Draft Quarto document

Clemens Wittenebcher

targets::tar\_config\_set(store = here::here("\_targets"))  
library(tidyverse)

Warning: package 'tidyverse' was built under R version 4.3.2

Warning: package 'ggplot2' was built under R version 4.3.2

Warning: package 'tibble' was built under R version 4.3.2

Warning: package 'tidyr' was built under R version 4.3.2

Warning: package 'readr' was built under R version 4.3.2

Warning: package 'purrr' was built under R version 4.3.2

Warning: package 'dplyr' was built under R version 4.3.2

Warning: package 'stringr' was built under R version 4.3.2

Warning: package 'forcats' was built under R version 4.3.2

Warning: package 'lubridate' was built under R version 4.3.2

── Attaching core tidyverse packages ──────────────────────── tidyverse 2.0.0 ──  
✔ dplyr 1.1.3 ✔ readr 2.1.4  
✔ forcats 1.0.0 ✔ stringr 1.5.0  
✔ ggplot2 3.4.4 ✔ tibble 3.2.1  
✔ lubridate 1.9.3 ✔ tidyr 1.3.0  
✔ purrr 1.0.2   
── Conflicts ────────────────────────────────────────── tidyverse\_conflicts() ──  
✖ dplyr::filter() masks stats::filter()  
✖ dplyr::lag() masks stats::lag()  
ℹ Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to become errors

library(targets)

Warning: package 'targets' was built under R version 4.3.2

library(tidymodels)

Warning: package 'tidymodels' was built under R version 4.3.2

── Attaching packages ────────────────────────────────────── tidymodels 1.1.1 ──  
✔ broom 1.0.5 ✔ rsample 1.2.0  
✔ dials 1.2.0 ✔ tune 1.1.2  
✔ infer 1.0.5 ✔ workflows 1.1.3  
✔ modeldata 1.2.0 ✔ workflowsets 1.0.1  
✔ parsnip 1.1.1 ✔ yardstick 1.2.0  
✔ recipes 1.0.8

Warning: package 'broom' was built under R version 4.3.2

Warning: package 'dials' was built under R version 4.3.2

Warning: package 'scales' was built under R version 4.3.2

Warning: package 'infer' was built under R version 4.3.2

Warning: package 'modeldata' was built under R version 4.3.2

Warning: package 'parsnip' was built under R version 4.3.2

Warning: package 'recipes' was built under R version 4.3.2

Warning: package 'rsample' was built under R version 4.3.2

Warning: package 'tune' was built under R version 4.3.2

Warning: package 'workflows' was built under R version 4.3.2

Warning: package 'workflowsets' was built under R version 4.3.2

Warning: package 'yardstick' was built under R version 4.3.2

── Conflicts ───────────────────────────────────────── tidymodels\_conflicts() ──  
✖ scales::discard() masks purrr::discard()  
✖ dplyr::filter() masks stats::filter()  
✖ recipes::fixed() masks stringr::fixed()  
✖ dplyr::lag() masks stats::lag()  
✖ yardstick::spec() masks readr::spec()  
✖ recipes::step() masks stats::step()  
• Learn how to get started at https://www.tidymodels.org/start/

source(here::here("R/functions.R"))  
lipidomics <- tar\_read(lipidomics)

## Results

## Descriptive statistics table

targets::tar\_read(df\_stats\_by\_metabolite) %>%   
 mutate(MeanSD = glue::glue("{value\_mean} ({value\_sd})")) %>%  
 select(Metabolite = metabolite, `Mean (SD)` = MeanSD) %>%  
 knitr::kable(caption = "Descriptive statistics of the metabolites.")

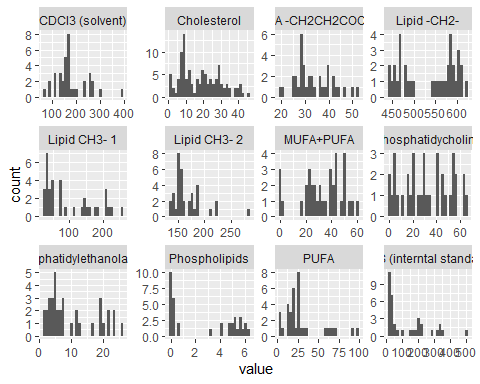
Descriptive statistics of the metabolites.

| Metabolite | Mean (SD) |
| --- | --- |
| CDCl3 (solvent) | 180 (67) |
| Cholesterol | 18.6 (11.4) |
| FA -CH2CH2COO- | 33.6 (7.8) |
| Lipid -CH2- | 536.6 (61.9) |
| Lipid CH3- 1 | 98.3 (73.8) |
| Lipid CH3- 2 | 168.2 (29.2) |
| MUFA+PUFA | 32.9 (16.1) |
| PUFA | 30 (24.1) |
| Phosphatidycholine | 31.7 (20.5) |
| Phosphatidylethanolamine | 10 (7.6) |
| Phospholipids | 2.7 (2.6) |
| TMS (interntal standard) | 123 (130.4) |

## Univariate metabolite distributions

tar\_read(fig\_metabolite\_distribution)

`stat\_bin()` using `bins = 30`. Pick better value with `binwidth`.



## Running multiple models

targets::tar\_read(df\_model\_estimates) %>%  
 dplyr::select(-term) %>%   
 dplyr::arrange(p.value) %>%   
 knitr::kable(caption = "Metabolite outcome associations")

Metabolite outcome associations

| metabolite | estimate | std.error | statistic | p.value |
| --- | --- | --- | --- | --- |
| TMS (interntal standard) | 0.0561975 | 9.898652e-01 | -2.9083580 | 0.0036333 |
| CDCl3 (solvent) | 0.0869604 | 8.649502e-01 | -2.8236342 | 0.0047483 |
| Lipid CH3- 1 | 44.4730379 | 1.406299e+00 | 2.6984901 | 0.0069655 |
| Phosphatidylethanolamine | 26.8810059 | 1.323904e+00 | 2.4861474 | 0.0129134 |
| Cholesterol | 2.9682992 | 4.578064e-01 | 2.3765265 | 0.0174765 |
| PUFA | 3.2688029 | 5.602082e-01 | 2.1142565 | 0.0344934 |
| Lipid -CH2- | 0.0025921 | 3.138898e+00 | -1.8972514 | 0.0577948 |
| MUFA+PUFA | 0.4555963 | 4.487599e-01 | -1.7518235 | 0.0798042 |
| FA -CH2CH2COO- | 1.5241884 | 3.871097e-01 | 1.0887409 | 0.2762682 |
| Lipid CH3- 2 | 0.8848907 | 3.605017e-01 | -0.3392247 | 0.7344405 |
| Phosphatidycholine | 0.0000000 | 1.166281e+05 | -0.0023670 | 0.9981114 |
| Phospholipids | 0.0000000 | 6.896422e+04 | -0.0006217 | 0.9995039 |

### Figure of model estimates

tar\_read(fig\_model\_estimates)

