X-Ray Photoelectron Spectroscopy – Principal Component Analysis
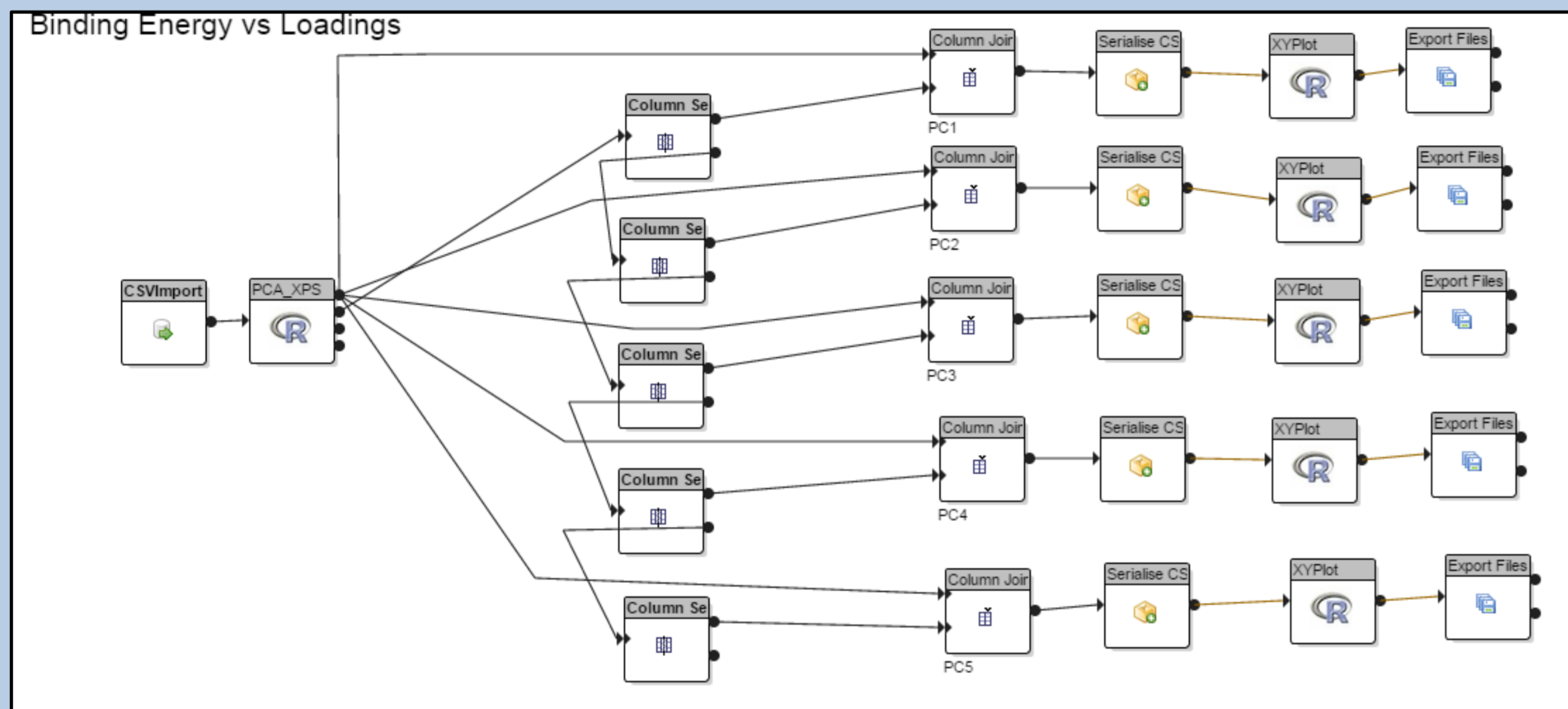
Aims:
-To create a block in the e-science central system to process XPS data and produce separate outputs for scores, loading and Binding Energy
-To manipulate the outputs of the created block to acquire the individual principal components
-To implement this block into a workflow in e-science to produce required plots for Principal Component Analysis of XPS data

An example of the workflow produced for Binding Energy vs Loadings
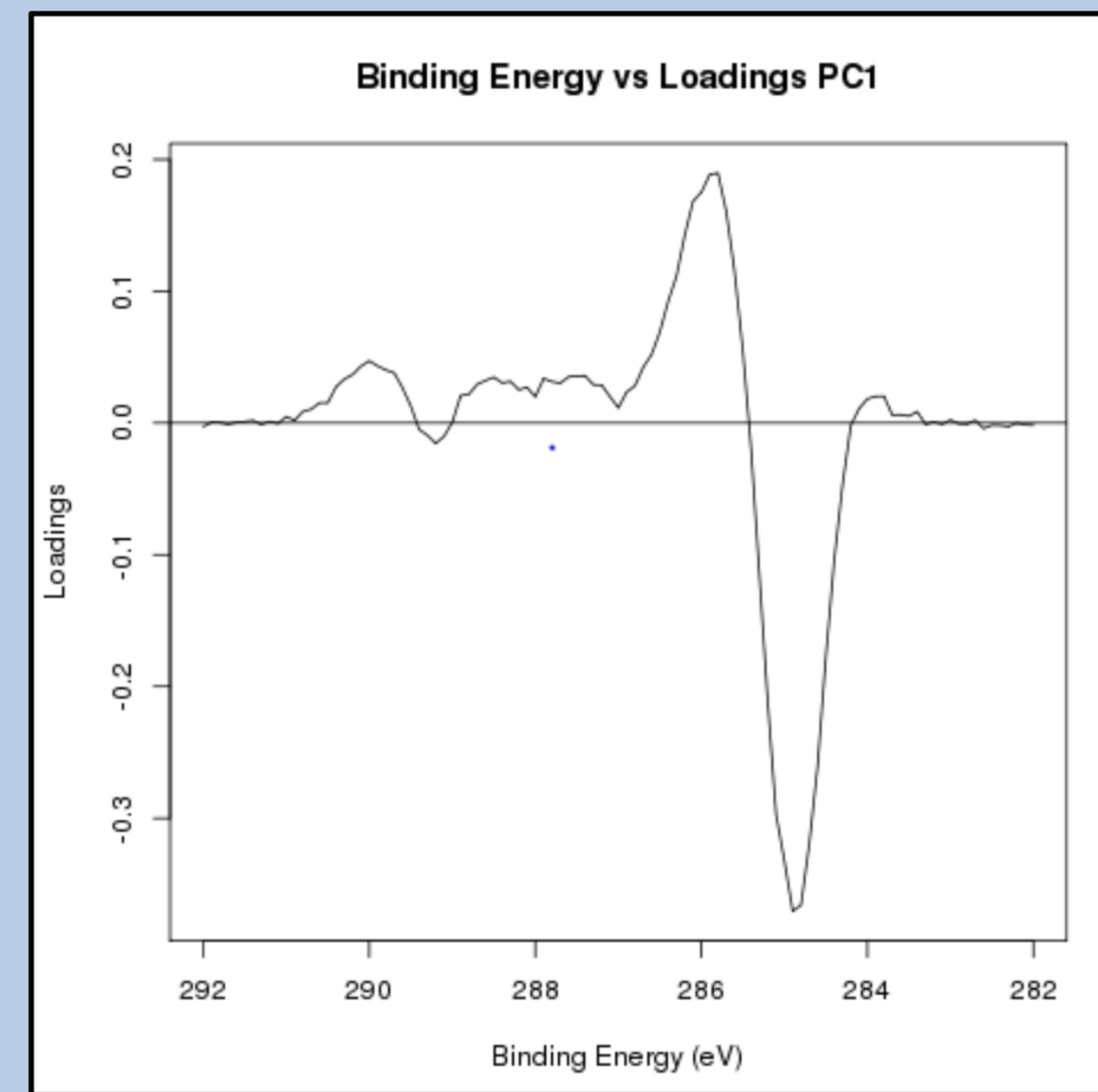
Example of the plots produced by Binding Energy vs Loadings Workflow

As shown in the 2 workflows the column select block already in the e-science system can be used to select the 1st column (PC1), the remaining columns can then be filtered into another column select and PC2 can be selected by the same method, this can be repeated until the desired amount of principal components are selected.

There are existing blocks in e-science system for plotting these principal components against each other in an XY Plot.
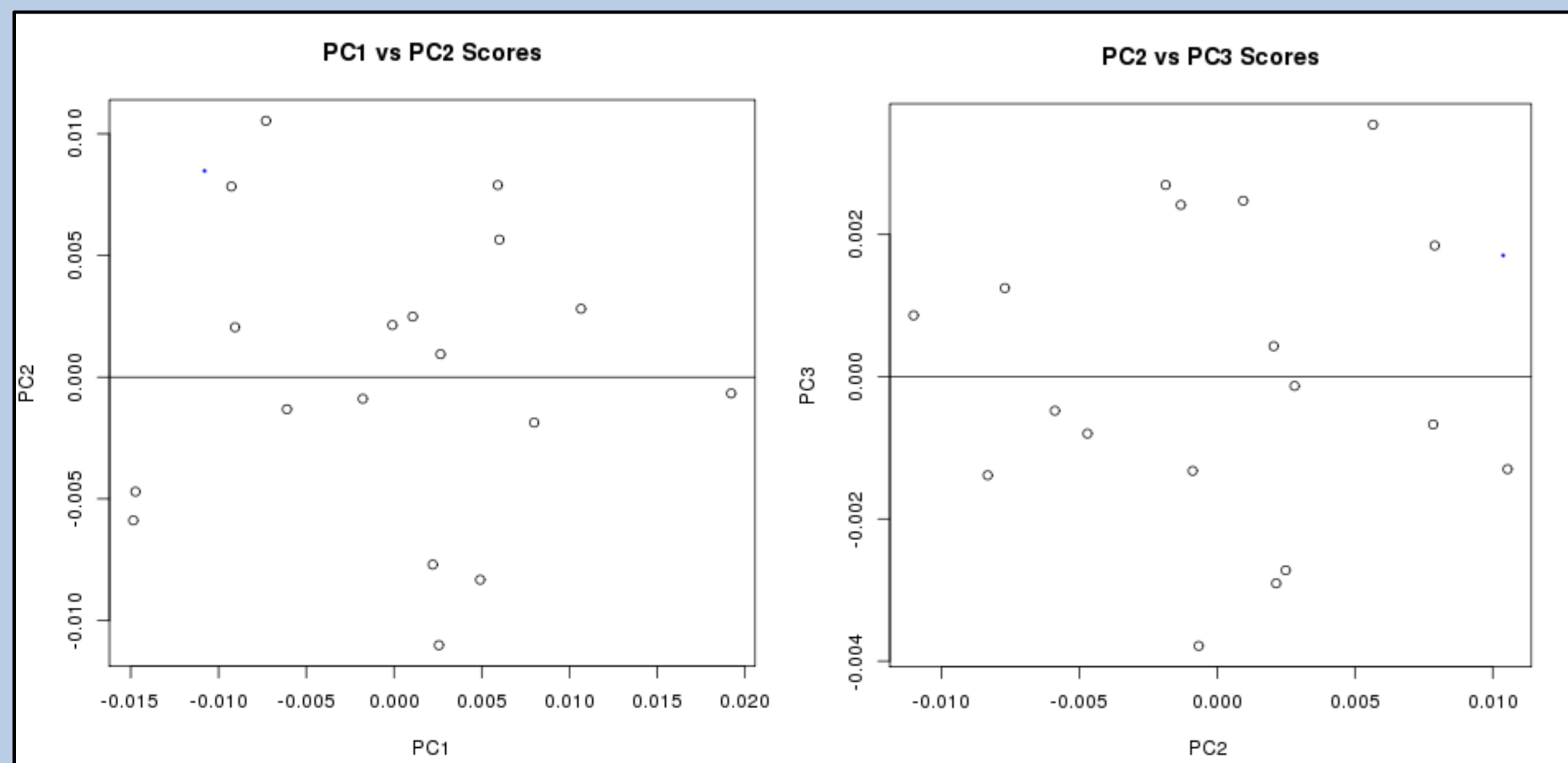
Score Plots created by the workflow PCA Scores
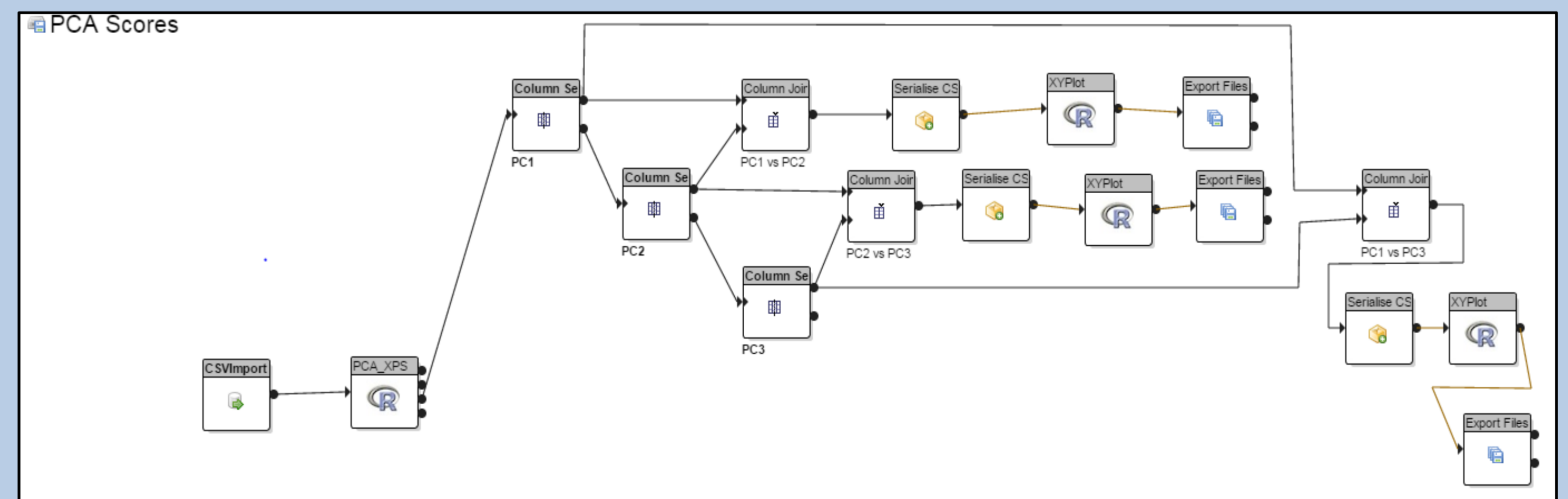
Workflow produced to produce score plots of various principal components against each other e.g pc1 vs pc2