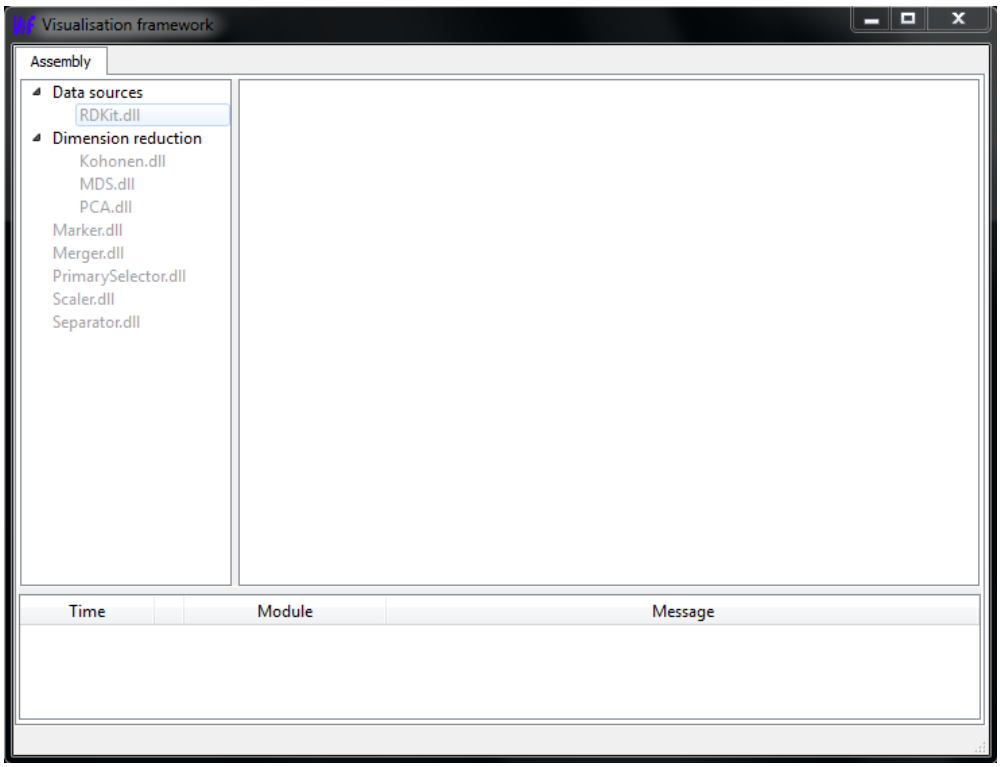
# FiVrame

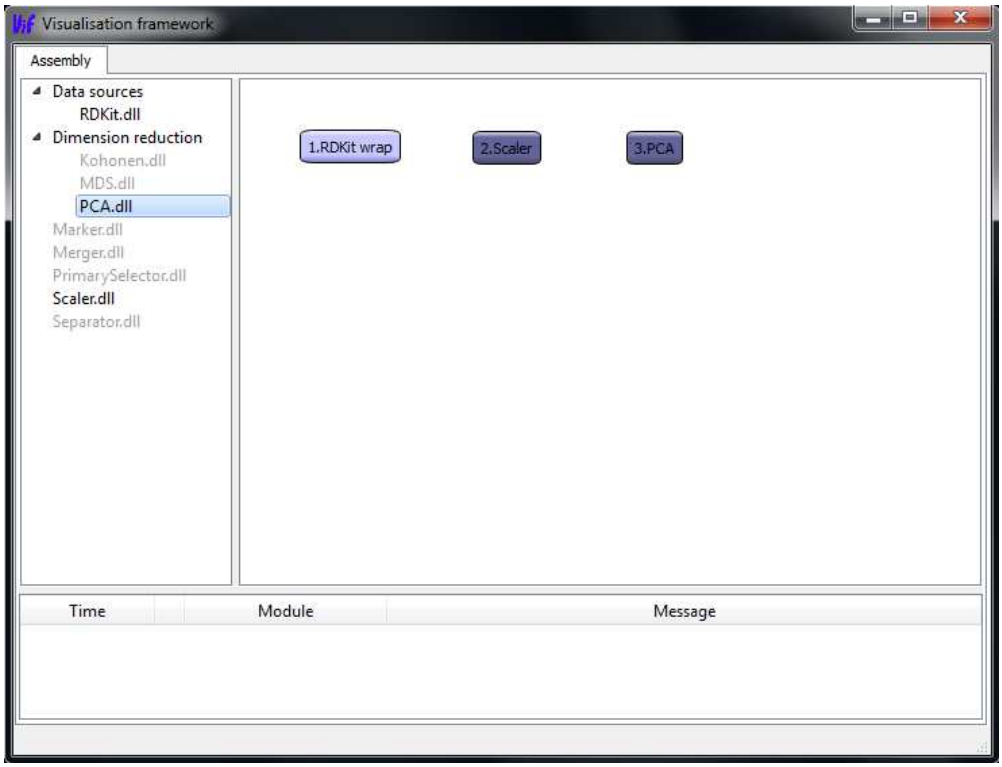
Quick usage guide

In this document we give a quick introduction into usage of 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 are exported as an image or in csv file.

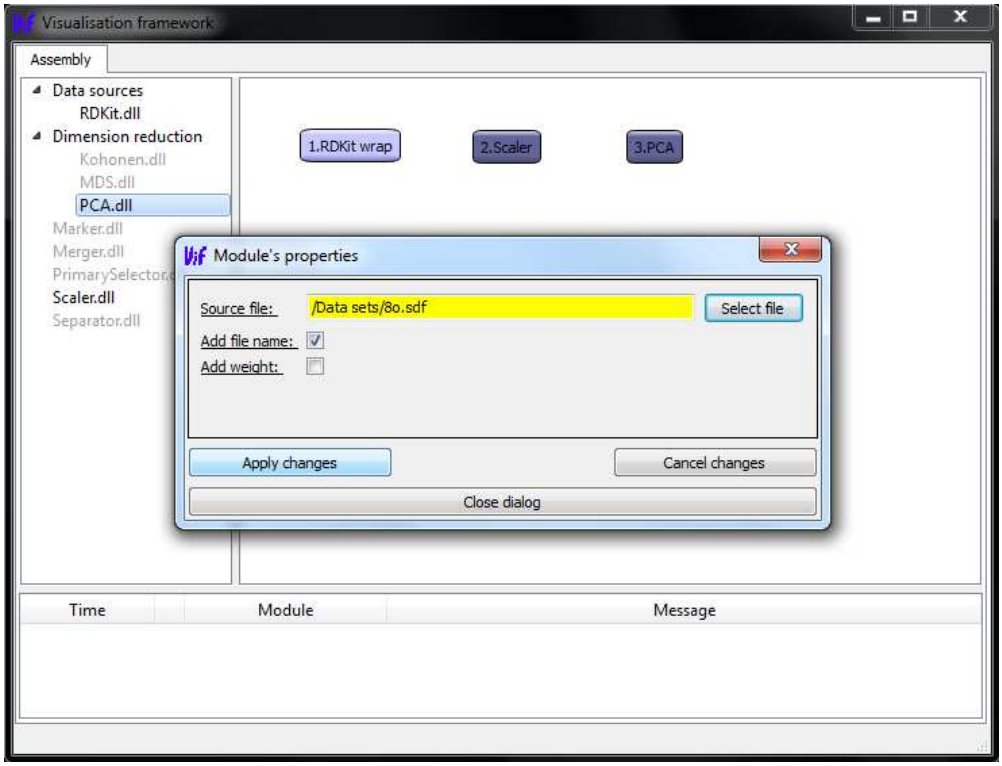
Start by opening the application. After application starts you should see similar image like the fallowing image.




In the left the tree view with modules presented in \Module subfolder is located. At the bottom the message view can be found. The last sub-windows is a assembly construction place. Here the assembly construction is done. By using drag and drop move RDKit.dll, Scaler.dll, PCA.dll into the assembly construction place. You should get image similar to the fallowing.



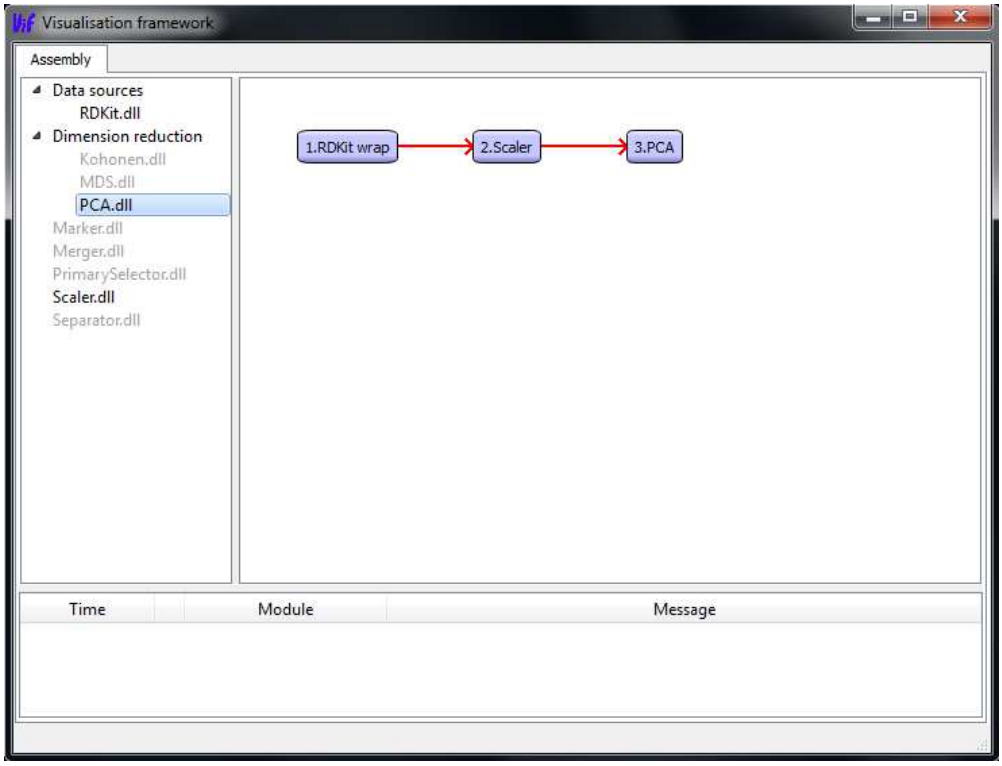

Now we set properties of 1.RDKit wrap module. Right click on the module and select Properties.



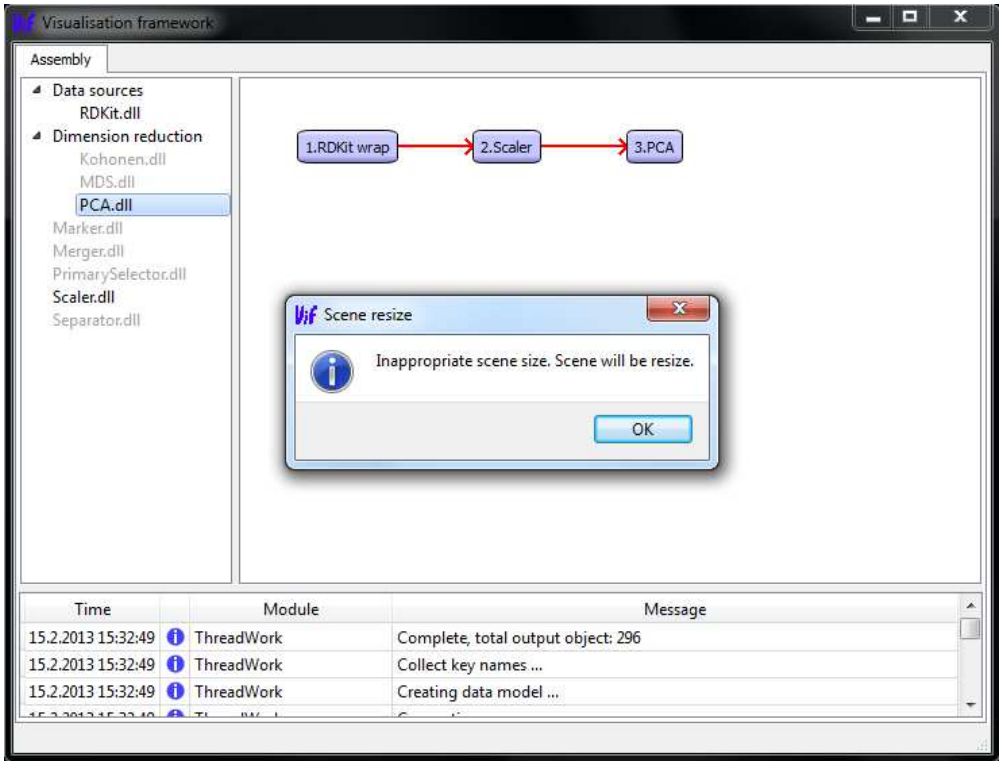

What you can see is Properties dialog; from here module properties can be set. We want to set Source file. Click on Select file and select 8o.sdf from data source folder. As you can see the text box with path to the selected file changed color. The yellow color means that value has not been saved. Click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

Now we connect modules together. Use drag and drop to move 1.RDKit wrap on the 2.Scalar. In the opened dialog click on Connect and then on Close button. The red line which appeared between modules indicates connection. The arrow indicates the direction of the connection.

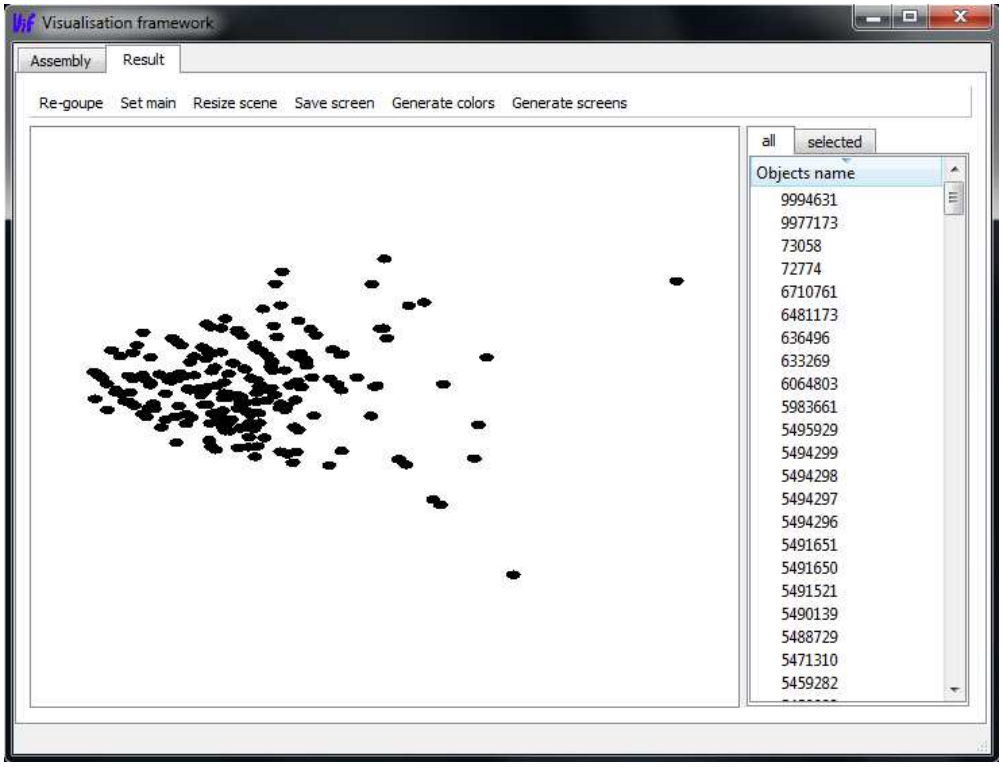
Repeat the same action for 2.Scaler and 3.PCA. On the end you should see something like on the next image.



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.



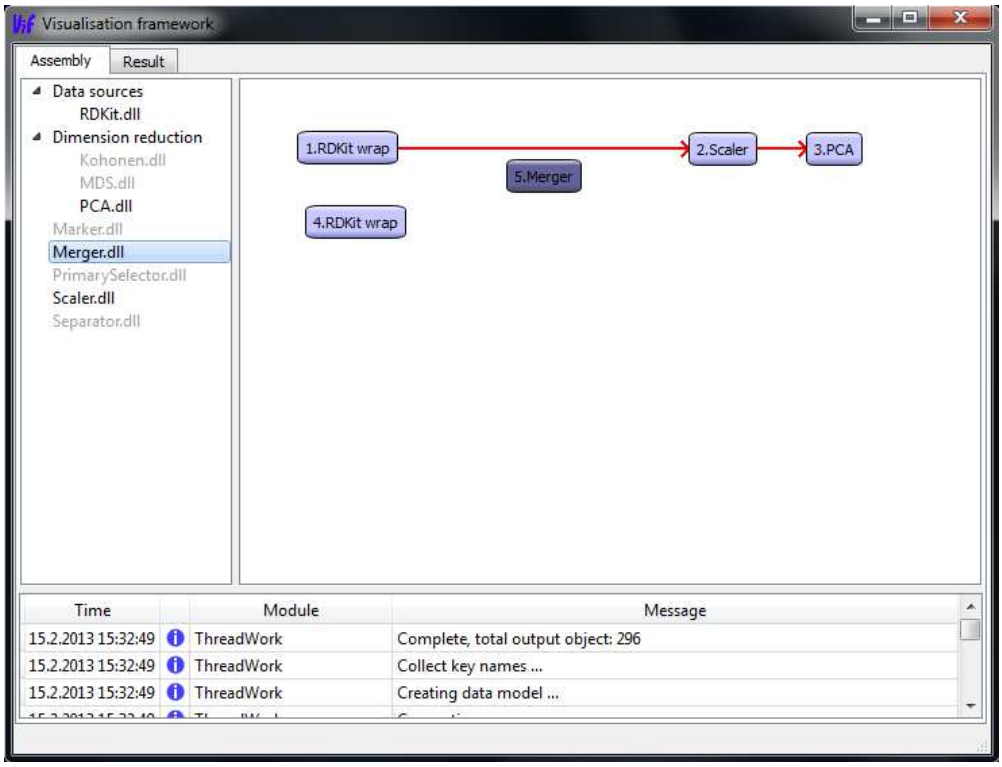

When the visualisation process ends then the dialog appears. The dialog says that the range of output data was “inappropriate” and so will be resize (scaled), press OK.
Then in the left top corner the tab named Result will appear. When you click on it you will see the results of visualisation.



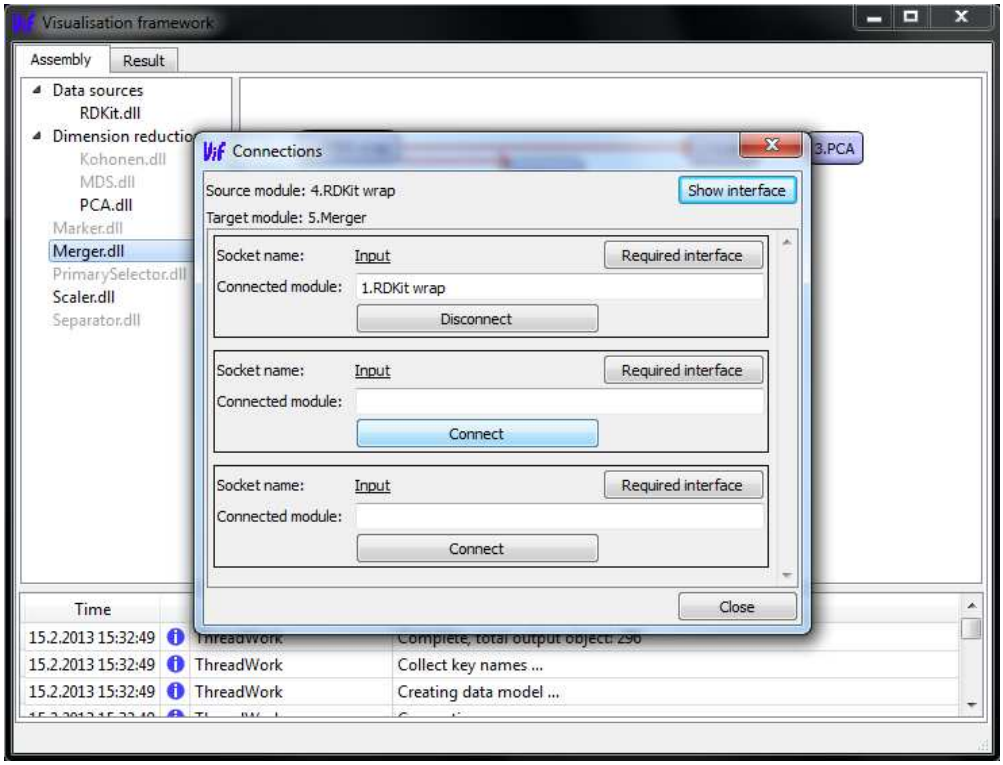

n the left part you can see the visualisation canvas. You can use mouse wheel to zoom in and out. If you press and hold the left button you can move left, right up and down above the visualised data. To prevent use lost or move out, there are borders which can be cross. In the visualisation canvas the results are visualised. 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.spf. After this you should see something like the fallowing image.

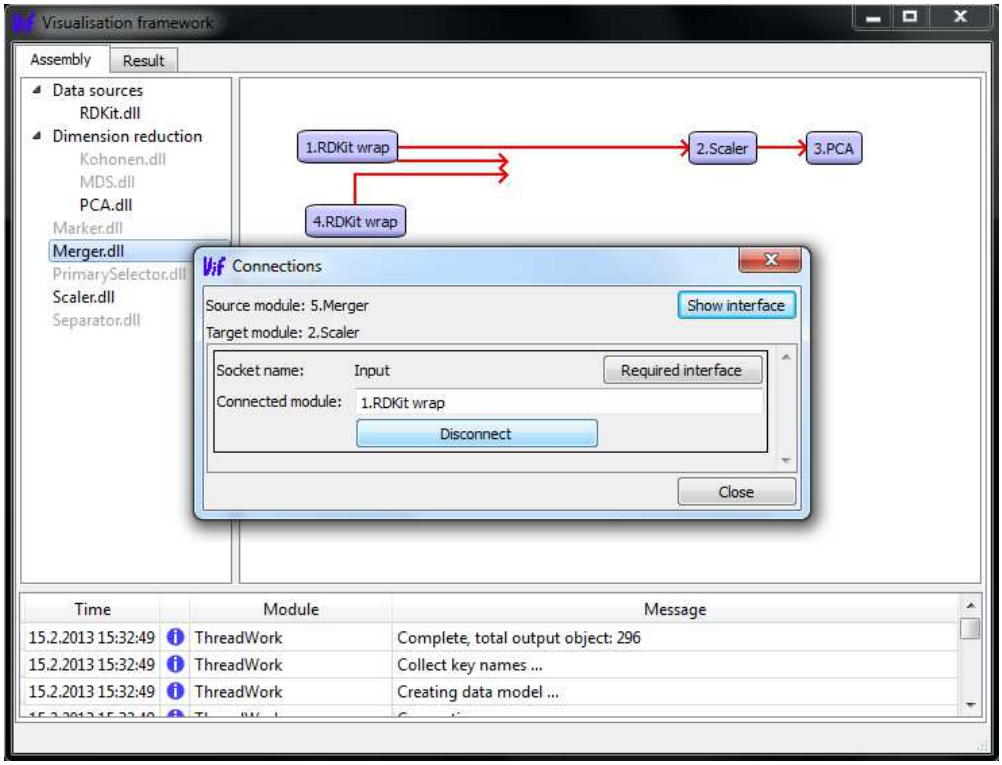



Now we reconnect connection between modules. First start by connecting 1.RDKit wrap to 5.Merger. Then connect 4.RDKit wrap module to 5.Merger. The module 5.Merger has multiple inputs choose one and click Connect. Module can generally have any number of inputs bud must have just one output.

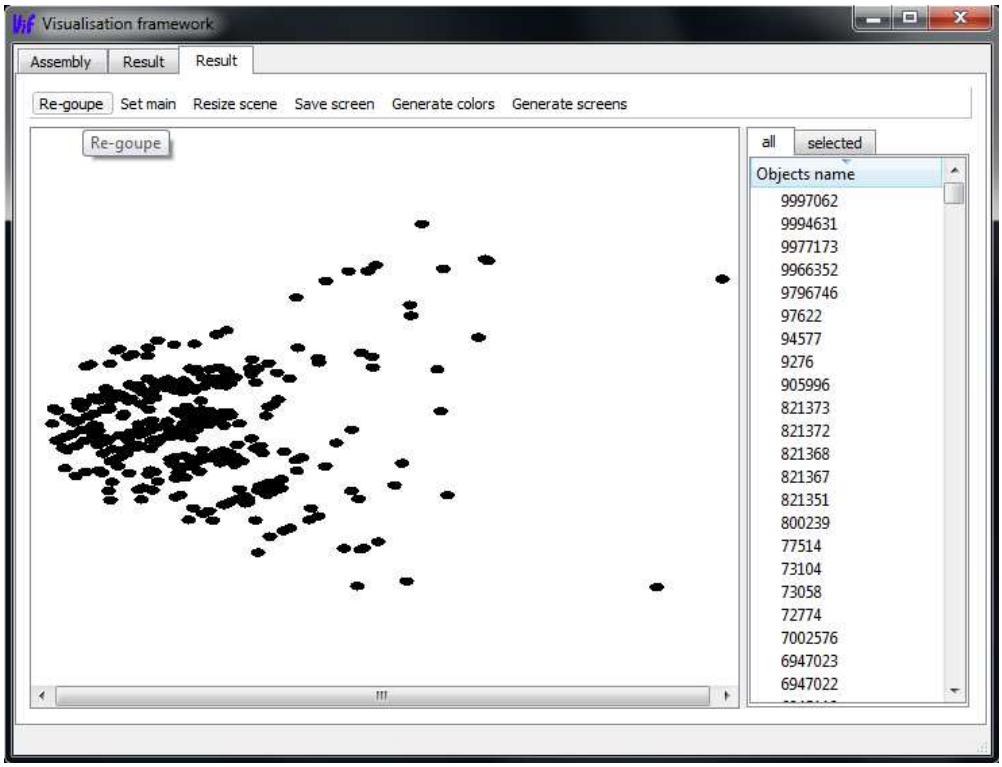



As you can see after connection is established module name is added and button is changed to Disconnect.

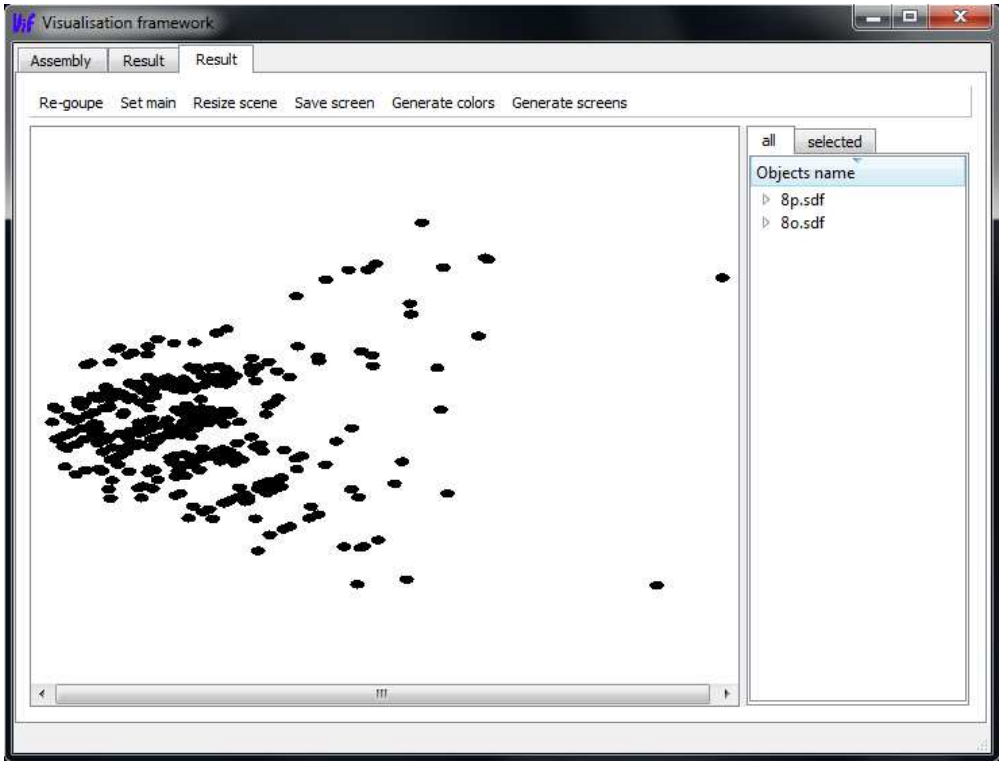
Now we disconnect 1.RDKit wrapper from 2.Scaler and connect 5.Merger instead. Just use drag and drop as previously. In dialog then click on Disconnect and Connect.



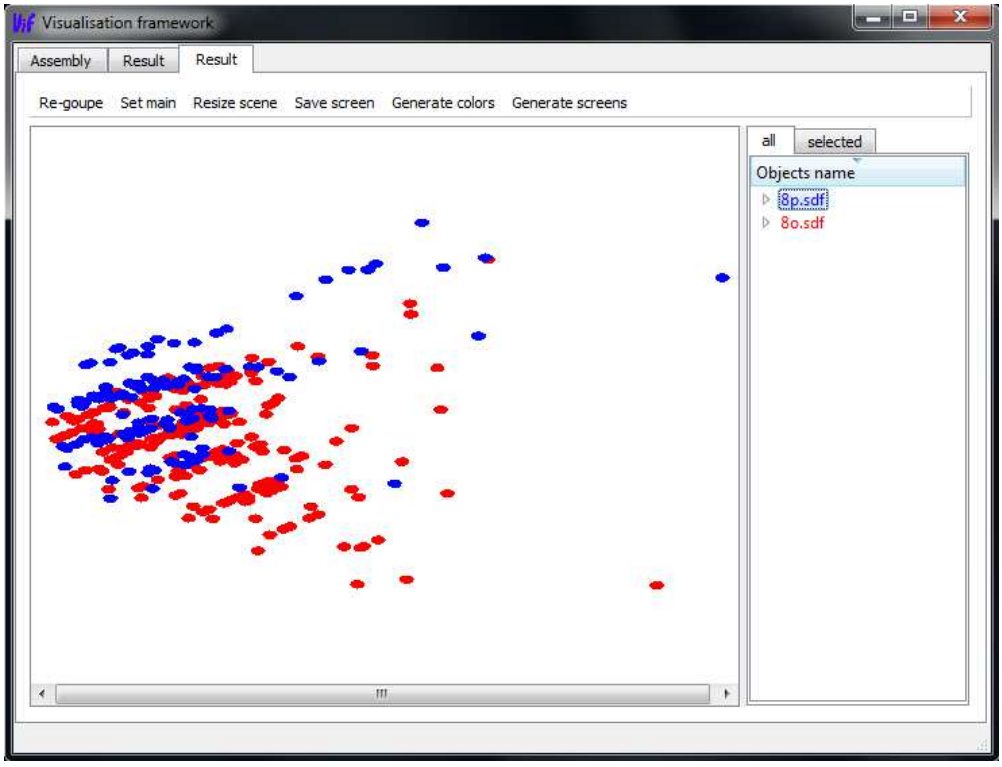

Now right click on the 3.PCA and select Run. After operation is finished a new tab named Result is added click on it. Like in previous case the dialog about resize is shown, just say ok. The dialog is shown because the data has too small range. If the original value is used then they are too close together.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




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

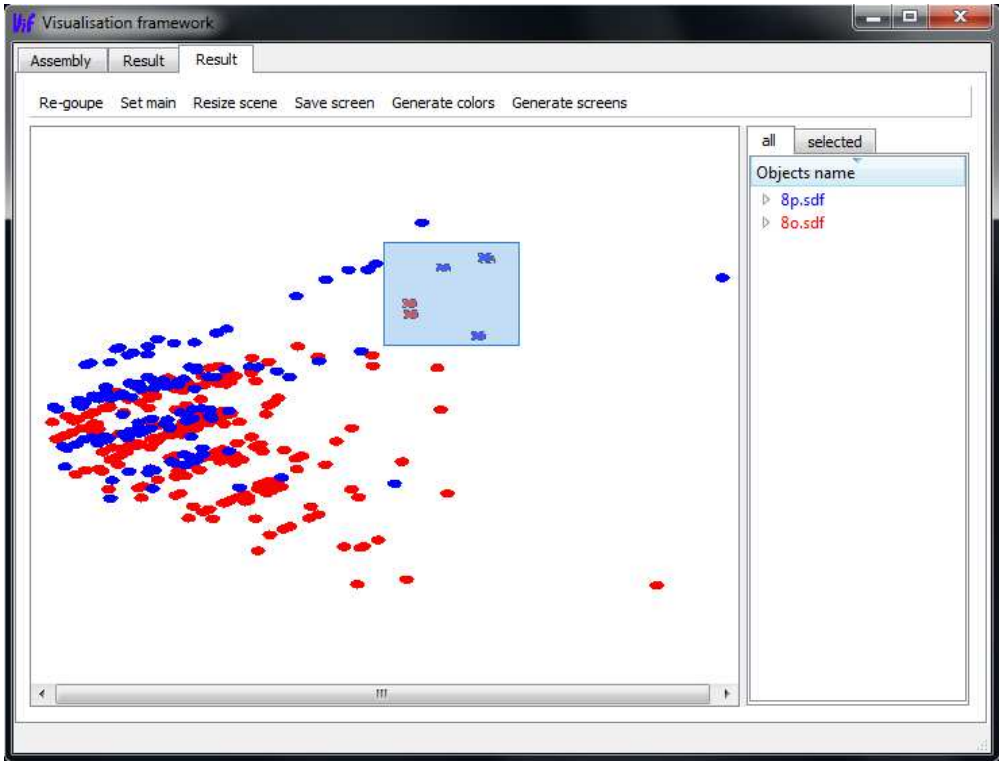



As you can see two group were created. This corresponds to the fact that we have two sources. Now right click on the group, for example 8p.sdf and select Set color and select color. Repeat the same for the second group. Now you could see which molecule belong to which source clearly.

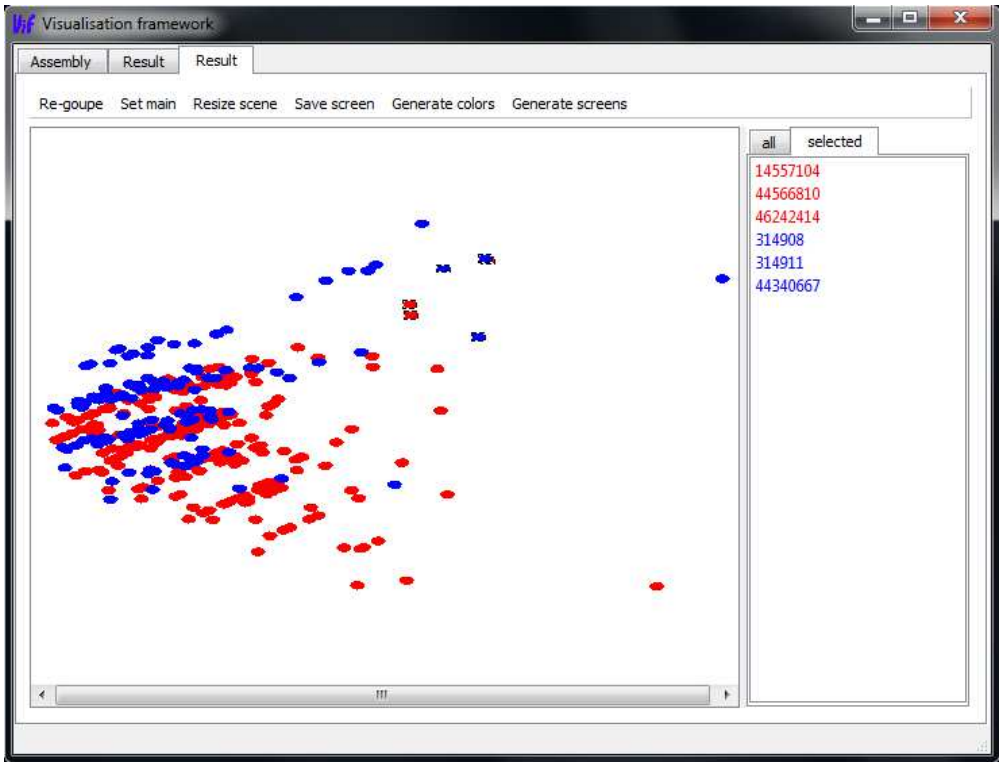



We now export current view into an image file. Click on Save image button, which is located in the top toolbar. If you want you can let place legend into output image. Then click ok and save image. If all goes well then you now exported a current view into selected file.

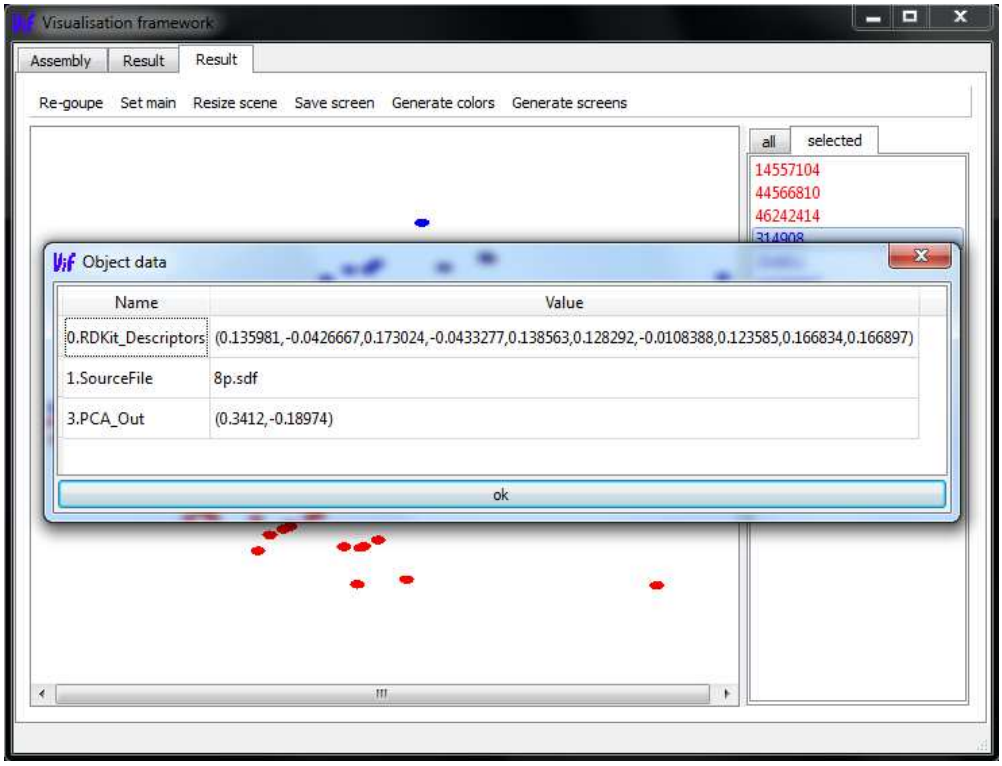
Now press and hold ctrl and select few molecules in the visualisation canvas. You can drag when do selection.




Now as you can see the molecules are highlighted. When you click on select tab (left). You can see the list of selected molecules.

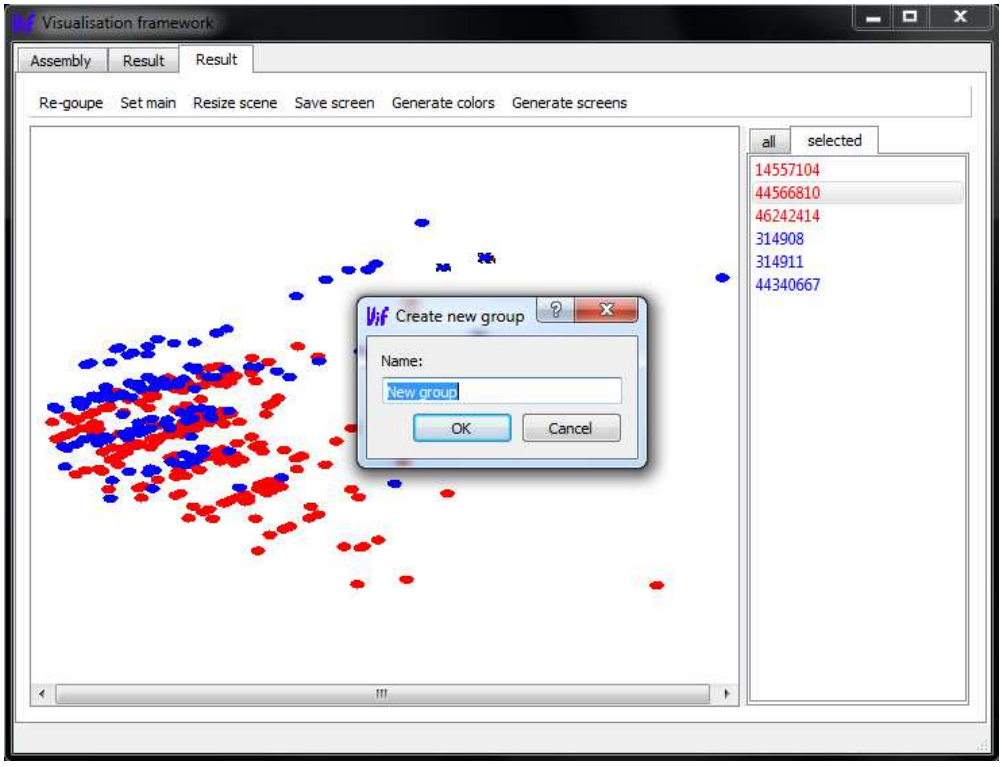



If you right click on molecule in all/selected list and select Show details a dialog with details about molecule will be shown as on the fallowing image.

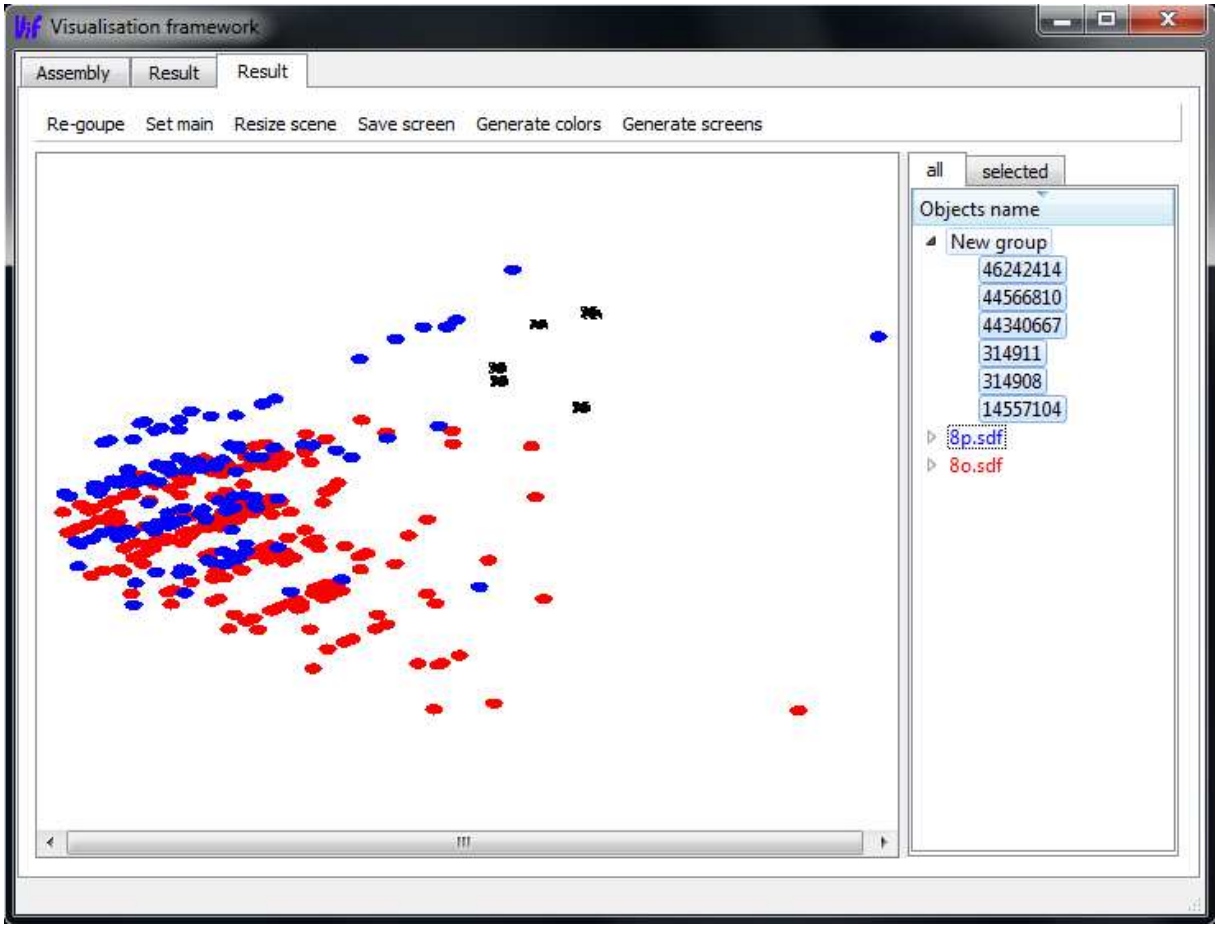



As you can see molecule can contains a number of different values. In this case molecule contain data from RDKit, that goes through scaling, SourceFile and PCA_Out. The PCA_Out is currently used value to determine position of the molecules on the visualisation canvas.  Close the dialog by pressing ok.

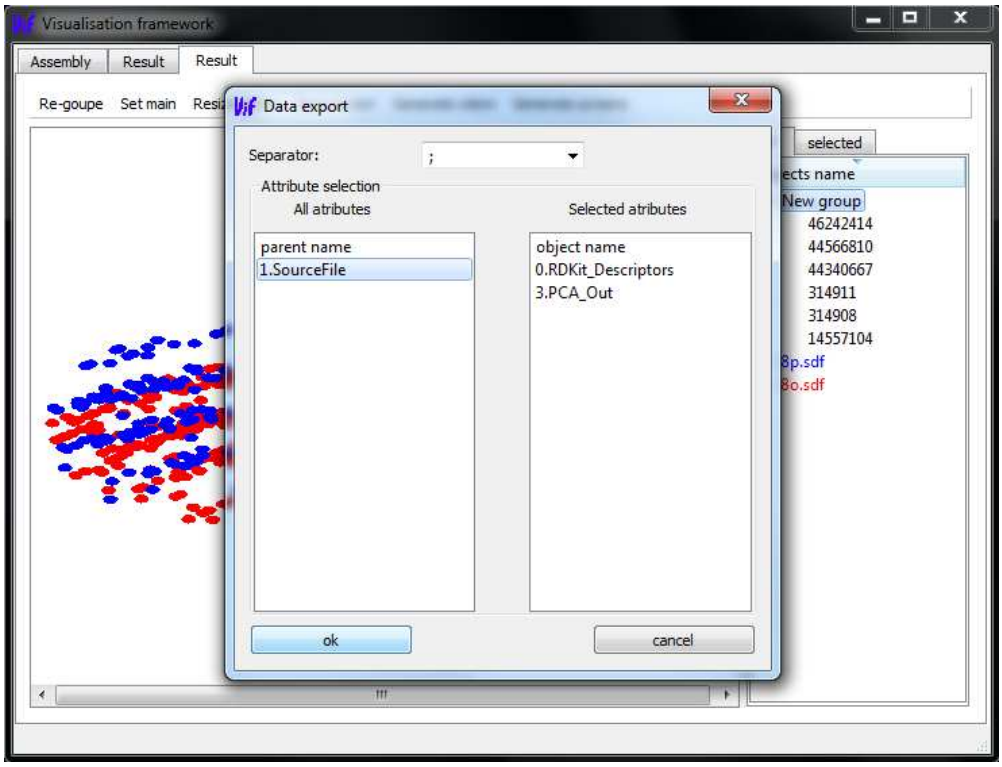
Now click to free space in the selected tab and press Move to new group. This will move all selected molecules into new group. You can specify the new group name, you can just press enter to continue.




The newly created group has default black color, because of that 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 click on the group's name select Export. Now the export dialog will appear (see the fallowing image). In 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 mention to be exported.




When you select desired attributes click on ok and select file where to store output. The selected attributes from selected molecules will be saved into given file.