

GAS Certification

TCM

Tuesday, July 21, 2014

Automated analysing submitted data for GAS based on defined outliers

Thomas Meisel (2014-08-03)

defining the RM and measurand to be analysed

```
refmat <- 'GAS' # defining the RM  
setwd("~/GitHub/GOMcertification")
```

opts_chunk\$set(dev="png", dev.args=list(type="cairo"), dpi=300) options(base64_images = 'inline') #####
general comments to the design

The data for this interlaboratory comparison based certification of property values were analysed by 36 labs following the nested design approached as proposed the IAG certification protocol. Participating labs received 3 packages of OKUM and MUH-1 respectively and one package of GAS. The latter was supplied as a "traceability" sample and is here used for quality control purposes. It was the task of the labs to prepare two independent sample preparations (i.e. digestions) of each packet and analyse the preparations on two different days. Labs thus should have submitted 12 values (3x2x2 PacketxPrepxDay). The outliers have been selected based in Youden plots, Mandel's k and detection limit criteria. In this file the property values and the uncertainties are calculated for all analytes of a specific candidate GAS

```
'%p%' <- function(x, y) {as.character(paste (x, y, sep =""))}  
df <- data.frame(cbind(0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0))  
names(df) <- c("date", "RM", "measurand", "mean.before", "mean.after", "median.before", "median.after",  
df <- df[!1,]  
write.table(df, "df3.txt", row.names=FALSE) # needed only the first time
```

```
# Data for certification project was gathered and joined in Excel. The files  
# were exported from Excel as xxxx.csv files to make them universally  
# readable. For this markdown the data is stored in the 'root/documents'  
# directory. Data is loaded ('GOMGather1.R') and merged ('GOMMerge.R') for  
# GAS, OKUM and MUH-1 are merged together with a methods file  
# ('OKUM.method') into a universal data.frame file named 'GOM'. All of this  
# happens in the 'Makefile.R'
```

```
setwd("~/GitHub/GOMcertification")  
source("Makefile.R")
```

importing the data and assigning factors

defining the function for plotting methods vs. measurand mass fraction. Sample preparation methods are also marked in the plot.

defining the function of Youden plots

```
## means over packets within lab
meanGOM <- function(x) mean(x, na.rm=TRUE) # defining a function for further calcuations
sdGOM <- function(x) sd(x, na.rm=TRUE) # defining a function for further calcuations, here for calculate
meanGOM.packet <- ddply(GOM, c("Lab", "Packet"), numcolwise(meanGOM)) # calculated the mean for each Pa
## mean over mean of packets within lab
GOM.mean <- ddply(meanGOM.packet, c("Lab")), numcolwise(meanGOM))
GOM.mean <- merge(GOM.mean, OKUM.methods, by="Lab")
```

```
## median over packets within lab
medianGOM <- function(x) median(x, na.rm=TRUE)
medianGOM.packet <- ddply(GOM, c("Lab", "Packet"), numcolwise(medianGOM))
GOM.sd <- ddply(medianGOM.packet, c("Lab"), numcolwise(sdGOM))
## median over median of packets within lab
GOM.median <- ddply(medianGOM.packet, c("Lab")), numcolwise(medianGOM))
GOM.median <- merge(GOM.median, OKUM.methods, by="Lab")
```

initial calculations with complete data set

plots before outlier removal and outlier removal

```
sequence <- seq(from = 1, to = length(names(GAS.outlier)), by = 3)
col <- GAS.outlier[,c(sequence)]
col.names <- colnames(col)
for (m in col.names) {
  measurand.name <- m
  switch(
    refmat,
    GAS = rm1 <- 2,
    MUH = rm1 <- 1,
    OKUM = rm1 <- 0
  )
  if(rm1 > 0)
  {measurand <- measurand.name %p% '.' %p% rm1
  } else
  {
    measurand <- measurand.name
  }
  MorT <- grep(measurand.name, colnames(GOM), fixed=TRUE) # finding the position of the measurand.name
  ifelse(MorT[1]< 21, MorT <- 'M', MorT<-'T') # testing if measurand is a major or trace element/componou
  ifelse(MorT == "T", unit <- 'mg/kg', unit <- 'g/100g') # testing which unit is needed
```

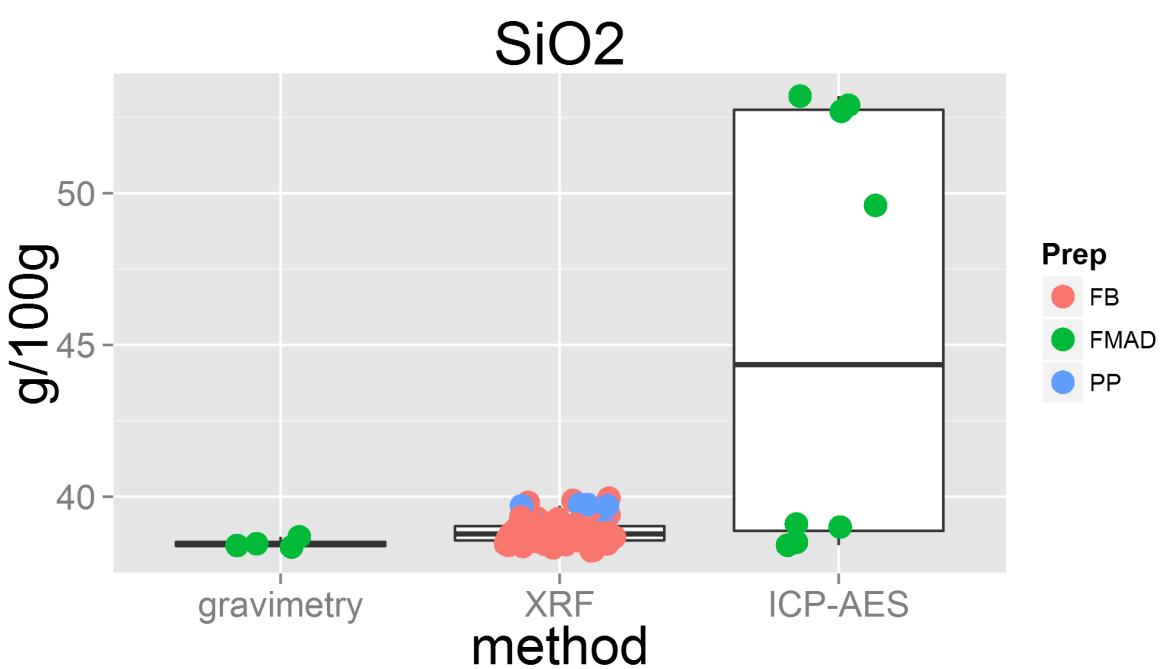
```
print(plot_method(measurand))

# outlier removal

outlier <- GAS.outlier[[measurand.name]]
outlier <- na.omit(outlier)
leng <- length(outlier) ## counting the number of outliers for loop
for(i in seq(leng)) ## looping
{
  GOM[[measurand]] <- ifelse(GOM$Lab==outlier[i], NA, GOM[[measurand]]) ## replacing values of outlying
  message("Lab ", outlier[i], " was removed")
# print(summary(GOM[[measurand]]), na.rm=TRUE, digits=4))
}
}

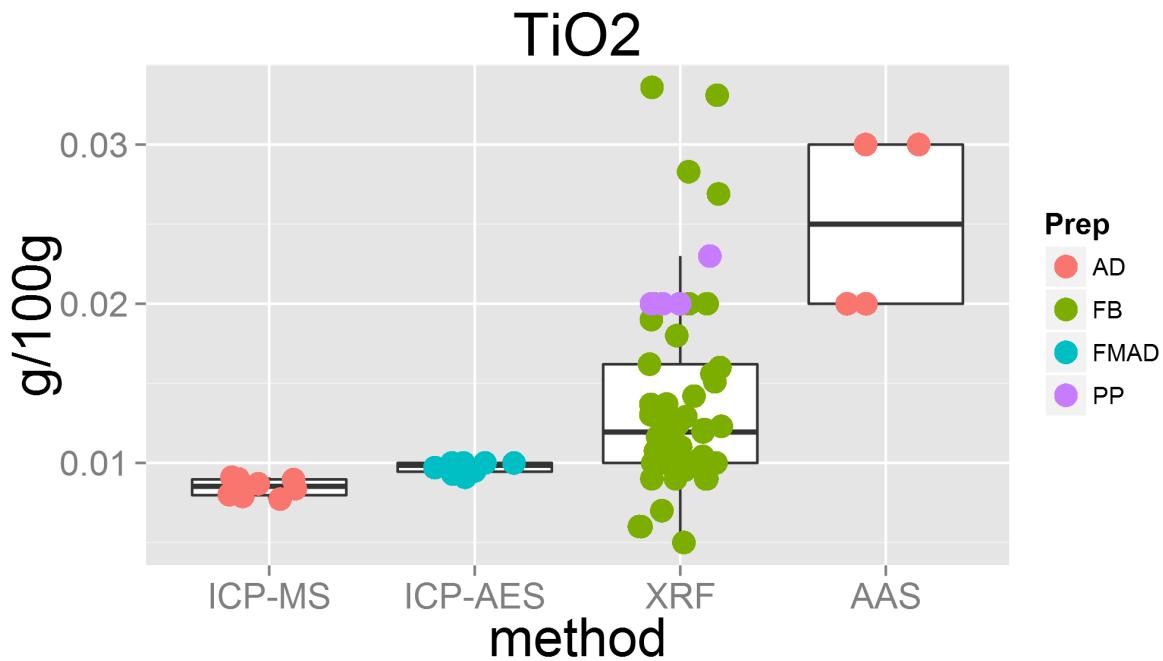
## Warning: Removed 6 rows containing missing values (geom_point).

## Lab 16 was renamed
```



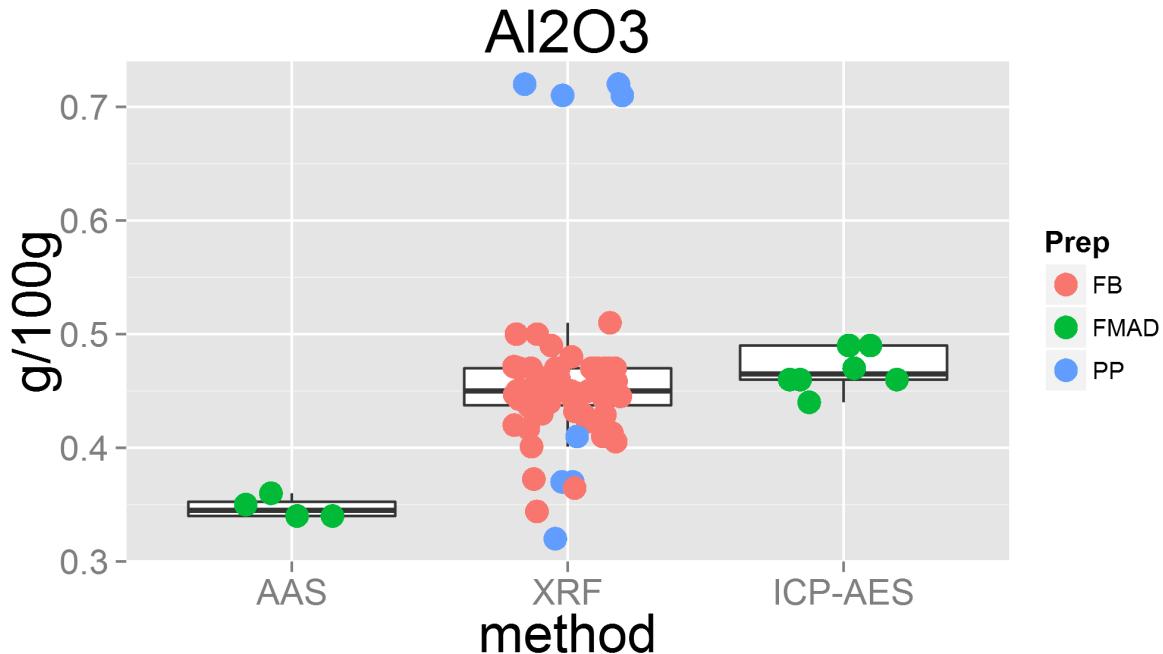
Warning: Removed 4 rows containing missing values (geom_point).

```
## Lab 7 was removed  
## Lab 12 was removed  
## Lab 23 was removed
```



```
## Warning: Removed 10 rows containing missing values (geom_point).
```

```
## Lab 12 was removed
## Lab 14 was removed
## Lab 7 was removed
## Lab 33 was removed
```

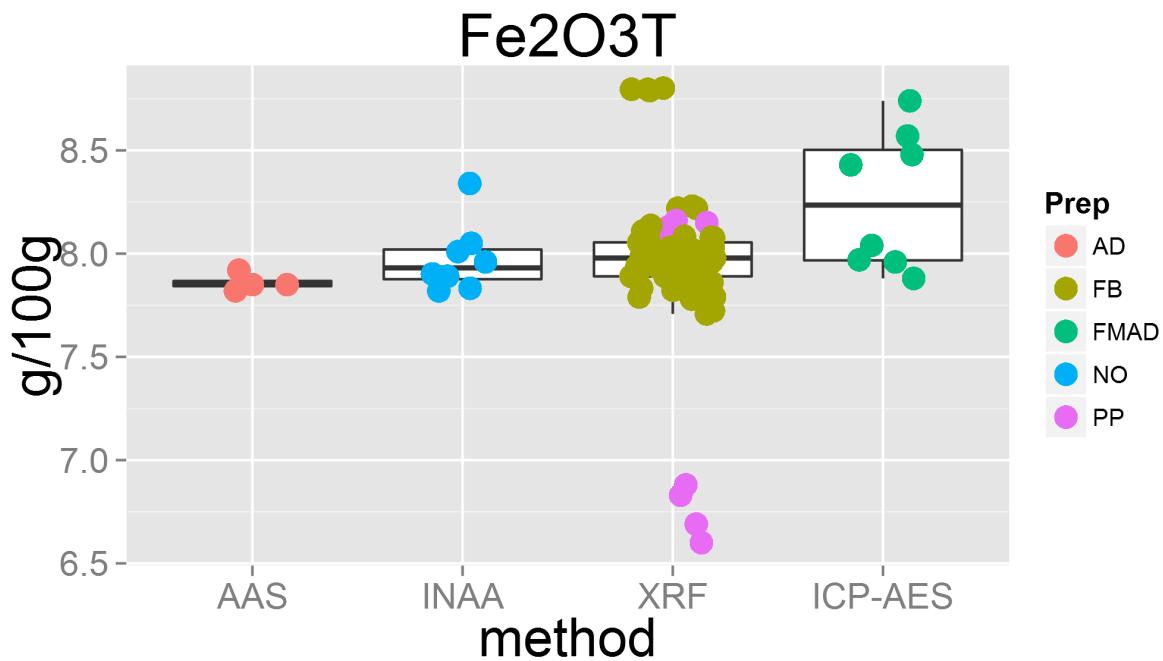


```

## Warning: Removed 1 rows containing missing values (geom_point).
## Warning: Removed 1 rows containing missing values (geom_point).
## Warning: Removed 8 rows containing missing values (geom_point).

## Lab 12 was removed
## Lab 16 was removed
## Lab 31 was removed

```

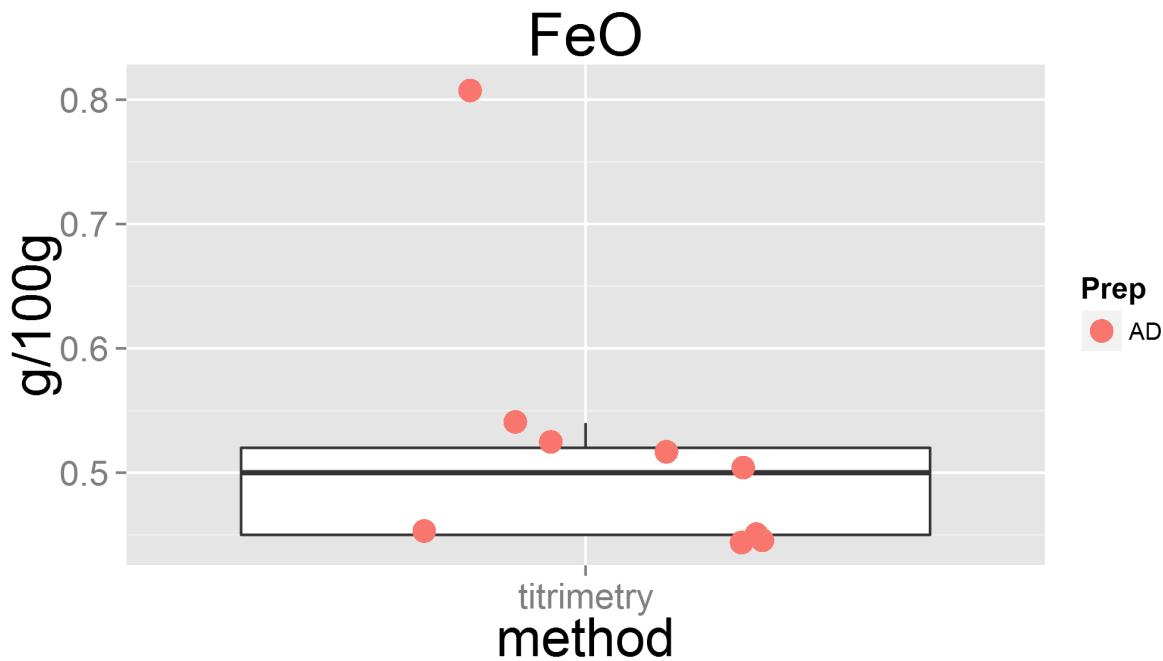


```

## Warning: Removed 1 rows containing missing values (geom_point).

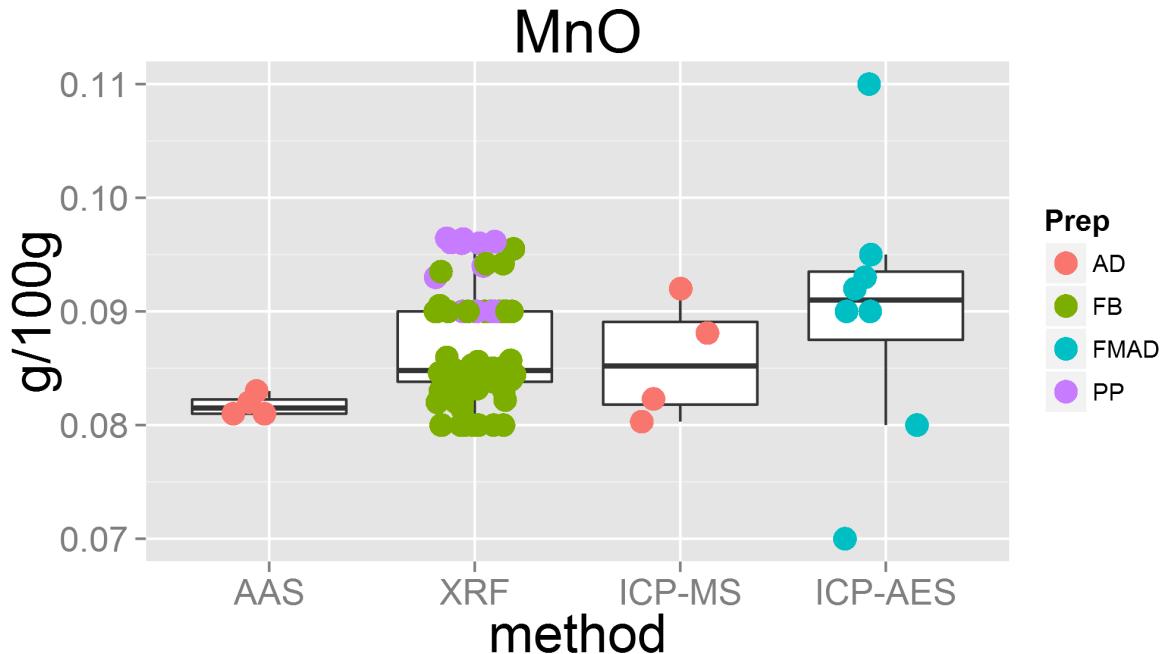
## Lab 0 was removed

```

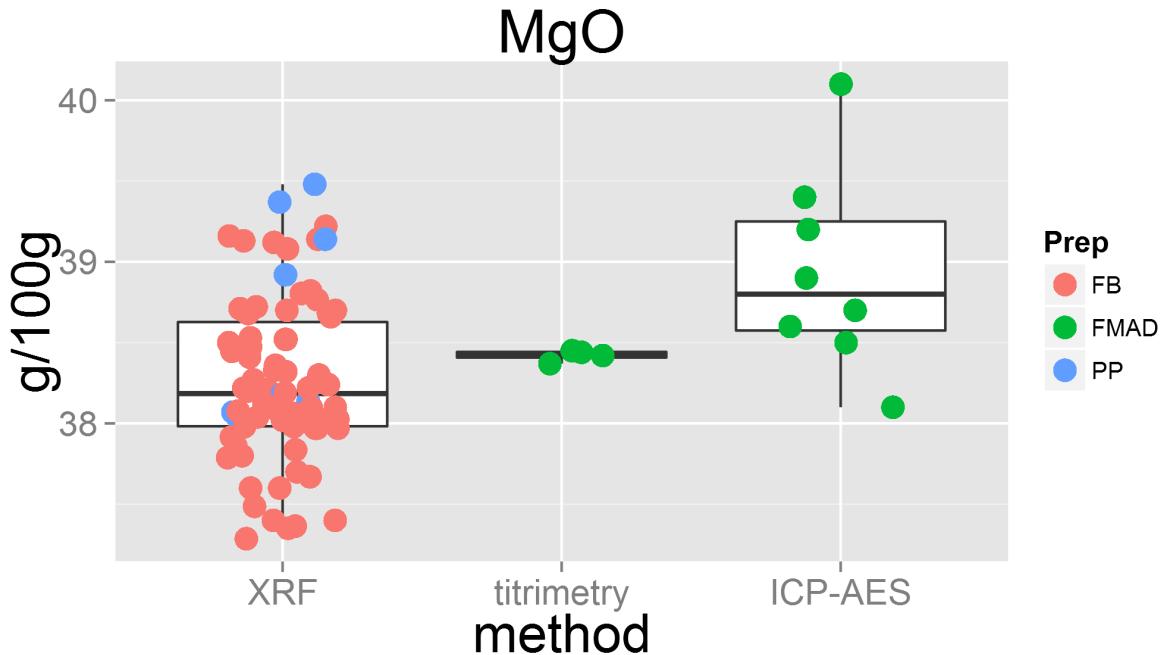


```
## Warning: Removed 2 rows containing missing values (geom_point).
```

```
## Lab 12 was removed
## Lab 16 was removed
## Lab 23 was removed
## Lab 24 was removed
```

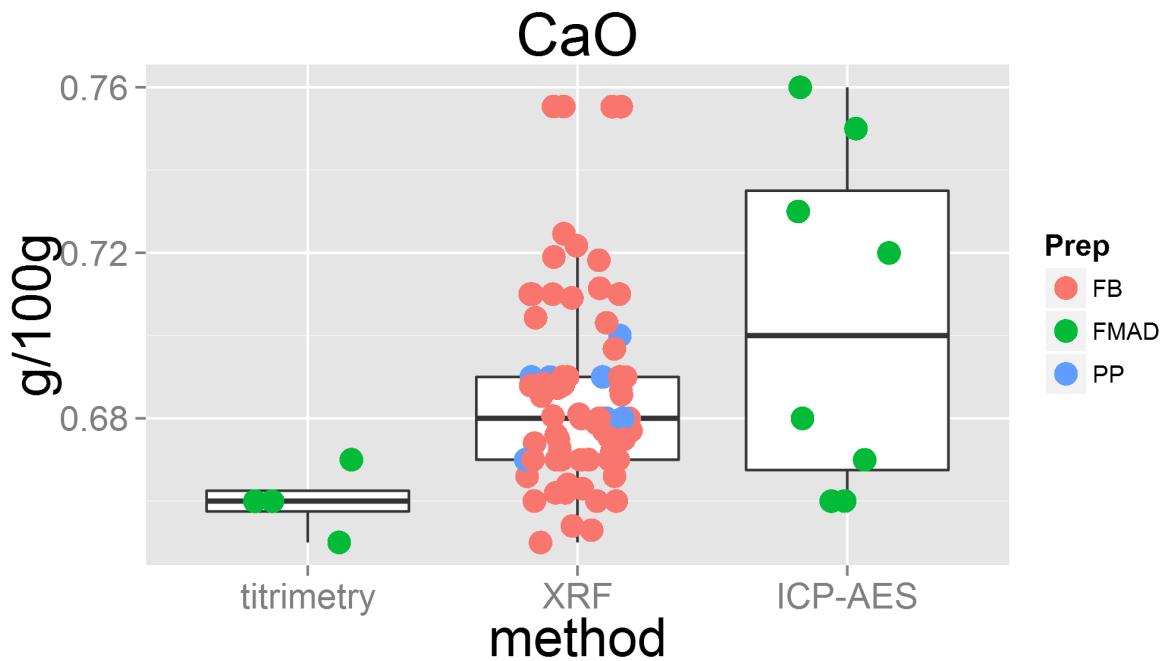


```
## Lab 10 was removed  
## Lab 12 was removed  
## Lab 16 was removed  
## Lab 32 was removed
```



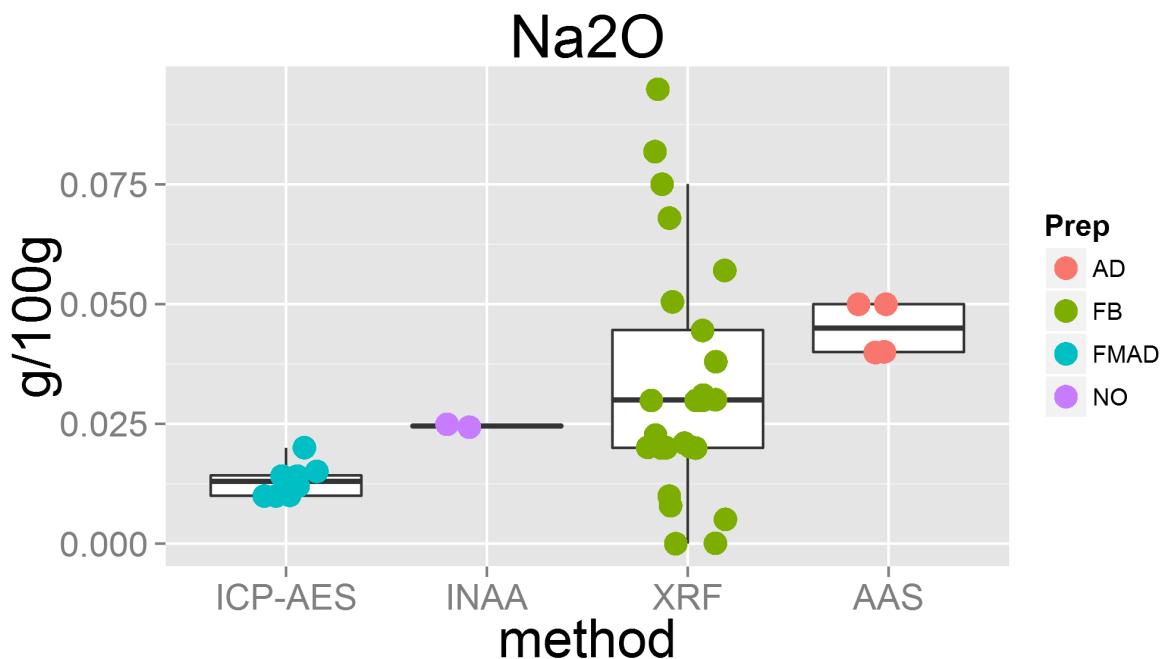
```
## Warning: Removed 1 rows containing missing values (geom_point).  
## Warning: Removed 6 rows containing missing values (geom_point).
```

```
## Lab 16 was removed  
## Lab 30 was removed
```



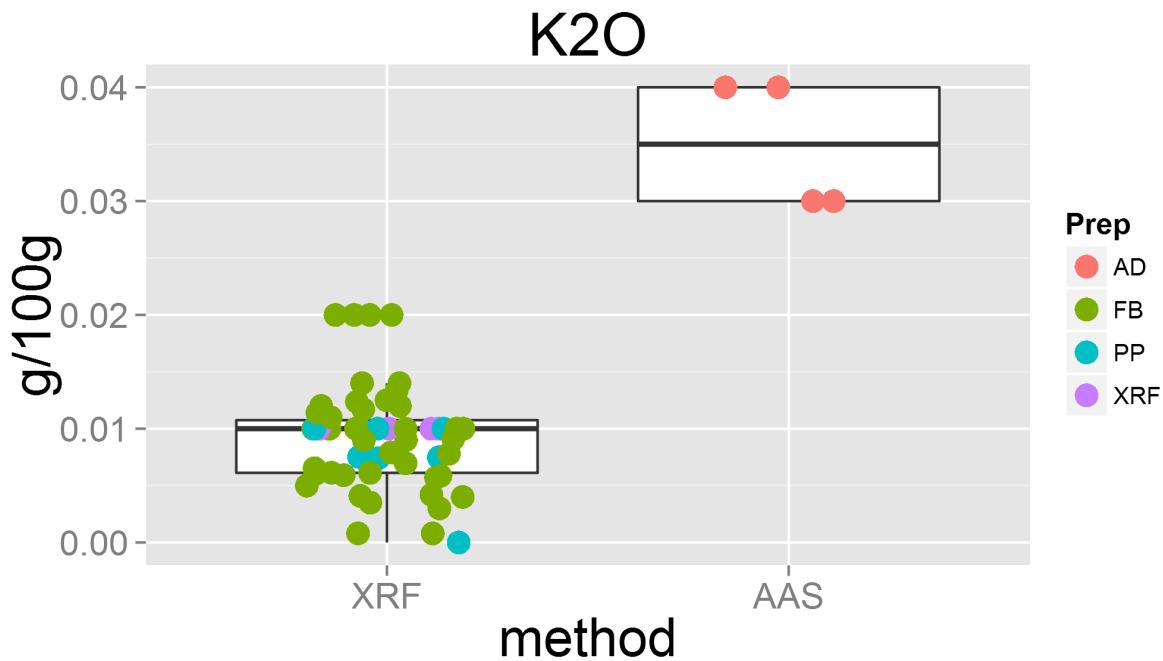
```
## Warning: Removed 2 rows containing missing values (geom_point).
```

```
## Lab 33 was removed
```



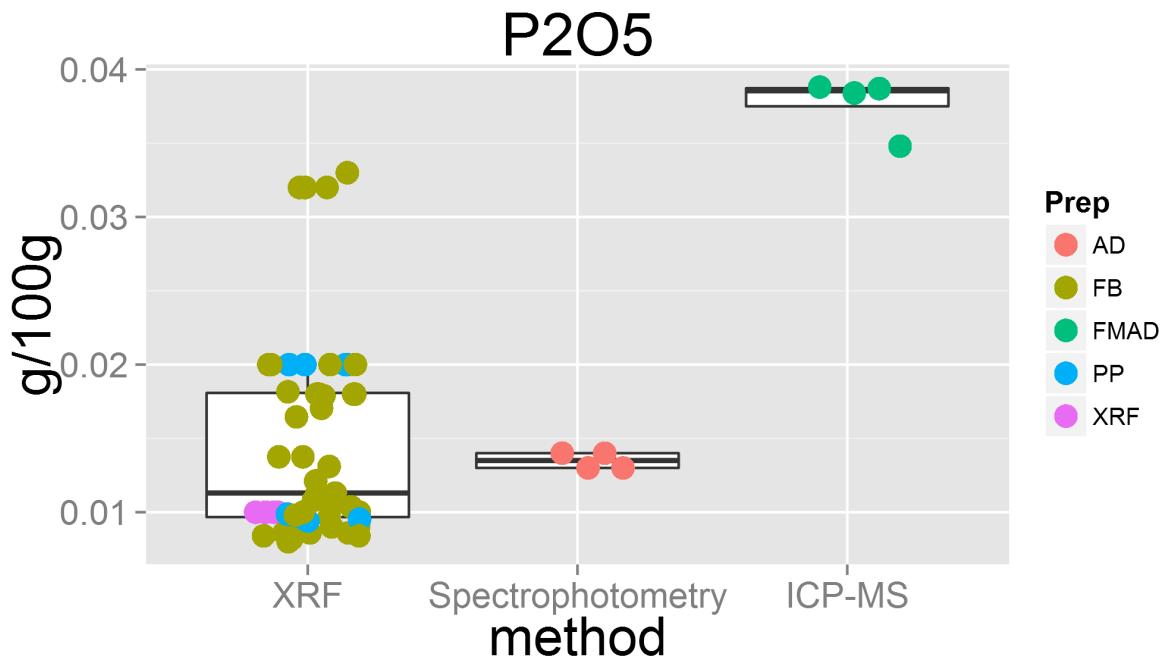
```
## Warning: Removed 4 rows containing missing values (geom_point).
```

```
## Lab 7 was removed
```



```
## Warning: Removed 4 rows containing missing values (geom_point).
## Warning: Removed 1 rows containing missing values (geom_point).
```

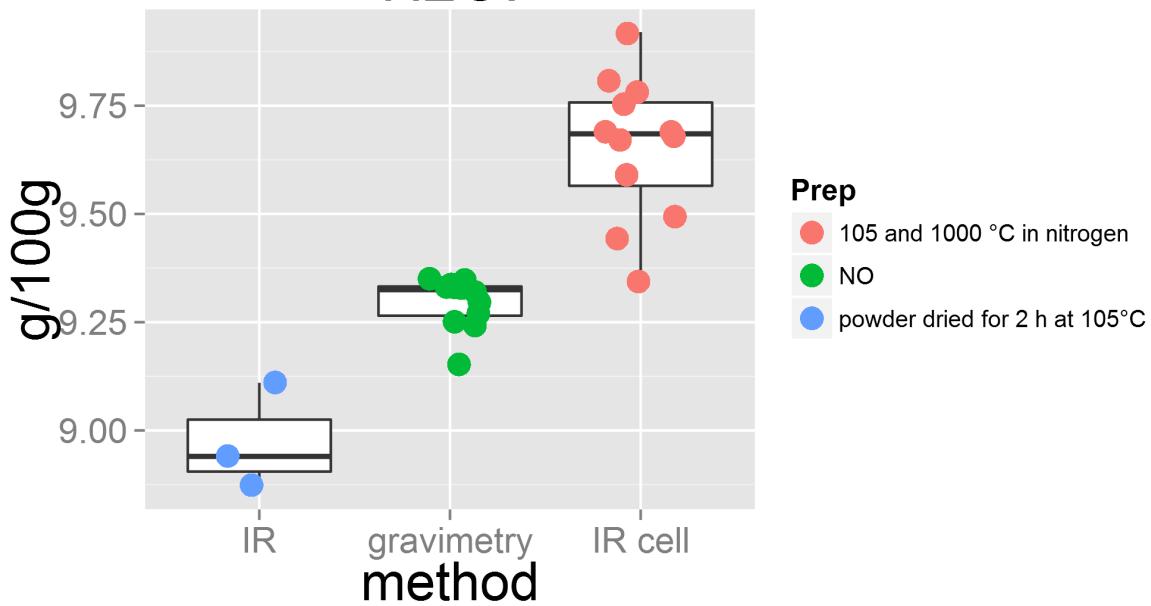
```
## Lab 6 was removed
## Lab 33 was removed
```



```
## Warning: Removed 1 rows containing missing values (geom_point).
```

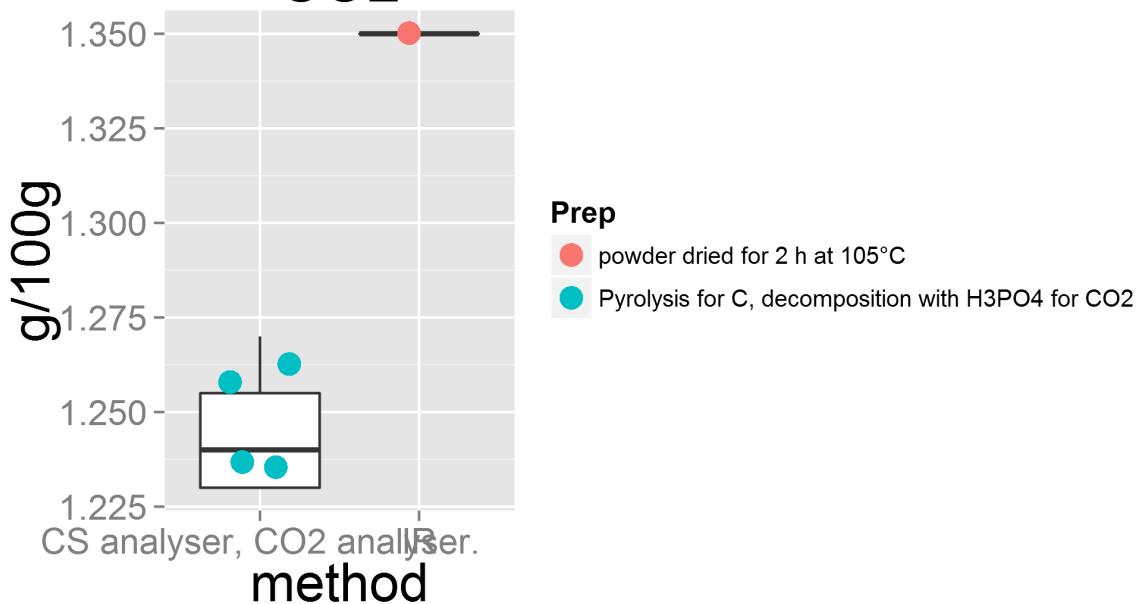
Lab 0 was removed

H2O.

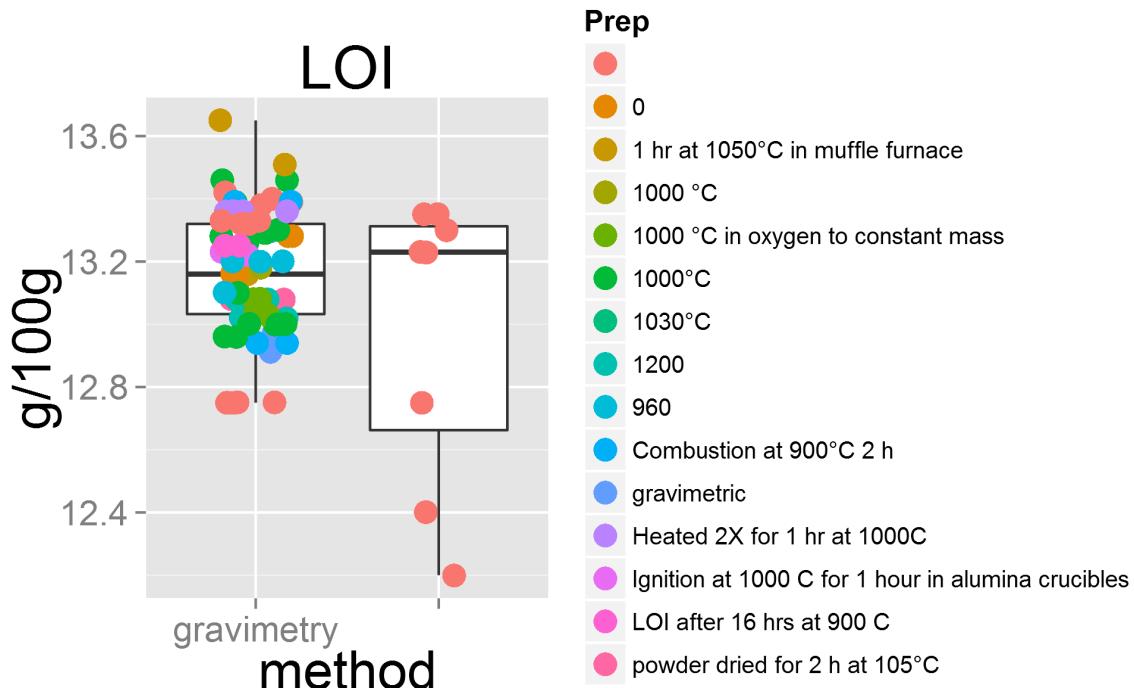


Lab 0 was removed

CO₂

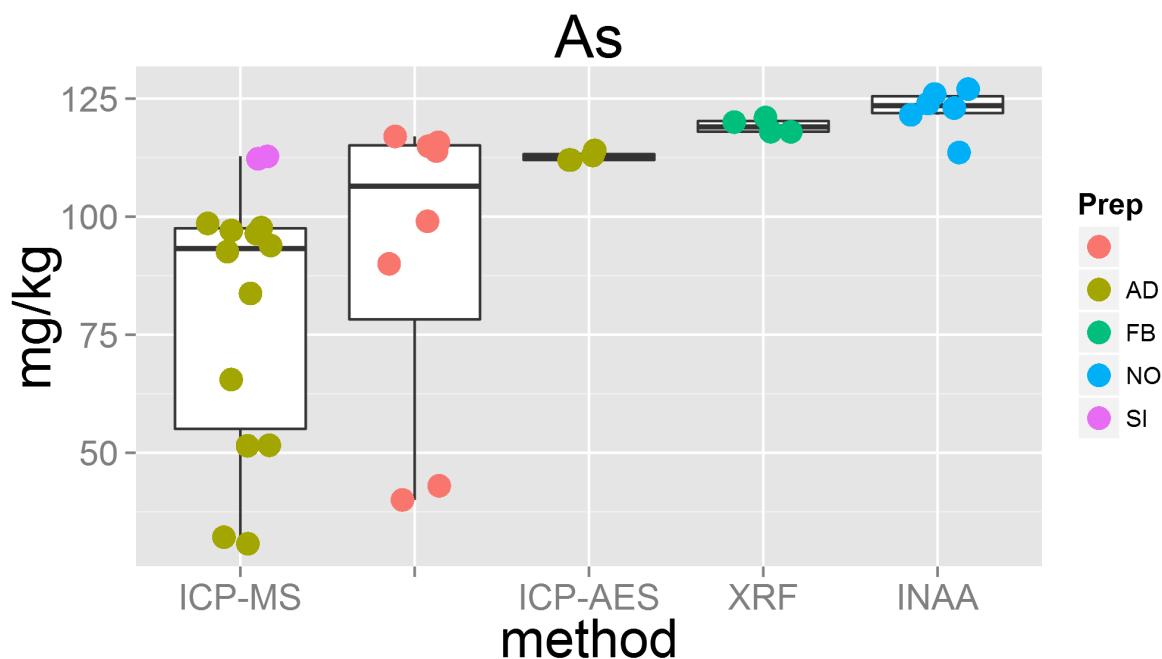


Lab 0 was removed



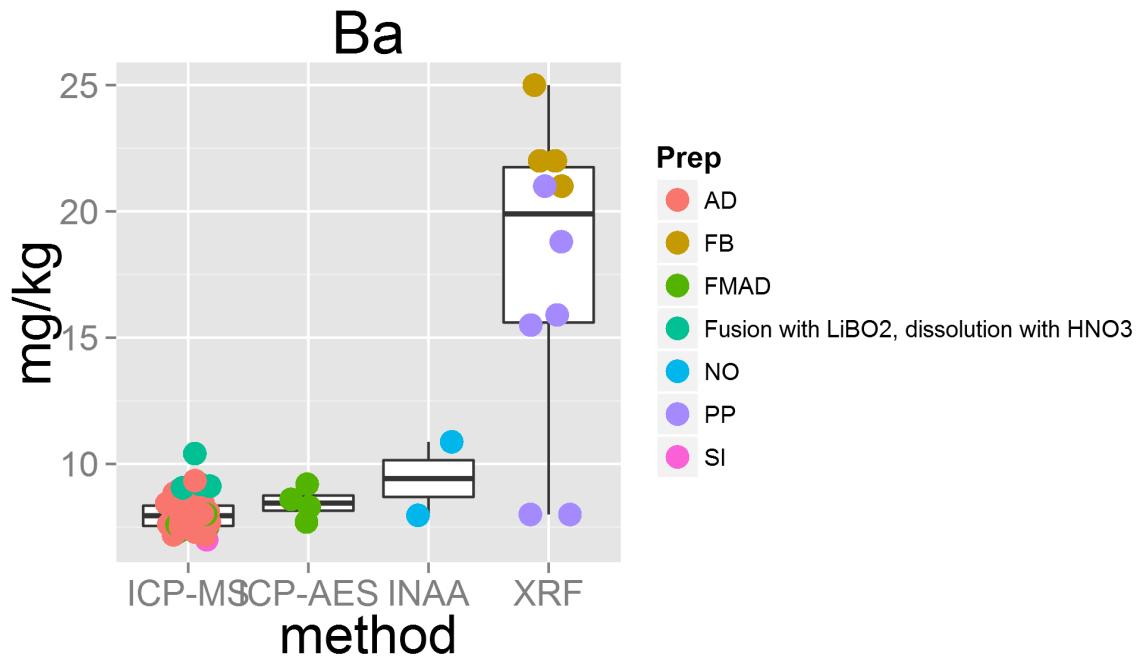
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 18 was removed
```



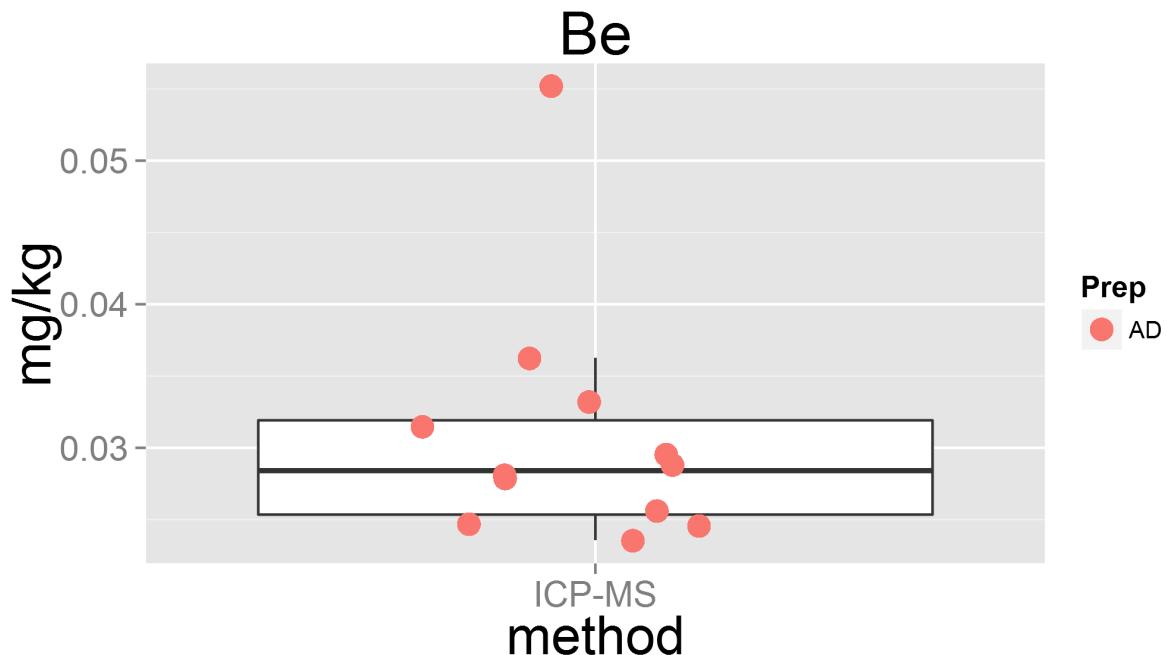
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 14 was removed  
## Lab 26 was removed
```



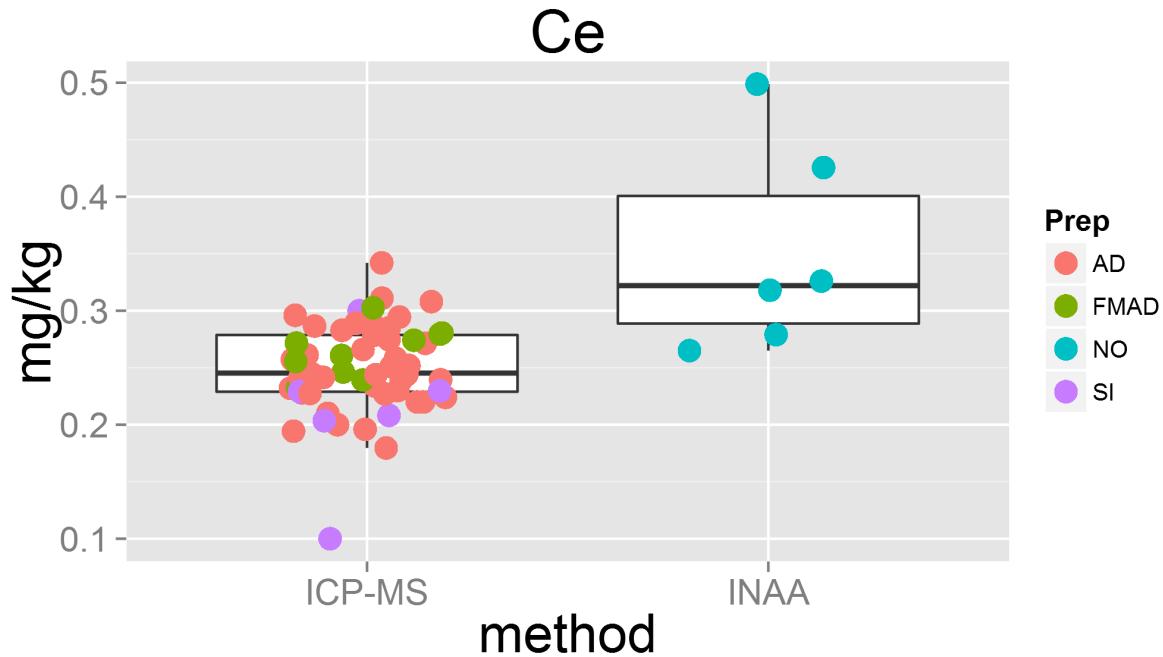
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 0 was removed
```



```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 29 was removed
```



```
## Warning: Removed 2 rows containing missing values (geom_point).
```

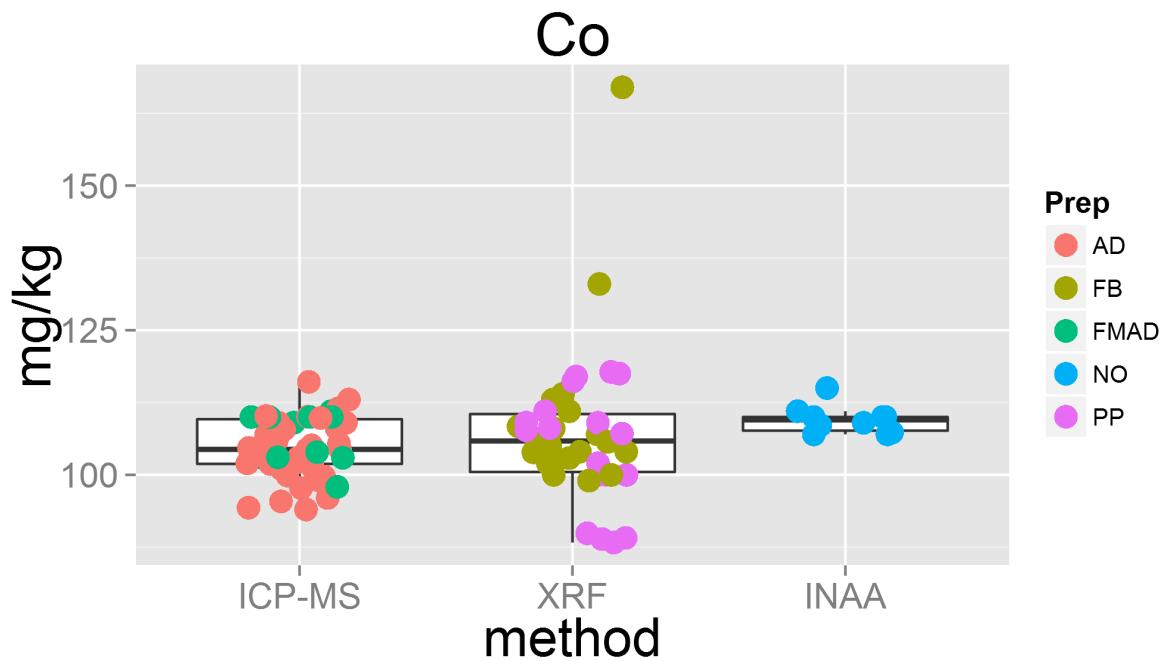
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 12 was removed
```

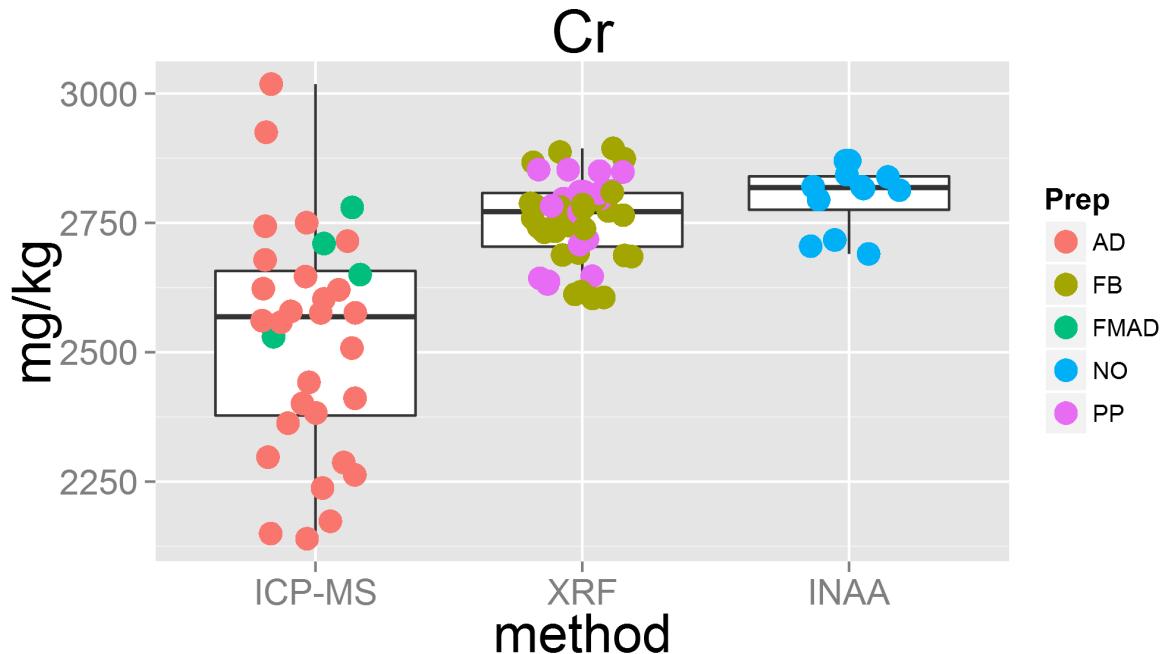
```
## Lab 24 was removed
```

```
## Lab 5 was removed
```

```
## Lab 26 was removed
```

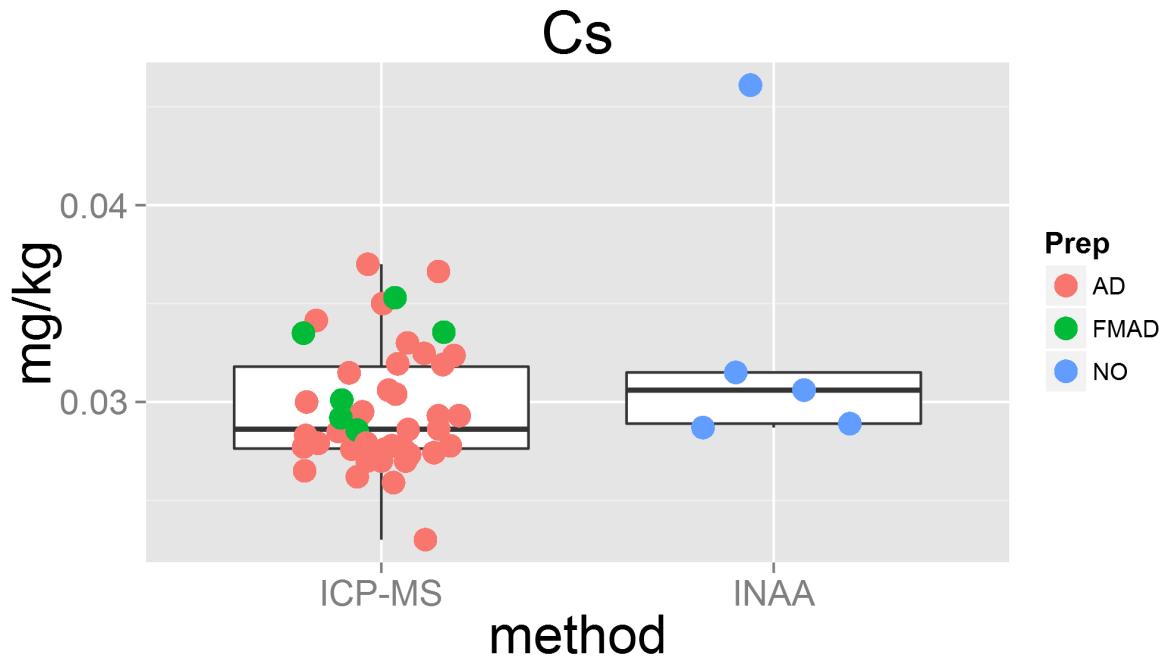


```
## Lab 8 was removed
## Lab 12 was removed
## Lab 16 was removed
## Lab 18 was removed
```



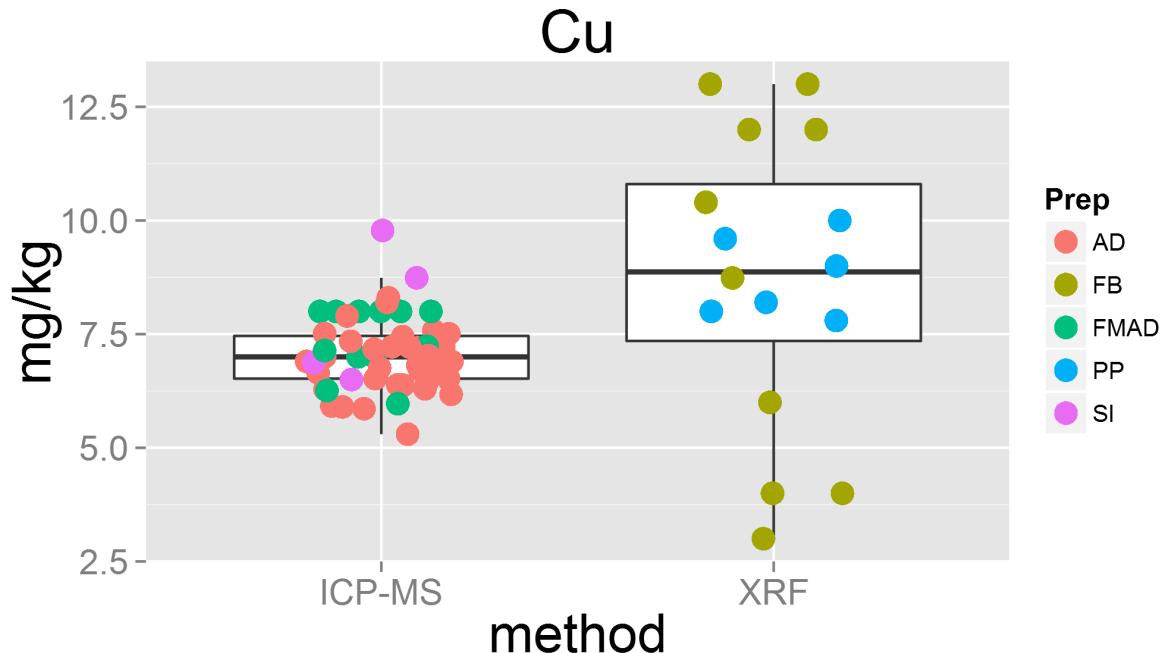
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 29 was removed
```



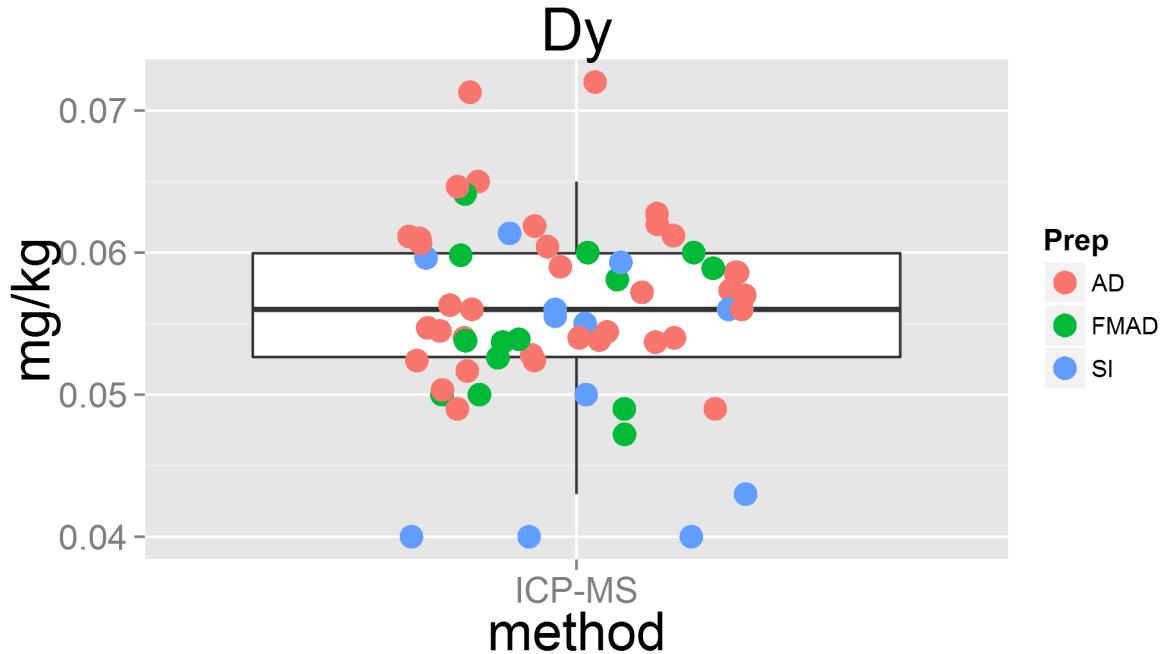
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 3 was removed  
## Lab 14 was removed
```



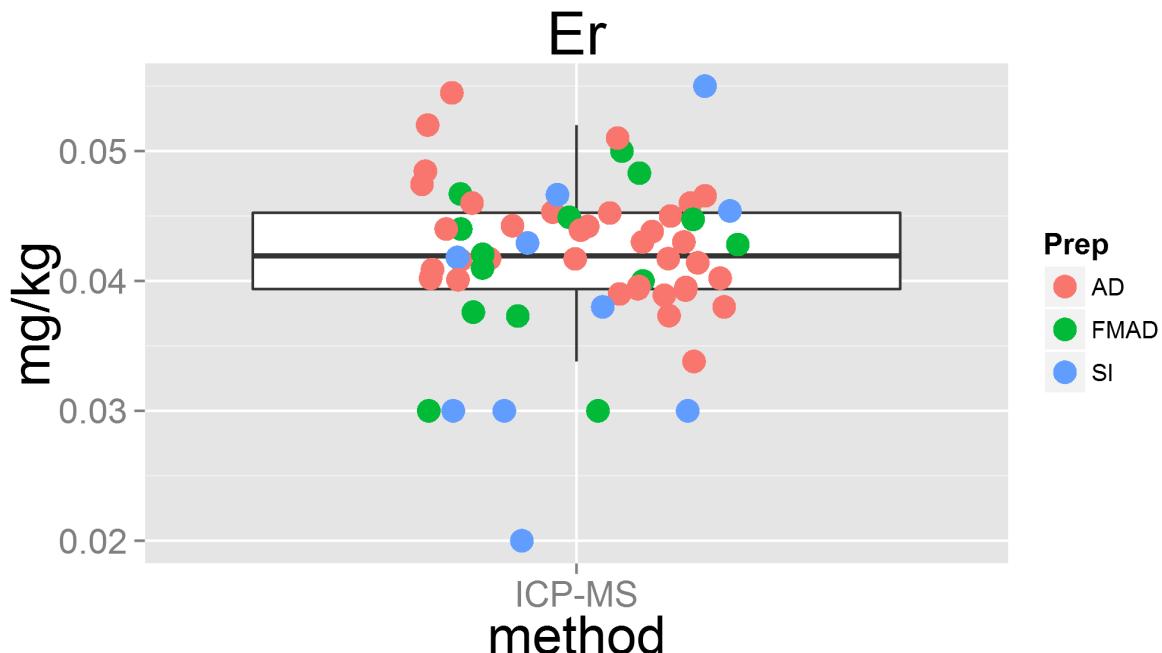
```
## Warning: Removed 5 rows containing missing values (geom_point).
```

```
## Lab 31 was removed
```



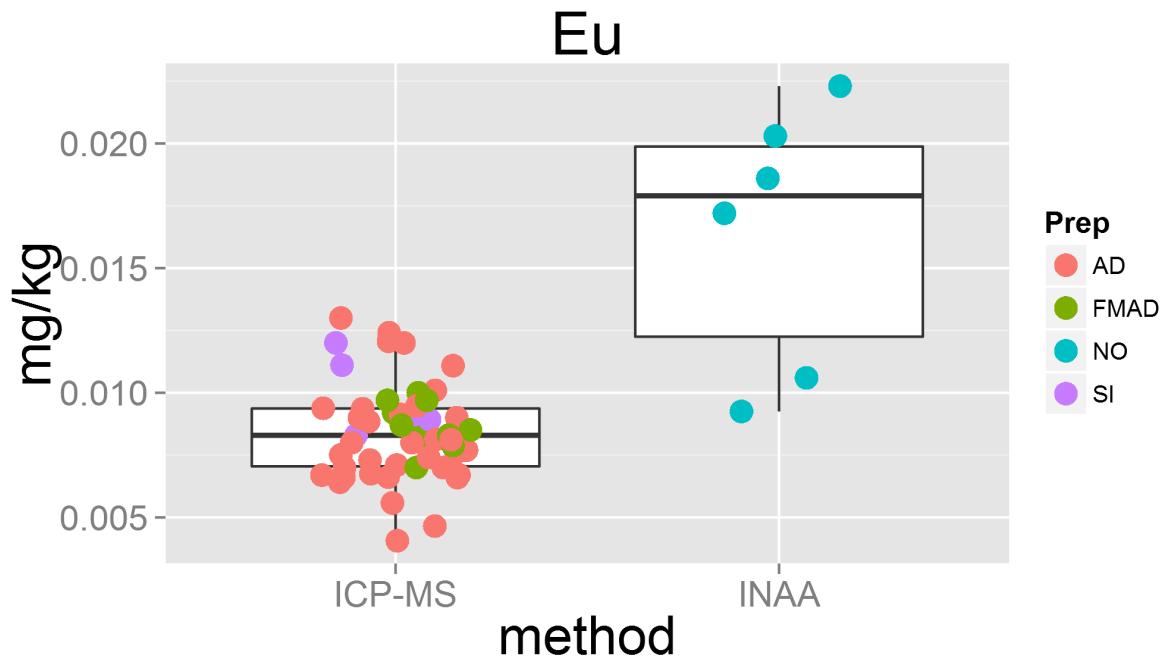
```
## Warning: Removed 8 rows containing missing values (geom_point).
```

```
## Lab 31 was removed
```



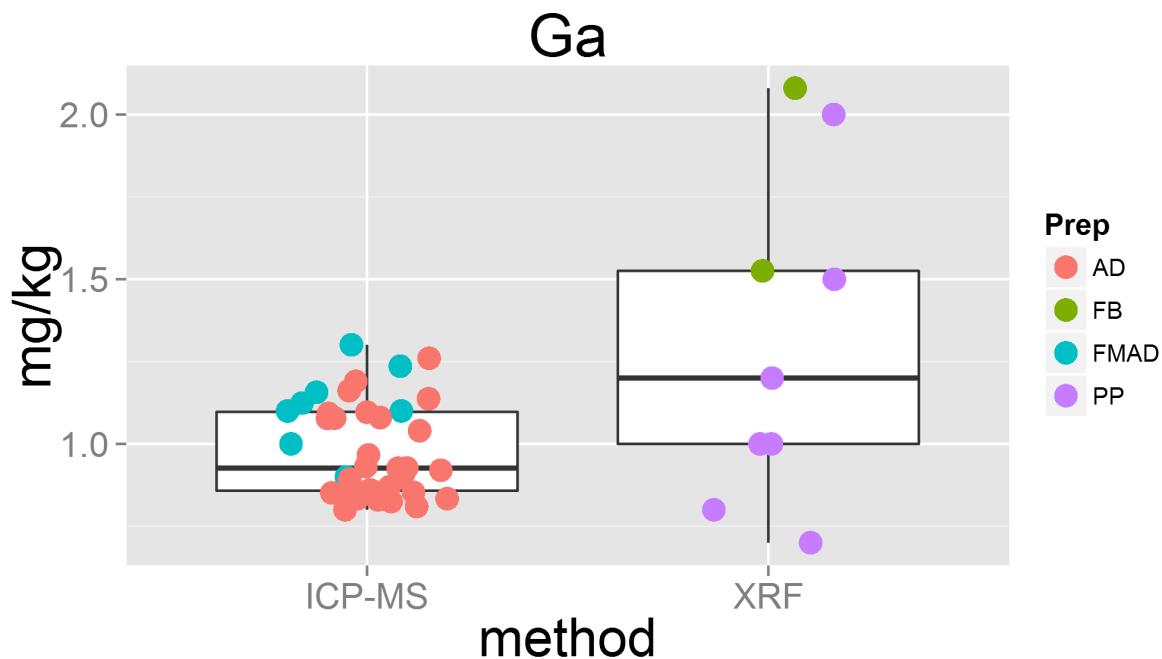
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 31 was removed
```



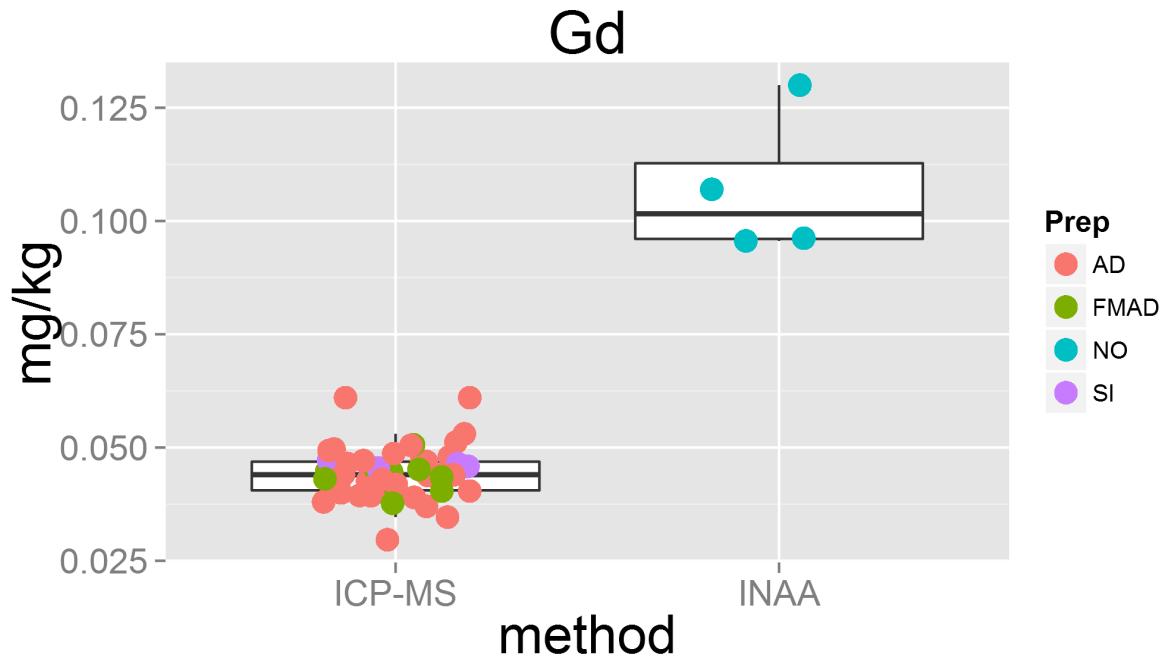
```
## Lab 4 was removed
```

```
## Lab 35 was removed
```



```
## Warning: Removed 3 rows containing missing values (geom_point).
```

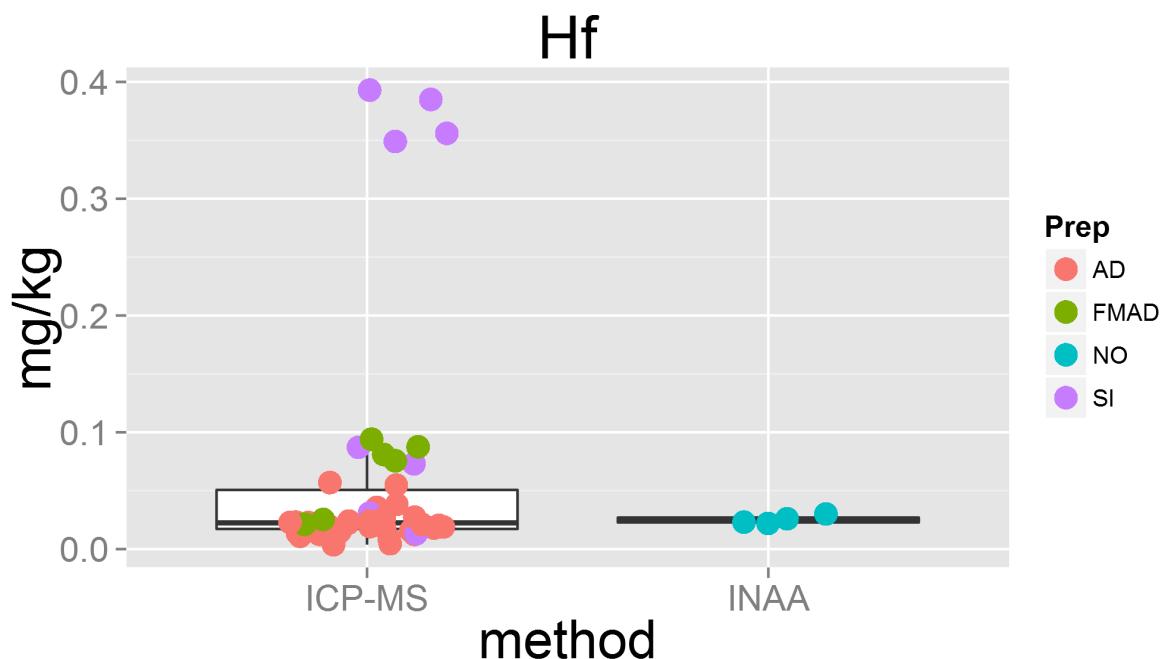
```
## Lab 31 was removed
```



```
## Warning: Removed 4 rows containing missing values (geom_point).
```

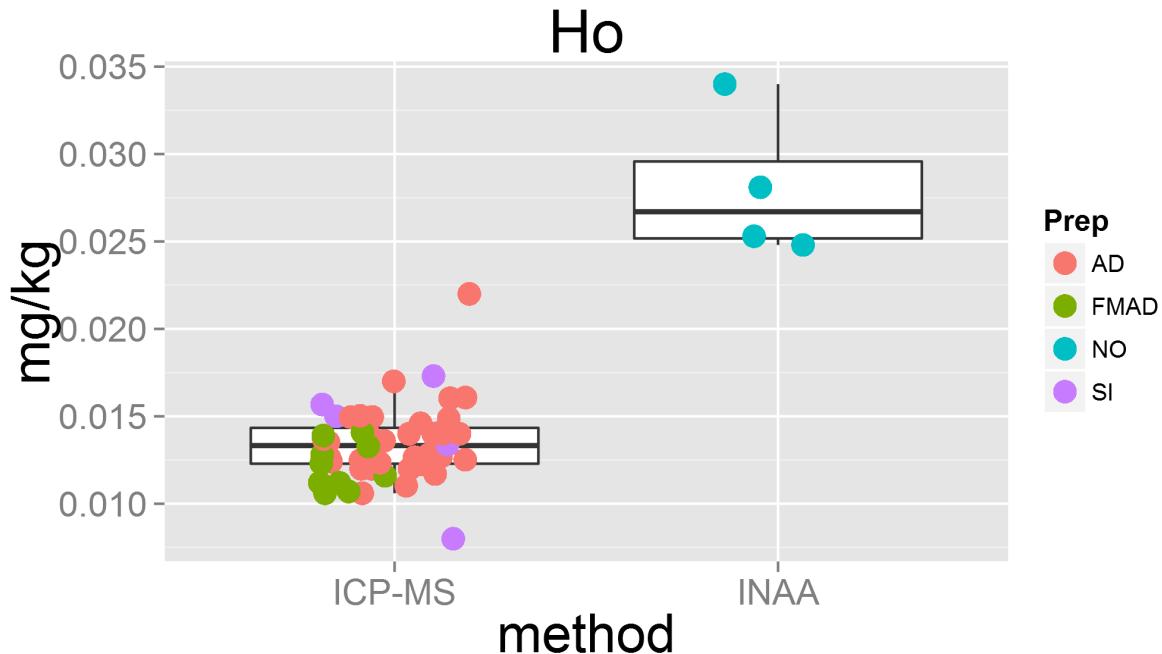
```
## Lab 14 was removed
```

```
## Lab 33 was removed
```



```
## Warning: Removed 2 rows containing missing values (geom_point).
```

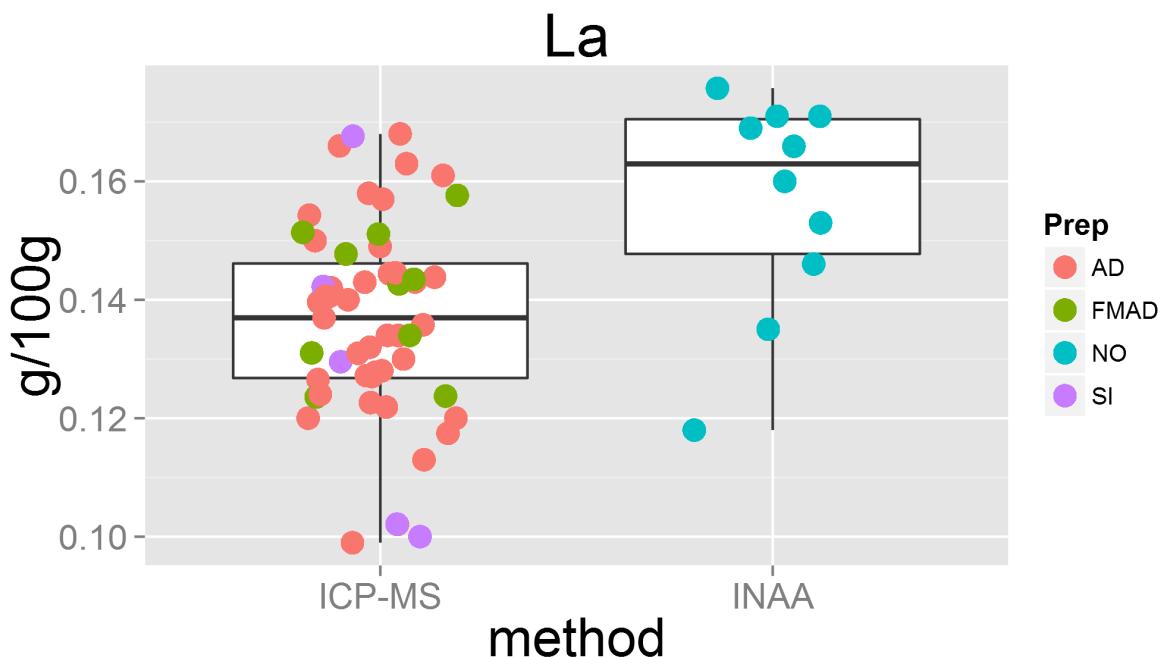
```
## Lab 31 was removed
```



```
## Lab 4 was removed
```

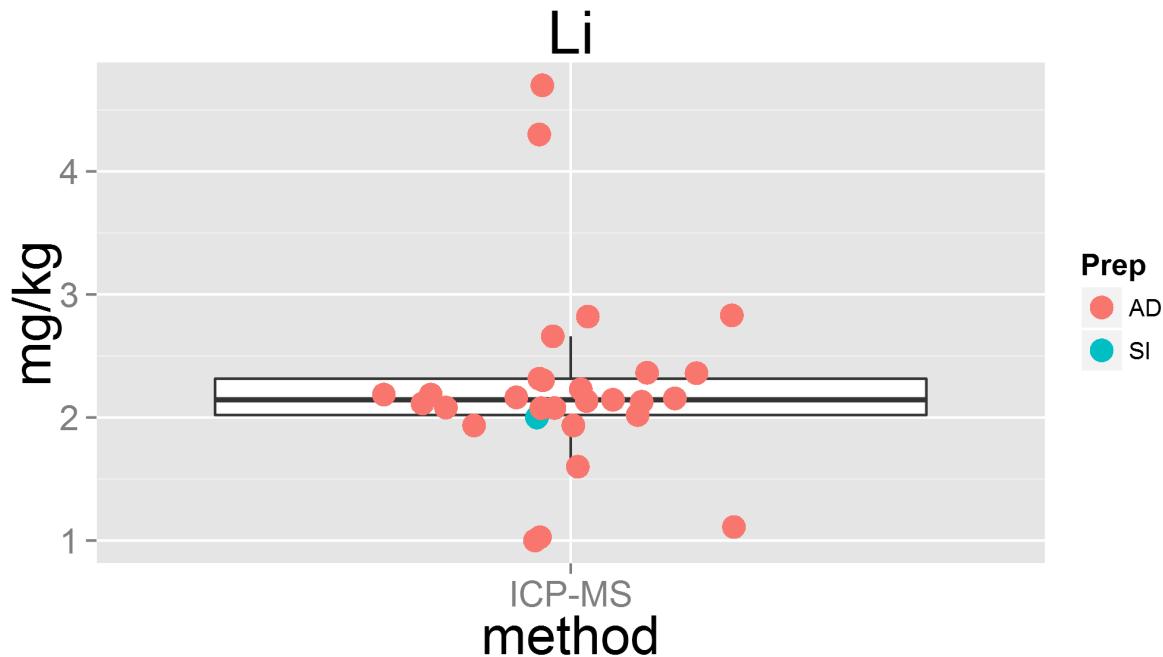
```
## Lab 16 was removed
```

```
## Lab 12 was removed
```



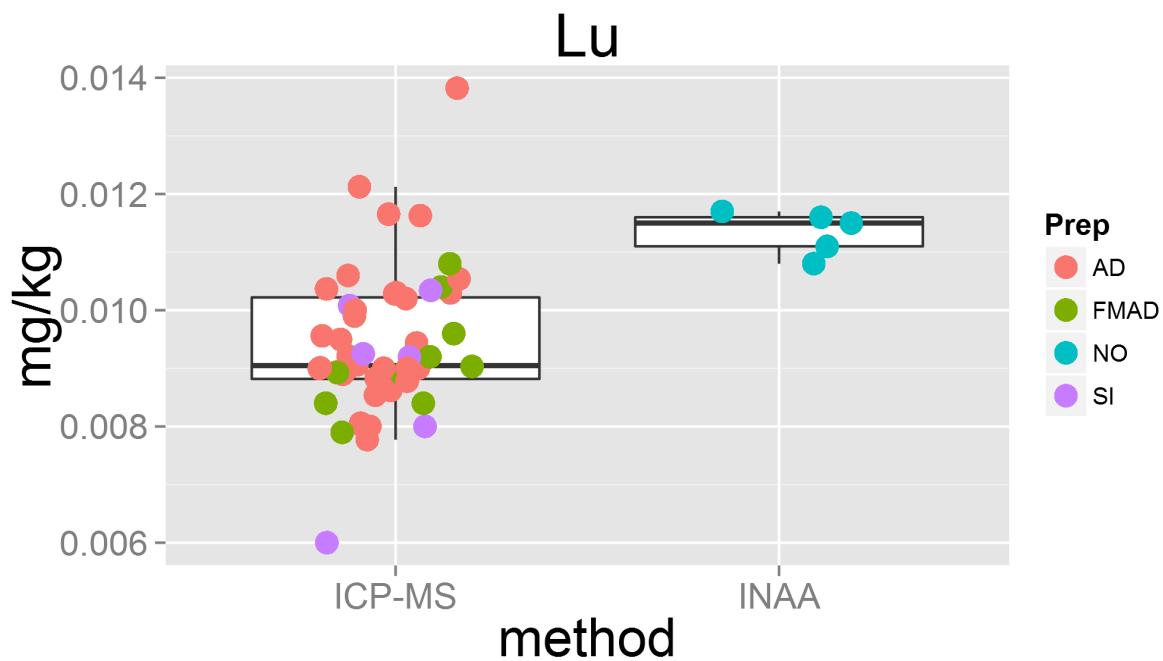
```
## Warning: Removed 7 rows containing missing values (geom_point).
```

```
## Lab 4 was removed  
## Lab 31 was removed
```



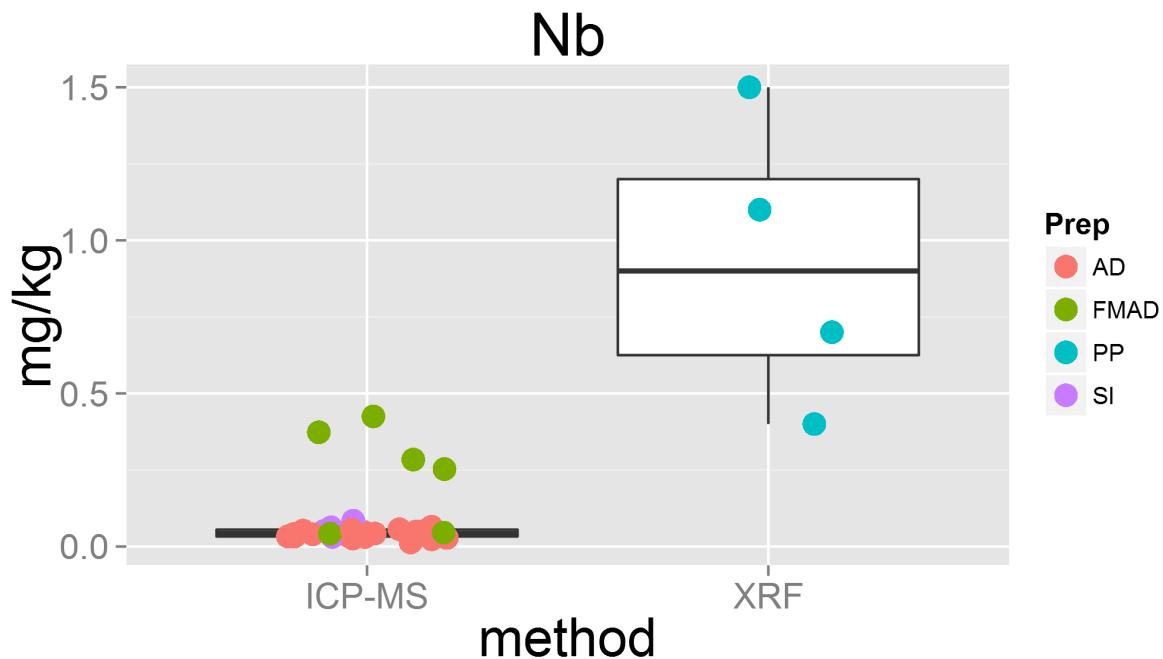
```
## Warning: Removed 2 rows containing missing values (geom_point).
```

```
## Lab 4 was removed
```



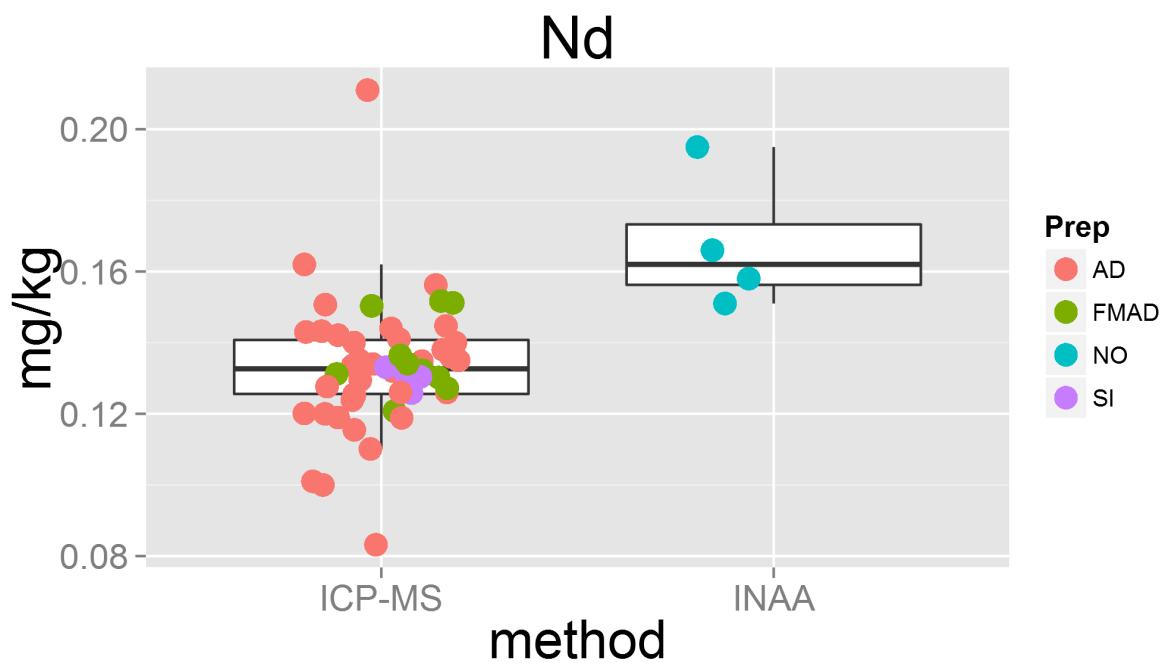
```
## Warning: Removed 4 rows containing missing values (geom_point).
```

```
## Lab 26 was removed  
## Lab 33 was removed
```



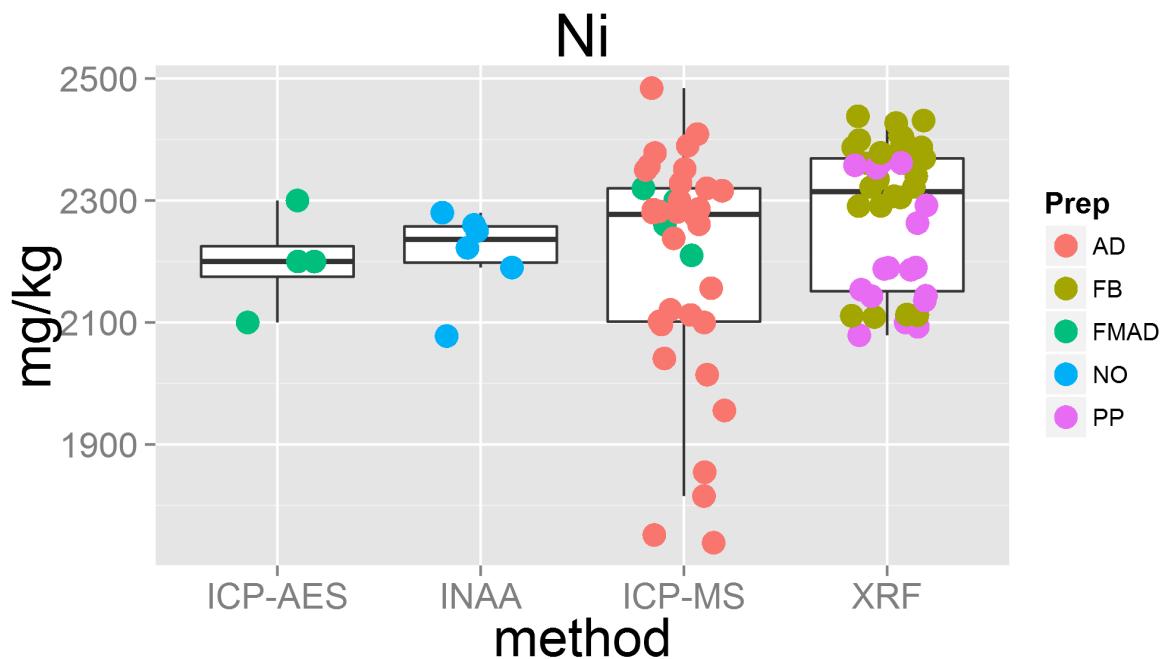
```
## Warning: Removed 4 rows containing missing values (geom_point).
```

```
## Lab 31 was removed
```



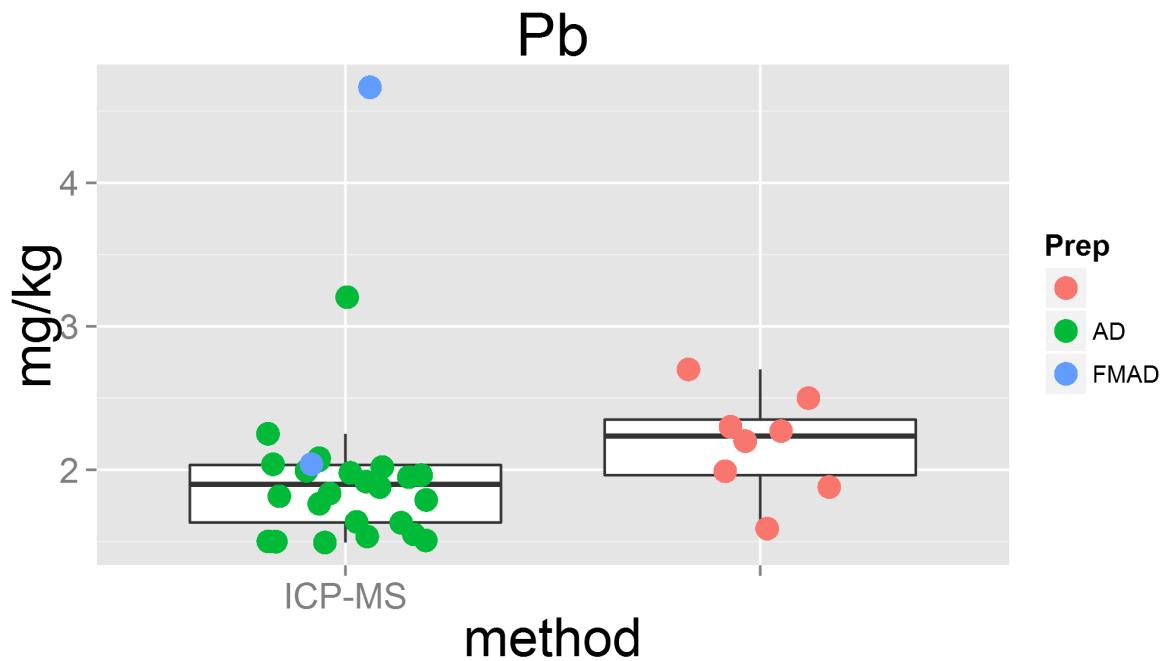
```
## Warning: Removed 1 rows containing missing values (geom_point).  
## Warning: Removed 2 rows containing missing values (geom_point).
```

```
## Lab 12 was removed  
## Lab 18 was removed  
## Lab 22 was removed
```



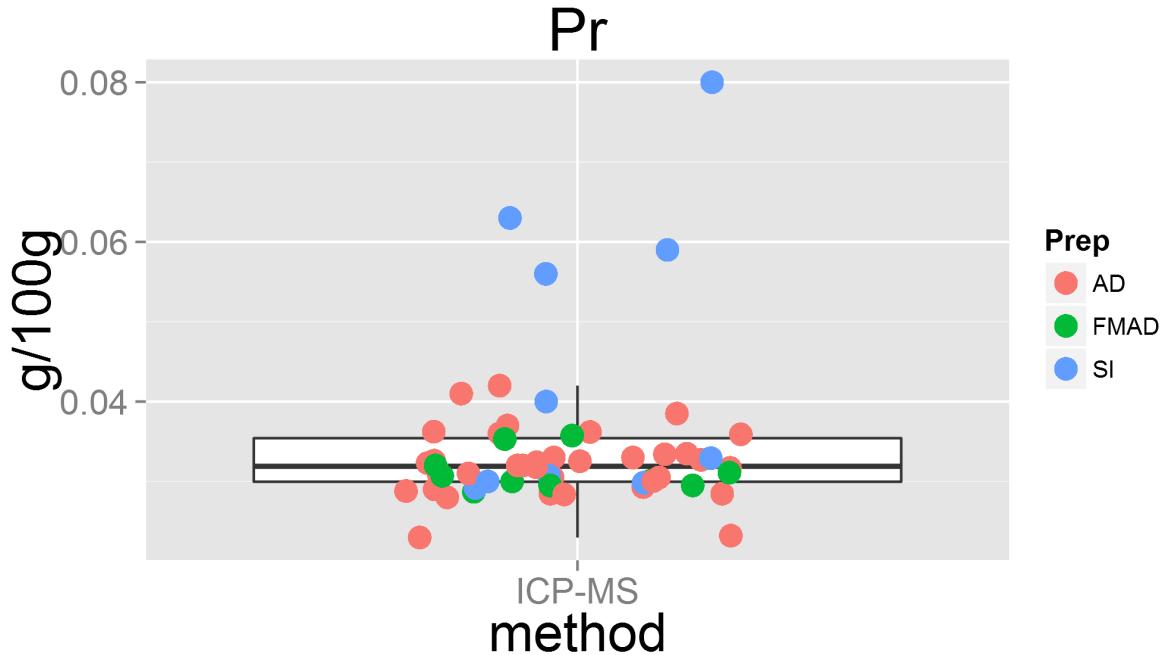
```
## Warning: Removed 2 rows containing missing values (geom_point).
```

```
## Lab 35 was removed
```



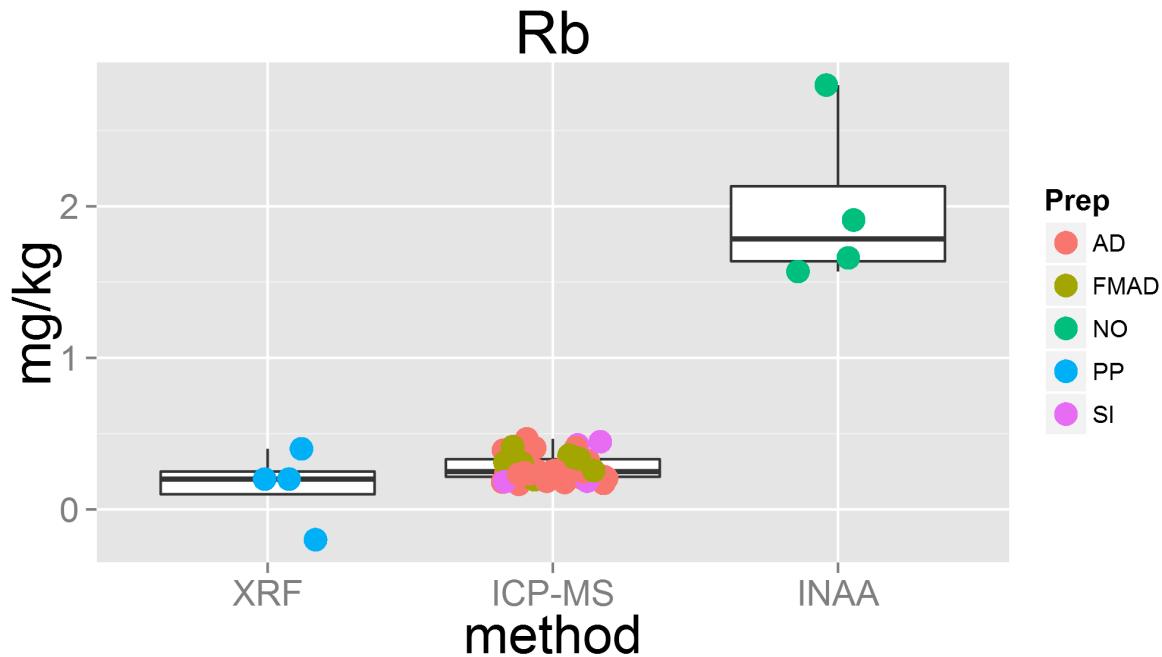
```
## Warning: Removed 4 rows containing missing values (geom_point).
```

```
## Lab 14 was removed
## Lab 31 was removed
```



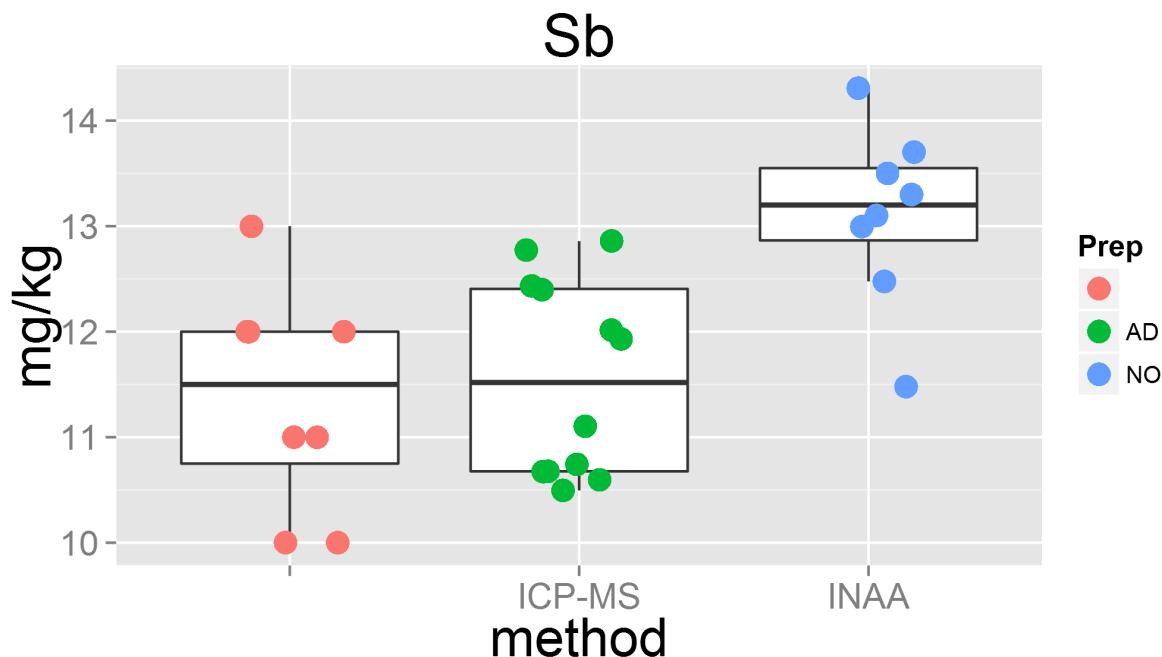
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 31 was removed  
## Lab 26 was removed
```



```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 0 was removed
```

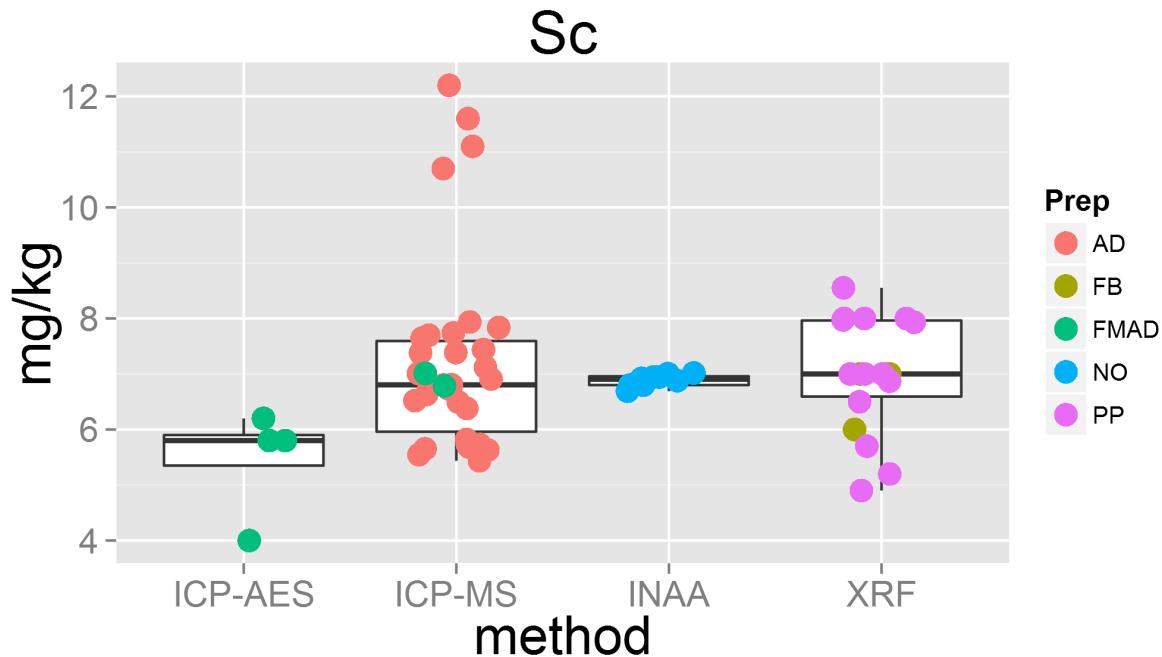


```

## Warning: Removed 1 rows containing missing values (geom_point).
## Warning: Removed 4 rows containing missing values (geom_point).

## Lab 8 was removed

```

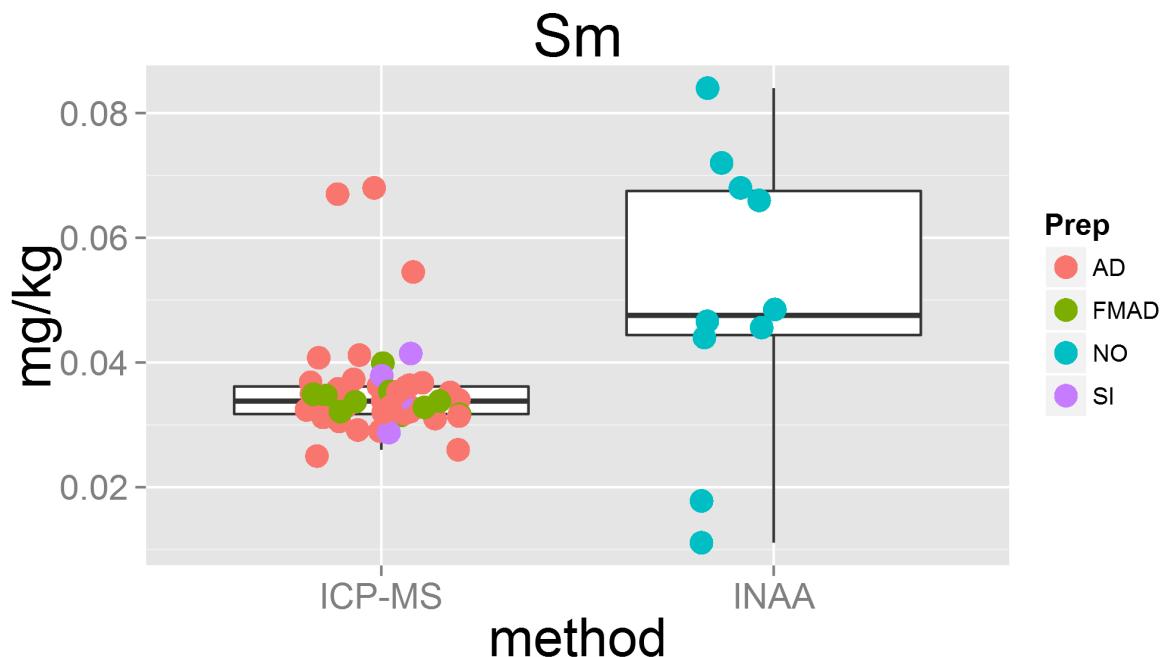


```

## Warning: Removed 4 rows containing missing values (geom_point).

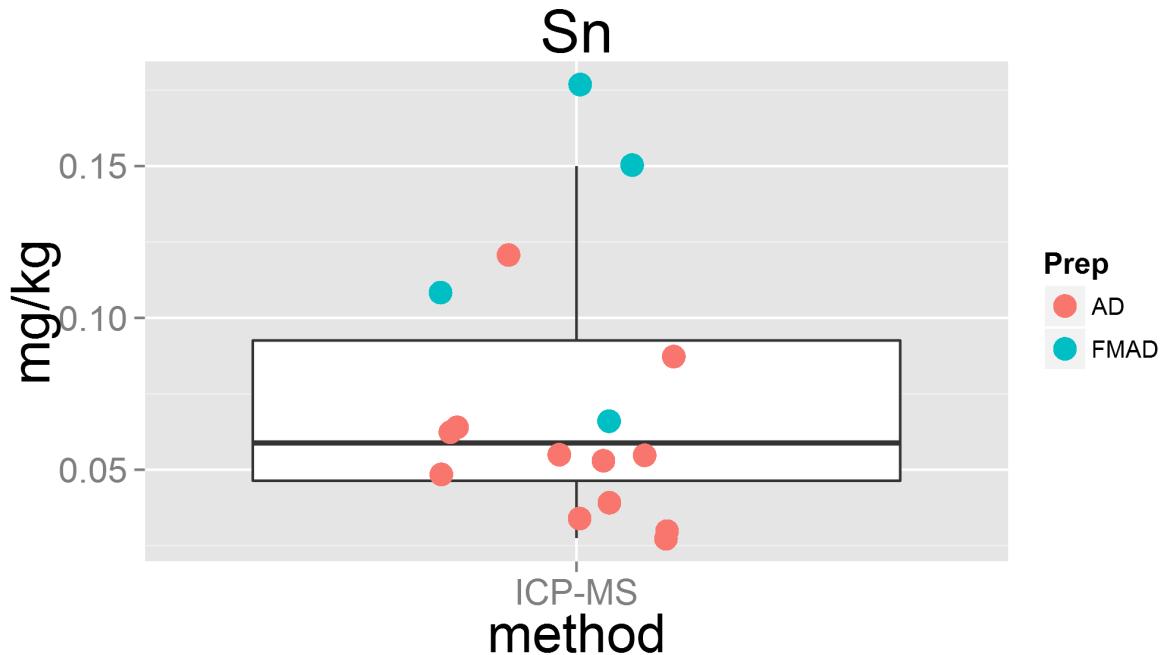
## Lab 0 was removed

```



```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 0 was removed
```

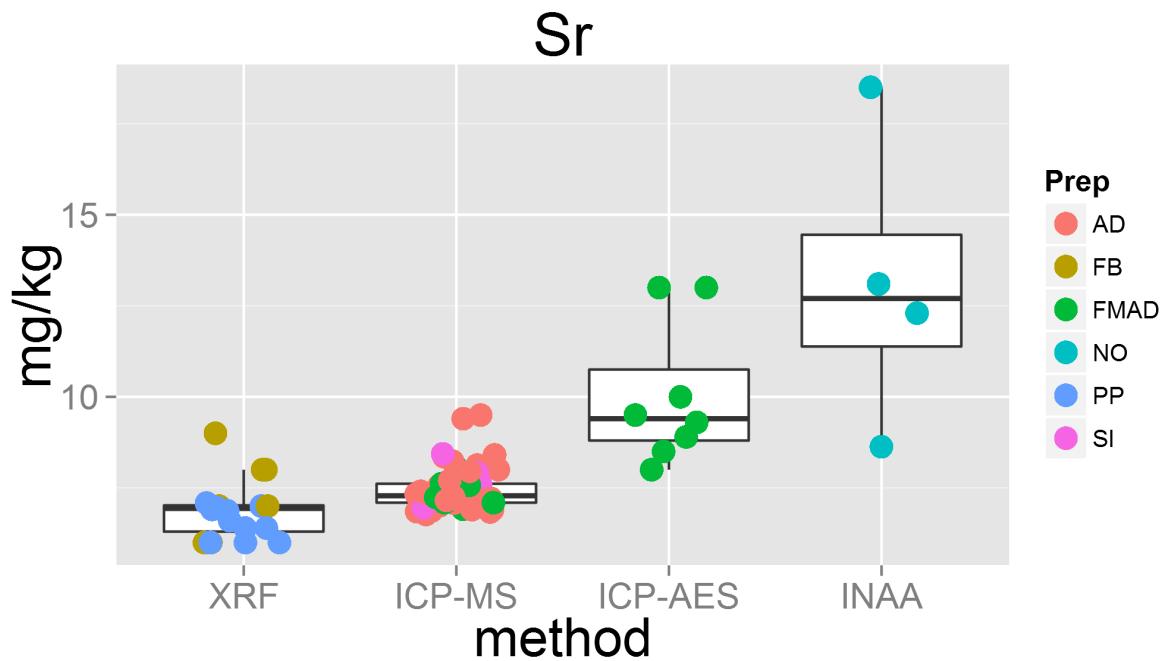


```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Warning: Removed 4 rows containing missing values (geom_point).
```

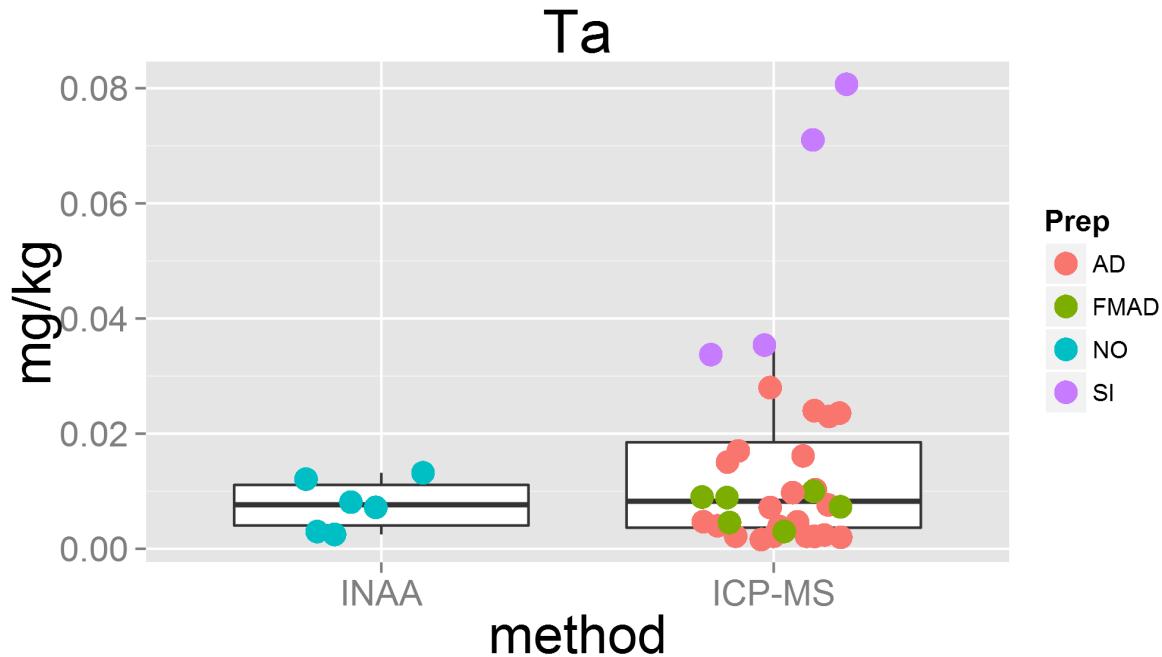
```
## Lab 5 was removed
```

```
## Lab 31 was removed
```



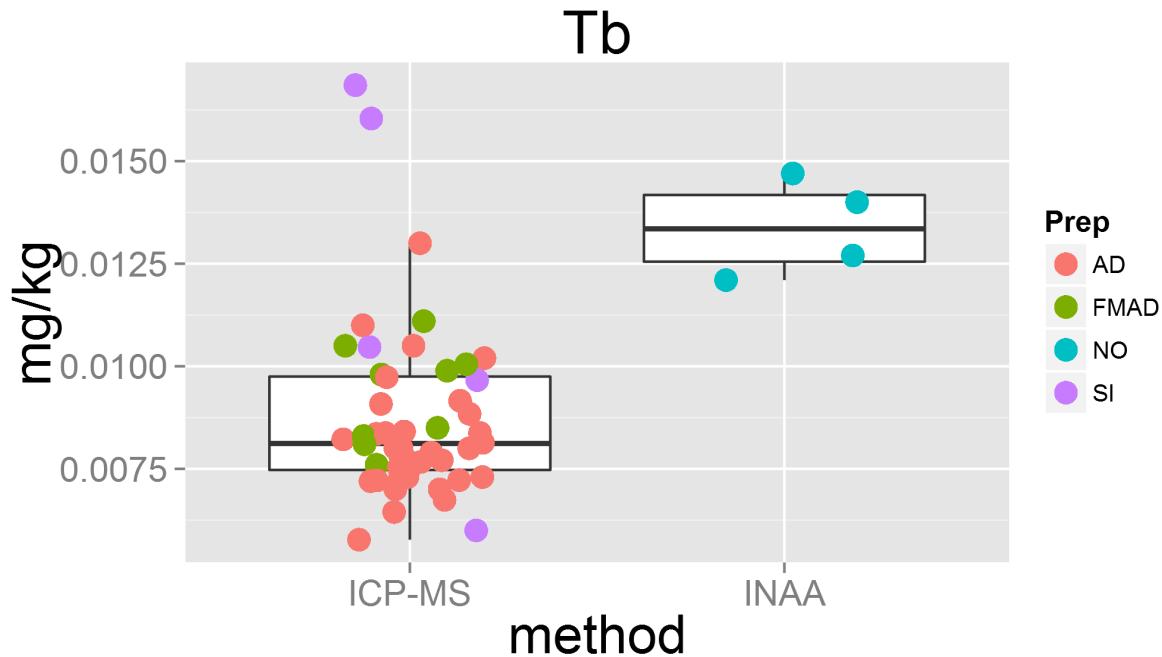
```
## Warning: Removed 2 rows containing missing values (geom_point).
```

```
## Lab 8 was removed
## Lab 21 was removed
```



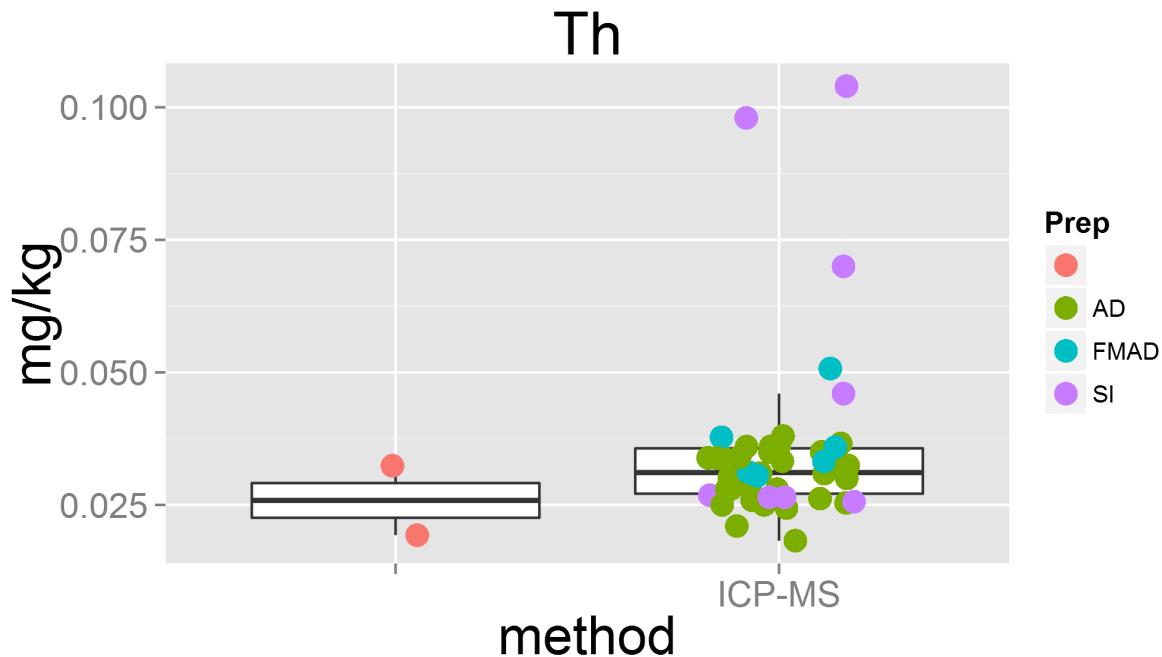
```
## Warning: Removed 2 rows containing missing values (geom_point).
```

```
## Lab 21 was removed  
## Lab 31 was removed
```



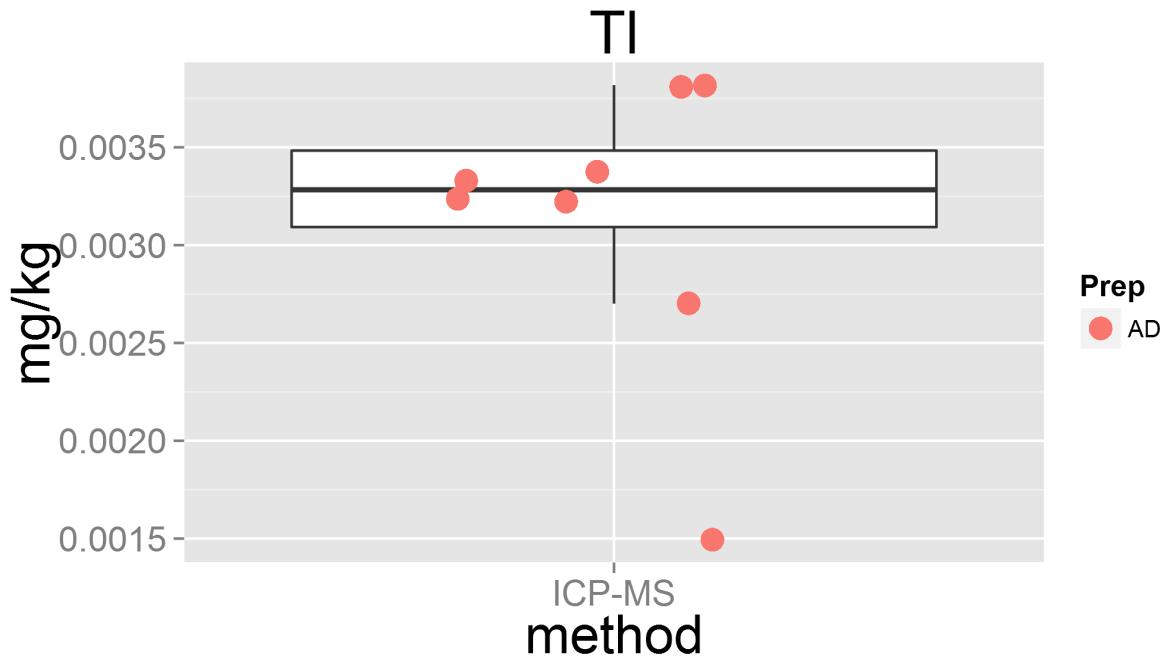
```
## Warning: Removed 4 rows containing missing values (geom_point).
```

```
## Lab 14 was removed
```



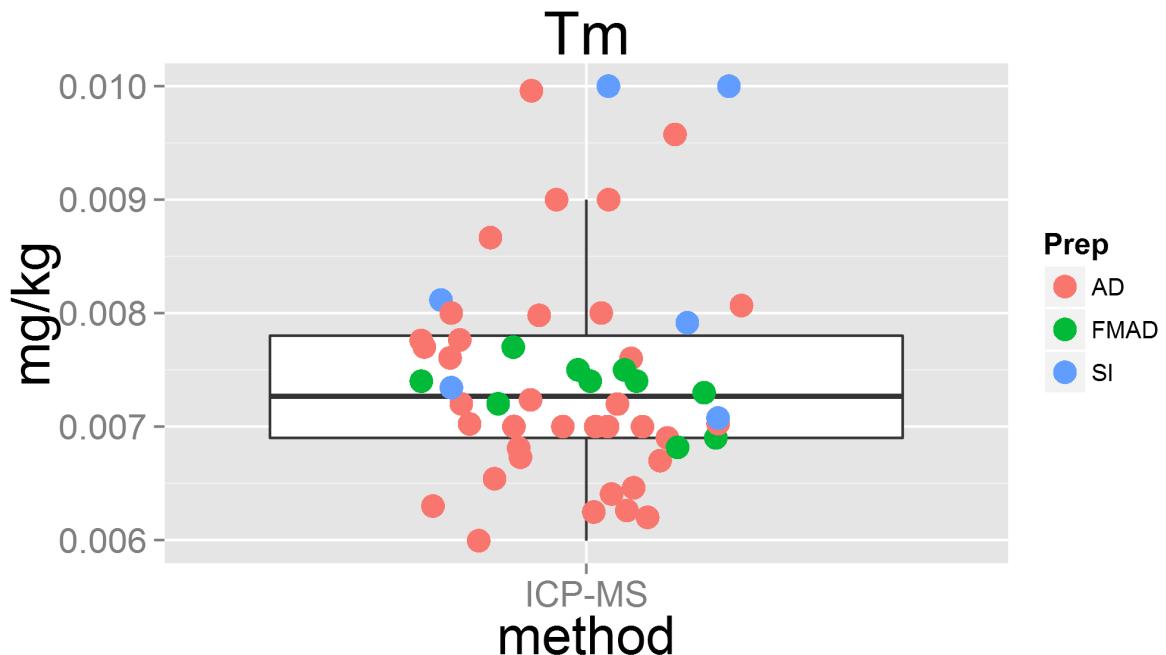
```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Lab 0 was removed
```



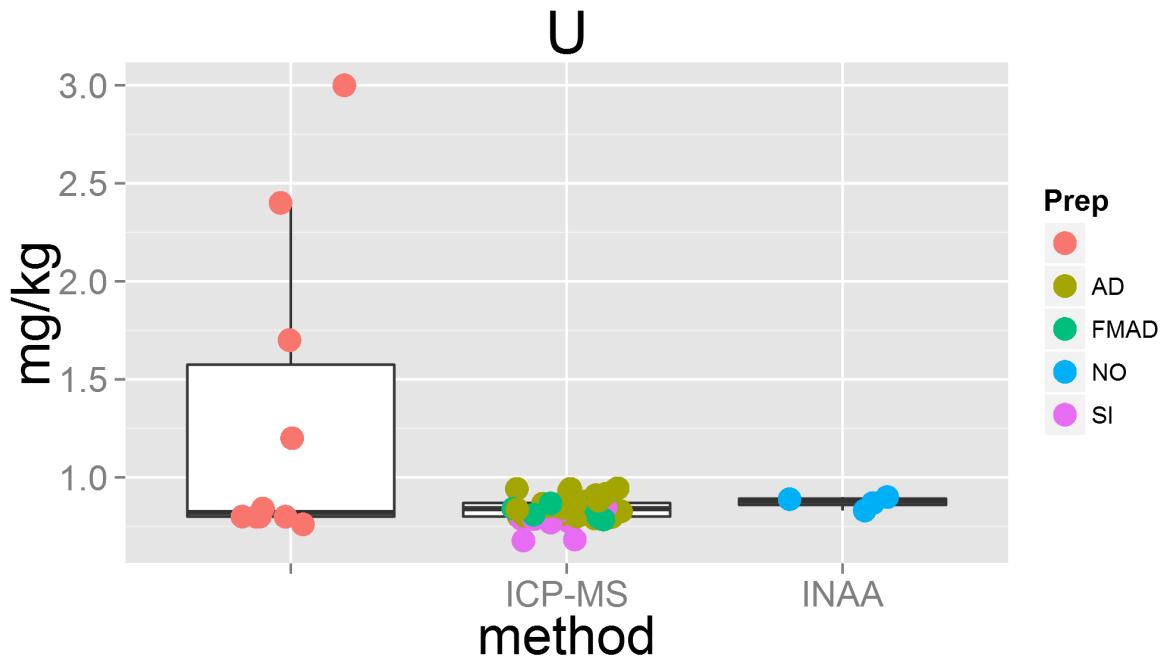
```
## Warning: Removed 4 rows containing missing values (geom_point).
```

```
## Lab 4 was removed
```

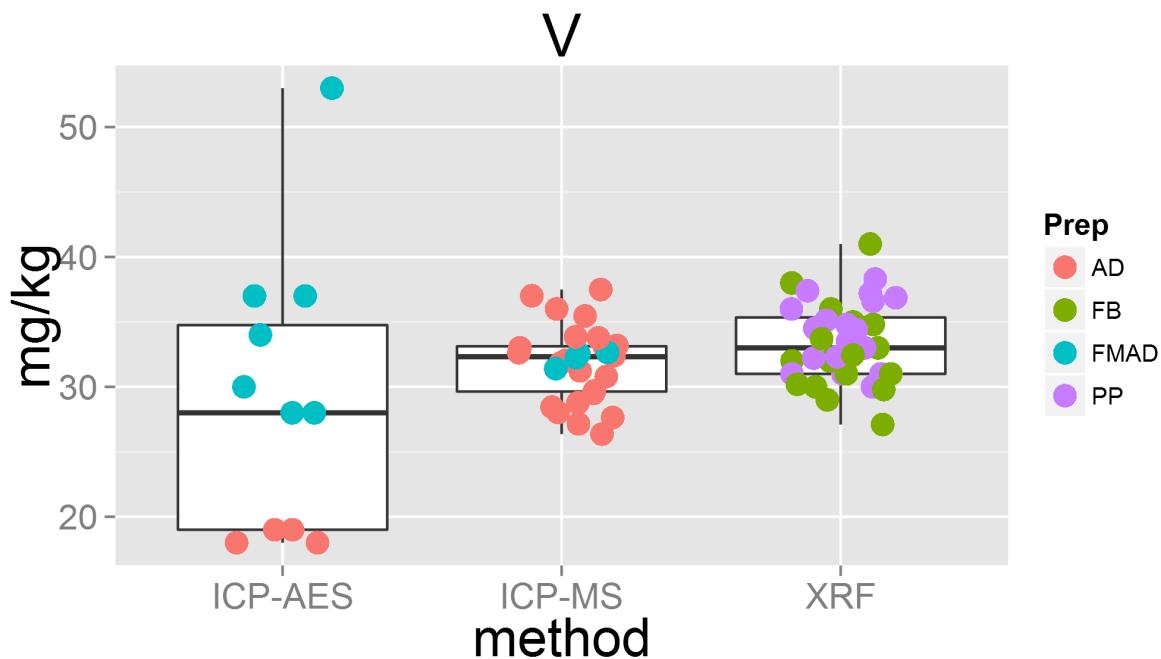


```
## Warning: Removed 1 rows containing missing values (geom_point).  
## Warning: Removed 2 rows containing missing values (geom_point).
```

```
## Lab 26 was removed
```

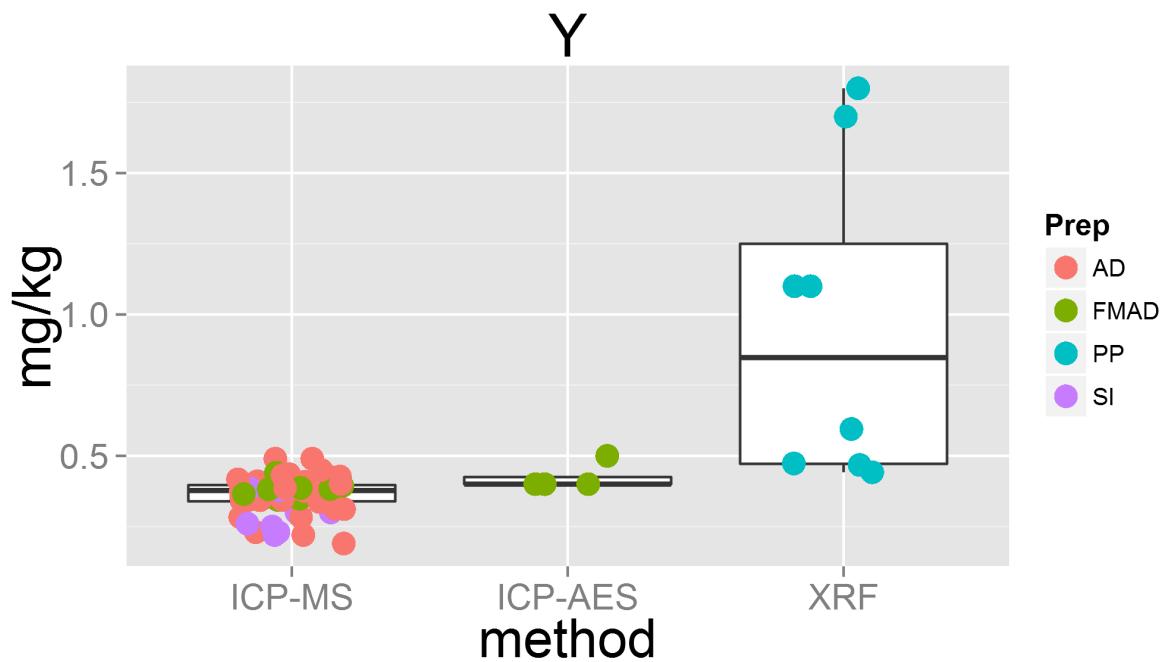


```
## Lab 31 was removed
```



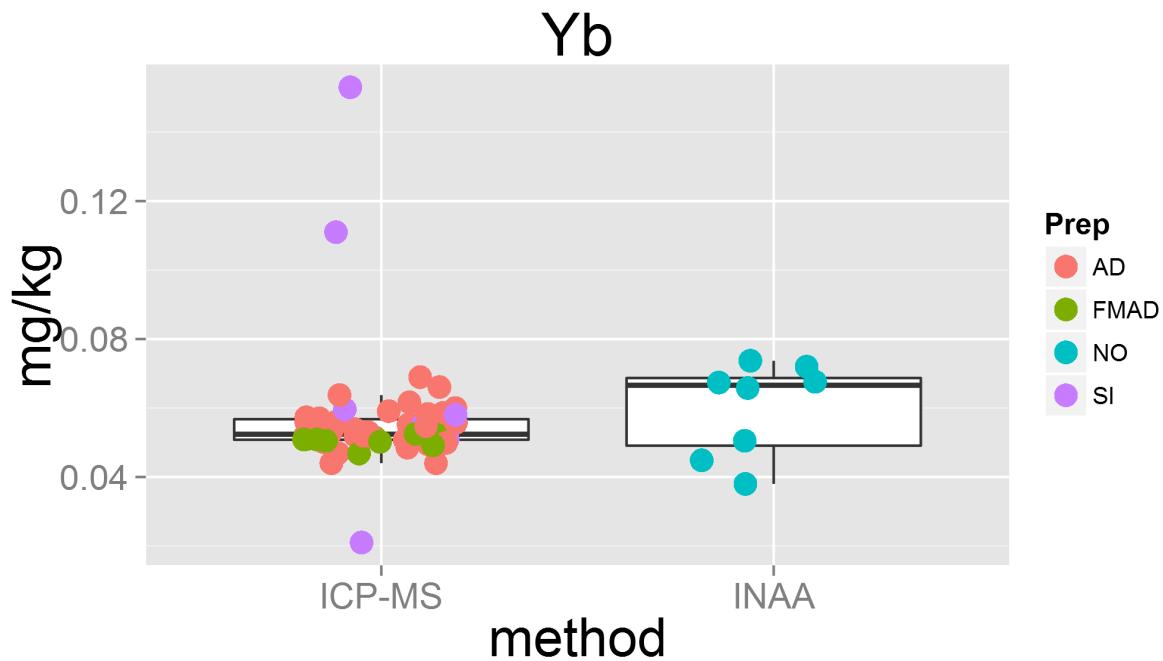
```
## Warning: Removed 9 rows containing missing values (geom_point).
## Warning: Removed 1 rows containing missing values (geom_point).

## Lab 26 was removed
## Lab 31 was removed
```

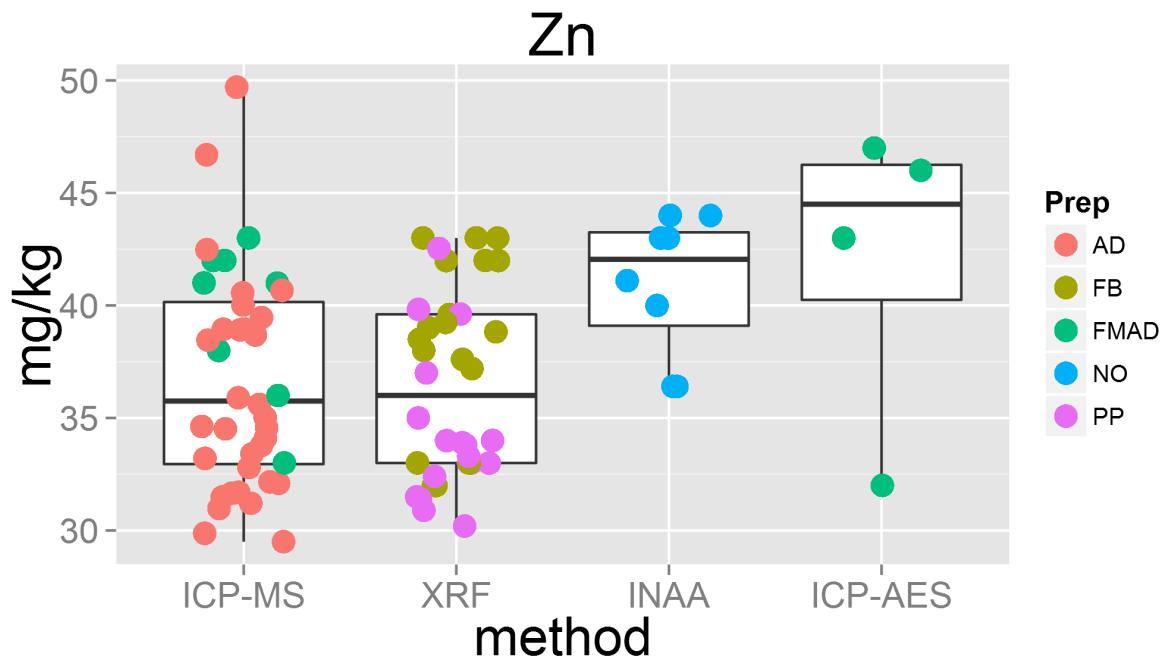


```
## Warning: Removed 5 rows containing missing values (geom_point).

## Lab 14 was removed
```

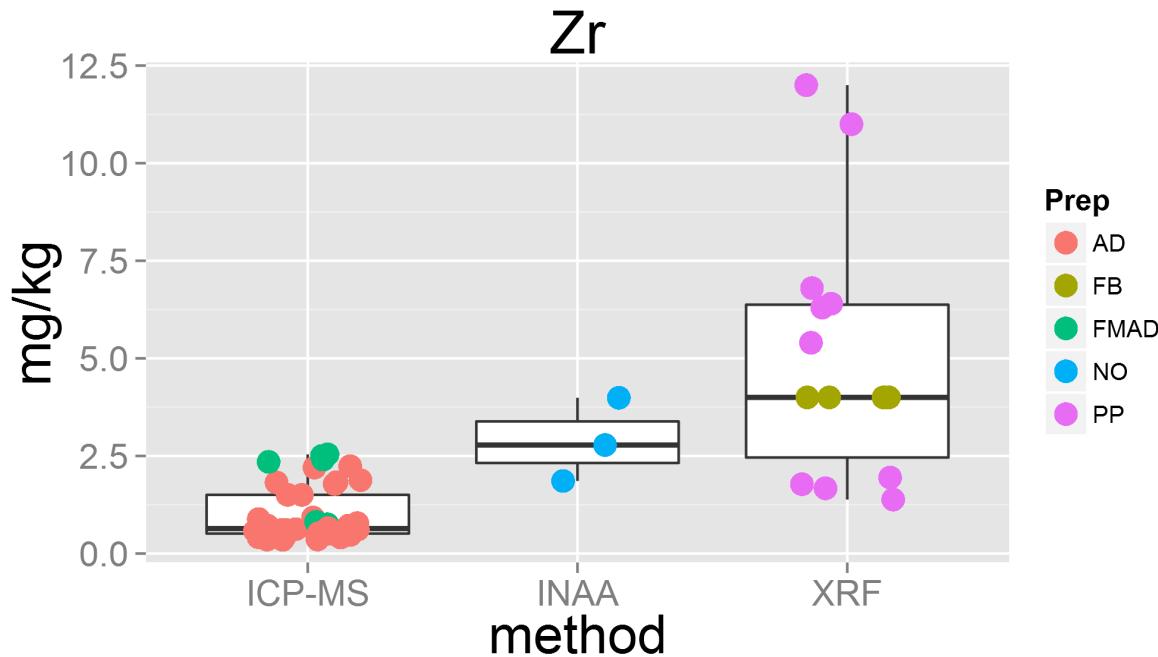


```
## Lab 0 was removed
```



```
## Lab 10 was removed
## Lab 6 was removed
## Lab 26 was removed
## Lab 33 was removed
```

```
## Lab 31 was removed
## Lab 24 was removed
```



```
medianGOM.packet.after <- ddply(GOM, c("Lab", "Packet"), numcolwise(medianGOM)) # median Lab and Packet
## median over median of packets within lab
GOM.median.after <- ddply(medianGOM.packet.after, c("Lab"), numcolwise(medianGOM)) # creating a new table
GOM.median.after <- merge(GOM.median.after, OKUM.methods, by="Lab")
GOM.median.after.df <- data.frame(apply(GOM.median.after[2:56], 2, median, na.rm=TRUE)) # creating a new table
names(GOM.median.after.df) <- c("mass fraction")
meanGOM.packet <- ddply(GOM, c("Lab", "Packet"), numcolwise(meanGOM))
meanGOM.packet.after <- ddply(GOM, c("Lab", "Packet"), numcolwise(meanGOM)) # mean Lab and Packets after
## mean over mean of packets within lab
GOM.mean.after <- ddply(meanGOM.packet.after, c("Lab"), numcolwise(meanGOM)) # creating a new table of mean
GOM.mean.after <- merge(GOM.mean.after, OKUM.methods, by="Lab")
GOM.mean.after.df <- data.frame(apply(GOM.mean.after[2:56], 2, mean, na.rm=TRUE)) # creating a new table
names(GOM.mean.after.df) <- c("mass fraction")
```

Nested random effects in data analysis: two way ANOVA

This model can be used when the results of the interlaboratory study are used to confirm the homogeneity of the material as well as to characterise it. The experimental scheme is illustrated in Fig X for the particular case of the IAG protocol. When the ILC consists of different methos, the result can be expressed by the equation

$$x_{ijk} = \mu + A_i + B_{ij} + \epsilon_{ijk}$$

where

x_{ijk} is the k th result of sample unit j reported from method/laboratory i ,

A_i is the error due to method/laboratory i ,

B_{ij} is the error due to the j th sample unit within method/laboratory i , ϵ_{ijk} is the measurement error.

The parameters to be estimated are the grand mean, the between-laboratory standard deviation s_L , the between-bottle standard deviation s_{bb} and the repeatability standard deviation s_r . They are related as follows

$$\begin{aligned}s_L &= \sqrt{\text{Var}(A_i)} \\ s_{bb} &= \sqrt{\text{Var}(B_{ij})} \\ s_r &= \sqrt{\text{Var}(\epsilon_{ijk})}\end{aligned}$$

The formulae for computing the above-mentioned estimates read as follows. The grand mean is computed using

$$\bar{x} = \frac{1}{\sum_{i=1}^p \sum_{j=1}^{b_i} n_{ij}} \sum_{i=1}^p \sum_{j=1}^{b_i} \sum_{k=1}^{n_{ij}} x_{ijk}$$

where p denotes the number of laboratories, b_i the number of bottles used by method/laboratory i , and n_{ij} is the number of replicates measured on bottle ij . The variances are computed as follows

$$\begin{aligned}\text{Var}(\epsilon_{ijk}) &= MS_{within} = s_r^2 \\ \text{Var}(B_{ij}) &= \frac{MS_{B \subset A} - MS_{within}}{n_0} = s_{bb}^2 \\ \text{Var}(A_i) &= \frac{MS_{among} - n'_0 \text{Var}(B_{ij}) - \text{Var}(\epsilon_{ijk})}{(nb)_0} = s_L^2\end{aligned}$$

where

$$\begin{aligned}MS_{among} &= \frac{\sum_{i=1}^p n_i (\bar{x}_A - \bar{x})^2}{p-1} \\ MS_{B \subset A} &= \frac{\sum_{i=1}^p \sum_{j=1}^{b_i} n_{ij} (\bar{x}_B - \bar{x}_A)^2}{\sum_{i=1}^p b_i - p} \\ MS_{within} &= \frac{\sum_{i=1}^p \sum_{j=1}^{b_i} \sum_{k=1}^{n_{ij}} (x_{ijk} - \bar{x}_B)^2}{\sum_{i=1}^p \sum_{j=1}^{b_i} n_{ij} - \sum_{i=1}^p b_i}\end{aligned}$$

and

$$\begin{aligned}n'_0 &= \frac{\sum_{i=1}^p \left(\frac{\sum_{j=1}^{b_i} n_{ij}^2}{\sum_{j=1}^{b_i} n_{ij}} \right) - \sum_{i=1}^p \sum_{j=1}^{b_i} n_{ij}^2}{p-1} \\ n_0 &= \frac{\sum_{i=1}^p \sum_{j=1}^{b_i} n_{ij} - \sum_{i=1}^p \left(\frac{\sum_{j=1}^{b_i} n_{ij}^2}{\sum_{j=1}^{b_i} n_{ij}} \right)}{\sum_{i=1}^p b_i - p} \\ (nb)_0 &= \frac{\sum_{i=1}^p \sum_{j=1}^{b_i} n_{ij} - \frac{\sum_{i=1}^p (\sum_{j=1}^{b_i} n_{ij})^2}{\sum_{i=1}^p \sum_{j=1}^{b_i} n_{ij}}}{p-1}\end{aligned}$$

solutions of the above equations in R

ANOVA is calculated based on a linear model using the "linear mixed effects models" of package nlme (lme {nlme})

GOM.lme <- lme(measurand ~ 1, random = ~ 1|Lab, data=DF.lme) # linear model with random effects

the variance components are extracted with package ape (varcomp {ape})

$$\begin{aligned}s_L^2 &= sL2 <- varcomp(GOM.lme, FALSE, FALSE)[[1]] \# between-laboratory variance \\ s_{bb}^2 &= sbb2 <- varcomp(GOM.lme, FALSE, FALSE)[[2]] \# between bottle variance \\ s_r^2 &= sr2 <- varcomp(GOM.lme, FALSE, FALSE)[[3]] \# repeatability standard deviation\end{aligned}$$

The characterisation uncertainty u_{char} is calculated

$$u1 <- sqrt(sL2/p+sbb2/p+r+sr2/p/r/4)$$

which is equivalent to

$$u_1 = \sqrt{\frac{s_L^2}{p} - \frac{s_r^2}{np} - \frac{s_{bb}^2}{npr}}$$

This approach is not completely correct as it assumes 4 replicates per bottle

```
u2 <- attr(GOM.lme$fixDF, "varFixFact") # this approach takes unbalanced data into account and is used for all further calculations.
```

The between day variance is neglected here but the uncertainty component due to inhomogeneity is taken into account through the s_{bb}^2 component.

```
for (m in col.names) {
  measurand.name <- m
  switch(
    reformat,
    GAS = rm1 <- 2,
    MUH = rm1 <- 1,
    OKUM = rm1 <- 0
  )
  if(rm1 > 0)
  {measurand <- measurand.name %p% '.' %p% rm1
  } else
  {
    measurand <- measurand.name
  }
  MorT <- grep(measurand.name, colnames(GOM), fixed=TRUE) # finding the position of the measurand.name
  ifelse(MorT[1] < 21, MorT <- 'M', MorT<-'T') # testing if measurand is a major or trace element/compound
  ifelse(MorT == "T", unit <- 'mg/kg', unit <- 'g/100g') # testing which unit is needed
  ## calculating method parameters
  # '%p%' <- function(x, y) {as.character(paste(x, y, sep = ""))}
  mean <- mean(tapply(GOM[[measurand]], GOM$Lab, mean, na.rm=TRUE), na.rm=TRUE)
  mean.before <- mean(GOM.mean[[measurand]], na.rm=TRUE)
  median.before <- median(GOM.median[[measurand]], na.rm=TRUE)
  median.after <- median(GOM.median.after[[measurand]], na.rm=TRUE) # median of the individual measurand
  prep <- 'Prep.'
  method <- 'Method.'
  anal.prep <- prep %p% measurand.name
  anal.method <- method %p% measurand.name
  anal <- GOM.median.after[[measurand]]
  anal.prep <- GOM.median.after[[anal.prep]]
  anal.method <- GOM.median.after[[anal.method]]
  analyte <- data.frame(GOM.median.after$Lab, GOM.median.after$names, anal, anal.prep, anal.method)
  analyte <- na.omit(analyte)

  bymethod.n <- dplyr::summarise(analyte, c("anal.method"), summarise,
    N=length(anal),
    mean = round(mean(anal), 3),
    median = round(median(anal), 3),
    sd = round(sd(anal), 3),
    se = round(sd/sqrt(N), 3))

  meanGOM.packet.after$Lab <- as.factor(meanGOM.packet$Lab) # using only the median of the 3 packages per
  meanGOM.packet.after$Packet <- as.factor(meanGOM.packet$Packet)
  anal <- meanGOM.packet.after[[measurand]]
  DF.lme <- data.frame(meanGOM.packet.after$Lab, meanGOM.packet.after$Packet, meanGOM.packet.after[[measurand]])
  DF.lme <- na.omit(DF.lme)
```

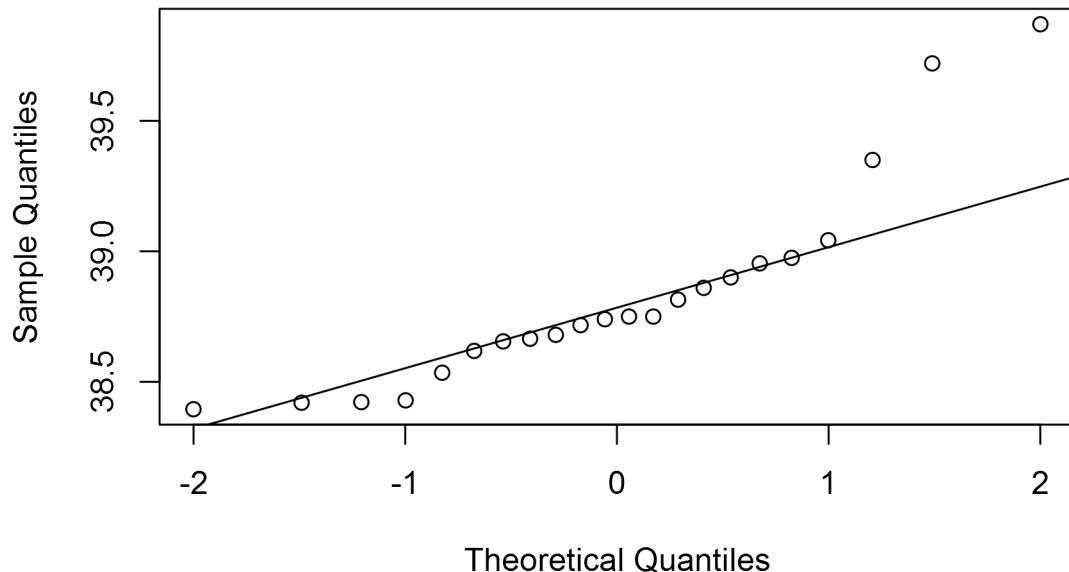
```

names(DF.lme) <- c("Lab", "Packet", "measurand")
GOM.lme <- lme(measurand ~ 1, random = ~ 1|Lab, data=DF.lme) # linear model with random effects
sL2.a <- varcomp(GOM.lme, FALSE, FALSE)[[1]] # between-laboratory variance
sbb2.a <- varcomp(GOM.lme, FALSE, FALSE)[[2]] # between bottle standard deviation
#sr2.a <- varcomp(GOM.lme, FALSE, FALSE)[[3]] # repeatability standard deviation
n.p <- dim(DF.lme)[1] # number of observations
p <- length(unique(DF.lme$Lab)) # haven't found a better way how to extract the number of labs (number of
r <- length(unique(DF.lme$Packet))
t.value <- qt(0.975,df=p-1)
u1.a <- sqrt(sL2.a/p+sbb2.a/p/r) # calculating the standard uncertainty of characterization
u2.a <- attr(GOM.lme$fixDF,"varFixFact") # gives the same results as u1, amazing!
# plot(DF.lme)
analyte.noPP <- subset(analyte, analyte$anal.prep!="PP") # Removing all PP preparations for comparison
median.after.noPP <- median(analyte.noPP$anal)
outlier <- ifelse(outlier=="0", "X", outlier)
print(measurand)
qqnorm(GOM.median.after[[measurand]])
qqline(GOM.median.after[[measurand]])
reference.line <- median.after
u.Ulim <- median.after + u2.a*t.value
l.Ulim <- median.after - u2.a*t.value
bymethod <- ggplot(bymethod.n, aes(x=anal.method, y=median))+geom_point(size=4)+geom_errorbar(aes(ymin=,
plot.lab <- plot_lab(measurand, MorT, horw = FALSE, u = TRUE)
# grid.arrange(bymethod, plot.lab, ncol=2)
print(plot.lab)
# print(bymethod.n)
outlier.type.name <- measurand.name %p% ".outlier.type" # defining if outlier is selected ("Y" or NA)
outlier.dist.type <- measurand.name %p% ".dist.type" # defining if outlier is based on Y = Youden plot,
out.measurand <- data.frame(GAS.outlier[[measurand.name]], GAS.outlier[[outlier.type.name]], GAS.outlier[[outlier.dist.type]])
# out.measurand <- cbind(GAS.outlier[[measurand.name]], GAS.outlier[[outlier.type.name]])
names(out.measurand) <- c("outlier.lab", "outlier.type", "outlier.dist" )
property.value.dist.type <- out.measurand[1,3]
property.value <- ifelse(property.value.dist.type == "median", median.after, mean)
df <- data.frame(Sys.Date(), refmat, measurand.name, signif(mean.before, 4), signif(mean,4), signif(med,
write.table(df, "df3.txt", row.names=FALSE, append=TRUE, col.names=FALSE)
}

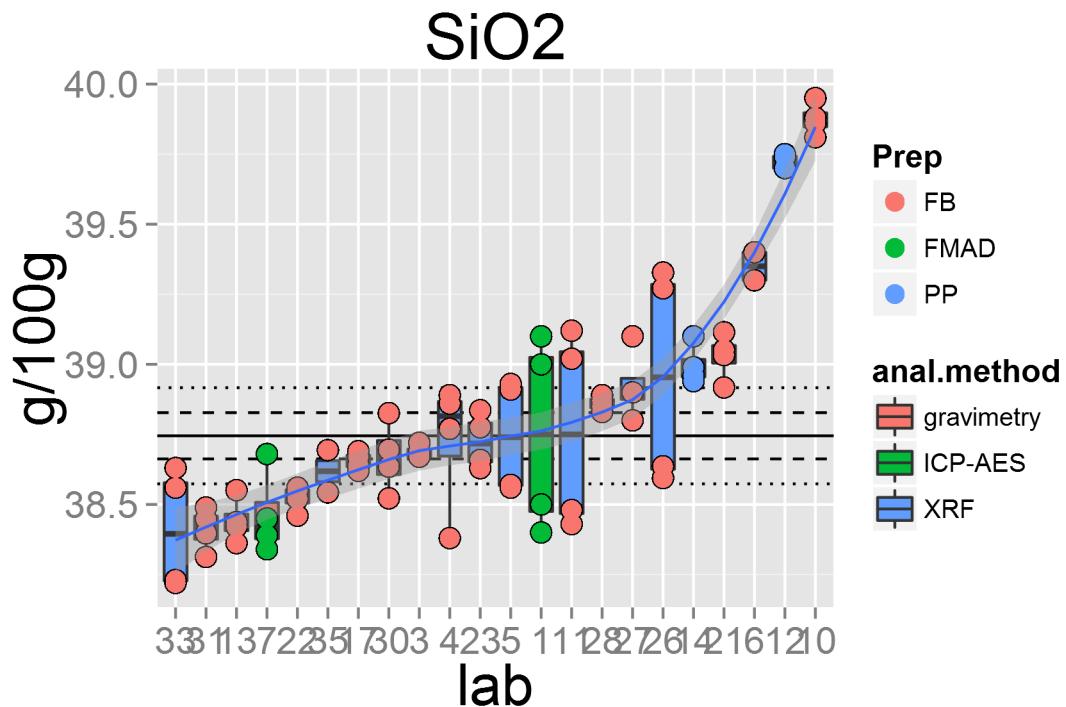
## [1] "Si02.2"

```

Normal Q-Q Plot

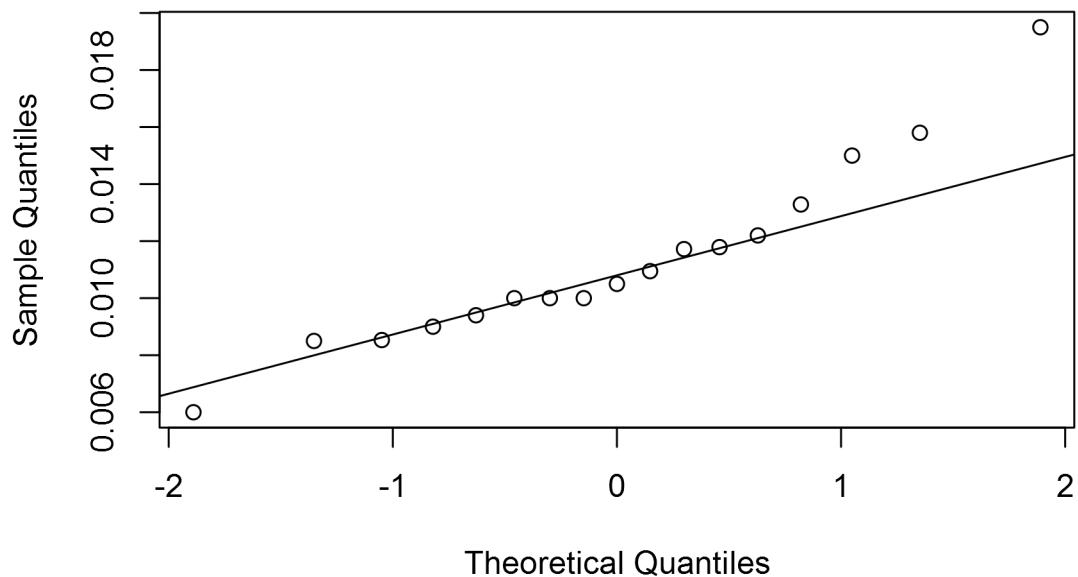


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

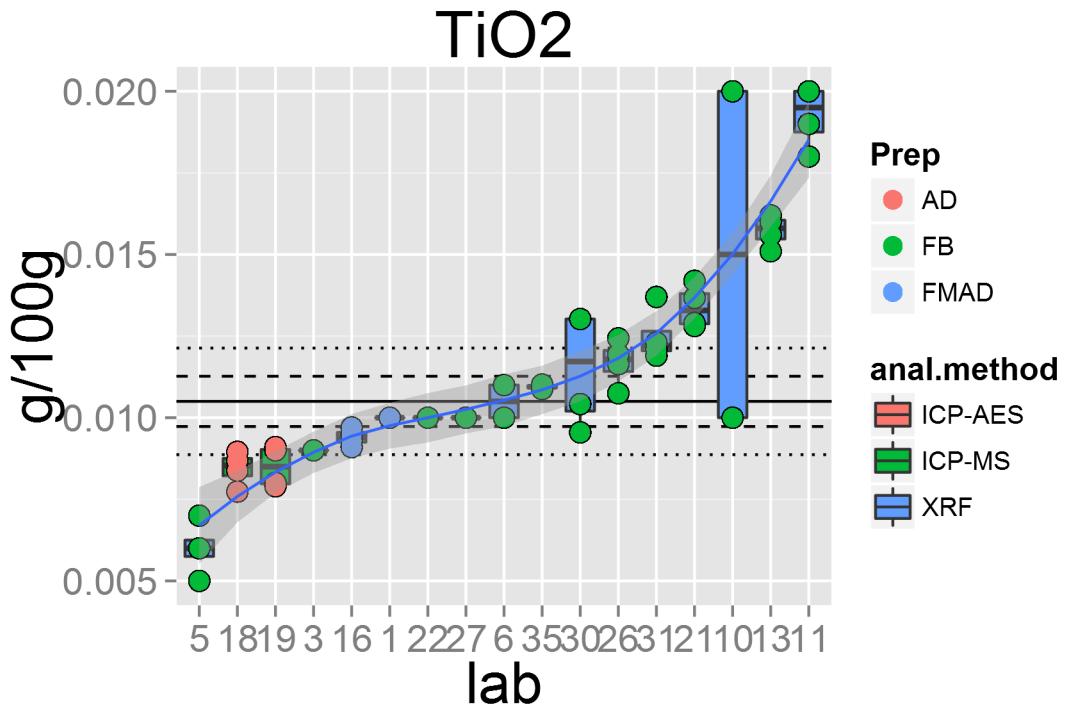


```
## [1] "Ti02.2"
```

Normal Q-Q Plot

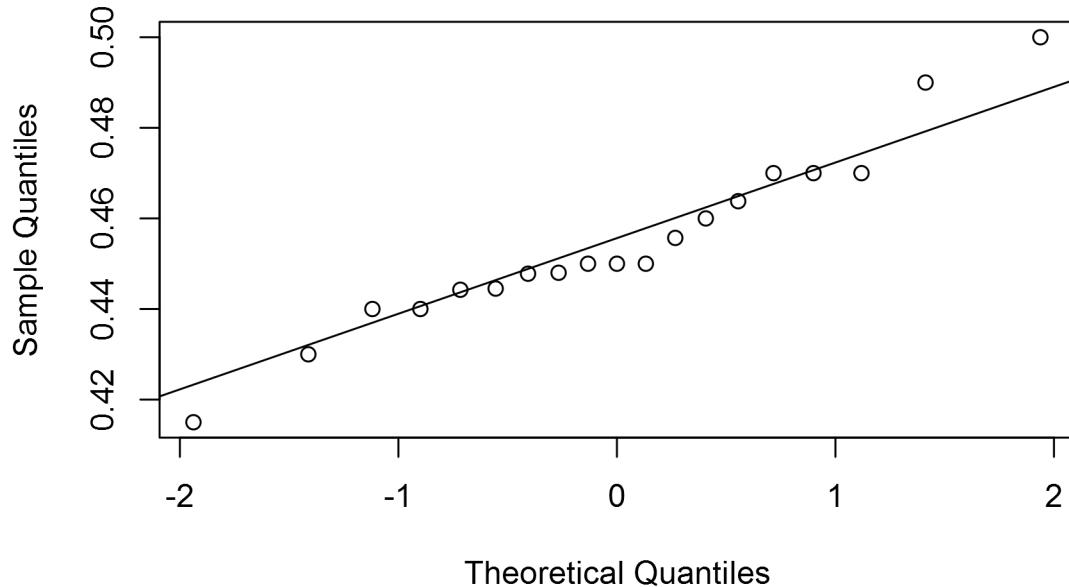


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

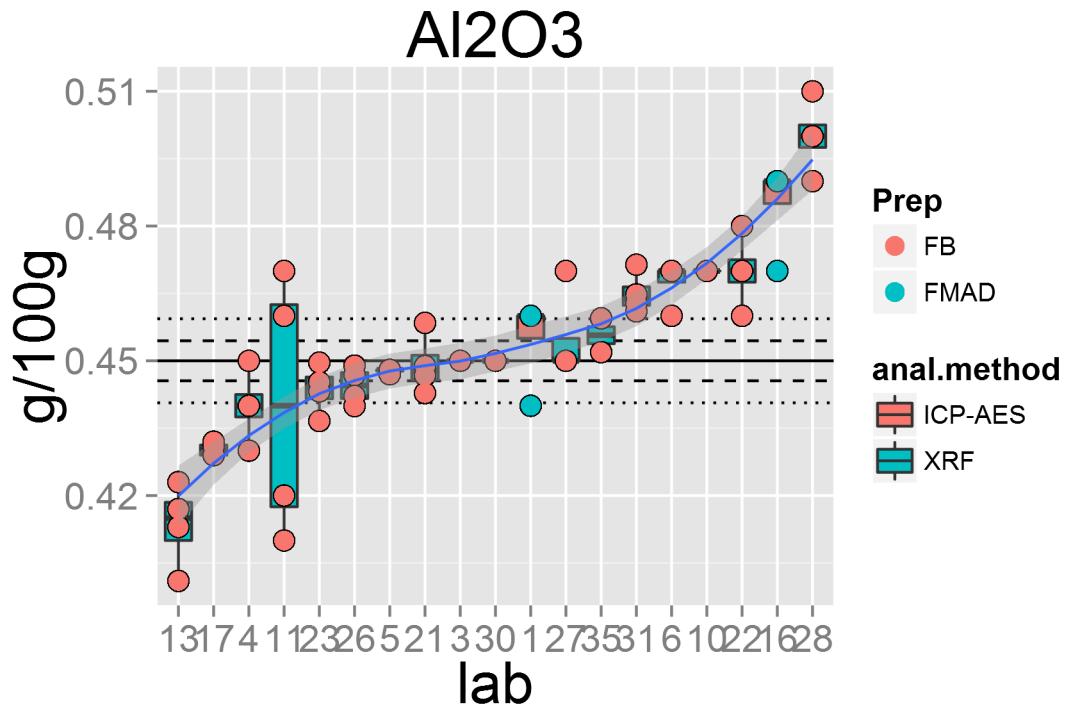


```
## [1] "Al203.2"
```

Normal Q-Q Plot

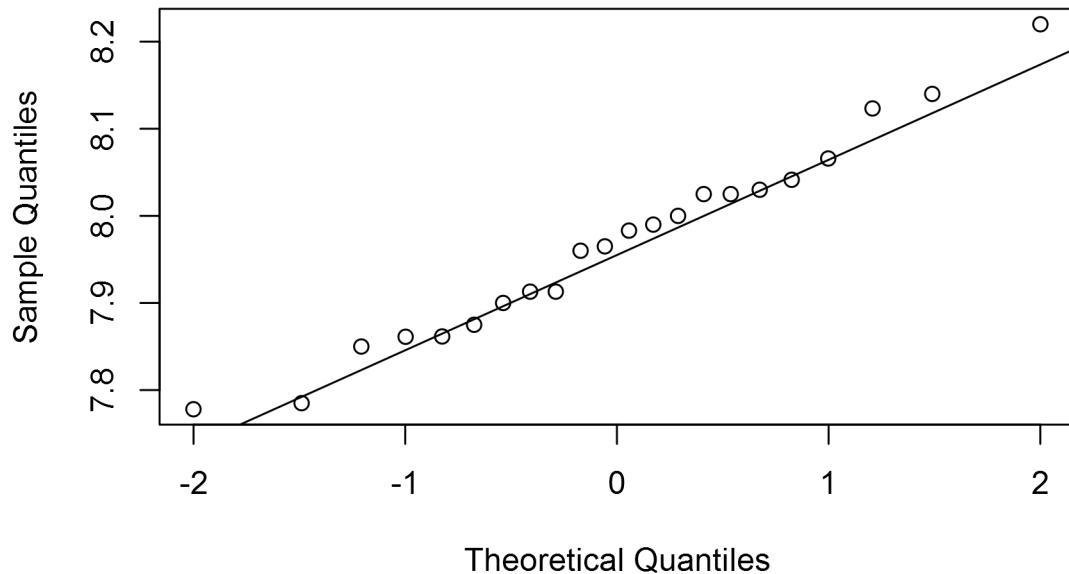


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

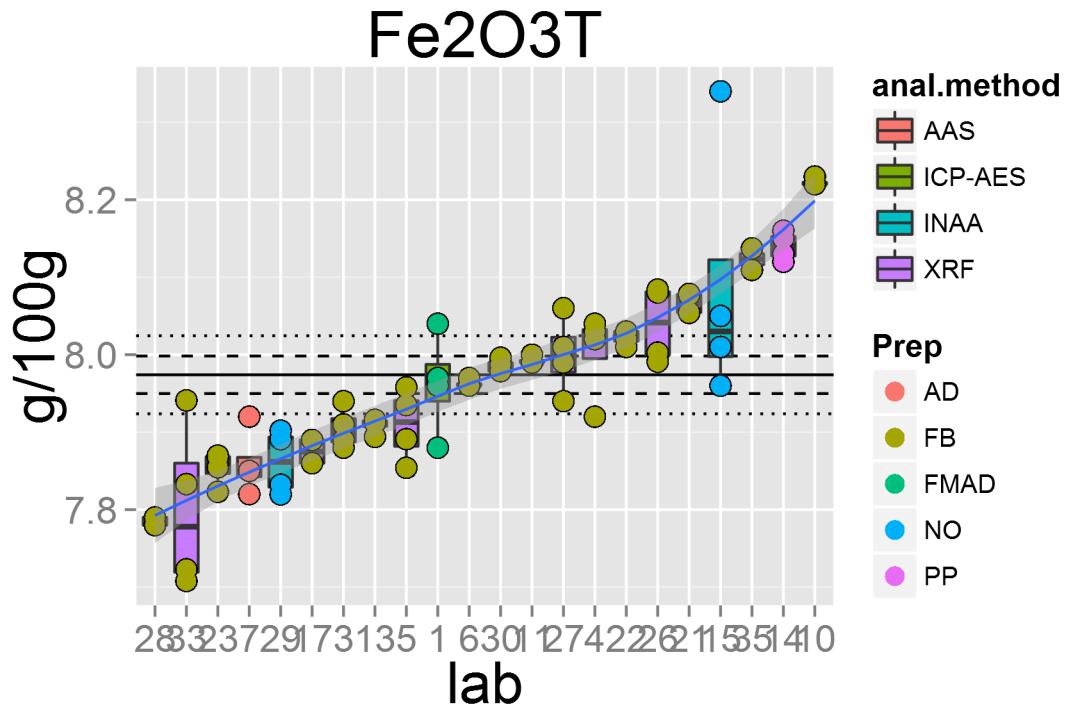


```
## [1] "Fe203T.2"
```

Normal Q-Q Plot

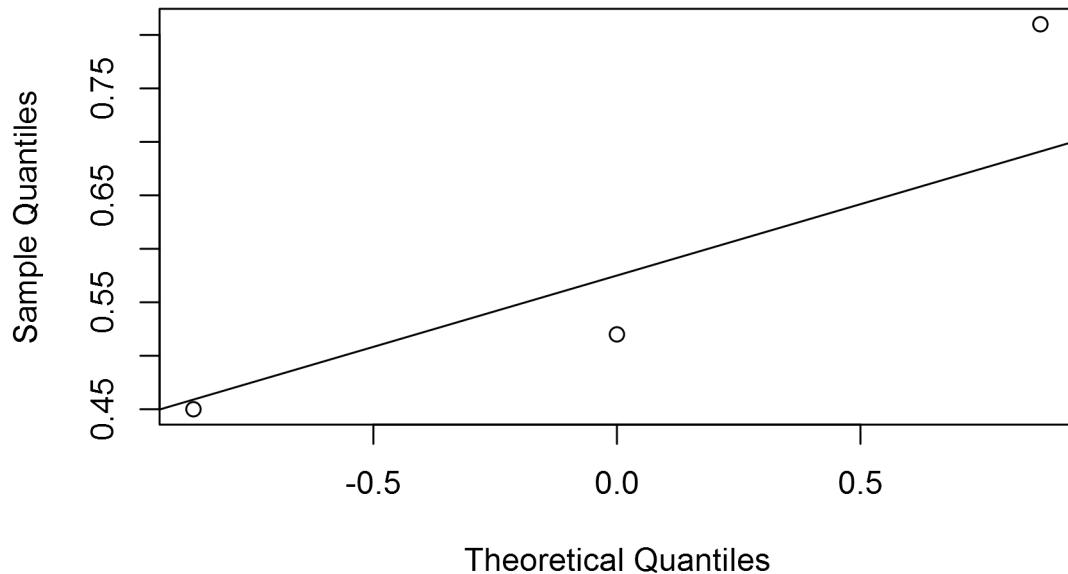


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

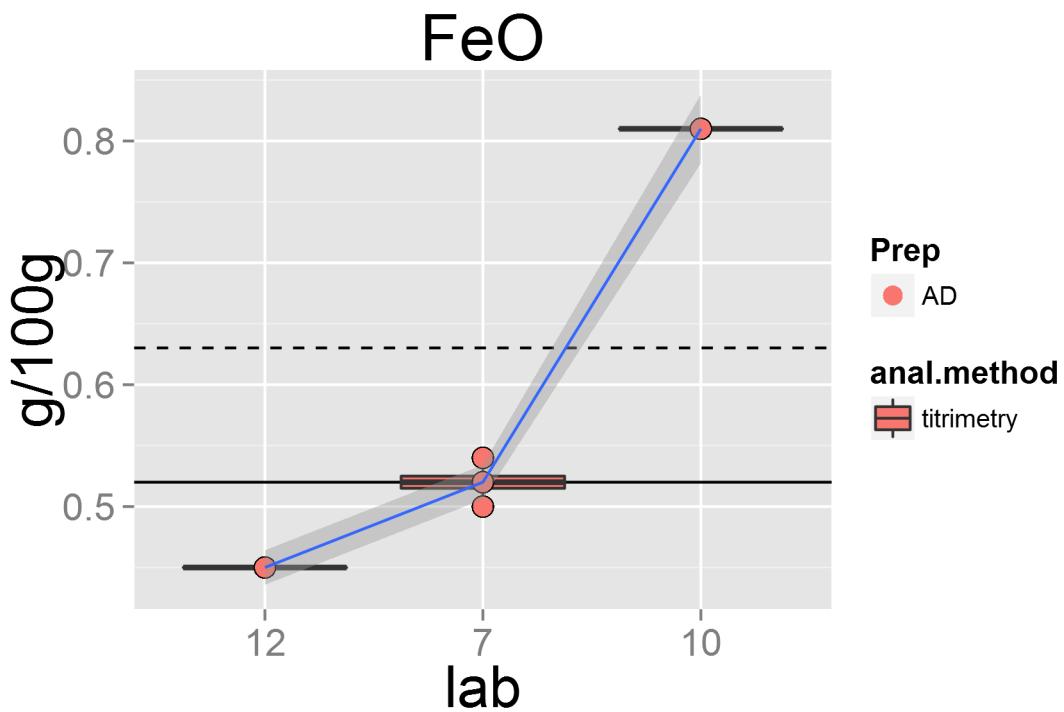


```
## [1] "FeO.2"
```

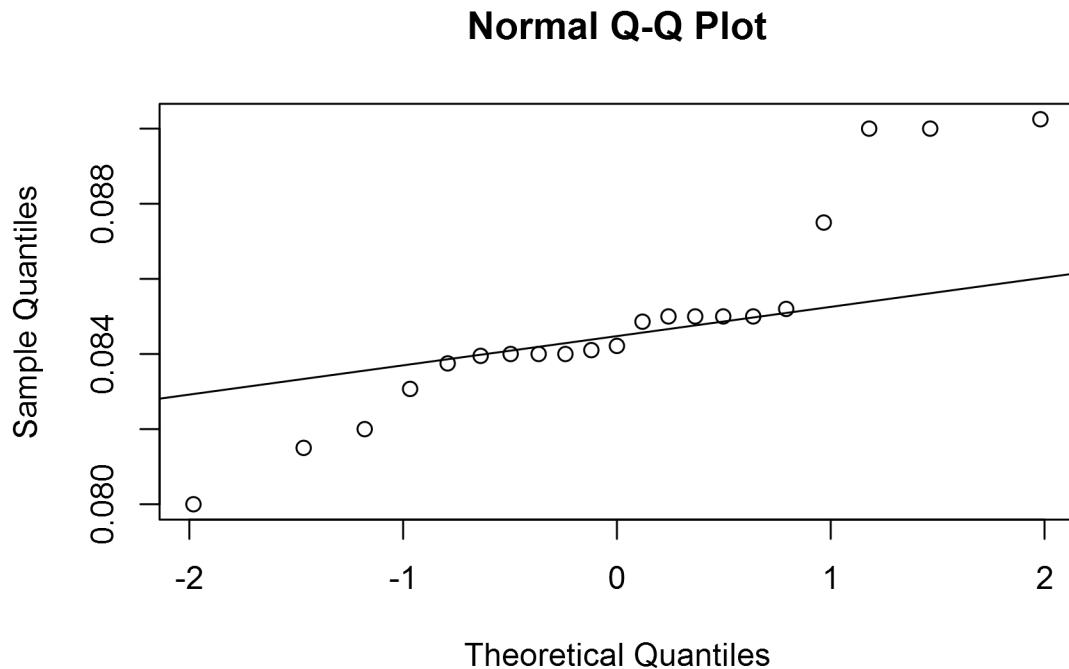
Normal Q-Q Plot



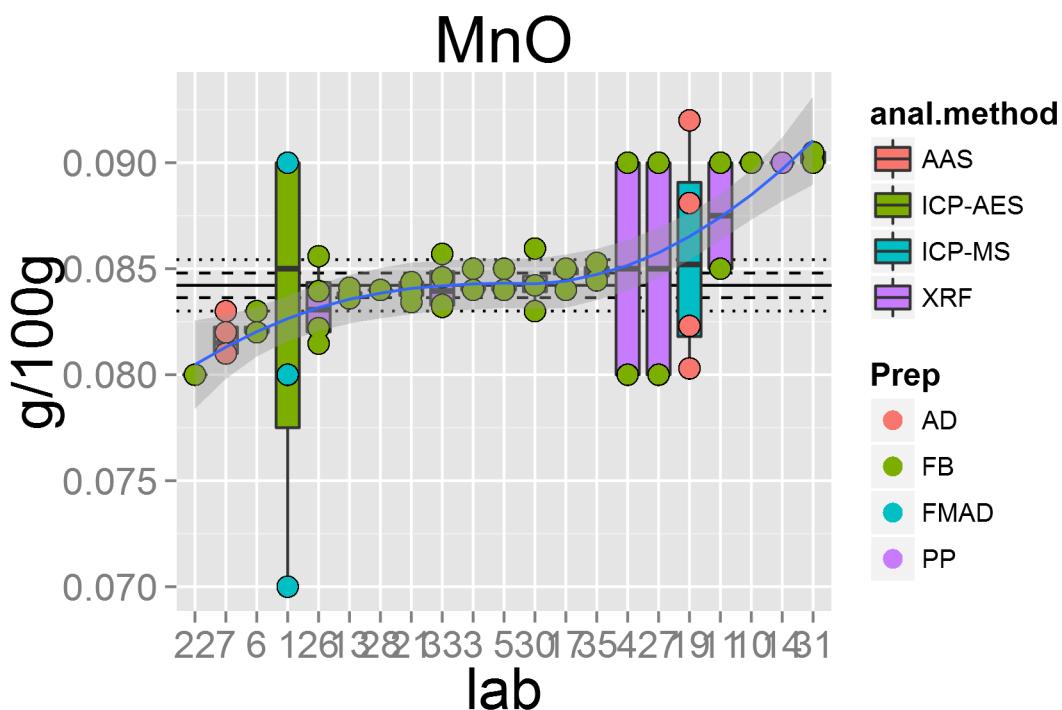
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c  
## Warning: pseudoinverse used at 0.99  
## Warning: neighborhood radius 1.01  
## Warning: reciprocal condition number  0  
## Warning: There are other near singularities as well. 4.0401  
## Warning: pseudoinverse used at 0.99  
## Warning: neighborhood radius 1.01  
## Warning: reciprocal condition number  0  
## Warning: There are other near singularities as well. 4.0401
```



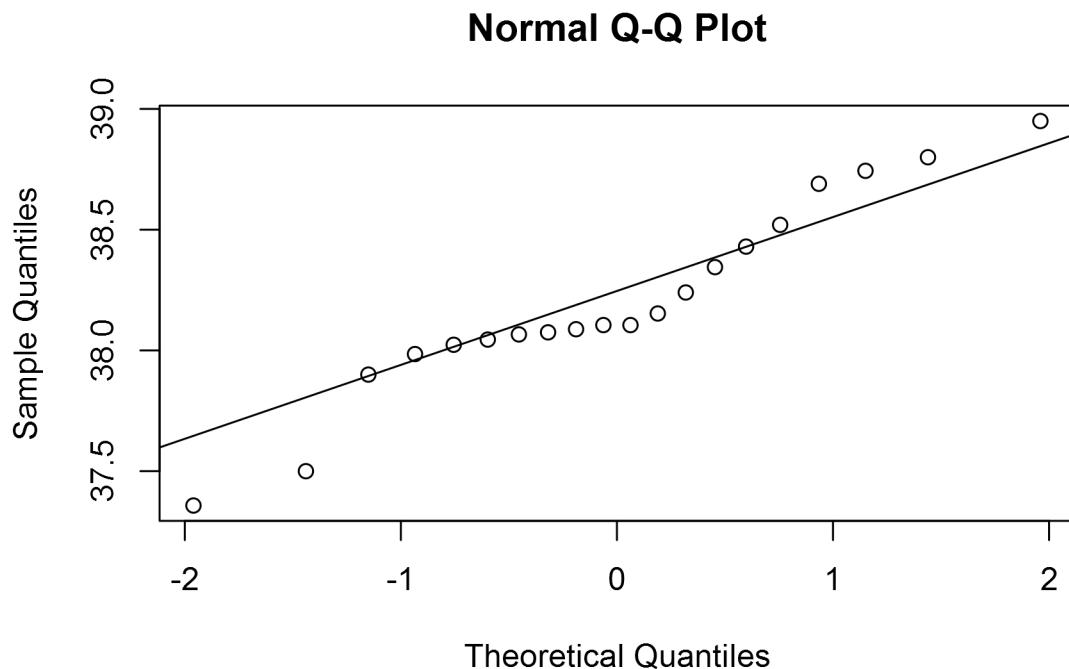
```
## [1] "Mn0.2"
```



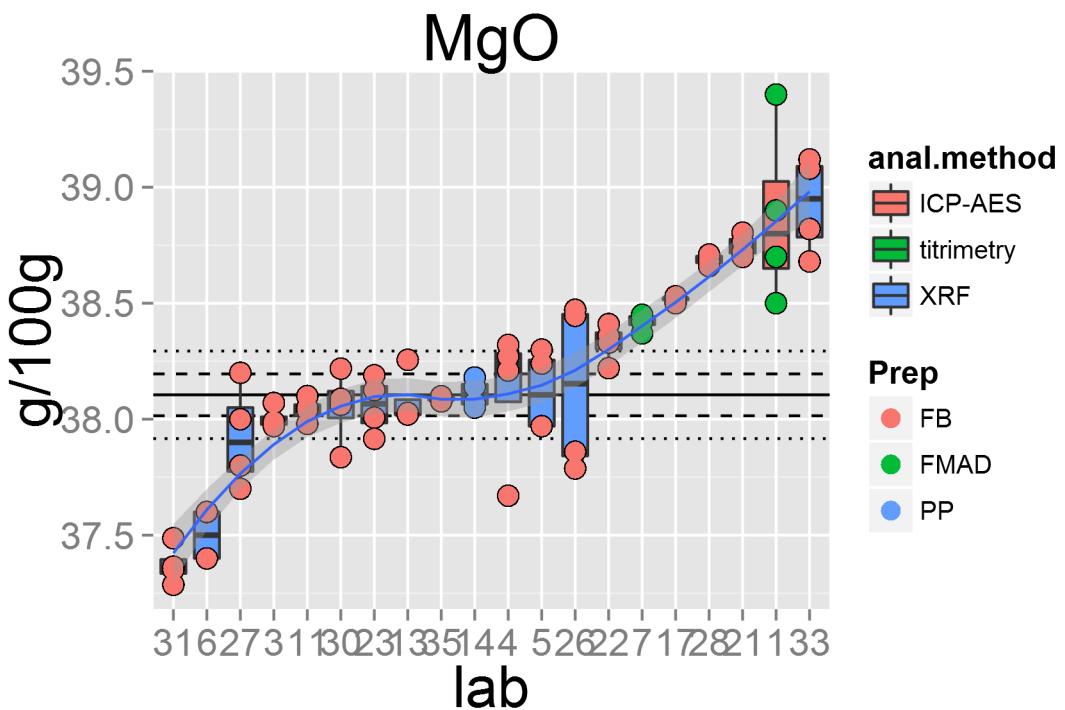
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



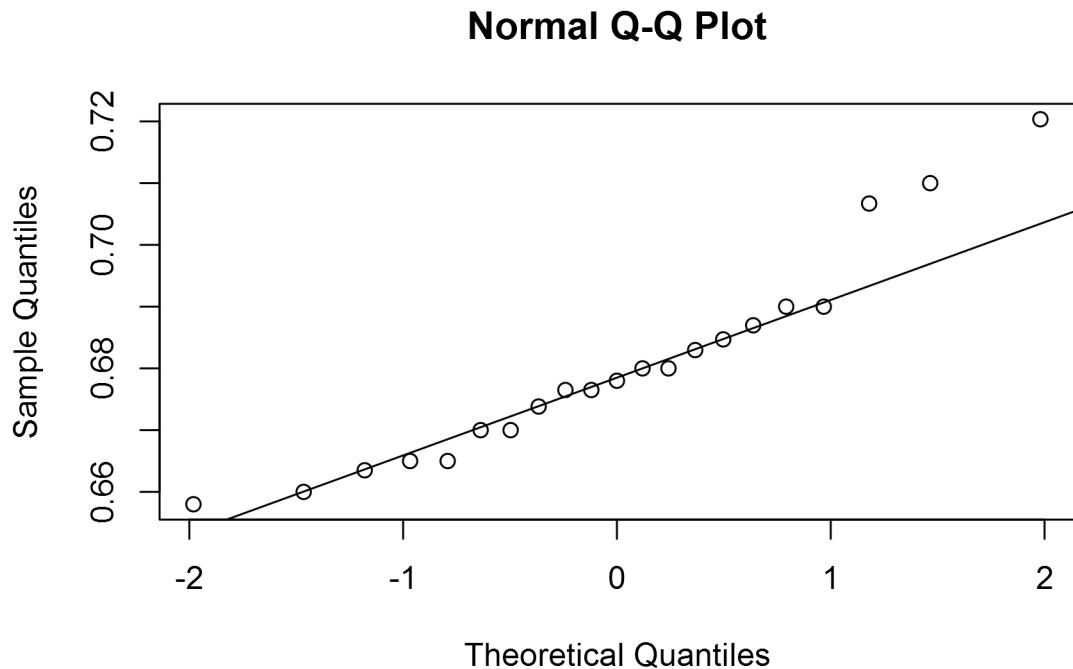
```
## [1] "Mg0.2"
```



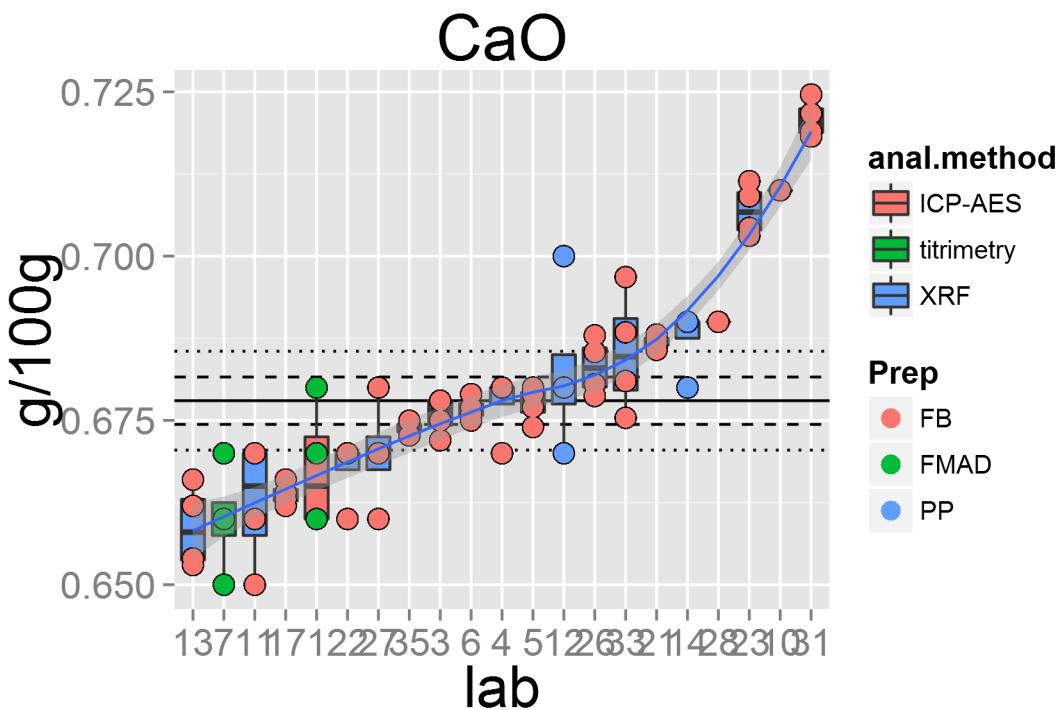
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



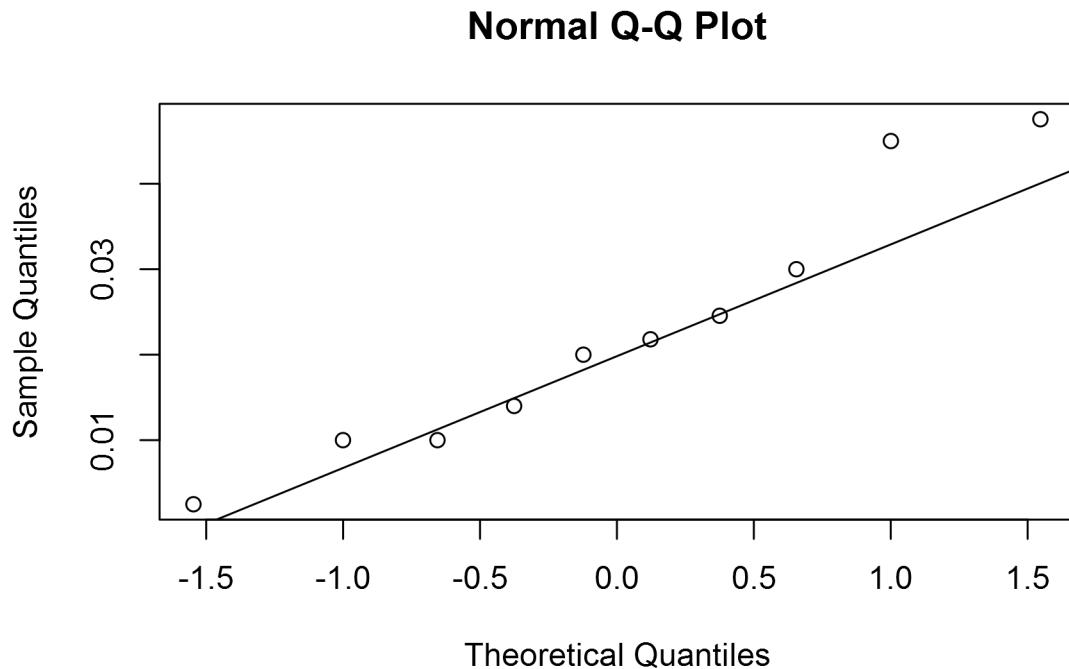
```
## [1] "Ca0.2"
```



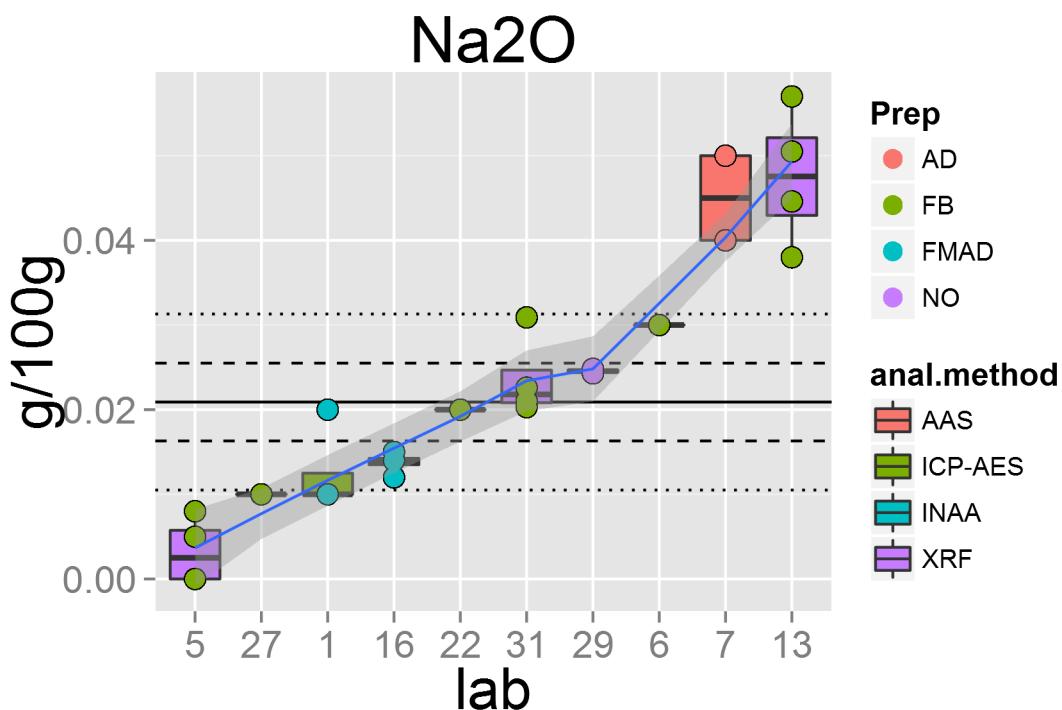
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



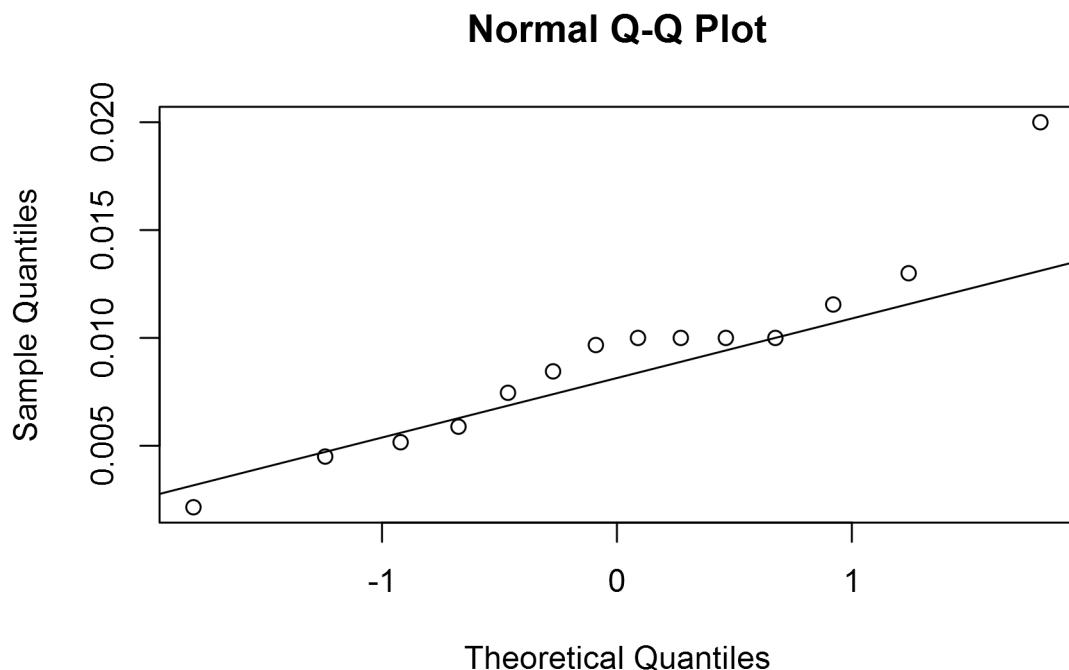
```
## [1] "Na20.2"
```



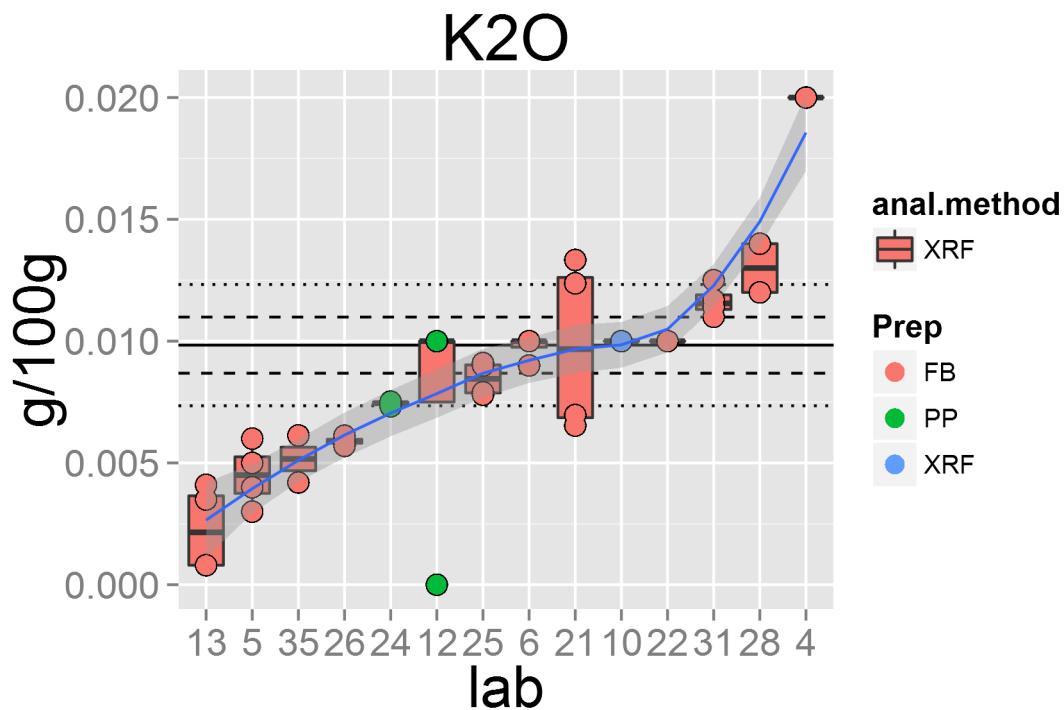
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



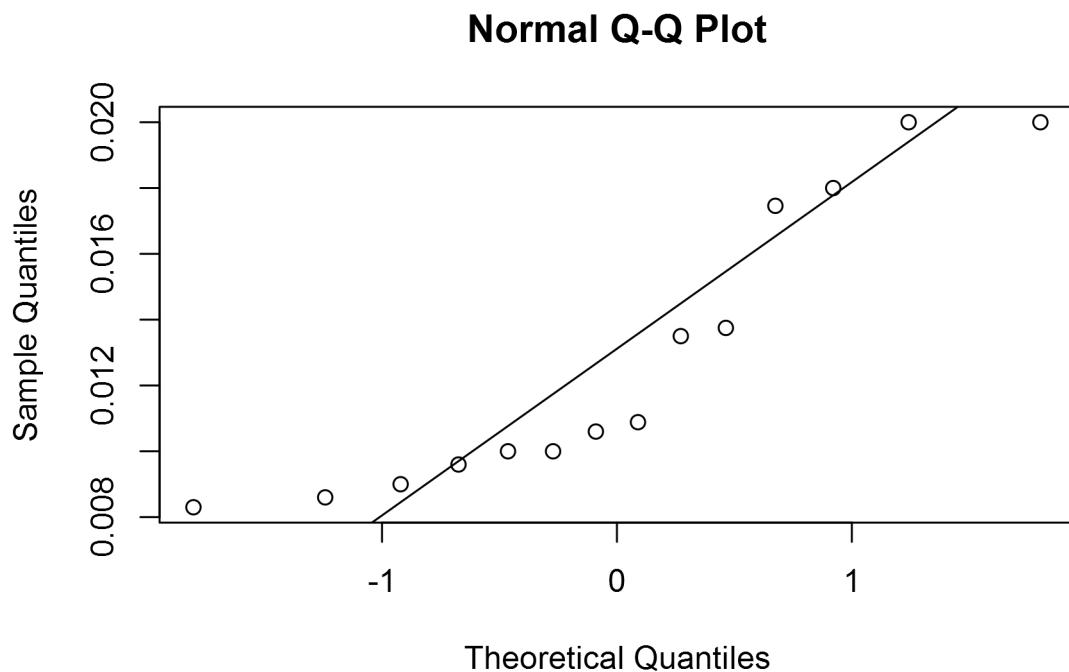
```
## [1] "K20.2"
```



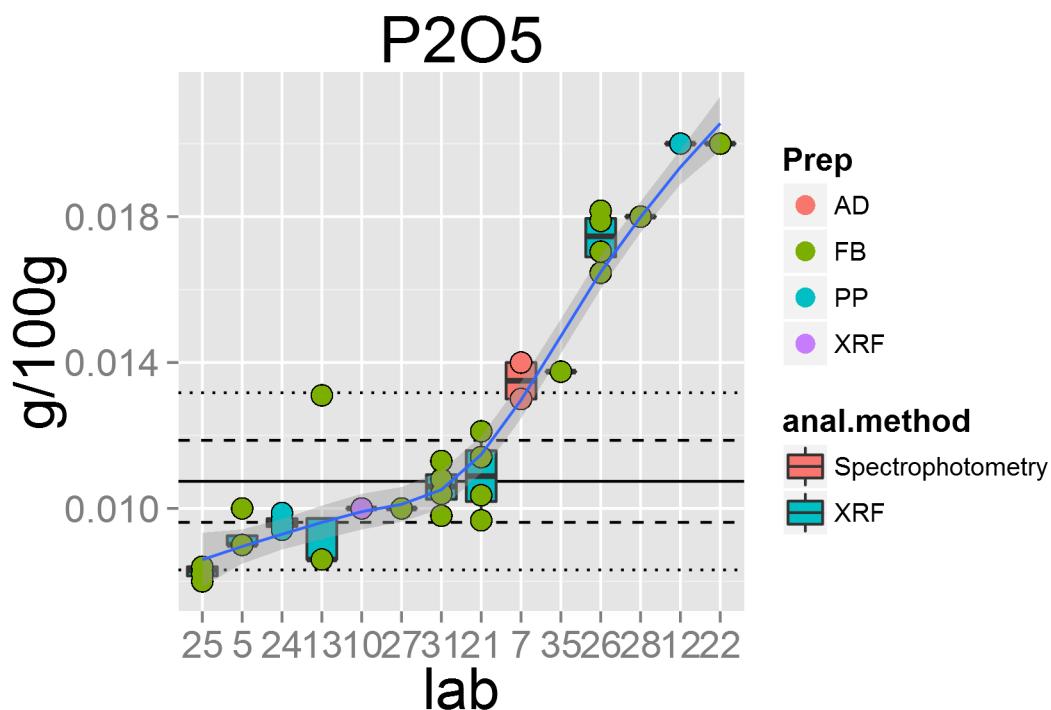
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



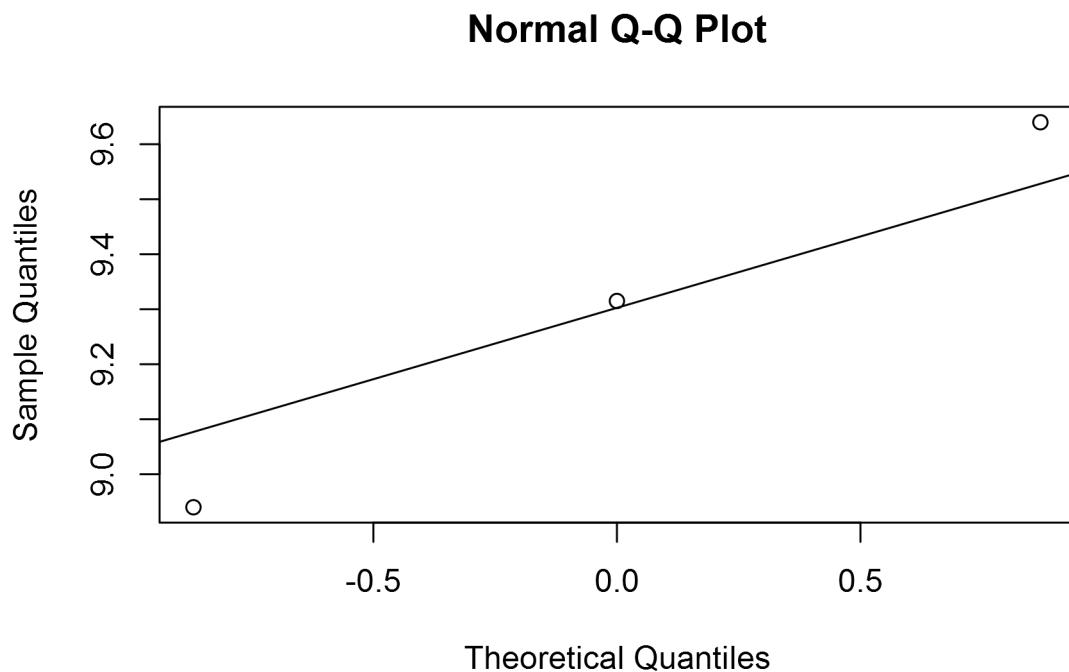
```
## [1] "P205.2"
```



```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



```
## [1] "H2O..2"
```

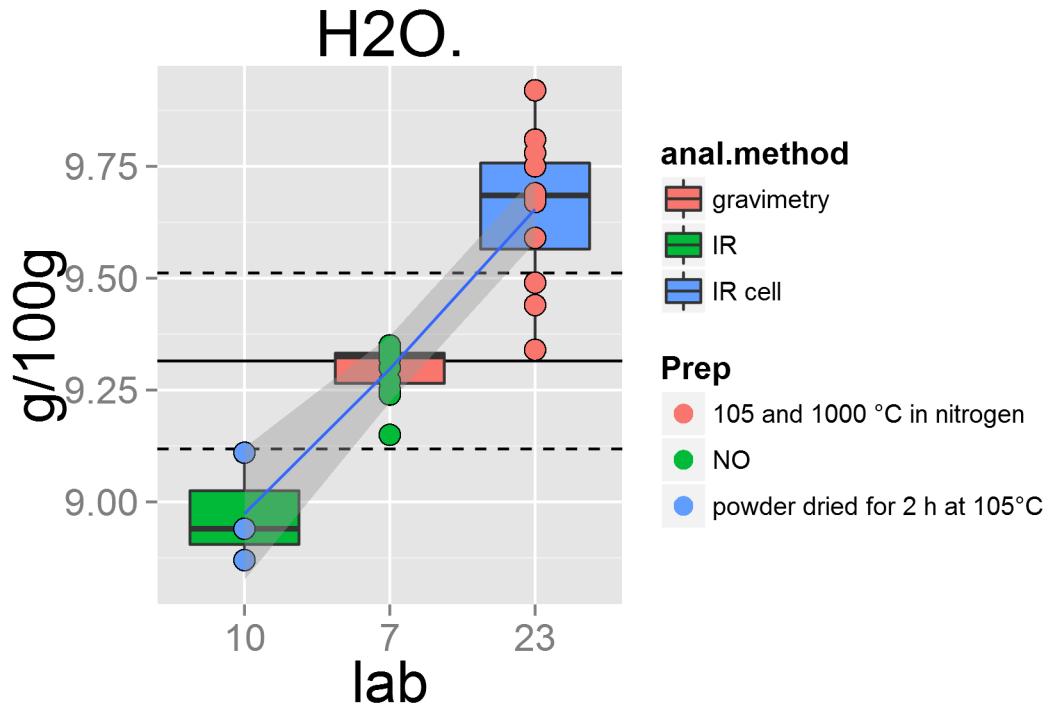


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

```

## Warning: pseudoinverse used at 0.99
## Warning: neighborhood radius 2.01
## Warning: reciprocal condition number 1.3327e-016
## Warning: There are other near singularities as well. 1.0201
## Warning: pseudoinverse used at 0.99
## Warning: neighborhood radius 2.01
## Warning: reciprocal condition number 1.3327e-016
## Warning: There are other near singularities as well. 1.0201

```

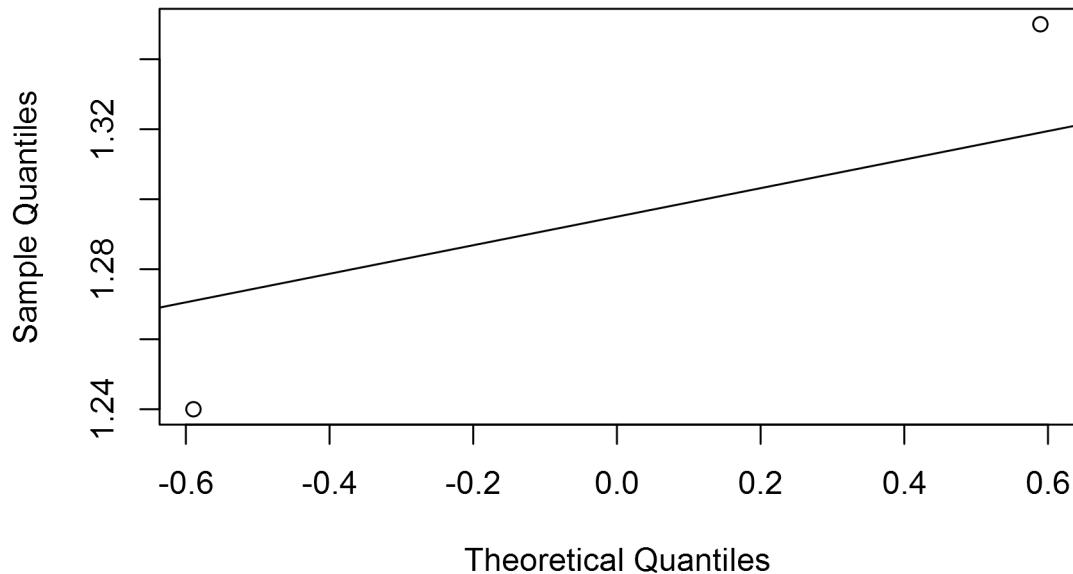


```

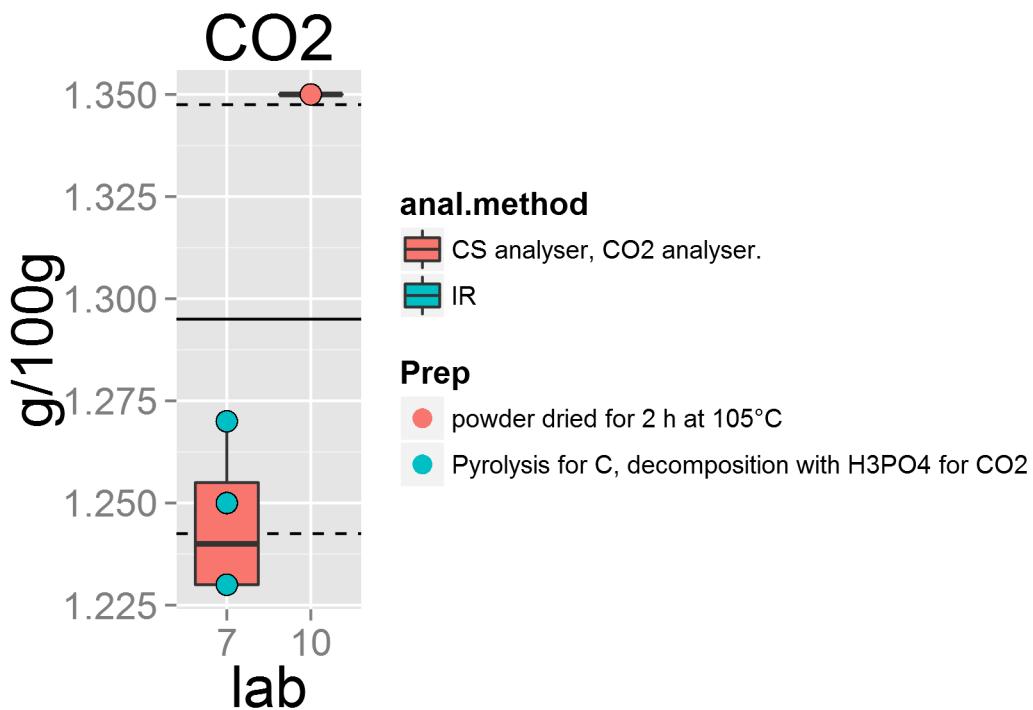
## [1] "CO2.2"

```

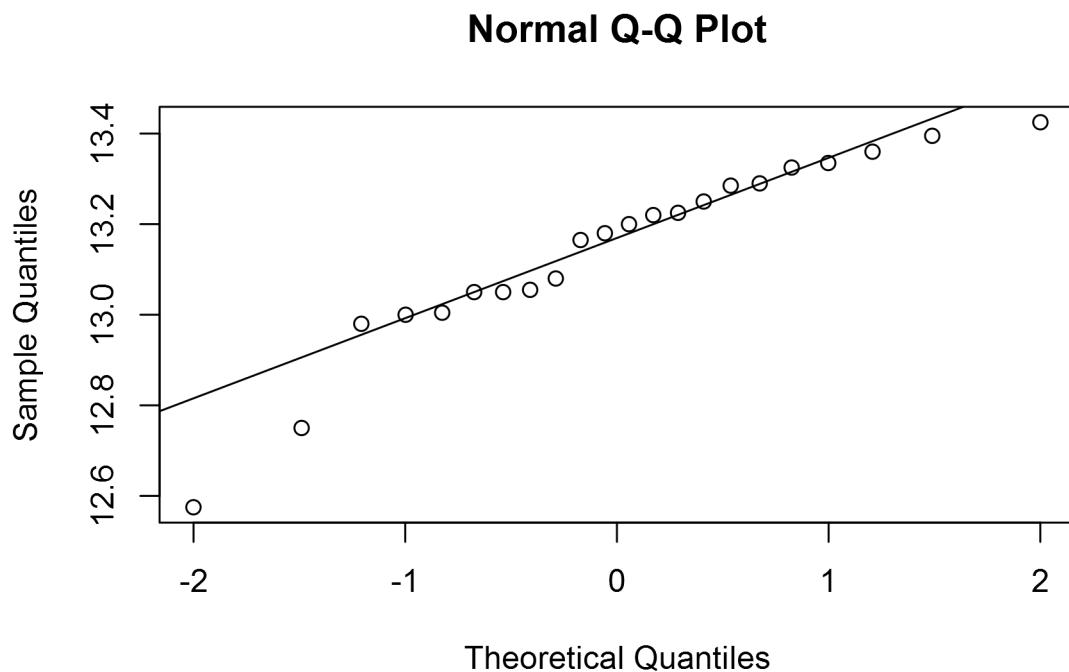
Normal Q-Q Plot



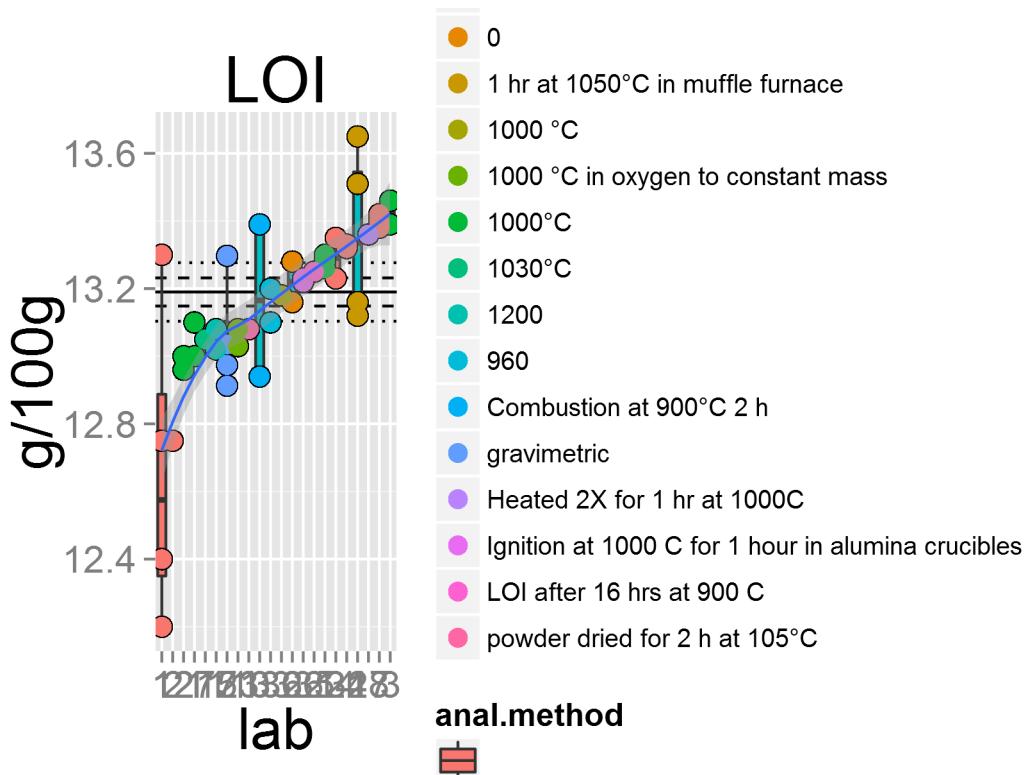
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
## Warning: span too small. fewer data values than degrees of freedom.
## Warning: at 0.995
## Warning: radius 2.5e-005
## Warning: all data on boundary of neighborhood. make span bigger
## Warning: pseudoinverse used at 0.995
## Warning: neighborhood radius 0.005
## Warning: reciprocal condition number 1
## Warning: There are other near singularities as well. 1.01
## Warning: zero-width neighborhood. make span bigger
```



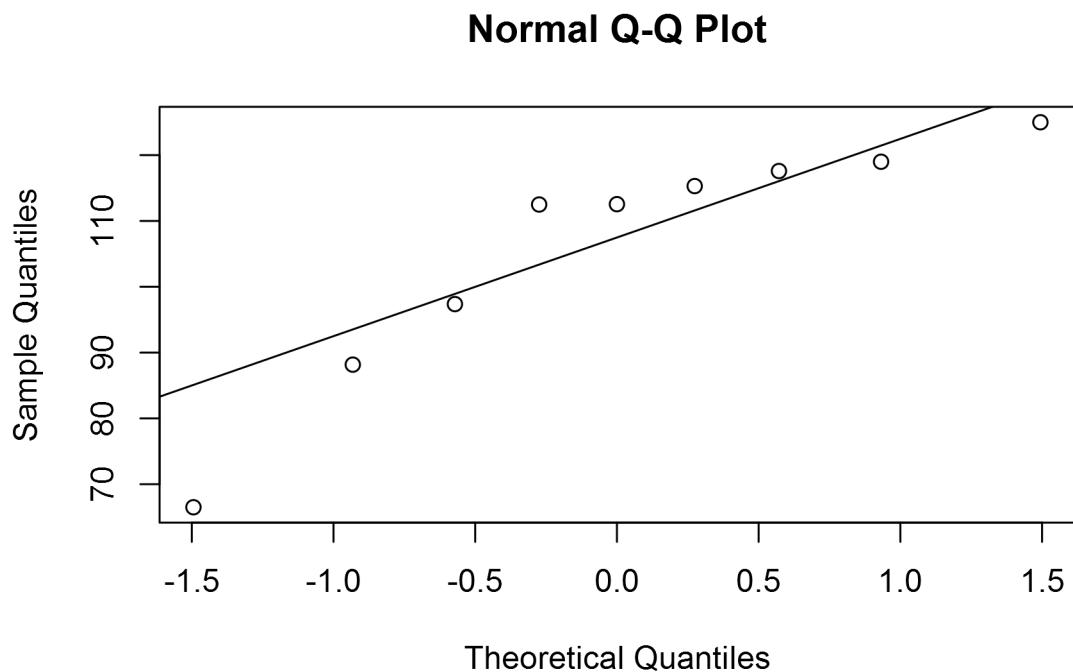
```
## [1] "LOI.2"
```



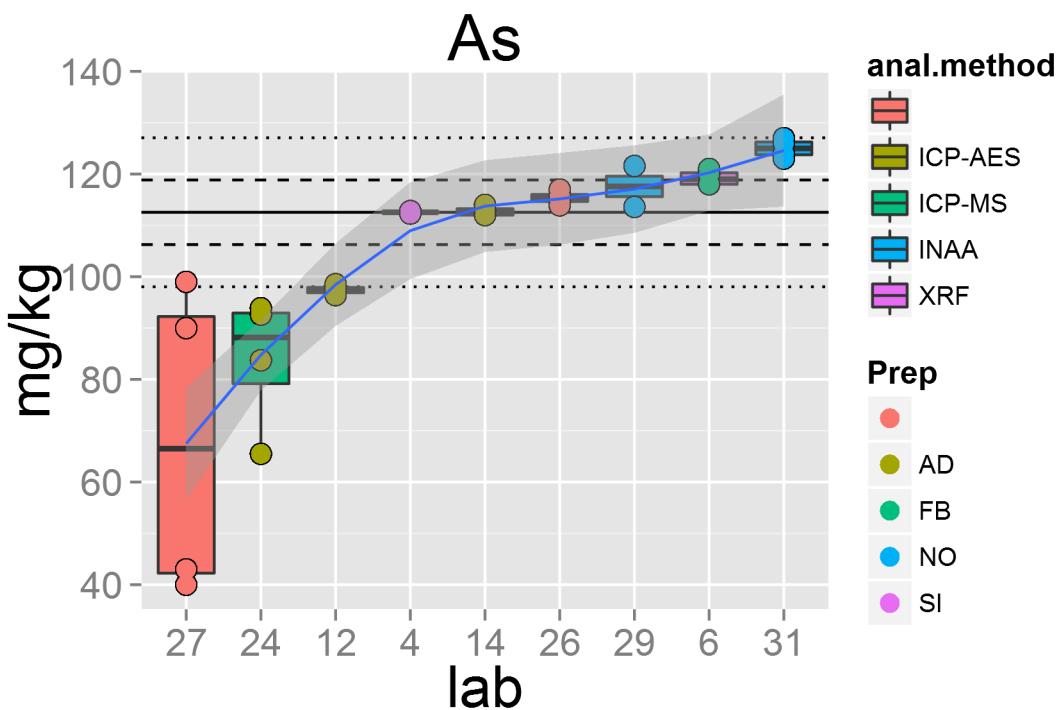
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



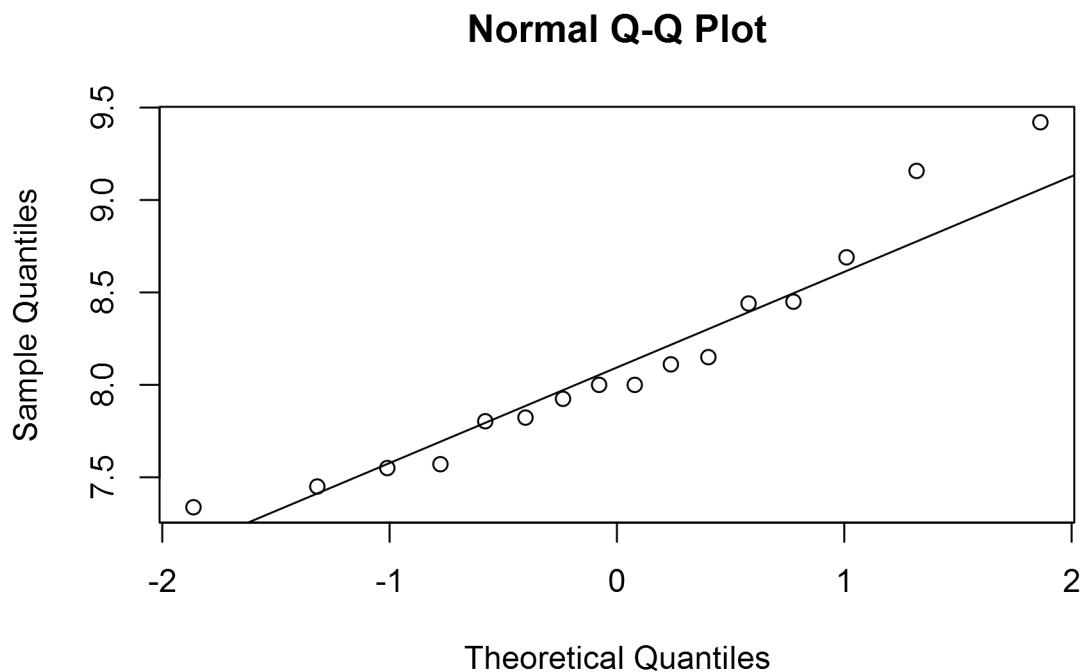
```
## [1] "As.2"
```



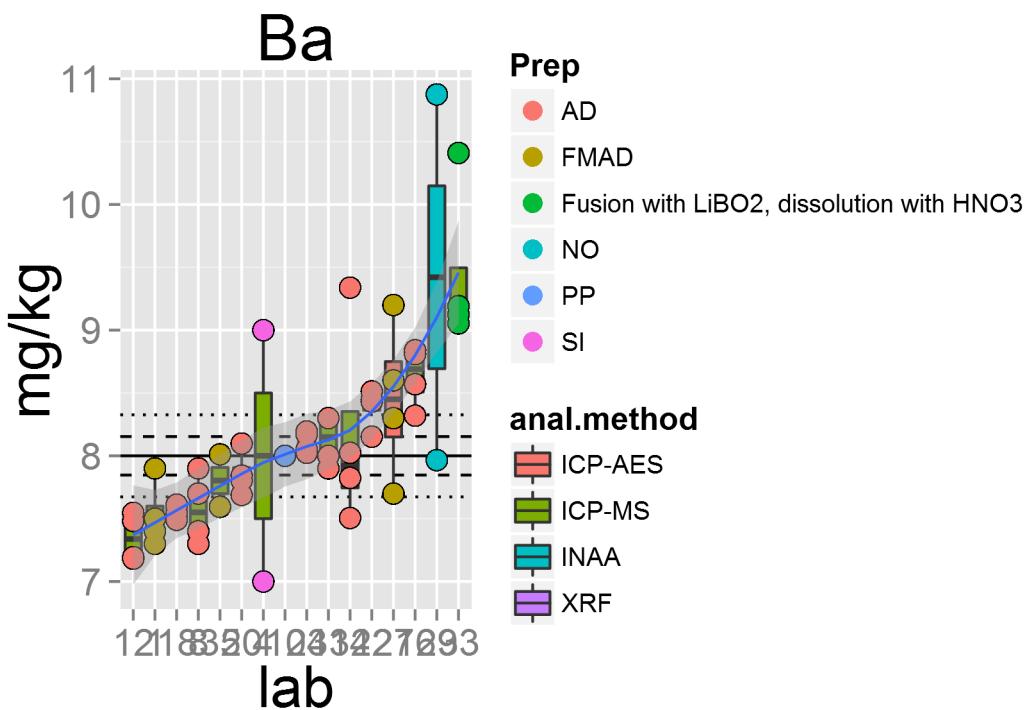
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



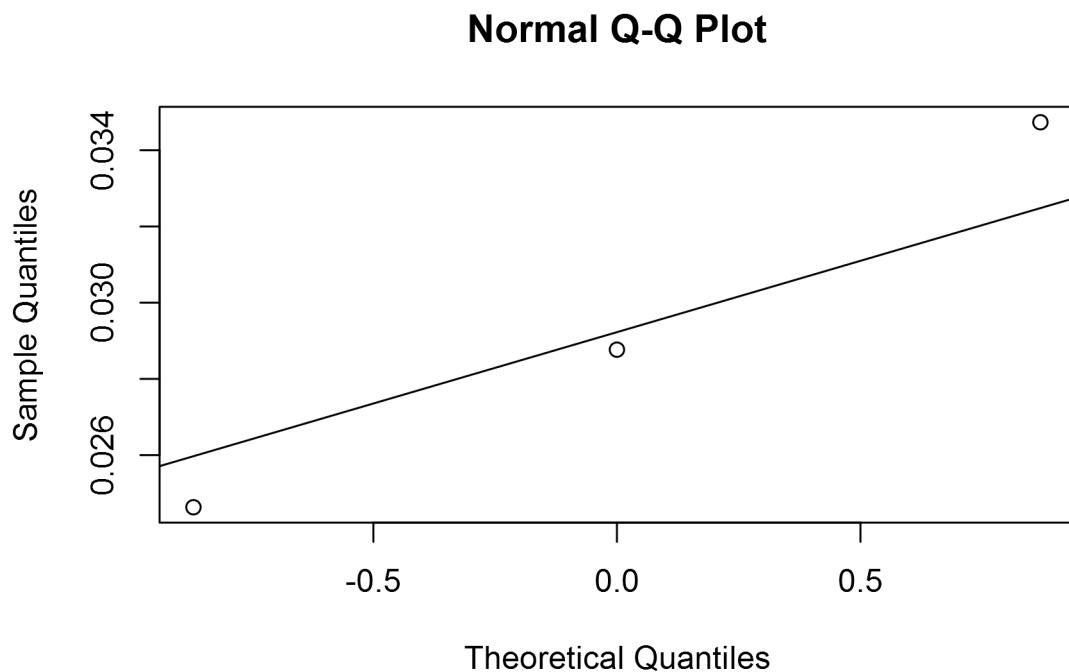
```
## [1] "Ba.2"
```



```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



```
## [1] "Be.2"
```

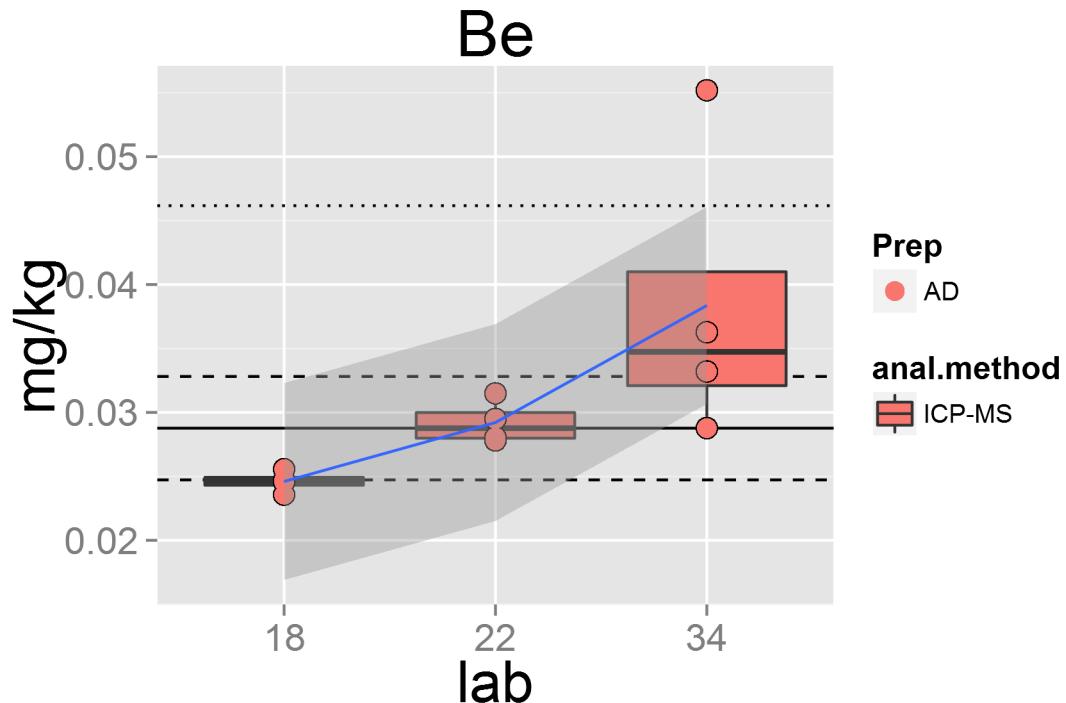


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

```

## Warning: pseudoinverse used at 0.99
## Warning: neighborhood radius 2.01
## Warning: reciprocal condition number 5.2085e-017
## Warning: There are other near singularities as well. 4.0401
## Warning: pseudoinverse used at 0.99
## Warning: neighborhood radius 2.01
## Warning: reciprocal condition number 5.2085e-017
## Warning: There are other near singularities as well. 4.0401

```

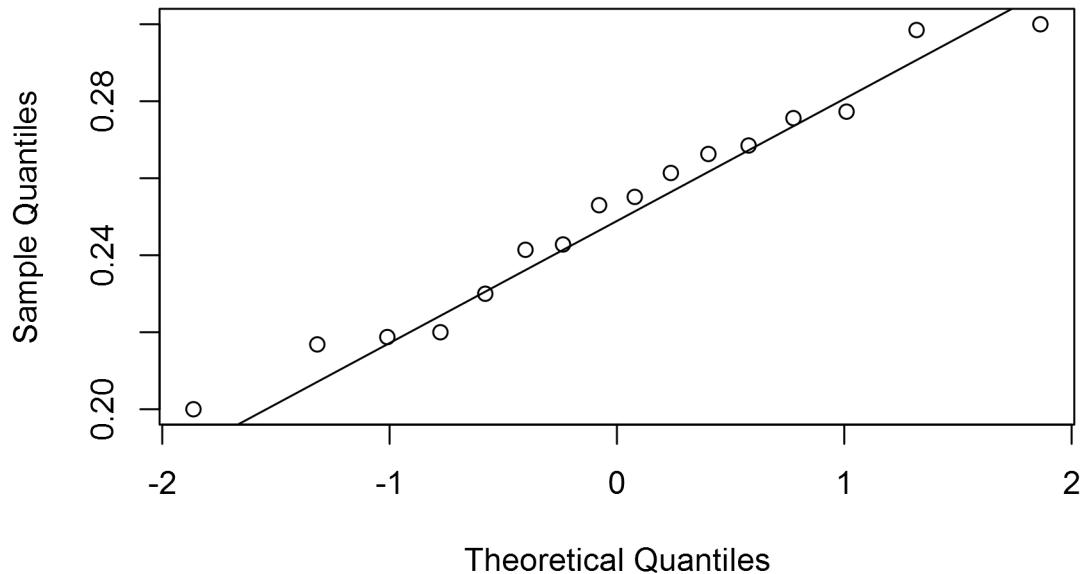


```

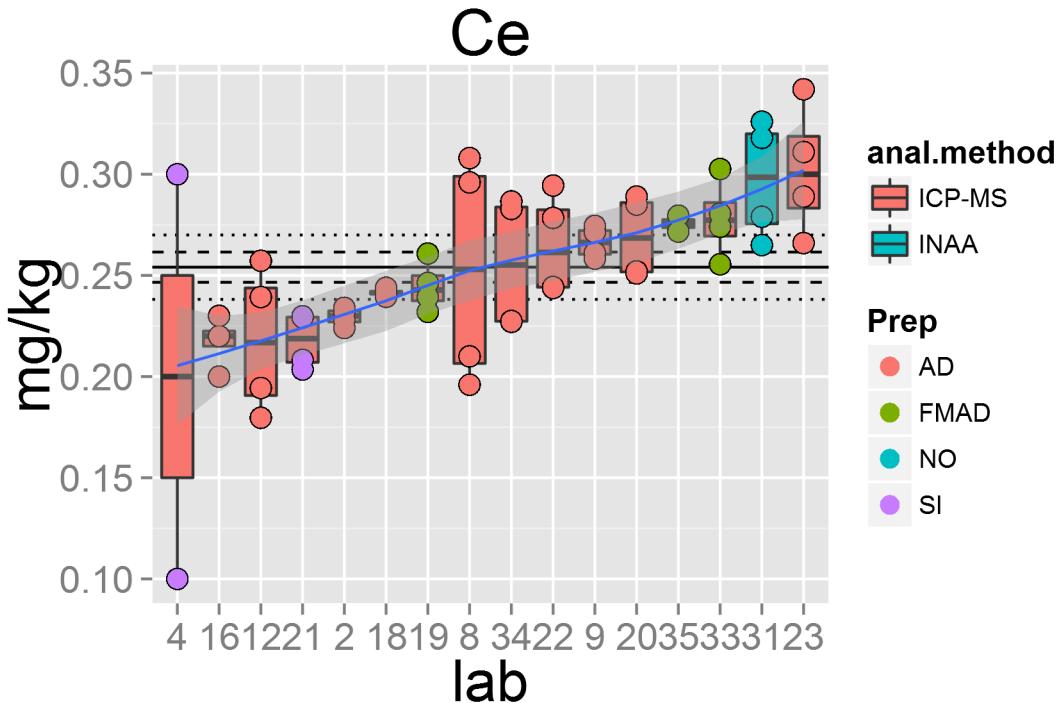
## [1] "Ce.2"

```

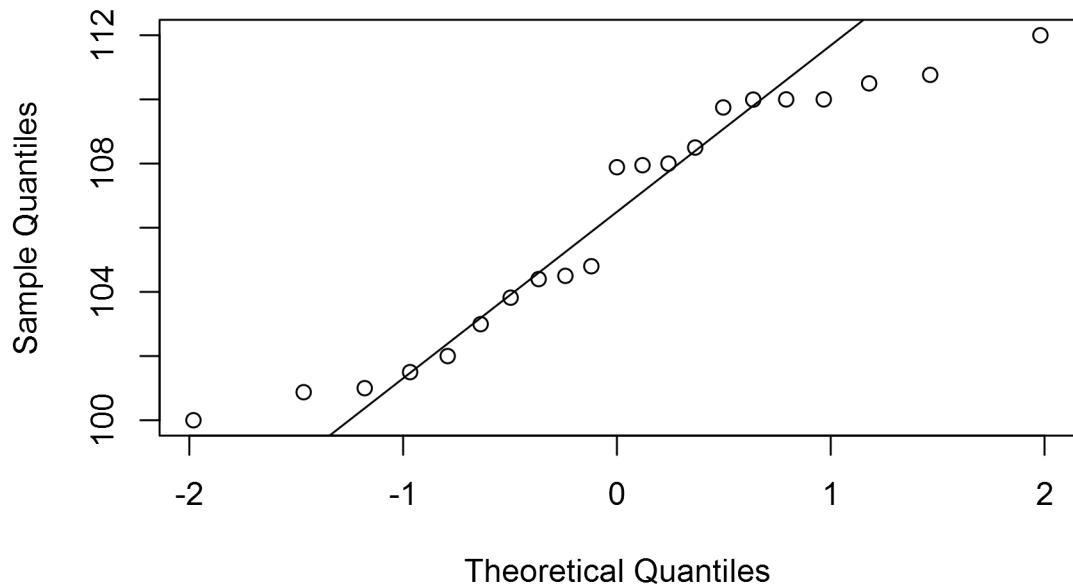
Normal Q-Q Plot



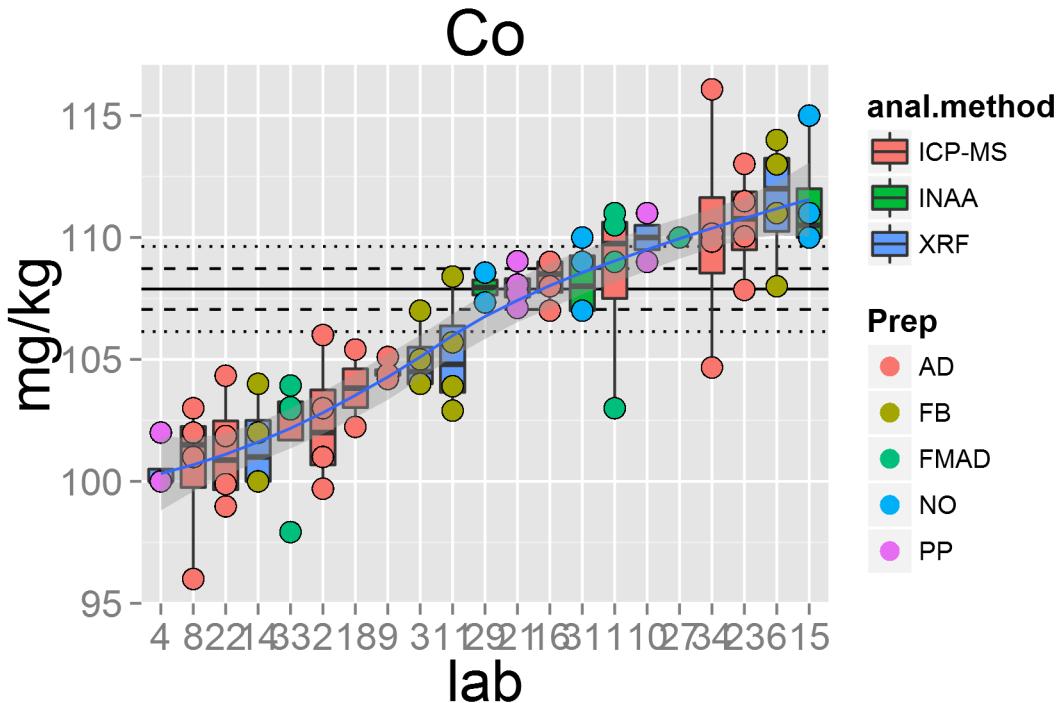
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



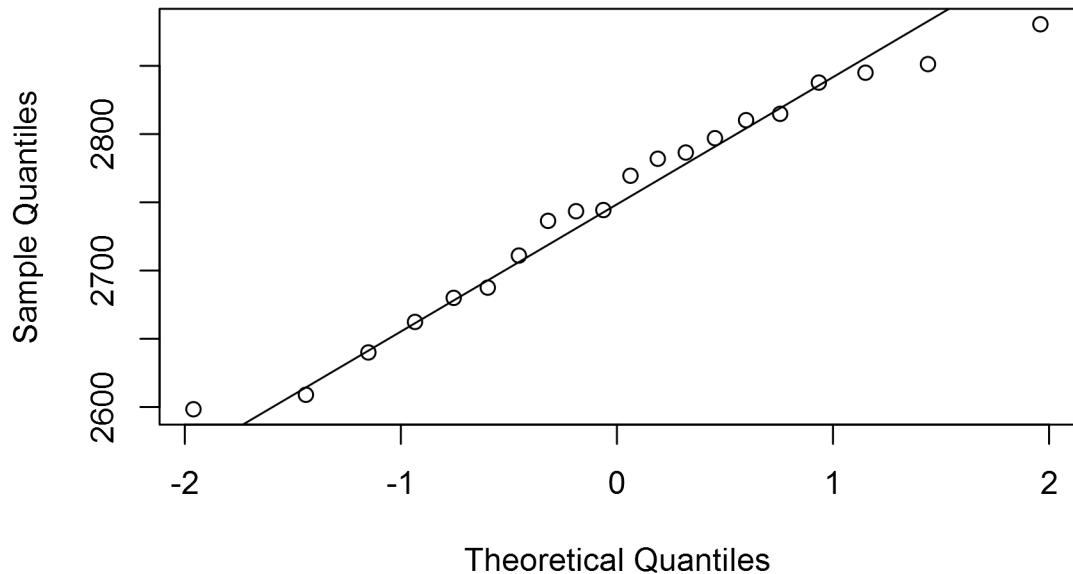
Normal Q-Q Plot



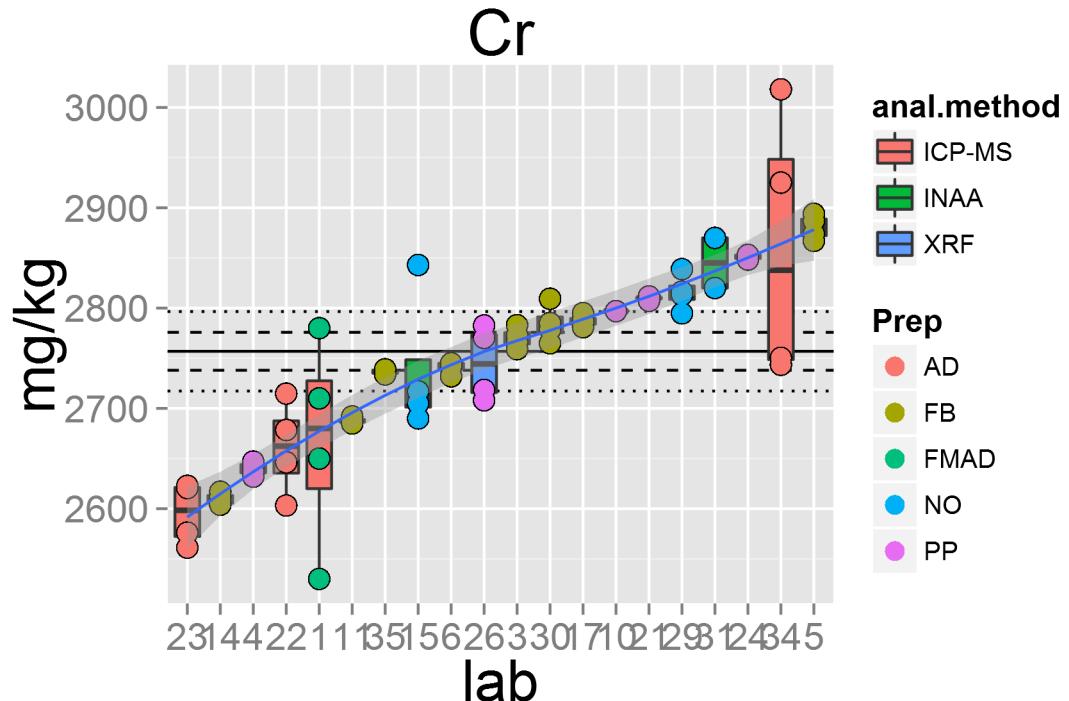
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



Normal Q-Q Plot

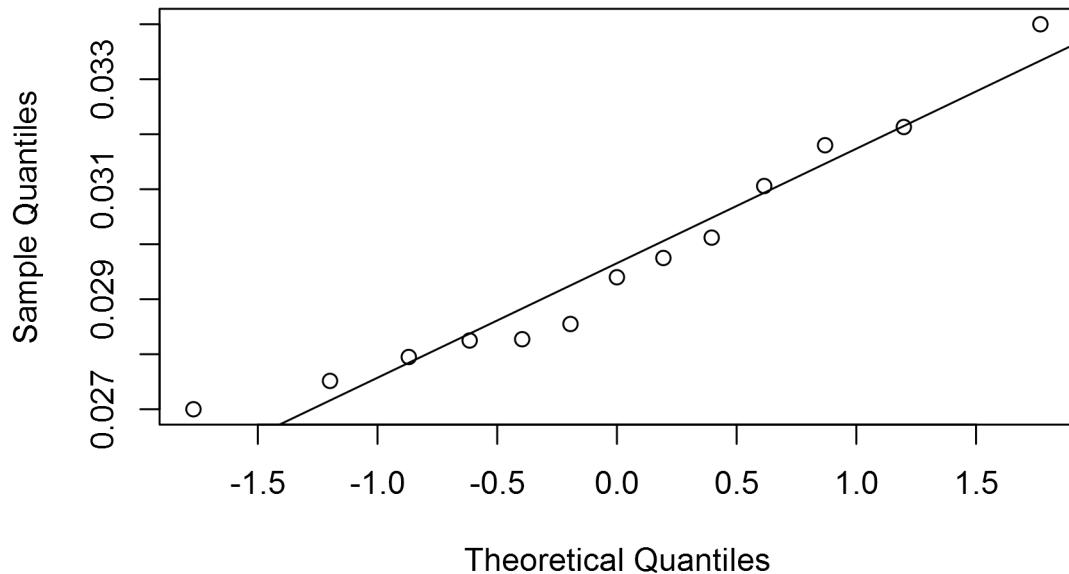


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

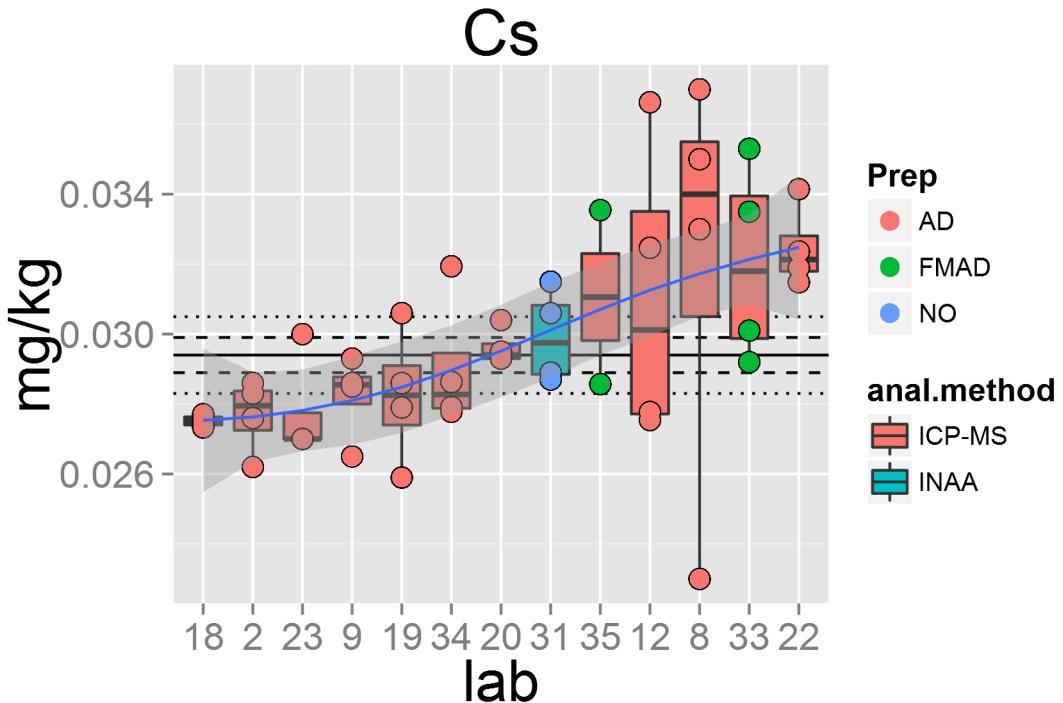


```
## [1] "Cs.2"
```

Normal Q-Q Plot

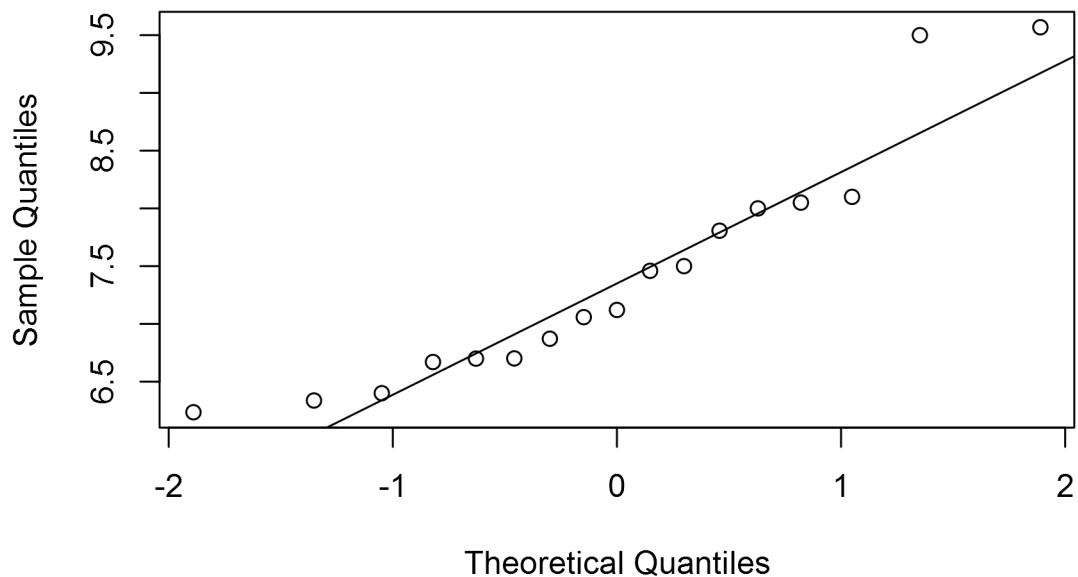


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

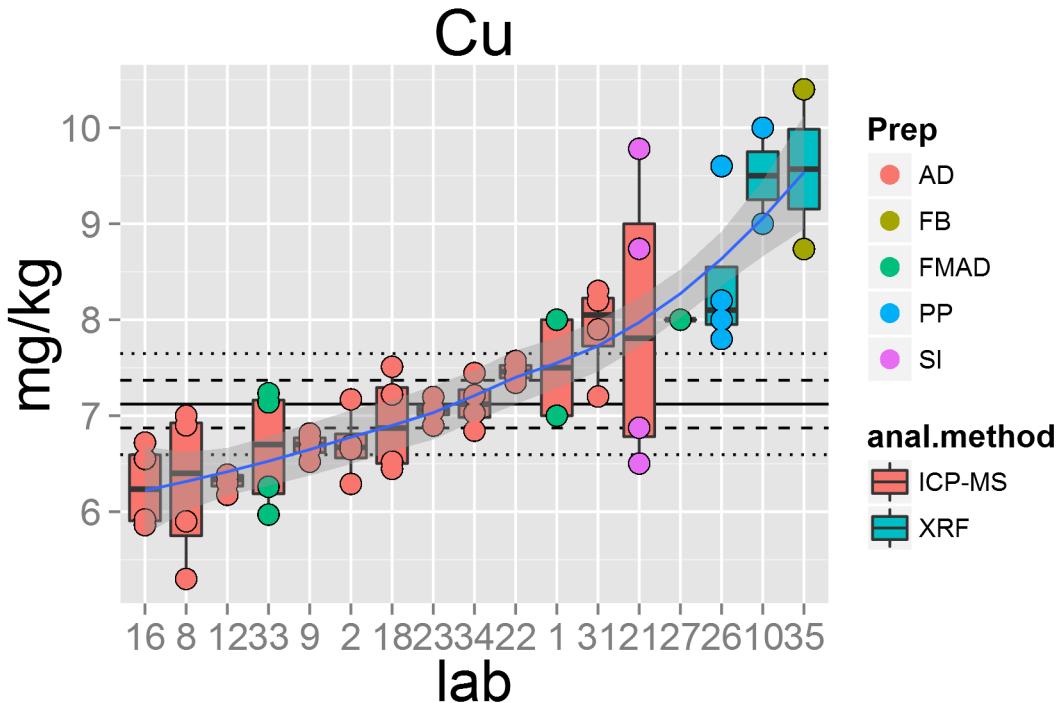


```
## [1] "Cu.2"
```

Normal Q-Q Plot

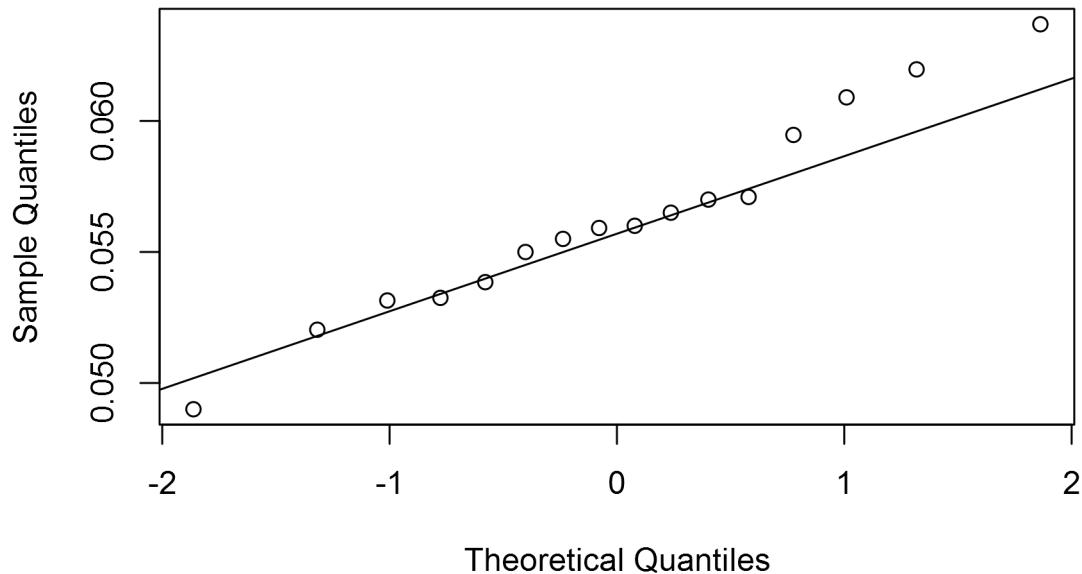


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

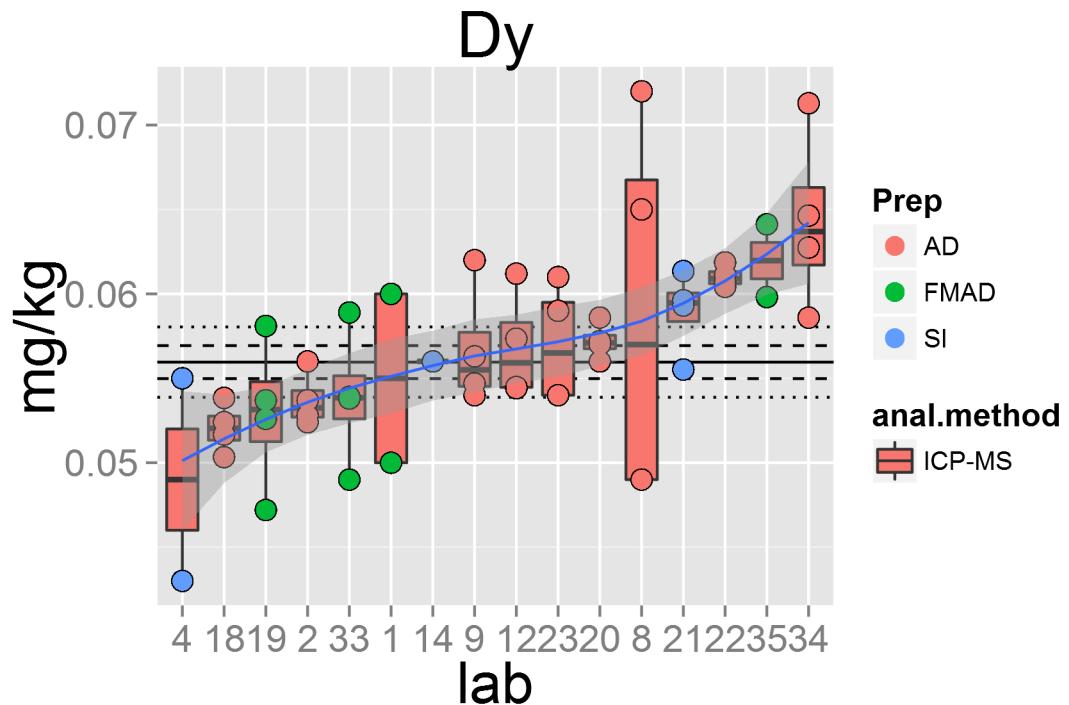


```
## [1] "Dy .2"
```

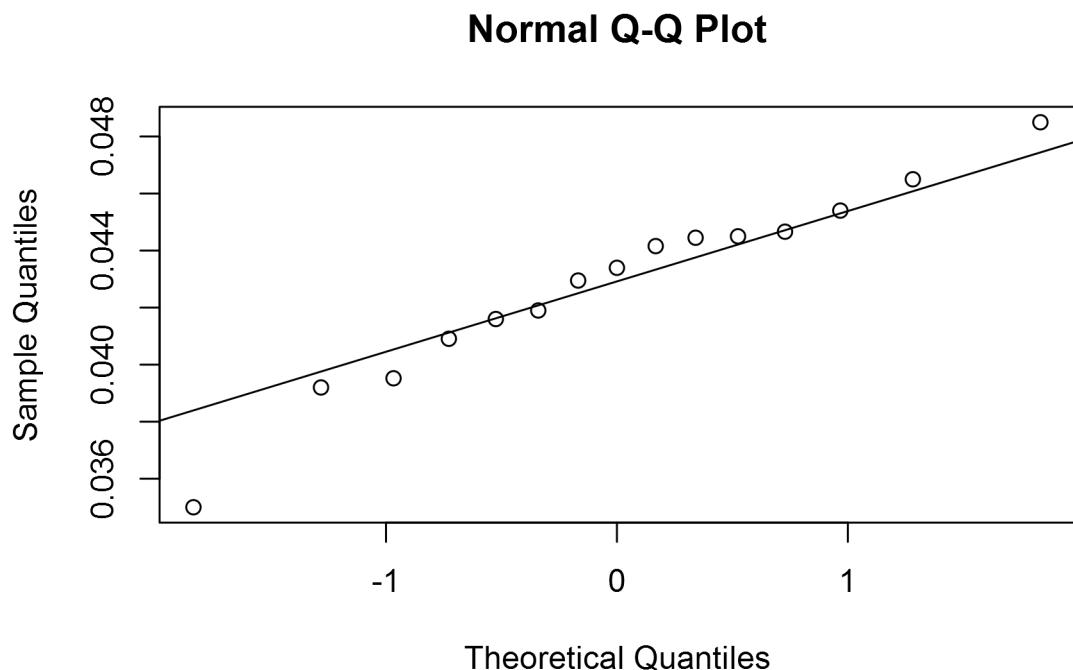
Normal Q-Q Plot



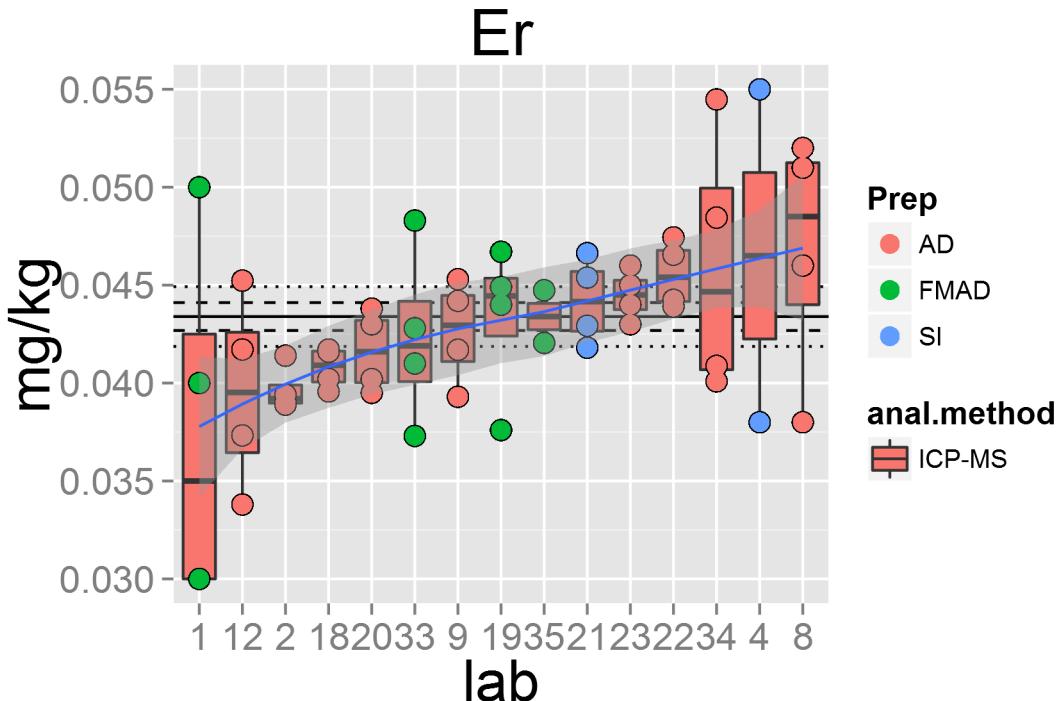
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



```
## [1] "Er.2"
```

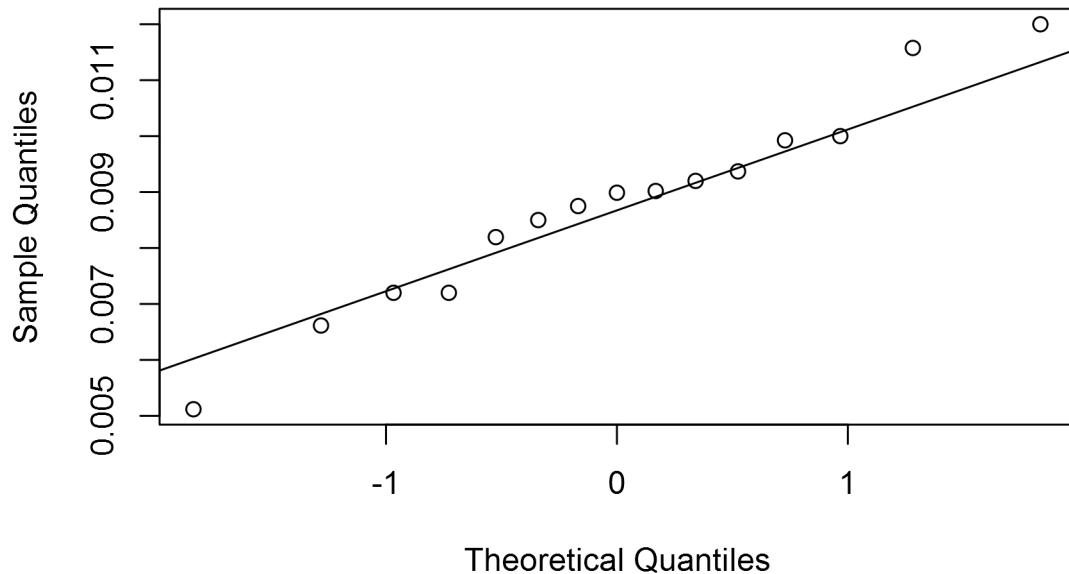


geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change.

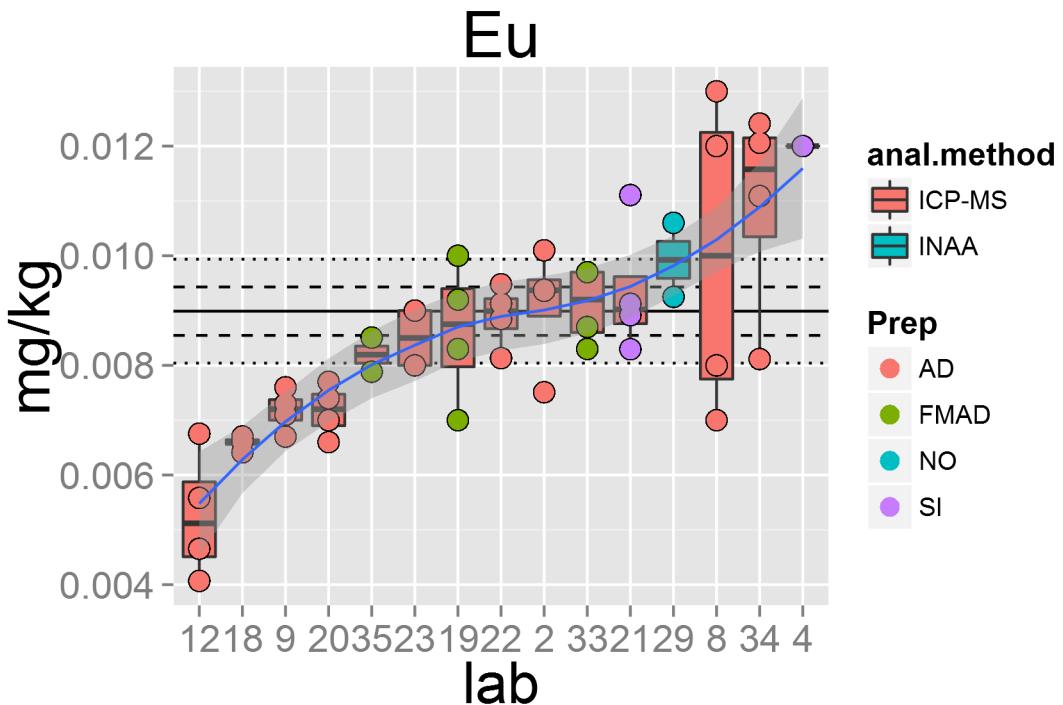


```
## [1] "Eu.2"
```

Normal Q-Q Plot

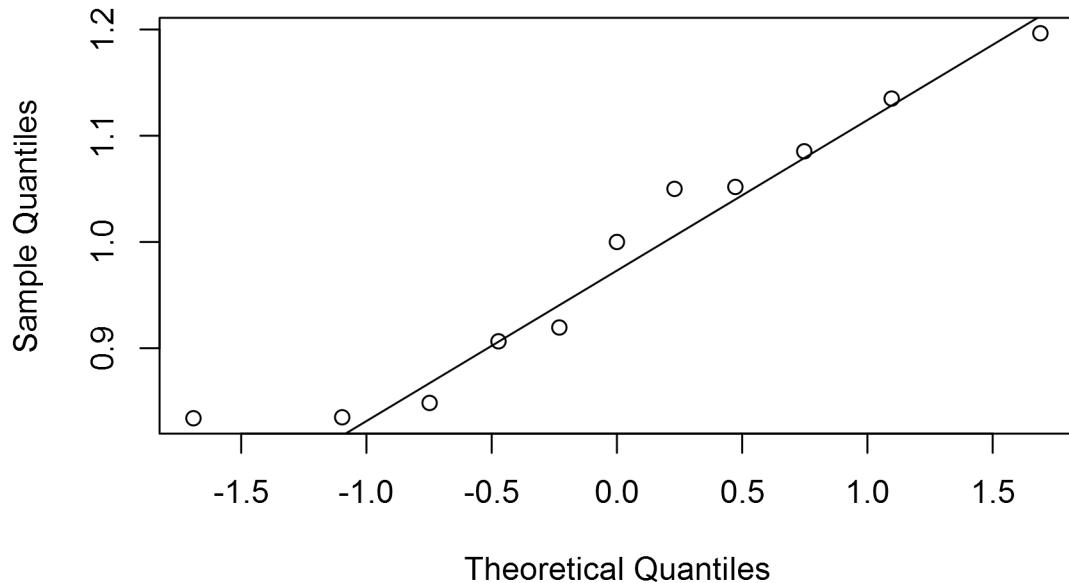


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

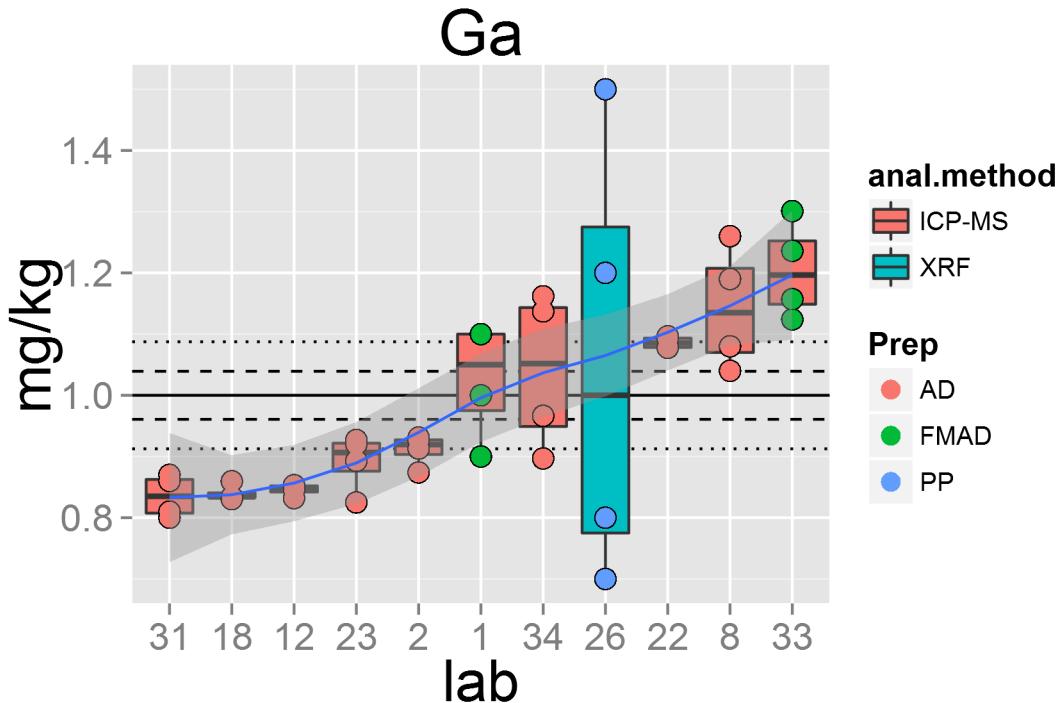


```
## [1] "Ga.2"
```

Normal Q-Q Plot

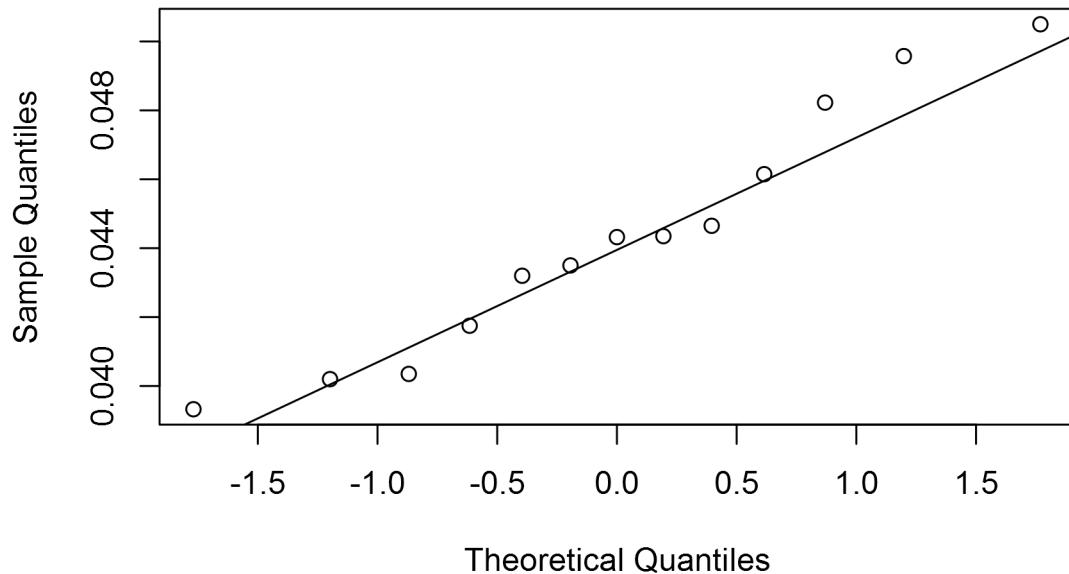


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

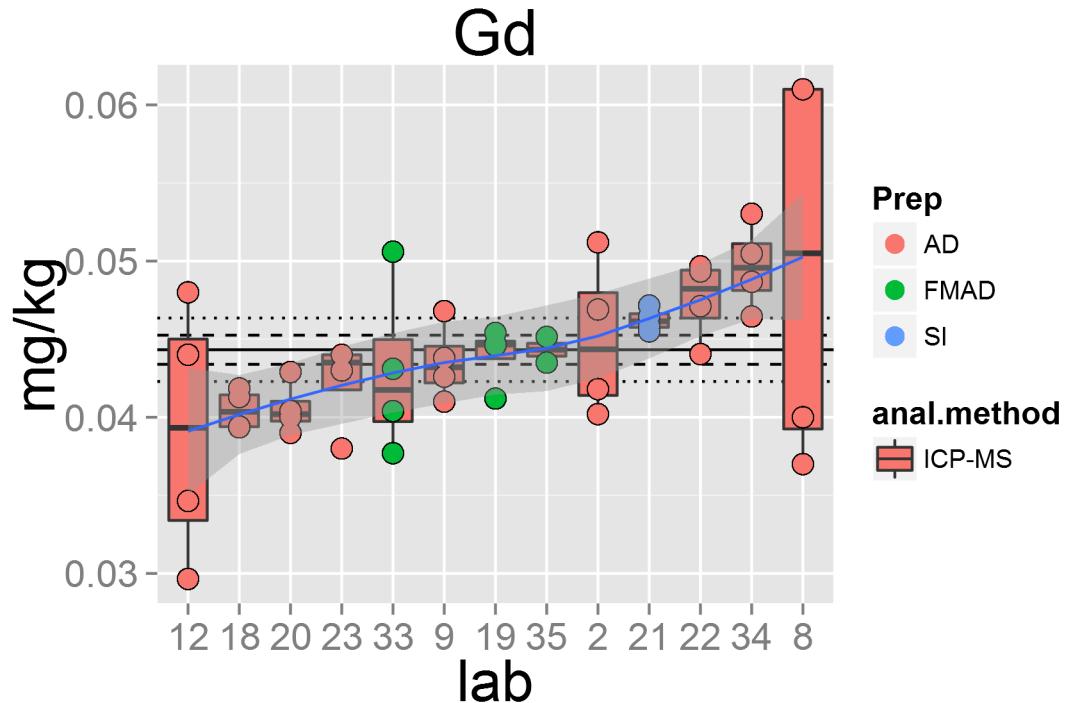


```
## [1] "Gd.2"
```

Normal Q-Q Plot

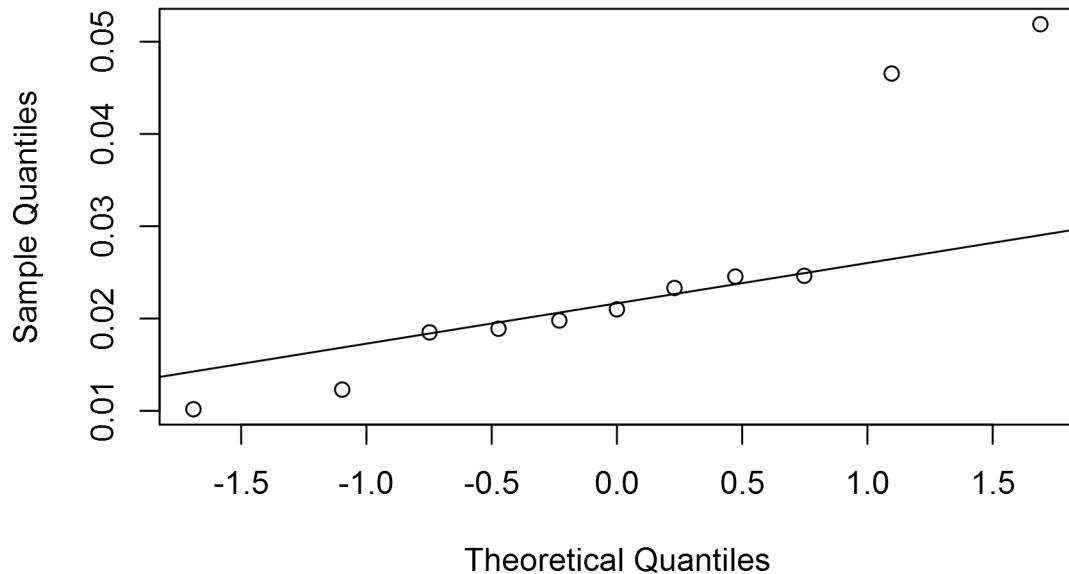


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

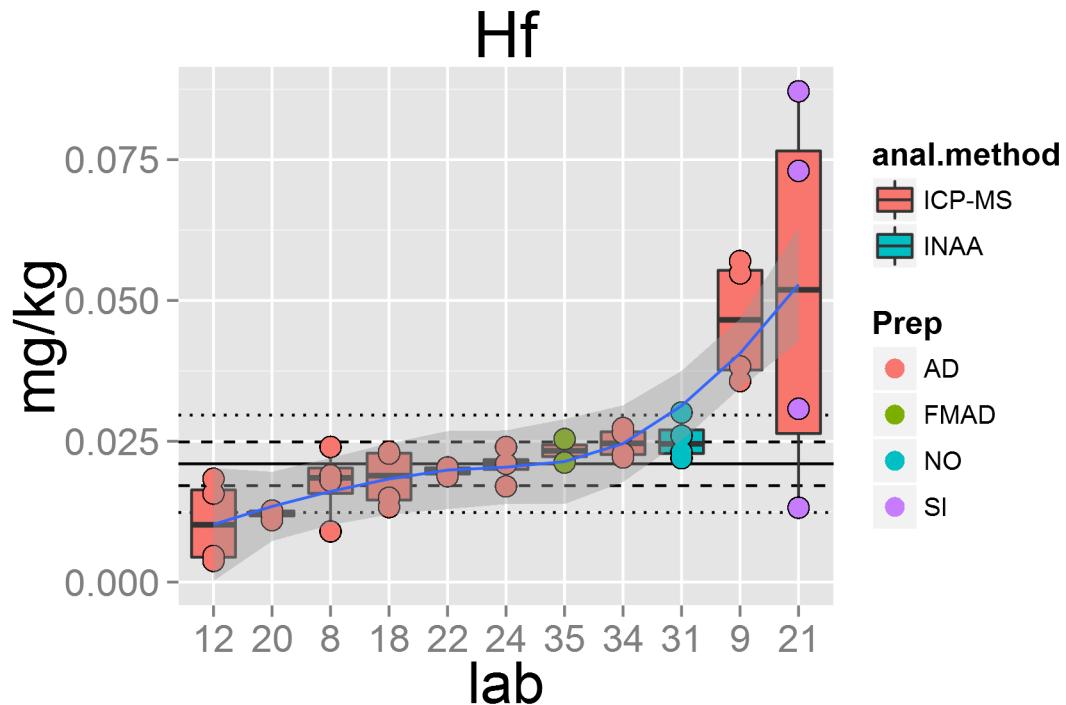


```
## [1] "Hf.2"
```

Normal Q-Q Plot

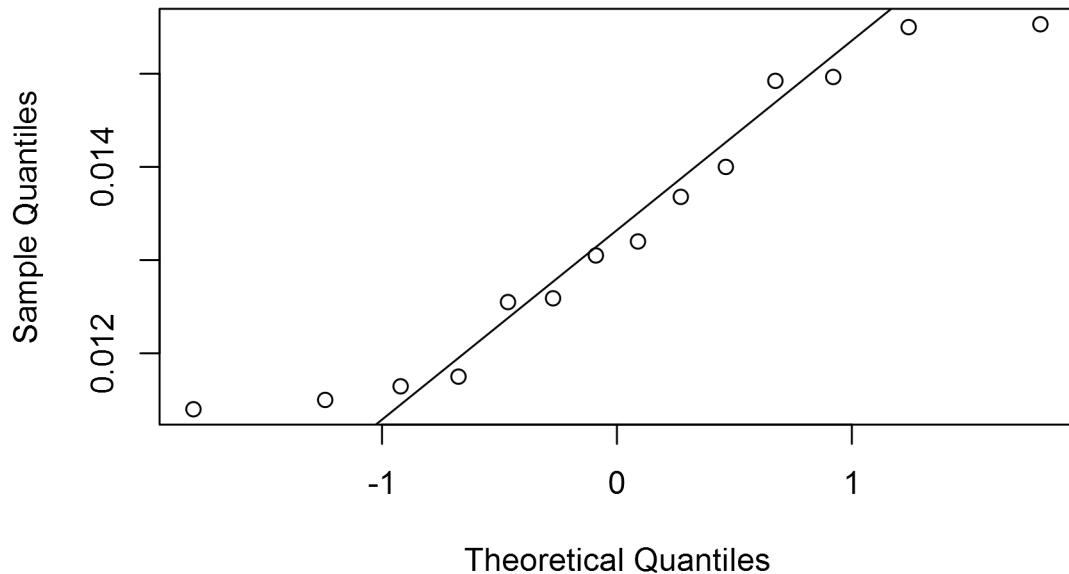


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

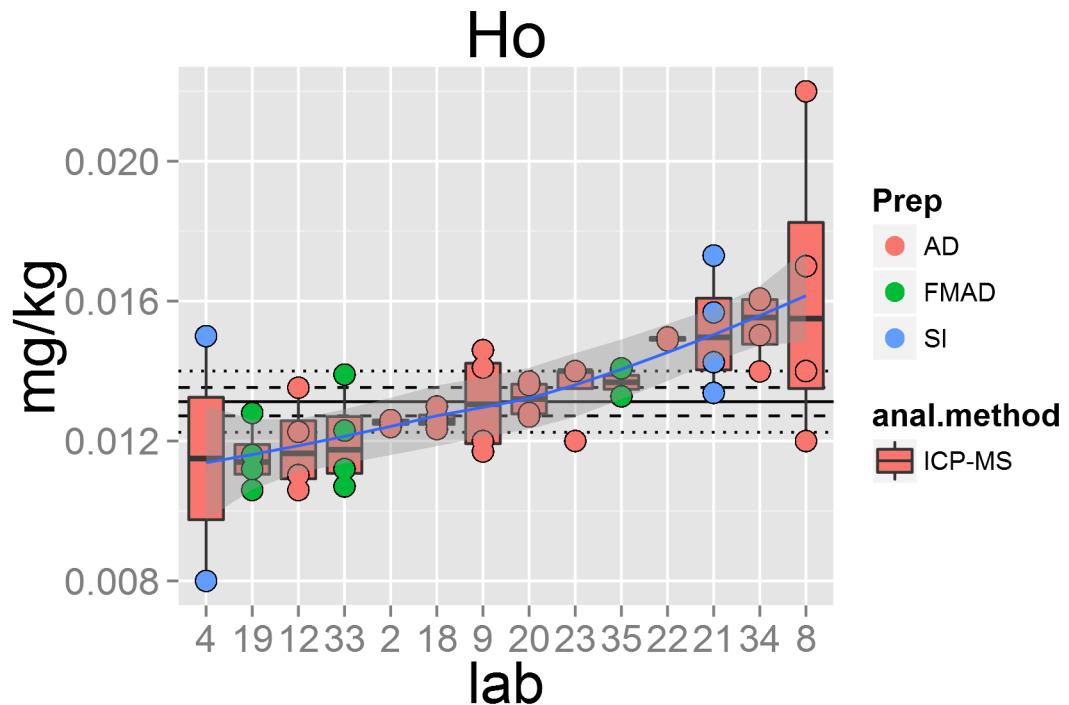


```
## [1] "Ho .2"
```

Normal Q-Q Plot

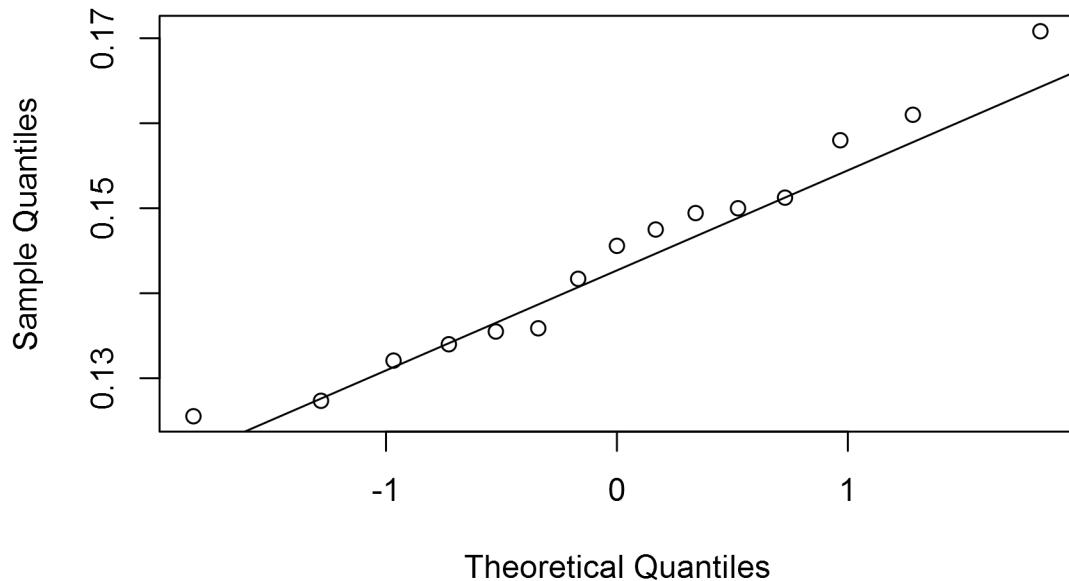


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

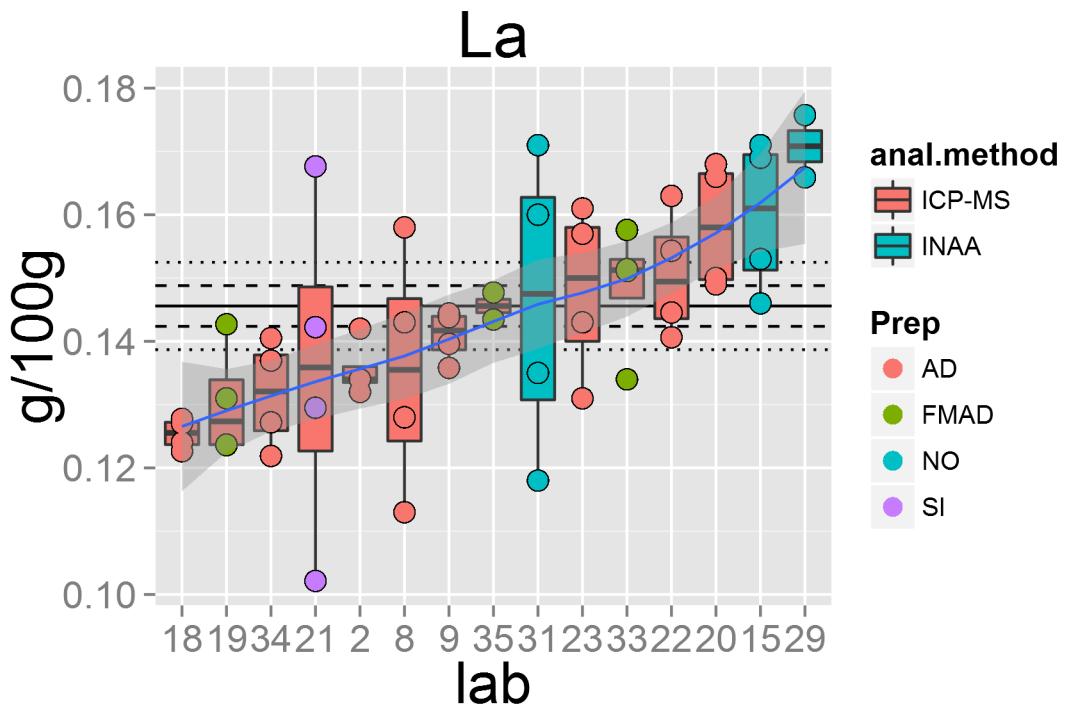


```
## [1] "La.2"
```

Normal Q-Q Plot

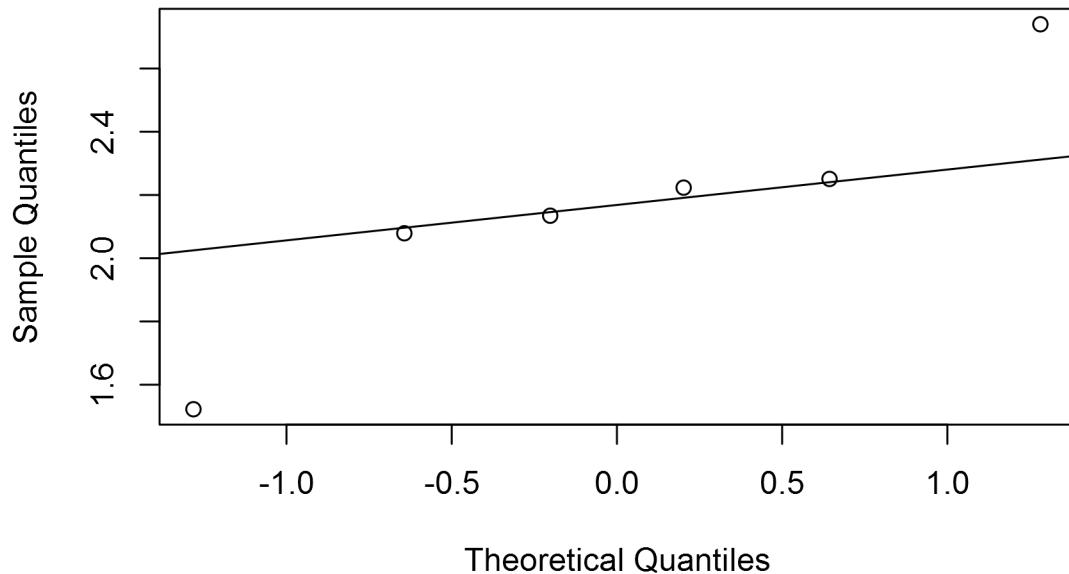


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

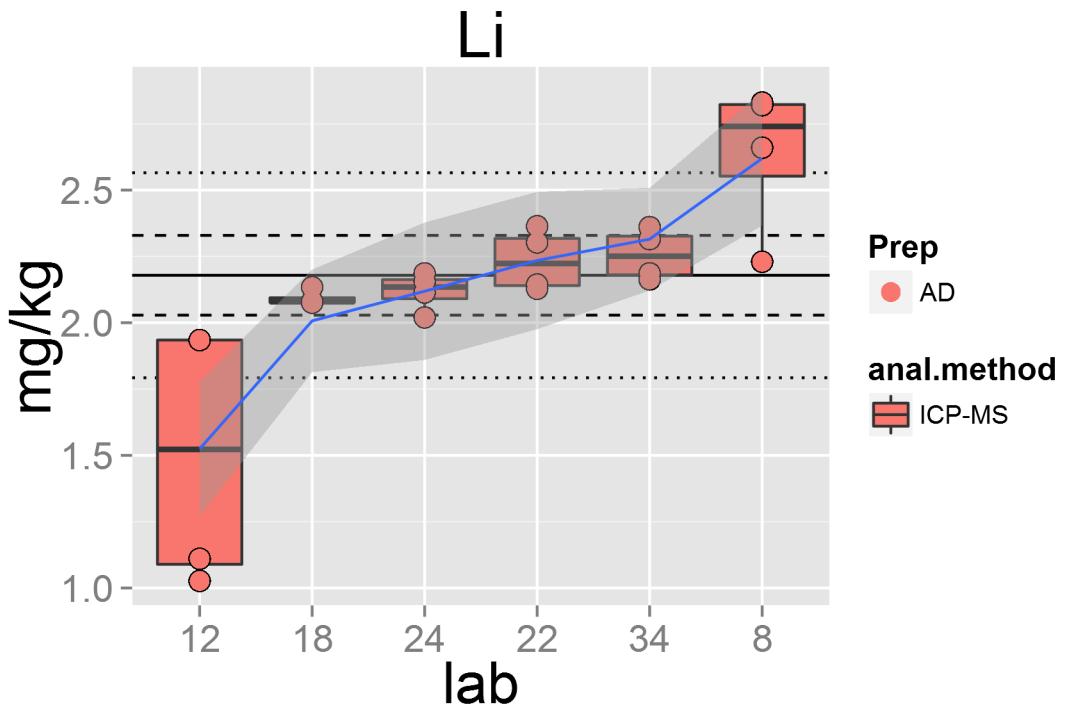


```
## [1] "Li.2"
```

Normal Q-Q Plot

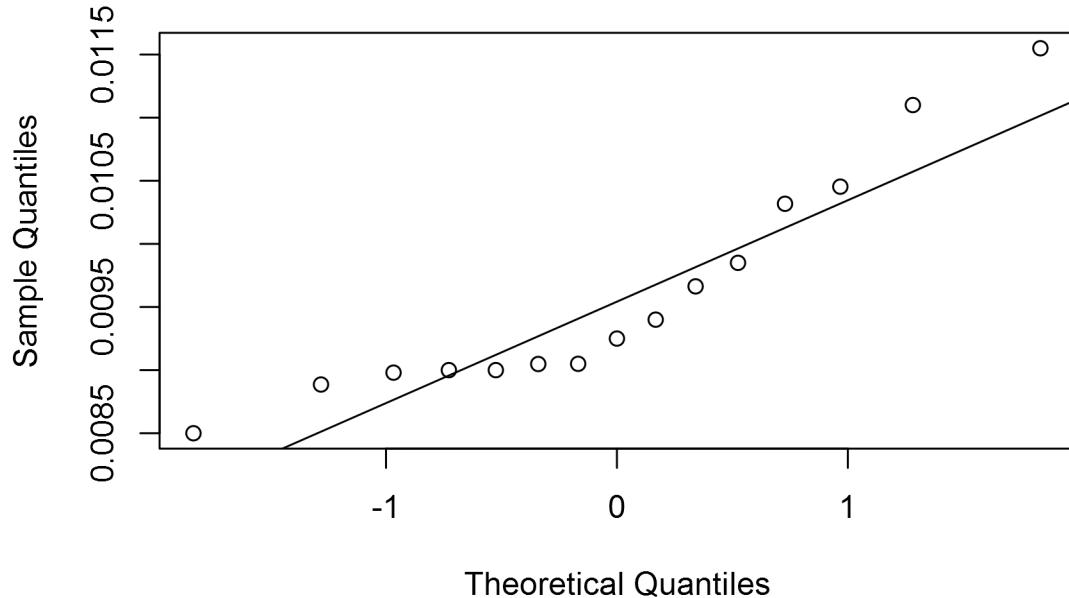


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

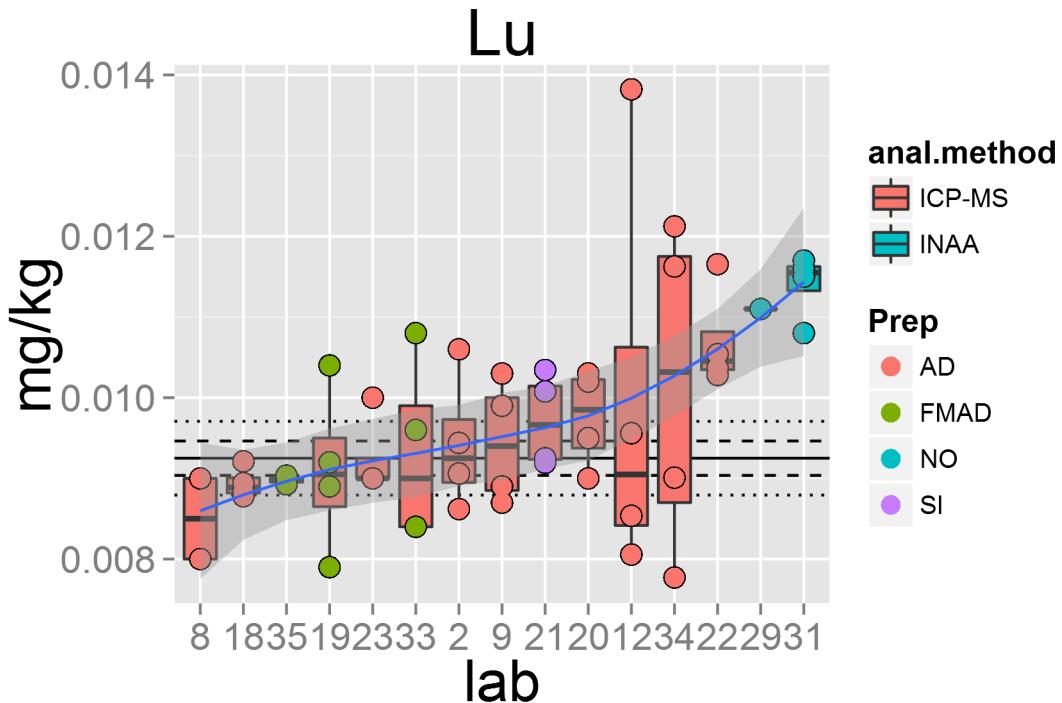


```
## [1] "Lu.2"
```

Normal Q-Q Plot

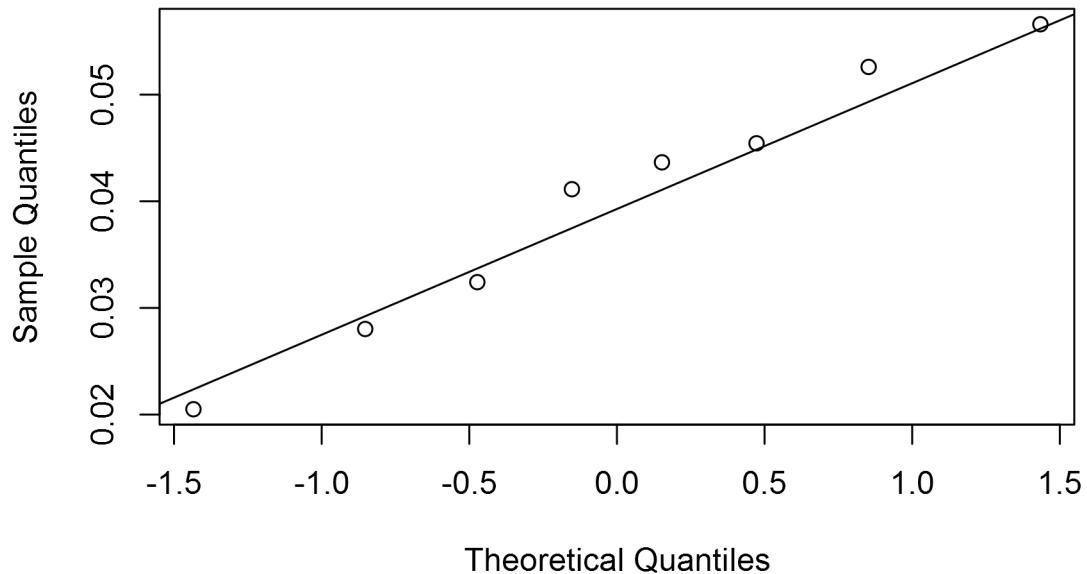


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

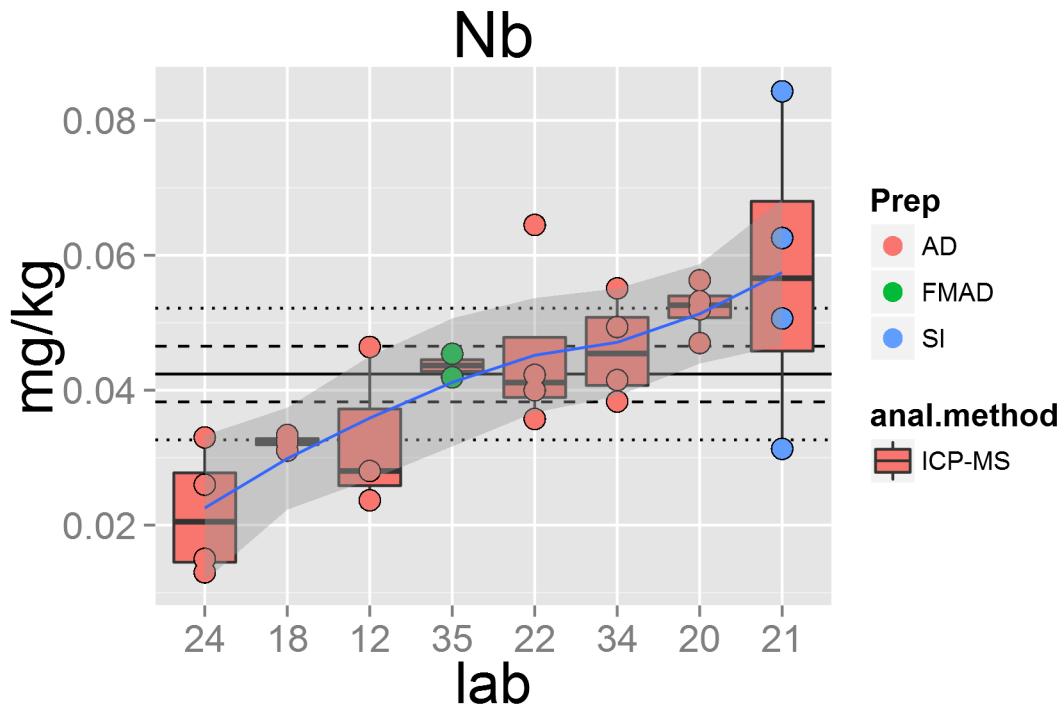


```
## [1] "Nb. 2"
```

Normal Q-Q Plot

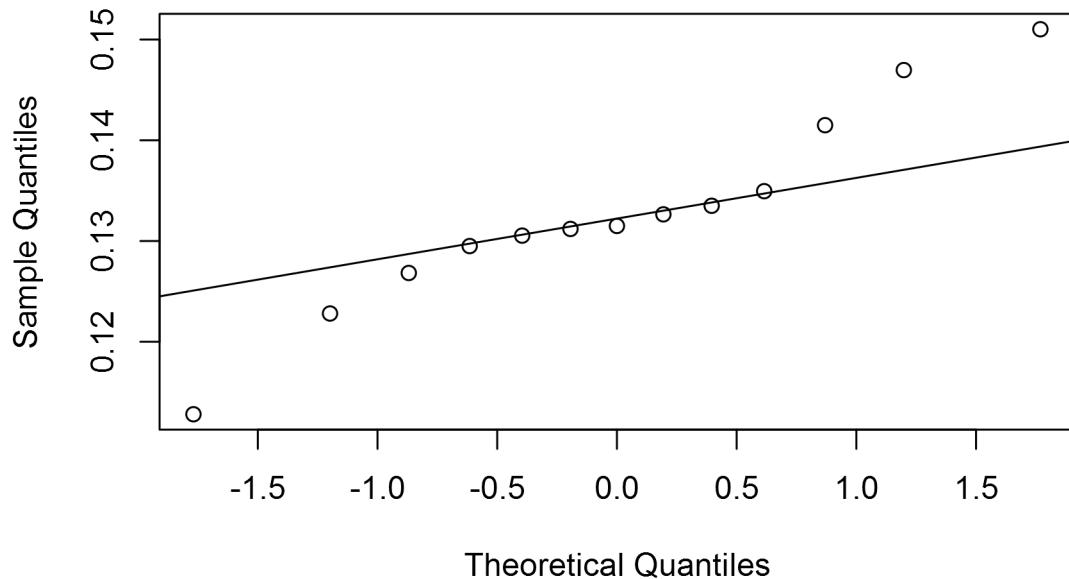


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

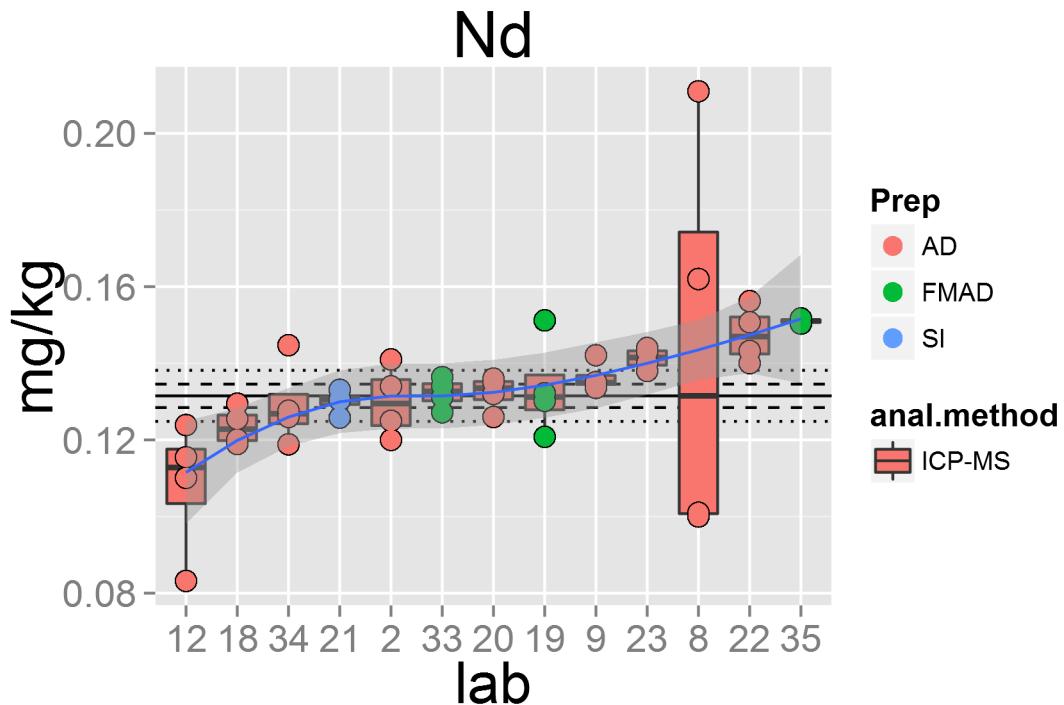


```
## [1] "Nd.2"
```

Normal Q-Q Plot

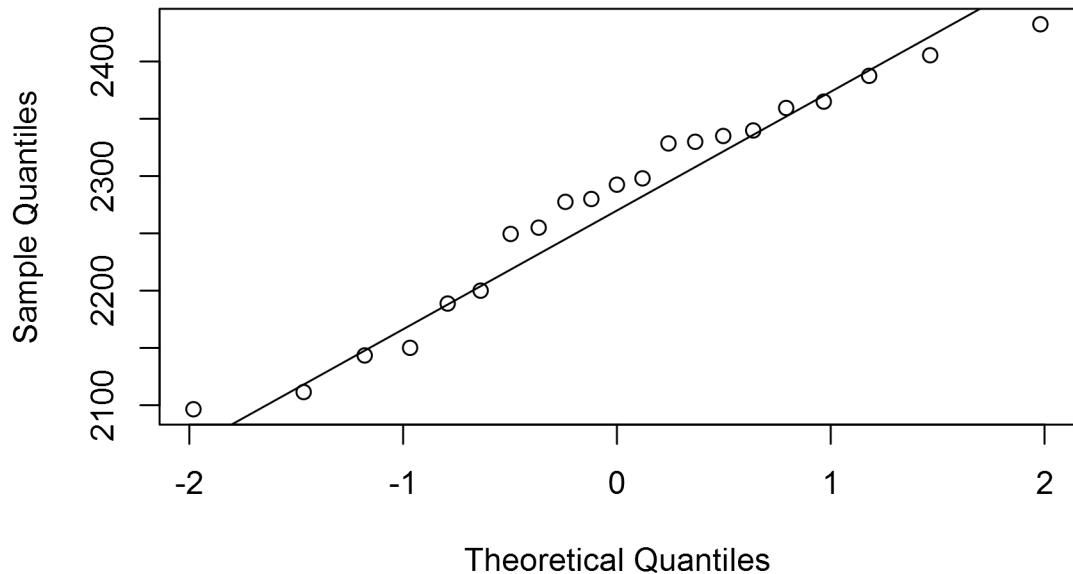


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

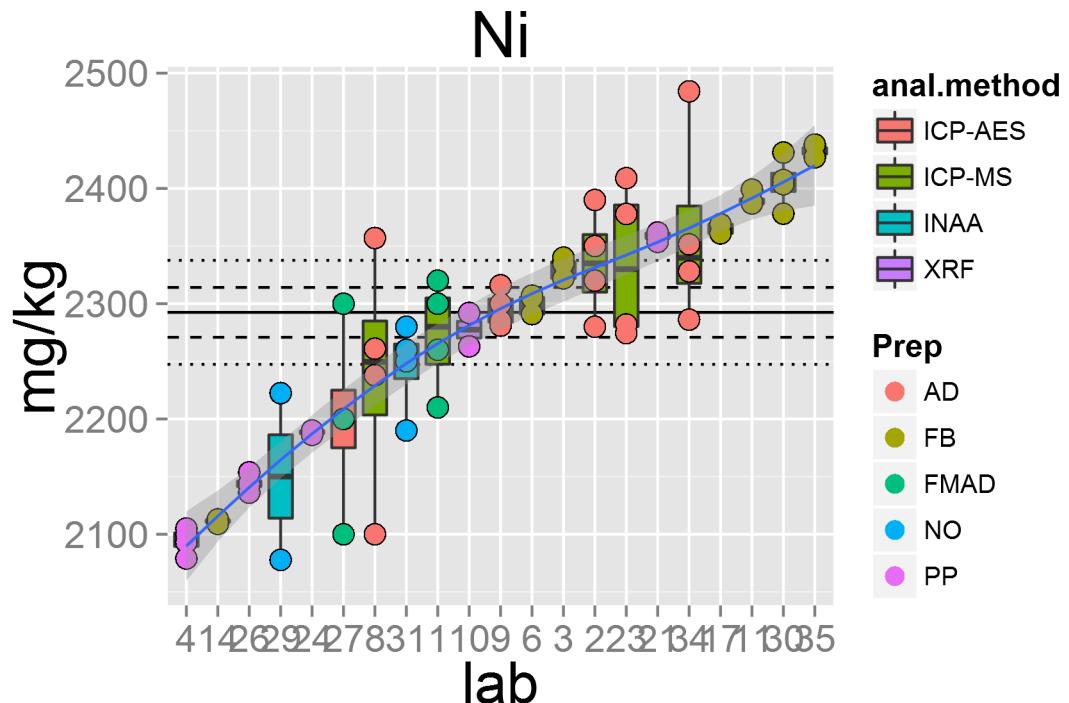


```
## [1] "Ni.2"
```

Normal Q-Q Plot

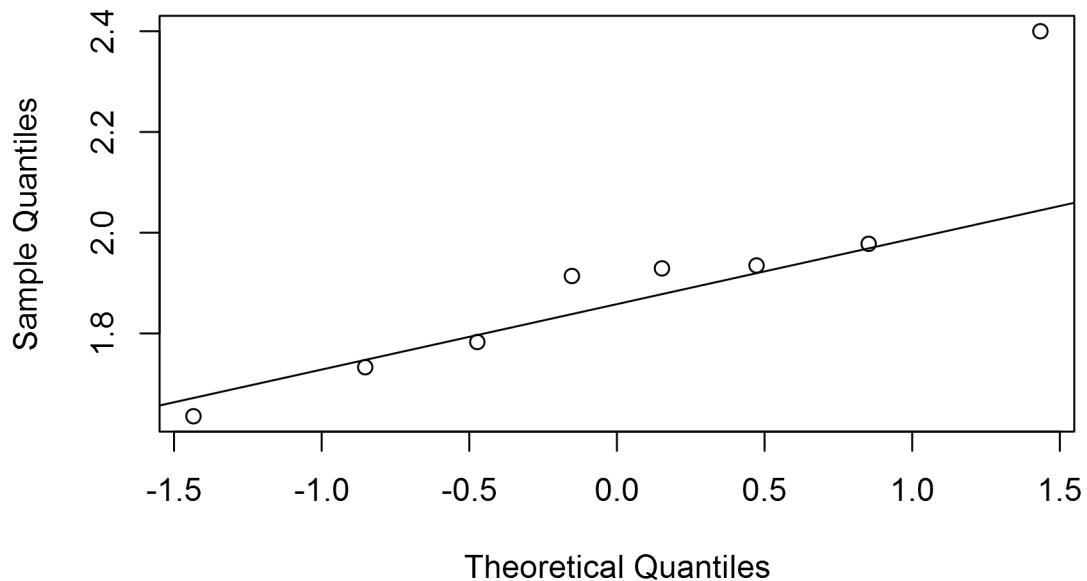


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

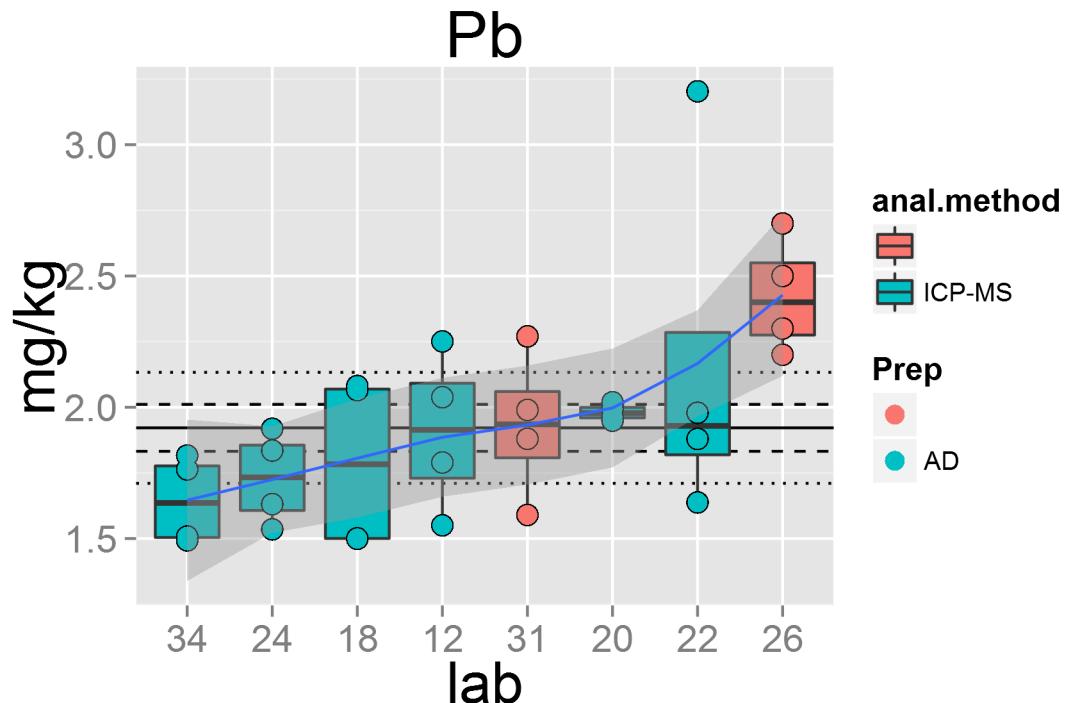


```
## [1] "Pb.2"
```

Normal Q-Q Plot

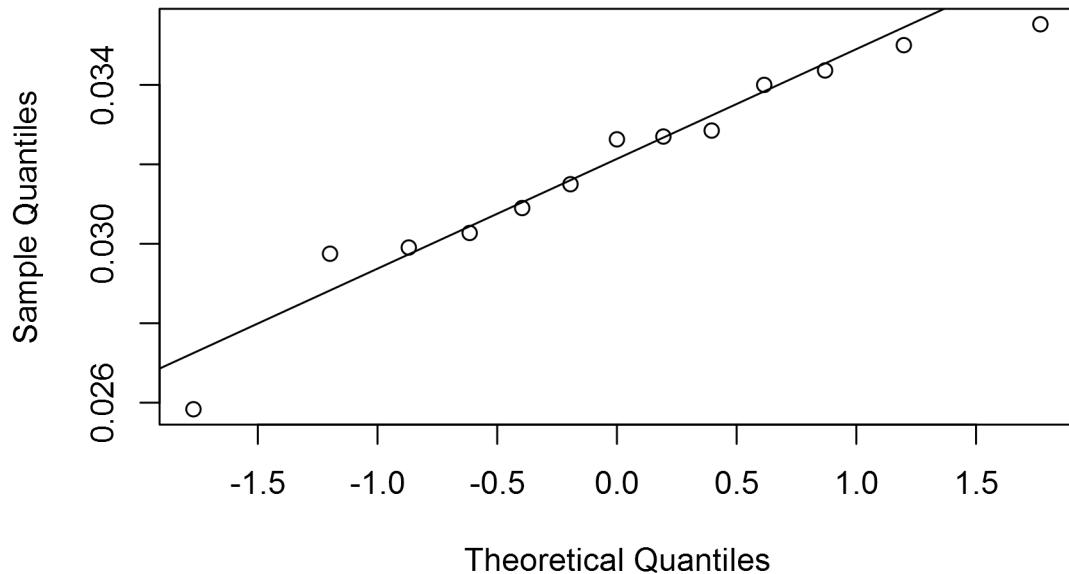


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

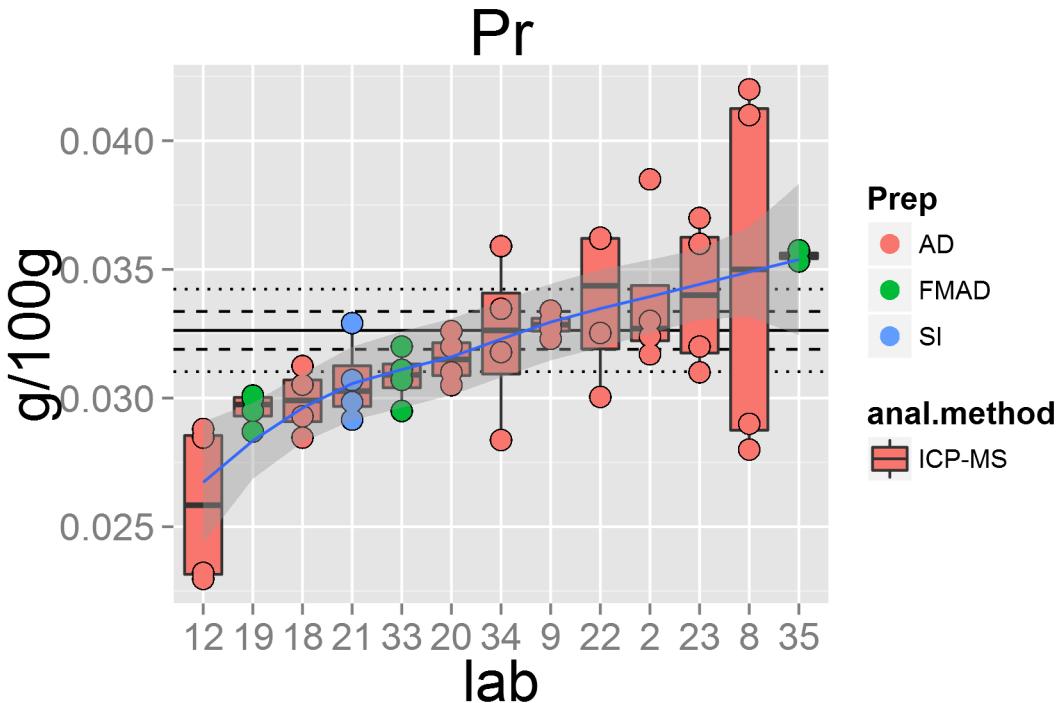


```
## [1] "Pr. 2"
```

Normal Q-Q Plot

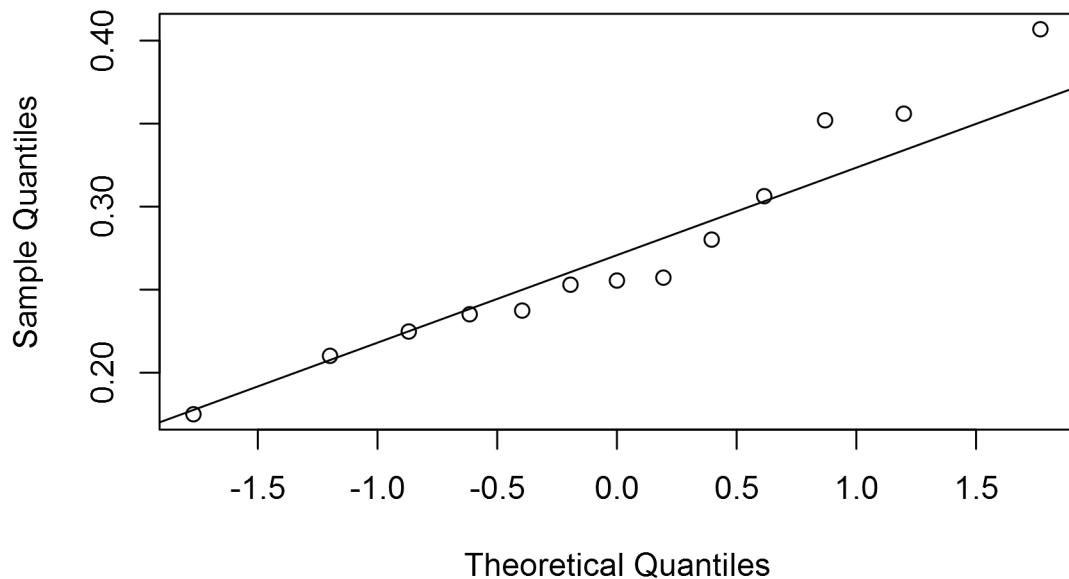


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

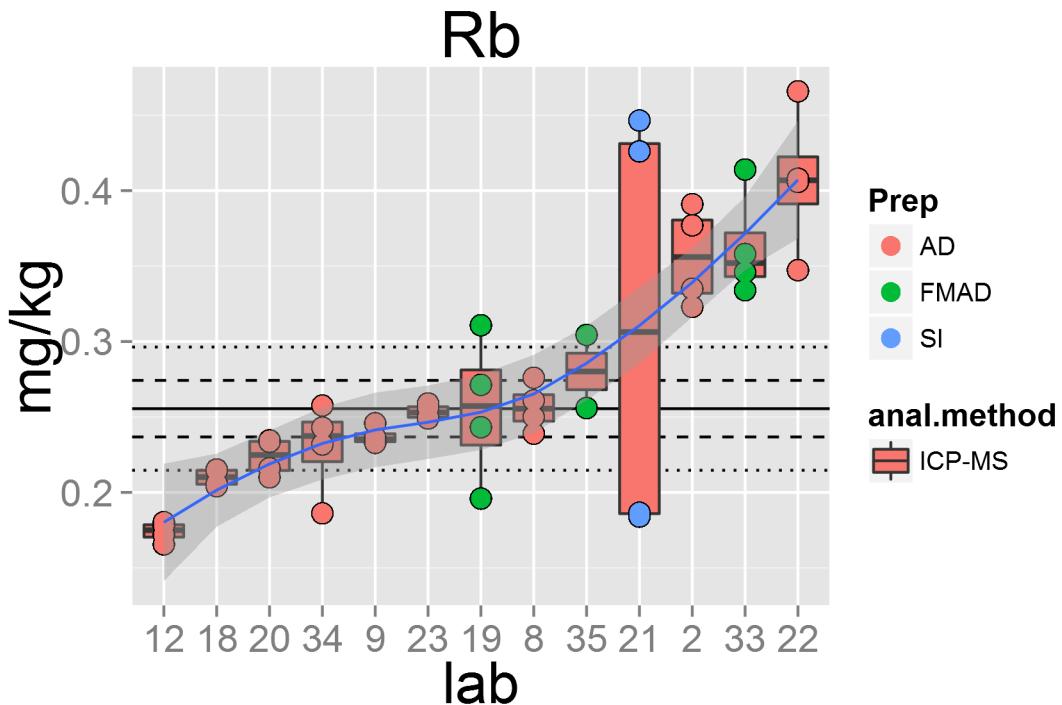


```
## [1] "Rb.2"
```

Normal Q-Q Plot

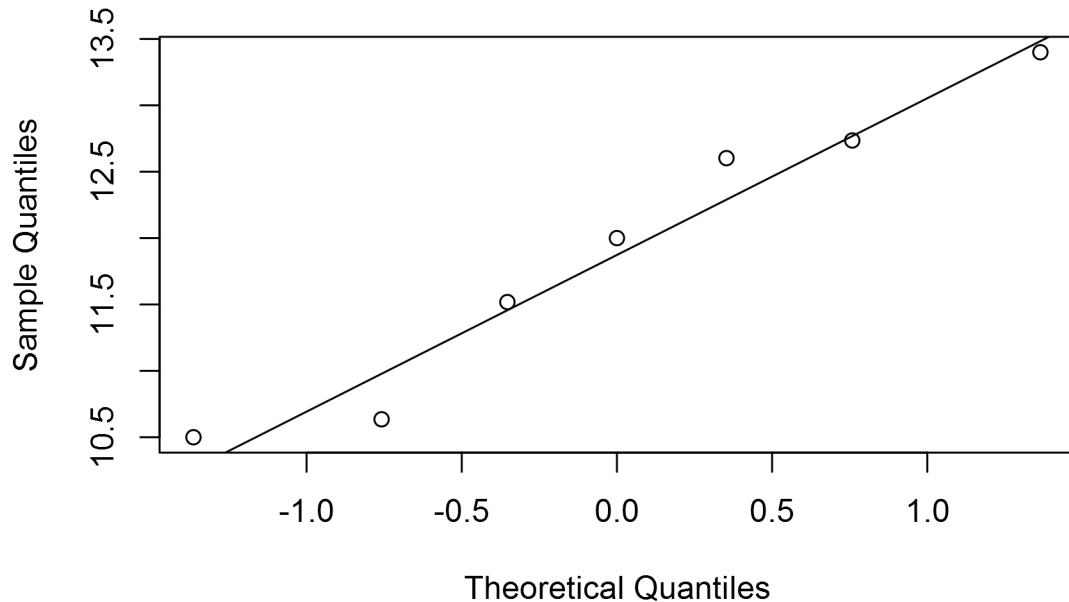


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

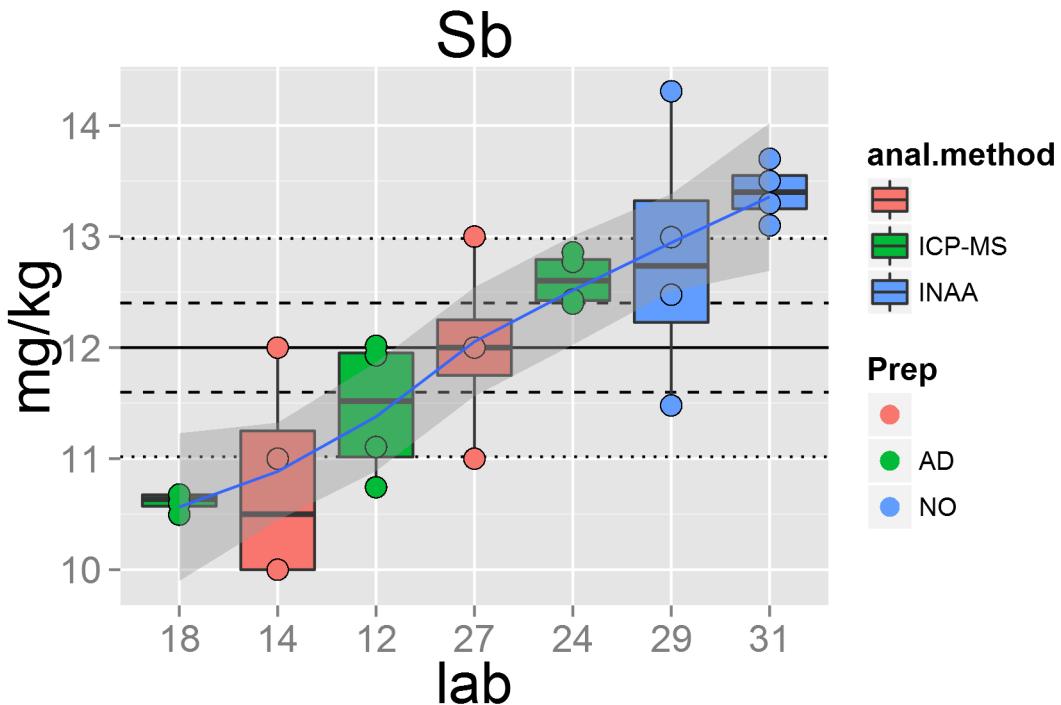


```
## [1] "Sb.2"
```

Normal Q-Q Plot

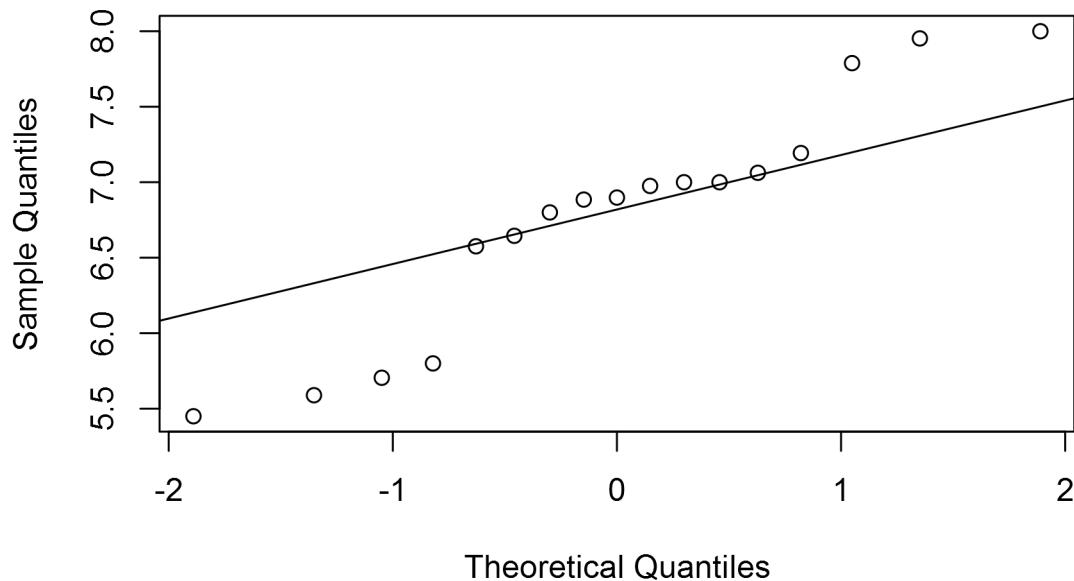


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

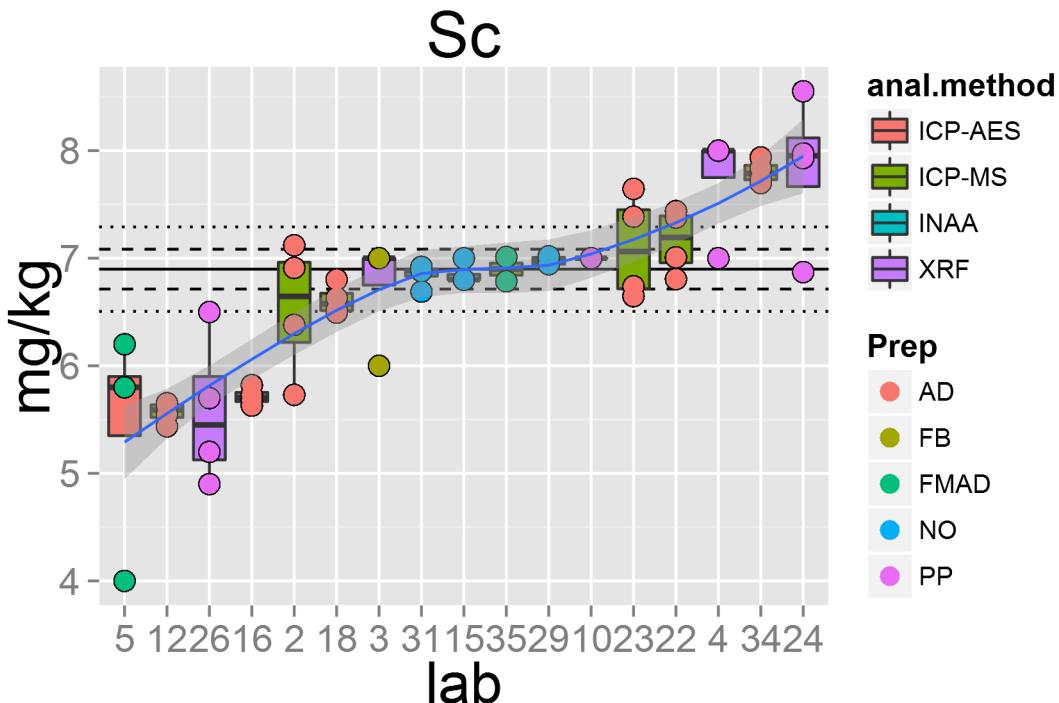


```
## [1] "Sc.2"
```

Normal Q-Q Plot

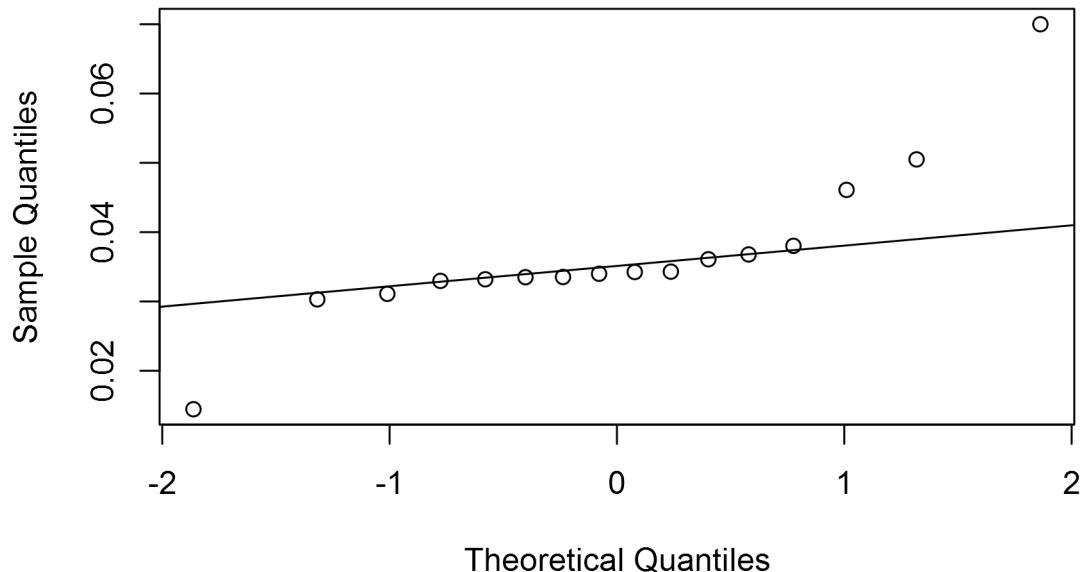


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

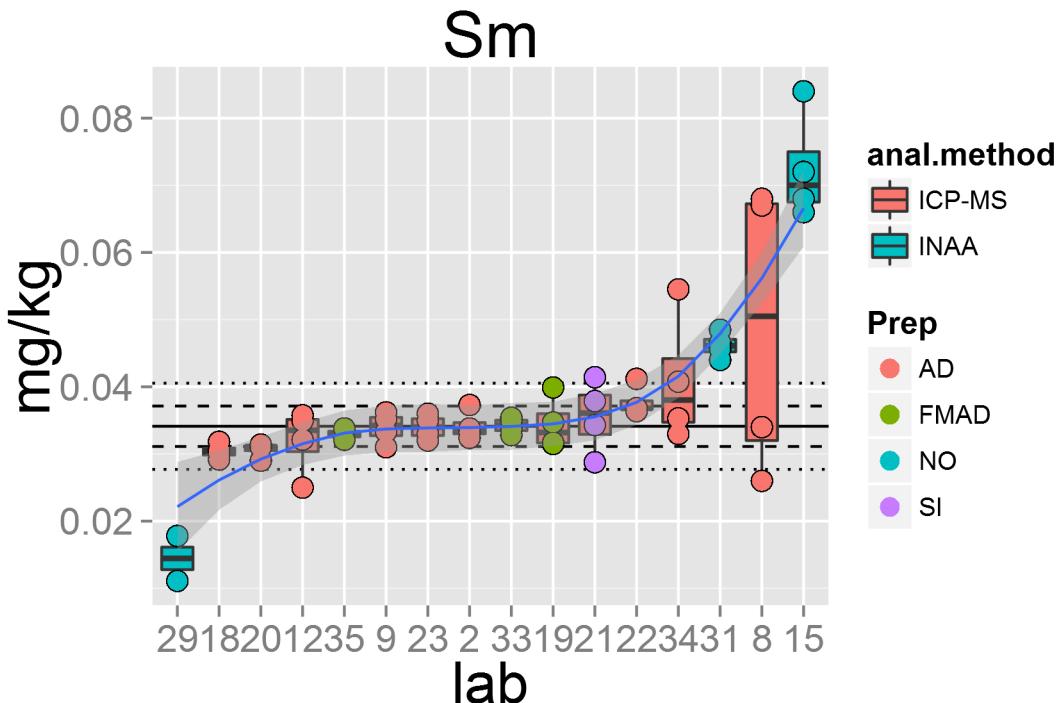


```
## [1] "Sm.2"
```

Normal Q-Q Plot

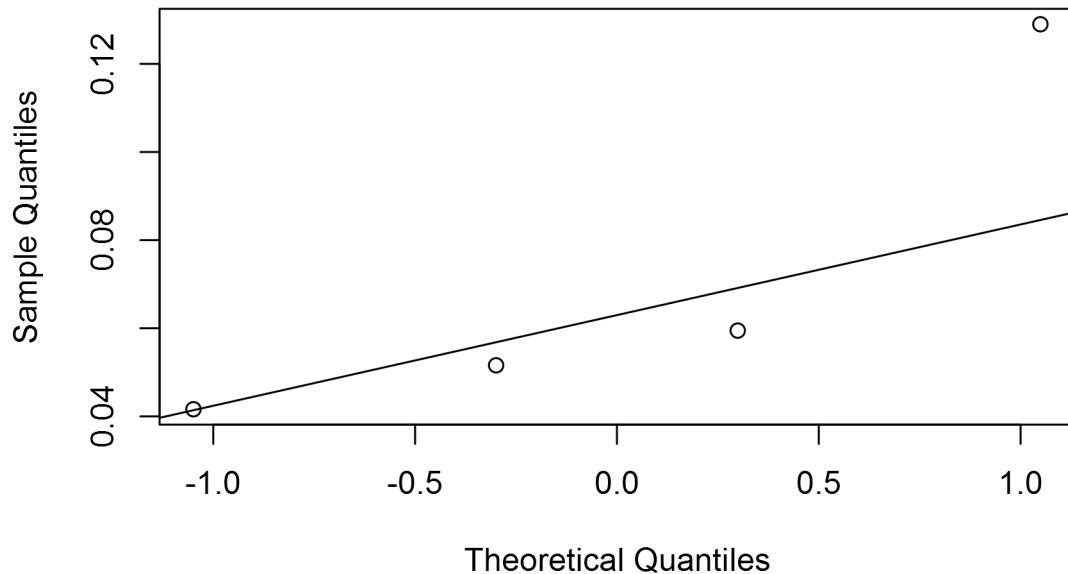


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```

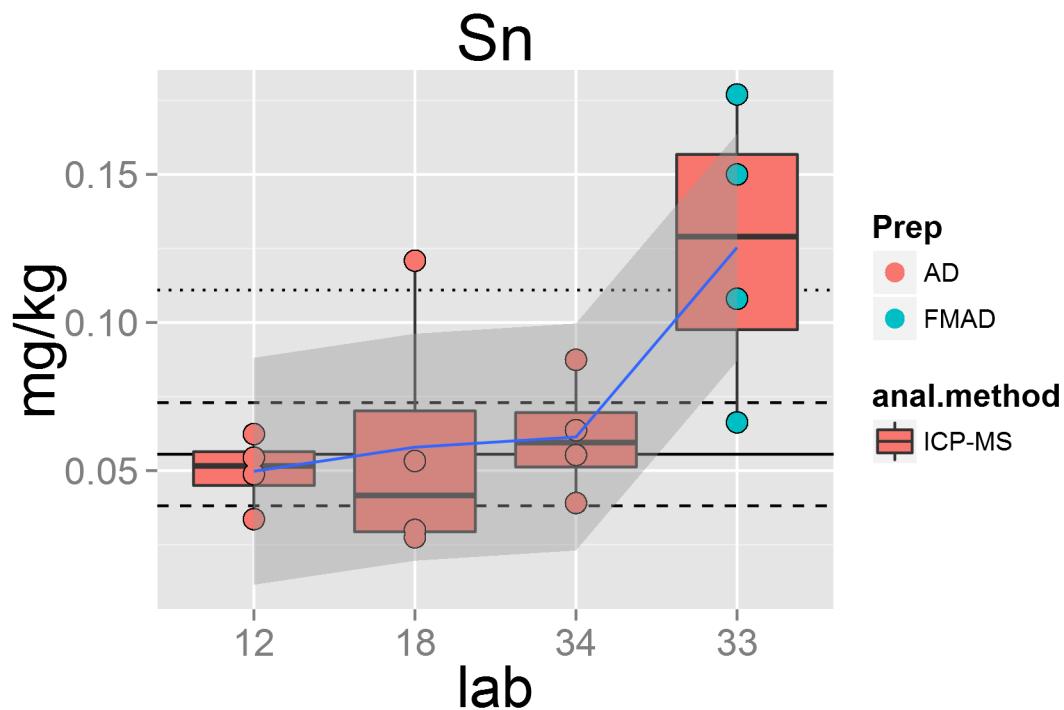


```
## [1] "Sn.2"
```

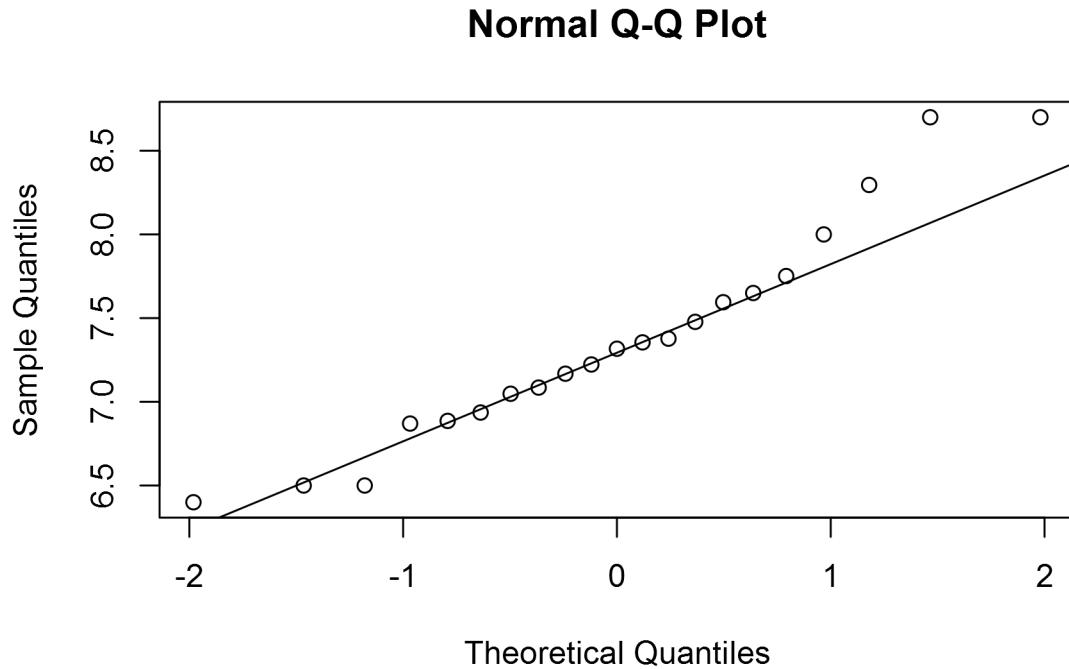
Normal Q-Q Plot



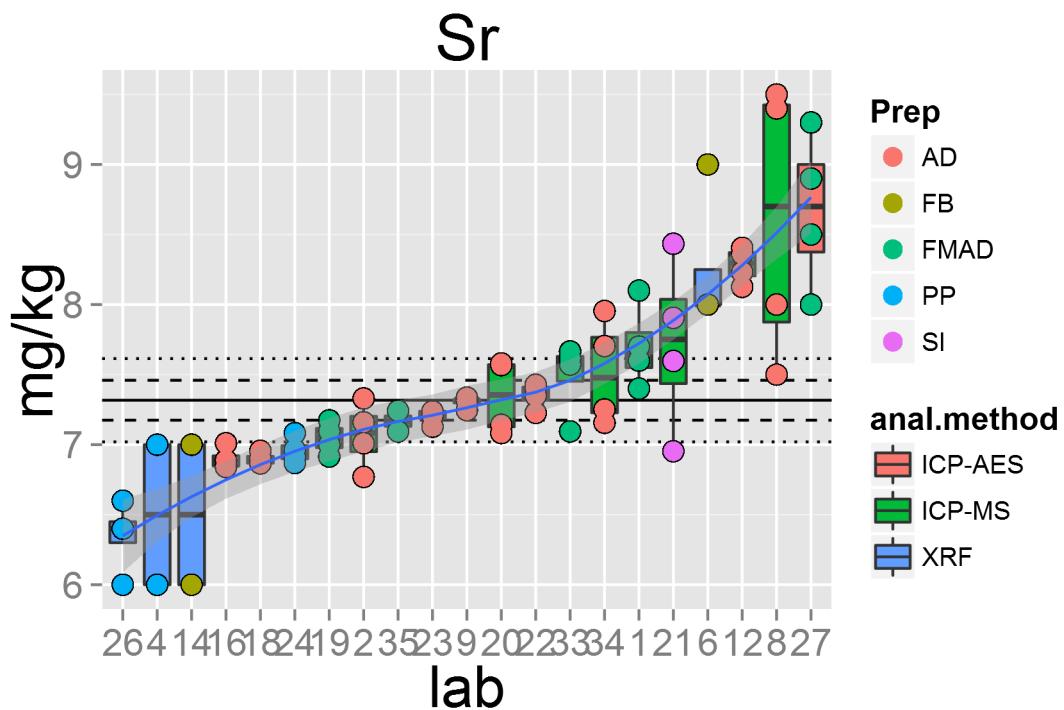
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
## Warning: pseudoinverse used at 0.985
## Warning: neighborhood radius 2.015
## Warning: reciprocal condition number 5.193e-017
## Warning: There are other near singularities as well. 4.0602
## Warning: pseudoinverse used at 0.985
## Warning: neighborhood radius 2.015
## Warning: reciprocal condition number 5.193e-017
## Warning: There are other near singularities as well. 4.0602
```



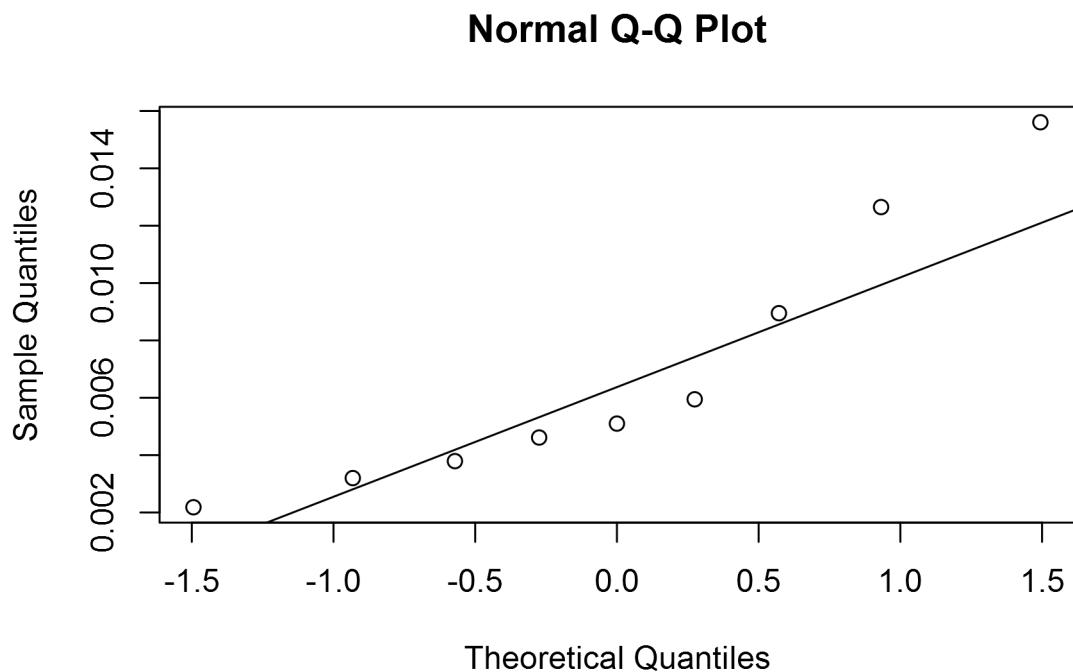
```
## [1] "Sr.2"
```



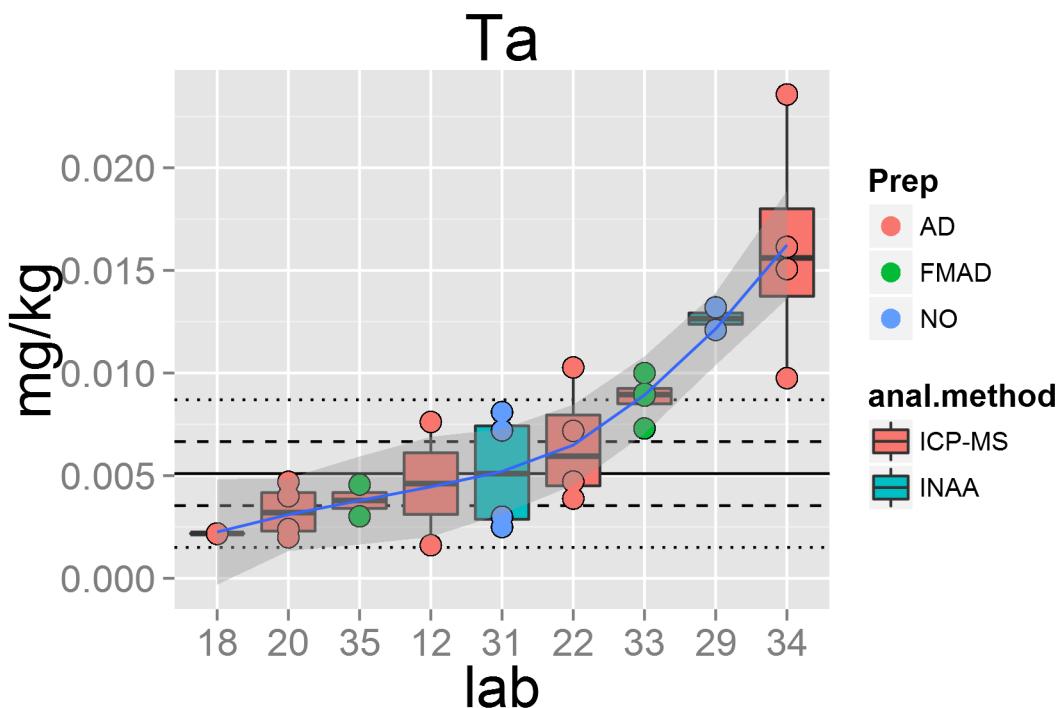
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



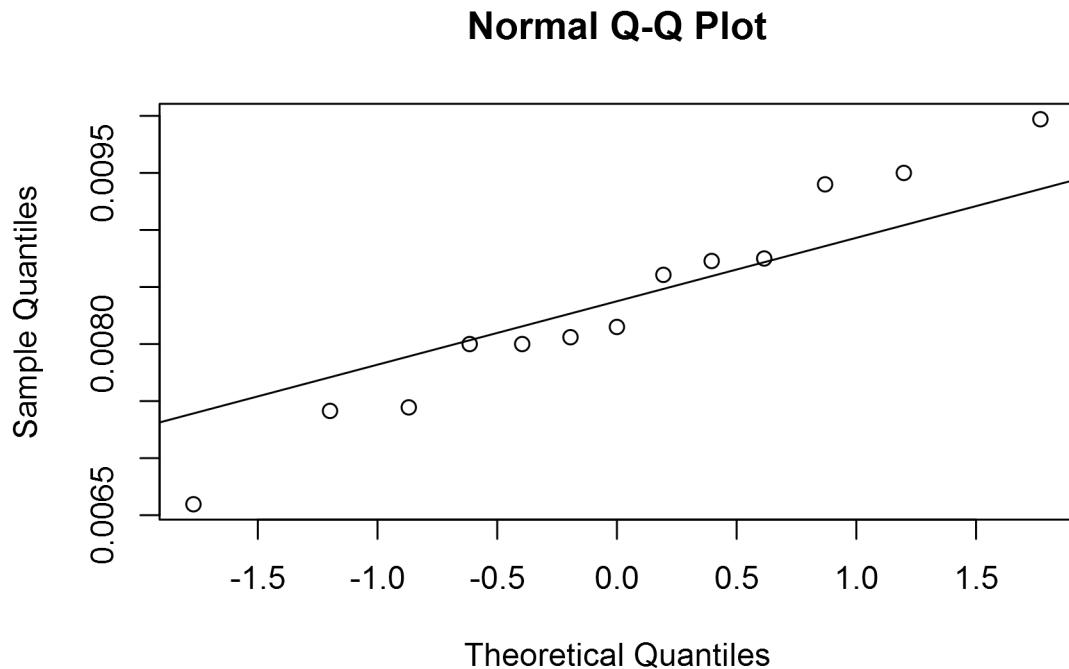
```
## [1] "Ta.2"
```



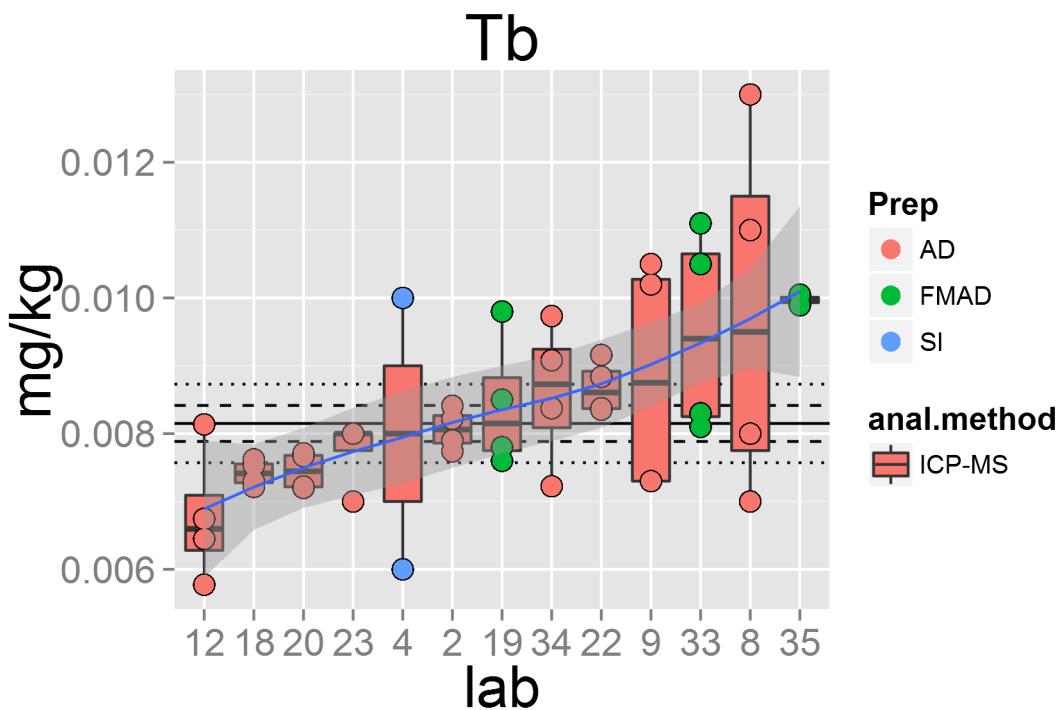
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



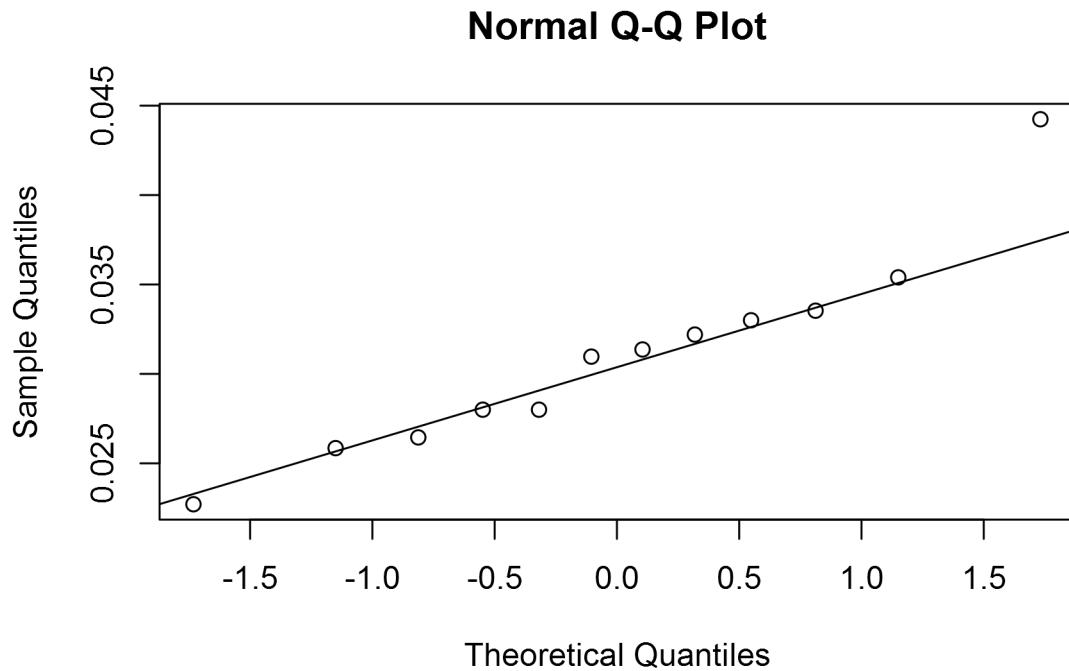
```
## [1] "Tb.2"
```



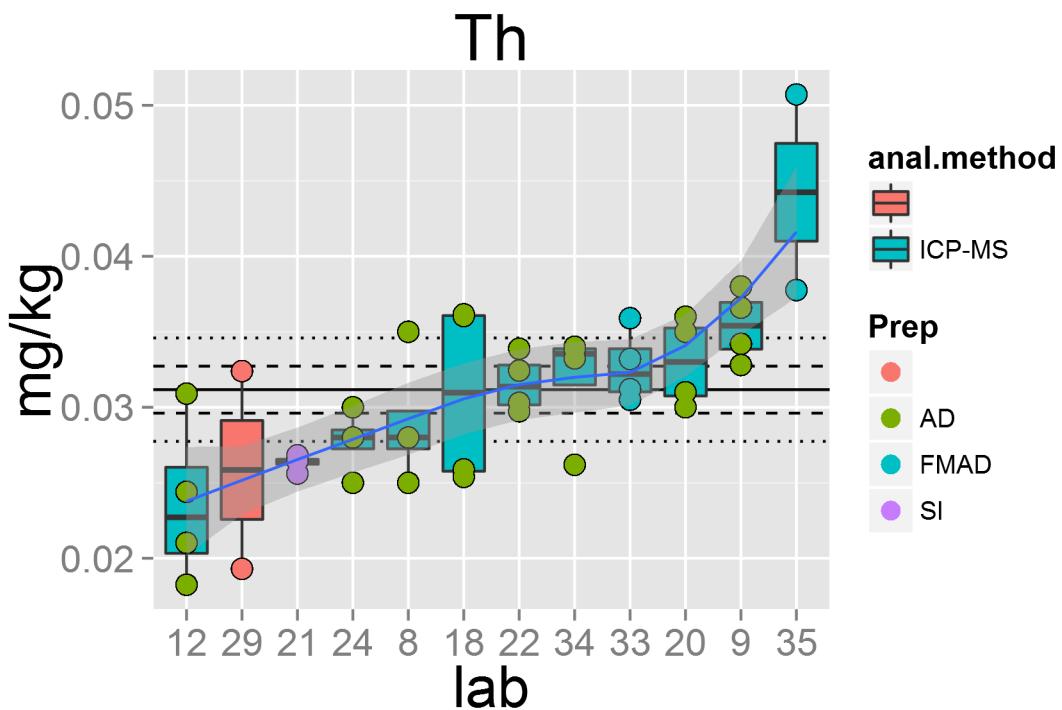
```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



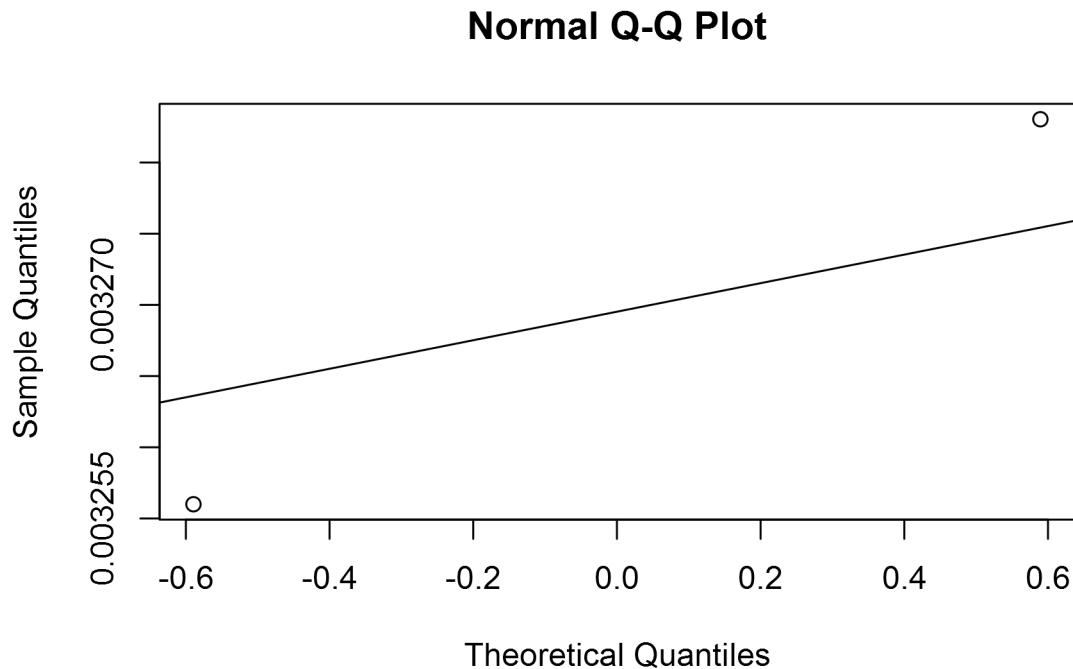
```
## [1] "Th.2"
```



```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```



```
## [1] "T1.2"
```

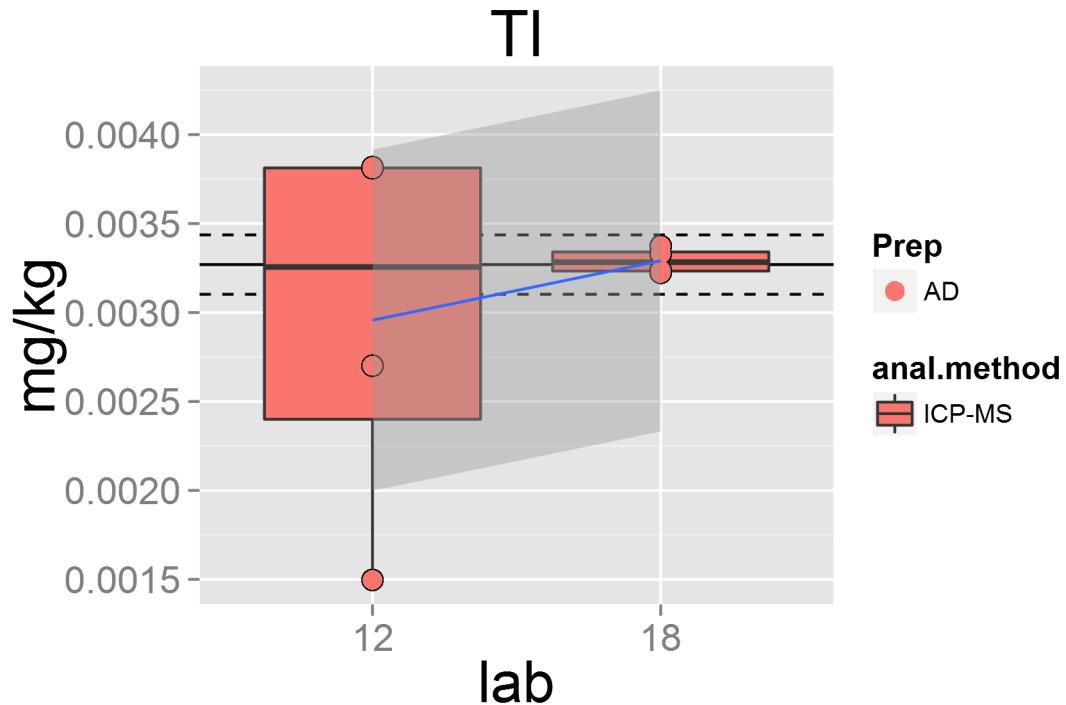


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

```

## Warning: pseudoinverse used at 0.995
## Warning: neighborhood radius 1.005
## Warning: reciprocal condition number  0
## Warning: There are other near singularities as well. 1.01
## Warning: pseudoinverse used at 0.995
## Warning: neighborhood radius 1.005
## Warning: reciprocal condition number  0
## Warning: There are other near singularities as well. 1.01

```

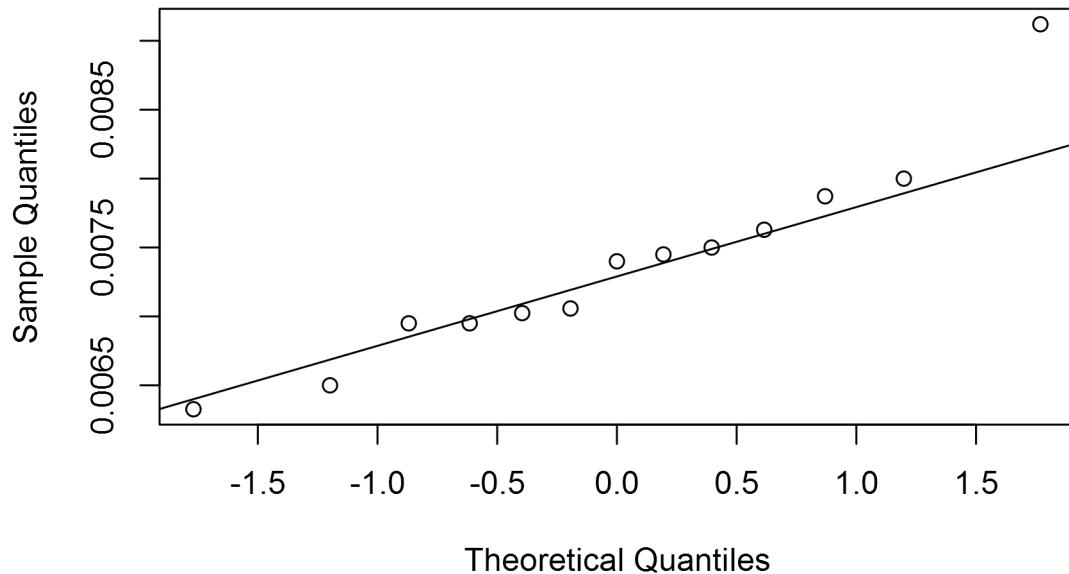


```

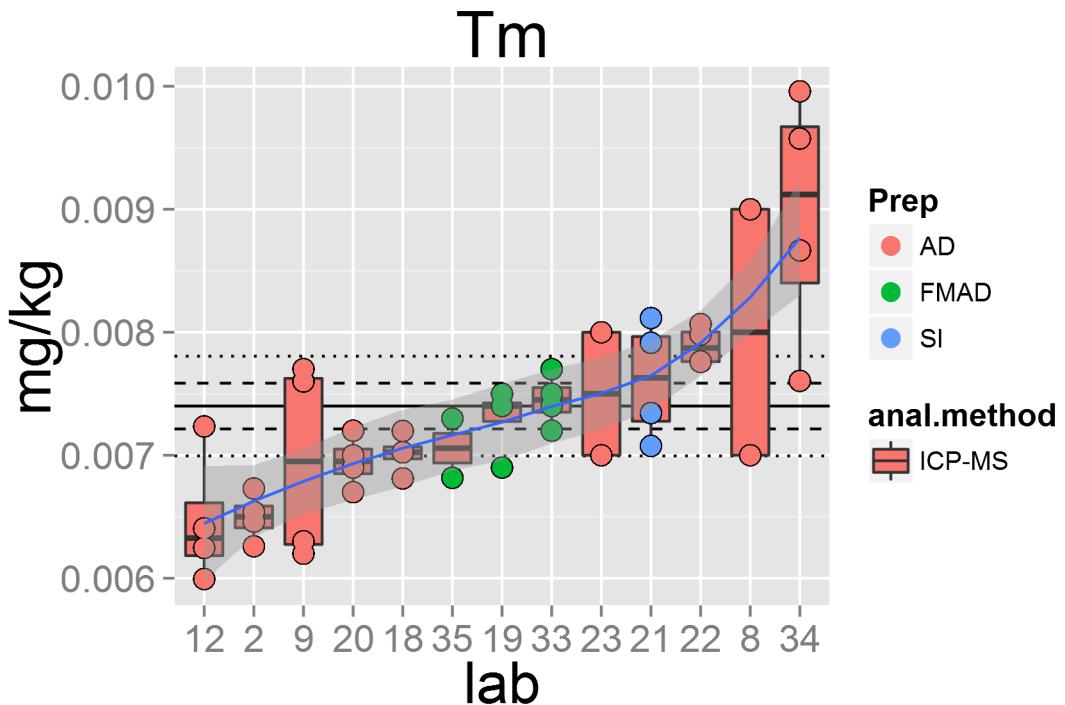
## [1] "Tm.2"

```

Normal Q-Q Plot

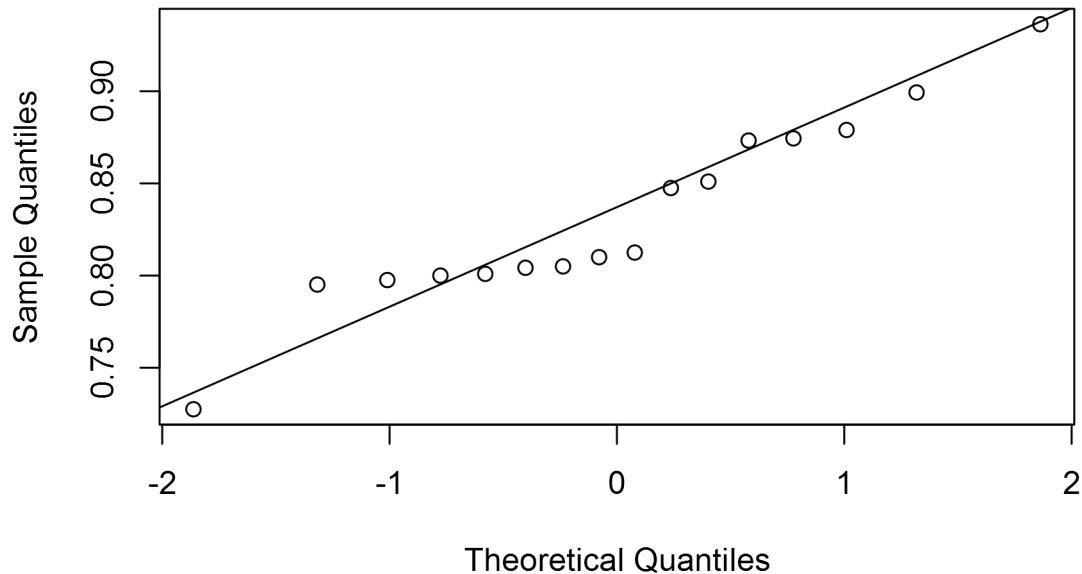


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

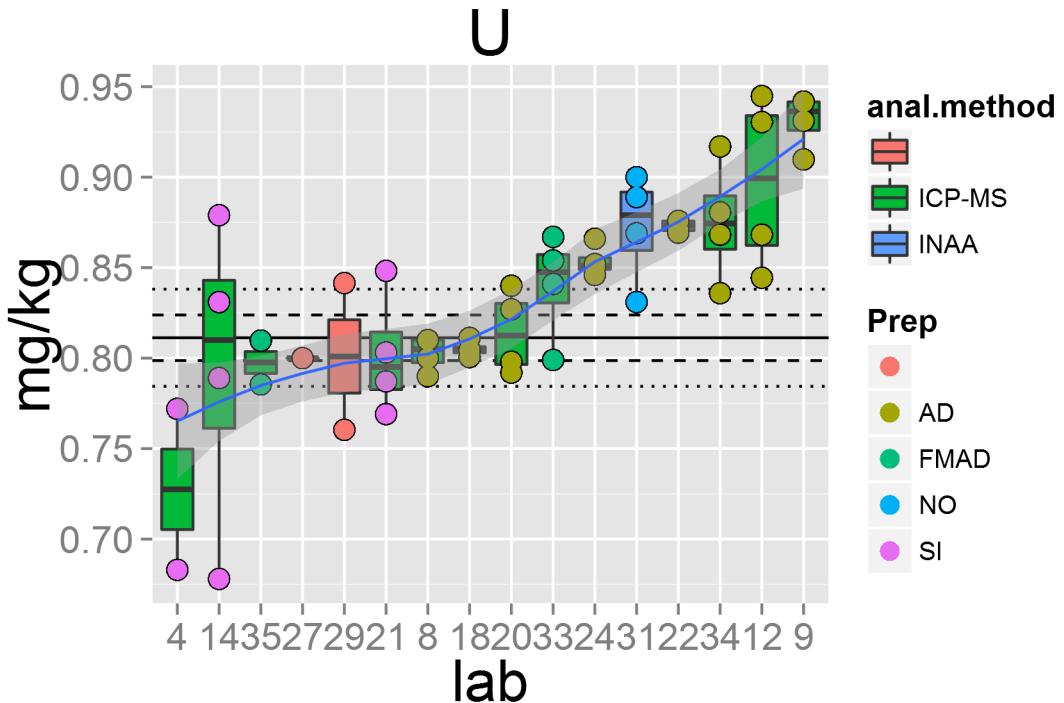


```
## [1] "U.2"
```

Normal Q-Q Plot

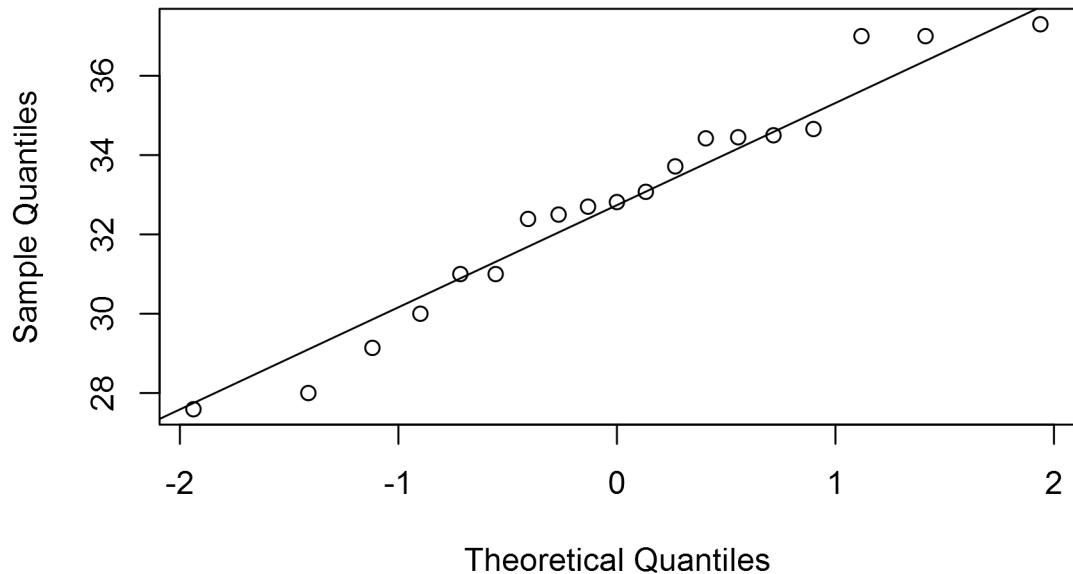


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

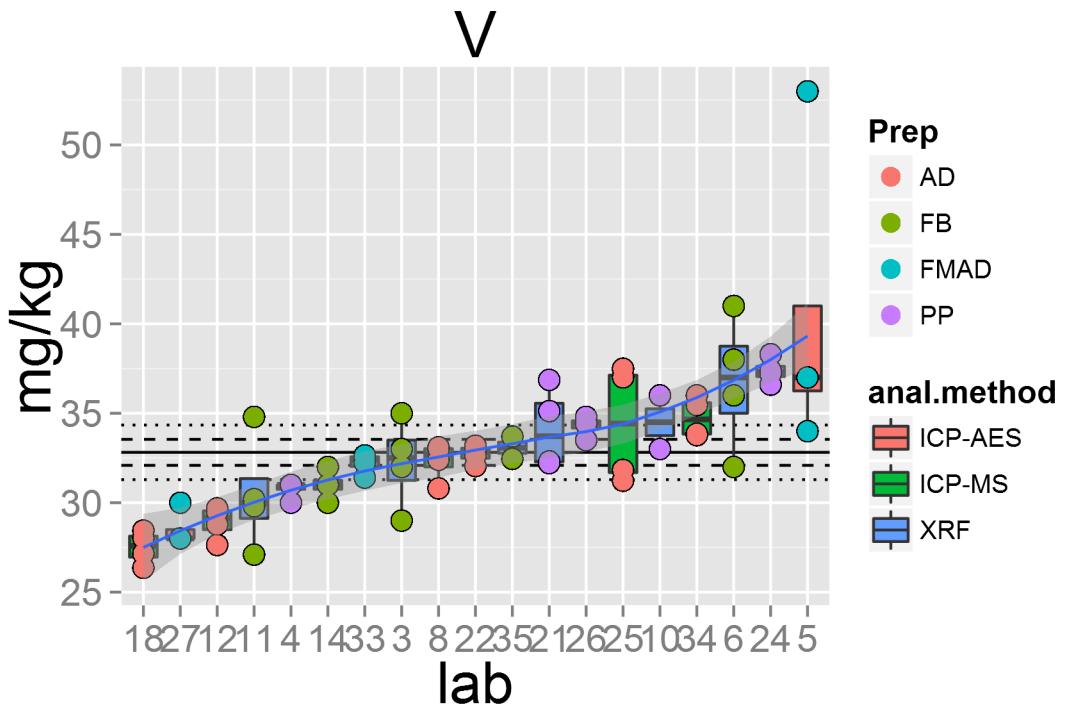


```
## [1] "V.2"
```

Normal Q-Q Plot

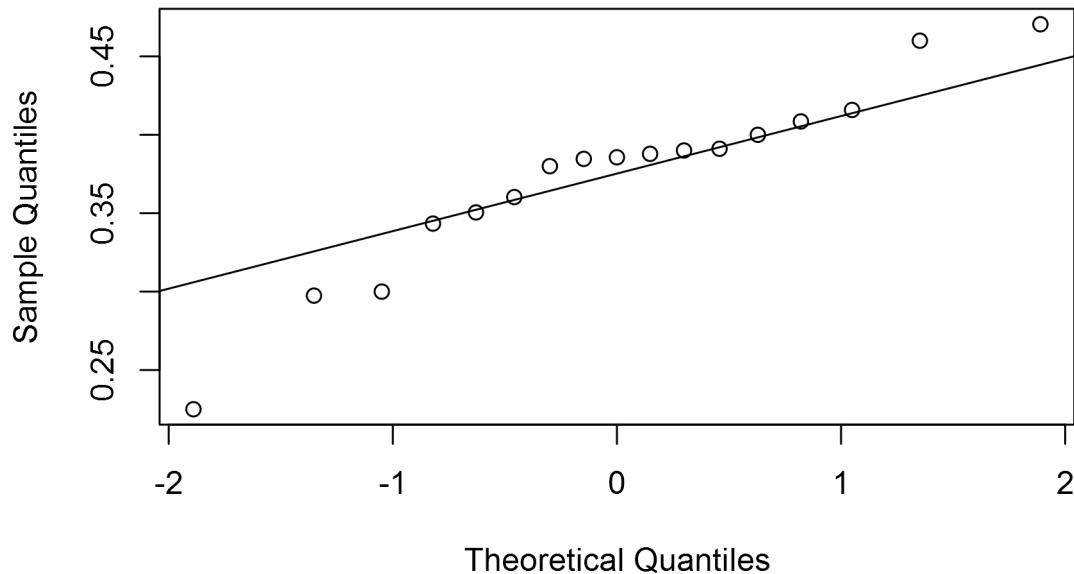


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

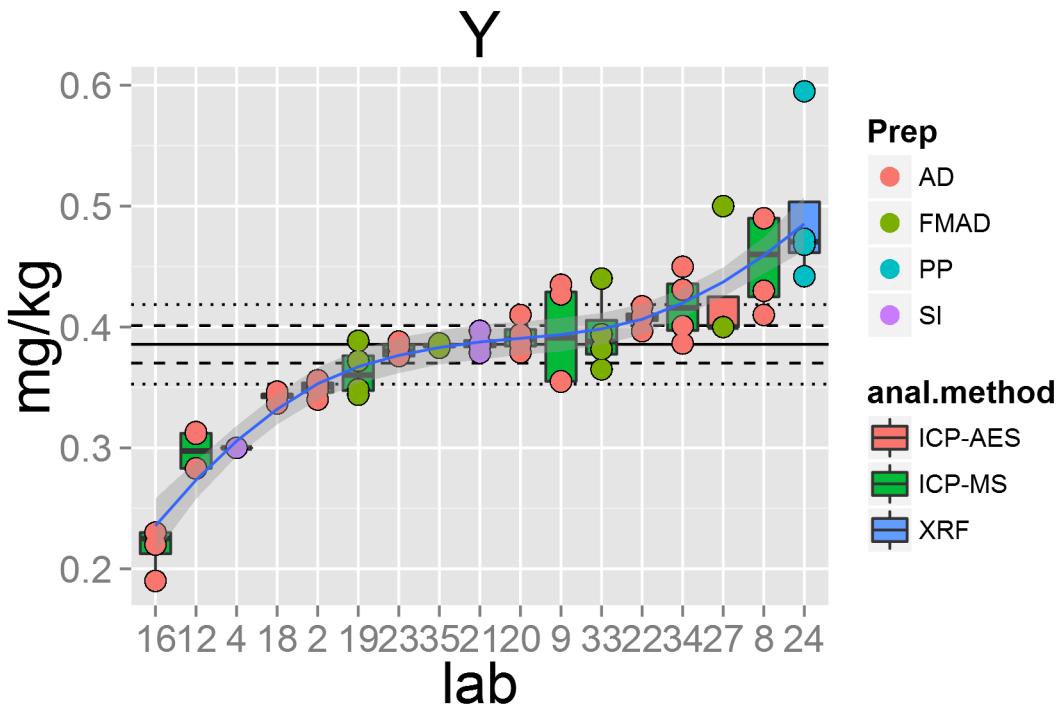


```
## [1] "Y.2"
```

Normal Q-Q Plot

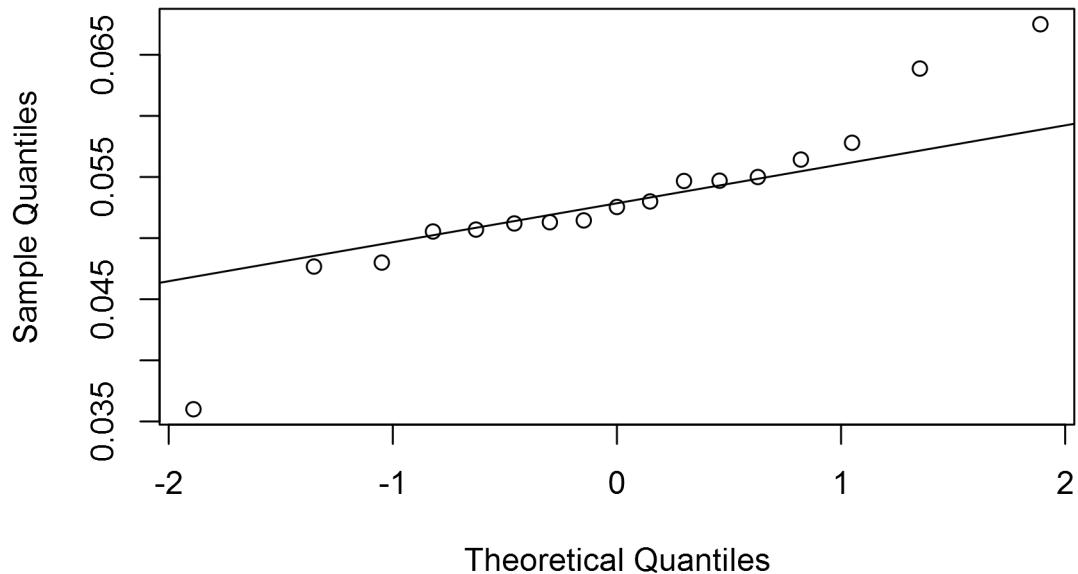


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

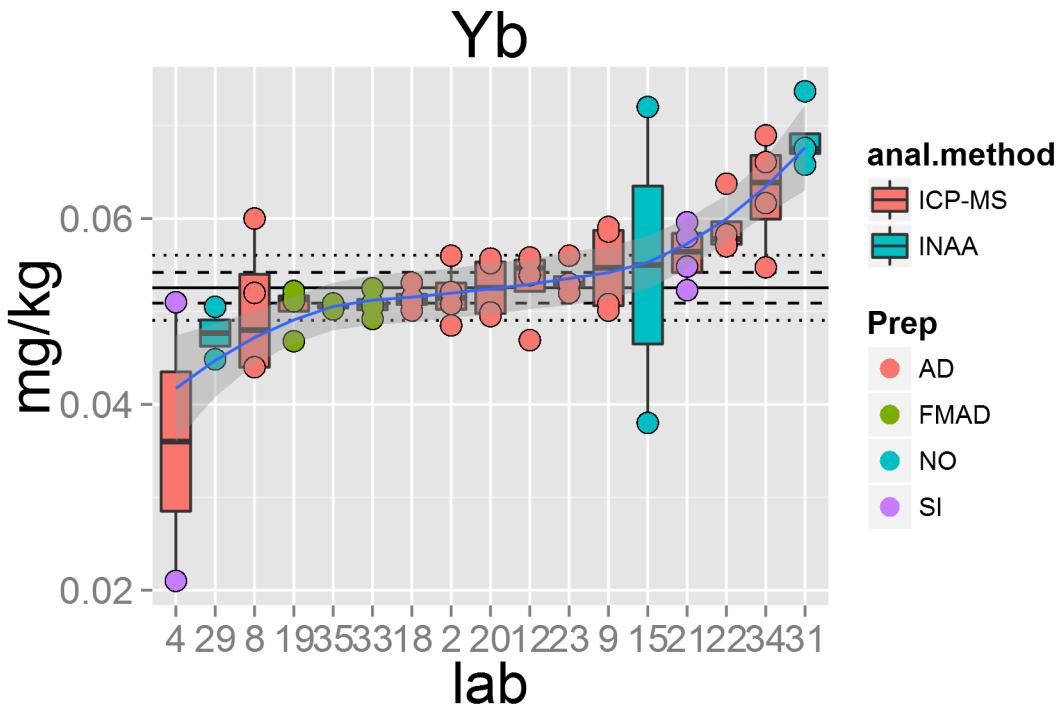


```
## [1] "Yb.2"
```

Normal Q-Q Plot

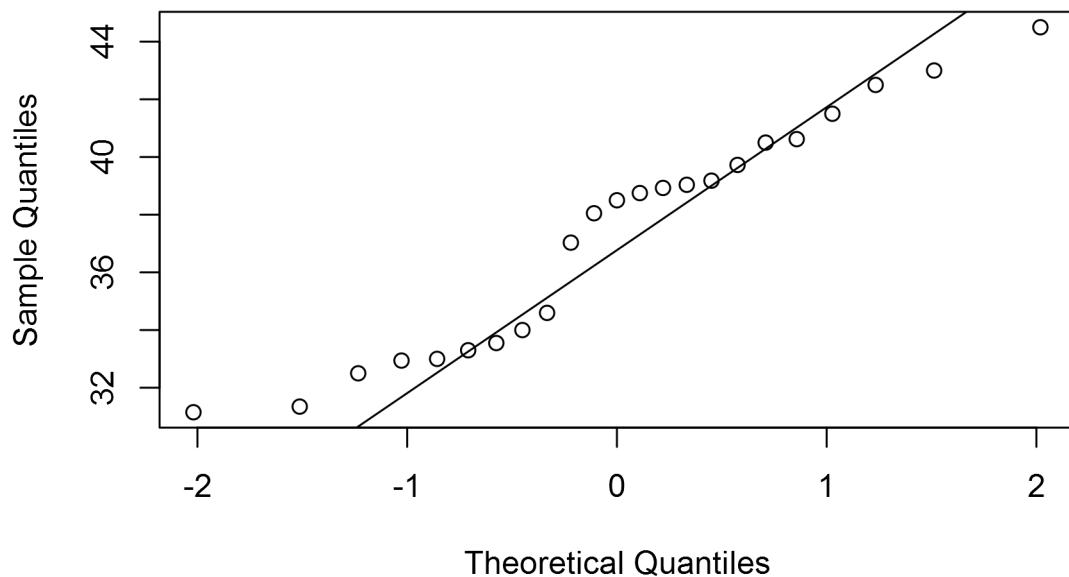


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

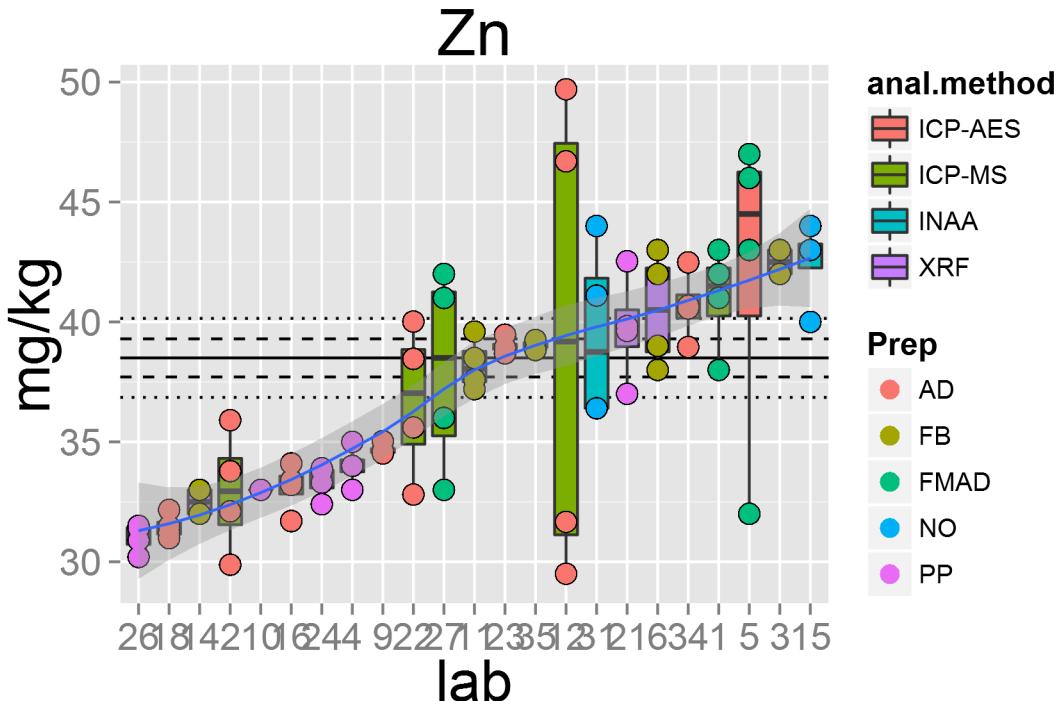


```
## [1] "Zn.2"
```

Normal Q-Q Plot

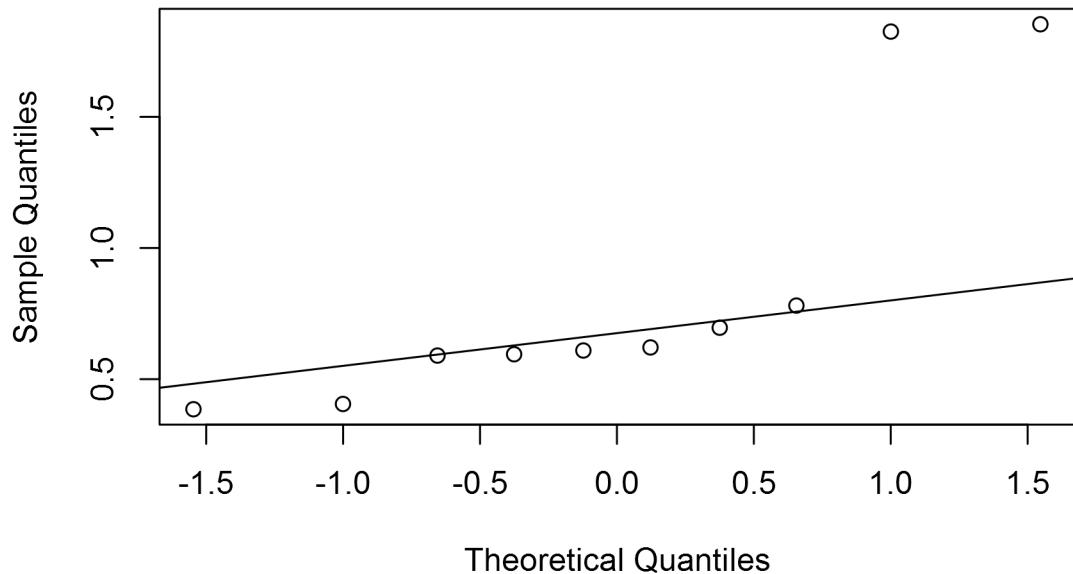


```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to change this.
```

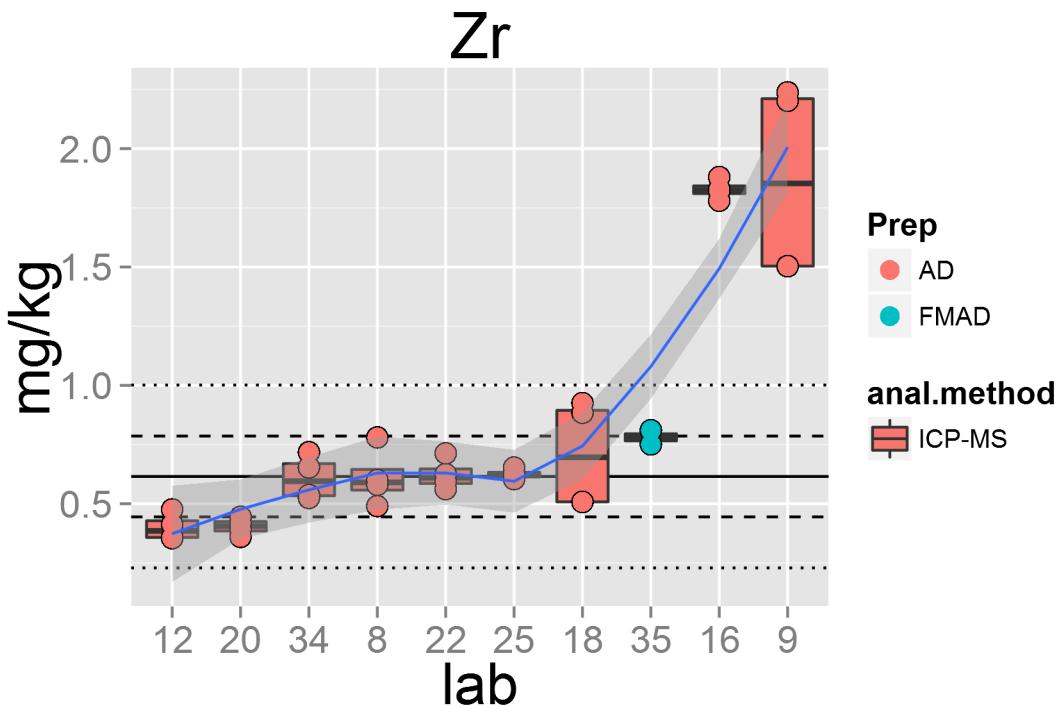


```
## [1] "Zr.2"
```

Normal Q-Q Plot



```
## geom_smooth: method="auto" and size of largest group is <1000, so using loess. Use 'method = x' to c
```



```

df3 <- read.table("~/GitHub/GOMcertification/df3.txt", header=T, quote="")
final <- ddply(df3, c("date", "RM", "measurand", "based.on", "unit"), numcolwise(meanGOM))
write.csv(final, "GASall.csv")

```

```

# kable(final, format = "markdown", padding=0, digits=c(0,0,0,0,3,3,3,3,3,3,3,4,4,4,0,0,3,3,0))
#library(xtable)
#xt <- xtable(final, digits=c(0,0,0,0,0,3,3,3,3,3,3,3,3,3,2,0,0,3,3,0))
#print(xt, type="html")
#library(Gmisc)
# htmlTable(final)

```

```

certified.values <- data.frame(final$date, final$RM, final$measurand, final$t.value, final$lab.remainin
names(certified.values) <- c("date", "RM", "measurand", "t.value", "n", "PV", "U", "unit")
write.table(certified.values, "CV1.txt", row.names=FALSE)
CV2 <- subset.data.frame(certified.values, n >= 10) # CV based on IAG protocol with n >= 10
CV3 <- subset.data.frame(certified.values, n < 10) # Information value based on IAG protocol with n < 10
write.table(CV2, "CV2.txt", row.names=FALSE) # just CV
write.table(CV3, "CV3.txt", row.names=FALSE, append=TRUE, col.names=FALSE) # CV and IV
CV <- read.table("C:/Data/projects/R/certification/CV2.txt", header=TRUE, quote="")
#xtCV <- xtable(CV, digits=c(0,0,0,0,2,0,4,4,0))
#print(xtCV, type="html")
kable(CV, digits=c(0,0,0,2,2,4,4,0), padding=1)

```

| date | RM | measurand | t.value | n | PV | U | unit |
|------------|------|-----------|---------|----|-----------|---------|--------|
| 2014-07-21 | OKUM | Al2O3 | 2.08 | 22 | 7.9780 | 0.0394 | g/100g |
| 2014-07-21 | OKUM | Ba | 2.13 | 16 | 6.1610 | 0.3960 | mg/kg |
| 2014-07-21 | OKUM | CaO | 2.09 | 20 | 7.8510 | 0.0573 | g/100g |
| 2014-07-21 | OKUM | Ce | 2.11 | 18 | 1.2790 | 0.0339 | mg/kg |
| 2014-07-21 | OKUM | Co | 2.07 | 23 | 89.4000 | 1.1400 | mg/kg |
| 2014-07-21 | OKUM | Cr | 2.08 | 22 | 2456.0000 | 31.0000 | mg/kg |
| 2014-07-21 | OKUM | Cs | 2.18 | 13 | 0.1831 | 0.0034 | mg/kg |
| 2014-07-21 | OKUM | Cu | 2.09 | 20 | 43.3400 | 1.2200 | mg/kg |
| 2014-07-21 | OKUM | Dy | 2.12 | 17 | 1.6050 | 0.0393 | mg/kg |
| 2014-07-21 | OKUM | Er | 2.11 | 18 | 1.0430 | 0.0143 | mg/kg |
| 2014-07-21 | OKUM | Eu | 2.10 | 19 | 0.3019 | 0.0068 | mg/kg |
| 2014-07-21 | OKUM | Fe2O3T | 2.08 | 22 | 11.8100 | 0.0484 | g/100g |
| 2014-07-21 | OKUM | Ga | 2.12 | 17 | 8.8650 | 0.1640 | mg/kg |
| 2014-07-21 | OKUM | Gd | 2.13 | 16 | 1.1720 | 0.0425 | mg/kg |
| 2014-07-21 | OKUM | Hf | 2.14 | 15 | 0.5565 | 0.0228 | mg/kg |
| 2014-07-21 | OKUM | Ho | 2.14 | 15 | 0.3529 | 0.0085 | mg/kg |
| 2014-07-21 | OKUM | K2O | 2.13 | 16 | 0.0436 | 0.0020 | g/100g |

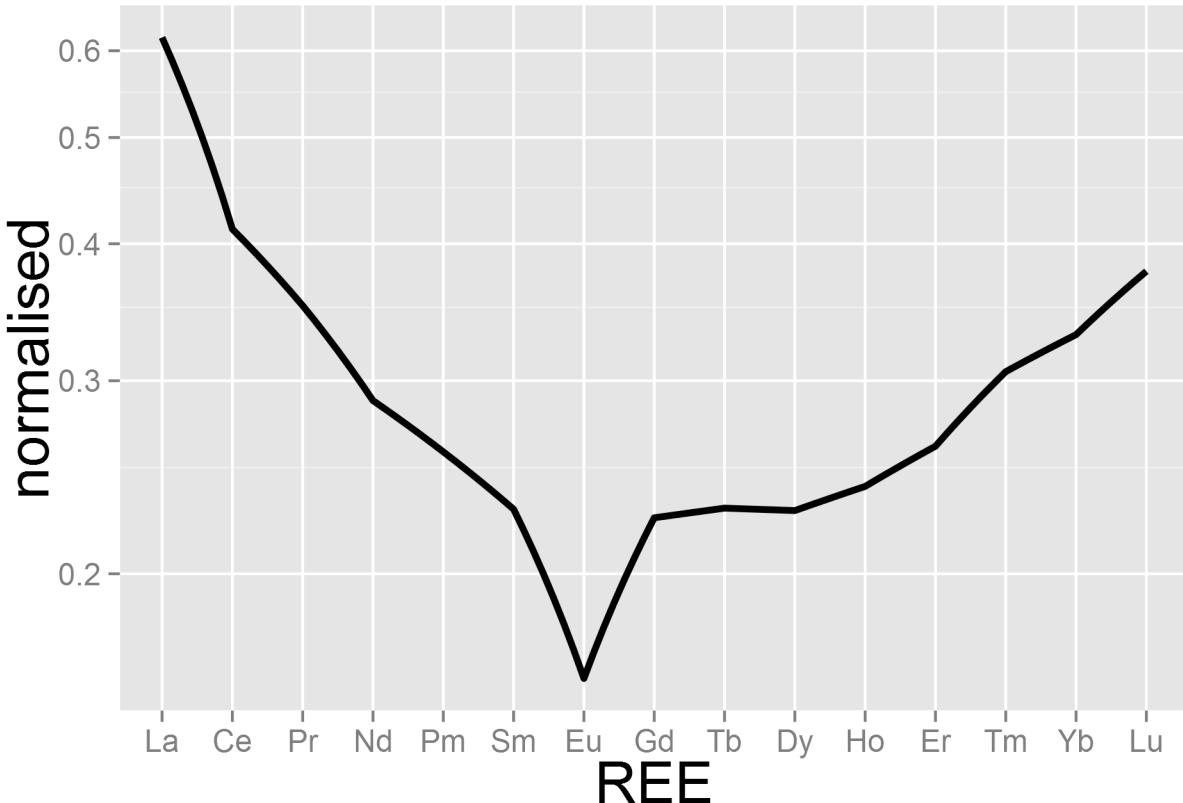
| date | RM | measurand | t.value | n | PV | U | unit |
|------------|------|-----------|---------|----|----------|---------|--------|
| 2014-07-21 | OKUM | La | 2.11 | 18 | 0.4086 | 0.0170 | g/100g |
| 2014-07-21 | OKUM | LOI | 2.08 | 22 | 4.6900 | 0.1190 | g/100g |
| 2014-07-21 | OKUM | Lu | 2.10 | 19 | 0.1488 | 0.0047 | mg/kg |
| 2014-07-21 | OKUM | MgO | 2.09 | 21 | 21.3000 | 0.0972 | g/100g |
| 2014-07-21 | OKUM | MnO | 2.07 | 23 | 0.1800 | 0.0027 | g/100g |
| 2014-07-21 | OKUM | Na2O | 2.08 | 22 | 1.1480 | 0.0215 | g/100g |
| 2014-07-21 | OKUM | Nb | 2.23 | 11 | 0.3525 | 0.0589 | mg/kg |
| 2014-07-21 | OKUM | Nd | 2.13 | 16 | 1.4990 | 0.0204 | mg/kg |
| 2014-07-21 | OKUM | Ni | 2.09 | 21 | 880.5000 | 10.3000 | mg/kg |
| 2014-07-21 | OKUM | P2O5 | 2.12 | 17 | 0.0265 | 0.0023 | g/100g |
| 2014-07-21 | OKUM | Pr | 2.12 | 17 | 0.2416 | 0.0080 | g/100g |
| 2014-07-21 | OKUM | Rb | 2.16 | 14 | 0.9400 | 0.0563 | mg/kg |
| 2014-07-21 | OKUM | Sc | 2.09 | 21 | 28.5000 | 0.8750 | mg/kg |
| 2014-07-21 | OKUM | SiO2 | 2.08 | 22 | 44.1400 | 0.1350 | g/100g |
| 2014-07-21 | OKUM | Sm | 2.11 | 18 | 0.7138 | 0.0113 | mg/kg |
| 2014-07-21 | OKUM | Sr | 2.07 | 23 | 16.3500 | 0.3110 | mg/kg |
| 2014-07-21 | OKUM | Ta | 2.20 | 12 | 0.0276 | 0.0038 | mg/kg |
| 2014-07-21 | OKUM | Tb | 2.11 | 18 | 0.2286 | 0.0056 | mg/kg |
| 2014-07-21 | OKUM | Th | 2.23 | 11 | 0.0285 | 0.0036 | mg/kg |
| 2014-07-21 | OKUM | TiO2 | 2.07 | 23 | 0.3781 | 0.0042 | g/100g |
| 2014-07-21 | OKUM | Tm | 2.13 | 16 | 0.1549 | 0.0037 | mg/kg |
| 2014-07-21 | OKUM | U | 2.20 | 12 | 0.0121 | 0.0026 | mg/kg |
| 2014-07-21 | OKUM | V | 2.10 | 19 | 169.5000 | 3.0500 | mg/kg |
| 2014-07-21 | OKUM | Y | 2.10 | 19 | 8.9980 | 0.2900 | mg/kg |
| 2014-07-21 | OKUM | Yb | 2.09 | 20 | 1.0080 | 0.0225 | mg/kg |
| 2014-07-21 | OKUM | Zn | 2.08 | 22 | 61.8000 | 1.8600 | mg/kg |
| 2014-07-21 | OKUM | Zr | 2.13 | 16 | 17.1200 | 1.2100 | mg/kg |
| 2014-07-21 | OKUM | As | 2.45 | 7 | 0.3725 | 0.2260 | mg/kg |
| 2014-07-21 | OKUM | Be | 2.57 | 6 | 0.0660 | 0.0041 | mg/kg |
| 2014-07-21 | OKUM | CO2 | 12.71 | 2 | 0.2000 | 0.5450 | g/100g |
| 2014-07-21 | OKUM | FeO | 4.30 | 3 | 8.0950 | 0.1650 | g/100g |
| 2014-07-21 | OKUM | H2O. | 4.30 | 3 | 5.7100 | 0.3100 | g/100g |
| 2014-07-21 | OKUM | Li | 2.36 | 8 | 4.3520 | 0.2590 | mg/kg |
| 2014-07-21 | OKUM | Pb | 2.45 | 7 | 0.2626 | 0.0210 | mg/kg |
| 2014-07-21 | OKUM | Sb | 2.78 | 5 | 0.0780 | 0.0124 | mg/kg |
| 2014-07-21 | OKUM | Sn | 2.78 | 5 | 0.2580 | 0.0228 | mg/kg |

| date | RM | measurand | t.value | n | PV | U | unit |
|------------|------|-----------|---------|---|--------|--------|-------|
| 2014-07-21 | OKUM | Tl | 4.30 | 3 | 0.0143 | 0.0019 | mg/kg |

```

REE.chondrites <- read.csv("~/GitHub/REE/REE.chondrites.csv", sep=";") # reading chondrite normalising values
REE.chondrites <- rename(REE.chondrites, c("norm"= "REE")) # renaming the column to make it suitable for merging
REE <- c("La", "Ce", "Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb", "Dy", "Ho", "Er", "Tm", "Yb", "Lu") # needed REE elements
RM <- read.table("~/GitHub/GOMcertification/CV2.txt", header=TRUE, quote="\") # reading all the finalised RM values
RM.REE <- subset(RM, measurand %in% REE, select=c(RM,measurand,PV)) # extracting only the REE values
RM.REE <- rename(RM.REE, c("measurand"="REE")) # renaming the column head suitable for merging
RM.REE <- merge(REE.chondrites, RM.REE, by = "REE", all.x=TRUE) # merging the data set so that element names are common
RM.normalised <- ddply(RM.REE, c("RM"), transform, normalised = PV/chondrite) # adding a chondrite normalised column
RM.normalised[15,5] <- (RM.normalised[9,5]+RM.normalised[11,5])/2
REEtheme <- theme_grey() + theme(plot.title = element_text(colour = "black", size = rel(2)))+ theme(axis.ticks = element_text(size=10))
p <- ggplot(data=RM.normalised, aes(x=REE, y=normalised, group=1)) + geom_line(size= 1.2)
p + scale_x_discrete(limits=c("La", "Ce", "Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb", "Dy", "Ho", "Er", "Tm", "Yb", "Lu"))

```



```
sessionInfo()
```

```

## R version 3.1.1 (2014-07-10)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
##

```

```
## locale:  
## [1] LC_COLLATE=German_Austria.1252 LC_CTYPE=German_Austria.1252  
## [3] LC_MONETARY=German_Austria.1252 LC_NUMERIC=C  
## [5] LC_TIME=German_Austria.1252  
##  
## attached base packages:  
## [1] grid      stats     graphics grDevices utils     datasets  methods  
## [8] base  
##  
## other attached packages:  
## [1] knitr_1.6      plyr_1.8.1      nlme_3.1-117    ape_3.1-4  
## [5] metRology_0.9-17 plotflow_1.0      gridExtra_0.9.1 ggplot2_1.0.0  
##  
## loaded via a namespace (and not attached):  
## [1] colorspace_1.2-4 digest_0.6.4      evaluate_0.5.5  
## [4] formatR_0.10      gtable_0.1.2      htmltools_0.2.4  
## [7] labeling_0.2       lattice_0.20-29    MASS_7.3-33  
## [10] munsell_0.4.2     numDeriv_2012.9-1 proto_0.3-10  
## [13] Rcpp_0.11.2       reshape2_1.4      rmarkdown_0.2.50  
## [16] scales_0.2.4      stringr_0.6.2     tools_3.1.1  
## [19] yaml_2.1.13
```