

User Menu

This software tool has a set of functions dedicated to the visualization of complex protein-protein interactions and protein structures for use in computational biology. This tool is organized with six tabbed panels. The first three panels are for network generation and display. In the fourth panel, the BallSticks mode is to output the atom display in Protein Data Bank (PDB) file format and the spacefill mode is to output the space structure of the protein correlated partners. The fifth panel shows the protein structure information recorded in the PDB database. The sixth is the summarized table about the child nodes, the names of the corresponding proteins and the IDs of the nodes. The complex mechanism of protein interaction is not intuitive in 2D viewer. Especially, the protein structure information in 2D viewer can not help researchers to get the overview and space picture of the protein. Therefore, it is urgent for a computer application to visualize these complex structures. The following is a brief description of the components of this tool and the user guide. The overall interface of the tool is shown in Figure 1.

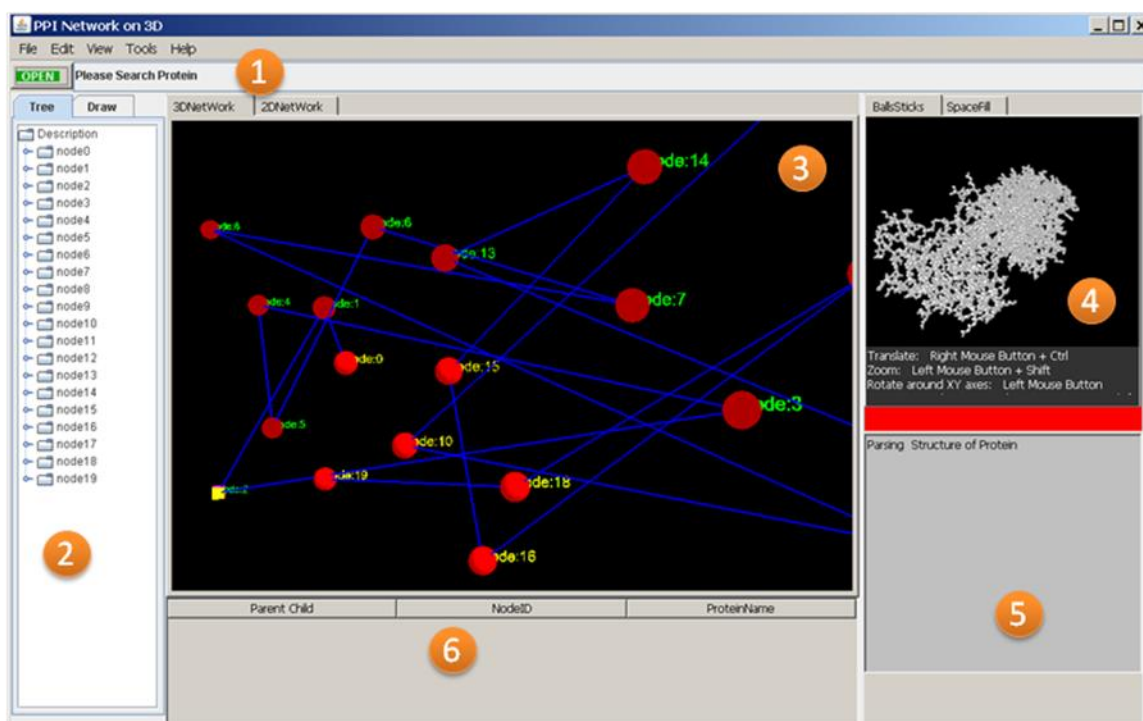


Figure 1. The interface of the tool

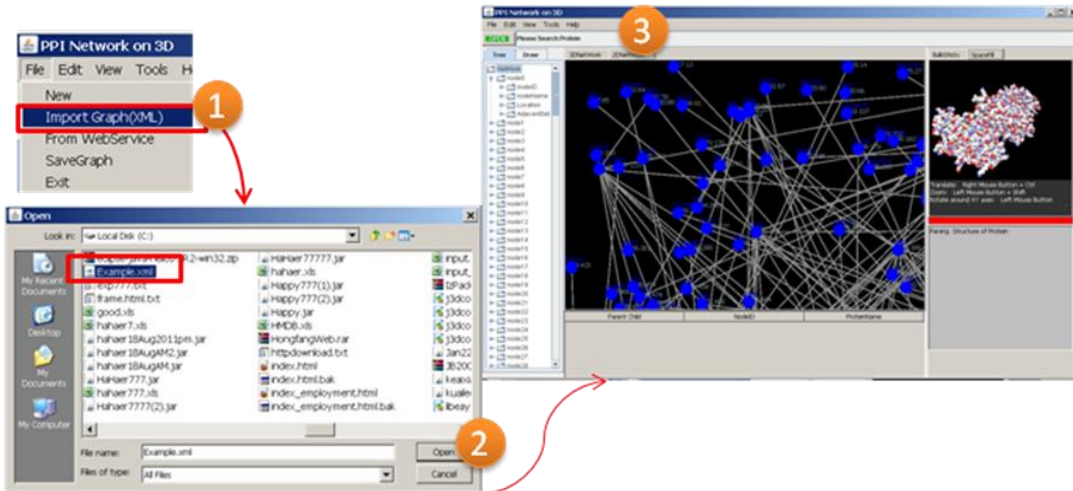
There are six functional panels in the tool. 1. The first top panel is the file menu and protein search area. Their functions will be introduced in detail later. 2. The left panel is node management and network manual drawing area. 3. The left middle panel is for 3D or 2D network viewers. 4. The right top panel is under the 3D viewer to display atoms in *BallStick* mode which can be used for special rendering or in spacefill mode. 5. The right bottom panel is the summary area of the queried protein structure information including the PDB ID of the protein, the number of chains, atoms and molecular center information about the protein. 6. The bottom panel is the statistics table about the child nodes, their corresponding protein names and node IDs in the network.

1. File drop-down menu

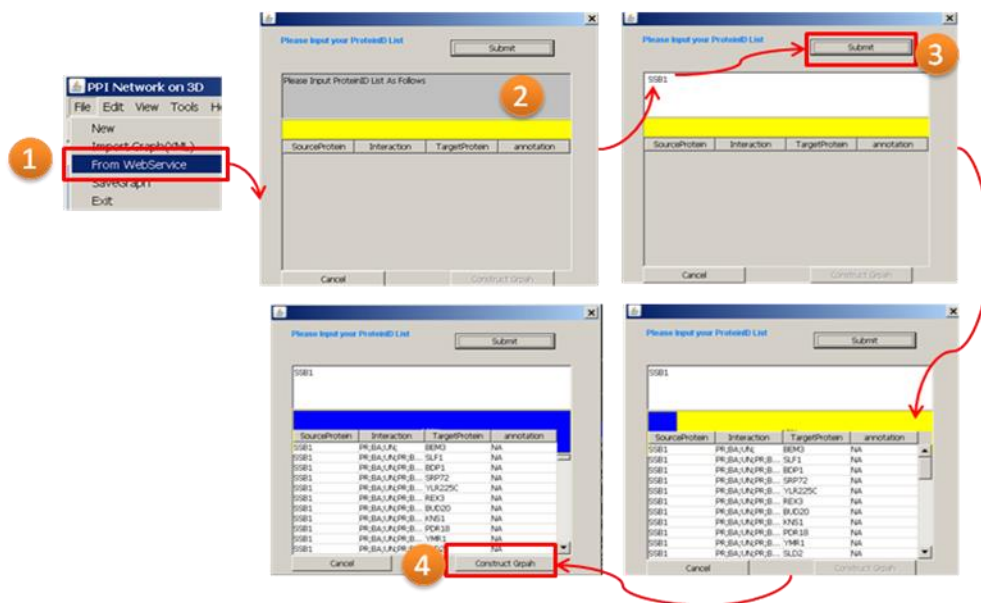
As shown in Figure 2 A, the File menu has five drop-down components: New, Import Graph (XML), From Webservice, SaveGraph and Exit. 'New' is for constructing a new network with manual drawing. 'Import Graph' is used for importing a graph file in .xml. As shown in Figure 2 B, when clicking Import Graph (XML), the .xml file will be imported into the tool and the network structure of the networks will be displayed. 'From Webservice' is used for constructing specific protein-protein interaction network. When inputting the name or the PDB ID of the protein in the query area of the tool, the interacted proteins of the queried protein will be grasped dynamically and the interaction network of the queried protein will be displayed in the 3D or 2D viewers. The process of 'From Webservice' is shown in Figure 2C. Figure 2D demonstrates the exported graph in the format of .xml.



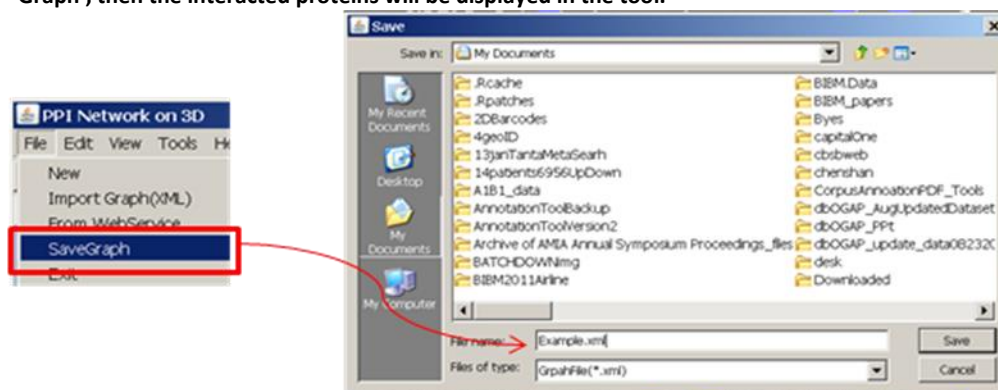
A. File Menu



B. Import Graph in the format of .xml. When clicking 'Import Graph' and opening the local file folder containing a .xml file, the network structure will be displayed in the tool.



- C. The process of dynamically grasping the interacted proteins of the queried protein. Clicking 'From Web Service', a small window will pop up. Then after inputting the name of the queried protein such as SSB1 in the blank area, click 'Submit' button, a blue bar will show the progress of getting information from PDB. In addition, each protein that interacts with SSB1 will be displayed in the table with the source information, target proteins and interaction types. Once the blue bar is 100% filled, click the 'Construct Graph', then the interacted proteins will be displayed in the tool.



- D. Save a graph in the format of .xml. After clicking 'SaveGraph', opening a local fold to save the graph, and then clicking 'Save', the graph will be saved in a file in .xml format.

Figure 2. The file pull down menu of the tool

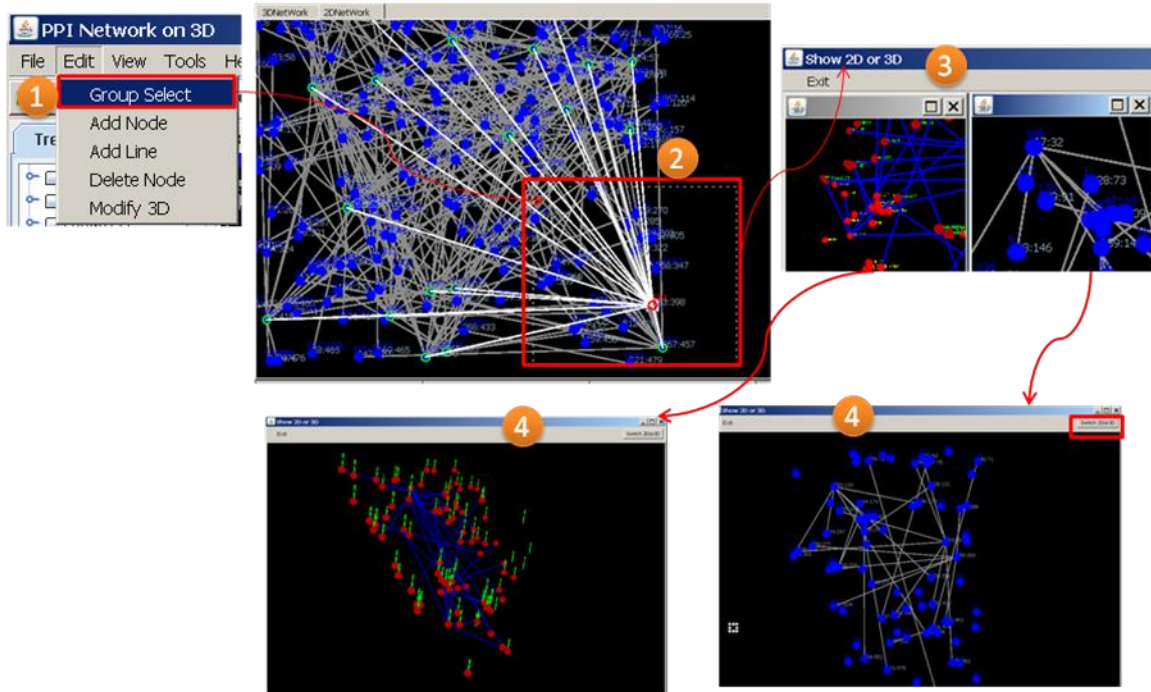
2. Edit pull-down menu

The 'Edit' menu contains five components as shown in Figure 3. 'Group Select' is used for selecting sub networks. When drag the mouse in the 2D or 3D viewer and select the area in the network, a window will pop up to show the sub-network structure in both 2D and 3D viewers. Users can switch the 2D and 3D viewers by clicking the top right button of '2D or 3D switch'. Functions of editing nodes are offered in the 'Edit' menu. Extra nodes or edges in the network can be added by clicking the 'Add nodes' or 'Add lines' in the 'Edit' menu. In particular, after adding nodes in the 2D viewer, the network can be transited from the 2D viewer to the 3D viewer by clicking the 'Save graph' menu.

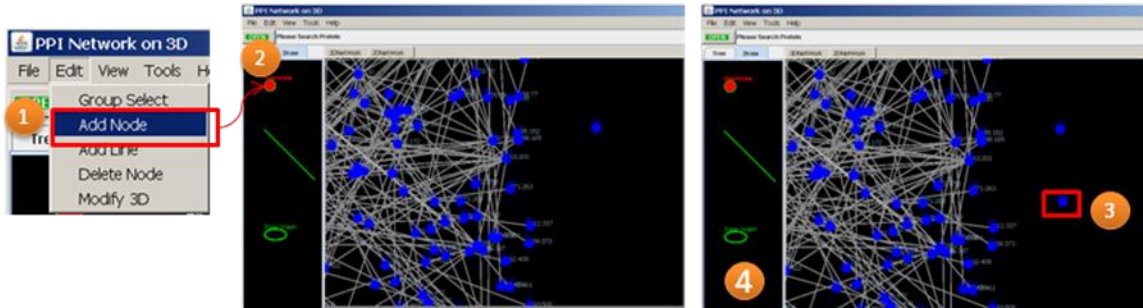
Nodes can also be deleted by selecting the 'Delete nodes' menu or by right clicking the mouse in the network viewer. When delete an edge, the nodes linking to the edge will be deleted automatically.



A. Edit Menu



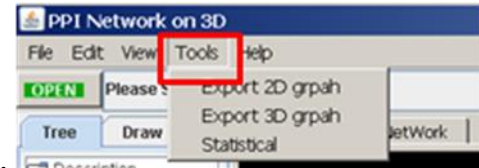
B. Sub network selection. When click the 'Group Select', press left button of mouse, and drag the mouse in the 2D or the 3D viewer, the window of 'show 2D or 3D' will pop up. When maximize the window of the 2D or the 3D viewer, the sub-network structure will be enlarged and will be displayed clearly. By clicking the 'Switch 2D or 3D' menu, the structure of the sub network will be displayed and transited between the 2D viewer and the 3D viewer.



- C. Edit nodes in the network. The 'Add Node' component in the edit menus is for adding extra nodes in the existing network. When clicking the 'Add node' menu, the network will switch to 2D viewer and the nodes and edges will be displayed in the left panel. Using the left mouse button to click the red node image in the left panel, and then click the left mouse button in the 2D viewer, the node will be displayed in the network. After adding the nodes, by clicking 'Save graph' in the left panel, the information of the graph in the 2D viewer will be transformed to the 3D viewer automatically.



View Menu



Tools Menu

