library(xcms)

library(multtest)

library(BiocParallel)

xset <- xcmsSet(method='centWave', ppm=10, BPPARAM = SerialParam(), snthresh=10,

prefilter=c(4,200), scanrange = c(40,1000), peakwidth = c(5,30),

integrate=1,fitgauss=F,verbose.columns=T)

####Key points/notes####

- ‘ppm=10’ maximum error (deviation in m/z in consecutive scans) allowed for mass

acquisition in parts per million (ppm).

- ‘BPPARAM = SerialParam()’ analyses peaks one after the other instead of in parallel

to lessen computing power required

- ‘snthresh=10’ the cutoff for the signal to noise ratio.

- ‘prefilter=c(4,200)’ Only retains mass traces if they contain at least k (4) peaks with

intensity >= I (200).

- ‘scanrange = c(40,1000)’ gives the range of masses to be considered

- ‘peakwidth = c(5,12)’ range of acceptable peak width (in seconds).

- ‘integrate=1’ integration method (to find area under MS curve) which is less prone to

signal noise but potentially less exact (than integrate=2).

- ‘fitgauss=F’ means that a Gaussian is not fitted to normalise the peak.

- ‘verbose.columns=T’ returns additional peak metadata.

##################################

xset

xset <- group(xset)

xset2 <- retcor(xset, family="s", plottype="m")

### family=”s” only keeps symmetric peaks###

xset2 <- group(xset2, bw=10)

### bw=10 removes peaks that have not been grouped correctly ###

xset3<- fillPeaks(xset2)

reporttab <- diffreport((xset3, 'myClass1', 'myClass2', 'myResultDir', 20, metlin = 0.15)

###this is where you specify output file names and location ####