

Assignment02 - Feature Extraction

General Instructions – Must Read

- ❑ **Number of Questions:** 01
- ❑ **Submission Guidelines:** You need to submit single R file.
 - Single R (.r) file | File Name must be <YourRollNum>.r | Example: **10155.r**
- ❑ Your program must be run from **command line** only:
 - **Usages:** rscript <program.r> <InputDataFile>
 - **Example:** rscript 10155.r input.csv
- ❑ **Output File Name:** <output>-<YourRollNum>.csv
 - **Example:** output-10155.csv
- Your program must be capable to handle exception/error (if any) and write to **log file**:
 - Correct number of parameters (inputFileName).
 - Show the appropriate message for wrong inputs.
 - Handling of “File not Found” exception
 - Many sequences are missing in the input file, handle them (ignore them).
 - If any issue with the input record, it must be write to a log file

1. Write a R program that extract the features (aliphatic index, Boman index, hmoment index, peptide charge, etc) of each “Peptide Sequence” given in the input file and create a feature matrix given below. [Input file is available in “Input for Assignment02” folder]

Peptide Sequence	len	Aliphatic_index	Boman_index	hmoment_index	peptide_chrage	molecular_weight	Target
TLYGPQLSQKIVQIN	15	123.33	0.68	0.51	1.00	1701.98	0
PSWGLVVTMFAWGYL	24	101.25	-0.28	0.44	-0.91	2764.26	1
TMIKTAVAVV	10	146.00	-1.23	0.40	1.00	1032.31	1
AGISLIIDPNPMFV	15	130.00	-0.64	0.23	-1.00	1573.87	1
DPMIVGVLFIEIHMM	15	142.67	-1.24	0.13	-1.91	1745.19	0
ELNNALQNLARTISE	15	117.33	2.44	0.73	-1.00	1685.85	1
AGILLGLFYLVAVAR	15	188.67	-1.86	0.23	1.00	1575.96	0
GKAGCQTYKWETFLTSE	20	44.00	1.02	0.30	-0.06	2216.49	0
QLSAEYASTAAELSG	15	78.67	0.94	0.26	-2.00	1497.58	1
AAVVRFQEAANKQKQ	15	65.33	2.52	0.52	2.00	1687.92	1

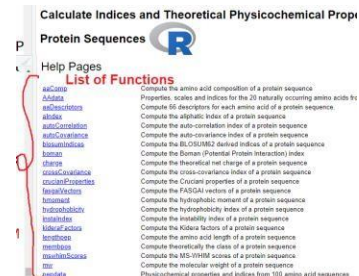
Please note: Steps for feature extraction

1. First, install two packages: 'Peptides' and 'peptider'

```
install.packages('Peptides')
```

```
install.packages('peptider')
```

2. Explore all the functions of both the packages:



3. Give the sequence to these functions, get the value, merge them and write to the output file.

4. Sample Code

```
library(Peptides)
library(peptider)
mydata = read.table("input.csv") # Reading the sequence file
for (sequence in mydata$V1){
  F1 <- aIndex(sequence)          # F1: aliphaticIndex
  F2 <- boman(sequence)           # F2: bomanIndex
  F3 <- instaIndex(sequence)       # F3: instaIndex
  F4 <- ppeptide(sequence, libscheme = "NNK", N=10^8) # F4: probabilityDetectionPeptide
  allFeatures = data.frame(F1,F2,F3,F4) # Merging all features
  # Write and append allFeatures to the file
  write.table(allFeatures, "output-10155.csv", sep = ",", row.names=F, col.names = F, append = T)
}
cat("Done")
```