

Pathways

QuetzallyMed

2025-06-11

```
getwd()
```

```
## [1] "C:/Program Files/Git/Camda25_gut"
```

```
path <- read.csv("DataSets/CAMDA_2025/pathways.txt", sep = "\t")
samp <- read.csv("DataSets/CAMDA_2025/metadata_corrected_final.txt", sep = "\t")
type_path <- read.csv("DataSets/CAMDA_2025/Pathways_Types_complete.txt", sep = "\t")
```

```
t <- t(path)

colnames(t) <- as.character(t[1, ])
t <- t[-1, ]
t <- as.data.frame(t)

t <- rownames_to_column(t, var = "sample")

merg <- samp %>% select(sample, Group) %>%
  merge(t, by = "sample")

long <- merg %>%
  pivot_longer(
    cols = matches("."),
    names_to = "Object.ID",
    values_to = "value"
  )
```

```
joined <- long %>%
  regex_left_join(
    type_path %>% select(Object.ID, General_Pathway_Type),
    by = c("Object.ID" = "Object.ID") # Coincidencia parcial
  )
```

```
no_match <- joined %>%
  filter(is.na(General_Pathway_Type))
```

```
unique(no_match$Object.ID.x)
```

```
## character(0)
```

```

# Agrupar y sumar los valores por sample, group y type
joined$value <- as.numeric(joined$value)

grouped <- joined %>%
  group_by(sample, Group, General_Pathway_Type) %>%
  summarise(total = sum(value), .groups = "drop")

# Volver a formato ancho
Path_grouped <- grouped %>%
  pivot_wider(
    names_from = General_Pathway_Type,
    values_from = total
  )

# Crear carpeta si no existe
if (!dir.exists("DataSets/CAMDA_2025/densidad_pathways")) {
  dir.create("DataSets/CAMDA_2025/densidad_pathways")
}

write.table(Path_grouped, file = "DataSets/CAMDA_2025/Path_agrupados.txt", row.names = FALSE, quote = F)

# Lista de columnas numéricas a graficar
columns_to_plot <- unique(grouped$General_Pathway_Type)

# Loop para crear una gráfica por variable
for (col_name in columns_to_plot) {
  p <- ggplot(Path_grouped %>% filter(Group != "delete"),
    aes_string(x = col_name, fill = "Group", color = "Group")) +
    geom_density(alpha = 0.4) +
    labs(
      title = paste (col_name),
      x = "Total de valores",
      y = "Densidad"
    ) +
    theme_minimal()

  ggsave(
    filename = paste0("DataSets/CAMDA_2025/densidad_pathways/", gsub("[^a-zA-Z0-9]", "_", col_name), ".pdf"),
    plot = p,
    width = 8, height = 5
  )

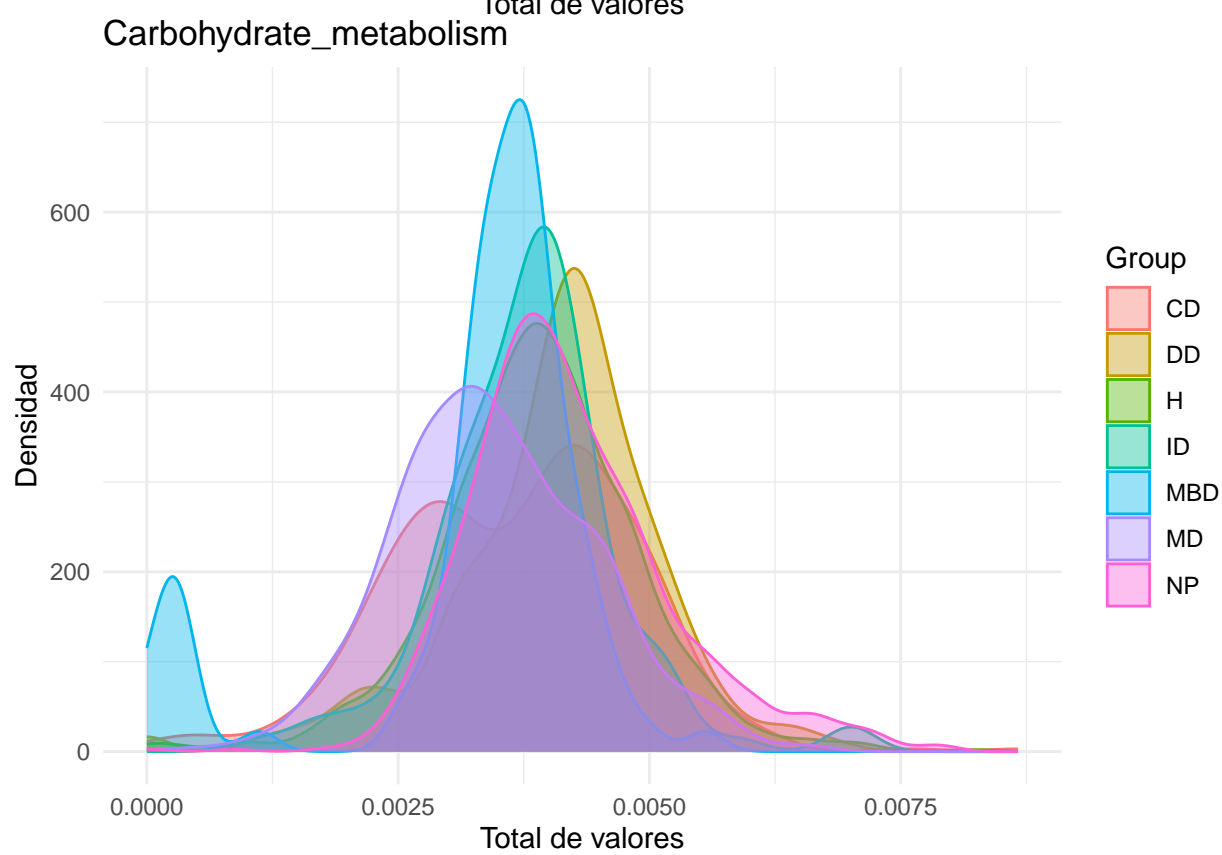
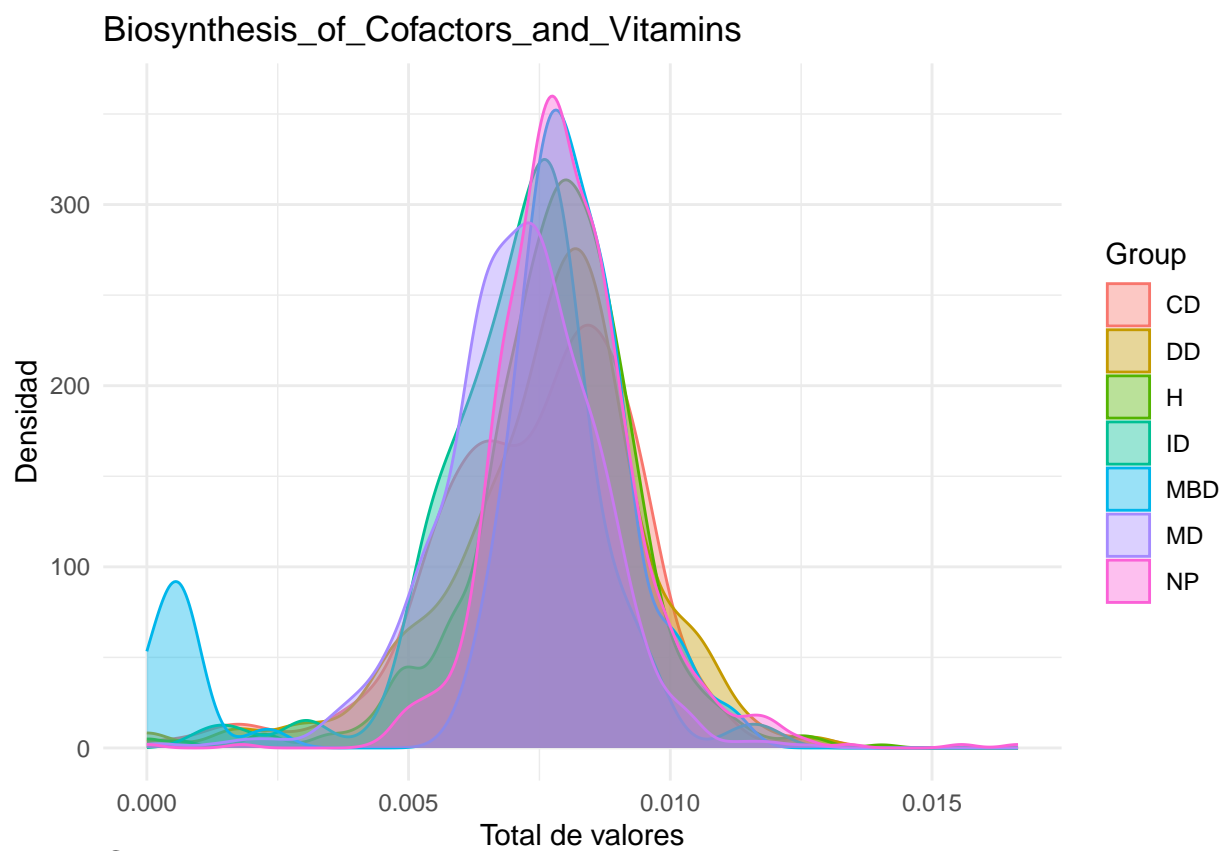
  print(p)
}

```

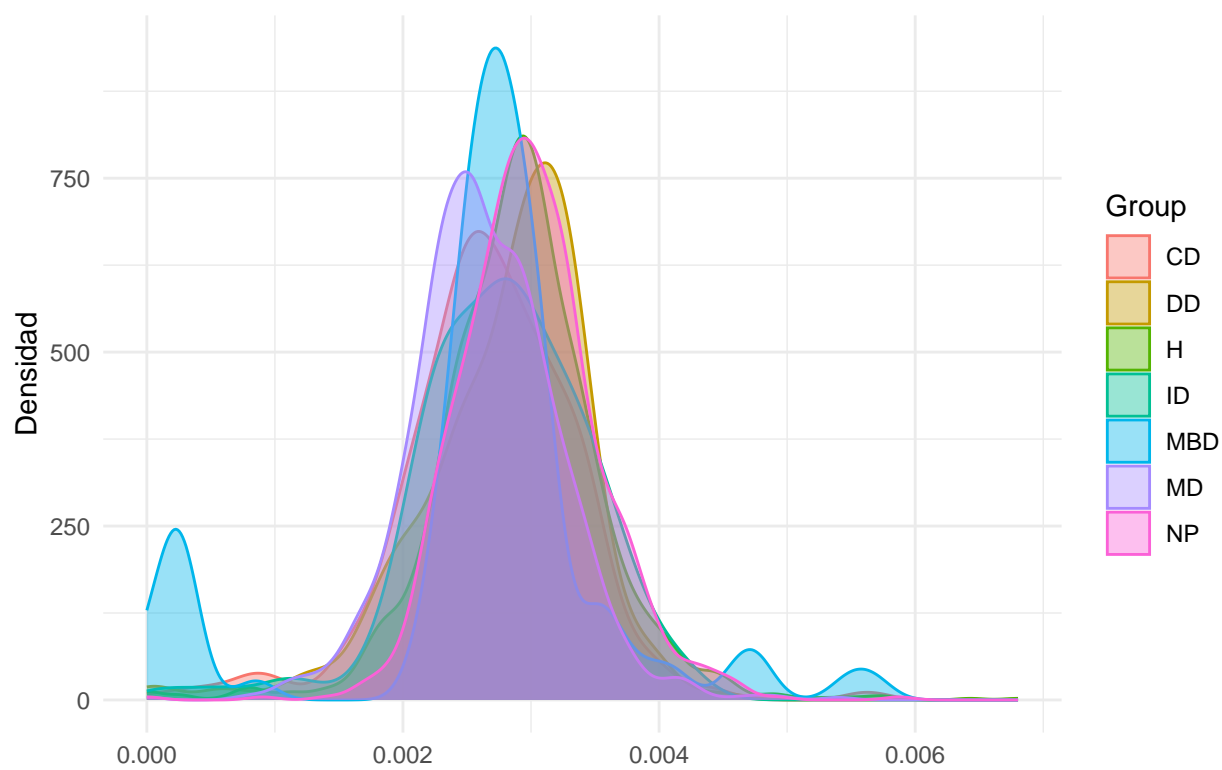
```

## Warning: 'aes_string()' was deprecated in ggplot2 3.0.0.
## i Please use tidy evaluation idioms with 'aes()'.
## i See also 'vignette("ggplot2-in-packages")' for more information.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.

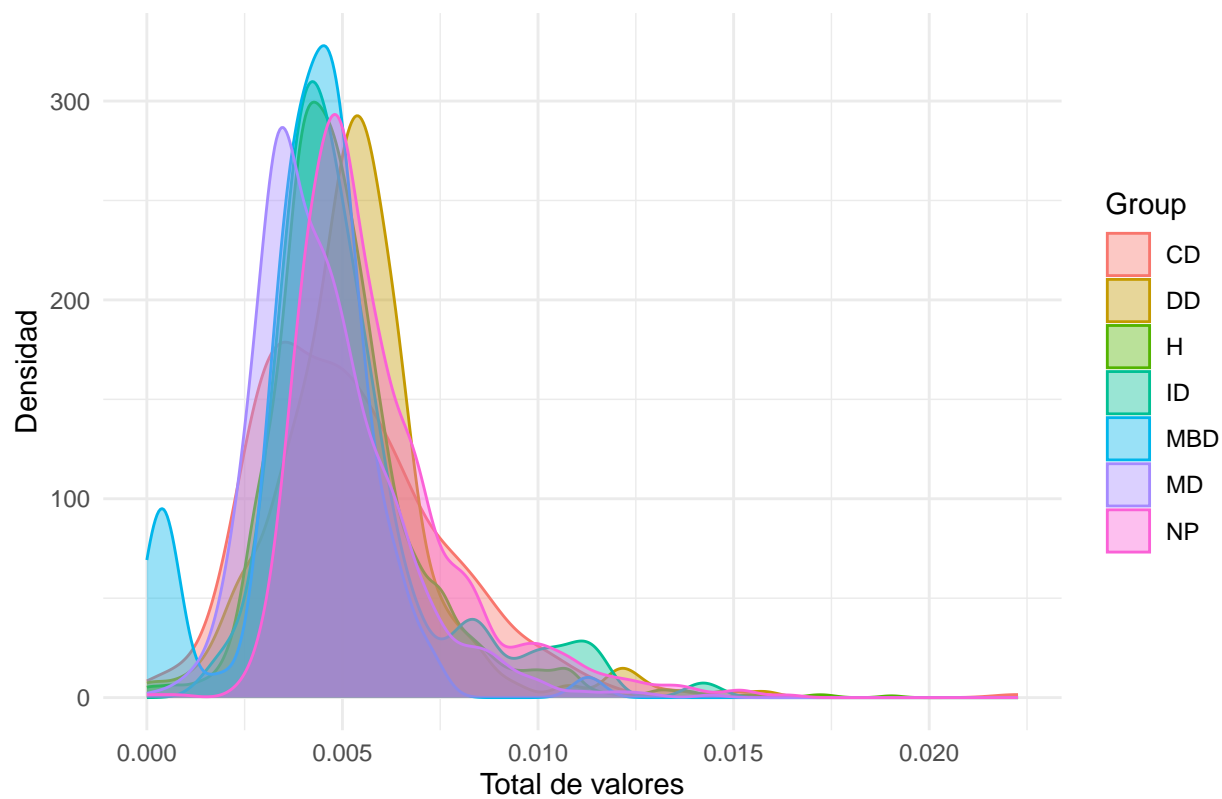
```

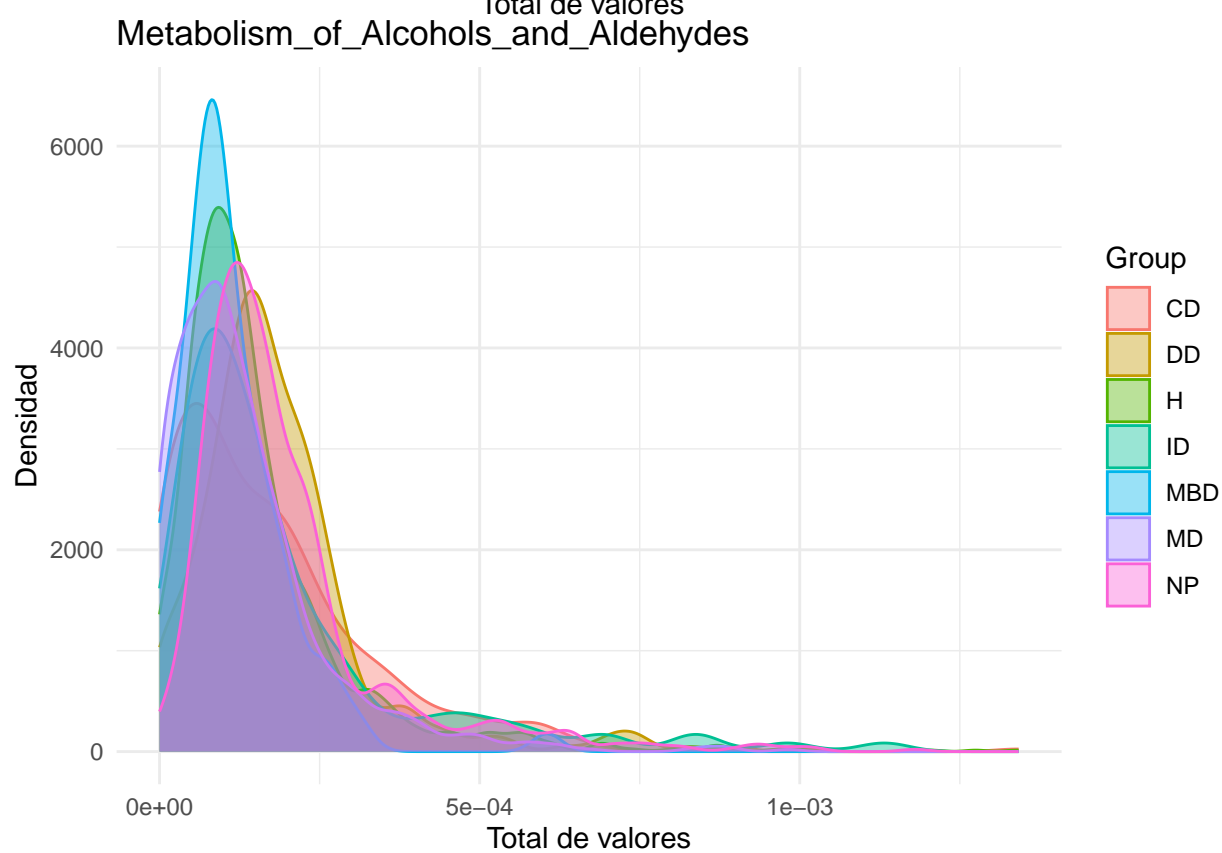
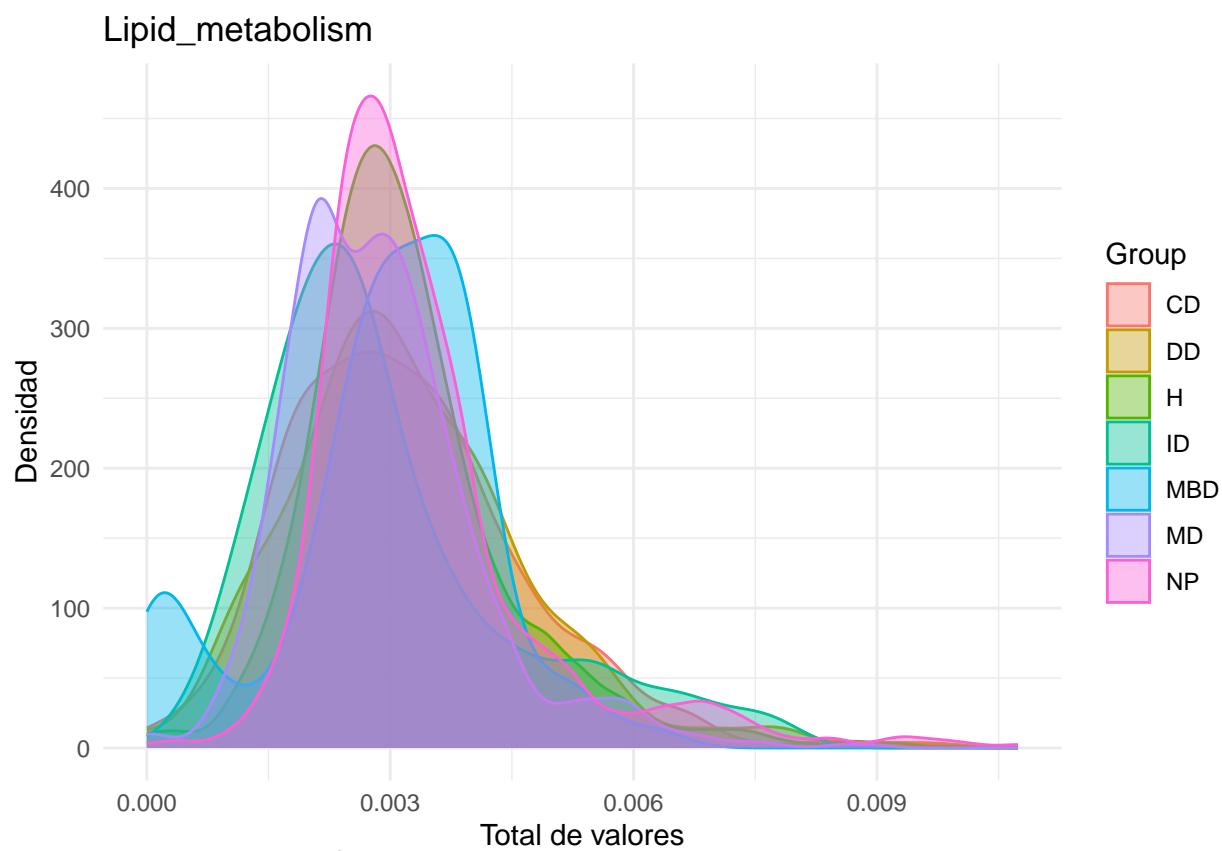


Cellular_Structure_and_Modification_of_Macromolecules

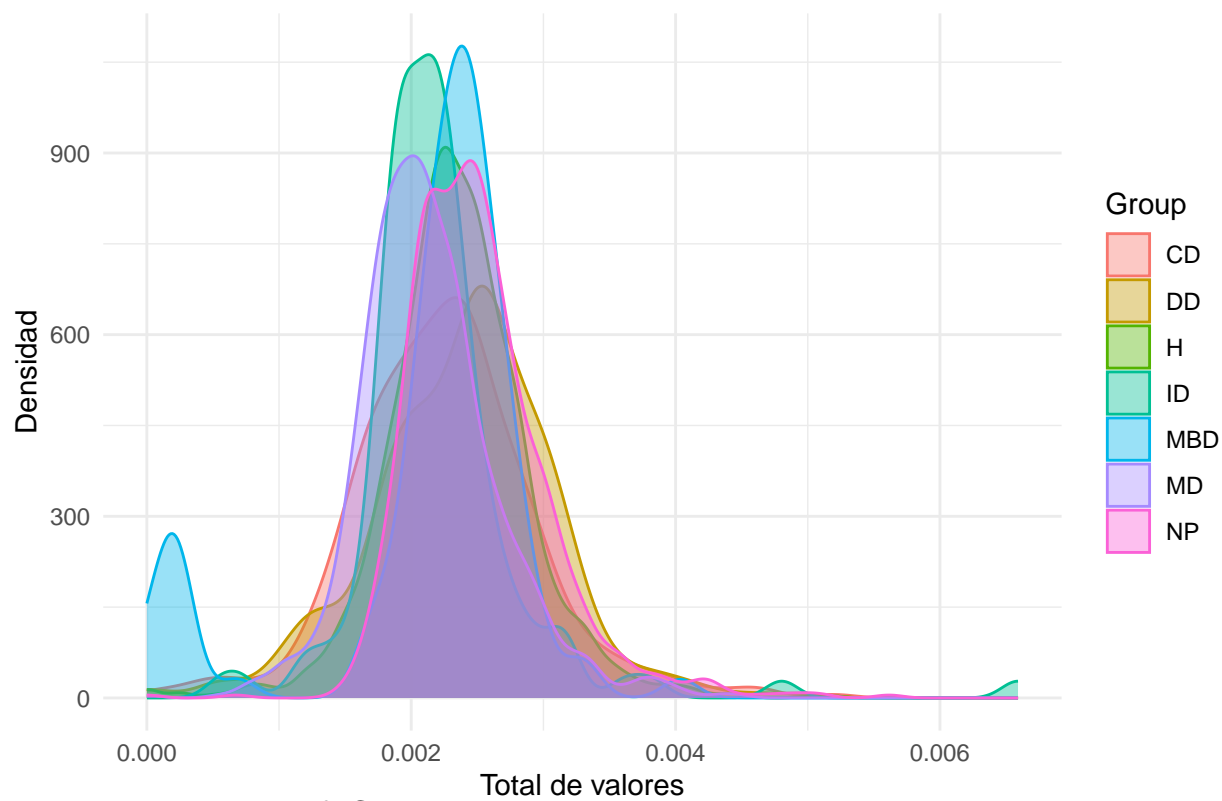


Central_metabolism_and_energy

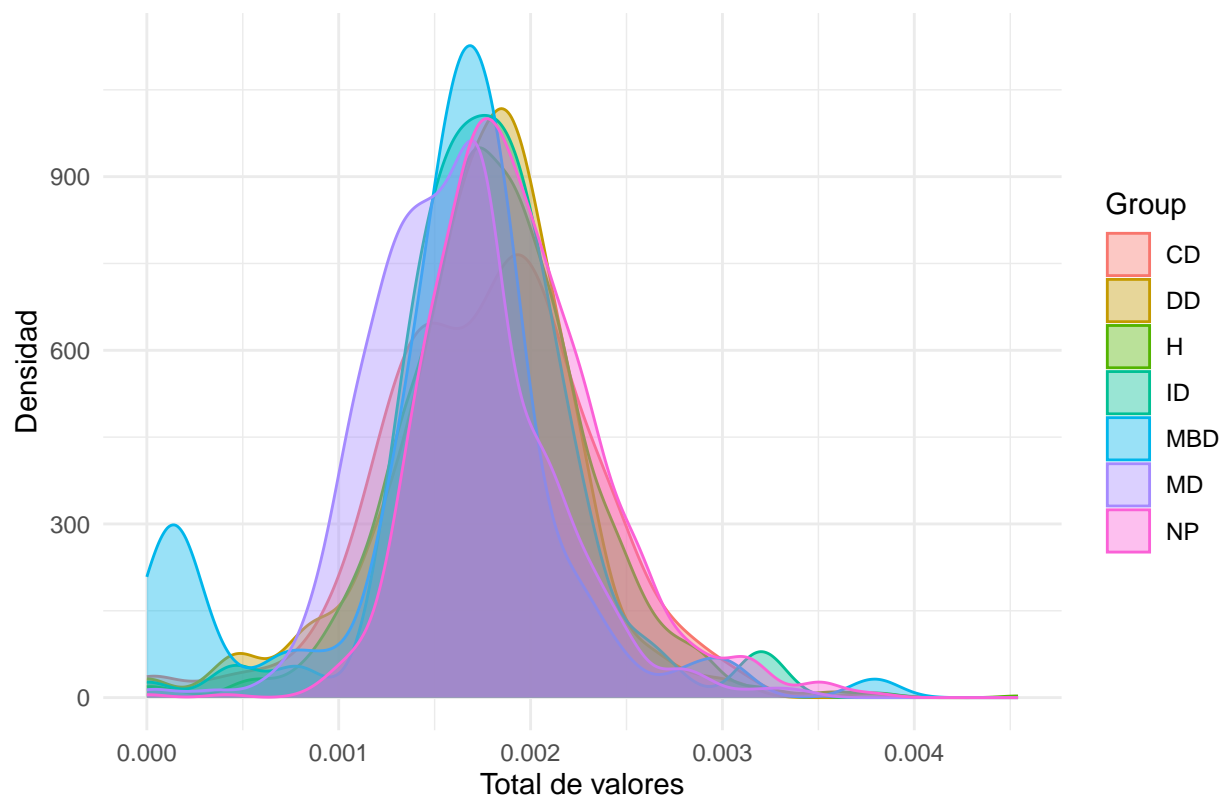


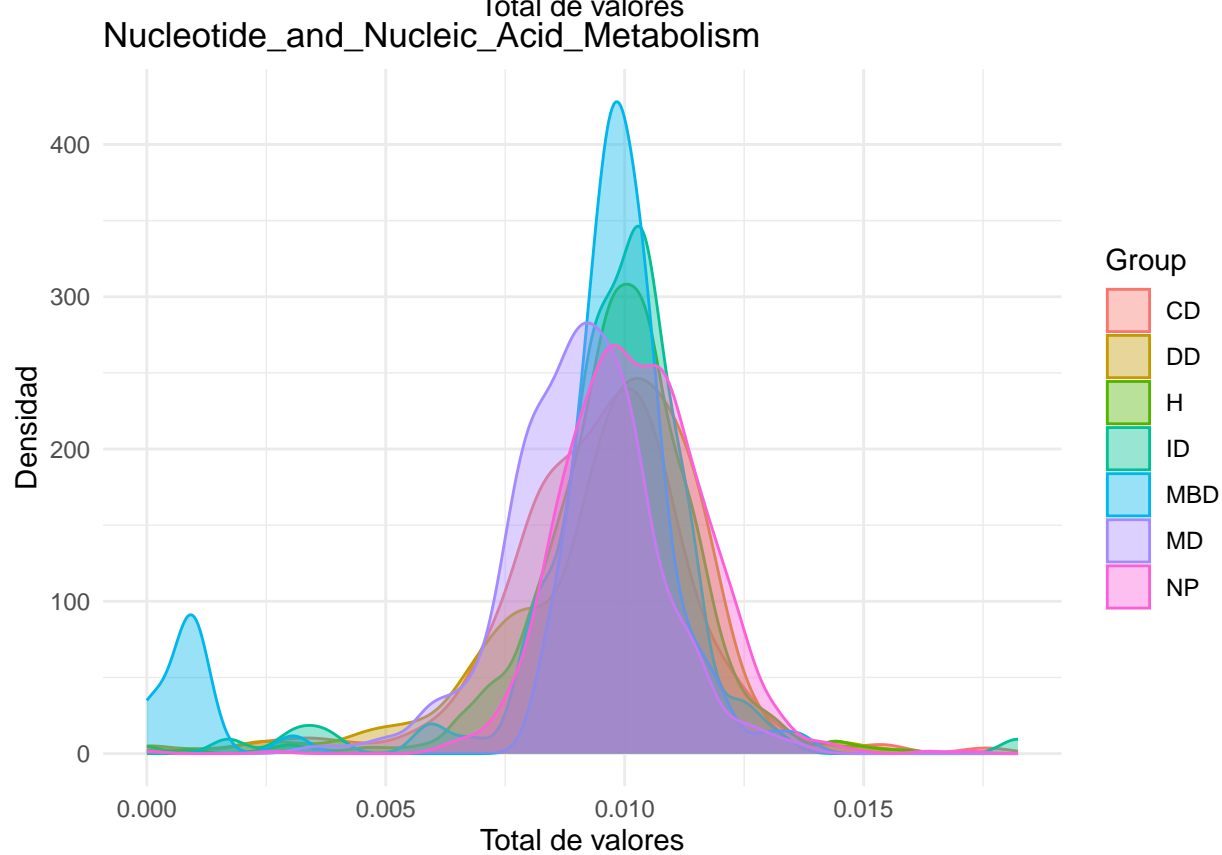
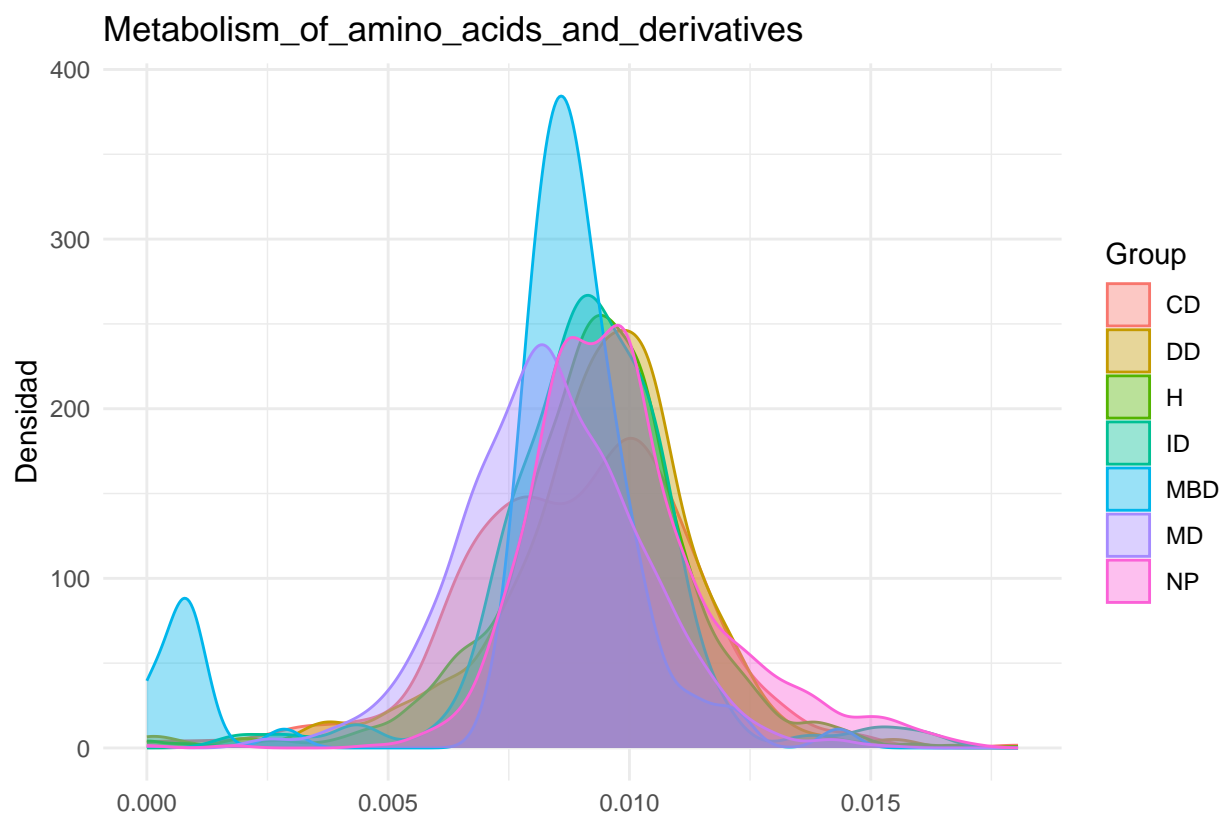


Metabolism_of_Aromatic_Compounds_and_Xenobiotics

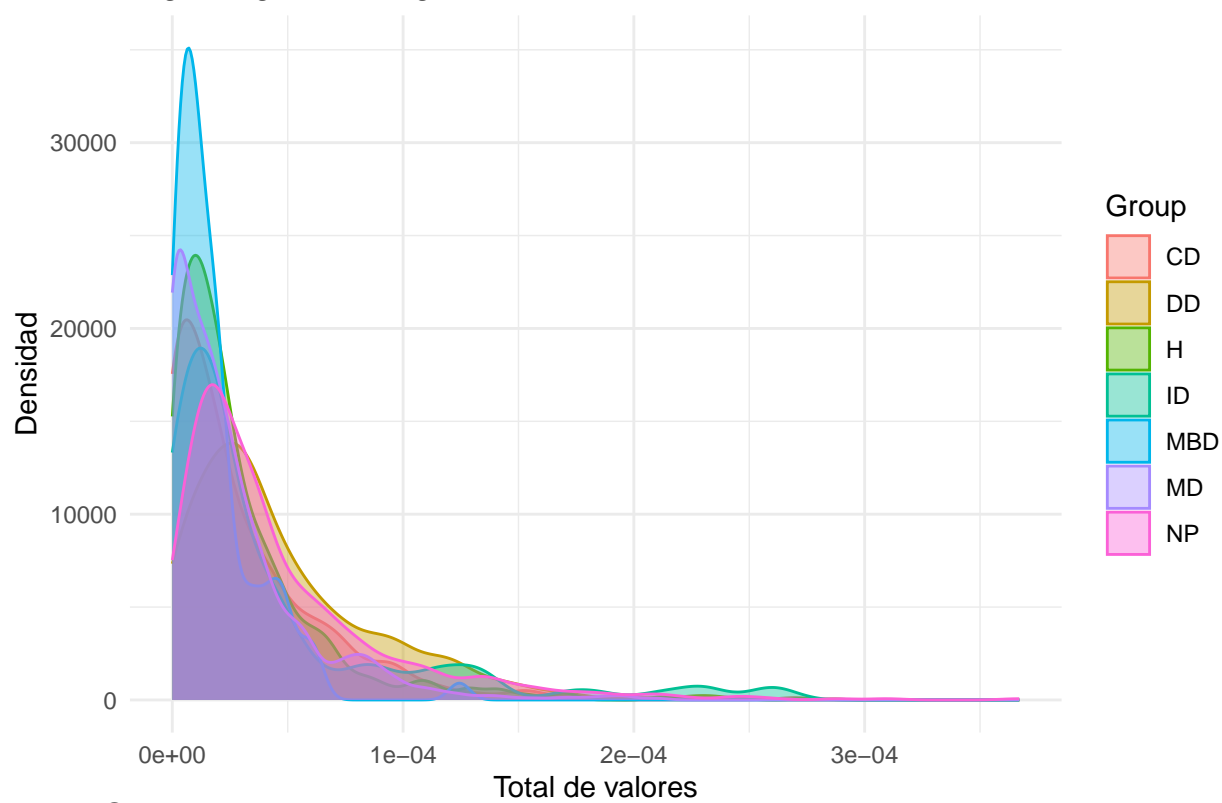


Metabolism_of_Carboxylic_Acids

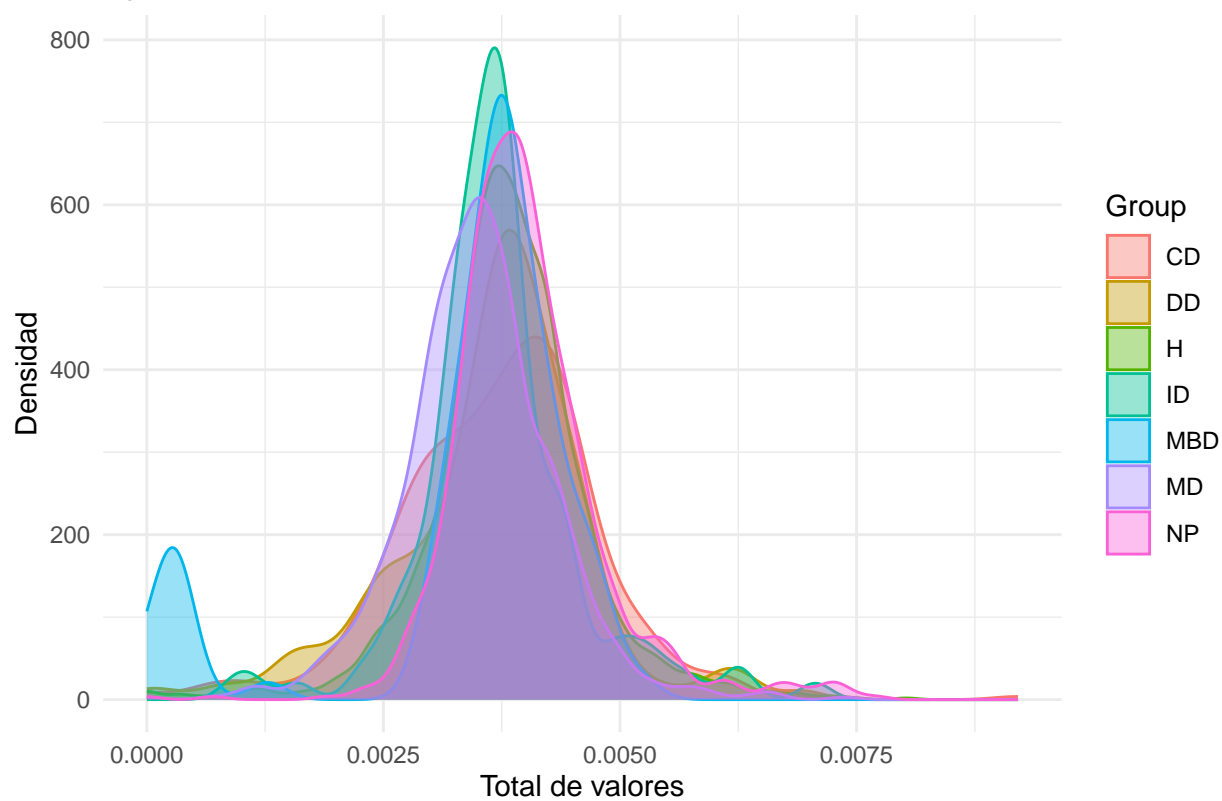




Signaling_and_Regulation_Metabolism



Specialized_and_Miscellaneous_Routes




```

joined_Parental <- long %>%
  regex_left_join(
    type_path %>% select(Object.ID, Parental.Ontology.pathway_type),
    by = c("Object.ID" = "Object.ID") # Coincidencia parcial
  )

# Agrupar y sumar los valores por sample, group y type

joined_Parental$value <- as.numeric(joined_Parental$value)

grouped_Parental <- joined_Parental %>%
  group_by(sample, Group, Parental.Ontology.pathway_type) %>%
  summarise(total = sum(value), .groups = "drop")

# Volver a formato ancho
Path_grouped_P <- grouped_Parental %>%
  pivot_wider(
    names_from = Parental.Ontology.pathway_type,
    values_from = total
  )

# Crear carpeta si no existe
if (!dir.exists("DataSets/CAMDA_2025/densidad_pathways")) {
  dir.create("DataSets/CAMDA_2025/densidad_pathways")
}

write.table(Path_grouped_P, file = "DataSets/CAMDA_2025/Path_agrupados_Parental.txt", sep = "\t", row.names = FALSE)

# Lista de columnas numéricas a graficar
columns_to_plot <- unique(grouped_Parental$Parental.Ontology.pathway_type)

# Loop para crear una gráfica por variable
for (col_name in columns_to_plot) {
  p <- ggplot(Path_grouped_P %>% filter(Group != "delete"),
    aes_string(x = col_name, fill = "Group", color = "Group")) +
    geom_density(alpha = 0.4) +
    labs(
      title = paste (col_name),
      x = "Total de valores",
      y = "Densidad"
    ) +
    theme_minimal()

  ggsave(
    filename = paste0("DataSets/CAMDA_2025/densidad_pathways/", gsub("[^a-zA-Z0-9]", "_", col_name), "P", col_name, ".pdf"),
    plot = p,
    width = 8, height = 5
  )

  print(p)
}

```

