

Supplementary Text 1. R script for peak picking for GC-MS data

```
# Peak Picking.R
# EM Sogin
# Description: R script to pick peaks from GC-MS data

library(xcms)
library(CAMERA)

## PEAK PICKING, RETENTION TIME GROUPING & CORRECTION WITH XCMS
setwd('home/path/to/files')
files<-list.files(pattern='.mzXML', recursive = T, full.names=T)
xs <- xcmsSet(files, method = "matchedFilter", fwhm = 8.4, snthresh = 1, step= 0.25, steps= 2, sigma =
3.56718192627824, max= 500, mzdif= 1, index= FALSE)
xset1 <- group(xs, method = "density", bw=2, mzwid= 1, minfrac = 0.3, minsamp = 1, max = 500) ##
Initial peak grouping
xset2 <- retcor(xset1)
xset2 <- group(xset2, method = "density", bw=2, mzwid= 1, minfrac = 0.3, minsamp = 1, max = 500)
xset<-fillPeaks(xset2)

## Group peaks in to pseudo-spectra using CAMERA
an<-xsAnnotate(xset)
xsF<-groupFWHM(an, perfwHM=3)

peaks<-getPeaklist(xsF)
peaks[is.na(peaks)]<-0

save.image('Peak_Picking_Results.RData')
# End
```