Instructions for workshop 1/4

Data

- Download csv-files of detailed protein data (http://computproteomics.bmb.sdu.dk/tmp/PMC3316730.csv) and the file formated for upload to the apps (http://computproteomics.bmb.sdu.dk/tmp/PMC3316730_cut_reordered.csv)
- The files provide protein abundances described in the paper
  Comparative Proteomic Analysis of Eleven Common Cell Lines Reveals Ubiquitous but Varying Expression of Most Proteins (http://www.mcponline.org/content/11/3/M111.014050)
- What do the rows and the columns contain?
- How many replicates and conditions do we have?
- What is the order of the samples in the reordered file?

Instructions for workshop 2/4: VSClust

http://computproteomics.bmb.sdu.dk/Apps/VSClust (http://computproteomics.bmb.sdu.dk/Apps/VSClust)

Important The app can handle only one active user, so please arrange with the other participant when it is your turn to press one of the “Run” or “Estimate paramters” buttons.

- Load the file into VSClust and set the correct parameters. Download the results from the limma test. Filter for most significant proteins when comparing to the first condition
- Provide 3 different cluster numbers that are good candidates for the clustering
- Apply clustering and compare the number of proteins between variance-sensitive and standard fuzzy c-means
- Download results and try to understand the content of the table. What are membership values? How are they related to being part of a cluster and cluster number?
- Take the proteins in a cluster and look for GO terms and pathways (e.g. in DAVID, gProfileR or GOrilla)

  In case you are not able to obtain the VSClust output: http://computproteomics.bmb.sdu.dk/tmp/VSClustOut.csv (http://computproteomics.bmb.sdu.dk/tmp/VSClustOut.csv)

Instructions for workshop 3/4

ComplexBrowser

http://computproteomics.bmb.sdu.dk/Apps/ComplexBrowser (http://computproteomics.bmb.sdu.dk/Apps/ComplexBrowser)

- Upload the same file as for VSClust and look into the QC. Try out different normalizations. Which one gives the lowest mean/median CVs? What do the most deviating samples have in common?
- For the complexes, go to *Analysis* and press the button “run analysis” to investigate changes of protein complexes.
- Do you understand the meaning of the different figures?
- Look into the details of the 40S ribosomal subunit. What does the “Protein correlations heatmap” tell you?
- In honour to this venue, select the *SKI complex*. Given the expression profiles of its subunits, they seem to be co-regulated in the considered cells types.

Instructions for workshop 4/4

CoExpresso

http://computproteomics.bmb.sdu.dk/Apps/CoExpresso (http://computproteomics.bmb.sdu.dk/Apps/CoExpresso)

- Select the 40S ribosomal subunit (you will need to remove one protein from the list). Its proteins are highly co-regulated (with a few exceptions). Do you see a similar pattern as in ComplexBrowser for the cell line data? Reduce the list to the same proteins as measured and shown in ComplexBrowser. Do you see the same grouping?
- Select the SKI complex. Is this complex highly co-regulated in human cells when looking at the significance scores?
- Take the most changing complexes from ComplexBrowser and investigate their general behavior in human cells
- Take the 20 proteins with the highest membership values to a particular cluster and look into their co-regulation in human cells