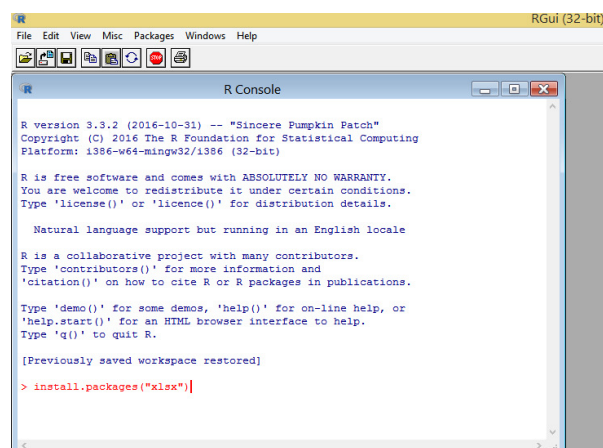


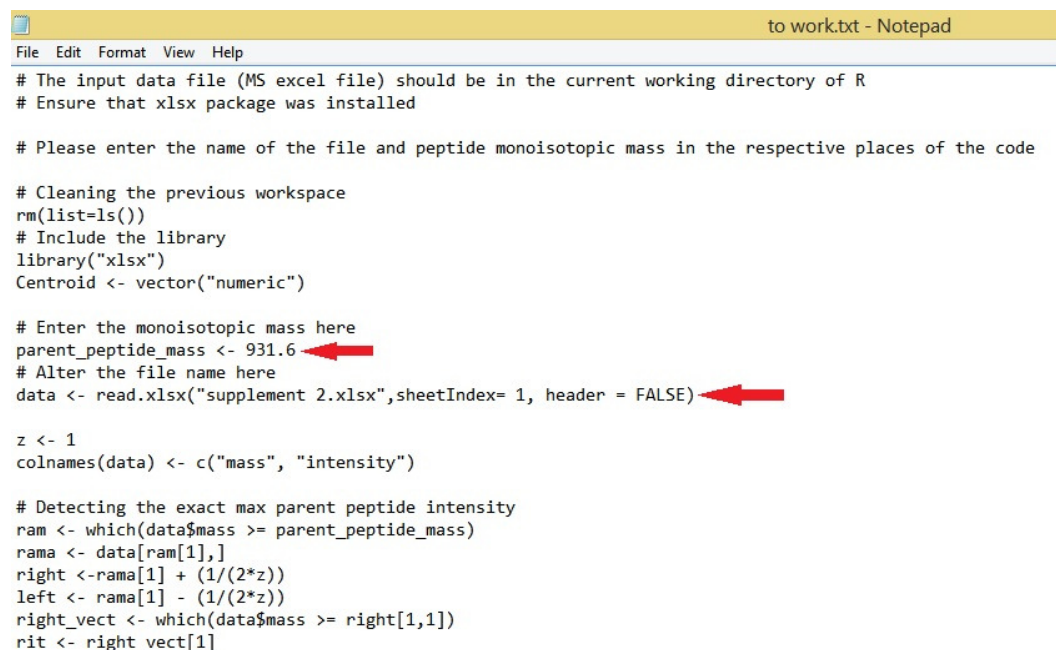
SUPPLEMENT 1

Instructions for using the code:

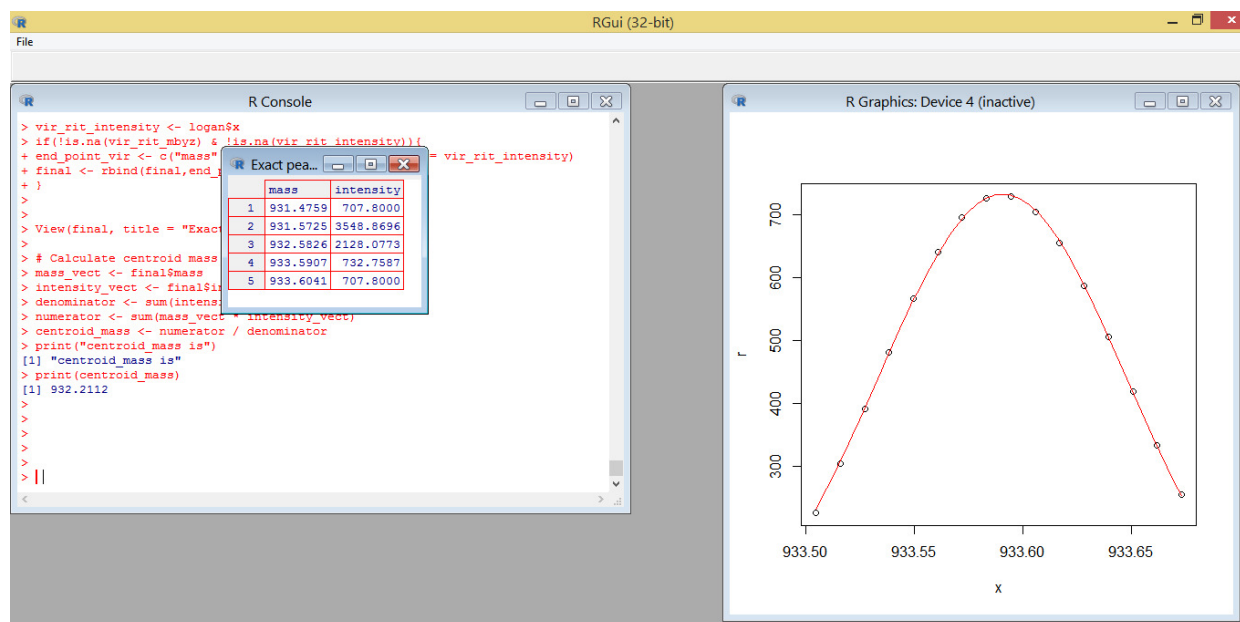
1. Download and install the latest version of R software from <https://www.r-project.org/>
2. Open 32-bit version of the software and install the package “xlsx” using the command `install.packages()` for the first time. If there is any error installing the package, install the dependent packages “rJava” and “xlsxjars” and retry installing xlsx.



3. Transfer the input excel file containing the data to the current working directory of R. A sample data file has been provided as supplement 2.
4. Edit the code in notepad to enter the excel file name and monoisotopic mass of peptide in respective places.



5. Copy the entire code and paste it in R console. A window with the exact peak values after fitting will be displayed along with two virtual points at the start and at the end. The individual fitted peaks will be shown in separate windows. Only 63 such windows could be opened simultaneously. The centroid mass is printed out in the console.



Program code

```
# The input data file (MS excel file) should be in the current working directory of R
# Ensure that xlsx package was installed
# Please enter the name of the file and peptide monoisotopic mass in the respective places of the code
# Cleaning the previous workspace
rm(list=ls())
# Include the library
library("xlsx")
Centroid <- vector("numeric")
```

```
# Enter the monoisotopic mass here
parent_peptide_mass <- 931.6
# Alter the file name here
data <- read.xlsx("supplement 2.xlsx",sheetIndex= 1, header = FALSE)
```

```
z <- 1
colnames(data) <- c("mass", "intensity")
```

```
# Detecting the exact max parent peptide intensity
ram <- which(data$mass >= parent_peptide_mass)
rama <- data[ram[1],]
right <- rama[1] + (1/(2*z))
left <- rama[1] - (1/(2*z))
right_vect <- which(data$mass >= right[1,1])
rit <- right_vect[1]
left_vect <- which(data$mass <= left[1,1])
lft <- left_vect[length(left_vect)]
interval <- data[lft:rit,]
```

```
kri <- max(interval$intensity)
bal <- which(interval$intensity == kri)
kal <- interval[bal,]
```

```

ppm_exp <- kal[1,1]

# Assign the experimental parent peptide mass value to another variable 'peak_mid_grab'
peak_mid_grab <- ppm_exp

# Perform a loop to describe the peaks
a <- 1:1000
b <- 1:1000
peaks <- vector("numeric")
for(a in b){
  ram <- which(data$mass >= peak_mid_grab)
  rama <- data[ram[1],]
  right <- rama[1] + (1/(2*z))
  left <- rama[1] - (1/(2*z))
  right_vect <- which(data$mass >= right[1,1])
  rit <- right_vect[1]
  left_vect <- which(data$mass <= left[1,1])
  lft <- left_vect[length(left_vect)]
  interval <- data[lft:rit,]

  kri <- max(interval$intensity)
  bal <- which(interval$intensity == kri)
  kal <- interval[bal,]
  ppm_mid <- kal[1,1]

## Trace the left half of distribution
position_mbyz <- which(data$mass >= ppm_mid)
click <- position_mbyz
i <- 1:1000
t <- 1:1000
for(i in t){
  del1 <- data$intensity[click]
  del2 <- data$intensity[click - 1]
  if(del2>del1){
    break
  }
  click <- click - 1
}

## Trace the right half of distribution
right_click <- position_mbyz
i <- 1:1000
t <- 1:1000
for(i in t){
  acer1 <- data$intensity[right_click]
  acer2 <- data$intensity[right_click + 1]
  if(acer2 > acer1){
    break
  }
  right_click <- right_click + 1
}

## Subset the entire datapoints corresponding to the single peak
peak_dist <- data[click:right_click,]
#plot(peak_dist)
#windows()

```

```

## Calculate maximum of peak intensity and check if it is increasing again
peak_max <- max(peak_dist$intensity)
peaks <- c(peaks, peak_max)
## Increment the mid mbyz value
peak_mid_grab <- peak_mid_grab + 1
}
#View(peaks, title = "entire peak list")

# Type1 : The envelope intensity is like - 50,40,30,20,10.
# Type2 : The envelope intensity is like - 20,30,50,40,30,20,10.
# Type3 : The envelope intensity is like - 20,20,30,50,40,30,20,10.
#           or 50,50,40,30,20,10.
# Create a major loop to decide on the path and to retrieve the end peak position
# of the envelope as 'empire'

u <- 1:length(peaks)
p <- 1:(length(peaks)-1)
l <- 1
o <- l+1
if(peaks[l] > peaks[o]){
  for(p in u){
    if(peaks[l] > peaks[o]){
      empire <- l+1
      l <- l+1
      o <- o+1
    }
    else{
      empire <- l
    }
  }
}

# Type2
if(peaks[l] < peaks[o]){
  for(p in u){
    if(peaks[l] < peaks[o]){
      empire <- l+1
      l <- l+1
      o <- o+1
    }
  }
}

for(p in u){
  if(peaks[l] > peaks[o]){
    empire <- l+1
    l <- l+1
    o <- o+1
  }
}

# Type3
if(peaks[l] == peaks[o]){
  if(peaks[2] < peaks[3]){
    l <- 2
    o <- l+1
  }
}

```

```

for(p in u){
  if(peaks[l] < peaks[o]){
    empire <- l+1
    l <- l+1
    o <- o+1
  }
}
else{
  if(peaks[2] > peaks[3]){
    l <- 2
    o <- l+1
    for(p in u){
      if(peaks[l] > peaks[o]){
        empire <- l+1
        l <- l+1
        o <- o+1
      }
    }
  }
}
}
}
}
}
}
}
}

```

```
print(empire)
```

```

# Construct the envelope data.frame
## Find the starting point using the exp max of parent peptide mass
position_mbyz <- which(data$mass == ppm_exp)
click <- position_mbyz
i <- 1:1000
t <- 1:1000
for(i in t){
  del1 <- data$intensity[click]
  del2 <- data$intensity[click - 1]
  if(del2>del1){
    break
  }
  click <- click - 1
}

```

```

## Find the ending point using the max peak intensity corresponding to 'empire' value
## Find the times of increment in mbyz value to reach the point
end_incre <- empire - 1
middlle_mbyz_of_end <- ppm_exp + (end_incre * (1/z))
rama <- middlle_mbyz_of_end
right <- rama + (1/(2*z))
left <- rama - (1/(2*z))
right_vect <- which(data$mass >= right)
rit <- right_vect[1]
left_vect <- which(data$mass <= left)
lft <- left_vect[length(left_vect)]
interval <- data[lft:rit,]

```

```

kri <- max(interval$intensity)
bal <- which(interval$intensity == kri)
kal <- interval[bal,]

```

```

middle_mbyz_of_end_exp <- kal[1,1]

position_mbyz <- which(data$mass == middle_mbyz_of_end_exp)
right_click <- position_mbyz
i <- 1:1000
t <- 1:1000
for(i in t){
  acer1 <- data$intensity[right_click]
  acer2 <- data$intensity[right_click + 1]
  if(acer2 > acer1){
    break
  }
  right_click <- right_click + 1
}

## name the new data.frame as 'frame1'
frame1 <- data[click:right_click,]

# Find the base peak intensity from 'frame1'
bp <- max(frame1$intensity)
bp_mbyz <- frame1$mass[which(frame1$intensity == bp)[1]]
cut_off <- 0.20 * bp

## Refine the envelope and store it in 'frame2'
### Perform a loop to describe the peaks
peak_mid_grab <- ppm_exp
vibe <- data.frame()
peak_max1 <- min(data$intensity)
a <- 1:1000
b <- 1:1000
peaks <- vector("numeric")
peaksr <- vector("numeric")
for(a in b){
  ### Define the distribution of the peak according to condition 1 : successive point intensity
  ### should be less than the preceeding intensity
  ### Grab the exact middle mbyz based on maximum intensity

  ram <- which(data$mass >= peak_mid_grab)
  rama <- data[ram[1],]
  right <- rama[1] + (1/(2*z))
  left <- rama[1] - (1/(2*z))
  right_vect <- which(data$mass >= right[1,1])
  rit <- right_vect[1]
  left_vect <- which(data$mass <= left[1,1])
  lft <- left_vect[length(left_vect)]
  interval <- data[lft:rit,]

  kri <- max(interval$intensity)
  bal <- which(interval$intensity == kri)
  kal <- interval[bal,]
  ppm_mid <- kal[1,1]

  ##### Trace the left half of distribution
  position_mbyz <- which(data$mass >= ppm_mid)
  click <- position_mbyz

```

```

i <- 1:1000
t <- 1:1000
for(i in t){
  del1 <- data$intensity[click]
  del2 <- data$intensity[click - 1]
  if(del2>del1){
    break
  }
  click <- click - 1
}

#### Trace the right half of distribution
right_click <- position_mbyz
i <- 1:1000
t <- 1:1000
for(i in t){
  acer1 <- data$intensity[right_click]
  acer2 <- data$intensity[right_click + 1]
  if(acer2 > acer1){
    break
  }
  right_click <- right_click + 1
}

### Subset the entire datapoints corresponding to the single peak
peak_dist <- data[click:right_click,]
#plot(peak_dist)
#windows()
### Calculate maximum of peak intensity and check if it is increasing again
peak_max <- max(peak_dist$intensity)
vibe_mbyz <- peak_dist$mass[peak_dist$intensity == peak_max]
flash_peak <- data[data$mass == vibe_mbyz[1],]
if(peak_dist$mass[1] > bp_mbyz & (peak_max1 < peak_max | peak_max < cut_off)){
  break
}
peaks <- c(peaks, peak_max)
vibe <- rbind(vibe, flash_peak)
### Increment the mid mbyz value
peak_mid_grab <- peak_mid_grab + (1/z)
peak_max1 <- peak_max
}

##
## Trace the starting point of 'frame2'
#####$
re_vibe <- data.frame()
peak_max1 <- data$intensity[data$mass == bp_mbyz]
a <- 1:1000
b <- 1:1000
peak_mid_grab <- bp_mbyz
for(a in b){

### Grab the exact middle mbyz based on maximum intensity
ram <- which(data$mass >= peak_mid_grab)
rama <- data[ram[1],]
right <- rama[1] + (1/(2*z))

```

```

left <- rama[1] - (1/(2*z))
right_vect <- which(data$mass >= right[1,1])
rit <- right_vect[1]
left_vect <- which(data$mass <= left[1,1])
lft <- left_vect[length(left_vect)]
interval <- data[lft:rit,]

kri <- max(interval$intensity)
bal <- which(interval$intensity == kri)
kal <- interval[bal,]
ppm_mid <- kal[1,1]

# Should stop if it extends beyond low mbyz of parent peptide
if(ppm_mid < ppm_exp){
  break
}

#### Trace the left half of distribution
position_mbyz <- which(data$mass >= ppm_mid)
click <- position_mbyz
i <- 1:1000
t <- 1:1000
for(i in t){
  del1 <- data$intensity[click]
  del2 <- data$intensity[click - 1]
  if(del2>del1){
    break
  }
  click <- click - 1
}

#### Trace the right half of distribution
right_click <- position_mbyz
i <- 1:1000
t <- 1:1000
for(i in t){
  acer1 <- data$intensity[right_click]
  acer2 <- data$intensity[right_click + 1]
  if(acer2 > acer1){
    break
  }
  right_click <- right_click + 1
}

### Subset the entire datapoints corresponding to the single peak
peak_distr <- data[click:right_click,]
#plot(peak_dist)
#windows()
### Calculate maximum of peak intensity and check if it is increasing again
peak_max <- max(peak_distr$intensity)
re_vibe_mbyz <- peak_distr$mass[peak_distr$intensity == peak_max]
reverse_flash_peak <- data[data$mass == re_vibe_mbyz[1],]

if(peak_distr$mass[1] < bp_mbyz & (peak_max1 < peak_max | peak_max < cut_off)){
  if(peak_max == bp){
    peaksr <- c(peaksr, peak_max)
  }
}

```

```

break
}
break
}

peaksr <- c(peaksr, peak_max)
re_vibe <- rbind(re_vibe, reverse_flash_peak)
### Decrement the mid mbyz value
peak_mid_grab <- peak_mid_grab - (1/z)
peak_max1 <- peak_max
}

## Trace the end point of frame2
wall <- length(peaks)
fence <- vibe$mass[wall]
f2_end_pk <- which(data$mass == fence)
right_click <- f2_end_pk
i <- 1:1000
t <- 1:1000
for(i in t){
  acer1 <- data$intensity[right_click]
  acer2 <- data$intensity[right_click + 1]
  if(acer2 > acer1){
    break
  }
  right_click <- right_click + 1
}

## Trace the exact starting point for 'frame2'
wallr <- length(peaksr)
fencer <- re_vibe$mass[wallr]
f2_start_pk <- which(data$mass == fencer)
click <- f2_start_pk
i <- 1:1000
t <- 1:1000
for(i in t){
  del1 <- data$intensity[click]
  del2 <- data$intensity[click - 1]
  if(del2 > del1){
    break
  }
  click <- click - 1
}

#####

frame2 <- data[click:right_click,]

# Do the fitting
# Assign the mbyz value of the first peak in frame2 to peak_mid_grab
peak_mid_grab <- data$mass[data$mass == fencer]

# Perform a loop to describe the peaks
a <- 1:1000
b <- 1:1000
peaks <- vector("numeric")

```

```

iso_peak <- vector("numeric")
iso_mass <- vector("numeric")
opt_sigma <- vector("numeric")
for(a in b){
  ram <- which(data$mass >= peak_mid_grab)
  rama <- data[ram[1],]
  right <- rama[1] + (1/(2*z))
  left <- rama[1] - (1/(2*z))
  right_vect <- which(data$mass >= right[1,1])
  rit <- right_vect[1]
  left_vect <- which(data$mass <= left[1,1])
  lft <- left_vect[length(left_vect)]
  interval <- data[lft:rit,]

  kri <- max(interval$intensity)
  bal <- which(interval$intensity == kri)
  kal <- interval[bal,]
  ppm_mid <- kal[1,1]

  ## Trace the left half of distribution
  position_mbyz <- which(data$mass == ppm_mid)
  click <- position_mbyz
  i <- 1:1000
  t <- 1:1000
  for(i in t){
    del1 <- data$intensity[click]
    del2 <- data$intensity[click - 1]
    if(del2>del1){
      break
    }
    click <- click - 1
  }

  ## Trace the right half of distribution
  right_click <- position_mbyz
  i <- 1:1000
  t <- 1:1000
  for(i in t){
    acer1 <- data$intensity[right_click]
    acer2 <- data$intensity[right_click + 1]
    if(acer2 > acer1){
      break
    }
    right_click <- right_click + 1
  }

  ## Subset the entire datapoints corresponding to the single peak
  peak_dist <- data[click:right_click,]
  #plot(peak_dist)
  #windows()

  # Fit it in the gaussian curve to find the maximum value
  tab1 <- data.frame(x=peak_dist$mass, r=peak_dist$intensity)
  xmax <- tab1$x[tab1$r == max(tab1$r)]
  r_at_fwtm <- 0.3 * (max(tab1$r))
  tab <- tab1[which(tab1$r >= r_at_fwtm),]

```

```

plot(tab$x, tab$r, xlab = "mass", ylab = "intensity")
b <- round(mean(tab$x))
a <- max(tab$r)
xmax <- tab$x[tab$r == max(tab$r)]
x1 <- tab$x[tab$x < xmax][which.min(abs(tab$r[tab$x < xmax] - max(tab$r)/2))]
x2 <- tab$x[tab$x > xmax][which.min(abs(tab$r[tab$x > xmax] - max(tab$r)/2))]
c <- ((x2 - x1)/2.3)
print(c)

fg <- 1:1000
for(h in fg){
  (res <- nls( r ~ k*exp(-1/2*(x-mu)^2/sigma^2), start=c(mu=b,sigma=c,k=a) , data = tab, trace = TRUE, control =
  nls.control(printEval = TRUE, warnOnly = TRUE)))
  c <- c + 0.1
  if(res$convInfo$stopCode == 0){
    break
  }
}
print(summary(res))
v <- summary(res)$parameters[, "Estimate"]

plot(r~x, data=tab)
plot(function(x) v[3]*exp(-1/2*(x-v[1])^2/v[2]^2), col=2, add=T, xlim = range(tab$x))
windows()

iso_mass1 <- summary(res)$parameters[1, "Estimate"]
iso_peak1 <- summary(res)$parameters[3, "Estimate"]
sigma1 <- summary(res)$parameters[2, "Estimate"]

iso_peak <- c(iso_peak, iso_peak1)
iso_mass <- c(iso_mass, iso_mass1)
opt_sigma <- c(opt_sigma, sigma1)

print(tab)

## Calculate maximum of peak intensity and check if it is increasing again
peak_max <- max(peak_dist$intensity)
peaks <- c(peaks, peak_max)

## Include the stop point corresponding to the extent of frame2
jolly <- nrow(frame2)
if(tab1$x[nrow(tab1)] == frame2$mass[jolly]){
  break
}

## Increment the mid mbyz value
peak_mid_grab <- peak_mid_grab + (1/z)
}

final <- data.frame(iso_mass, iso_peak)
names(final) <- c("mass", "intensity")

# Include the virtual points to balance the envelope
## Trace the left virtual point
tom <- which(frame2$mass <= final[1, 1])
hunter <- frame2[1:length(tom), ]
###select A point

```

```

AA <- which(hunter$intensity <= cut_off)
A <- hunter[length(AA),]$mass
A1 <- hunter[length(AA),]$intensity
###select B point
B <- final[1,1]
B1 <- final[1,2]
print(A)
print(A1)
print(B)
print(B1)
###find the left virtual point
walley <- approx(x=c(A1,B1), y=c(A,B), method="linear",xout=cut_off)
vir_lft_mbyz <- walley$y
vir_lft_intensity <- walley$x
if(!is.na(vir_lft_mbyz) & !is.na(vir_lft_intensity)){
start_point_vir <- c("mass" = vir_lft_mbyz,"intensity" = vir_lft_intensity)
final <- rbind(start_point_vir,final)
}

```

```

## Trace the right virtual point
jerry <- which(frame2$mass>=final[nrow(final),1])
thawne <- frame2[jerry[1]:jerry[length(jerry)],]
###select A point
A <- final[length(final$mass), 1]
A1 <- final[length(final$mass), 2]
###select B point
BB <- which(thawne$intensity <= cut_off)
B <- thawne[BB[1],]$mass
B1 <- thawne[BB[1],]$intensity
print(A)
print(A1)
print(B)
print(B1)
###find the right virtual point
logan <- approx(x=c(A1,B1), y=c(A,B), method="linear",xout=cut_off)
vir_rit_mbyz <- logan$y
vir_rit_intensity <- logan$x
if(!is.na(vir_rit_mbyz) & !is.na(vir_rit_intensity)){
end_point_vir <- c("mass" = vir_rit_mbyz, "intensity" = vir_rit_intensity)
final <- rbind(final,end_point_vir)
}

```

```

View(final, title = "Exact peak values")

```

```

# Calculate centroid mass
mass_vect <- final$mass
intensity_vect <- final$intensity
denominator <- sum(intensity_vect)
numerator <- sum(mass_vect * intensity_vect)
centroid_mass <- numerator / denominator
print("centroid_mass is")
print(centroid_mass)

```

SUPPLEMENT 2

930.0145	6.56E+00
930.0257	6.87E+00
930.0369	7.24E+00
930.0482	7.61E+00
930.0594	7.92E+00
930.0705	8.10E+00
930.0817	8.14E+00
930.093	8.02E+00
930.1042	7.79E+00
930.1154	7.51E+00
930.1266	7.23E+00
930.1378	7.02E+00
930.149	6.87E+00
930.1602	6.80E+00
930.1714	6.75E+00
930.1827	6.70E+00
930.1939	6.60E+00
930.2051	6.44E+00
930.2162	6.25E+00
930.2275	6.07E+00
930.2387	5.98E+00
930.2499	6.05E+00
930.2612	6.33E+00
930.2724	6.88E+00
930.2835	7.70E+00
930.2947	8.83E+00
930.306	1.03E+01
930.3172	1.21E+01
930.3284	1.44E+01
930.3397	1.75E+01
930.3509	2.18E+01
930.362	2.77E+01
930.3732	3.58E+01
930.3845	4.65E+01
930.3957	6.00E+01
930.4069	7.61E+01
930.4182	9.40E+01
930.4294	1.12E+02
930.4405	1.30E+02

930.4517	1.44E+02
930.463	1.54E+02
930.4742	1.58E+02
930.4855	1.56E+02
930.4967	1.48E+02
930.5079	1.35E+02
930.5192	1.18E+02
930.5303	1.00E+02
930.5415	8.24E+01
930.5527	6.59E+01
930.564	5.19E+01
930.5752	4.08E+01
930.5864	3.24E+01
930.5977	2.65E+01
930.6088	2.25E+01
930.62	1.98E+01
930.6312	1.79E+01
930.6425	1.65E+01
930.6537	1.53E+01
930.6649	1.41E+01
930.6761	1.30E+01
930.6874	1.20E+01
930.6985	1.11E+01
930.7097	1.06E+01
930.7209	1.03E+01
930.7322	1.03E+01
930.7434	1.06E+01
930.7546	1.11E+01
930.7659	1.17E+01
930.7771	1.24E+01
930.7882	1.30E+01
930.7994	1.36E+01
930.8107	1.39E+01
930.8219	1.41E+01
930.8331	1.40E+01
930.8444	1.38E+01
930.8556	1.35E+01
930.8668	1.30E+01
930.8779	1.25E+01
930.8892	1.20E+01
930.9004	1.15E+01

930.9116	1.11E+01
930.9229	1.07E+01
930.9341	1.04E+01
930.9454	1.02E+01
930.9566	1.01E+01
930.9678	1.02E+01
930.9789	1.03E+01
930.9902	1.07E+01
931.0014	1.11E+01
931.0126	1.17E+01
931.0239	1.23E+01
931.0351	1.29E+01
931.0463	1.35E+01
931.0576	1.39E+01
931.0688	1.42E+01
931.0799	1.43E+01
931.0911	1.43E+01
931.1024	1.41E+01
931.1136	1.38E+01
931.1248	1.35E+01
931.136	1.32E+01
931.1473	1.29E+01
931.1585	1.26E+01
931.1697	1.24E+01
931.181	1.22E+01
931.1921	1.21E+01
931.2033	1.20E+01
931.2145	1.20E+01
931.2258	1.21E+01
931.237	1.23E+01
931.2482	1.26E+01
931.2595	1.29E+01
931.2707	1.35E+01
931.2819	1.42E+01
931.2932	1.51E+01
931.3043	1.64E+01
931.3155	1.81E+01
931.3267	2.03E+01
931.338	2.29E+01
931.3492	2.56E+01
931.3604	2.78E+01

931.3716	2.91E+01
931.3829	2.91E+01
931.3942	2.88E+01
931.4054	3.09E+01
931.4165	4.10E+01
931.4277	6.83E+01
931.439	1.25E+02
931.4502	2.26E+02
931.4614	3.85E+02
931.4727	6.14E+02
931.4839	9.18E+02
931.4951	1.29E+03
931.5063	1.72E+03
931.5176	2.17E+03
931.5288	2.61E+03
931.54	3.00E+03
931.5511	3.31E+03
931.5624	3.49E+03
931.5736	3.54E+03
931.5848	3.45E+03
931.5961	3.23E+03
931.6073	2.90E+03
931.6185	2.51E+03
931.6298	2.08E+03
931.641	1.66E+03
931.6522	1.26E+03
931.6635	9.15E+02
931.6747	6.32E+02
931.6858	4.13E+02
931.697	2.54E+02
931.7083	1.45E+02
931.7195	7.64E+01
931.7307	3.65E+01
931.7419	1.59E+01
931.7532	7.10E+00
931.7644	4.88E+00
931.7756	5.74E+00
931.7869	7.72E+00
931.7981	9.85E+00
931.8093	1.17E+01
931.8206	1.33E+01

931.8318	1.47E+01
931.843	1.58E+01
931.8542	1.69E+01
931.8654	1.79E+01
931.8766	1.88E+01
931.8879	1.95E+01
931.8991	1.99E+01
931.9103	2.01E+01
931.9216	2.00E+01
931.9328	1.97E+01
931.944	1.93E+01
931.9553	1.87E+01
931.9665	1.82E+01
931.9777	1.77E+01
931.989	1.74E+01
932.0002	1.71E+01
932.0113	1.69E+01
932.0225	1.67E+01
932.0338	1.65E+01
932.045	1.63E+01
932.0562	1.60E+01
932.0674	1.56E+01
932.0787	1.52E+01
932.0899	1.47E+01
932.1011	1.43E+01
932.1124	1.39E+01
932.1236	1.36E+01
932.1348	1.35E+01
932.1461	1.35E+01
932.1573	1.35E+01
932.1685	1.36E+01
932.1797	1.38E+01
932.191	1.39E+01
932.2021	1.41E+01
932.2133	1.43E+01
932.2245	1.45E+01
932.2358	1.48E+01
932.247	1.51E+01
932.2582	1.54E+01
932.2695	1.56E+01
932.2807	1.58E+01

932.292	1.59E+01
932.3032	1.61E+01
932.3145	1.63E+01
932.3257	1.66E+01
932.3369	1.73E+01
932.3481	1.81E+01
932.3594	1.92E+01
932.3706	2.02E+01
932.3818	2.08E+01
932.3931	2.11E+01
932.4043	2.14E+01
932.4155	2.34E+01
932.4268	3.05E+01
932.438	4.79E+01
932.4491	8.30E+01
932.4603	1.44E+02
932.4716	2.41E+02
932.4828	3.78E+02
932.494	5.60E+02
932.5052	7.82E+02
932.5165	1.04E+03
932.5277	1.31E+03
932.5389	1.57E+03
932.5502	1.80E+03
932.5614	1.98E+03
932.5726	2.09E+03
932.5839	2.12E+03
932.5951	2.07E+03
932.6063	1.93E+03
932.6176	1.74E+03
932.6288	1.50E+03
932.64	1.25E+03
932.6512	9.90E+02
932.6625	7.52E+02
932.6737	5.44E+02
932.6849	3.74E+02
932.6962	2.42E+02
932.7074	1.47E+02
932.7186	8.21E+01
932.7299	4.22E+01
932.7411	2.01E+01

932.7524	9.87E+00
932.7636	6.74E+00
932.7748	7.28E+00
932.7861	9.25E+00
932.7973	1.14E+01
932.8084	1.32E+01
932.8196	1.45E+01
932.8309	1.53E+01
932.8421	1.59E+01
932.8533	1.64E+01
932.8646	1.69E+01
932.8758	1.74E+01
932.887	1.78E+01
932.8983	1.83E+01
932.9095	1.88E+01
932.9207	1.92E+01
932.9319	1.96E+01
932.9432	1.99E+01
932.9544	2.02E+01
932.9656	2.04E+01
932.9769	2.05E+01
932.9881	2.05E+01
932.9993	2.03E+01
933.0106	2.01E+01
933.0218	1.98E+01
933.033	1.95E+01
933.0443	1.91E+01
933.0555	1.88E+01
933.0667	1.84E+01
933.0779	1.81E+01
933.0892	1.79E+01
933.1004	1.77E+01
933.1116	1.75E+01
933.1229	1.75E+01
933.1341	1.76E+01
933.1453	1.78E+01
933.1566	1.81E+01
933.1678	1.84E+01
933.179	1.86E+01
933.1902	1.88E+01
933.2015	1.89E+01

933.2128	1.88E+01
933.224	1.88E+01
933.2352	1.88E+01
933.2465	1.90E+01
933.2577	1.93E+01
933.2689	1.97E+01
933.2802	2.02E+01
933.2914	2.07E+01
933.3026	2.10E+01
933.3138	2.12E+01
933.3251	2.13E+01
933.3363	2.12E+01
933.3475	2.11E+01
933.3588	2.09E+01
933.37	2.08E+01
933.3812	2.06E+01
933.3925	2.04E+01
933.4037	2.03E+01
933.4149	2.05E+01
933.4261	2.19E+01
933.4374	2.58E+01
933.4486	3.40E+01
933.4598	4.91E+01
933.4711	7.38E+01
933.4823	1.11E+02
933.4935	1.62E+02
933.5048	2.27E+02
933.516	3.05E+02
933.5272	3.92E+02
933.5385	4.82E+02
933.5497	5.67E+02
933.5609	6.41E+02
933.5721	6.96E+02
933.5834	7.26E+02
933.5946	7.29E+02
933.6058	7.05E+02
933.6171	6.56E+02
933.6283	5.87E+02
933.6395	5.06E+02
933.6508	4.20E+02
933.662	3.34E+02

933.6733	2.55E+02
933.6845	1.86E+02
933.6957	1.30E+02
933.7071	8.75E+01
933.7183	5.68E+01
933.7296	3.66E+01
933.7408	2.46E+01
933.752	1.84E+01
933.7632	1.59E+01
933.7745	1.55E+01
933.7857	1.59E+01
933.7969	1.65E+01
933.8082	1.71E+01
933.8194	1.76E+01
933.8306	1.81E+01
933.8419	1.86E+01
933.8531	1.93E+01
933.8643	2.00E+01
933.8755	2.05E+01
933.8868	2.08E+01
933.898	2.08E+01
933.9092	2.05E+01
933.9205	2.00E+01
933.9317	1.95E+01
933.9429	1.92E+01
933.9542	1.90E+01
933.9654	1.90E+01
933.9766	1.91E+01
933.9879	1.93E+01
933.9991	1.94E+01
934.0103	1.93E+01
934.0215	1.90E+01
934.0328	1.85E+01
934.044	1.79E+01
934.0552	1.74E+01
934.0665	1.70E+01
934.0778	1.68E+01
934.0891	1.69E+01
934.1003	1.71E+01
934.1116	1.76E+01
934.1228	1.81E+01

934.134	1.86E+01
934.1453	1.90E+01
934.1565	1.92E+01
934.1677	1.93E+01
934.179	1.93E+01
934.1902	1.91E+01
934.2014	1.88E+01
934.2126	1.86E+01
934.2239	1.84E+01
934.2351	1.82E+01
934.2463	1.82E+01
934.2576	1.83E+01
934.2688	1.84E+01
934.28	1.86E+01
934.2913	1.89E+01
934.3025	1.92E+01
934.3138	1.95E+01
934.3251	2.00E+01
934.3363	2.05E+01
934.3475	2.11E+01
934.3588	2.18E+01
934.37	2.26E+01
934.3812	2.36E+01
934.3925	2.46E+01
934.4037	2.57E+01
934.4149	2.71E+01
934.4261	2.88E+01
934.4374	3.12E+01
934.4486	3.48E+01
934.4598	4.00E+01
934.4711	4.73E+01
934.4823	5.73E+01
934.4935	7.00E+01
934.5048	8.52E+01
934.5161	1.03E+02
934.5273	1.21E+02
934.5386	1.40E+02
934.5498	1.57E+02
934.5611	1.72E+02
934.5723	1.83E+02
934.5836	1.89E+02

934.5948	1.89E+02
934.606	1.84E+02
934.6172	1.74E+02
934.6285	1.59E+02
934.6397	1.41E+02
934.6509	1.20E+02
934.6622	9.95E+01
934.6734	7.99E+01
934.6848	6.26E+01
934.696	4.82E+01
934.7072	3.70E+01
934.7184	2.90E+01
934.7297	2.36E+01
934.7409	2.03E+01
934.7521	1.84E+01
934.7634	1.74E+01
934.7746	1.70E+01
934.7858	1.69E+01
934.7971	1.70E+01
934.8083	1.72E+01
934.8195	1.73E+01
934.8307	1.74E+01
934.8421	1.72E+01
934.8533	1.67E+01
934.8646	1.59E+01
934.8758	1.50E+01
934.887	1.39E+01
934.8983	1.30E+01
934.9095	1.25E+01
934.9207	1.23E+01
934.9319	1.26E+01
934.9432	1.34E+01
934.9544	1.44E+01
934.9656	1.54E+01
934.977	1.64E+01
934.9882	1.72E+01
934.9995	1.77E+01
935.0107	1.79E+01
935.022	1.79E+01
935.0332	1.79E+01
935.0444	1.78E+01

935.0557	1.77E+01
935.0669	1.78E+01
935.0781	1.78E+01
935.0894	1.78E+01
935.1007	1.77E+01
935.1119	1.74E+01
935.1232	1.69E+01
935.1344	1.62E+01
935.1456	1.56E+01
935.1569	1.50E+01
935.1681	1.46E+01
935.1793	1.45E+01
935.1906	1.46E+01
935.2018	1.50E+01
935.213	1.55E+01
935.2244	1.58E+01
935.2356	1.60E+01
935.2468	1.59E+01
935.2581	1.55E+01
935.2693	1.50E+01
935.2805	1.45E+01
935.2917	1.41E+01
935.303	1.41E+01
935.3142	1.44E+01
935.3254	1.51E+01
935.3368	1.62E+01
935.348	1.74E+01
935.3593	1.88E+01
935.3705	2.00E+01
935.3817	2.10E+01
935.3929	2.17E+01
935.4042	2.22E+01
935.4154	2.26E+01
935.4266	2.31E+01
935.4379	2.40E+01
935.4492	2.54E+01
935.4604	2.75E+01
935.4717	3.02E+01
935.483	3.34E+01
935.4942	3.69E+01
935.5054	4.04E+01

935.5167	4.38E+01
935.5279	4.68E+01
935.5391	4.94E+01
935.5505	5.15E+01
935.5617	5.30E+01
935.5729	5.40E+01
935.5842	5.43E+01
935.5954	5.38E+01
935.6066	5.23E+01
935.6179	4.99E+01
935.6291	4.66E+01
935.6404	4.26E+01
935.6517	3.83E+01
935.6629	3.39E+01
935.6741	2.97E+01
935.6854	2.59E+01
935.6966	2.26E+01
935.7078	1.97E+01
935.7191	1.74E+01
935.7303	1.54E+01
935.7416	1.38E+01
935.7529	1.26E+01
935.7641	1.18E+01
935.7753	1.13E+01
935.7866	1.12E+01
935.7978	1.14E+01
935.809	1.18E+01
935.8203	1.24E+01
935.8316	1.29E+01
935.8428	1.33E+01
935.8541	1.35E+01
935.8653	1.36E+01
935.8765	1.35E+01
935.8878	1.32E+01
935.899	1.29E+01
935.9102	1.25E+01
935.9216	1.23E+01
935.9329	1.22E+01
935.9441	1.23E+01
935.9553	1.27E+01
935.9666	1.33E+01

935.9778	1.39E+01
935.989	1.46E+01
936.0004	1.52E+01
936.0116	1.55E+01
936.0228	1.56E+01
936.0341	1.53E+01
936.0453	1.48E+01
936.0565	1.40E+01
936.0677	1.31E+01
936.0791	1.22E+01
936.0903	1.13E+01
936.1016	1.07E+01
936.1128	1.02E+01
936.124	1.01E+01
936.1353	1.03E+01
936.1465	1.08E+01
936.1577	1.15E+01
936.1691	1.23E+01
936.1803	1.33E+01
936.1915	1.43E+01
936.2028	1.52E+01
936.214	1.60E+01
936.2252	1.65E+01
936.2366	1.68E+01
936.2478	1.69E+01
936.259	1.66E+01
936.2703	1.62E+01
936.2815	1.56E+01
936.2927	1.50E+01
936.304	1.44E+01
936.3153	1.39E+01
936.3265	1.37E+01
936.3378	1.37E+01
936.349	1.40E+01
936.3602	1.47E+01
936.3715	1.57E+01
936.3828	1.72E+01
936.3941	1.91E+01
936.4053	2.15E+01
936.4166	2.41E+01
936.4278	2.69E+01

936.439	2.97E+01
936.4503	3.22E+01
936.4616	3.43E+01
936.4728	3.58E+01
936.4841	3.67E+01
936.4953	3.68E+01
936.5065	3.64E+01
936.5178	3.54E+01
936.5291	3.40E+01
936.5403	3.24E+01
936.5516	3.05E+01
936.5628	2.85E+01
936.574	2.64E+01
936.5853	2.42E+01
936.5965	2.19E+01
936.6078	1.97E+01
936.6191	1.76E+01
936.6303	1.57E+01
936.6415	1.39E+01
936.6528	1.24E+01
936.664	1.13E+01
936.6754	1.04E+01
936.6866	9.94E+00
936.6978	9.72E+00
936.709	9.67E+00
936.7203	9.71E+00
936.7316	9.72E+00
936.7429	9.67E+00
936.7541	9.55E+00
936.7653	9.37E+00
936.7766	9.19E+00
936.7878	9.06E+00
936.7991	9.04E+00
936.8104	9.12E+00
936.8216	9.28E+00
936.8328	9.49E+00
936.8441	9.69E+00
936.8553	9.84E+00
936.8667	9.94E+00
936.8779	9.96E+00
936.8892	9.92E+00

936.9004	9.82E+00
936.9116	9.66E+00
936.9229	9.48E+00
936.9342	9.26E+00
936.9454	9.05E+00
936.9567	8.85E+00
936.9679	8.68E+00
936.9791	8.55E+00
936.9905	8.42E+00
937.0017	8.27E+00
937.0129	8.07E+00
937.0242	7.79E+00
937.0354	7.44E+00
937.0468	7.05E+00
937.058	6.70E+00
937.0692	6.43E+00
937.0804	6.33E+00
937.0917	6.41E+00
937.1029	6.65E+00
937.1143	7.00E+00
937.1255	7.42E+00
937.1367	7.83E+00
937.1479	8.23E+00
937.1592	8.60E+00
937.1705	8.97E+00
937.1818	9.38E+00
937.193	9.83E+00
937.2042	1.03E+01
937.2155	1.07E+01
937.2268	1.11E+01
937.238	1.13E+01
937.2493	1.14E+01
937.2605	1.14E+01
937.2717	1.13E+01
937.2831	1.12E+01
937.2944	1.11E+01
937.3056	1.11E+01
937.3168	1.11E+01
937.3281	1.11E+01
937.3394	1.13E+01
937.3506	1.15E+01

937.3619	1.19E+01
937.3731	1.25E+01
937.3843	1.35E+01
937.3957	1.48E+01
937.4069	1.63E+01
937.4182	1.80E+01
937.4294	1.97E+01
937.4406	2.13E+01
937.452	2.26E+01
937.4632	2.36E+01
937.4744	2.42E+01
937.4857	2.45E+01
937.4969	2.46E+01
937.5082	2.45E+01
937.5195	2.42E+01
937.5307	2.37E+01
937.5419	2.30E+01
937.5532	2.21E+01
937.5645	2.09E+01
937.5757	1.94E+01
937.587	1.78E+01
937.5982	1.61E+01
937.6096	1.45E+01
937.6208	1.31E+01
937.632	1.19E+01
937.6432	1.10E+01
937.6545	1.04E+01
937.6658	9.89E+00
937.6771	9.46E+00
937.6883	9.04E+00
937.6995	8.60E+00
937.7108	8.17E+00
937.7221	7.79E+00
937.7333	7.50E+00
937.7446	7.32E+00
937.7559	7.24E+00
937.7672	7.23E+00
937.7784	7.23E+00
937.7897	7.20E+00
937.8009	7.11E+00
937.8121	6.97E+00

937.8235	6.82E+00
937.8347	6.71E+00
937.8459	6.70E+00
937.8572	6.81E+00
937.8685	7.03E+00
937.8798	7.33E+00
937.891	7.64E+00
937.9022	7.86E+00
937.9136	7.93E+00
937.9248	7.80E+00
937.936	7.45E+00
937.9473	6.91E+00
937.9585	6.25E+00
937.9698	5.55E+00
937.9811	4.91E+00
937.9923	4.42E+00
938.0035	4.17E+00
938.0149	4.18E+00
938.0261	4.45E+00
938.0374	4.96E+00
938.0486	5.61E+00
938.0599	6.30E+00
938.0712	6.93E+00
938.0824	7.41E+00
938.0936	7.67E+00
938.1049	7.70E+00
938.1162	7.54E+00
938.1274	7.24E+00
938.1387	6.90E+00
938.1499	6.60E+00
938.1613	6.43E+00
938.1725	6.41E+00
938.1837	6.54E+00
938.1949	6.81E+00
938.2064	7.16E+00
938.2176	7.53E+00
938.2288	7.88E+00
938.2401	8.15E+00
938.2514	8.34E+00
938.2626	8.42E+00
938.2739	8.41E+00

938.2851	8.32E+00
938.2964	8.20E+00
938.3077	8.10E+00
938.3189	8.08E+00
938.3301	8.23E+00
938.3415	8.62E+00
938.3527	9.36E+00
938.364	1.06E+01
938.3752	1.23E+01
938.3865	1.48E+01
938.3978	1.80E+01
938.409	2.20E+01
938.4202	2.67E+01
938.4316	3.20E+01
938.4428	3.75E+01
938.454	4.28E+01
938.4653	4.74E+01
938.4766	5.09E+01
938.4879	5.29E+01
938.4991	5.31E+01
938.5103	5.17E+01
938.5217	4.89E+01
938.5329	4.50E+01
938.5441	4.06E+01
938.5554	3.60E+01
938.5667	3.17E+01
938.5779	2.78E+01
938.5892	2.44E+01
938.6005	2.15E+01
938.6118	1.90E+01
938.623	1.67E+01
938.6342	1.46E+01
938.6456	1.27E+01
938.6569	1.11E+01
938.6681	9.64E+00
938.6793	8.45E+00
938.6907	7.48E+00
938.7019	6.71E+00
938.7131	6.10E+00
938.7244	5.60E+00
938.7357	5.19E+00

938.7469	4.84E+00
938.7582	4.55E+00
938.7695	4.34E+00
938.7808	4.19E+00
938.792	4.12E+00
938.8032	4.10E+00
938.8146	4.12E+00
938.8258	4.18E+00
938.837	4.24E+00
938.8483	4.30E+00
938.8596	4.36E+00
938.8708	4.42E+00
938.8821	4.50E+00
938.8934	4.60E+00
938.9047	4.72E+00
938.9159	4.87E+00
938.9271	5.04E+00
938.9385	5.24E+00
938.9497	5.46E+00
938.9609	5.68E+00
938.9723	5.89E+00
938.9835	6.06E+00
938.9948	6.18E+00
939.006	6.21E+00
939.0173	6.13E+00
939.0286	5.93E+00
939.0398	5.64E+00
939.051	5.28E+00
939.0624	4.91E+00
939.0736	4.60E+00
939.0848	4.40E+00
939.0962	4.33E+00
939.1074	4.41E+00
939.1187	4.62E+00
939.1301	4.92E+00
939.1413	5.25E+00
939.1525	5.58E+00
939.1638	5.89E+00
939.1751	6.18E+00
939.1863	6.46E+00
939.1976	6.76E+00

939.2089	7.11E+00
939.2202	7.48E+00
939.2314	7.85E+00
939.2426	8.18E+00
939.254	8.41E+00
939.2652	8.48E+00
939.2764	8.40E+00
939.2878	8.17E+00
939.299	7.87E+00
939.3102	7.56E+00
939.3215	7.34E+00
939.3328	7.31E+00
939.3441	7.56E+00
939.3553	8.18E+00
939.3666	9.25E+00
939.3779	1.09E+01
939.3891	1.31E+01
939.4005	1.61E+01
939.4117	1.98E+01
939.4229	2.41E+01
939.4343	2.89E+01
939.4455	3.38E+01
939.4567	3.84E+01
939.468	4.22E+01
939.4793	4.49E+01
939.4905	4.61E+01
939.5018	4.57E+01
939.5131	4.38E+01
939.5244	4.07E+01
939.5356	3.68E+01
939.5469	3.25E+01
939.5582	2.82E+01
939.5695	2.43E+01
939.5808	2.09E+01
939.592	1.80E+01
939.6033	1.56E+01
939.6145	1.36E+01
939.6259	1.19E+01
939.6371	1.04E+01
939.6483	9.07E+00
939.6597	7.94E+00

939.6709	6.97E+00
939.6821	6.18E+00
939.6935	5.55E+00
939.7047	5.06E+00
939.7159	4.69E+00
939.7273	4.42E+00
939.7385	4.24E+00
939.7498	4.12E+00
939.7611	4.06E+00
939.7723	4.06E+00
939.7836	4.09E+00
939.7949	4.14E+00
939.8062	4.21E+00
939.8174	4.27E+00
939.8286	4.31E+00
939.84	4.36E+00
939.8512	4.41E+00
939.8624	4.48E+00
939.8738	4.59E+00
939.885	4.76E+00
939.8962	4.95E+00
939.9076	5.15E+00
939.9188	5.31E+00
939.9301	5.36E+00
939.9414	5.27E+00
939.9526	5.03E+00
939.9639	4.65E+00
939.9752	4.18E+00
939.9865	3.67E+00
939.9977	3.20E+00
940.009	2.81E+00
940.0203	2.53E+00
940.0316	2.35E+00
940.0429	2.24E+00
940.0541	2.17E+00
940.0654	2.11E+00
940.0767	2.06E+00
940.088	2.01E+00
940.0992	2.00E+00
940.1105	2.06E+00
940.1218	2.20E+00

940.133	2.46E+00
940.1443	2.81E+00
940.1556	3.26E+00
940.1668	3.77E+00
940.1782	4.31E+00
940.1894	4.86E+00
940.2006	5.38E+00
940.212	5.85E+00
940.2232	6.24E+00
940.2344	6.53E+00
940.2458	6.72E+00
940.257	6.77E+00
940.2684	6.71E+00

SUPPLEMENT 3

Table. Centroid mass of H/D exchanged peptic peptides of deoxy HbA at various time points

Origin of peptide and amino acid sequence	0 min	10 min	20 min	40 min	50 min	60 min	75 min	90 min	120 min	140 min	160 min	180 min	360 min
β130-146 YQKVVAGVANA LAHKYH	1870. 244	1870. 686	1870. 676	1870. 980	1871. 102	1871. 190	1871. 169	1871. 137	1871. 122	1871. 580	1871. 076	1871. 240	1871. 637
β1-14 VHLTPEEKSAVT AL	1495. 613	1498. 647	1498. 778	1499. 342	1499. 667	1499. 635	1499. 594	1499. 397	1499. 477	1499. 681	1499. 197	1499. 521	1499. 746
α34-46 LSFPTTKTYFPH F	1588. 025	1588. 915	1588. 576	1588. 766	1588. 387	1589. 094	1589. 091	1588. 044	1588. 792	1589. 277	1588. 401	1588. 819	1589. 654
β86-102 ATLSELHCDKLH VDPEN	1922. 119	1923. 359	1923. 615	1924. 070	1924. 176	1924. 587	1924. 535	1924. 230	1924. 002	1924. 881	1923. 936	1924. 663	1925. 242
β32-41 LVVYPWTQRF	1309. 492	1309. 805	1309. 868	1309. 962	1310. 004	1310. 045	1310. 054	1310. 066	1310. 090	1310. 158	1310. 096	1310. 169	1310. 451
β32-40 LVVYPWTQR	1163. 435	1163. 793	1163. 332	1163. 974	1165. 390	1164. 432	1164. 807	1164. 068	1164. 274	1166. 440	1164. 218	1164. 147	1163. 699
α110-141 AAHLPAEFTPAV HASLDKFLASVS TVLTSKYR	3429. 718	3432. 567	3432. 805	3433. 572	3433. 527	3433. 712	3433. 727	3433. 656	3433. 711	3433. 813	3433. 319	3433. 753	3435. 129
β103-110 FRLLGNVL	932.2 25	932.2 15	932.2 40	932.2 74	932.2 80	932.2 90	932.2 99	932.3 02	932.3 29	932.3 42	932.3 56	932.3 60	932.6 81

β15-31 WGKVNVDVVG GEALGRL	1800. 033	1801. 775	1801. 851	1802. 536	1802. 818	1802. 821	1802. 737	1802. 410	1802. 600	1802. 811	1802. 003	1802. 456	1802. 659
α1-29 VLSPADKTNVK AAWGKVGAAH GEYGAEAL	2912. 185	2915. 669	2915. 812	2916. 501	2916. 736	2917. 129	2917. 074	2916. 841	2916. 638	2917. 419	2916. 400	2914. 704	2918. 646
β22-31 EVGGGEALGRL	1000. 949	1003. 042	1002. 884	1003. 339	1003. 404	1003. 725	1003. 677	1003. 427	1003. 568	1003. 764	1003. 186	1003. 422	1003. 420
α1-32 VLSPADKTNVK AAWGKVGAAH GEYGAEALERM	3328. 507	3331. 833	3331. 992	3332. 907	3332. 819	3333. 267	3333. 168	3333. 039	3332. 772	3333. 492	3332. 569	3333. 145	3335. 427
α1-33 VLSPADKTNVK AAWGKVGAAH GEYGAEALERM F	3475. 641	3478. 934	3479. 141	3480. 099	3479. 935	3480. 388	3480. 281	3480. 181	3479. 899	3480. 599	3479. 701	3480. 289	3482. 691
β111-129 VCVLAHHFGKE FTPPVQAA	2052. 318	2053. 518	2053. 646	2053. 863	2053. 851	2054. 187	2054. 166	2054. 156	2053. 972	2054. 283	2053. 962	2054. 545	2054. 661

SUPPLEMENT 4

Table. Centroid mass of H/D exchanged peptic peptides of oxy HbA at various time points

Origin of peptide and amino acid sequence	0 min	10 min	20 min	40 min	50 min	60 min	75 min	90 min	120 min	140 min	160 min	180 min	360 min
β 130-146 YQKVVAGVANALA HKYH	1870. 131	1870. 637	1870. 792	1871. 189	1871. 094	1871. 189	1871. 209	1871. 173	1871. 286	1871. 113	1871. 330	1871. 517	1871. 615
β 1-14 VHLTPEEKSAVTAL	1496. 841	1497. 279	1498. 144	1498. 809	1498. 727	1498. 934	1499. 175	1499. 126	1499. 302	1498. 817	1499. 580	1499. 305	1499. 710
α 34-46 LSFPTTKTYFPHF	1586. 989	1588. 137	1587. 632	1589. 364	1588. 581	1589. 521	1588. 763	1589. 115	1588. 919	1588. 931	1588. 860	1589. 253	1590. 140
β 86-102 ATLSELHCDKLHVD PEN	1922. 092	1923. 496	1924. 228	1925. 741	1925. 145	1925. 227	1925. 185	1925. 300	1925. 175	1924. 617	1925. 637	1926. 197	1926. 255
β 32-41 LVVYPWTQRF	1309. 496	1309. 974	1310. 141	1310. 518	1310. 516	1310. 565	1310. 642	1310. 621	1310. 732	1310. 640	1310. 774	1310. 742	1310. 798
β 32-40 LVVYPWTQR	1162. 365	1163. 132	1163. 546	1164. 426	1164. 373	1166. 319	1164. 451	1164. 487	1165. 867	1164. 576	1164. 431	1164. 513	1164. 249
α 110-141 AAHLPAEFTPAVHA SLDKFLASVSTVLT SKYR	3429. 702	3431. 936	3432. 514	3432. 852	3432. 520	3432. 705	3433. 130	3432. 964	3433. 494	3433. 082	3433. 610	3434. 064	3435. 159
β 103-110 FRLGNVL	932.2 11	932.2 06	932.2 59	932.3 37	932.3 41	932.3 72	932.3 97	932.4 09	932.4 61	932.4 34	932.4 96	932.5 06	932.8 30
β 15-31 WGKVNVDVEVGGE	1800. 014	1801. 103	1801. 710	1802. 291	1801. 962	1802. 383	1802. 611	1802. 570	1802. 727	1802. 233	1803. 014	1802. 773	1802. 849

ALGRL													
α1-29 VLSPADKTNVKAA WGKVGAHAGEYG AEAL	2912. 130	2915. 153	2916. 263	2917. 346	2916. 811	2917. 283	2917. 842	2917. 491	2918. 116	2917. 125	2918. 284	2918. 207	2919. 673
β22-31 EVGGEALGRL	1001. 181	1002. 294	1002. 816	1003. 319	1002. 946	1003. 520	1003. 399	1003. 333	1003. 702	1003. 237	1003. 645	1003. 676	1003. 712
α1-32 VLSPADKTNVKAA WGKVGAHAGEYG AEALERM	3328. 483	3331. 774	3332. 672	3333. 806	3333. 051	3333. 585	3334. 065	3333. 887	3334. 422	3333. 383	3334. 388	3334. 472	3336. 160
α1-33 VLSPADKTNVKAA WGKVGAHAGEYG AEALERMF	3475. 908	3478. 997	3479. 805	3480. 949	3480. 219	3480. 645	3481. 263	3481. 062	3481. 550	3480. 581	3481. 862	3481. 699	3483. 381
β111-129 VCVLAHHFGKEFT PPVQAA	2052. 284	2053. 050	2053. 280	2053. 737	2053. 727	2053. 798	2053. 927	2053. 896	2054. 460	2054. 689	2054. 857	2054. 302	2054. 755

SUPPLEMENT 5

Table. Comparison of centroid mass calculated by three softwares for an isotopic distribution

S. No.	Monoisotopic mass	Average mass calculated by MS- Product	Centroid mass calculated using customized program	Centroid mass calculated using HX- Express
1	931.6	932.161	932.211	932.131
2	1000.6	1001.134	1001.181	1001.142
3	1161.7	1162.385	1162.365	1162.377
4	1308.7	1309.563	1309.496	1309.529
5	1494.9	1495.726	1496.841	1495.671
6	1585.9	1586.842	1586.989	1587.043
7	1799.0	1800.037	1800.014	1800.002
8	1869.1	1870.178	1870.131	1870.117
9	1921.0	1922.137	1922.092	1922.105
10	2051.1	2052.420	2052.284	2052.298
11	2910.6	2912.295	2912.13	2912.089
12	3326.8	3328.798	3328.483	3328.533
13	3428.0	3429.969	3429.702	3429.797
14	3473.9	3475.976	3475.908	3475.526