ICPMSCode

ArielleSherbak

10/29/2020

library(readr)  
library(tidyverse)

## ── Attaching packages ─────────────────────────────────────── tidyverse 1.3.0 ──

## ✓ ggplot2 3.3.2 ✓ dplyr 1.0.2  
## ✓ tibble 3.0.4 ✓ stringr 1.4.0  
## ✓ tidyr 1.1.2 ✓ forcats 0.5.0  
## ✓ purrr 0.3.4

## ── Conflicts ────────────────────────────────────────── tidyverse\_conflicts() ──  
## x dplyr::filter() masks stats::filter()  
## x dplyr::lag() masks stats::lag()

library(janitor)

##   
## Attaching package: 'janitor'

## The following objects are masked from 'package:stats':  
##   
## chisq.test, fisher.test

icpms\_data<- read.csv("~/ICPMSArielle/Data/ICPMS\_Data.csv", skip= 1, na= "N/A")  
  
sample\_key <- read.csv("~/ICPMSArielle/Data/Sample\_Key.csv", skip= 0)  
  
RSD\_data<-icpms\_data %>%  
 #first the rsd columns are selected and renamed with the approptiate metal isotope  
 select(Cr52 = CPS.RSD,  
 Cr53 = CPS.RSD.1,  
 As76 = CPS.RSD.2,  
 Cd111 = CPS.RSD.3,  
 Cd114 = CPS.RSD.4,  
 Pb208 = CPS.RSD.5,  
 Ge\_RSD = CPS.RSD.7,  
 Sample.Key)%>%  
   
 pivot\_longer(1:6,   
 names\_to="metal",   
 values\_to = "RSD")  
  
  
ICPMS\_tidy <- icpms\_data %>%  
 select(Cr52 = CPS,  
 Cr53 = CPS.1,  
 As76 = CPS.2,  
 Cd111 = CPS.3,  
 Cd114 = CPS.4,  
 Pb208 = CPS.5,  
 Ge72 = CPS.7,  
 Sample.Key)%>%  
   
 pivot\_longer(1:6,   
 names\_to="metal",   
 values\_to = "CPS")%>%  
  
mutate(RSD = RSD\_data$RSD/RSD\_data$Ge\_RSD,  
 CPS=CPS/Ge72)%>%  
 select(-Ge72)  
  
  
all(RSD\_data$Sample.Key==ICPMS\_tidy$Sample.Key, RSD\_data$metal==ICPMS\_tidy$metal)

## [1] TRUE

ICPMS\_merged <- merge(ICPMS\_tidy, sample\_key) %>%  
 clean\_names()

### rm(list=setdiff(ls(), "ICPMS\_merged"))  
write.csv(ICPMS\_merged, file = "~/ICPMSArielle/Data/ICPMS\_merged")

AA\_Data <- read\_csv("~/ICPMSArielle/Data/AA\_Data.csv", skip = 4)

##   
## ── Column specification ────────────────────────────────────────────────────────  
## cols(  
## `Sample Key` = col\_character(),  
## `Mean Abs.` = col\_double(),  
## `%RSD` = col\_character()  
## )

AA\_tidy<-AA\_Data%>%  
 rename(Sample.Key ="Sample Key")%>%  
 rename(percentRSD = "%RSD")  
  
  
AA\_tidy$percentRSD[AA\_tidy$percentRSD == "HIGH"] <- 999.99  
  
AA\_tidy$Sample.Key[AA\_tidy$Sample.Key == "check10"] <- 80  
AA\_tidy$Sample.Key[AA\_tidy$Sample.Key == "Sample Blank"] <- 90  
  
AA\_tidy$Sample.Key <- as.numeric(AA\_tidy$Sample.Key)  
AA\_tidy$percentRSD <- as.numeric(AA\_tidy$percentRSD)  
  
  
AA\_merge<-merge(sample\_key, AA\_tidy)  
  
  
##clean\_names(AA\_tidy, case="snake")  
   
  
write.csv(AA\_merge, file = "~/ICPMSArielle/Data/AAData.csv")

AA\_imported <- read\_csv("~/ICPMSArielle/Data/AA\_Data.csv",  
 skip = 4,  
 na = "N/A")

##   
## ── Column specification ────────────────────────────────────────────────────────  
## cols(  
## `Sample Key` = col\_character(),  
## `Mean Abs.` = col\_double(),  
## `%RSD` = col\_character()  
## )

AA\_imported <- AA\_imported %>%  
 rename(Sample.Key = "Sample Key")  
sample\_key <- read.csv("~/ICPMSArielle/Data/Sample\_Key.csv",   
 skip = 0)

AA\_merged <- merge(AA\_imported, sample\_key) %>%  
 clean\_names()

write.csv(AA\_merged, "~/ICPMSArielle/Data/AA\_data2.csv")