Draft Quarto document

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## Header 1

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

Warning: package 'tidyverse' was built under R version 4.2.3

Warning: package 'ggplot2' was built under R version 4.2.3

Warning: package 'tibble' was built under R version 4.2.3

Warning: package 'tidyr' was built under R version 4.2.3

Warning: package 'readr' was built under R version 4.2.3

Warning: package 'purrr' was built under R version 4.2.3

Warning: package 'dplyr' was built under R version 4.2.3

Warning: package 'stringr' was built under R version 4.2.3

Warning: package 'forcats' was built under R version 4.2.3

Warning: package 'lubridate' was built under R version 4.2.3

── 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 4.2.3

library(tidymodels)

Warning: package 'tidymodels' was built under R version 4.2.3

── 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 4.2.3

Warning: package 'dials' was built under R version 4.2.3

Warning: package 'scales' was built under R version 4.2.3

Warning: package 'infer' was built under R version 4.2.3

Warning: package 'modeldata' was built under R version 4.2.3

Warning: package 'parsnip' was built under R version 4.2.3

Warning: package 'recipes' was built under R version 4.2.3

Warning: package 'rsample' was built under R version 4.2.3

Warning: package 'tune' was built under R version 4.2.3

Warning: package 'workflows' was built under R version 4.2.3

Warning: package 'workflowsets' was built under R version 4.2.3

Warning: package 'yardstick' was built under R version 4.2.3

── 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()  
• Search for functions across packages at https://www.tidymodels.org/find/

source(here::here("R/functions.R"))  
lipidomics <- tar\_read(lipidomics)  
#| include: false  
# knitr::opts\_chunk$set(echo = TRUE)

#Results

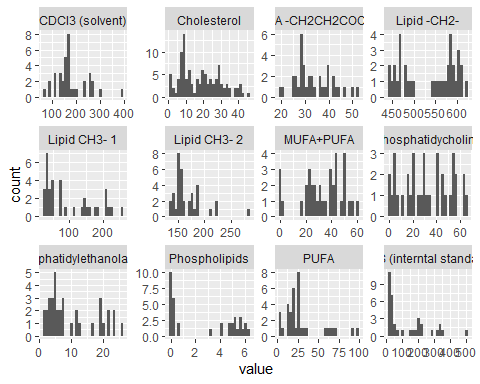
tar\_read(df\_stats\_by\_metabolite) %>%  
 mutate(MeanSD = glue::glue("{value\_mean} (SUM 24  
value\_sd})")) %>%  
 select(Metabolite = metabolite, `Mean SD` = MeanSD) %>%  
 knitr::kable(caption = "Description statistics of the metabolites")

Description statistics of the metabolites

| Metabolite | Mean SD |
| --- | --- |
| CDCl3 (solvent) | 180 (SUM 24 |
| value\_sd}) |  |
| Cholesterol | 18.6 (SUM 24 |
| value\_sd}) |  |
| FA -CH2CH2COO- | 33.6 (SUM 24 |
| value\_sd}) |  |
| Lipid -CH2- | 536.6 (SUM 24 |
| value\_sd}) |  |
| Lipid CH3- 1 | 98.3 (SUM 24 |
| value\_sd}) |  |
| Lipid CH3- 2 | 168.2 (SUM 24 |
| value\_sd}) |  |
| MUFA+PUFA | 32.9 (SUM 24 |
| value\_sd}) |  |
| PUFA | 30 (SUM 24 |
| value\_sd}) |  |
| Phosphatidycholine | 31.7 (SUM 24 |
| value\_sd}) |  |
| Phosphatidylethanolamine | 10 (SUM 24 |
| value\_sd}) |  |
| Phospholipids | 2.7 (SUM 24 |
| value\_sd}) |  |
| TMS (interntal standard) | 123 (SUM 24 |
| value\_sd}) |  |

tar\_read(fig\_metabolite\_distribution)

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



log\_reg\_specs <- logistic\_reg() %>%  
 set\_engine("glm")  
log\_reg\_specs

Logistic Regression Model Specification (classification)  
  
Computational engine: glm

lipidomics %>% column\_values\_to\_snake\_case(metabolite)

# A tibble: 504 × 6  
 code gender age class metabolite value  
 <chr> <chr> <dbl> <chr> <chr> <dbl>  
 1 ERI109 M 25 CT tms\_interntal\_standard 208.   
 2 ERI109 M 25 CT cholesterol 19.8   
 3 ERI109 M 25 CT lipid\_ch\_3\_1 44.1   
 4 ERI109 M 25 CT lipid\_ch\_3\_2 147.   
 5 ERI109 M 25 CT cholesterol 27.2   
 6 ERI109 M 25 CT lipid\_ch\_2 587.   
 7 ERI109 M 25 CT fa\_ch\_2\_ch\_2\_coo 31.6   
 8 ERI109 M 25 CT pufa 29.0   
 9 ERI109 M 25 CT phosphatidylethanolamine 6.78  
10 ERI109 M 25 CT phosphatidycholine 41.7   
# ℹ 494 more rows

lipidomics %>% metabolites\_to\_wider()

# A tibble: 36 × 16  
 code gender age class metabolite\_TMS (interntal …¹ metabolite\_Cholesterol  
 <chr> <chr> <dbl> <chr> <dbl> <dbl>  
 1 ERI109 M 25 CT 208. 18.6   
 2 ERI111 M 39 CT 219. 20.8   
 3 ERI163 W 58 CT 57.1 15.5   
 4 ERI375 M 24 CT 19.2 10.2   
 5 ERI376 M 26 CT 35.4 13.5   
 6 ERI391 M 31 CT 30.4 9.53  
 7 ERI392 M 24 CT 21.7 9.87  
 8 ERI79 W 26 CT 185. 17.6   
 9 ERI81 M 52 CT 207. 17.0   
10 ERI83 M 25 CT 322. 19.7   
# ℹ 26 more rows  
# ℹ abbreviated name: ¹​`metabolite\_TMS (interntal standard)`  
# ℹ 10 more variables: `metabolite\_Lipid CH3- 1` <dbl>,  
# `metabolite\_Lipid CH3- 2` <dbl>, `metabolite\_Lipid -CH2-` <dbl>,  
# `metabolite\_FA -CH2CH2COO-` <dbl>, metabolite\_PUFA <dbl>,  
# metabolite\_Phosphatidylethanolamine <dbl>,  
# metabolite\_Phosphatidycholine <dbl>, metabolite\_Phospholipids <dbl>, …

lipidomics\_wider <- lipidomics %>%  
 column\_values\_to\_snake\_case(metabolite) %>%  
 metabolites\_to\_wider()

recipe(class ~ metabolite\_lipid\_ch\_3\_1 + age + gender,  
 data = lipidomics\_wider  
)

── Recipe ──────────────────────────────────────────────────────────────────────

── Inputs

Number of variables by role

outcome: 1  
predictor: 3

recipe(lipidomics\_wider) %>%  
 update\_role(metabolite\_lipid\_ch\_3\_1, age, gender,  
 new\_role = "predictor"  
 ) %>%  
 update\_role(class, new\_role = "outcome") %>%  
 step\_normalize(starts\_with("metabolite\_"))

── Recipe ──────────────────────────────────────────────────────────────────────

── Inputs

Number of variables by role

outcome: 1  
predictor: 3  
undeclared role: 12

── Operations

• Centering and scaling for: starts\_with("metabolite\_")

recipe\_specs <- lipidomics\_wider %>%  
 create\_recipe\_spec(metabolite\_lipid\_ch\_3\_1)  
recipe\_specs

── Recipe ──────────────────────────────────────────────────────────────────────

── Inputs

Number of variables by role

outcome: 1  
predictor: 3  
undeclared role: 12

── Operations

• Centering and scaling for: tidyselect::starts\_with("metabolite\_")

workflow() %>%  
 add\_model(log\_reg\_specs) %>%  
 add\_recipe(recipe\_specs)

══ Workflow ════════════════════════════════════════════════════════════════════  
Preprocessor: Recipe  
Model: logistic\_reg()  
  
── Preprocessor ────────────────────────────────────────────────────────────────  
1 Recipe Step  
  
• step\_normalize()  
  
── Model ───────────────────────────────────────────────────────────────────────  
Logistic Regression Model Specification (classification)  
  
Computational engine: glm

model\_workflow <- create\_model\_workflow(  
 logistic\_reg() %>%  
 set\_engine("glm"),  
 lipidomics\_wider %>%  
 create\_recipe\_spec(metabolite\_lipid\_ch\_3\_1)  
)  
  
model\_workflow

══ Workflow ════════════════════════════════════════════════════════════════════  
Preprocessor: Recipe  
Model: logistic\_reg()  
  
── Preprocessor ────────────────────────────────────────────────────────────────  
1 Recipe Step  
  
• step\_normalize()  
  
── Model ───────────────────────────────────────────────────────────────────────  
Logistic Regression Model Specification (classification)  
  
Computational engine: glm

fitted\_model <- model\_workflow %>%  
 fit(lipidomics\_wider)  
  
fitted\_model

══ Workflow [trained] ══════════════════════════════════════════════════════════  
Preprocessor: Recipe  
Model: logistic\_reg()  
  
── Preprocessor ────────────────────────────────────────────────────────────────  
1 Recipe Step  
  
• step\_normalize()  
  
── Model ───────────────────────────────────────────────────────────────────────  
  
Call: stats::glm(formula = ..y ~ ., family = stats::binomial, data = data)  
  
Coefficients:  
 (Intercept) genderW age   
 1.93190 0.82191 -0.04312   
metabolite\_lipid\_ch\_3\_1   
 3.79488   
  
Degrees of Freedom: 35 Total (i.e. Null); 32 Residual  
Null Deviance: 49.91   
Residual Deviance: 19.93 AIC: 27.93

fitted\_model %>%  
 extract\_fit\_parsnip() %>%  
 broom::tidy(exponentiate = TRUE)

# A tibble: 4 × 5  
 term estimate std.error statistic p.value  
 <chr> <dbl> <dbl> <dbl> <dbl>  
1 (Intercept) 6.90 2.17 0.891 0.373   
2 genderW 2.27 1.25 0.657 0.511   
3 age 0.958 0.0558 -0.772 0.440   
4 metabolite\_lipid\_ch\_3\_1 44.5 1.41 2.70 0.00697

fitted\_model %>% tidy\_model\_output()

# A tibble: 4 × 5  
 term estimate std.error statistic p.value  
 <chr> <dbl> <dbl> <dbl> <dbl>  
1 (Intercept) 6.90 2.17 0.891 0.373   
2 genderW 2.27 1.25 0.657 0.511   
3 age 0.958 0.0558 -0.772 0.440   
4 metabolite\_lipid\_ch\_3\_1 44.5 1.41 2.70 0.00697

create\_model\_workflow(  
 logistic\_reg() %>%  
 set\_engine("glm"),  
 lipidomics\_wider %>%  
 create\_recipe\_spec(metabolite\_lipid\_ch\_3\_1)  
) %>%  
 fit(lipidomics\_wider) %>%  
 tidy\_model\_output()

# A tibble: 4 × 5  
 term estimate std.error statistic p.value  
 <chr> <dbl> <dbl> <dbl> <dbl>  
1 (Intercept) 6.90 2.17 0.891 0.373   
2 genderW 2.27 1.25 0.657 0.511   
3 age 0.958 0.0558 -0.772 0.440   
4 metabolite\_lipid\_ch\_3\_1 44.5 1.41 2.70 0.00697

##Running multiple models

split\_by\_metabolite(lipidomics)

[[1]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_cd\_cl\_3\_solvent  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 166.  
 2 ERI111 M 39 CT 171.  
 3 ERI163 W 58 CT 262.  
 4 ERI375 M 24 CT 172.  
 5 ERI376 M 26 CT 300.  
 6 ERI391 M 31 CT 241.  
 7 ERI392 M 24 CT 172.  
 8 ERI79 W 26 CT 148.  
 9 ERI81 M 52 CT 168.  
10 ERI83 M 25 CT 253.  
# ℹ 26 more rows  
  
[[2]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_cholesterol  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 18.6   
 2 ERI111 M 39 CT 20.8   
 3 ERI163 W 58 CT 15.5   
 4 ERI375 M 24 CT 10.2   
 5 ERI376 M 26 CT 13.5   
 6 ERI391 M 31 CT 9.53  
 7 ERI392 M 24 CT 9.87  
 8 ERI79 W 26 CT 17.6   
 9 ERI81 M 52 CT 17.0   
10 ERI83 M 25 CT 19.7   
# ℹ 26 more rows  
  
[[3]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_fa\_ch\_2\_ch\_2\_coo  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 31.6  
 2 ERI111 M 39 CT 28.9  
 3 ERI163 W 58 CT 36.6  
 4 ERI375 M 24 CT 39.4  
 5 ERI376 M 26 CT 52.1  
 6 ERI391 M 31 CT 42.8  
 7 ERI392 M 24 CT 39.9  
 8 ERI79 W 26 CT 32.7  
 9 ERI81 M 52 CT 28.4  
10 ERI83 M 25 CT 26.5  
# ℹ 26 more rows  
  
[[4]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_lipid\_ch\_2  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 587.  
 2 ERI111 M 39 CT 585.  
 3 ERI163 W 58 CT 558.  
 4 ERI375 M 24 CT 606.  
 5 ERI376 M 26 CT 554.  
 6 ERI391 M 31 CT 597.  
 7 ERI392 M 24 CT 607.  
 8 ERI79 W 26 CT 546.  
 9 ERI81 M 52 CT 593.  
10 ERI83 M 25 CT 606.  
# ℹ 26 more rows  
  
[[5]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_lipid\_ch\_3\_1  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 44.1  
 2 ERI111 M 39 CT 28.1  
 3 ERI163 W 58 CT 75.1  
 4 ERI375 M 24 CT 22.0  
 5 ERI376 M 26 CT 29.5  
 6 ERI391 M 31 CT 38.0  
 7 ERI392 M 24 CT 34.8  
 8 ERI79 W 26 CT 109.   
 9 ERI81 M 52 CT 49.6  
10 ERI83 M 25 CT 29.9  
# ℹ 26 more rows  
  
[[6]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_lipid\_ch\_3\_2  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 147.  
 2 ERI111 M 39 CT 153.  
 3 ERI163 W 58 CT 144.  
 4 ERI375 M 24 CT 220.  
 5 ERI376 M 26 CT 282.  
 6 ERI391 M 31 CT 220.  
 7 ERI392 M 24 CT 215.  
 8 ERI79 W 26 CT 153.  
 9 ERI81 M 52 CT 150.  
10 ERI83 M 25 CT 153.  
# ℹ 26 more rows  
  
[[7]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_mufa\_pufa  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 50.6   
 2 ERI111 M 39 CT 53.2   
 3 ERI163 W 58 CT 60.7   
 4 ERI375 M 24 CT 0.532  
 5 ERI376 M 26 CT 1.15   
 6 ERI391 M 31 CT 0.602  
 7 ERI392 M 24 CT 0.422  
 8 ERI79 W 26 CT 36.3   
 9 ERI81 M 52 CT 40.1   
10 ERI83 M 25 CT 39.3   
# ℹ 26 more rows  
  
[[8]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_phosphatidycholine  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 41.7  
 2 ERI111 M 39 CT 52.9  
 3 ERI163 W 58 CT 35.3  
 4 ERI375 M 24 CT 66.9  
 5 ERI376 M 26 CT 32.7  
 6 ERI391 M 31 CT 62.9  
 7 ERI392 M 24 CT 64.3  
 8 ERI79 W 26 CT 41.0  
 9 ERI81 M 52 CT 56.1  
10 ERI83 M 25 CT 57.8  
# ℹ 26 more rows  
  
[[9]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_phosphatidylethanolamine  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 6.78  
 2 ERI111 M 39 CT 3.66  
 3 ERI163 W 58 CT 3.59  
 4 ERI375 M 24 CT 3.59  
 5 ERI376 M 26 CT 2.33  
 6 ERI391 M 31 CT 1.46  
 7 ERI392 M 24 CT 2.00  
 8 ERI79 W 26 CT 4.93  
 9 ERI81 M 52 CT 5.20  
10 ERI83 M 25 CT 5.01  
# ℹ 26 more rows  
  
[[10]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_phospholipids  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 5.58  
 2 ERI111 M 39 CT 6.16  
 3 ERI163 W 58 CT 5.19  
 4 ERI375 M 24 CT 4.20  
 5 ERI376 M 26 CT 3.27  
 6 ERI391 M 31 CT 4.71  
 7 ERI392 M 24 CT 4.14  
 8 ERI79 W 26 CT 5.70  
 9 ERI81 M 52 CT 5.46  
10 ERI83 M 25 CT 4.89  
# ℹ 26 more rows  
  
[[11]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_pufa  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 29.0   
 2 ERI111 M 39 CT 27.4   
 3 ERI163 W 58 CT 35.5   
 4 ERI375 M 24 CT 6.92  
 5 ERI376 M 26 CT 3.22  
 6 ERI391 M 31 CT 3.43  
 7 ERI392 M 24 CT 3.52  
 8 ERI79 W 26 CT 18.7   
 9 ERI81 M 52 CT 20.7   
10 ERI83 M 25 CT 18.2   
# ℹ 26 more rows  
  
[[12]]  
# A tibble: 36 × 5  
 code gender age class metabolite\_tms\_interntal\_standard  
 <chr> <chr> <dbl> <chr> <dbl>  
 1 ERI109 M 25 CT 208.   
 2 ERI111 M 39 CT 219.   
 3 ERI163 W 58 CT 57.1  
 4 ERI375 M 24 CT 19.2  
 5 ERI376 M 26 CT 35.4  
 6 ERI391 M 31 CT 30.4  
 7 ERI392 M 24 CT 21.7  
 8 ERI79 W 26 CT 185.   
 9 ERI81 M 52 CT 207.   
10 ERI83 M 25 CT 322.   
# ℹ 26 more rows

model\_estimates <- lipidomics %>%  
 split\_by\_metabolite() %>%  
 map(generate\_model\_results) %>%  
 list\_rbind() %>%   
 filter(str\_detect(term, "metabolite\_"))

Warning: glm.fit: algorithm did not converge

Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred  
  
Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

model\_estimates

# A tibble: 12 × 5  
 term estimate std.error statistic p.value  
 <chr> <dbl> <dbl> <dbl> <dbl>  
 1 metabolite\_cd\_cl\_3\_solvent 8.70e- 2 0.865 -2.82 0.00475  
 2 metabolite\_cholesterol 2.97e+ 0 0.458 2.38 0.0175   
 3 metabolite\_fa\_ch\_2\_ch\_2\_coo 1.52e+ 0 0.387 1.09 0.276   
 4 metabolite\_lipid\_ch\_2 2.59e- 3 3.14 -1.90 0.0578   
 5 metabolite\_lipid\_ch\_3\_1 4.45e+ 1 1.41 2.70 0.00697  
 6 metabolite\_lipid\_ch\_3\_2 8.85e- 1 0.361 -0.339 0.734   
 7 metabolite\_mufa\_pufa 4.56e- 1 0.449 -1.75 0.0798   
 8 metabolite\_phosphatidycholine 1.28e-120 116628. -0.00237 0.998   
 9 metabolite\_phosphatidylethanolamine 2.69e+ 1 1.32 2.49 0.0129   
10 metabolite\_phospholipids 2.39e- 19 68964. -0.000622 1.00   
11 metabolite\_pufa 3.27e+ 0 0.560 2.11 0.0345   
12 metabolite\_tms\_interntal\_standard 5.62e- 2 0.990 -2.91 0.00363

model\_estimates= lipidomics %>%  
 mutate(term = metabolite) %>%  
 column\_values\_to\_snake\_case(term) %>%  
 mutate(term = str\_c("metabolite\_", term)) %>%  
 distinct(term, metabolite) %>%  
 right\_join(model\_estimates, by = "term")  
model\_estimates

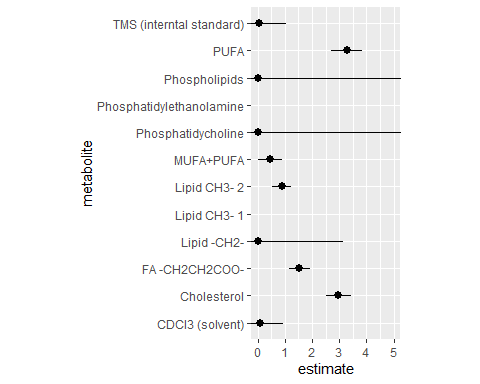
# A tibble: 12 × 6  
 term metabolite estimate std.error statistic p.value  
 <chr> <chr> <dbl> <dbl> <dbl> <dbl>  
 1 metabolite\_tms\_interntal\_st… TMS (inte… 5.62e- 2 9.90e-1 -2.91 0.00363  
 2 metabolite\_cholesterol Cholester… 2.97e+ 0 4.58e-1 2.38 0.0175   
 3 metabolite\_lipid\_ch\_3\_1 Lipid CH3… 4.45e+ 1 1.41e+0 2.70 0.00697  
 4 metabolite\_lipid\_ch\_3\_2 Lipid CH3… 8.85e- 1 3.61e-1 -0.339 0.734   
 5 metabolite\_lipid\_ch\_2 Lipid -CH… 2.59e- 3 3.14e+0 -1.90 0.0578   
 6 metabolite\_fa\_ch\_2\_ch\_2\_coo FA -CH2CH… 1.52e+ 0 3.87e-1 1.09 0.276   
 7 metabolite\_pufa PUFA 3.27e+ 0 5.60e-1 2.11 0.0345   
 8 metabolite\_phosphatidyletha… Phosphati… 2.69e+ 1 1.32e+0 2.49 0.0129   
 9 metabolite\_phosphatidycholi… Phosphati… 1.28e-120 1.17e+5 -0.00237 0.998   
10 metabolite\_phospholipids Phospholi… 2.39e- 19 6.90e+4 -0.000622 1.00   
11 metabolite\_mufa\_pufa MUFA+PUFA 4.56e- 1 4.49e-1 -1.75 0.0798   
12 metabolite\_cd\_cl\_3\_solvent CDCl3 (so… 8.70e- 2 8.65e-1 -2.82 0.00475

### Figure of model estimates

model\_estimates <- tar\_read(df\_model\_estimates)  
model\_estimates

# A tibble: 12 × 6  
 term metabolite estimate std.error statistic p.value  
 <chr> <chr> <dbl> <dbl> <dbl> <dbl>  
 1 metabolite\_tms\_interntal\_st… TMS (inte… 5.62e- 2 9.90e-1 -2.91 0.00363  
 2 metabolite\_cholesterol Cholester… 2.97e+ 0 4.58e-1 2.38 0.0175   
 3 metabolite\_lipid\_ch\_3\_1 Lipid CH3… 4.45e+ 1 1.41e+0 2.70 0.00697  
 4 metabolite\_lipid\_ch\_3\_2 Lipid CH3… 8.85e- 1 3.61e-1 -0.339 0.734   
 5 metabolite\_lipid\_ch\_2 Lipid -CH… 2.59e- 3 3.14e+0 -1.90 0.0578   
 6 metabolite\_fa\_ch\_2\_ch\_2\_coo FA -CH2CH… 1.52e+ 0 3.87e-1 1.09 0.276   
 7 metabolite\_pufa PUFA 3.27e+ 0 5.60e-1 2.11 0.0345   
 8 metabolite\_phosphatidyletha… Phosphati… 2.69e+ 1 1.32e+0 2.49 0.0129   
 9 metabolite\_phosphatidycholi… Phosphati… 1.28e-120 1.17e+5 -0.00237 0.998   
10 metabolite\_phospholipids Phospholi… 2.39e- 19 6.90e+4 -0.000622 1.00   
11 metabolite\_mufa\_pufa MUFA+PUFA 4.56e- 1 4.49e-1 -1.75 0.0798   
12 metabolite\_cd\_cl\_3\_solvent CDCl3 (so… 8.70e- 2 8.65e-1 -2.82 0.00475

plot\_estimates(model\_estimates)



tar\_read(fig\_model\_estimates)

