

# **TRGN 527: Applied Data Science and Bioinformatics**

### **UNIT I. Introduction and Basic Data Science**

## Week 4 – Assignment 4

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- Instructions: Please answer the following questions, first 14 questions worth 7 points and last 2 questions worth 1 point (Total: 100 points).
- Load the file "TRGN599\_A4.mzXML" in your R-Studio.
  - For example, using the following code:

```
45 library(mzR)
46 library(msdata)
47 library(magrittr)
48
49 TRGN599_MS_file <- 'TRGN599_A4.mzXML'
50
51 my.data <- openMSfile(TRGN599_MS_file)
52
```

- In order to answer the following questions you should
- 1) create an R markdown file as explained during the last class,
- 2) copy/paste & run with the new data file (TRGN599\_A4.mzXML) the first 129 lines of code of the case study 1 Rmarkdown file (proteomics analysis) that you can find in Blackboard/Lecture 4:
  - File name: Rmarkdown\_TRGN\_599\_Week\_4\_Proteomics\_Analysis.Rmd.

### • Question 1

- Which of the following R commands gives you access to the measurement-metadata?
  - A) runInfo(my.data)
  - B) openMSfile(my.data)
  - C) boxplot(my.data)
  - D) plot(my.data)

- Which is the number of actual spectra in the set by using the "runInfo(my.data)\$scanCount" function?
  - A) 10
  - B) 5
  - C) 2
  - D) 7

### Question 3

- Which is the ion source for the experiment by using the "instrumentInfo(my.data)\$ionisation" function?
  - A) hybridization ionization
  - B) fluorescence ionization
  - C) electrophoresis ionization
  - D) electrospray ionization

### • Question 4

- How many columns you have in your data when use the header(my.data) function?
  - A) 50
  - B) 26
  - C) 31
  - D) 33

### • Question 5

- When you plot the spectrum using the "plot(pl, type="h")" function how many peaks you observe greater than 4e+07?
  - A) 20
  - B) 10
  - C) 3
  - D) 9

- When you pick up the 15 strongest peaks using the function
  - "topnum <- 15
  - pl.top <- pl[pl[,2] %in% head(sort(pl[,2],decreasing=T),topnum),1]"</li>
- Which of the following is the highest peak?
  - A) 464.8184
  - B) 924.7365
  - C) 395.8215
  - D) 789.7467

#### • Question 7

- When you pick up the 15 strongest peaks using the function
  - "topnum <- 15
  - pl.top <- pl[pl[,2] %in% head(sort(pl[,2],decreasing=T),topnum),1]"</li>
- Which of the following is the lowest peak?
  - A) 464.8184
  - B) 924.7365
  - C) 395.8215
  - D) 789.7467

- When you pick up the 20 strongest peaks using the function
  - "topnum <- 15
  - pl.top <- pl[pl[,2] %in% head(sort(pl[,2],decreasing=T),topnum),1]"</li>
- Which of the following is the highest peak?
  - A) 333.6765
  - B) 924.7365
  - C) 395.8215
  - D) 789.7467

#### • Question 9

- When you pick up the 20 strongest peaks using the function:
  - "topnum <- 15
  - pl.top <- pl[pl[,2] %in% head(sort(pl[,2],decreasing=T),topnum),1]"</li>
- Which of the following is the lowest peak?
  - A) 333.6765
  - B) 924.7365
  - C) 395.8215
  - D) 789.7467

- When you plot the peak differences using the function:
  - peakdiff <- outer(pl.top, pl.top, '-')</li>
  - plot(density(abs(peakdiff)))
- Which of the following is the probability function of the graph:
  - A) Probability density function (PDF)
  - B) Probability mass function (PMF)
  - C) Poisson distribution
  - D) Random distribution

#### • Question 11

- When you plot the peak differences using the function:
  - peakdiff <- outer(pl.top, pl.top, '-')</li>
  - plot(density(abs(peakdiff)))
- Which of the following would be the most suitable description of the observed curve distributions:
  - A) One can observe that the curve is a composition of two wide distributions.
  - B) One can observe that the curve is a composition of three wide distributions.
  - C) One can observe that the curve is a composition of one wide distributions.
  - D) One can observe that the curve is a composition of five wide distributions.

- When you plot the peak differences using the function:
  - peakdiff <- outer(pl.top, pl.top, '-')</li>
  - plot(density(abs(peakdiff)))
- And previously used the 20 strongest peaks using the functions:
  - topnum <- 20
  - pl.top <- pl[pl[,2] %in% head(sort(pl[,2],decreasing=T),topnum),1]</li>
  - pl.top
- Which of the following would be the most suitable description of the peakdiff matrix:
  - A) It is by itself a 20x20 matrix containing the differences among the elements of the pl.top vector
  - B) It is by itself a 60x60 matrix containing the differences among the elements of the pl.top vector
  - C) It is by itself a 10x10 matrix containing the differences among the elements of the pl.top vector
  - D) It is by itself a 15x15 matrix containing the differences among the elements of the pl.top vector

### • Question 13

- When you plot the peak differences using the function:
  - peakdiff <- outer(pl.top, pl.top, '-')</li>
  - plot(density(abs(peakdiff)))
- And previously used the 20 strongest peaks using the functions:
  - topnum <- 20
  - pl.top <- pl[pl[,2] %in% head(sort(pl[,2],decreasing=T),topnum),1]</li>
  - pl.top
- Which of the following numbers is the sample size of the plot?
  - A) N = 200
  - B) N = 300
  - C) N = 500
  - D) N = 400

### • Question 14

- When you plot the peak differences using the function:
  - peakdiff <- outer(pl.top, pl.top, '-')</li>
  - plot(density(abs(peakdiff)))
- And previously used the 20 strongest peaks using the functions:
  - topnum <- 20
  - pl.top <- pl[pl[,2] %in% head(sort(pl[,2],decreasing=T),topnum),1]</li>
  - pl.top
- Which of the following numbers is the bandwidth of your plot?
  - A) Bandwidth = 32.53
  - B) Bandwidth = 53.52
  - C) Bandwidth = 22.53
  - D) Bandwidth = 52.53

### • Question 15

- Which of the following is an analytic technique that produces mass-to-charge ratio spectra of peptide fragment in samples:
  - A) Microarrays
  - B) Mass spectrometry (MS)
  - C) Messenger RNA (mRNA)
  - D) Proteomics

- Regarding the different file formats for MS data, which file format you are using in your proteomic analysis when uploading data through the mzR package from Bioconductor?
  - A) mzML
  - B) netCDF
  - C) mzXML
  - D) mzCDF