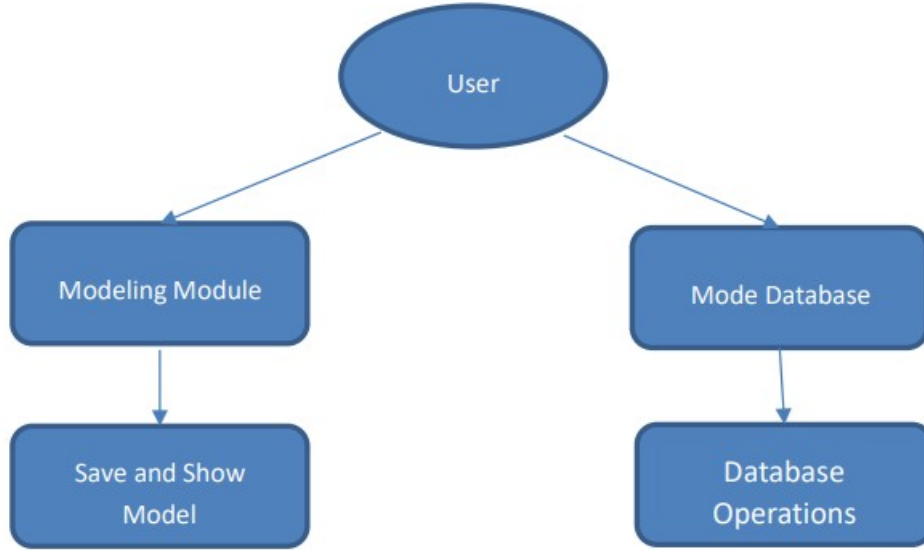   2) View and search the model database

1.2.2 Architecture

Figure 1: The architecture of NCRV tool.

1) User-friendly non-coding RNA icon, Protein icon, cell icon, etc.
2) Easy to build a strong non-coding RNA network.
3) Formal analysis based on graph theory.
4) Link non-coding RNA to Kinetic model based on Snoopy.

2 Modeling

This section will present a general step-by-step procedure for how to construct an NCRV model.This part of the model is just to show the function, without specific practical significance

2.1 Main interface

Figure 2 shows the main interface of the software. The menu and tool bar is on the top. The tools from left to right include "File", "Edit", "Options", "View","Tool", "Search", and "Help". Click"New" to create a new file, click "Save" to save the current page,and click "Open" to import the existing model of the computer.
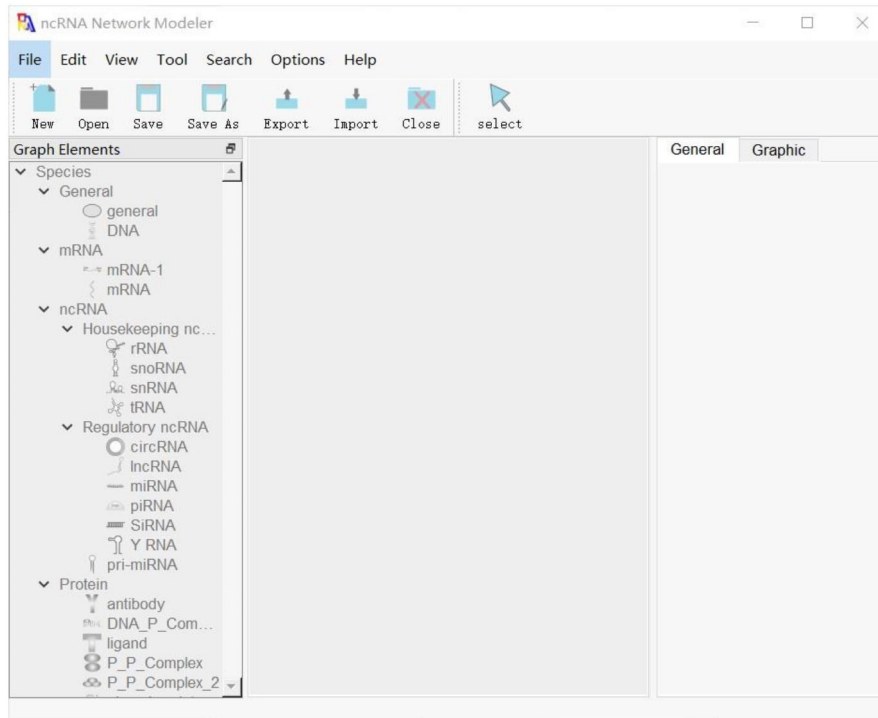
Figure 2: Main interface of NCRV tool.

2.2 Add nodes

Click on the element on the left side of the page to draw. There are two ways to add a node, one is to click the node (add one by one), or double-click the node (add continuously).
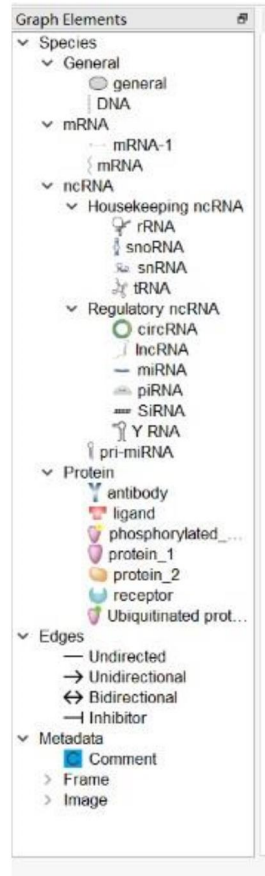
Figure 3: Graph elements

2.3 Node attributes

After adding a node, there is general attributes of the node on the right as show in Figure 4. Then user can change some attribute as show in Figure 5. The ID and Type(marked in red) in the attribute cannot be modified. Name, Standard Name, Alias Name (blue label) in the attribute can change the name. Among them, different names of Alias Name need to be separated by semicolon ";". Logic attribute bar binds multiple attributes together, only their positions are different, all other attributes are the same, including the name. Node Graphic attributes are show in Figure 6.

Figure 4: Node General attributes

Figure 5: The ID and Type (marked in red) in the attribute cannot be modified. Name, Standard Name, Alias Name (blue label) in the attribute can change the name.Among them, different names of Alias Name need to be separated by semicolon ";".

Figure 6: Node Graphic attributes

2.4 Frame attributes

Frame has no name by default, users can define the name. The type and ID cannot be changed. The width and height in graphic attributes cannot be changed.
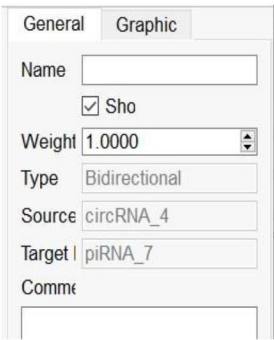

Figure 7: Frame General attributes

Figure 8: Frame Graphic attributes

2.5 Line attributes
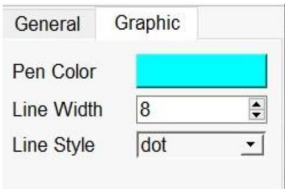
Figure 9: Line General attributes
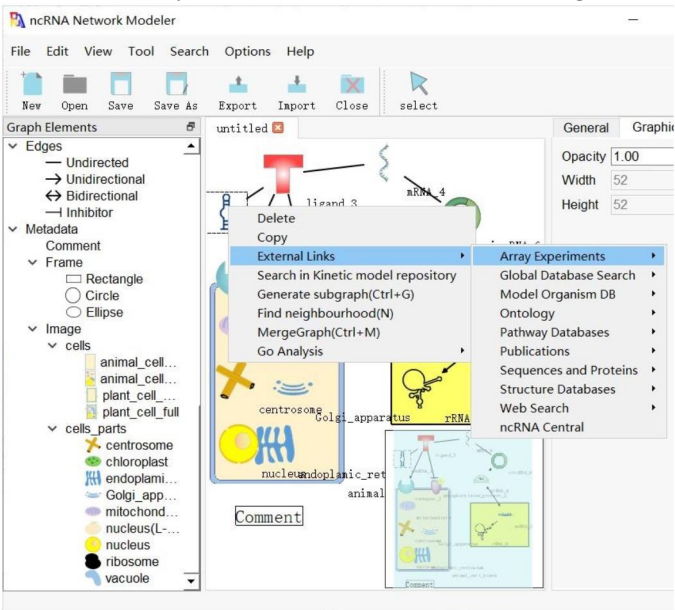

Figure 10: Line Graphic attributes

2.6 External database

Right-click the node icon and click "External Links" to display the external link database. You cannaccess the external database of information you are interested in.Showed in Figure 11.
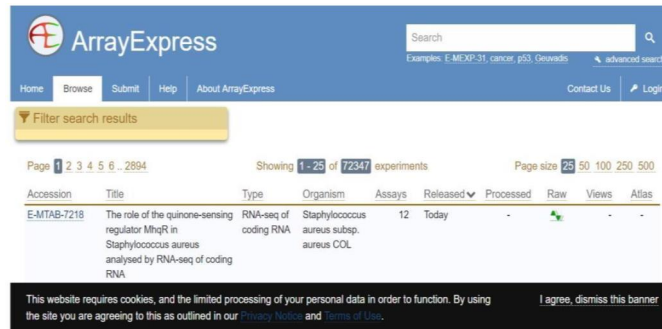
Figure 11: Access the external database.

2.7 Molecular information sheet

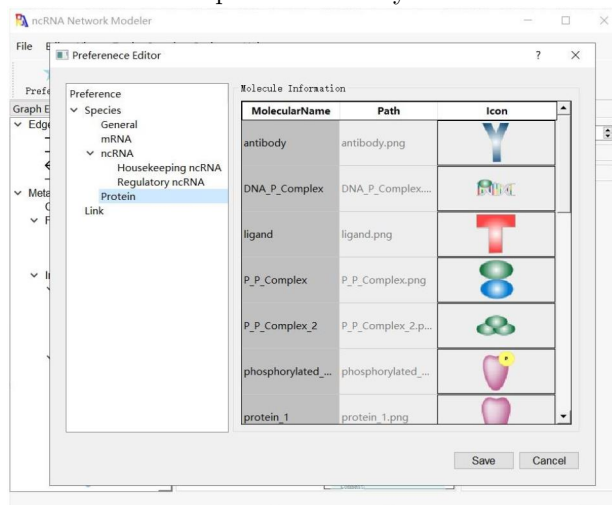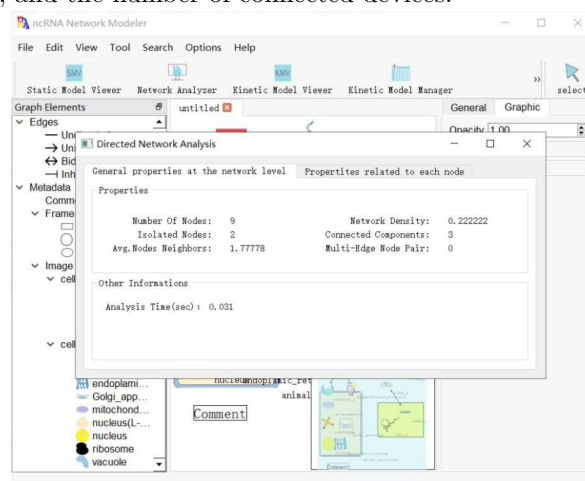Double-click the node, click on the node's preference and you can view the analysis information table.

Figure 12: Molecular information sheet

2.8 Network analysis

Click the image analysis button to view the image analysis results. There are the number of nodes,the number of discrete nodes, and the number of connected devices.
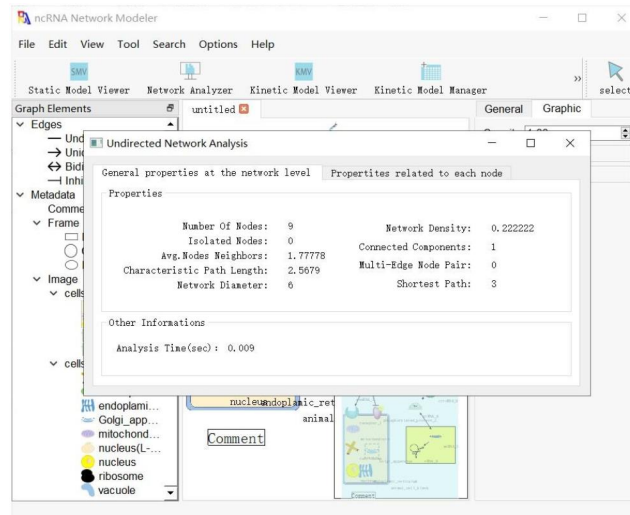
Figure 13: Network analysis function

2.9 Node analysis

Click the DegreeAnalyzer button to view the node analysis results. You can choose to show the degree of nodes by size and color.
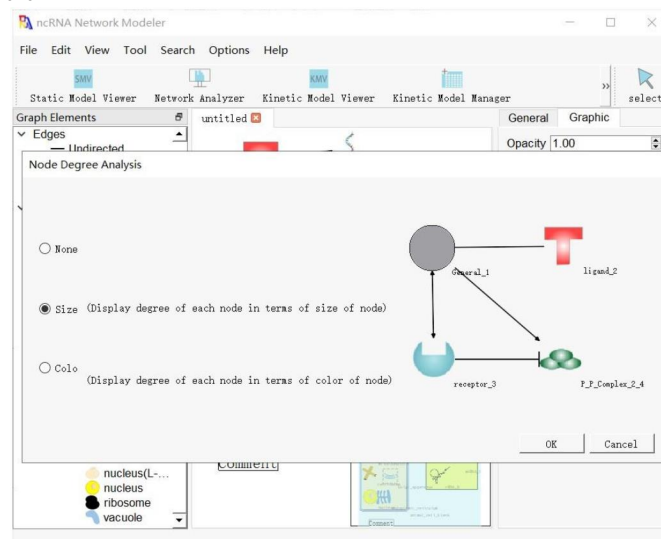

Figure 14: Node analysis function

2.10 Search Kenitic Repository

Select node and click the search kenitic repository button. All lists containing this mRNA can be listed.
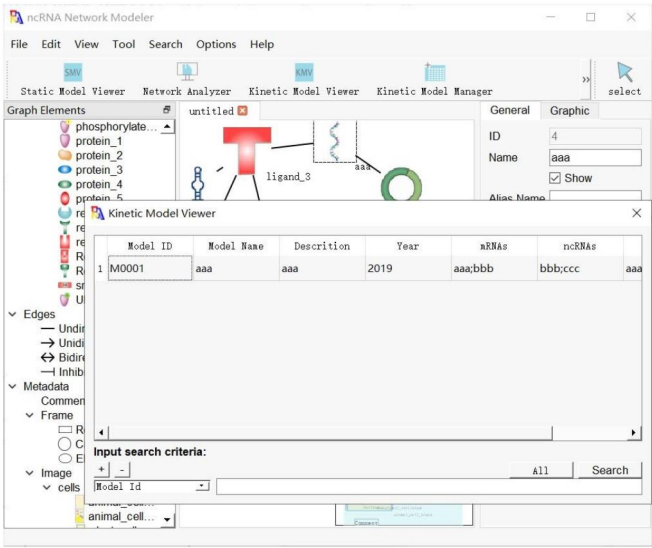

Figure 15: Search Kenitic Repository function

2.11 Layout

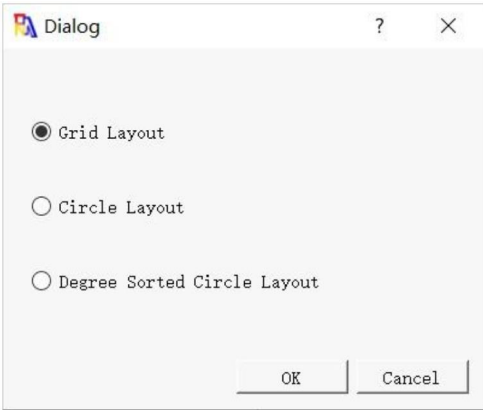Users can freely choose three layout modes
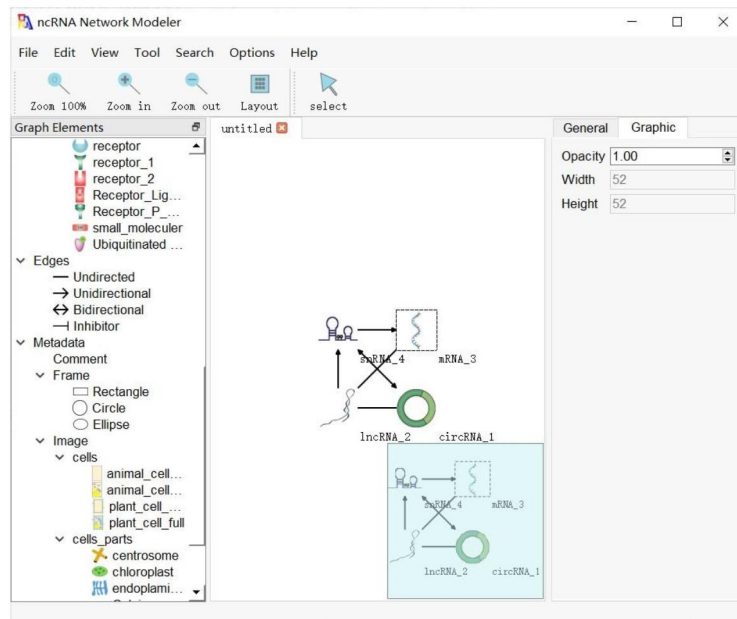

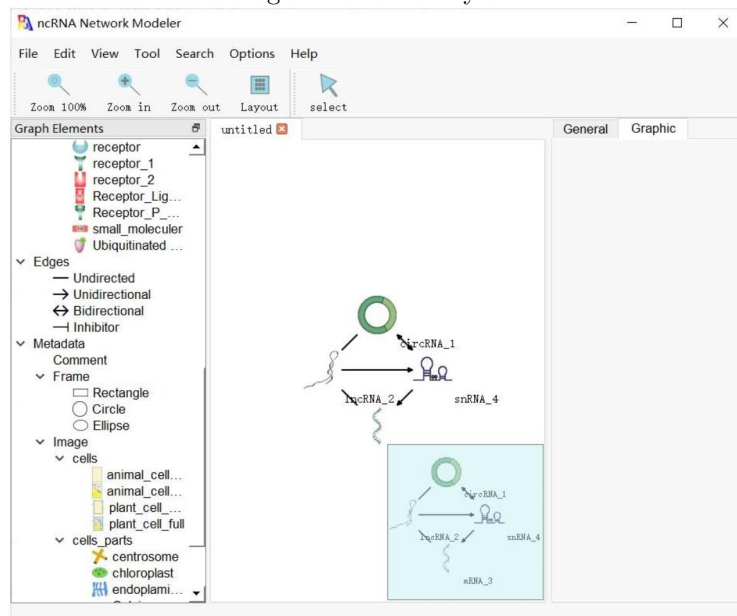Figure 16: Layout function
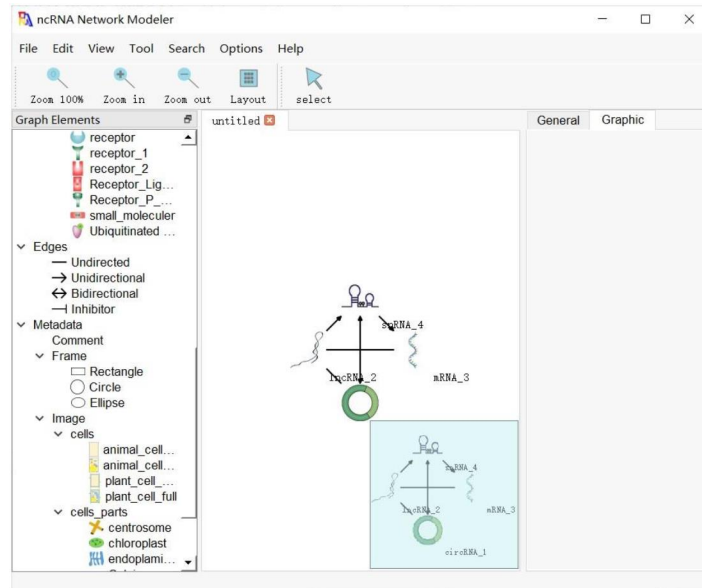
Figure 17: Grid Layout

Figure 18: Circle Layout

Figure 19: Degree Sorted Circle Layout

2.12 Search Nodes

Search nodes function can be found in the top menu. With the searching nodes function, users can focus on a certain ncRNA, protein or gene node easily by giving name or ID of the node.
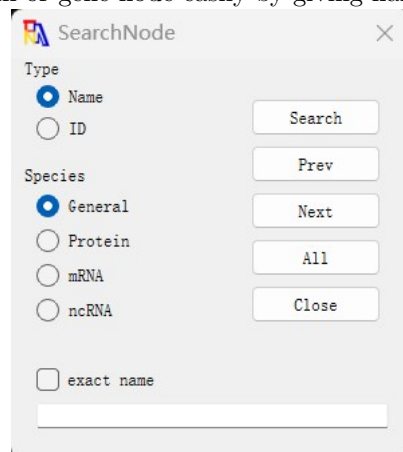

Figure 20: Search function

Let's use an example to show how to use this function. For example, when you want to focus on ncRNA nodes that names contain "uc", you can select the species options of ncRNA and enter "uc" in the input field. Then click the "Search" button, a node with name contains "uc" will be selected as the Figure 21.
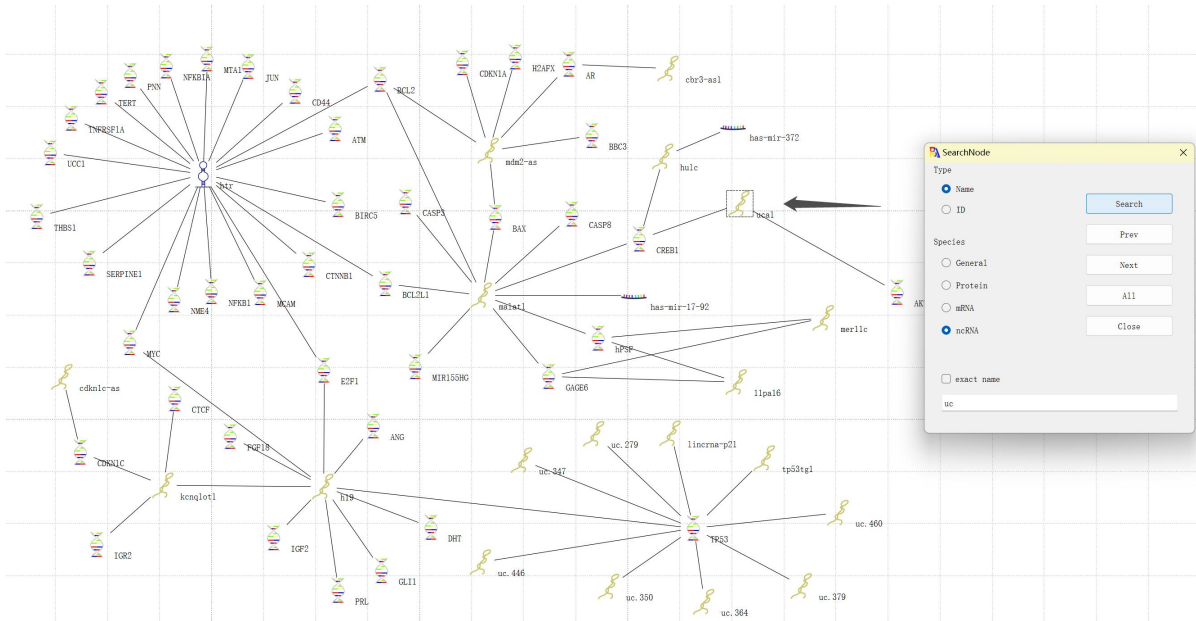
Figure 21: Search nodes example

You can use more operation buttons to select different that were found by the previous search. Such as "All" button to select all nodes whose name contains "uc"

3 Kinetic model viewing and management

Model database button are on the top of page as show in Figure 14. Click "Kinetic Model Viewer"to enter the database viewing page. Click "Kinetic Model Manager" to enter the database management page, then click add, fill in the information, add the database model, and finally click add to complete the addition of the dynamic model. To edit model, users can click "Kinetic Model Manager" to enter the database management page, then click specific items, click edit, modify the dynamic model information in the database here. Click on a specific entry and then click delete to delete the target model in the database. You can enter the target dynamic model data you want to query in the search bar below, then click Search to query the target dynamic model, or click the target dynamic model you want to view detailed information on this page to enter the target The detailed data page of the model.
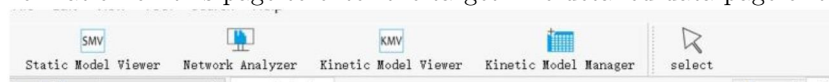

Figure 22: Model database button. Click "Kinetic Model Viewer" to enter the database viewing page.

Click "Kinetic Model Manager" to enter the database management page.

3.1 Kinetic Model Manager

Click "Kinetic Model Manager" to enter the database management page, then click "add", fill in the information, add the database model, and finally click "add" to complete the addition of the dynamic model.
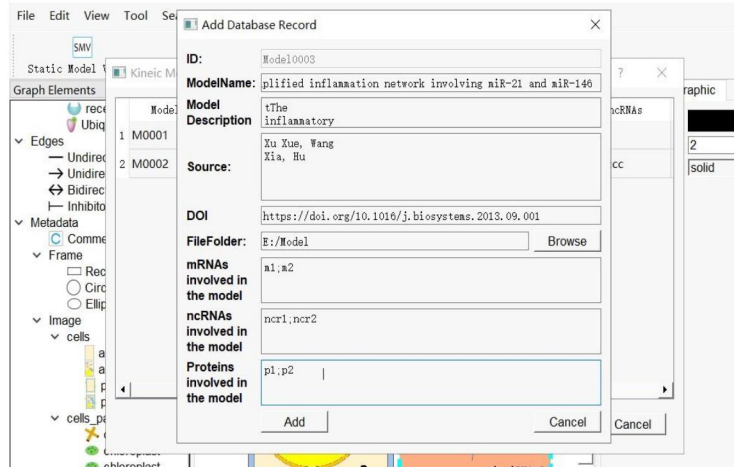
14

Figure 23: add database model

Click "Kinetic Model Manager" to enter the database management page, then click specific items, click edit, you can modify the dynamic model information in the database here.
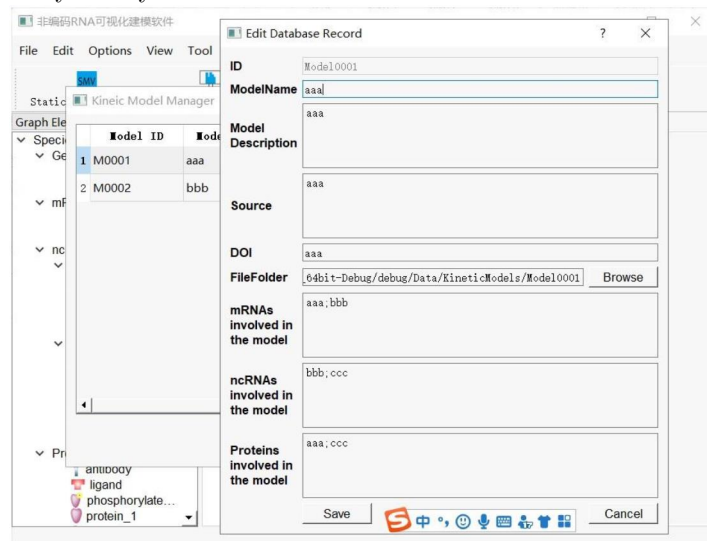

Figure 24: edit database model.

Click a specific entry and then click Delete to delete the target model in the database
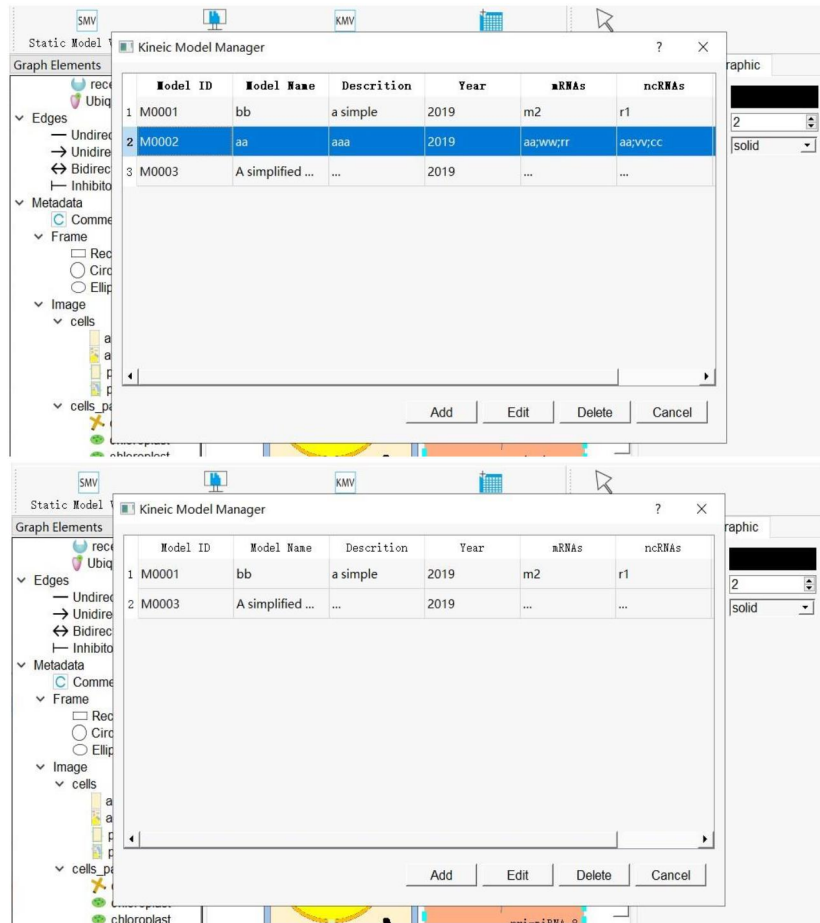
Figure 25: edit database model.

3.2 Kinetic Model Viewer

Click the kinetic model viewer button to enter the dynamic model database viewing page, where the brief information of the model in the database will be printed.

You can enter the target dynamic model data you want to query in the search bar below, and then click search to find the target dynamic model, or click the target dynamic model you want to view the detailed information in this page to enter the detailed data page of the target model.
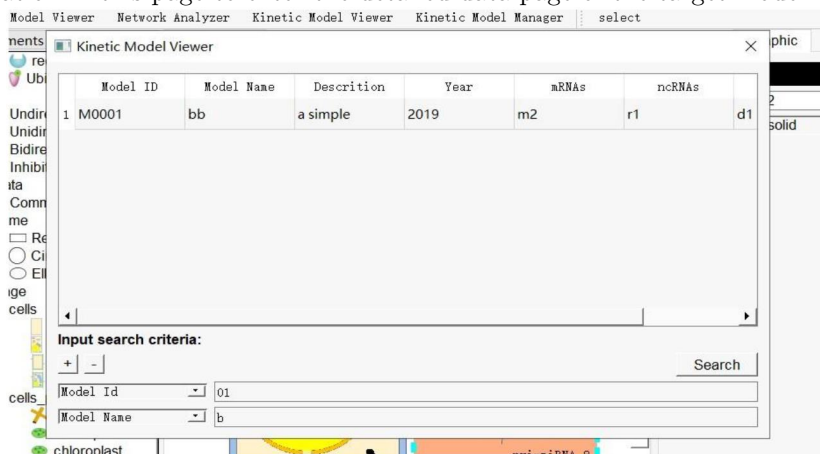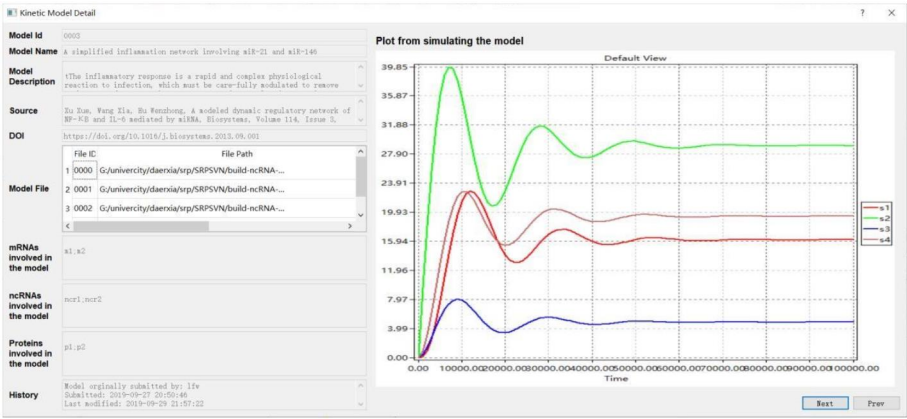
Figure 26: search database model.

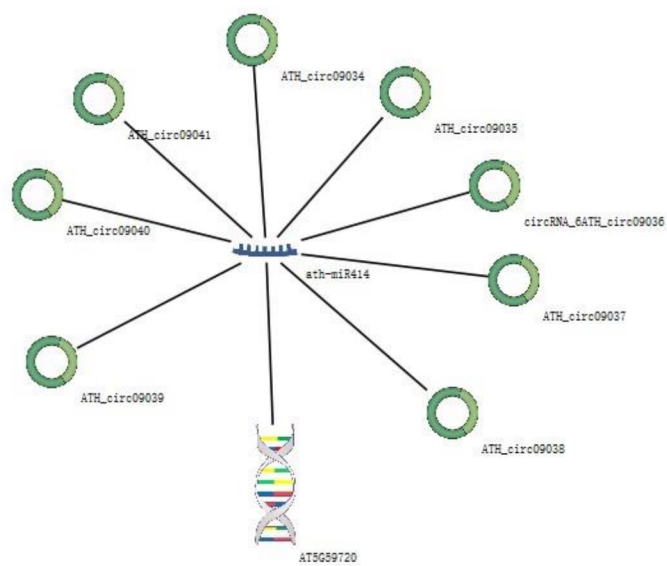Figure 27: view model information

4 Examples

Figure 28: Arabidopsis thaliana

Figure 29: Human