Figure 2D

```
library(RColorBrewer)
library(dplyr)
library(graphics)
install.packages("plotrix")#pie3D
library(plotrix)
df <- data.frame(value = c(20.15,14.67,12.30,11.70,9.92,8.89,7.11,6.81,5.63,2.67,0.15),
                         group = c('Lipids',
                                   'Others',
                                   'Amino acids and derivatives',
                                   'Phenolic acids',
                                   'Organic acids',
                                   'Nucleotides and derivatives',
                                   'Flavonoids',
                                   'Alkaloids',
                                   'Terpenoids',
                                   'Lignins and Coumarins',
                                   'Tannins'))
df <-arrange(df,value)
labs <- paste0(round(df$value/sum(df$value)*100,2), "%")
#mycolors<- brewer.pal(11,"Set3")
pie(df$value,labels=labs, init.angle=90,
      col = c("#8DD3C8",
                "#FEFFB3",
                "#BEBBDA",
                "#FB8071",
                "#80B1D2",
                "#FDB062",
                "#B3DE6A",
                "#FDCDE5",
                "#D9D9D9",
                "#BC80BC",
                "#CCEAC4"),
      border="white",
      edges = 10000)
      #explode=0.1)
group = c('Amino acids and derivatives',
            'Phenolic acids',
            'Flavonoids',
            'Lignins and Coumarins',
            'Nucleotides and derivatives',
            'Alkaloids',
            'Terpenoids',
            'Organic acids',
```

```
                'Lipids',
                'Tannins',
                'Others')
legend("topright", group, cex=1.5, fill=c("#8DD3C8",
                                                    "#FEFFB3",
                                                    "#BEBBDA",
                                                    "#FB8071",
                                                    "#80B1D2",
                                                    "#FDB062",
                                                    "#B3DE6A",
                                                    "#FDCDE5",
                                                    "#D9D9D9",
                                                    "#BC80BC",
                                                    "#CCEAC4"),border = NA)
zz <- data.frame(value = c(44.73,0,55.26),
                            group = c('down','up','insignificnat'))
zz <-arrange(zz,value)
labs <- paste0(round(zz$value/sum(zz$value)*100,2), "%")
```

Figure 3B

```
library(ggplot2)
library(ggrepel)
df2=read.csv("d:/R/df2.csv",sep=',',header=T)
df2[which(df2$VIP >= 1 & df2$logFC <= -1),'sig'] <- 'Down'
df2[which(df2$VIP >= 1 & df2$logFC >= 1),'sig'] <- 'Up'
df2[which(df2$VIP <= 1 | abs(df2$logFC) < 1),'sig'] <- 'insignificant'
p <- ggplot(df2, aes(x = logFC, y = VIP, color = sig)) +
   geom_point(size = 2) +
   scale_colour_manual(values    = c('red2', 'blue2', 'gray'), limits = c('Up', 'Down', 'insignificant'))
+
   theme(panel.grid = element_blank(), panel.background = element_rect(color = 'black', fill =
'transparent'), plot.title = element_text(hjust = 0.5)) +
   theme(legend.key = element_rect(fill = 'transparent'), legend.background = element_rect(fill =
'transparent'), legend.position = c(0.9, 0.93)) +
   geom_vline(xintercept = c(-1, 1), color = 'gray', size = 0.3) +
   geom_hline(yintercept = 1, color = 'gray', size = 0.3) +
   xlim(-18, 25) + ylim(0, 2) +
   labs(x = '\nLog2 Fold Change', y = 'Variable Importance in Projection(VIP)\n', color = '')+
   scale_x_continuous(breaks=seq(-18,25,6))
P
```

Figure 3C

```
pie(zz$value,labels=labs, init.angle=90,
      col = c("blue2",
                "red2",
                "grey"),
      border="white",
      edges = 10000,
      radius=0.5)
#explode=0.1)

library(openxlsx)
```

Figure 3D

```
KEGG=read.xlsx("d:/R/KEGG.xlsx",sep = '\t',check.names = F)
library(ggplot2)
KEGG1 <- ggplot(data = KEGG,mapping = aes(x = Rich_Factor,y = Kegg_pathway))+
  geom_point(aes(color= pvalue,size = Metabolite_number)) +
  scale_colour_gradient(high = 'green',low = 'red') +
  theme_bw()+
  labs(title = 'Statistics of KEGG Enrichment',
       x = 'Rich Factor',
       y = 'kegg pathways')+
  xlim(0.5,1)
KEGG1
```

Figure S3

```
#pheatmap
install.packages("pheatmap")
library(pheatmap)
library(openxlsx)
df4=read.xlsx("d:/R/df4.xlsx",rowNames=T)
annotation_row = data.frame(Class=factor(
  rep(c("Arachidonic acid metabolism",
        "Linoleic acid metabolism",
        "Alpha-Linolenic acid metabolism",
        "Flavone and flavonol biosynthesis",
        "Phenylpropanoid biosynthesis"),
      c(5, 6, 5, 4, 7))))
row.names(annotation_row)
row.names(annotation_row)<-rownames(df4)
ann_colors = list(
  Class = c(`Arachidonic acid metabolism`="blue",
            `Linoleic acid metabolism`= "green",
            `Alpha-Linolenic acid metabolism` = "red",
```

```
                `Flavone and flavonol biosynthesis`="orange",
                `Phenylpropanoid biosynthesis`="black"))
pheatmap(df4,scale="row",
         cellheight = 10,cellwidth = 20,
         treeheight_row = 50,
         fontsize_col = 10,fontsize = 8,angle_col=45,
         border_color = "white",
         cluster_cols = F,cluster_rows = F,
         annotation_row    = annotation_row,
         annotation_colors = ann_colors,
         color = colorRampPalette(c("blue", "white","red"))(100))
row.names(df4)
colnames(df4)
pheatmap(df1,annotation_row = annotation_row,scale = "row")
pheatmap(df1, scale='row',annotation_row = annotation_row, annotation_col = annotation_col,cluster_rows = FALSE, gaps_row = c(24, 38))
```