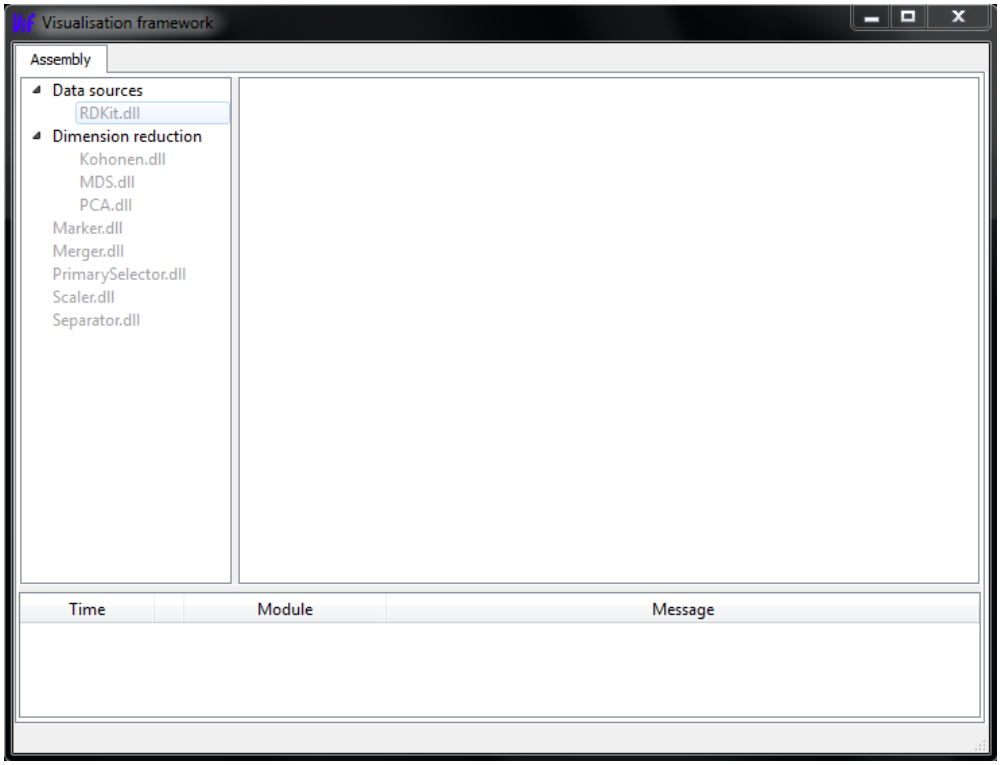
FiVrame

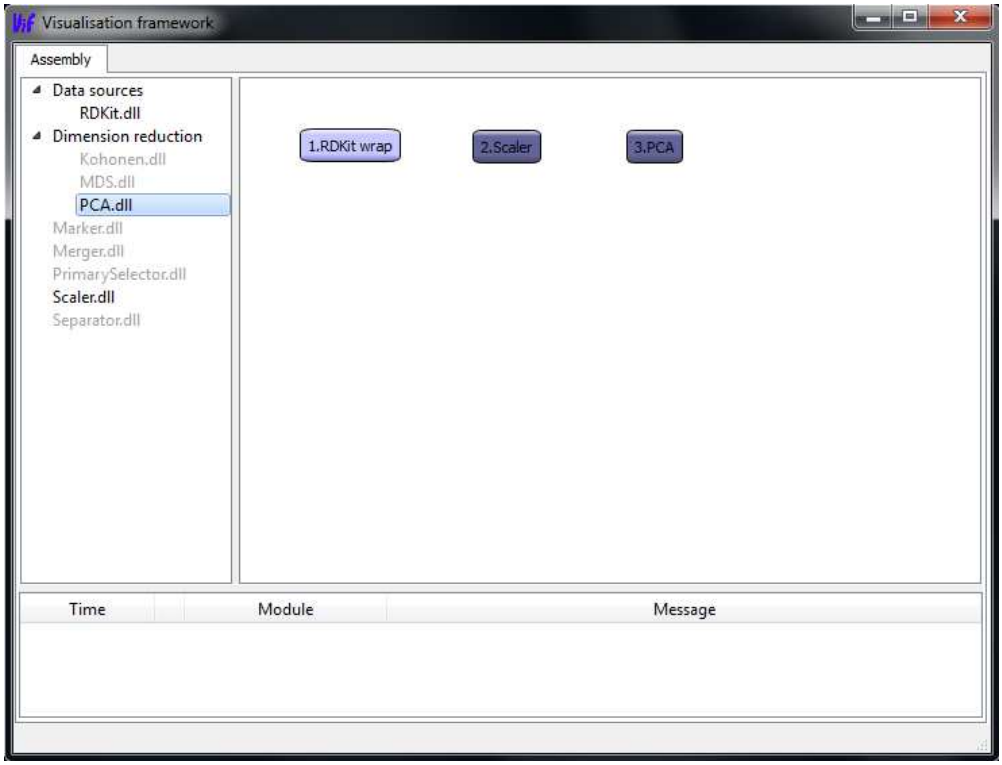
Quick usage guide

In this document we give a quick introduction to the usage of the ViFrame application. The document illustrates assembling a simple visualisation pipeline with multiple sources, running visualisation, simple work with visualisation output and exporting the results. The results can be exported as an image or in a form of a csv file.

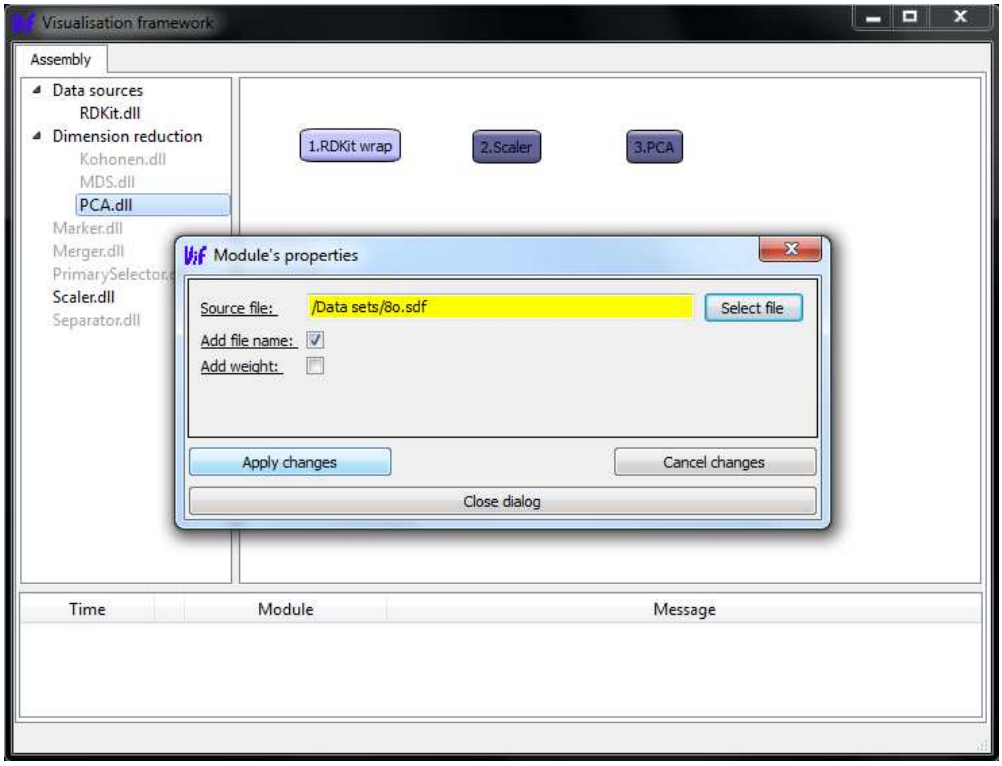
Start by opening the application. After the application starts you should see similar image to the following one.



On the left the tree view with modules which are located in the \Module application subfolder. At the bottom the message view can be found. The last sub-window is the assembly construction area. Here the assembly construction is done. By using dragand drop move RDKit.dll, Scaler.dll, PCA.dll into the assembly construction area. You should get image similar to the following.



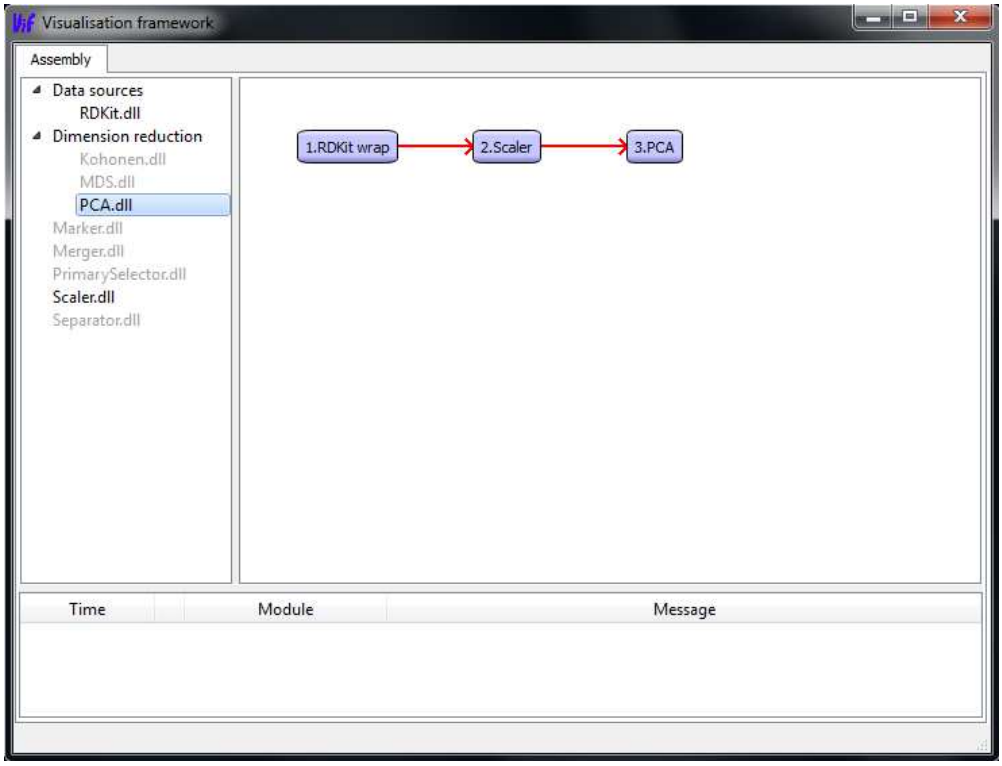
Now we set properties of 1.RDKit wrap module. Right click on the module and select Properties.



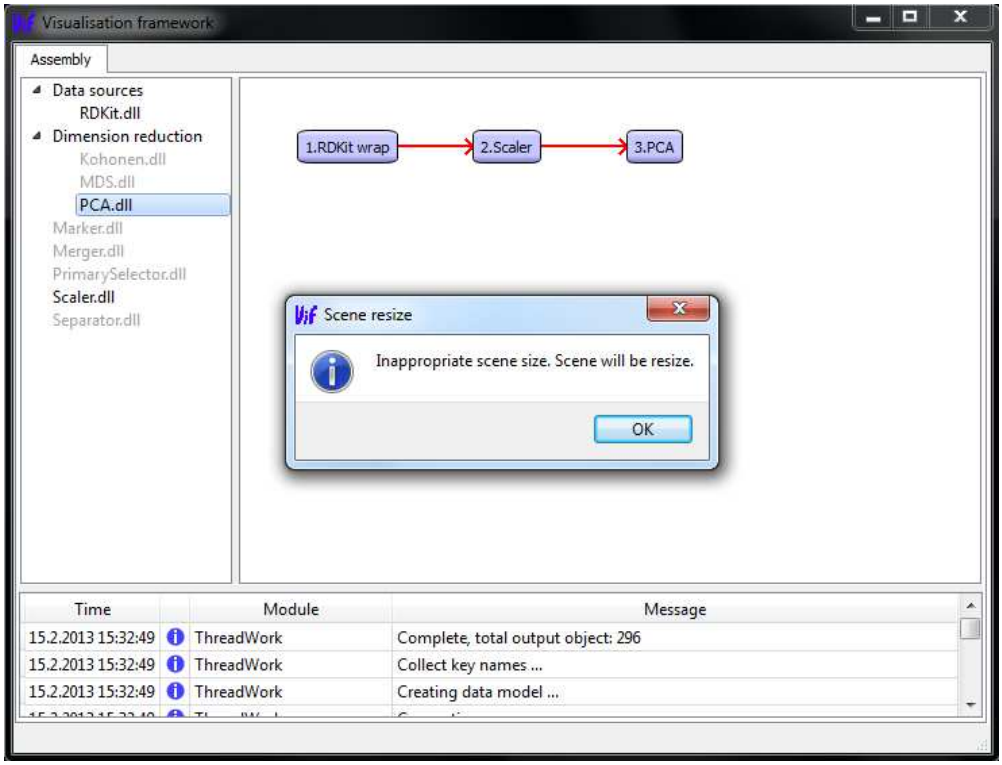
What you can see is *Properties* dialog - here the module properties can be set. We want to set *Source file*. Click on *Select file* and select *8o.sdf* from data source folder. As you can see the text box with the path to the selected file changed color. The yellow color means that value has not been saved. Click on Apply change to save it. Then close the dialog by clicking on *Close dialog*.
If the save operation fail then the color turns into red and an error message is shown.

Now we interconnect the modules. Use drag and drop to move *1.RDKit wrap* on the *2.Scalar*. In the dialog which appears, click on *Connect* and then on *Close* button. The red line which appears between the modules indicates their connection. The arrow indicates the direction of the connection.

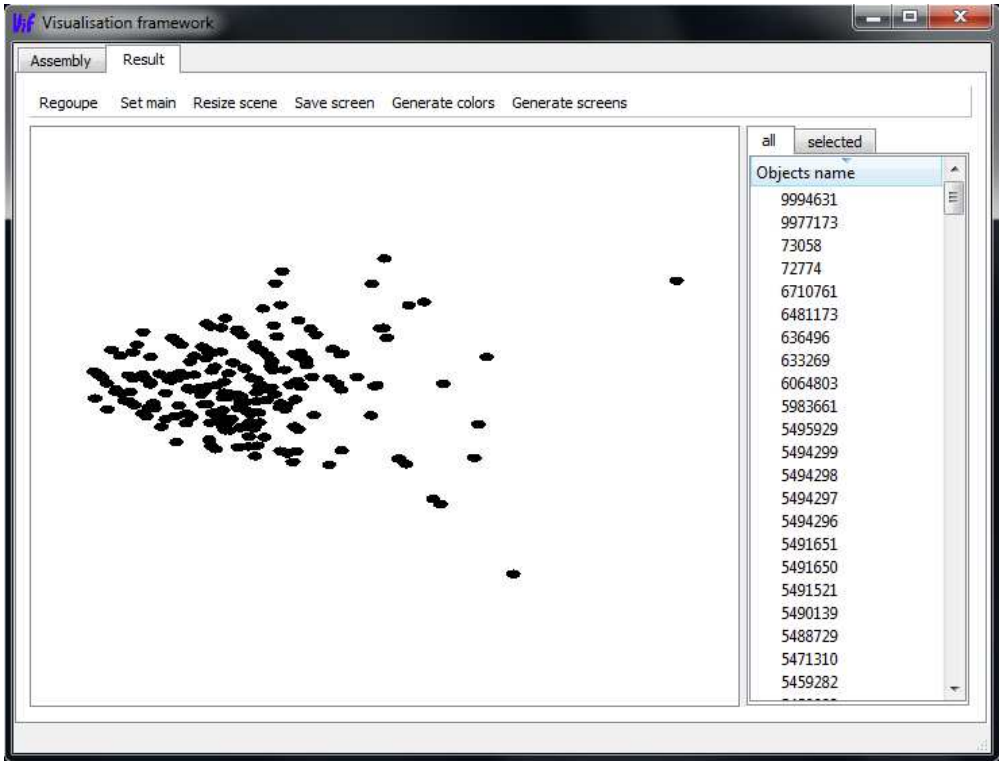
Repeat the same action for *2.Scaler* and *3.PCA*. In the end you should get following screen.



You have now successfully assembled your first pipeline in ViFrame. Now right click on *3.PCA* module and select *run*. You may see the green progress bar over *1.RDKit wrap*. The progress bar indicates progress as reported by the module. In the message view you can see messages from modules.



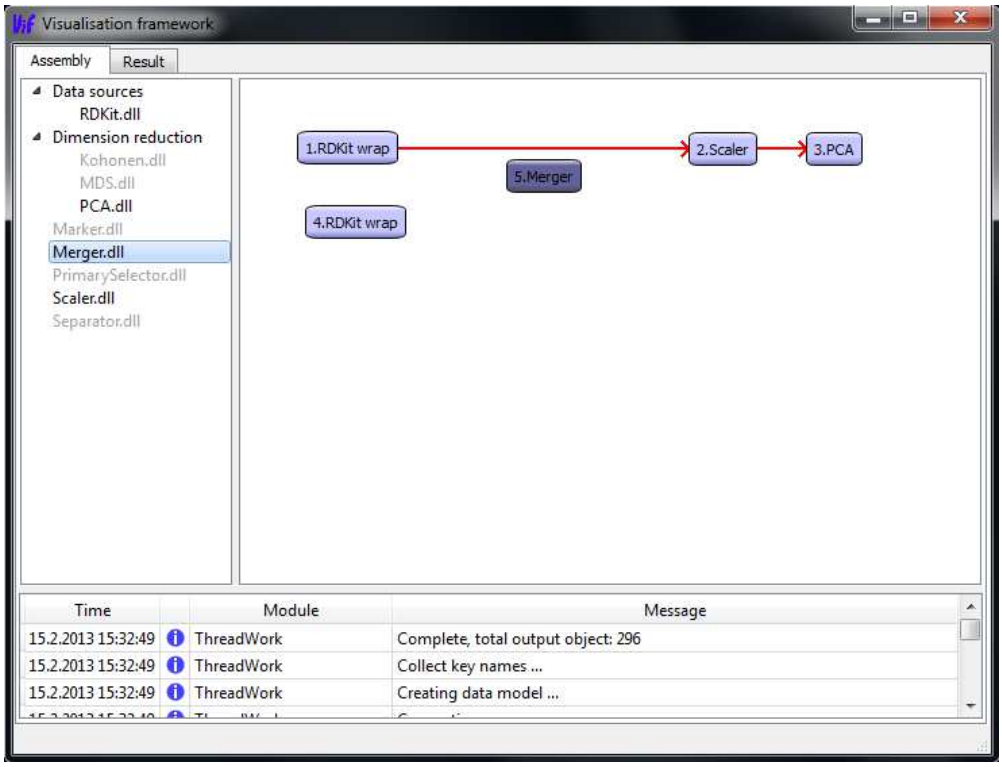
When the visualisation process ends then a dialog appears. The dialog says that the range of output data was "inappropriate" and so will be resize (scaled), press OK.
Then in the left top corner a tab called *Result*will appear. When you click on it you will see the results of the visualisation.



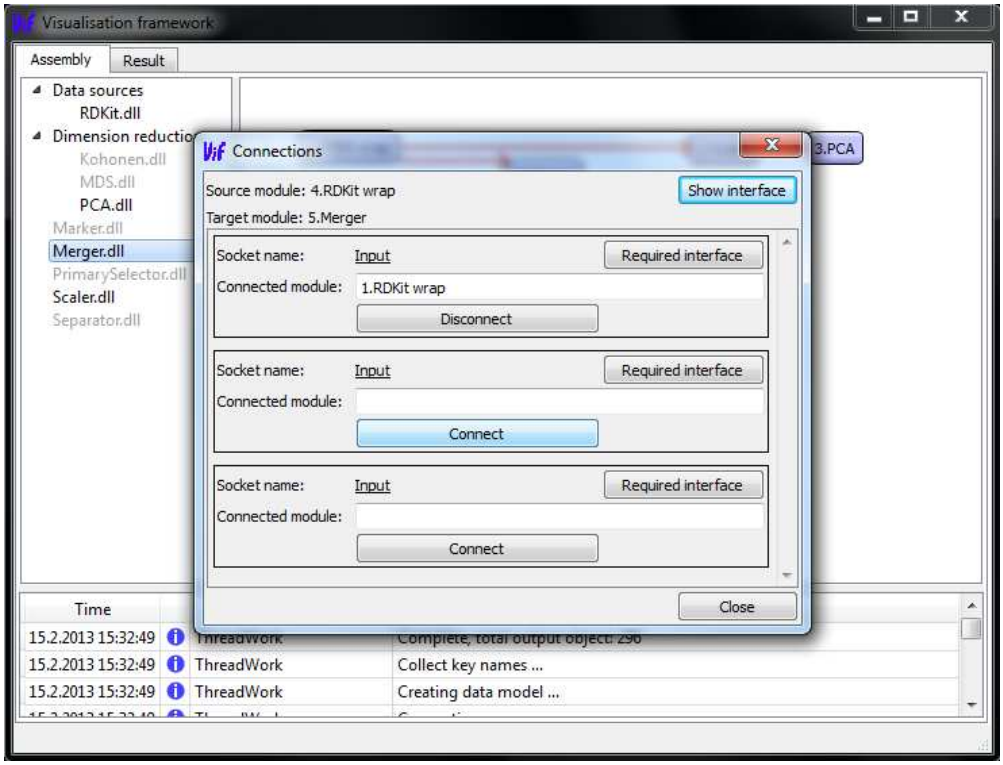
In the left part of the screen you can see the visualisation canvas where the results are visualised. You can use mouse wheel to zoom in and out. If you press and hold the left button you can move left, right up and down. To prevent moving out of the picture, there are borders which can be crossed.On the right side of the window the list of

all\selected molecules visualised is located. What you can see are the names of the molecules as loaded from sdf file.

Now we reassemble visualisation pipeline to use two sources. Return to Assembly tab. Add *RDKit.ddl* and *Merger.dll* modules. Set added *RDKit* source to *8p.sdf*. After this you should screen similar to the following image.

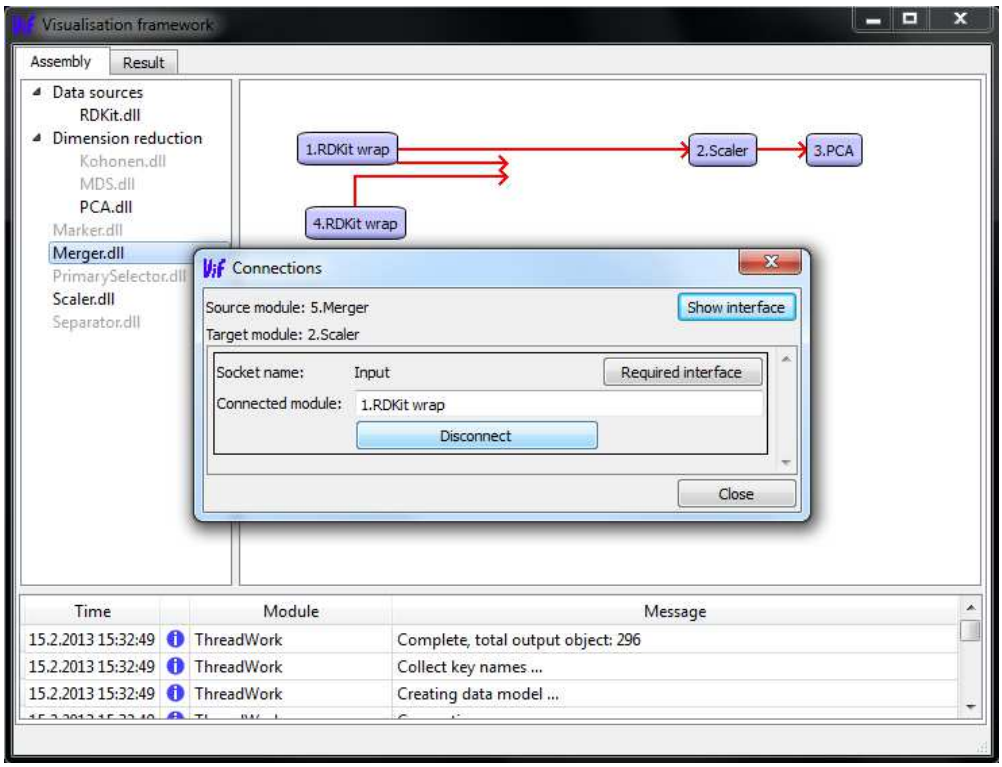


Now we reset connection between the modules. First start by connecting *1.RDKit* wrap to *5.Merger*. Then connect *4.RDKit wrap* module to *5.Merger*. The module *5.Merger* has multiple inputs, choose one and click *Connect*.A module can generally have any number of inputs but must have just one output.

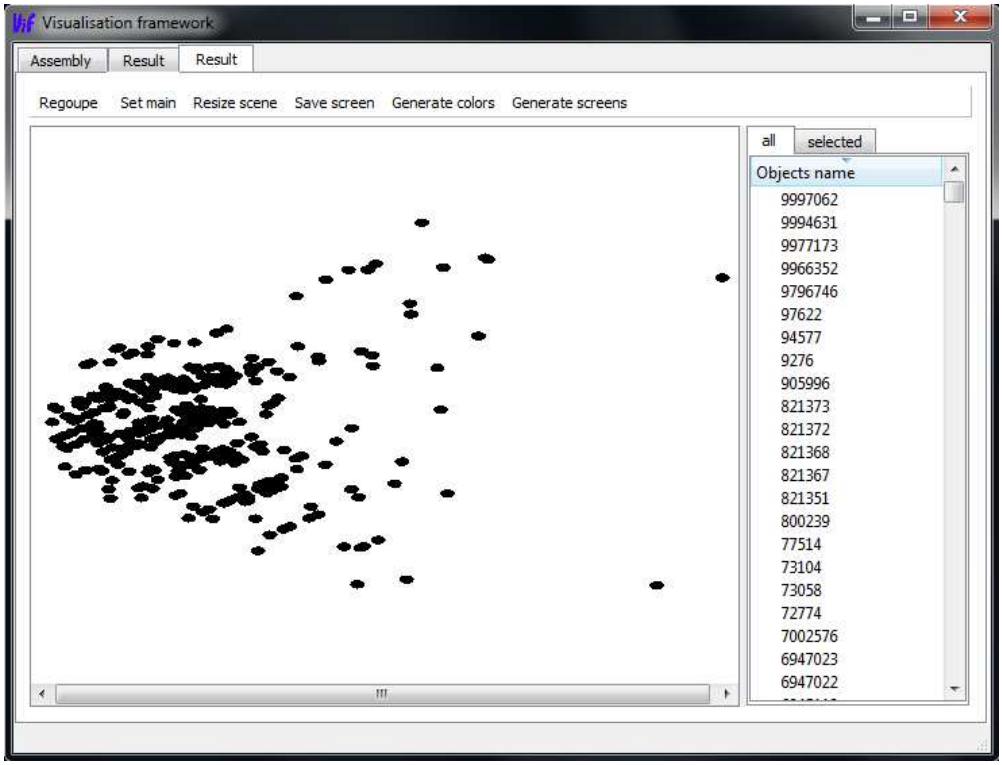


As you can see, after the connection is established the module name appears and the button is changed to *Disconnect*.

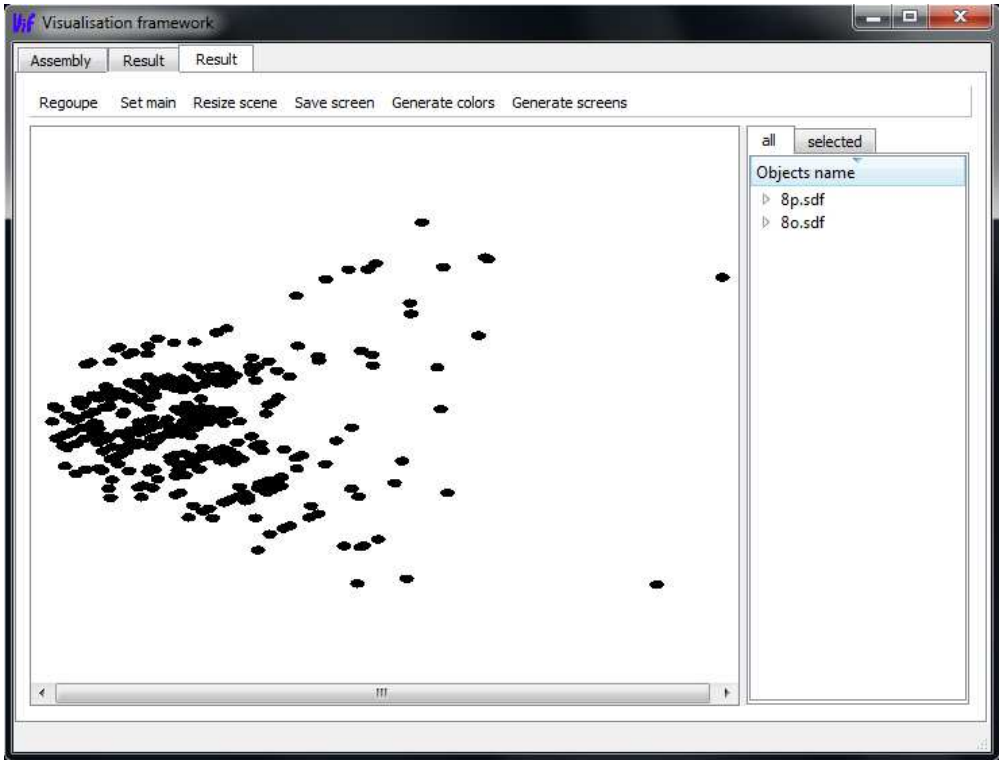
Now we disconnect *1.RDKit* wrapper from *2.Scaler* and connect *5.Merger* instead. Just use drag and drop as previously. In dialog then click on *Disconnect* and *Connect*.



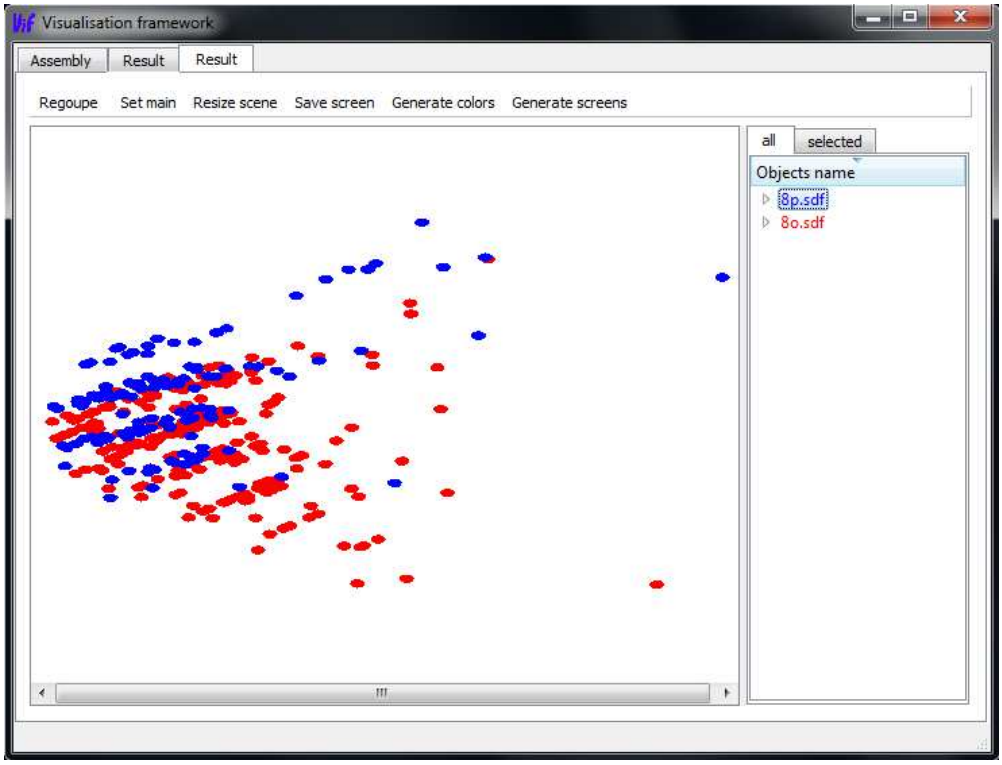
Now right click on the *3.PCA* and select *Run*. After the operation is finished a new tab called *Result* is added. Click on it. Like in previous case the dialog about resize is shown, just say OK. The dialog is shown because the data has too small range. If the original value was used then they would be too close together. So the application multiplies all coordinates with an appropriate constant. The data in objects remain the same because the rescale is done over a copy of the data.



As you can see the view is different from the first visualised case. But it's not possible to simply identify from which source a given moleculeis. To improve this click on *Re-group*, in the dialog select *Source file* and then click *OK*. Now the data are split to groups according to *Source file* value.

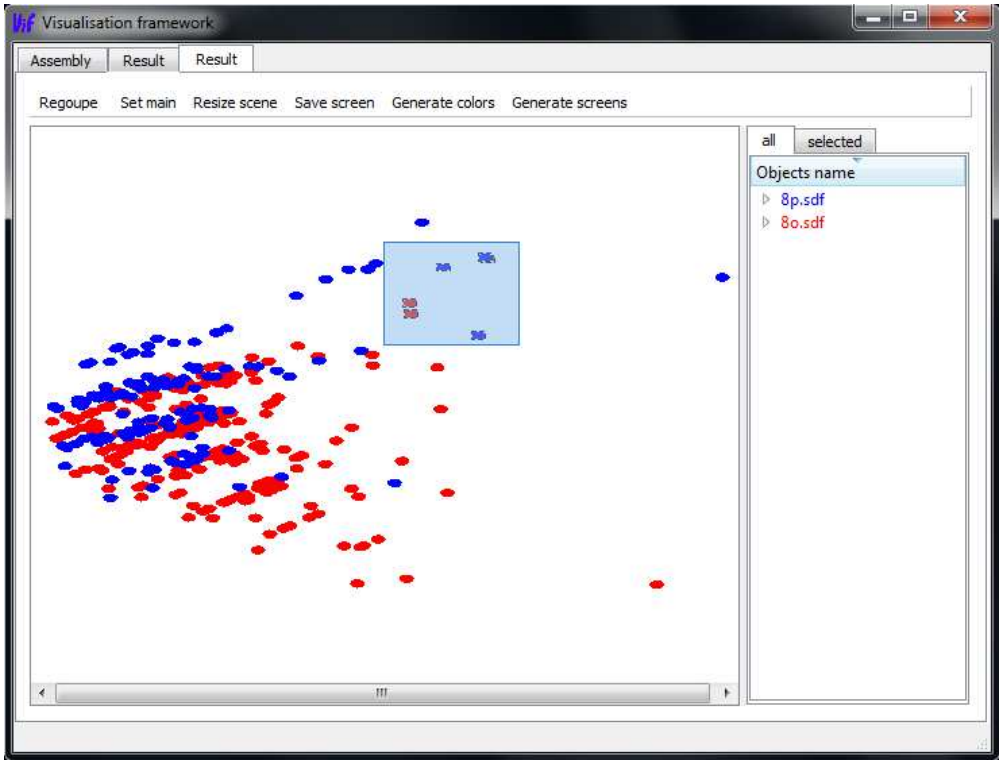


As you can see, two groups were created. This corresponds to the fact that we have two sources. Now right click on a group, for example 8p.sdf, and select *Set color* and select a color. Repeat the same for the second group. Now you should see which molecule belong to which source clearly.

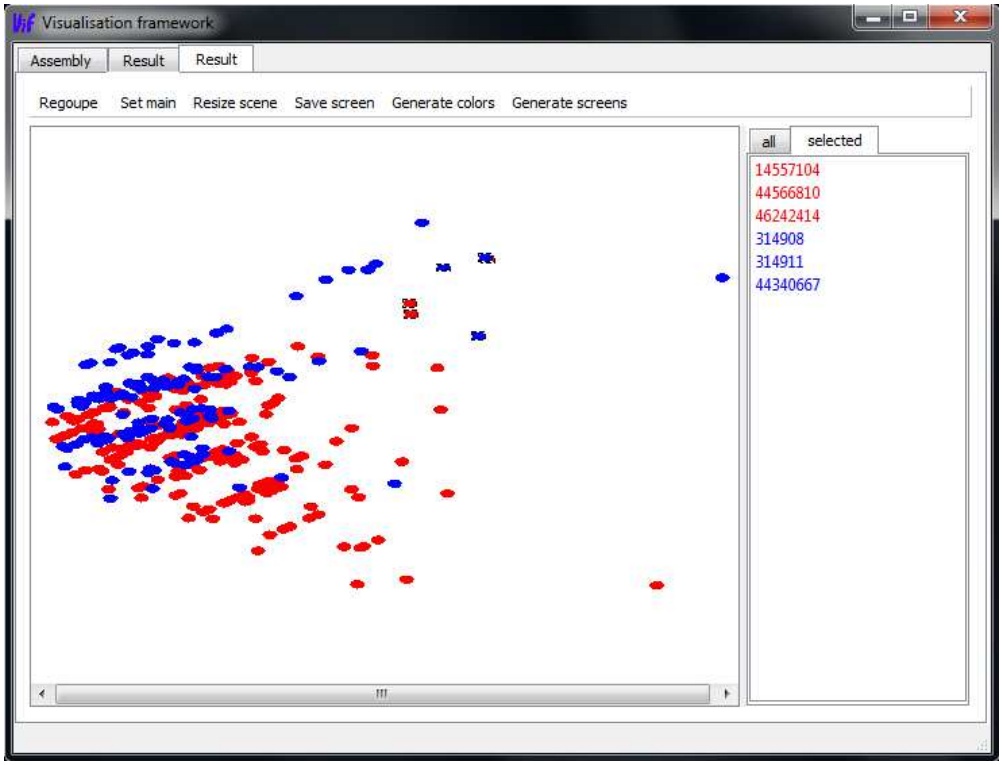


We now export the current view into an image file. Click on *Saveimage* button which is located in the top toolbar. If you want you can place legend into the output image. Then click *OK* and save image. If all goes well then you now exported a current view into the selected file.

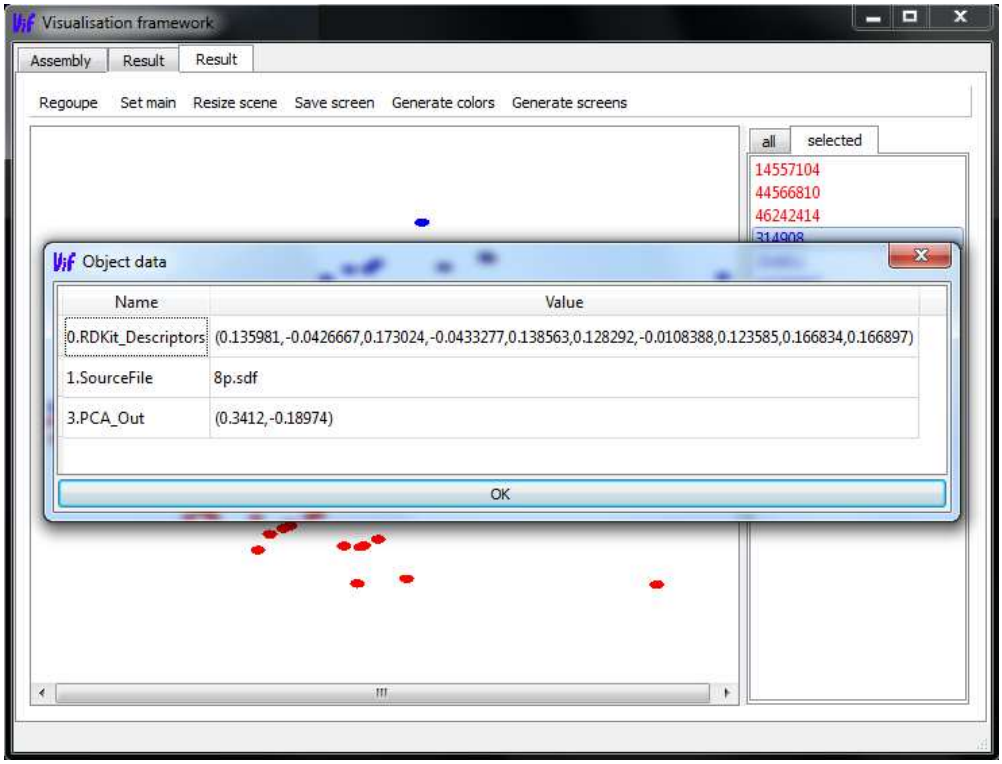
Now press and hold ctrl and select few molecules in the visualisation canvas. You can drag when do selection.



Now as you can see the molecules are highlighted. When you click on the *selected* tab you can see the list of selected molecules.

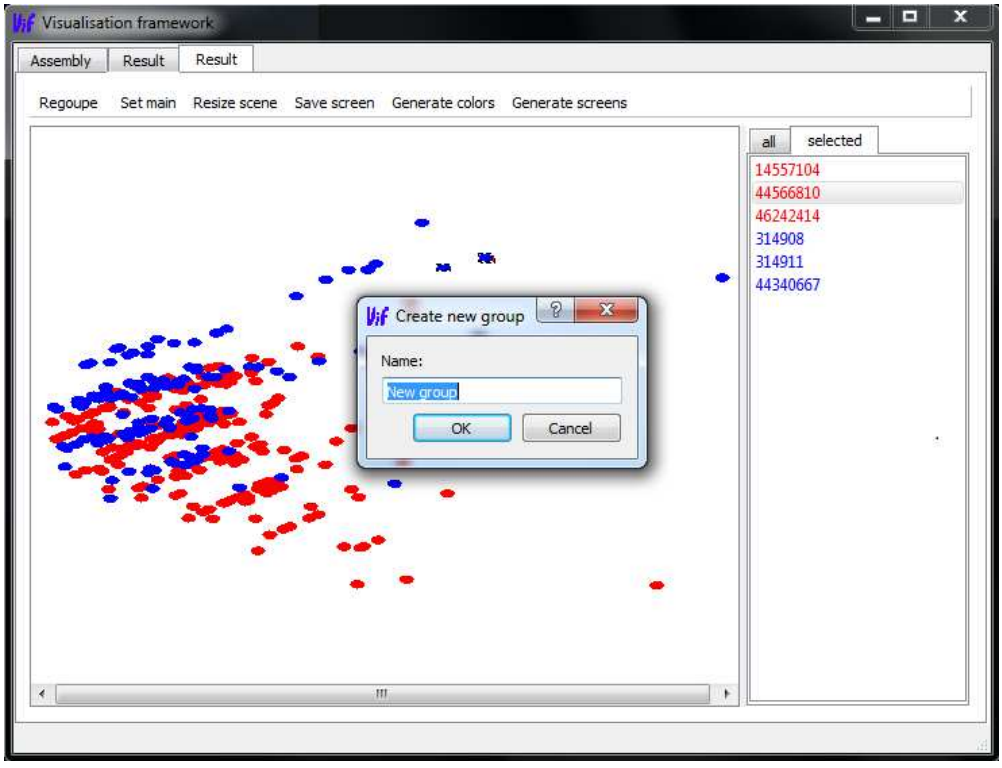


If you right click on a molecule in *all/selected* list and select *Show details* a dialog with details about the molecule will be shown as on the following image.

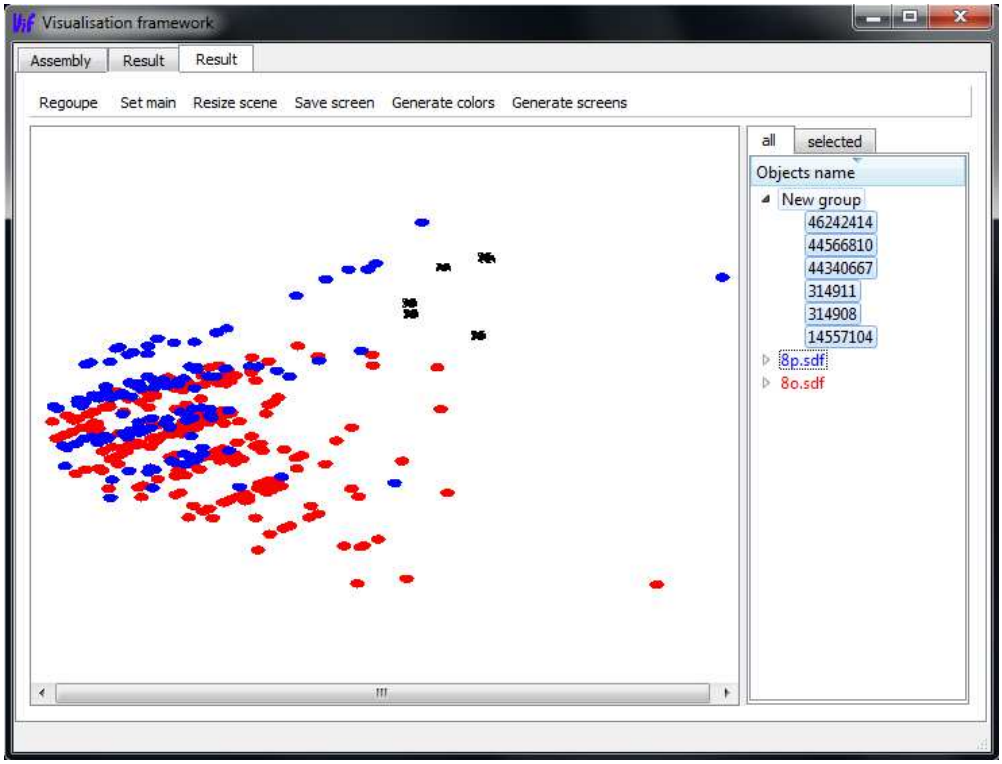


As you can see a molecule can contain a number of different values. In this case the molecule contains data from RDKit that goes through scaling, *SourceFile* and *PCA_Out*. The *PCA_Out* is currently used value to determine position of the molecules on the visualisation canvas. Close the dialog by pressing *OK*.

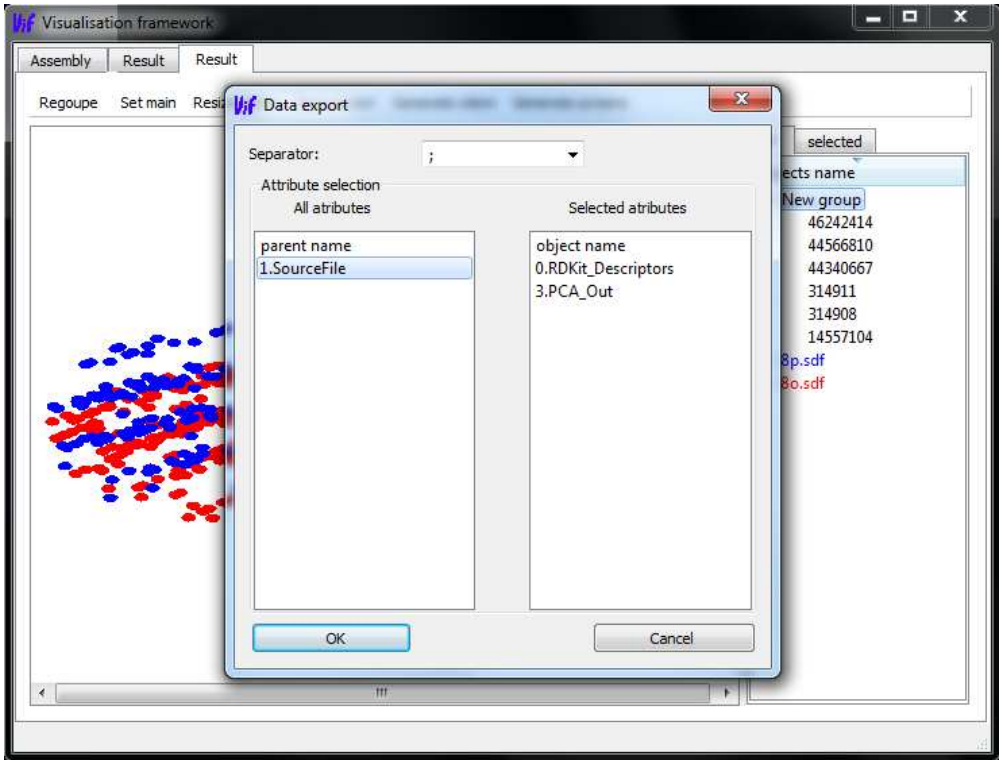
Now click on free space in the *selected* tab and press *Move to new group*. This will move all selected molecules into a new group. You can specify the new group's name or you can just press enter to continue.



The newly created group has black color as default which is why the selected molecules changed color to black. If you switch back on all list, you can see the new group.



Select the *New group* and after right clicking on the group's name select *Export*. Now the export dialog appears (see the following image). On the left, all attributes' names of selected molecule are listed. Use drag and drop to move attributes names from the left to the right list. The attributes in the right list are to be exported.



When you select the attributes click *OK* and select file where to store the output. The selected attributes from selected molecules will be saved into the given file.