# Supplemental Data 2

## R Code for Simulated Data Generation

```
#Set name of results file.
result_file <- "2LAG_30.txt"

#Indicate concentration levels to be used.
#x <- c(5, 10, 15, 50, 75, 100, 400, 500, 1000) #2G
x <- c(5, 10, 15, 40, 200, 400, 550, 800, 850, 1000) #PPT
#x <- c(10, 30, 50, 100, 250, 400, 500, 800, 1000) #SWG

#Number of levels.
n <- length(x)

#Setting calibration parameters.
b0 <- 0.0024
b1 <- 0.0912
b2 <- 0
#b2 <- -0.0000516

#Generation of predicted responses.
y <- (b2*x*x) + (b1*x) + b0

#Generation of standard deviation for each level.
#For all weight, program is set to generate a maximum of 20% RSD, but this can be changed in
     max=.
#For a w=1 (no weight) model, uncomment the following lines.
percent <- 12
absolute <- (percent/100)*y[1]
sd <- rep(absolute, n)
RSD <- sd/y*100

#For a w=1/x model, uncomment the following lines.
#percent <- 12
#varabs <- ((percent/100)*y[1])
#zsq <- varabs/sqrt(x[1])
#sd <- zsq*sqrt(x)
#RSD <- sd/y*100

#For a w=1/(x^2) model, uncomment the following lines.
#percent <- 2
#sd <- (percent/100)*y
#RSD <- sd/y*100

#Generation of an experimental data matrix.
#Set number of replicates.
rep = 7

```

```
#Create empty matrix to store the results.
T <- matrix(nrow=n, ncol=rep)

#Generation of random normally distributed measurements and storage in T matrix.
for(i in 1:n)
{
     Temp <- rnorm(rep, y[i], sd[i])
     T[i,] <- Temp
}

#Append the concentrations to the results.
R <- cbind(x, T)

#Save data matrix as .txt file.
write.table (R, result_file, sep="\t", row.names=F, col.names=F)

#Save parameters in a second file.
P <- cbind(x, n, rep, b0, b1, b2, sd, RSD)
parameters_file <- paste("P", result_file, sep="_")
write.table (P, parameters_file, sep="\t", row.names=F)
```