

# Day 2 – 00 Prepare Dataset

## Seminar plotting walk-through

This notebook converts the raw Day 2 file (`second_day_part2/data/dataset1.csv`) into the tidy CSVs used throughout the course:

- `second_day_part2/data/dataset1_subset.csv` / `dataset1_subset_long.csv`: only the two spotlight genomes (Akkermansia + Bacteroides).
- `second_day_part2/data/dataset2_subset.csv` / `dataset2_subset_long.csv`: the same table but with a third genome (Turicimonas) added for the exercises track.

Everything is written with base R so that you can explain each step to beginners. Run it from the repository root:

```
R -e "rmarkdown::render('second_day_part2/data/00_prepare_dataset.Rmd')"
```

### 1. Define input/output paths

```
input_path <- 'dataset1.csv'  
subset_path <- 'dataset1_subset.csv'  
long_path <- 'dataset1_subset_long.csv'  
subset2_path <- 'dataset2_subset.csv'  
long2_path <- 'dataset2_subset_long.csv'  
group_map_path <- 'mouse_group_mapping.csv'
```

### 2. Load the raw CSV and inspect

```
raw_df <- read.csv(  
  input_path,  
  check.names = FALSE,  
  stringsAsFactors = FALSE,  
  fileEncoding = 'UTF-8-BOM'  
)  
  
cat('Rows:', nrow(raw_df), '\nColumns:', ncol(raw_df), '\n')
```

```
## Rows: 71 \nColumns: 69 \n  
colnames(raw_df)
```

```
## [1] "Genome"      "Position"     "Alternative"   "Reference"    "Feature"  
## [6] "1683-0"       "1683-4"       "1683-9"        "1683-14"      "1683-18"  
## [11] "1683-23"      "1683-30"      "1683-37"       "1683-44"      "1683-49"  
## [16] "1683-53"      "1683-58"      "1683-63"       "1683-67"      "1683-72"  
## [21] "1683-79"      "1688-0"       "1688-4"        "1688-9"       "1688-14"  
## [26] "1688-18"      "1688-23"      "1688-30"       "1688-37"      "1688-44"  
## [31] "1688-49"      "1688-53"      "1688-58"       "1688-63"      "1688-67"  
## [36] "1688-72"      "1688-79"      "1692-0"        "1692-4"       "1692-9"  
## [41] "1692-14"      "1692-18"      "1692-23"       "1692-30"      "1692-37"
```

```

## [46] "1692-44"      "1692-49"      "1692-53"      "1692-58"      "1692-63"
## [51] "1692-67"      "1692-72"      "1692-79"      "1699-0"       "1699-4"
## [56] "1699-9"        "1699-14"      "1699-18"      "1699-23"      "1699-30"
## [61] "1699-37"      "1699-44"      "1699-49"      "1699-53"      "1699-58"
## [66] "1699-63"      "1699-67"      "1699-72"      "1699-79"

head(raw_df[, 1:8])

##                                     Genome Position Alternative Reference
## 1 Akkermansia_muciniphila_YL44 239840          C          G
## 2 Akkermansia_muciniphila_YL44 241793          A          G
## 3 Akkermansia_muciniphila_YL44 355328          A          T
## 4 Akkermansia_muciniphila_YL44 356291          C          A
## 5 Akkermansia_muciniphila_YL44 2351445         C          T
## 6 Bacteroides_caecimuris_I48 1601848         T          C
##                                         Feature 1683-0
## 1 autotransporter-associated beta strand repeat-containing protein 0.000000
## 2 autotransporter-associated beta strand repeat-containing protein 0.049587
## 3                                         protein kinase 0.138182
## 4                                         protein kinase 0.000000
## 5 protein phosphatase 2C domain-containing protein 0.000000
## 6 TonB-dependent receptor 0.041609
##   1683-4   1683-9
## 1 0.000000 0.000000
## 2 0.031414 0.076271
## 3 0.132275 0.138211
## 4 0.000000 0.000000
## 5 0.000000 0.000000
## 6 0.000000 0.038251

```

Explain that every row is a SNP call with many sample columns (e.g., 1683-0).

### 3. Helper to build wide + long subsets

```

build_subset <- function(genomes, wide_out, long_out) {
  message('Preparing subset for genomes: ', paste(genomes, collapse = ', '))
  subset_df <- raw_df[raw_df$Genome %in% genomes, , drop = FALSE]
  if (nrow(subset_df) == 0) {
    stop('No rows left after filtering for ', paste(genomes, collapse = ', '))
  }

  subset_df$snp_id <- paste(subset_df$Position,
                            subset_df$Alternative,
                            subset_df$Reference,
                            sep = '-')
}

sample_cols <- setdiff(names(subset_df),
                       c('Genome', 'snp_id', 'Position',
                         'Alternative', 'Reference', 'Feature'))

wide_df <- subset_df[, c('Genome', 'snp_id', 'Position', sample_cols), drop = FALSE]
write.csv(wide_df, wide_out, row.names = FALSE)
message('Saved: ', wide_out)

long_parts <- list()

```

```

for (col in sample_cols) {
  long_parts[[length(long_parts) + 1]] <- data.frame(
    Genome = wide_df$Genome,
    snp_id = wide_df$snp_id,
    Position = wide_df$Position,
    sample = col,
    value = wide_df[[col]],
    stringsAsFactors = FALSE
  )
}

long_df <- do.call(rbind, long_parts)
split_ids <- strsplit(long_df$sample, '-', fixed = TRUE)
long_df$mouse_id <- vapply(split_ids, function(x) x[[1]], character(1))
long_df$day <- as.integer(vapply(split_ids,
                                   function(x) if (length(x) >= 2) x[[2]] else NA_character_,
                                   character(1)))
long_df$sample <- NULL

# Attach treatment group information (if available)
if (file.exists(group_map_path)) {
  group_map <- read.csv(group_map_path, stringsAsFactors = FALSE, check.names = FALSE)
  group_map$Mouse <- as.character(group_map$Mouse)
  group_map$Day <- as.integer(group_map$Day)
  long_df <- merge(
    long_df,
    group_map[, c('Mouse', 'Day', 'Group')],
    by.x = c('mouse_id', 'day'),
    by.y = c('Mouse', 'Day'),
    all.x = TRUE
  )
  names(long_df)[names(long_df) == 'Group'] <- 'treatment_group'
  long_df <- long_df[, c('Genome', 'snp_id', 'Position', 'value', 'mouse_id', 'day', 'treatment_group')]
}

write.csv(long_df, long_out, row.names = FALSE)
message('Saved: ', long_out)

list(wide = wide_df, long = long_df)
}

```

#### 4. Dataset 1 – two spotlight genomes

```

primary_genomes <- c('Akkermansia_muciniphila_YL44', 'Bacteroides_caecimuris_I48')
dataset1 <- build_subset(primary_genomes, subset_path, long_path)

## Preparing subset for genomes: Akkermansia_muciniphila_YL44, Bacteroides_caecimuris_I48
## Saved: dataset1_subset.csv
## Saved: dataset1_subset_long.csv
head(dataset1$wide[, 1:5])

```

	Genome	snp_id	Position	1683-0	1683-4
##					

```

## 1 Akkermansia_muciniphila_YL44 239840-C-G 239840 0.000000 0.000000
## 2 Akkermansia_muciniphila_YL44 241793-A-G 241793 0.049587 0.031414
## 3 Akkermansia_muciniphila_YL44 355328-A-T 355328 0.138182 0.132275
## 4 Akkermansia_muciniphila_YL44 356291-C-A 356291 0.000000 0.000000
## 5 Akkermansia_muciniphila_YL44 2351445-C-T 2351445 0.000000 0.000000
## 6 Bacteroides_caecimuris_I48 1601848-T-C 1601848 0.041609 0.000000

head(dataset1$long)

##                                     Genome     snp_id Position   value mouse_id day
## 1 Akkermansia_muciniphila_YL44 239840-C-G 239840 0.000000 1683  0
## 2 Akkermansia_muciniphila_YL44 241793-A-G 241793 0.049587 1683  0
## 3 Akkermansia_muciniphila_YL44 355328-A-T 355328 0.138182 1683  0
## 4 Akkermansia_muciniphila_YL44 356291-C-A 356291 0.000000 1683  0
## 5 Akkermansia_muciniphila_YL44 2351445-C-T 2351445 0.000000 1683  0
## 6 Bacteroides_caecimuris_I48 1601848-T-C 1601848 0.041609 1683  0

## treatment_group
## 1      Control
## 2      Control
## 3      Control
## 4      Control
## 5      Control
## 6      Control

```

## 5. Dataset 2 – add Turicimonas for exercises

```

extended_genomes <- c('Akkermansia_muciniphila_YL44',
                      'Bacteroides_caecimuris_I48',
                      'Turicimonas_muris_YL45')
dataset2 <- build_subset(extended_genomes, subset2_path, long2_path)

## Preparing subset for genomes: Akkermansia_muciniphila_YL44, Bacteroides_caecimuris_I48, Turicimonas_muris_YL45
## Saved: dataset2_subset.csv
## Saved: dataset2_subset_long.csv

head(dataset2$long)

##                                     Genome     snp_id Position   value mouse_id day
## 1 Akkermansia_muciniphila_YL44 239840-C-G 239840 0.000000 1683  0
## 2 Akkermansia_muciniphila_YL44 241793-A-G 241793 0.049587 1683  0
## 3 Akkermansia_muciniphila_YL44 355328-A-T 355328 0.138182 1683  0
## 4 Akkermansia_muciniphila_YL44 356291-C-A 356291 0.000000 1683  0
## 5 Akkermansia_muciniphila_YL44 2351445-C-T 2351445 0.000000 1683  0
## 6 Bacteroides_caecimuris_I48 1601848-T-C 1601848 0.041609 1683  0

## treatment_group
## 1      Control
## 2      Control
## 3      Control
## 4      Control
## 5      Control
## 6      Control

```

With both CSV sets created, move on to `scripts/01_explore_data.Rmd` for the guided walkthrough, or try the exercises notebook (`scripts/01_explore_data_exercises.Rmd`, with `scripts/01_explore_data_exercises_solution.Rmd`)

as a key) that uses the three-genome dataset, and finally render `scripts/02_simple_heatmap.Rmd` for the visualization.