**Codes for Lipidr package to run successfully.**

dir\_path = getwd()

dir\_name = "/lipidr-demo-vs"

print(dir\_path)

dm\_path = paste(dir\_path,dir\_name,"/test\_data\_matrix.csv",

sep="")

ta\_path = paste(dir\_path,dir\_name,"/test\_annotation\_data.csv",

sep="")

test\_data\_matrix<-read.csv(file.choose(),header=T)

test\_annotation\_data<-read.csv(file.choose(),header=T)

if (!requireNamespace("BiocManager", quietly = TRUE))

d <- as\_lipidomics\_experiment(read.csv(file.choose(),header = T))

d <- add\_sample\_annotation(d, test\_annotation\_data)

install.packages("BiocManager")

a

BiocManager::install("lipidr")

plot\_samples(d, type="tic", log=TRUE)

d <- set\_logged(d, "Area", TRUE)

d <- set\_normalized(d, "Area", TRUE)

plot\_samples(d, "boxplot")

mvaresults = mva(d, measure="Area", method="PCA")

plot\_mva(mvaresults, color\_by="SampleType", components = c(1,2))

two\_group <- de\_analysis(d, Cancer-Benign, Cancer-Metastasis)

plot\_results\_volcano(two\_group)

mvaresults = mva(d, method = "OPLS-DA", group\_col = "SampleType", groups=c("Benign", "Cancer"))

plot\_mva(mvaresults, color\_by="SampleType")

plot\_mva\_loadings(mvaresults, color\_by="Class", top.n=10)

enrich\_results = lsea(two\_group, rank.by = "logFC")

significant\_lipidsets(enrich\_results)

plot\_enrichment(two\_group, significant\_lipidsets(enrich\_results), annotation="class")

plot\_enrichment(two\_group, significant\_lipidsets(enrich\_results), annotation="length")

plot\_trend(two\_group)