

R Notebook

```
library(dplyr)
```

```
##
## Attachement du package : 'dplyr'
## Les objets suivants sont masqués depuis 'package:stats':
##
##     filter, lag
## Les objets suivants sont masqués depuis 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
library(ggplot2)
```

```
DATA_ATP <- read.table("../Results/In_vitro/ATP_assay.csv", sep = "\t", col.names = c("Cell_line", "IDH", "Treatment", "Technique_replicat", "Biological_replicat", "Value"))
DATA_ATP$pheno <- paste(DATA_ATP$Cell_line, DATA_ATP$IDH, DATA_ATP$Treatment, DATA_ATP$Biological_replicat, DATA_ATP$Technique_replicat, DATA_ATP$Value)
Pulled_values <- sapply(unique(DATA_ATP$pheno), function(Pheno){
  tmp <- dplyr::filter(DATA_ATP, pheno == Pheno)
  mean(tmp[, "Value"])
})
Data_ATP_pulled <- DATA_ATP[DATA_ATP$Technique_replicat == 1, 1:5]
Data_ATP_pulled$Value <- Pulled_values
Data_ATP_pulled
```

	Cell_line	IDH	Treatment	Technique_replicat	Biological_replicat	Value
## 1	Molm13	WT	Combo	1	1	12319.667
## 4	Molm13	WT	Combo	1	2	5882.333
## 7	Molm13	WT	Combo	1	3	3994.667
## 10	Molm13	WT	FCCP	1	1	118661.667
## 13	Molm13	WT	FCCP	1	2	58662.000
## 16	Molm13	WT	FCCP	1	3	85467.000
## 19	Molm13	WT	Iodo	1	1	63011.667
## 22	Molm13	WT	Iodo	1	2	62746.333
## 25	Molm13	WT	Iodo	1	3	60636.667
## 28	Molm13	WT	OAA	1	1	91691.667
## 31	Molm13	WT	OAA	1	2	49346.333
## 34	Molm13	WT	OAA	1	3	83027.000
## 37	Molm13	WT	PBS	1	1	97746.000
## 40	Molm13	WT	PBS	1	2	100176.667
## 43	Molm13	WT	PBS	1	3	97891.000
## 46	K562	WT	Combo	1	1	22243.333
## 49	K562	WT	Combo	1	2	14499.333
## 52	K562	WT	Combo	1	3	11895.000
## 55	K562	WT	FCCP	1	1	224518.667
## 58	K562	WT	FCCP	1	2	251838.667
## 61	K562	WT	FCCP	1	3	141061.667
## 64	K562	WT	Iodo	1	1	143159.000
## 67	K562	WT	Iodo	1	2	126328.333

## 70	K562	WT	Iodo	1	3	73226.000
## 73	K562	WT	OAA	1	1	210353.667
## 76	K562	WT	OAA	1	2	241354.667
## 79	K562	WT	OAA	1	3	133493.333
## 82	K562	WT	PBS	1	1	204825.000
## 85	K562	WT	PBS	1	2	246443.000
## 88	K562	WT	PBS	1	3	141967.333
## 91	Molm13	IDH2	Combo	1	1	8428.333
## 94	Molm13	IDH2	Combo	1	2	5050.333
## 97	Molm13	IDH2	Combo	1	3	4881.667
## 100	Molm13	IDH2	FCCP	1	1	78454.667
## 103	Molm13	IDH2	FCCP	1	2	43391.333
## 106	Molm13	IDH2	FCCP	1	3	63466.000
## 109	Molm13	IDH2	Iodo	1	1	47639.667
## 112	Molm13	IDH2	Iodo	1	2	26885.000
## 115	Molm13	IDH2	Iodo	1	3	36107.000
## 118	Molm13	IDH2	OAA	1	1	71103.333
## 121	Molm13	IDH2	OAA	1	2	47409.667
## 124	Molm13	IDH2	OAA	1	3	67276.333
## 127	Molm13	IDH2	PBS	1	1	71178.333
## 130	Molm13	IDH2	PBS	1	2	51138.000
## 133	Molm13	IDH2	PBS	1	3	68965.667
## 136	K562	IDH2	Combo	1	1	24796.333
## 139	K562	IDH2	Combo	1	2	12528.667
## 142	K562	IDH2	Combo	1	3	11246.333
## 145	K562	IDH2	FCCP	1	1	217582.000
## 148	K562	IDH2	FCCP	1	2	158869.667
## 151	K562	IDH2	FCCP	1	3	169776.333
## 154	K562	IDH2	Iodo	1	1	160410.667
## 157	K562	IDH2	Iodo	1	2	87930.333
## 160	K562	IDH2	Iodo	1	3	96893.333
## 163	K562	IDH2	OAA	1	1	197636.000
## 166	K562	IDH2	OAA	1	2	150241.333
## 169	K562	IDH2	OAA	1	3	168278.000
## 172	K562	IDH2	PBS	1	1	203939.333
## 175	K562	IDH2	PBS	1	2	147892.000
## 178	K562	IDH2	PBS	1	3	181513.667
## 181	Molm13	IDH1	Combo	1	1	7491.667
## 184	Molm13	IDH1	Combo	1	2	2563.333
## 187	Molm13	IDH1	Combo	1	3	2582.667
## 190	Molm13	IDH1	FCCP	1	1	83305.000
## 193	Molm13	IDH1	FCCP	1	2	34561.333
## 196	Molm13	IDH1	FCCP	1	3	49968.667
## 199	Molm13	IDH1	Iodo	1	1	40887.000
## 202	Molm13	IDH1	Iodo	1	2	19807.667
## 205	Molm13	IDH1	Iodo	1	3	25821.333
## 208	Molm13	IDH1	OAA	1	1	59987.333
## 211	Molm13	IDH1	OAA	1	2	38880.333
## 214	Molm13	IDH1	OAA	1	3	44710.000
## 217	Molm13	IDH1	PBS	1	1	70143.667
## 220	Molm13	IDH1	PBS	1	2	55835.667
## 223	Molm13	IDH1	PBS	1	3	58646.000
## 226	K562	IDH1	Combo	1	1	25821.667
## 229	K562	IDH1	Combo	1	2	12467.333

## 232	K562	IDH1	Combo	1	3	14186.000
## 235	K562	IDH1	FCCP	1	1	222594.333
## 238	K562	IDH1	FCCP	1	2	206658.333
## 241	K562	IDH1	FCCP	1	3	188843.667
## 244	K562	IDH1	Iodo	1	1	134580.667
## 247	K562	IDH1	Iodo	1	2	105915.333
## 250	K562	IDH1	Iodo	1	3	87041.333
## 253	K562	IDH1	OAA	1	1	221051.667
## 256	K562	IDH1	OAA	1	2	159818.667
## 259	K562	IDH1	OAA	1	3	187083.000
## 262	K562	IDH1	PBS	1	1	231431.333
## 265	K562	IDH1	PBS	1	2	149879.333
## 268	K562	IDH1	PBS	1	3	198296.333

ATP_tot = PBS - Combo ATP_mito = (Iodo - Combo) / ATP_tot ATP_glyco = 1 - ATP_mito

```

ATP_assay <- lapply(1:3, function(Bio_replicat){
  dat <- dplyr::filter(Data_ATP_pulled, Biological_replicat == Bio_replicat)
  res <- lapply(c("Molm13", "K562"), function(cell_line){
    mIDH_cond <- lapply(c("WT", "IDH1", "IDH2"), function(mIDH){
      condition <- dplyr::filter(dat, Cell_line == cell_line & IDH == mIDH)
      PBS <- dplyr::filter(condition, Treatment == "PBS") %>% .$Value
      Combo <- dplyr::filter(condition, Treatment == "Combo") %>% .$Value
      Iodo <- dplyr::filter(condition, Treatment == "Iodo") %>% .$Value

      ATP_tot <- PBS - Combo
      ATP_mito <- (Iodo - Combo) / ATP_tot
      ATP_glyco <- 1 - ATP_mito
      list("PBS" = PBS, "Combo" = Combo, "Iodo" = Iodo,
           "ATP_Total" = ATP_tot, "ATP_mitochondrial" = ATP_mito, "ATP_glycolyse" = ATP_glyco)
    })
    names(mIDH_cond) <- c("WT", "IDH1", "IDH2")
    mIDH_cond
  })
  names(res) <- c("Molm13", "K562")
  res
})
names(ATP_assay) <- c("Biological_replicat_1", "Biological_replicat_2", "Biological_replicat_3")

ATP_mito <- lapply(c("Molm13", "K562"), function(Cell_line){
  lapply(c("WT", "IDH1", "IDH2"), function(mIDH){
    ATP_mito <- sapply(1:3, function(replicat){
      ATP_assay[[paste0("Biological_replicat_", replicat)]] [[Cell_line]] [[mIDH]] $ATP_mitochondrial
    }) %>% c %>% unname
    data.frame("Cell_line" = rep(Cell_line, 3),
               "mIDH" = rep(mIDH, 3),
               "Condition" = paste(Cell_line, mIDH, sep = "_"),
               "Biological_replicat" = 1:3,
               "ATP_mito" = ATP_mito)
  }) %>% data.table::rbindlist()
}) %>% data.table::rbindlist()

ATP_glyco <- lapply(c("Molm13", "K562"), function(Cell_line){
  lapply(c("WT", "IDH1", "IDH2"), function(mIDH){
    ATP_glyco <- sapply(1:3, function(replicat){

```

```

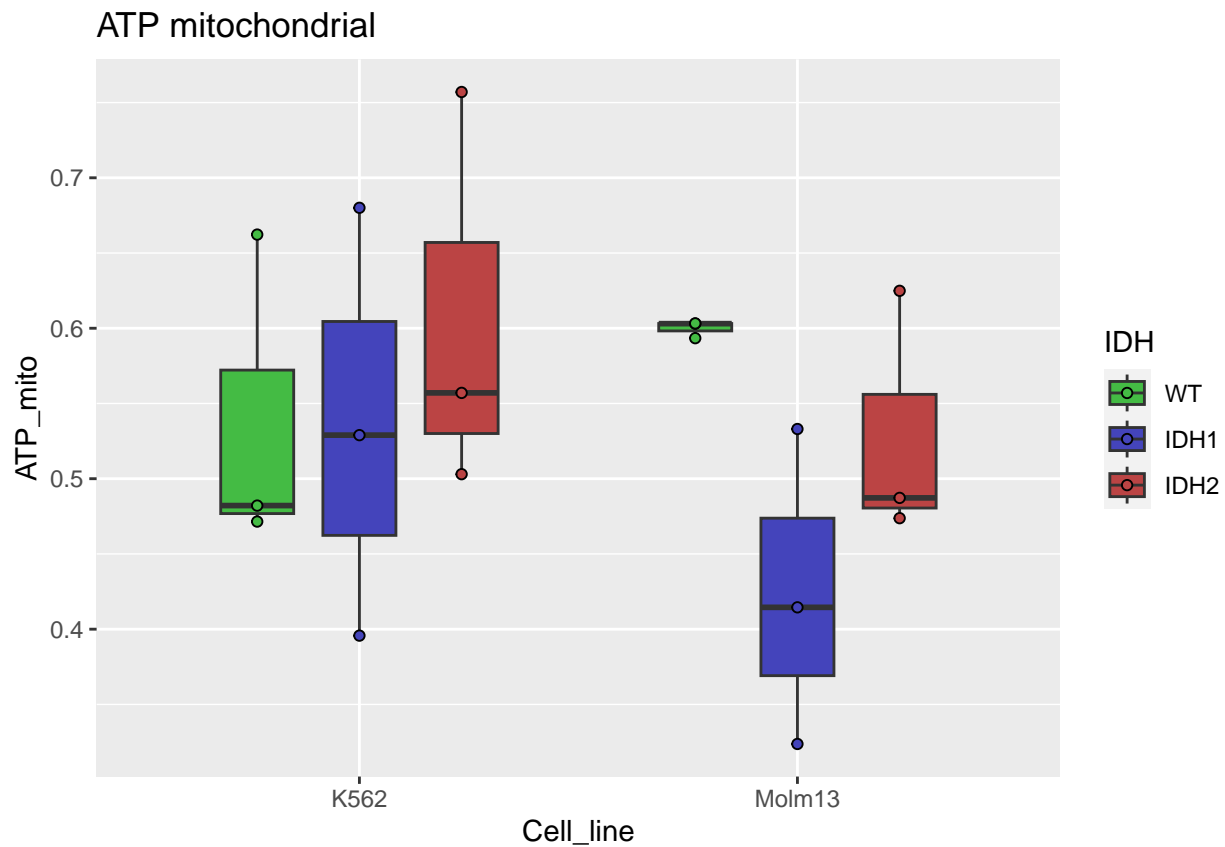
      ATP_assay[[paste0("Biological_replicat_", replicat)]] [[Cell_line]] [[mIDH]]$ATP_glycolyse
    }) %>% c %>% unname
    data.frame("Cell_line" = rep(Cell_line, 3),
              "mIDH" = rep(mIDH, 3),
              "Condition" = paste(Cell_line, mIDH, sep = "_"),
              "Biological_replicat" = 1:3,
              "ATP_glyco" = ATP_glyco)
  }) %>% data.table::rbindlist()
}) %>% data.table::rbindlist()

ATP_mito$Scaled <- 1:nrow(ATP_mito) %>% sapply(function(row){
  Ligne <- ATP_mito[row,]
  Wt_cond <- dplyr::filter(ATP_mito, Biological_replicat == Ligne$Biological_replicat & Cell_line == Ligne$Cell_line)
  mean <- Wt_cond$ATP_mito
  (Ligne$ATP_mito - mean)
})

ATP_glyco$Scaled <- 1:nrow(ATP_glyco) %>% sapply(function(row){
  Ligne <- ATP_glyco[row,]
  Wt_cond <- dplyr::filter(ATP_glyco, Biological_replicat == Ligne$Biological_replicat & Cell_line == Ligne$Cell_line)
  mean <- Wt_cond$ATP_glyco
  Ligne$ATP_glyco - mean
})

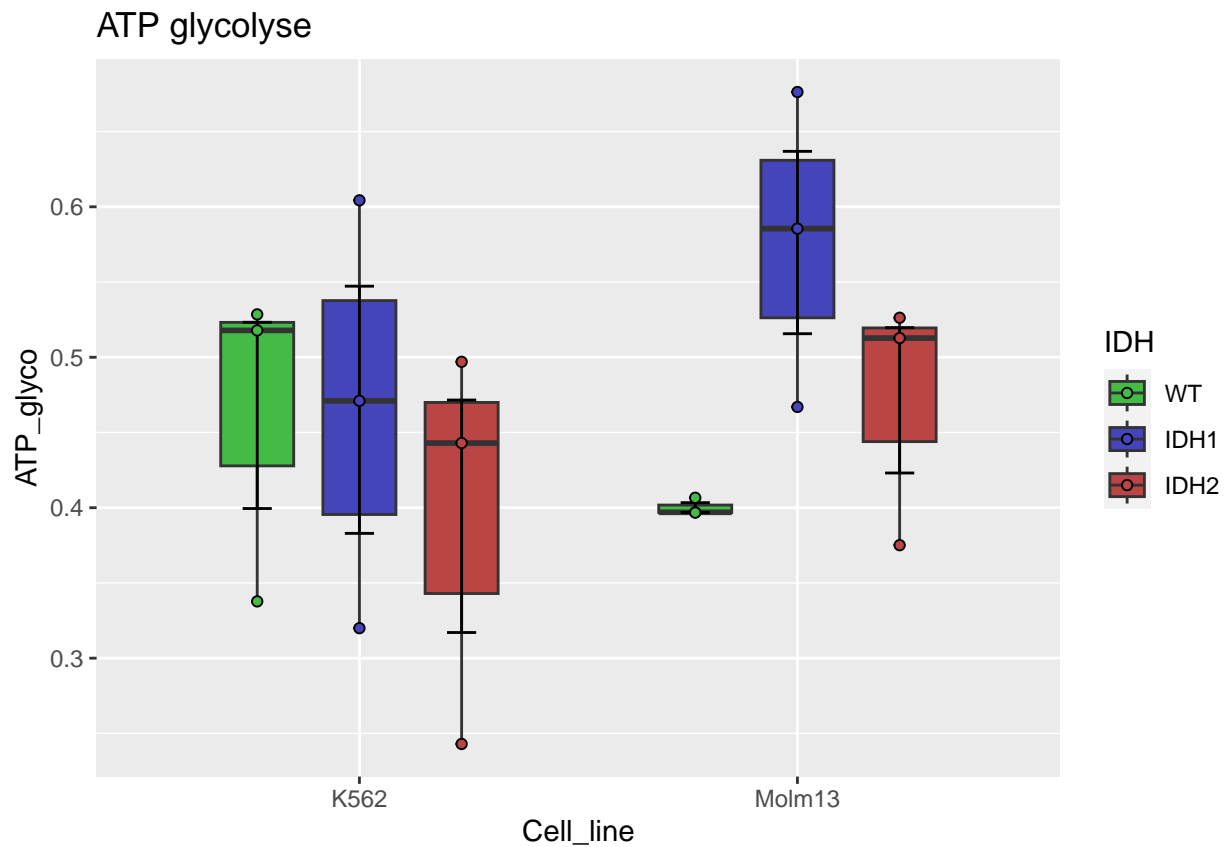
p <- ggplot(ATP_mito, aes(x = Cell_line, y = ATP_mito, fill = factor(mIDH, levels = c("WT", "IDH1", "IDH2"))))
p + geom_boxplot(position = position_dodge(width = 0.7), width = 0.5) +
  geom_point(aes(x = Cell_line), shape = 21, position = position_dodge(width = 0.7)) + labs(fill = c("WT", "IDH1", "IDH2"))
p + scale_fill_manual(values = c("#44BB44", "#4444BB", "#BB4444")) + ggtitle("ATP mitochondrial")

```

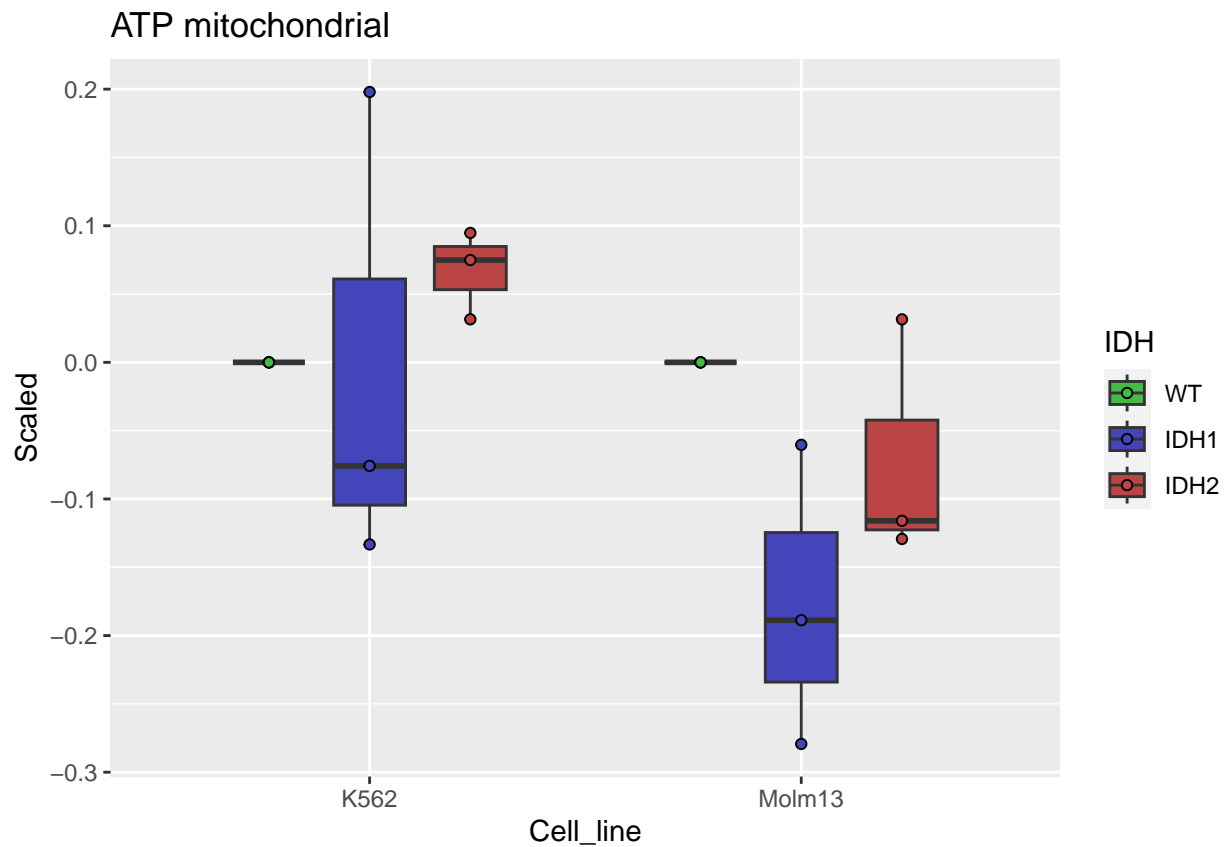


```
p <- ggplot(ATP_glyco, aes(x = Cell_line, y = ATP_glyco, fill = factor(mIDH, levels = c("WT", "IDH1", "IDH2")))) +
  p + geom_boxplot(position = position_dodge(width = 0.7), width = 0.5) +
  geom_errorbar(stat = 'summary', position = position_dodge(width = 0.7), width = 0.2) +
  geom_point(aes(x = Cell_line), shape = 21, position = position_dodge(width = 0.7)) + labs(fill = c("WT", "IDH1", "IDH2")) +
  scale_fill_manual(values = c("#44BB44", "#4444BB", "#BB4444")) + ggtitle("ATP glycolyse")
```

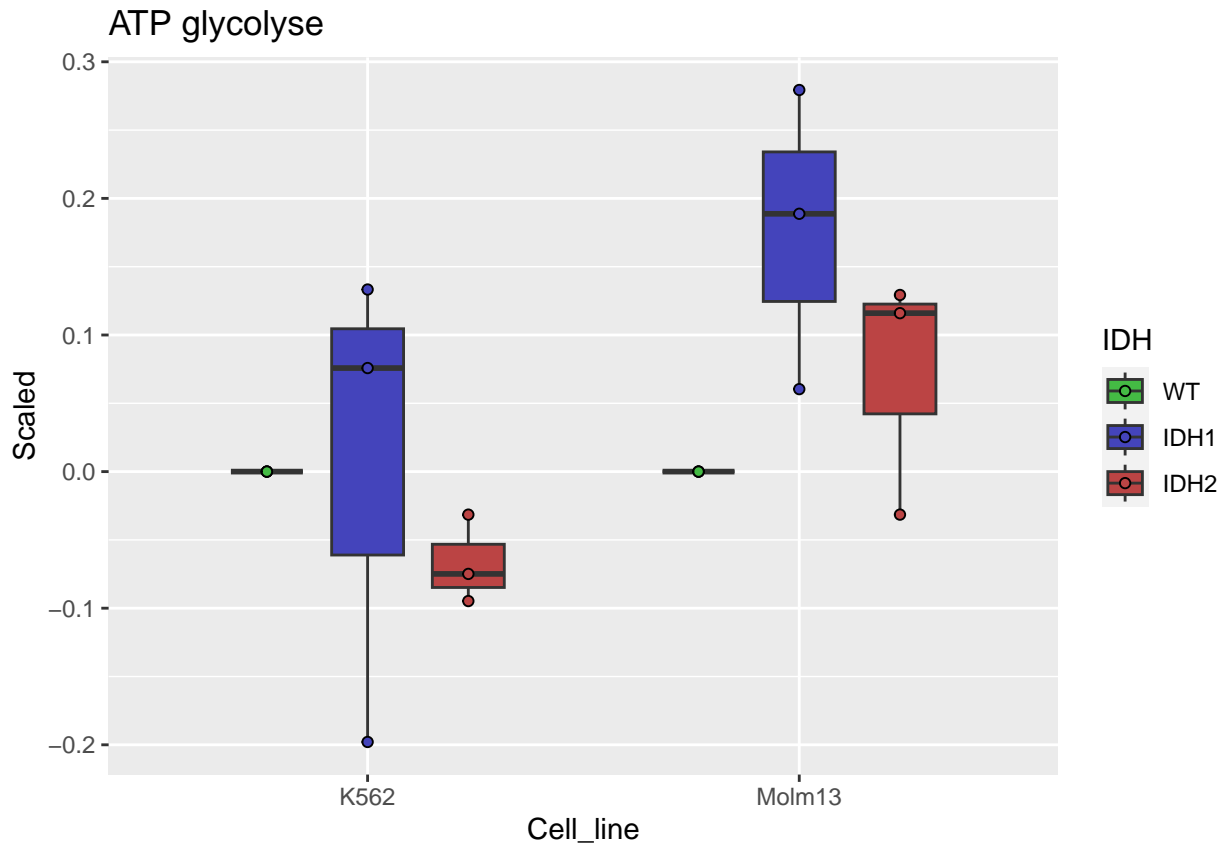
```
## No summary function supplied, defaulting to `mean_se()`
```



```
p <- ggplot(ATP_mito, aes(x = Cell_line, y = Scaled, fill = factor(mIDH, levels = c("WT", "IDH1", "IDH2"))))
p + geom_boxplot(position = position_dodge(width = 0.7), width = 0.5) +
  geom_point(aes(x = Cell_line), shape = 21, position = position_dodge(width = 0.7)) + labs(fill = c("WT", "IDH1", "IDH2"))
p + scale_fill_manual(values = c("#44BB44", "#4444BB", "#BB4444")) + ggtitle("ATP mitochondrial")
```



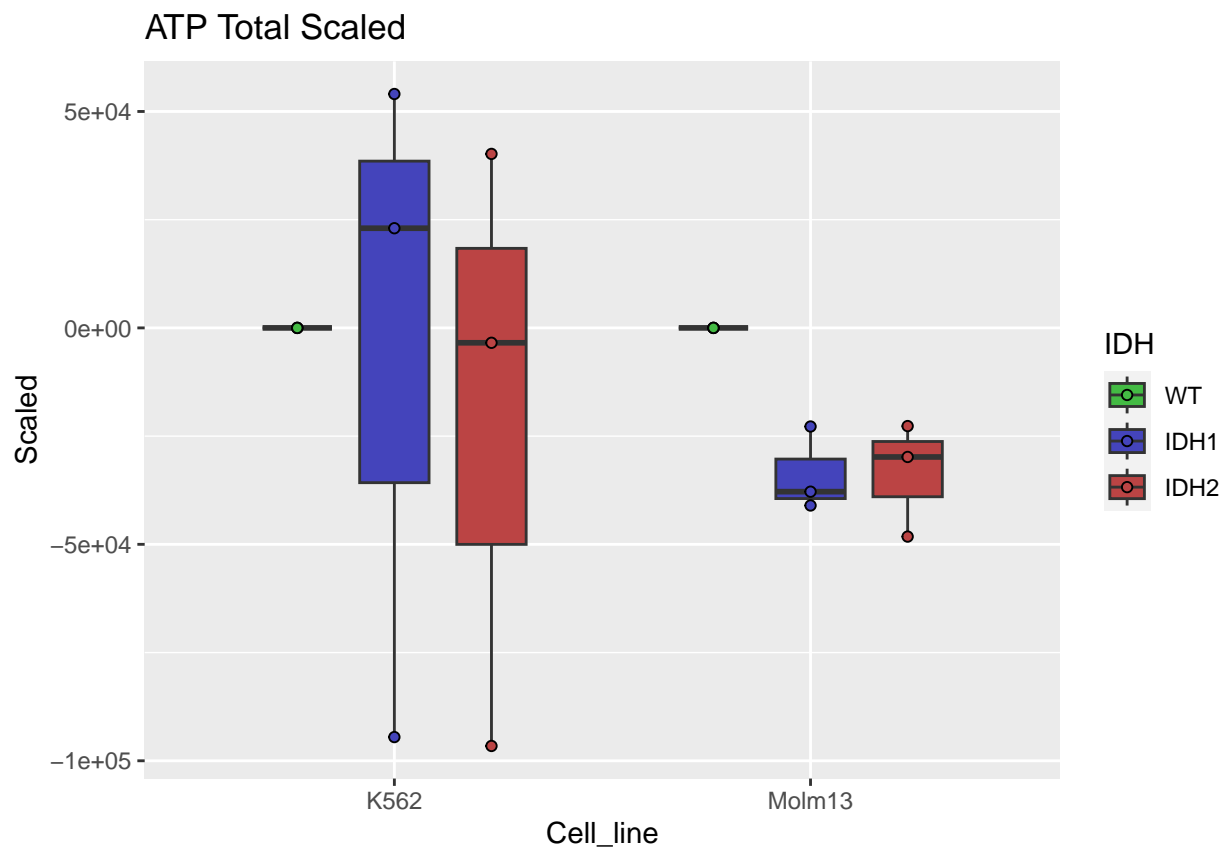
```
p <- ggplot(ATP_glyco, aes(x = Cell_line, y = Scaled, fill = factor(mIDH, levels = c("WT", "IDH1", "IDH2")))) +
p + geom_boxplot(position = position_dodge(width = 0.7), width = 0.5) +
  geom_point(aes(x = Cell_line), shape = 21, position = position_dodge(width = 0.7)) + labs(fill = c("WT", "IDH1", "IDH2")) +
  scale_fill_manual(values = c("#44BB44", "#4444BB", "#BB4444")) + ggtitle("ATP glycolyse")
```



```
ATP_total <- ATP_mito <- lapply(c("Molm13", "K562"), function(Cell_line){
  lapply(c("WT", "IDH1", "IDH2"), function(mIDH){
    ATP_Tot <- sapply(1:3, function(replicat){
      ATP_assay[[paste0("Biological_replicat_", replicat)]] [[Cell_line]] [[mIDH]]$ATP_Total
    }) %>% c %>% unname
    data.frame("Cell_line" = rep(Cell_line, 3),
              "mIDH" = rep(mIDH, 3),
              "Condition" = paste(Cell_line, mIDH, sep = "_"),
              "Biological_replicat" = 1:3,
              "ATP_Tot" = ATP_Tot)
  }) %>% data.table::rbindlist()
}) %>% data.table::rbindlist()
```

```
ATP_total$Scaled <- 1:nrow(ATP_total) %>% sapply(function(row){
  Ligne <- ATP_total[row,]
  Wt_cond <- dplyr::filter(ATP_total, Biological_replicat == Ligne$Biological_replicat & Cell_line == Ligne$Cell_line)
  mean <- Wt_cond$ATP_Tot
  (Ligne$ATP_Tot - mean)
})
```

```
p <- ggplot(ATP_total, aes(x = Cell_line, y = Scaled, fill = factor(mIDH, levels = c("WT", "IDH1", "IDH2")))) +
p + geom_boxplot(position = position_dodge(width = 0.7), width = 0.5) +
  geom_point(aes(x = Cell_line), shape = 21, position = position_dodge(width = 0.7)) + labs(fill = c("WT", "IDH1", "IDH2")) +
  scale_fill_manual(values = c("#44BB44", "#4444BB", "#BB4444")) + ggtitle("ATP Total Scaled")
```

```
p <- ggplot(ATP_total, aes(x = Cell_line, y = ATP_Tot, fill = factor(mIDH, levels = c("WT", "IDH1", "IDH2"))))
p + geom_boxplot(position = position_dodge(width = 0.7), width = 0.5) +
  geom_point(aes(x = Cell_line), shape = 21, position = position_dodge(width = 0.7)) + labs(fill = c("WT", "IDH1", "IDH2"))
p + scale_fill_manual(values = c("#44BB44", "#4444BB", "#BB4444")) + ggtitle("ATP Total")
```

