Figure1A_metabolomicsFedStarve

MOD

2023-08-09

```
### This part is important ####
starved <- readxl::read_xlsx('datasets/cest-1.2_MOGL_levels_starvation.xlsx') %>%
  select(1:6, contains("adult")) %>%
  pivot_longer(cols = contains("adult"), names_to = 'stage', values_to = 'AUC') %>%
  separate(stage, into = c("condition", "replicate"), sep = "adult...") %>%
  mutate(condition = case_when(
    condition == "starved" ~ "starved",
    TRUE ~ "fed"
  )) %>%
  mutate(anomeric_carbon = factor(case_when(
    str_detect(SMID, regex("^i\\glu", ignore_case=TRUE)) ~ "indole",
    str_detect(SMID, regex("tyglu", ignore_case=TRUE)) ~ "tyramine",
    str_detect(SMID, regex("angl#", ignore_case=TRUE)) ~ "anthranilate",
    str_detect(SMID, regex("bzglu", ignore_case=TRUE)) ~ "benzoic_acid",
    str_detect(SMID, regex("pyglu", ignore_case=TRUE)) ~ "pyrrolic_acid",
    str_detect(SMID, regex("mgglu", ignore_case=TRUE)) ~ "methyl_guanine",
    str_detect(SMID, regex("nglu", ignore_case=TRUE)) ~ "nicotinic_acid",
    str_detect(SMID, regex("oglu", ignore_case=TRUE)) ~ "octopamine",
    str_detect(SMID, regex("higlu", ignore_case=TRUE)) ~ "hydroxyindole",
    str_detect(SMID, regex("maglu", ignore_case=TRUE)) ~ "methyl_adenine",
    str_detect(SMID, regex("pyglu", ignore_case=TRUE)) ~ "pyrrolic_acid",
    str_detect(SMID, regex("tiglu", ignore_case=TRUE)) ~ "tiglic_acid"
  )),
  pathway = case_when(
    acylation1_2C %in% c("tiglic_acid",
                         "pyrrolic_acid",
                         "isovaleric_acid",
                         "propionic_acid",
                         "nicotinic_acid") ~ "AminoAcidCatabolism",
    TRUE ~ "other"
  ),
  nAcyl = case_when(
    cest_dep == "cest-1.2" & acylation2_6C != "none" ~ 2,
    cest_dep == "cest-1.2" & acylation1_2C != "none" & acylation2_6C == "none" ~ 1
  ))

### get an average, ratio and difference for each SMID in starved vs. fed #####
sumStarved <- starved %>% group_by(SMID, attachements, acylation1_2C, condition, cest_dep, anomeric_carb
  summarize(AUC = mean(AUC)) %>%
  pivot_wider(names_from = condition, values_from = AUC) %>%
  mutate(avg = (starved + fed) / 2,
         ratio = starved/fed,
```

```
         diff = starved - fed)

sumStarved <- sumStarved %>%
  filter(anomeric_carbon %in% c("tyramine", "indole", "octopamine","nicotinic_acid", "benzoic_acid", "ar
  mutate(anomeric_carbon = fct_relevel(anomeric_carbon, c("tyramine", "indole", "octopamine", "nicotini

#create a ranking for color schem based on the number of positive/negative ratios in the starved:fed av

CountPos <- sumStarved %>%
      filter(
        avg > 0.001,
        #cest_dep == "cest-1.2",
         !is.na(SMID),
         !is.na(acylation1_2C),
         !is.na(anomeric_carbon)) %>%
  mutate(change = case_when(
    ratio > 1 ~ "positive",
    ratio < 1 ~ "negative"
  )) %>%
  group_by(anomeric_carbon, change) %>%
  tally() %>%
  pivot_wider(names_from = change, values_from = n) %>%
  mutate(negOverPos = negative/positive) %>%
  mutate(negOverPos = case_when(
    is.na(negOverPos) ~ 1,
    TRUE ~ negOverPos
  )) %>%
  filter(anomeric_carbon %in% c("tyramine", "indole", "octopamine","nicotinic_acid", "benzoic_acid", "ar
  mutate(anomeric_carbon = fct_relevel(anomeric_carbon, c("tyramine", "indole", "octopamine", "nicotini
  pull(anomeric_carbon)

#get a colormap using viridis palette and the number of MOGL class types
# colors <- scales::viridis_pal(direction = -1)(6)
colors <- RColorBrewer::brewer.pal(length(unique(levels(CountPos))), "Paired")
#colors <- RColorBrewer::brewer.pal(6, "Set1")
colors <- colors[c(3,4,7,8,9,10)]
```

I created an object called “sumStarved”, it’s a tibble. I will now make a plot with it.

```
SMIDs_to_analyze <- sumStarved %>%
  pull(SMID)

SMID_data <- starved %>%
  filter(SMID %in% SMIDs_to_analyze) %>%
  full_join(., select(sumStarved, fed, avg, ratio)) %>%
  mutate(relAUC = AUC / fed,
         diffAUC = AUC - fed) %>%
    filter(avg > 0.001,
         cest_dep == "cest-1.2",
         condition == "starved",
         !is.na(SMID),
         !is.na(acylation1_2C),
         !is.na(anomeric_carbon),
```

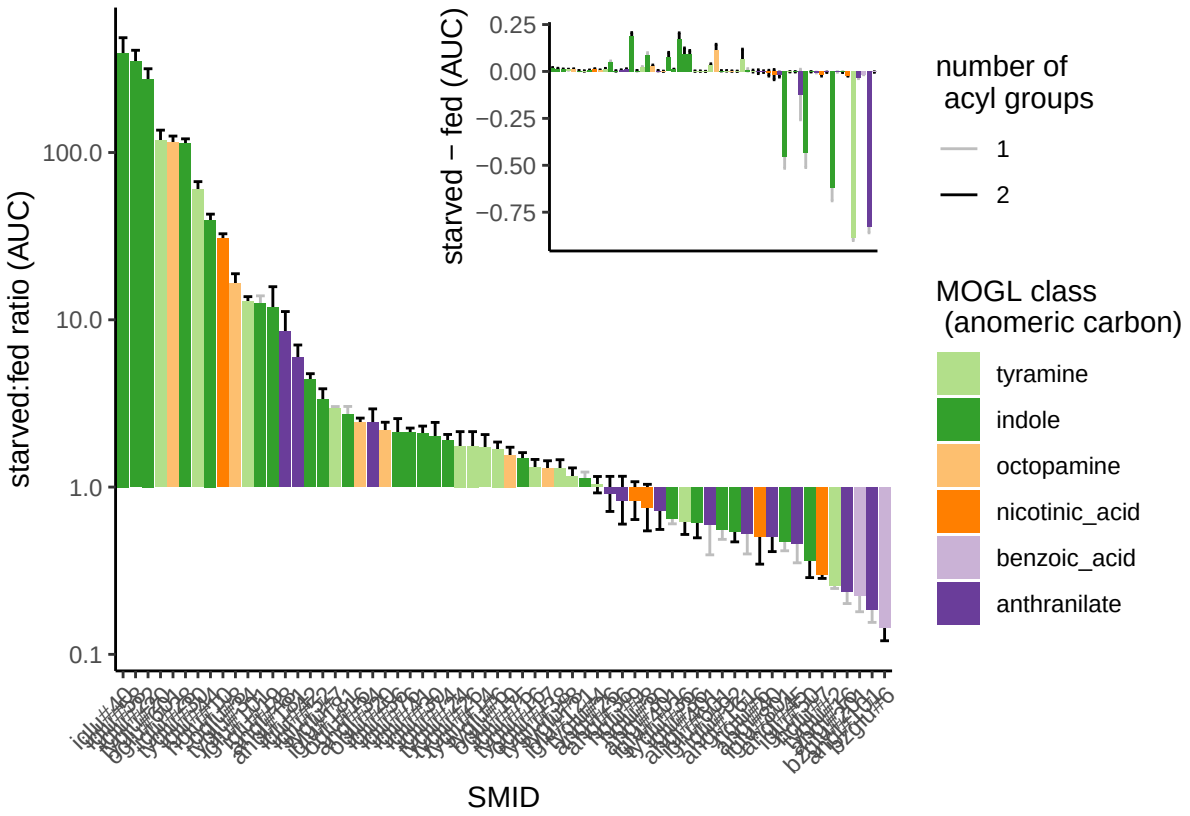
```
         !(SMID == "oglu#8" &
             attachements == "octopamine pyrrolic acid (x2)")
             ) %>%
  mutate(SMID = fct_reorder(SMID, log(relAUC), .fun = mean, .desc = TRUE))

plot_ratio <- SMID_data %>%
  ggplot(aes(x = SMID, y = relAUC)) +
  stat_summary(geom = "errorbar", fun.data = "mean_se", width = 0.7, aes(color = factor(nAcyl))) +
  stat_summary(geom = "bar", fun = "mean", aes(fill = anomeric_carbon)) +
  scale_y_log10() +
  scale_fill_manual(values = colors, breaks = levels(CountPos)) +
  scale_alpha_manual(values = c(0.75,1)) +
  scale_color_manual(values = c("grey", "black")) +
  guides(fill = guide_legend(title = "MOGL class \n (anomeric carbon)"),
         color = guide_legend(title = "number of \n acyl groups")) +
  theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
  labs(y = "starved:fed ratio (AUC)")

plot_diff <- SMID_data %>%
  ggplot(aes(x = SMID, y = diffAUC)) +
  stat_summary(geom = "errorbar", fun.data = "mean_se", width = 0.5, aes(color = factor(nAcyl))) +
  stat_summary(geom = "bar", fun = "mean", aes(fill = anomeric_carbon)) +
  #scale_y_log10() +
  scale_fill_manual(values = colors, breaks = levels(CountPos)) +
  scale_alpha_manual(values = c(0.75,1)) +
  scale_color_manual(values = c("grey", "black")) +
  guides(fill = guide_legend(title = "MOGL class")) +
  theme(axis.text.x =  element_blank(),
        axis.title.x = element_blank(),
        axis.ticks.x = element_blank()) +
  guides(fill = "none",
         color = "none") +
  labs(y = "starved - fed (AUC)")

inset_plot <- plot_ratio +
  inset_element(plot_diff, left = 0.4, bottom = 0.6, right = 1, top = 1)

inset_plot
```




```
plot_nAcyl1 <- SMID_data %>%
  mutate(relAUC = case_when(
    nAcyl == 1 ~ relAUC,
    TRUE ~ NA)) %>%
  ggplot(aes(x = SMID, y = relAUC)) +
  stat_summary(geom = "errorbar", fun.data = "mean_se", width = 0.5) +
  stat_summary(geom = "bar", fun = "mean", aes(fill = anomeric_carbon)) +
  #geom_bar(stat="identity", aes(fill = anomeric_carbon)) +
  scale_y_log10() +
  scale_fill_manual(values = colors, breaks = levels(CountPos)) +
  guides(fill = guide_legend(title = "MOGL class")) +
  theme(axis.text.x = element_text(angle = 45, hjust = 1))

plot_nAcyl2 <- SMID_data %>%
  mutate(relAUC = case_when(
    nAcyl == 2 ~ relAUC,
    TRUE ~ NA)) %>%
  ggplot(aes(x = SMID, y = relAUC)) +
  stat_summary(geom = "errorbar", fun.data = "mean_se", width = 0.5) +
  stat_summary(geom = "bar", fun = "mean", aes(fill = anomeric_carbon)) +
  #geom_bar(stat="identity", aes(fill = anomeric_carbon)) +
  scale_y_log10() +
  scale_fill_manual(values = colors, breaks = levels(CountPos)) +
  guides(fill = guide_legend(title = "MOGL class")) +
  theme(axis.text.x = element_text(angle = 45, hjust = 1))

    SMID_data %>%
  lm(formula = log(relAUC) ~ 0 + SMID ) %>%
```

```
  emmeans::ref_grid() %>%
  emmeans::contrast()
```

```
##  contrast         estimate    SE  df t.ratio p.value
##  iglu#40 effect     5.0977 0.179 124  28.475  <.0001
##  iglu#58 effect     4.9856 0.179 124  27.849  <.0001
##  iglu#22 effect     4.7402 0.179 124  26.478  <.0001
##  tyglu#20 effect    3.8943 0.179 124  21.753  <.0001
##  oglu#601 effect    3.8633 0.179 124  21.580  <.0001
##  iglu#28 effect     3.8481 0.179 124  21.495  <.0001
##  tyglu#30 effect    3.2169 0.179 124  17.969  <.0001
##  iglu#44 effect     2.7992 0.179 124  15.636  <.0001
##  nglu#10 effect     2.5495 0.179 124  14.241  <.0001
##  oglu#8 effect      1.9276 0.179 124  10.767  <.0001
##  tyglu#34 effect    1.6720 0.179 124   9.340  <.0001
##  iglu#101 effect    1.6490 0.179 124   9.211  <.0001
##  iglu#19 effect     1.5911 0.179 124   8.887  <.0001
##  angl#48 effect     1.2677 0.179 124   7.081  <.0001
##  angl#181 effect    0.9024 0.179 124   5.041  <.0001
##  iglu#42 effect     0.6001 0.179 124   3.352  0.0015
##  iglu#52 effect     0.3339 0.179 124   1.865  0.0816
##  tyglu#7 effect     0.2027 0.179 124   1.132  0.2982
##  iglu#181 effect    0.1263 0.179 124   0.705  0.5065
##  oglu#16 effect     0.0156 0.179 124   0.087  0.9383
##  angl#34 effect     0.0139 0.179 124   0.078  0.9383
##  oglu#20 effect    -0.0979 0.179 124  -0.547  0.6050
##  iglu#56 effect    -0.1291 0.179 124  -0.721  0.5046
##  iglu#76 effect    -0.1302 0.179 124  -0.727  0.5046
##  iglu#41 effect    -0.1422 0.179 124  -0.794  0.4745
##  iglu#30 effect    -0.1789 0.179 124  -0.999  0.3604
##  iglu#74 effect    -0.2337 0.179 124  -1.305  0.2271
##  tyglu#24 effect   -0.3110 0.179 124  -1.737  0.1012
##  tyglu#26 effect   -0.3110 0.179 124  -1.737  0.1012
##  tyglu#14 effect   -0.3260 0.179 124  -1.821  0.0881
##  tyglu#6 effect    -0.3533 0.179 124  -1.973  0.0654
##  oglu#10 effect    -0.4349 0.179 124  -2.429  0.0219
##  iglu#75 effect    -0.4838 0.179 124  -2.703  0.0106
##  tyglu#16 effect   -0.6105 0.179 124  -3.410  0.0012
##  oglu#17 effect    -0.6244 0.179 124  -3.488  0.0010
##  tyglu#38 effect   -0.6245 0.179 124  -3.488  0.0010
##  tyglu#8 effect    -0.7293 0.179 124  -4.074  0.0001
##  iglu#121 effect   -0.7578 0.179 124  -4.233  0.0001
##  tyglu#4 effect    -0.8436 0.179 124  -4.713  <.0001
##  angl#26 effect    -0.9707 0.179 124  -5.422  <.0001
##  angl#36 effect    -1.0571 0.179 124  -5.905  <.0001
##  nglu#9 effect     -1.0630 0.179 124  -5.938  <.0001
##  nglu#8 effect     -1.1590 0.179 124  -6.474  <.0001
##  angl#30 effect    -1.1938 0.179 124  -6.668  <.0001
##  iglu#401 effect   -1.3133 0.179 124  -7.336  <.0001
##  tyglu#36 effect   -1.3552 0.179 124  -7.570  <.0001
##  iglu#36 effect    -1.3628 0.179 124  -7.612  <.0001
##  angl#401 effect   -1.3996 0.179 124  -7.818  <.0001
##  iglu#601 effect   -1.4617 0.179 124  -8.165  <.0001
```

```
##  iglu#92 effect    -1.4842 0.179 124  -8.291  <.0001
##  angl#161 effect   -1.5114 0.179 124  -8.443  <.0001
##  nglu#6 effect     -1.5528 0.179 124  -8.674  <.0001
##  angl#40 effect    -1.5559 0.179 124  -8.691  <.0001
##  iglu#801 effect   -1.6320 0.179 124  -9.116  <.0001
##  angl#45 effect    -1.6606 0.179 124  -9.276  <.0001
##  iglu#50 effect    -1.8869 0.179 124 -10.540  <.0001
##  nglu#7 effect     -2.0775 0.179 124 -11.605  <.0001
##  tyglu#2 effect    -2.2294 0.179 124 -12.453  <.0001
##  angl#16 effect    -2.3168 0.179 124 -12.941  <.0001
##  bzglu#201 effect  -2.3655 0.179 124 -13.213  <.0001
##  angl#101 effect   -2.5610 0.179 124 -14.305  <.0001
##  bzglu#6 effect    -2.8050 0.179 124 -15.668  <.0001
##
## Results are given on the log (not the response) scale.
## P value adjustment: fdr method for 62 tests
```

```
  # )) %>%
  # ggplot(aes(x = SMID, y = relAUC)) +
  # stat_summary(geom = "errorbar", fun.data = "mean_se", width = 0.5) +
  # stat_summary(geom = "bar", fun = "mean", aes(fill = anomeric_carbon)) +
  # #geom_bar(stat="identity", aes(fill = anomeric_carbon)) +
  # scale_y_log10() +
  # scale_fill_manual(values = colors, breaks = levels(CountPos)) +
  # guides(fill = guide_legend(title = "MOGL class")) +
  # theme(axis.text.x = element_text(angle = 45, hjust = 1))
```

Now I'm going to use the relative paths in this directory to make a new folder with this example figure and example data in it, using the name of an object we entered in the header code chunk:

```
# SMID_data <- starved %>%
#   filter(SMID %in% SMIDs_to_analyze) %>%
#   full_join(., select(sumStarved, fed))

SMID_data %>%
  mutate(SMID = fct_relevel(SMID, "tyglu#4")) %>%
  lm(formula = log(relAUC) ~ SMID) %>%
  emmeans::emmeans("SMID", adjust = "fdr")
```

```
##  SMID      emmean   SE  df lower.CL upper.CL
##  tyglu#4    0.033 0.18 124  -0.5869   0.6530
##  iglu#40    5.974 0.18 124   5.3545   6.5944
##  iglu#58    5.862 0.18 124   5.2424   6.4823
##  iglu#22    5.617 0.18 124   4.9970   6.2369
##  tyglu#20   4.771 0.18 124   4.1510   5.3909
##  oglu#601   4.740 0.18 124   4.1200   5.3600
##  iglu#28    4.725 0.18 124   4.1048   5.3448
##  tyglu#30   4.094 0.18 124   3.4736   4.7136
##  iglu#44    3.676 0.18 124   3.0559   4.2959
##  nglu#10    3.426 0.18 124   2.8063   4.0462
##  oglu#8     2.804 0.18 124   2.1843   3.4243
##  tyglu#34   2.549 0.18 124   1.9288   3.1687
##  iglu#101   2.526 0.18 124   1.9057   3.1457
```

```
##  iglu#19    2.468 0.18 124   1.8478   3.0877
##  angl#48    2.144 0.18 124   1.5244   2.7643
##  angl#181   1.779 0.18 124   1.1591   2.3991
##  iglu#42    1.477 0.18 124   0.8568   2.0968
##  iglu#52    1.211 0.18 124   0.5907   1.8306
##  tyglu#7    1.079 0.18 124   0.4594   1.6994
##  iglu#181   1.003 0.18 124   0.3830   1.6229
##  oglu#16    0.892 0.18 124   0.2723   1.5123
##  angl#34    0.891 0.18 124   0.2706   1.5106
##  oglu#20    0.779 0.18 124   0.1588   1.3988
##  iglu#56    0.748 0.18 124   0.1276   1.3675
##  iglu#76    0.747 0.18 124   0.1265   1.3665
##  iglu#41    0.735 0.18 124   0.1145   1.3545
##  iglu#30    0.698 0.18 124   0.0779   1.3178
##  iglu#74    0.643 0.18 124   0.0230   1.2630
##  tyglu#24   0.566 0.18 124  -0.0543   1.1857
##  tyglu#26   0.566 0.18 124  -0.0543   1.1857
##  tyglu#14   0.551 0.18 124  -0.0693   1.1707
##  tyglu#6    0.523 0.18 124  -0.0966   1.1434
##  oglu#10    0.442 0.18 124  -0.1782   1.0618
##  iglu#75    0.393 0.18 124  -0.2271   1.0128
##  tyglu#16   0.266 0.18 124  -0.3537   0.8862
##  oglu#17    0.252 0.18 124  -0.3676   0.8723
##  tyglu#38   0.252 0.18 124  -0.3678   0.8721
##  tyglu#8    0.147 0.18 124  -0.4726   0.7673
##  iglu#121   0.119 0.18 124  -0.5011   0.7388
##  angl#26   -0.094 0.18 124  -0.7140   0.5259
##  angl#36   -0.180 0.18 124  -0.8004   0.4395
##  nglu#9    -0.186 0.18 124  -0.8063   0.4337
##  nglu#8    -0.282 0.18 124  -0.9022   0.3377
##  angl#30   -0.317 0.18 124  -0.9371   0.3029
##  iglu#401  -0.437 0.18 124  -1.0566   0.1834
##  tyglu#36  -0.479 0.18 124  -1.0985   0.1414
##  iglu#36   -0.486 0.18 124  -1.1060   0.1339
##  angl#401  -0.523 0.18 124  -1.1429   0.0970
##  iglu#601  -0.585 0.18 124  -1.2050   0.0350
##  iglu#92   -0.608 0.18 124  -1.2275   0.0124
##  angl#161  -0.635 0.18 124  -1.2547  -0.0148
##  nglu#6    -0.676 0.18 124  -1.2961  -0.0561
##  angl#40   -0.679 0.18 124  -1.2992  -0.0593
##  iglu#801  -0.755 0.18 124  -1.3753  -0.1353
##  angl#45   -0.784 0.18 124  -1.4038  -0.1639
##  iglu#50   -1.010 0.18 124  -1.6301  -0.3902
##  nglu#7    -1.201 0.18 124  -1.8208  -0.5808
##  tyglu#2   -1.353 0.18 124  -1.9727  -0.7327
##  angl#16   -1.440 0.18 124  -2.0600  -0.8201
##  bzglu#201 -1.489 0.18 124  -2.1087  -0.8688
##  angl#101  -1.684 0.18 124  -2.3042  -1.0643
##  bzglu#6   -1.928 0.18 124  -2.5483  -1.3083
##
## Results are given on the log (not the response) scale.
## Confidence level used: 0.95
## Conf-level adjustment: bonferroni method for 62 estimates
```

```
SMID_data %>%
  lm(formula = diffAUC ~ 0 + SMID + SMID) %>%
  emmeans::emmeans("SMID")
```

```
##  SMID         emmean     SE  df lower.CL upper.CL
##  iglu#40    0.017169 0.0263 124 -0.03485   0.0692
##  iglu#58    0.014967 0.0263 124 -0.03705   0.0670
##  iglu#22    0.011691 0.0263 124 -0.04032   0.0637
##  tyglu#20   0.010503 0.0263 124 -0.04151   0.0625
##  oglu#601   0.012705 0.0263 124 -0.03931   0.0647
##  iglu#28    0.004691 0.0263 124 -0.04732   0.0567
##  tyglu#30   0.002496 0.0263 124 -0.04952   0.0545
##  iglu#44    0.006819 0.0263 124 -0.04519   0.0588
##  nglu#10    0.013217 0.0263 124 -0.03880   0.0652
##  oglu#8     0.007144 0.0263 124 -0.04487   0.0592
##  tyglu#34   0.015232 0.0263 124 -0.03678   0.0672
##  iglu#101   0.050486 0.0263 124 -0.00153   0.1025
##  iglu#19    0.002789 0.0263 124 -0.04923   0.0548
##  angl#48    0.006936 0.0263 124 -0.04508   0.0590
##  angl#181   0.012172 0.0263 124 -0.03984   0.0642
##  iglu#42    0.187638 0.0263 124  0.13562   0.2397
##  iglu#52    0.004631 0.0263 124 -0.04738   0.0566
##  tyglu#7    0.024574 0.0263 124 -0.02744   0.0766
##  iglu#181   0.085363 0.0263 124  0.03335   0.1374
##  oglu#16    0.031333 0.0263 124 -0.02068   0.0833
##  angl#34    0.004270 0.0263 124 -0.04774   0.0563
##  oglu#20    0.001190 0.0263 124 -0.05082   0.0532
##  iglu#56    0.074407 0.0263 124  0.02239   0.1264
##  iglu#76    0.010923 0.0263 124 -0.04109   0.0629
##  iglu#41    0.172641 0.0263 124  0.12063   0.2247
##  iglu#30    0.094023 0.0263 124  0.04201   0.1460
##  iglu#74    0.095166 0.0263 124  0.04315   0.1472
##  tyglu#24   0.001701 0.0263 124 -0.05031   0.0537
##  tyglu#26   0.001701 0.0263 124 -0.05031   0.0537
##  tyglu#14   0.000651 0.0263 124 -0.05136   0.0527
##  tyglu#6    0.033382 0.0263 124 -0.01863   0.0854
##  oglu#10    0.113011 0.0263 124  0.06100   0.1650
##  iglu#75    0.003564 0.0263 124 -0.04845   0.0556
##  tyglu#16   0.003359 0.0263 124 -0.04866   0.0554
##  oglu#17    0.001860 0.0263 124 -0.05015   0.0539
##  tyglu#38   0.001090 0.0263 124 -0.05092   0.0531
##  tyglu#8    0.068489 0.0263 124  0.01647   0.1205
##  iglu#121   0.008540 0.0263 124 -0.04347   0.0606
##  tyglu#4    0.002029 0.0263 124 -0.04999   0.0540
##  angl#26   -0.001285 0.0263 124 -0.05330   0.0507
##  angl#36   -0.000893 0.0263 124 -0.05291   0.0511
##  nglu#9    -0.009272 0.0263 124 -0.06129   0.0427
##  nglu#8    -0.016900 0.0263 124 -0.06891   0.0351
##  angl#30   -0.016777 0.0263 124 -0.06879   0.0352
##  iglu#401  -0.456307 0.0263 124 -0.50832  -0.4043
##  tyglu#36  -0.001694 0.0263 124 -0.05371   0.0503
##  iglu#36   -0.001773 0.0263 124 -0.05379   0.0502
##  angl#401  -0.122898 0.0263 124 -0.17491  -0.0709
```

```
##  iglu#601  -0.431598 0.0263 124 -0.48361  -0.3796
##  iglu#92   -0.001831 0.0263 124 -0.05384   0.0502
##  angl#161  -0.005557 0.0263 124 -0.05757   0.0465
##  nglu#6    -0.017542 0.0263 124 -0.06956   0.0345
##  angl#40   -0.004157 0.0263 124 -0.05617   0.0479
##  iglu#801  -0.622177 0.0263 124 -0.67419  -0.5702
##  angl#45   -0.002842 0.0263 124 -0.05486   0.0492
##  iglu#50   -0.004932 0.0263 124 -0.05695   0.0471
##  nglu#7    -0.023741 0.0263 124 -0.07576   0.0283
##  tyglu#2   -0.887645 0.0263 124 -0.93966  -0.8356
##  angl#16   -0.036299 0.0263 124 -0.08831   0.0157
##  bzglu#201 -0.016324 0.0263 124 -0.06834   0.0357
##  angl#101  -0.826692 0.0263 124 -0.87871  -0.7747
##  bzglu#6   -0.003043 0.0263 124 -0.05506   0.0490
##
## Confidence level used: 0.95
```

```
# logistic regression on anomeric carbon either positive or negative based on starved:fed ratio
SMID_data %>%
  group_by(SMID, anomeric_carbon) %>%
  summarize(meanRatio = mean(relAUC)) %>%
  mutate(StarvedEffect = case_when(
    meanRatio > 1 ~ "Pos",
    meanRatio < 1 ~ "Neg"
  )) %>%
  group_by(anomeric_carbon, StarvedEffect) %>%
  tally() %>%
  pivot_wider(names_from = StarvedEffect, values_from = n) %>%
  glm(formula = cbind(Neg, Pos) ~ 0 + anomeric_carbon, family = "binomial") %>%
  summary()
```

```
## `summarise()` has grouped output by 'SMID'. You can override using the
## `.groups` argument.
```

```
##
## Call:
## glm(formula = cbind(Neg, Pos) ~ 0 + anomeric_carbon, family = "binomial",
##     data = .)
##
## Coefficients:
##                               Estimate Std. Error z value Pr(>|z|)
## anomeric_carbonanthranilate     1.0986     0.6667   1.648   0.0994 .
## anomeric_carbonindole          -1.0415     0.4749  -2.193   0.0283 *
## anomeric_carbonnicotinic_acid   1.3863     1.1180   1.240   0.2150
## anomeric_carbontyramine        -1.7918     0.7638  -2.346   0.0190 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance:  1.8474e+01  on 4  degrees of freedom
## Residual deviance: -4.4409e-16  on 0  degrees of freedom
##   (2 observations deleted due to missingness)
```

```
## AIC: 18.313
##
## Number of Fisher Scoring iterations: 4
```

```
### make a folder
fs::dir_create('../figures/',Figure_name)

## save the plot
ggsave(inset_plot,
       file = file.path('figures',
                 Figure_name,
                 paste0(Figure_name,'.pdf')),
       width = 12,
          height = 8)

## save the formatted edited tibble:
write_csv(sumStarved,
          file = file.path('figures',
                 Figure_name,
                 paste0(Figure_name,'.csv')))
```

figures/Figure1A/Figure1A.png