

NMF

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```
# load the packages
library(NMF)
library(tidyverse)
library(gridExtra)
library(readxl)
```

Reading the data

```
# read the radon data
# Old:
# hourly_radon <- readRDS("hourly_radon.rds")
# New:
hourly_data <- readRDS("../DataProcessing/Trailer_hourly_merge_20240905.rds")

# remove NAs
hourly_nona <- hourly_data %>% select(-c(temp_bb,rhi, esf_bb, distToLovi,inv_dist,
                                         distToLovi_wells, monthly_oil, monthly_gas)) %>% na.omit()

# retrieving the vocs, removing everything else except the vocs
hourly_vocs <- hourly_nona %>% select(c("ethane", "ethene", "propane", "propene",
                                         "1_3-butadiene", "i-butane", "n-butane",
                                         "acetylene", "cyclopentane", "i-pentane",
                                         "n-pentane", "n-hexane", "isoprene", "n-heptane",
                                         "benzene", "n-octane", "toluene", "ethyl-benzene",
                                         "m&p-xylene", "o-xylene"))

# retrieving the non-vocs: co2_ppm, nox, ch4, h2s, so2, o3
# double check this
non_vocs <- c('ch4', 'co2_ppm', 'co', 'h2s', 'so2', 'nox', 'o3')
hourly_non_vocs <- hourly_nona %>% select(all_of(non_vocs))

hourly_full_nona <- cbind(hourly_non_vocs, hourly_vocs)

# retrieve a vector of yearmonth
hourly_dates <- hourly_nona %>%
  mutate(yearmonth = substring(day, 0, 7)) %>%
  pull(yearmonth)
```

Data preprocessing

```
# Define LOD for each chemical
LOD_non_voc <- c('ch4' = 0.9,
```

```

      'co2_ppm' = 0.0433,
      'co' = 40,
      'h2s' = 0.4,
      'so2' = 0.4,
      'nox' = 0.05,
      'o3' = 1)

LOD_voc_monthly <- read_csv('../data/LNM_VOC_LOD_Rounded.csv') %>% select(-1)
# extract the yearmonth from date variables
LOD_voc_monthly <- LOD_voc_monthly %>%
  mutate(yearmonth = strptime(as.POSIXct(start_date, format = '%Y-%m-%d %H:%M:%S', tz = 'UTC'), '%Y-%m-%d %H:%M:%S'))

LOD_voc_monthly <- LOD_voc_monthly %>%
  select(-c(start_date, end_date)) %>%
  select(!any_of(ends_with('half_ldl')))

colnames(LOD_voc_monthly) <- str_replace_all(names(LOD_voc_monthly), '_ldl', '')

LOD_voc_avg <- read_xlsx('../data/LNM_VOC_Uncertainties.xlsx', skip = 1)
LOD_voc_avg <- LOD_voc_avg %>%
  select(1, 4) %>%
  rename('LOD' = 2, 'chemical' = 1) %>%
  head(20)

# find the min for background-levels
background_levels <- sapply(hourly_full_nona, min)
background_levels

##          ch4          co2_ppm          co          h2s          so2
##    1928.000        411.300        61.630         0.200         0.200
##          nox           o3          ethane          ethene          propane
##         0.025         0.500         0.916         0.011         0.224
##    propene 1_3-butadiene    i-butane    n-butane    acetylene
##         0.009         0.007         0.035         0.090         0.019
## cyclopentane    i-pentane    n-pentane    n-hexane    isoprene
##         0.005         0.038         0.042         0.021         0.005
##    n-heptane    benzene    n-octane    toluene ethyl-benzene
##         0.004         0.017         0.004         0.004         0.004
##    m&p-xylene    o-xylene
##         0.004         0.004

get_info <- function(column) {
  N <- length(column)
  background <- quantile(column, 0)
  quantile1 <- quantile(column, 0.01)
  quantile99 <- quantile(column, 0.99)
  return(c(N, quantile1, quantile99, background))
}

info_table <- hourly_full_nona %>%
  reframe(across(everything(), ~ get_info(.x)))

info_table <- info_table %>%
  mutate(rownames = c('N', '1st percentile', '99th percentile', 'Background')) %>%
  pivot_longer(-rownames) %>%

```

```

pivot_wider(names_from = rownames, values_from = value)

knitr::kable(info_table)

```

name	N	1st percentile	99th percentile	Background
ch4	4497	1963.40000	6318.81200	1928.000
co2_ppm	4497	417.09000	457.87120	411.300
co	4497	84.90720	444.04320	61.630
h2s	4497	0.20000	5.18084	0.200
so2	4497	0.20000	1.83896	0.200
nox	4497	0.22700	92.01080	0.025
o3	4497	0.50000	72.11200	0.500
ethane	4497	1.80852	536.67200	0.916
ethene	4497	0.01100	3.52212	0.011
propane	4497	0.81700	305.54000	0.224
propene	4497	0.00900	0.70228	0.009
1_3-butadiene	4497	0.00700	0.05904	0.007
i-butane	4497	0.14496	63.53760	0.035
n-butane	4497	0.34792	171.37600	0.090
acetylene	4497	0.04900	2.66204	0.019
cyclopentane	4497	0.00500	3.12356	0.005
i-pentane	4497	0.10396	51.02080	0.038
n-pentane	4497	0.10300	58.10280	0.042
n-hexane	4497	0.04196	18.32640	0.021
isoprene	4497	0.00500	0.03204	0.005
n-heptane	4497	0.01500	6.58924	0.004
benzene	4497	0.02700	3.87512	0.017
n-octane	4497	0.00400	2.01452	0.004
toluene	4497	0.01296	3.53640	0.004
ethyl-benzene	4497	0.00400	0.31604	0.004
m&p-xylene	4497	0.00400	1.31824	0.004
o-xylene	4497	0.00400	0.45912	0.004

```

#adjustments that were made according to paper
#William: I'm guessing this refers to Gunnar's paper section 2.2 and Guha 3.3
adjusting_neg_bg_from_lod <- function(chemical, LOD, background, hourly_data){
  # get min and max
  min_value <- min(hourly_data[chemical], na.rm = TRUE)
  max_value <- max(hourly_data[chemical], na.rm = TRUE)
  # if min less than double LOD or max > 100 times LOD
  # adjust to -100 (for entire column???)
  if (min_value < 2 * LOD & max_value > 100 * LOD ){
    return (0)
  }
  return (background)
}

# Check if background is negligible for non voc
# merge background and LOD
background_lod_non_voc <- tibble(chemical = non_vocs,
                                  LOD = LOD_non_voc,
                                  background = unname(background_levels[non_vocs]))
adjusted_background_non_voc <- background_lod_non_voc %>%

```

```

rowwise() %>%
mutate(min = min(hourly_data[chemical], na.rm = TRUE),
       LODx2 = 2 * LOD,
       criterion1 = min(hourly_data[chemical], na.rm = TRUE) < 2 * LOD,
       max = max(hourly_data[chemical], na.rm = TRUE),
       LODx100 = 100 * LOD,
       criterion2 = max(hourly_data[chemical], na.rm = TRUE) > 100 * LOD,
       adjusted_background = adjusting_neg_bg_from_lod(chemical, LOD, background, hourly_data))

# Check if background is negligible for voc
# merge background and LOD
background_lod_voc <- LOD_voc_avg %>%
  left_join(tibble(chemical = setdiff(names(background_levels), non_vocs),
                  background = background_levels[setdiff(names(background_levels), non_vocs)]))

## Joining with `by = join_by(chemical)`
adjusted_background_voc <- background_lod_voc %>%
  rowwise() %>%
  mutate(min = min(hourly_data[chemical], na.rm = TRUE),
         LODx2 = 2 * LOD,
         criterion1 = min(hourly_data[chemical], na.rm = TRUE) < 2 * LOD,
         max = max(hourly_data[chemical], na.rm = TRUE),
         LODx100 = 100 * LOD,
         criterion2 = max(hourly_data[chemical], na.rm = TRUE) > 100 * LOD,
         adjusted_background = adjusting_neg_bg_from_lod(chemical, LOD, background, hourly_data))

# So now we have the adjusted background concentrations
subtract_adj_bg <- function(column, chemical) {
  print(chemical)
  result <-
  return (result)
}
hourly_nona_bgrm <- hourly_full_nona %>%
  mutate(across(adjusted_background_non_voc$chemical, ~ .x - adjusted_background_non_voc$adjusted_backg
hourly_nona_bgrm <- hourly_nona_bgrm %>%
  mutate(across(adjusted_background_voc$chemical, ~ .x - adjusted_background_voc$adjusted_background[a

# look at zero values
colSums(hourly_nona_bgrm == 0)

##          ch4          co2_ppm          co          h2s          so2
##          1            1            1          777        3065
##          nox            o3          ethane          ethene          propane
##          0            0            1            0            1
##          propene 1_3-butadiene          i-butane          n-butane          acetylene
##          0          3126            1            1            0
##          cyclopentane          i-pentane          n-pentane          n-hexane          isoprene
##          0            1            1            0          2815
##          n-heptane          benzene          n-octane          toluene          ethyl-benzene
##          0            0            0            0            0
##          m&p-xylene          o-xylene
##          0            0

# replace negative values with random values between 0 and 0.5*LOD
set.seed(123)

```

```

replace_zero_with_random <- function(column, name, LOD_df){
  LOD <- LOD_df$LOD[LOD_df$chemical == name]
  column <- if_else(column == 0, round(runif(length(column), 0, 0.5 * LOD), 3), column)
  return (column)
}

hourly_nona_bgrm_zerorepl <- hourly_nona_bgrm %>%
  mutate(across(adjusted_background_non_voc$chemical, ~ replace_zero_with_random(.x, cur_column(), adjusted_background_non_voc$LOD[adjusted_background_non_voc$chemical == cur_column()]))

hourly_nona_bgrm_zerorepl <- hourly_nona_bgrm_zerorepl %>%
  mutate(across(adjusted_background_voc$chemical, ~ replace_zero_with_random(.x, cur_column(), adjusted_background_voc$LOD[adjusted_background_voc$chemical == cur_column()]))

```

Normalize the non-vocs

```

#normalizing function
normalize_column <- function(column){
  background <- quantile(column, 0)
  max <- quantile(column, 0.99)
  return ((column - background)/(max - background))
}

# normalize all
hourly_nona_bgrm_zerorepl_norm <- as_tibble(sapply(as.list(hourly_nona_bgrm_zerorepl), normalize_column))
summary(hourly_nona_bgrm_zerorepl_norm)

```

```

##          ch4          co2_ppm          co          h2s
## Min.      :0.00000  Min.      :0.0000  Min.      :0.0000  Min.      :0.00000
## 1st Qu.:0.04163  1st Qu.:0.2781  1st Qu.:0.1523  1st Qu.:0.05642
## Median :0.10679  Median :0.3635  Median :0.2377  Median :0.12909
## Mean     :0.19848  Mean     :0.3976  Mean     :0.2953  Mean     :0.19418
## 3rd Qu.:0.27300  3rd Qu.:0.4808  3rd Qu.:0.3721  3rd Qu.:0.25197
## Max.      :7.30686  Max.      :1.9903  Max.      :6.4901  Max.      :5.52116
##          so2          nox          o3          ethane
## Min.      :0.00000  Min.      :0.00000  Min.      :0.0000  Min.      :0.0000
## 1st Qu.:0.04088  1st Qu.:0.03208  1st Qu.:0.1355  1st Qu.:0.0314
## Median :0.08054  Median :0.10033  Median :0.3589  Median :0.1007
## Mean     :0.13442  Mean     :0.18181  Mean     :0.3732  Mean     :0.1976
## 3rd Qu.:0.12081  3rd Qu.:0.24866  3rd Qu.:0.5739  3rd Qu.:0.2917
## Max.      :5.11178  Max.      :4.92396  Max.      :1.2121  Max.      :3.8434
##          ethene          propane          propene          1_3-butadiene
## Min.      :0.00000  Min.      :0.00000  Min.      :0.00000  Min.      : 0.00000
## 1st Qu.:0.06294  1st Qu.:0.03571  1st Qu.:0.04616  1st Qu.: 0.03843
## Median :0.17459  Median :0.11131  Median :0.14857  Median : 0.09608
## Mean     :0.24709  Mean     :0.21527  Mean     :0.23032  Mean     : 0.17294
## 3rd Qu.:0.35373  3rd Qu.:0.32152  3rd Qu.:0.34474  3rd Qu.: 0.17294
## Max.      :4.83008  Max.      :3.96568  Max.      :7.96071  Max.      :23.05918
##          i-butane          n-butane          acetylene          cyclopentane
## Min.      :0.00000  Min.      :0.00000  Min.      :0.00000  Min.      :0.00000
## 1st Qu.:0.02802  1st Qu.:0.02682  1st Qu.:0.08853  1st Qu.:0.03143
## Median :0.08893  Median :0.08557  Median :0.16837  Median :0.09684
## Mean     :0.18128  Mean     :0.17406  Mean     :0.24305  Mean     :0.18948
## 3rd Qu.:0.25229  3rd Qu.:0.24489  3rd Qu.:0.33257  3rd Qu.:0.26903
## Max.      :4.67041  Max.      :3.13405  Max.      :3.19783  Max.      :4.31449
##          i-pentane          n-pentane          n-hexane          isoprene

```

```
## Min.      :0.00000 Min.      :0.00000 Min.      :0.00000 Min.      : 0.00000
## 1st Qu.:0.02579 1st Qu.:0.02494 1st Qu.:0.02376 1st Qu.: 0.03698
## Median :0.08349 Median :0.08124 Median :0.08052 Median : 0.07396
## Mean    :0.17550 Mean    :0.17463 Mean    :0.17907 Mean    : 0.13700
## 3rd Qu.:0.24496 3rd Qu.:0.24418 3rd Qu.:0.25118 3rd Qu.: 0.14793
## Max.    :4.23427 Max.    :4.45673 Max.    :5.09899 Max.    :13.20266
## n-heptane benzene n-octane toluene
## Min.      :0.00000 Min.      :0.00000 Min.      :0.00000 Min.      :0.00000
## 1st Qu.:0.02460 1st Qu.:0.03914 1st Qu.:0.02736 1st Qu.:0.03454
## Median :0.08276 Median :0.10186 Median :0.08704 Median :0.10588
## Mean    :0.18168 Mean    :0.18957 Mean    :0.18465 Mean    :0.19932
## 3rd Qu.:0.25481 3rd Qu.:0.26619 3rd Qu.:0.26013 3rd Qu.:0.28677
## Max.    :4.62641 Max.    :2.48644 Max.    :3.41355 Max.    :2.56851
## ethyl-benzene m&p-xylene o-xylene
## Min.      :0.00000 Min.      :0.00000 Min.      :0.00000
## 1st Qu.:0.01923 1st Qu.:0.01598 1st Qu.:0.00000
## Median :0.09614 Median :0.08902 Median :0.0813
## Mean    :0.18206 Mean    :0.18234 Mean    :0.1730
## 3rd Qu.:0.26279 3rd Qu.:0.26860 3rd Qu.:0.2571
## Max.    :2.97077 Max.    :2.37323 Max.    :2.0171
```

Combine and Transpose

```
normalized_matrix <- as.matrix(hourly_nona_bgrm_zerorepl_norm) #important: using the normalized VOCs for
# Transpose <- cbind(Normalized_Data, Merged_VOCs)
# rownames(Transpose) <- as.character(Transpose[,1]) # I'm not able to run this line, but it shouldn't
# transpose_normalized_matrix <- t(as.matrix(normalized_matrix))

number_row<- dim(normalized_matrix)[1] #store number of rows (used for checking)
number_column<- dim(normalized_matrix)[2] #store number of columns
```

NMF section

```
# compute weight matrix (uncertainties)
# Based on the Guha paper
# next comment is from the other nmf R file
weight_matrix <- matrix(0, nrow = nrow(normalized_matrix), ncol = ncol(normalized_matrix))
LOD_merged <- tibble(chemical = c(adjusted_background_non_voc$chemical, adjusted_background_voc$chemical),
                      LOD = c(adjusted_background_non_voc$LOD, adjusted_background_voc$LOD))

LOD_merged <- tibble(chemical = names(hourly_nona_bgrm_zerorepl_norm)) %>%
  left_join(LOD_merged)

## Joining with `by = join_by(chemical)`

# creating uncertainty Matrix
for (i in 1:number_row) {
  for (j in 1:number_column) {
    xij <- normalized_matrix[i, j]
    LOD <- LOD_merged$LOD[[j]]
    # Get LOD value for this row
    if (j == 1) {
      # based on equation 6, we sqrt ch4 (at column = 1) and times by 1

```

```

    weight_matrix[i, j] <- sqrt(xij)
  } else if (j == 2) {
    # 0.25 for co2
    weight_matrix[i, j] <- 0.25 * sqrt(xij)
  } else if (j == 3) {
    # 0.5 for CO
    weight_matrix[i, j] <- 0.5 * sqrt(xij)
  } else if (xij <= LOD) {
    weight_matrix[i, j] <- 2 * LOD # equation 5a) in reference paper
  } else {
    weight_matrix[i, j] <- sqrt(((0.1 * xij)**2 + LOD**2)) #equation 5c) in reference paper
  }
}
}

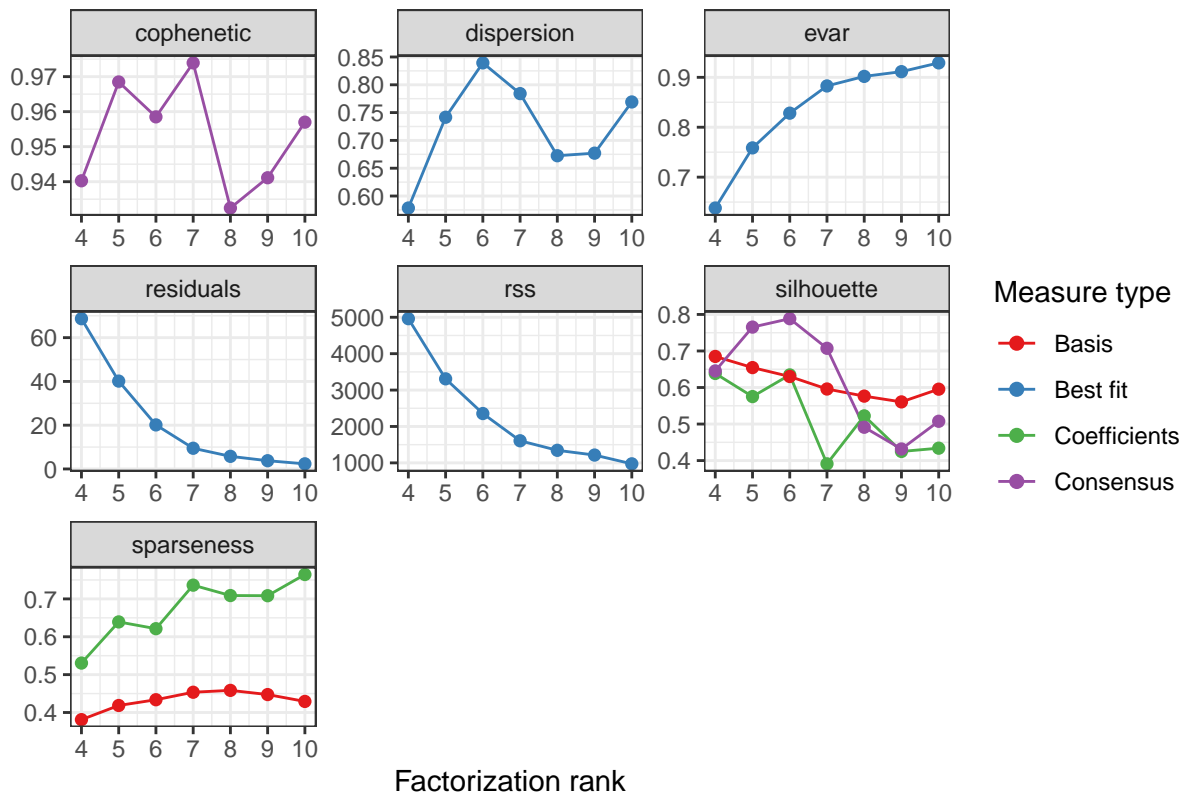
# set a seed for nmf
set.seed(123)
# #function below used to estimate the optimal rank and will be used in the nmf() function.
# # takes around 20-30 mins to run
# estimate_rank <- nmfEstimateRank(normalized_matrix, 4:10, method = "ls-nmf", weight = weight_matrix,
# # changing the range of rank to 2:20 from 4:20
# saveRDS(estimate_rank, 'estimate_rank.rds')

estimate_rank <- readRDS('estimate_rank.rds')
measures <- estimate_rank$measures
fit <- estimate_rank$fit
consensus <- estimate_rank$consensus

# plots the NMF rank survey
plot(estimate_rank)

```

NMF rank survey



```
# fitting the optimal rank based on the above plots
# the choice of the optimal rank needs to be discussed
output <- nmf(normalized_matrix, rank = 4, weight = weight_matrix, method = "ls-nmf")
W <- basis(output)
H <- coef(output)
```

Source contributions

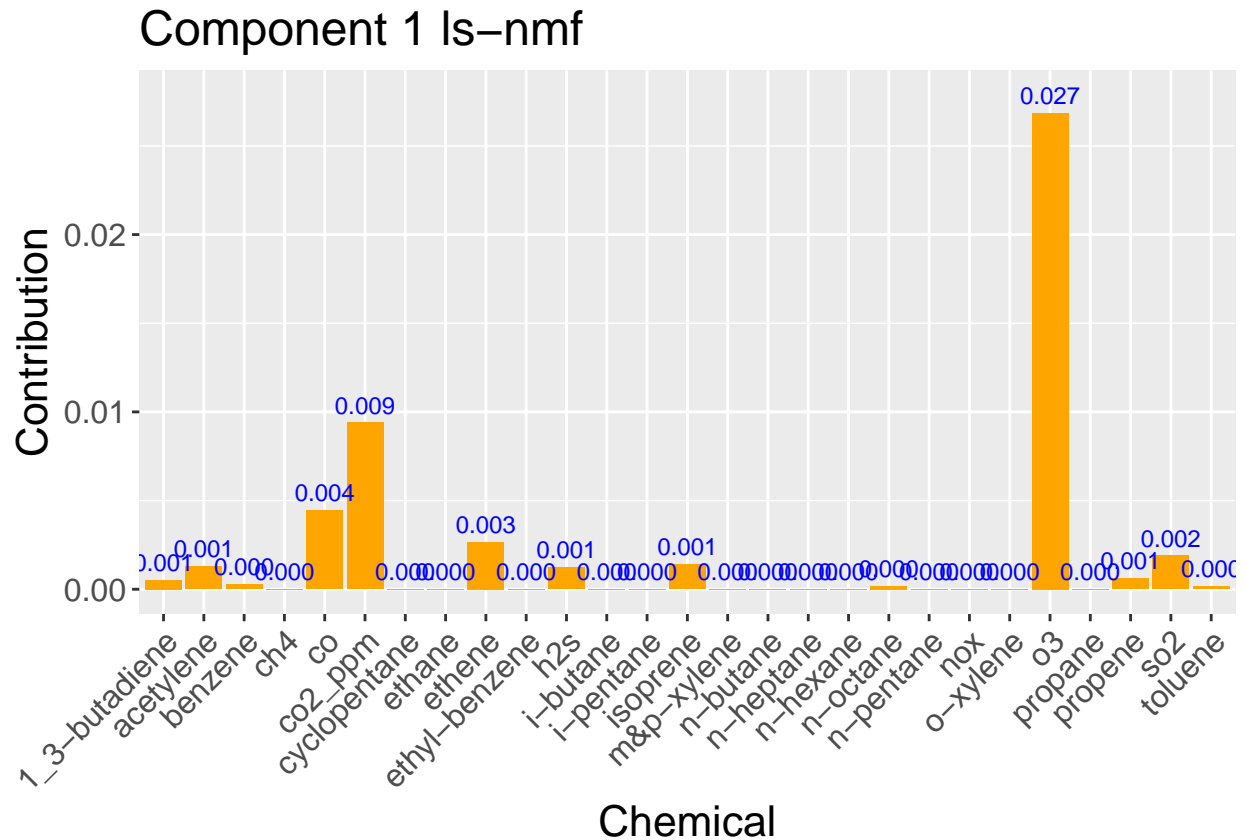
```
# Convert H to a data frame for ggplot
H_df <- as.data.frame(H)
# Add a column for component
H_df$Component <- names(as.data.frame(W))

# Reshape data to long format
H_long <- pivot_longer(H_df, cols = -Component, names_to = "Chemical", values_to = "Contribution")

NFM1 <- subset(H_long, Component == 'V1')
# Plot
nmfplt_1_ls <- ggplot(NFM1, aes(x = Chemical, y = Contribution)) +
  geom_bar(stat = "identity", position = "dodge", fill = "orange") +
  theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
  geom_text(aes(label = sprintf("%.3f", Contribution)), color = "blue", size = 3, nudge_y = 0.001) +
  labs(x = "Chemical", y = "Contribution", title = "Component 1 ls-nmf") +
  theme(
    text = element_text(size = 14), # Base text size for all text elements
    axis.title = element_text(size = 16), # Size of axis titles
```

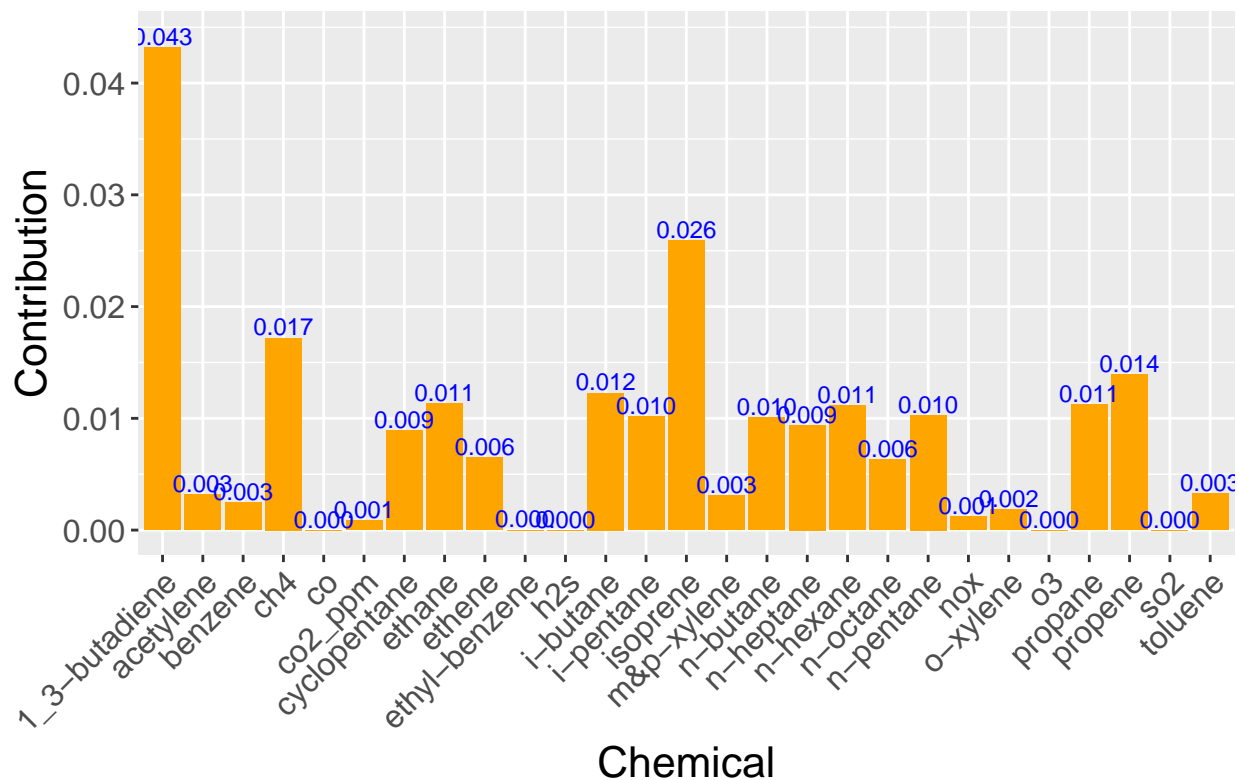


```
axis.text = element_text(size = 12), # Size of axis text (tick labels)
plot.title = element_text(size = 18) # Size of the plot title
)
nmfplt_1_ls
```



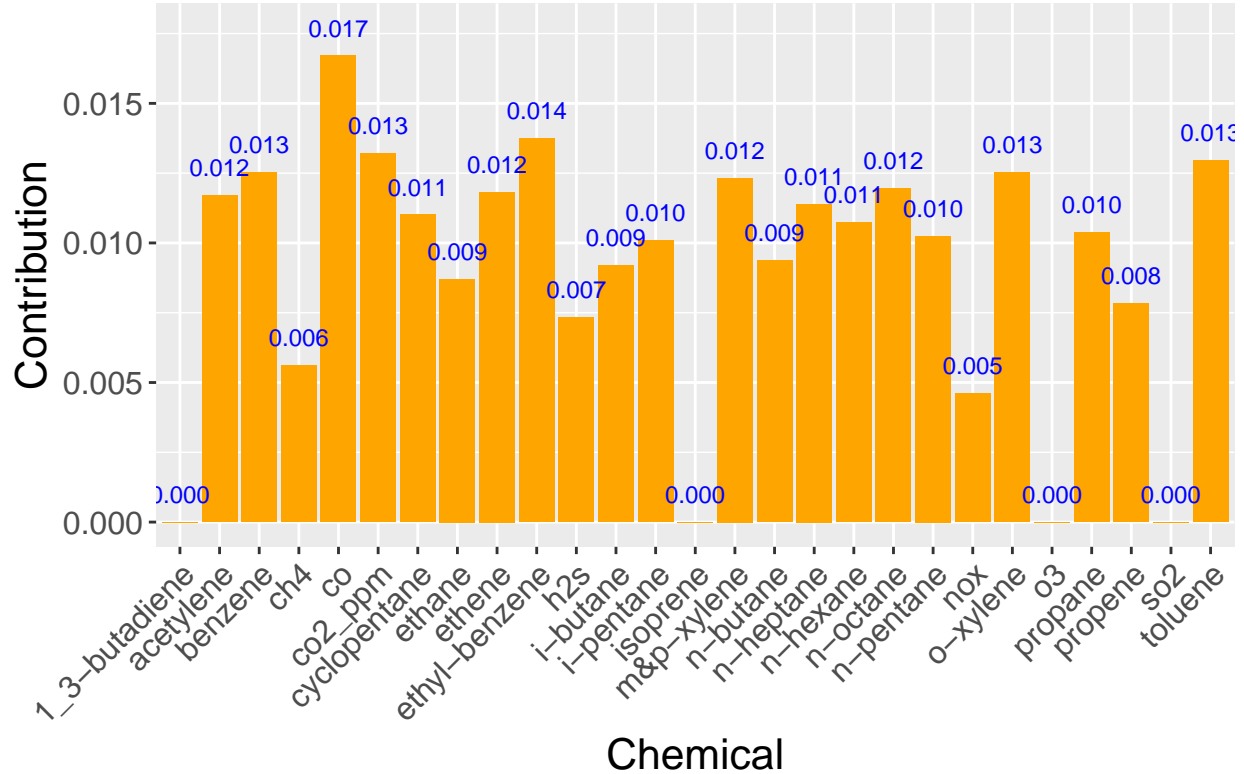
```
NFM2 <- subset(H_long, Component == 'V2')
# Plot
nmfplt_2_ls <- ggplot(NFM2, aes(x = Chemical, y = Contribution)) +
  geom_bar(stat = "identity", position = "dodge", fill = "orange") +
  theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
  geom_text(aes(label = sprintf("%.3f", Contribution)), color = "blue", size = 3, nudge_y = 0.001) +
  labs(x = "Chemical", y = "Contribution", title = "Component 2 ls-nmf")+
  theme(
    text = element_text(size = 14), # Base text size for all text elements
    axis.title = element_text(size = 16), # Size of axis titles
    axis.text = element_text(size = 12), # Size of axis text (tick labels)
    plot.title = element_text(size = 18) # Size of the plot title
  )
nmfplt_2_ls
```

Component 2 ls-nmf



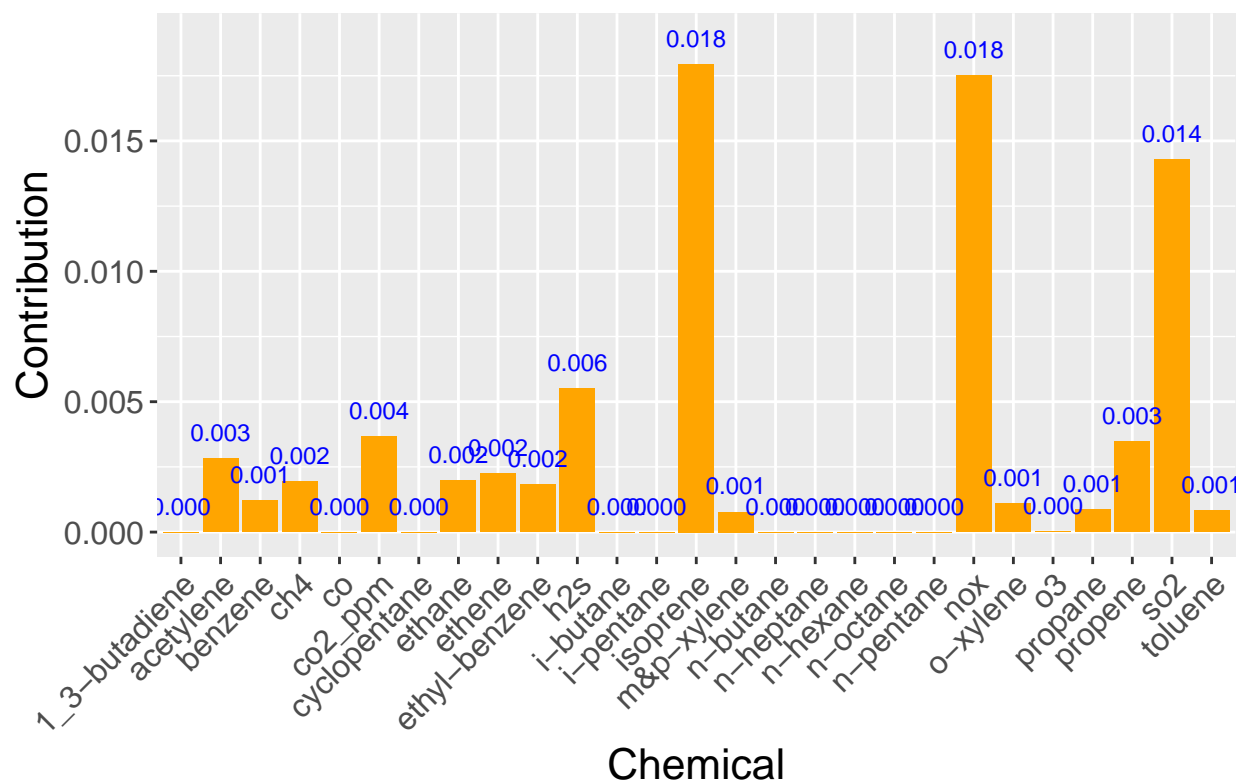
```
NFM3 <- subset(H_long, Component == 'V3')
# Plot
nmfplt_3_ls <- ggplot(NFM3, aes(x = Chemical, y = Contribution)) +
  geom_bar(stat = "identity", position = "dodge", fill = "orange") +
  theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
  geom_text(aes(label = sprintf("%.3f", Contribution)), color = "blue", size = 3, nudge_y = 0.001) +
  labs(x = "Chemical", y = "Contribution", title = "Component 3 ls-nmf") +
  theme(
    text = element_text(size = 14), # Base text size for all text elements
    axis.title = element_text(size = 16), # Size of axis titles
    axis.text = element_text(size = 12), # Size of axis text (tick labels)
    plot.title = element_text(size = 18) # Size of the plot title
  )
nmfplt_3_ls
```

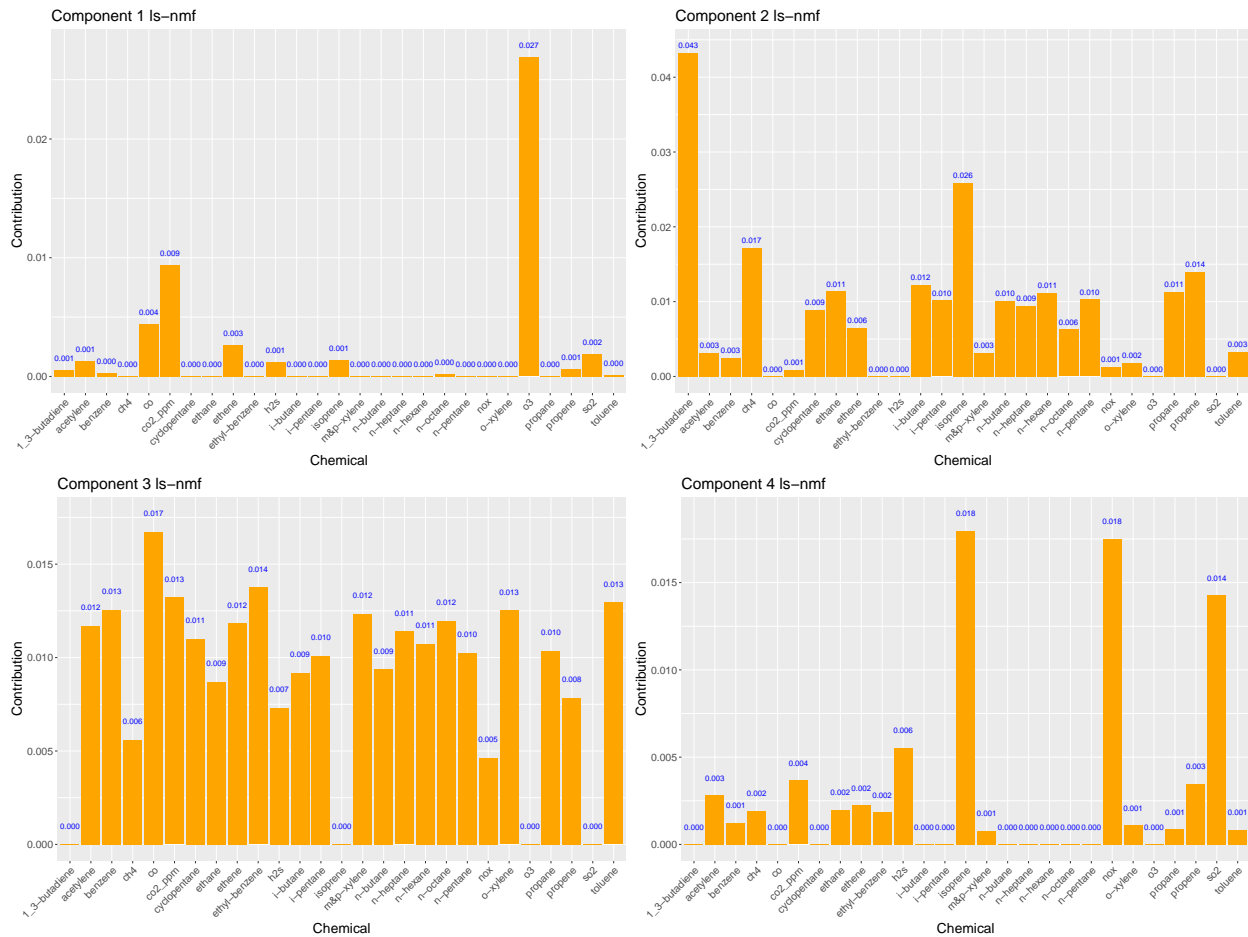
Component 3 ls-nmf



```
NFM4 <- subset(H_long, Component == 'V4')
# Plot
nmfplt_4_ls <- ggplot(NFM4, aes(x = Chemical, y = Contribution)) +
  geom_bar(stat = "identity", position = "dodge", fill = "orange") +
  theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
  geom_text(aes(label = sprintf("%.3f", Contribution)), color = "blue", size = 3, nudge_y = 0.001) +
  labs(x = "Chemical", y = "Contribution", title = "Component 4 ls-nmf") +
  theme(
    text = element_text(size = 14), # Base text size for all text elements
    axis.title = element_text(size = 16), # Size of axis titles
    axis.text = element_text(size = 12), # Size of axis text (tick labels)
    plot.title = element_text(size = 18) # Size of the plot title
  )
nmfplt_4_ls
```

Component 4 ls-nmf





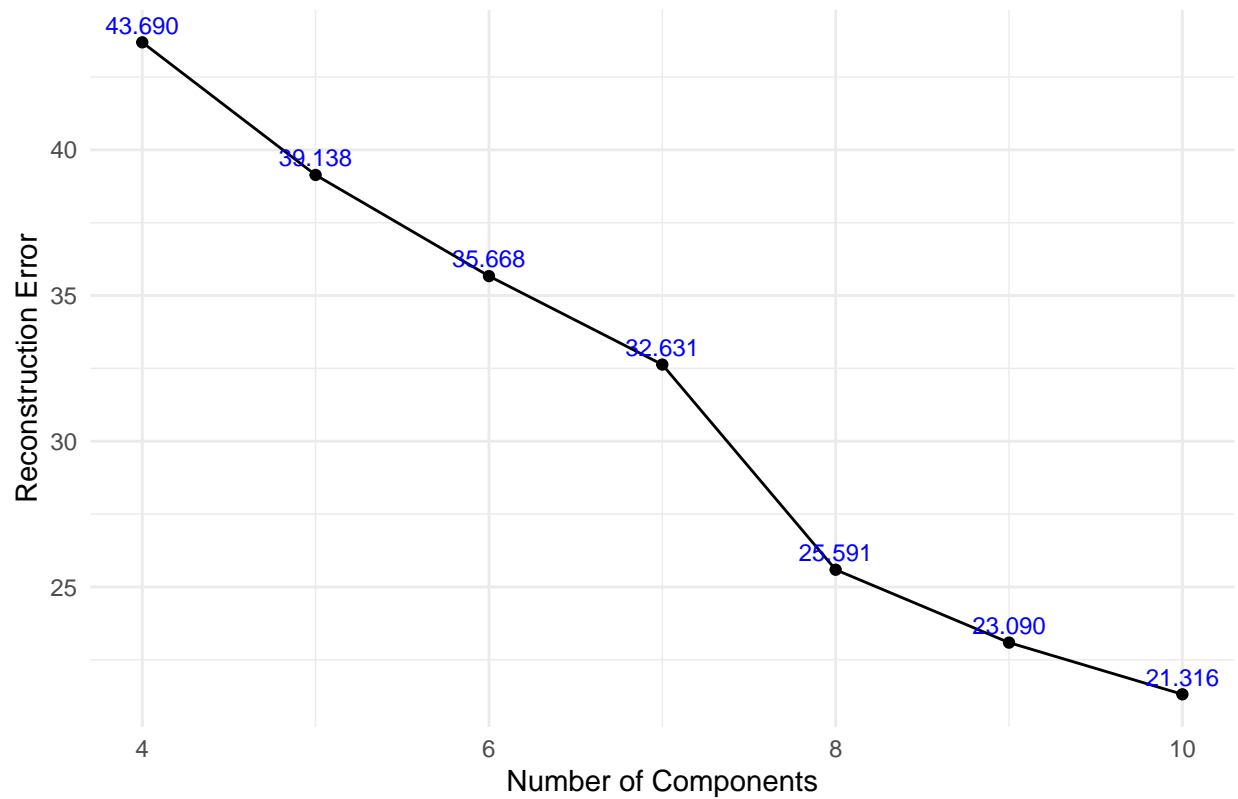
NMF - Eva

```
# Try Eva's approach
components <- 4:10
errors <- numeric(length(components) - 4)

# Loop over the number of components
# for (n in components) {
#   nmf_result <- nmf(normalized_matrix, rank = n, method = "KL", seed='nndsvd')
#   reconstruction <- basis(nmf_result) %*% coef(nmf_result)
#   error <- norm(normalized_matrix - reconstruction, type = "F")
#   errors[n-3] <- error
#   print(paste0('Completed ', n - 3, ' out of 7'))
# }
#
# saveRDS(errors, 'errors_norm.rds')

errors <- readRDS('errors_norm.rds')
```

NMF Reconstruction Error vs. Number of Components



```
## [1] 43.69019
```

```
## Warning in sqrt(S[i] * termn) * uun: Recycling array of length 1 in array-vector arithmetic is deprecated.
## Use c() or as.vector() instead.
```

```
## Warning in sqrt(S[i] * termn) * vvn: Recycling array of length 1 in array-vector arithmetic is deprecated.
## Use c() or as.vector() instead.
```

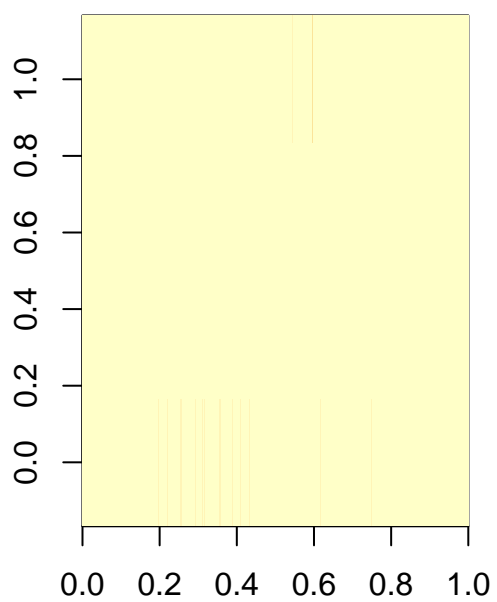
```
## Warning in sqrt(S[i] * termn) * uup: Recycling array of length 1 in array-vector arithmetic is deprecated.
## Use c() or as.vector() instead.
```

```
## Warning in sqrt(S[i] * termn) * vvp: Recycling array of length 1 in array-vector arithmetic is deprecated.
## Use c() or as.vector() instead.
```

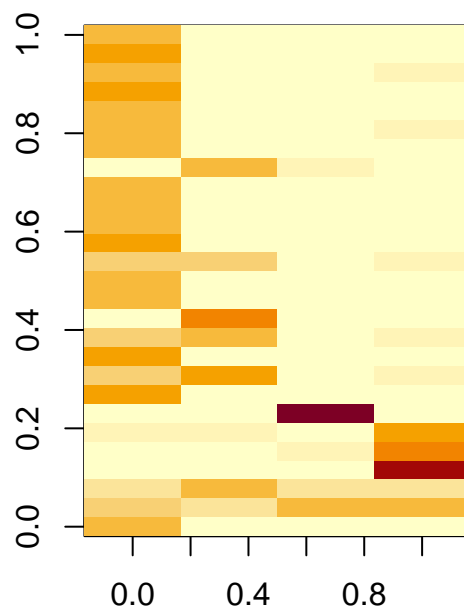
```
## Warning in sqrt(S[i] * termn) * uun: Recycling array of length 1 in array-vector arithmetic is deprecated.
## Use c() or as.vector() instead.
```

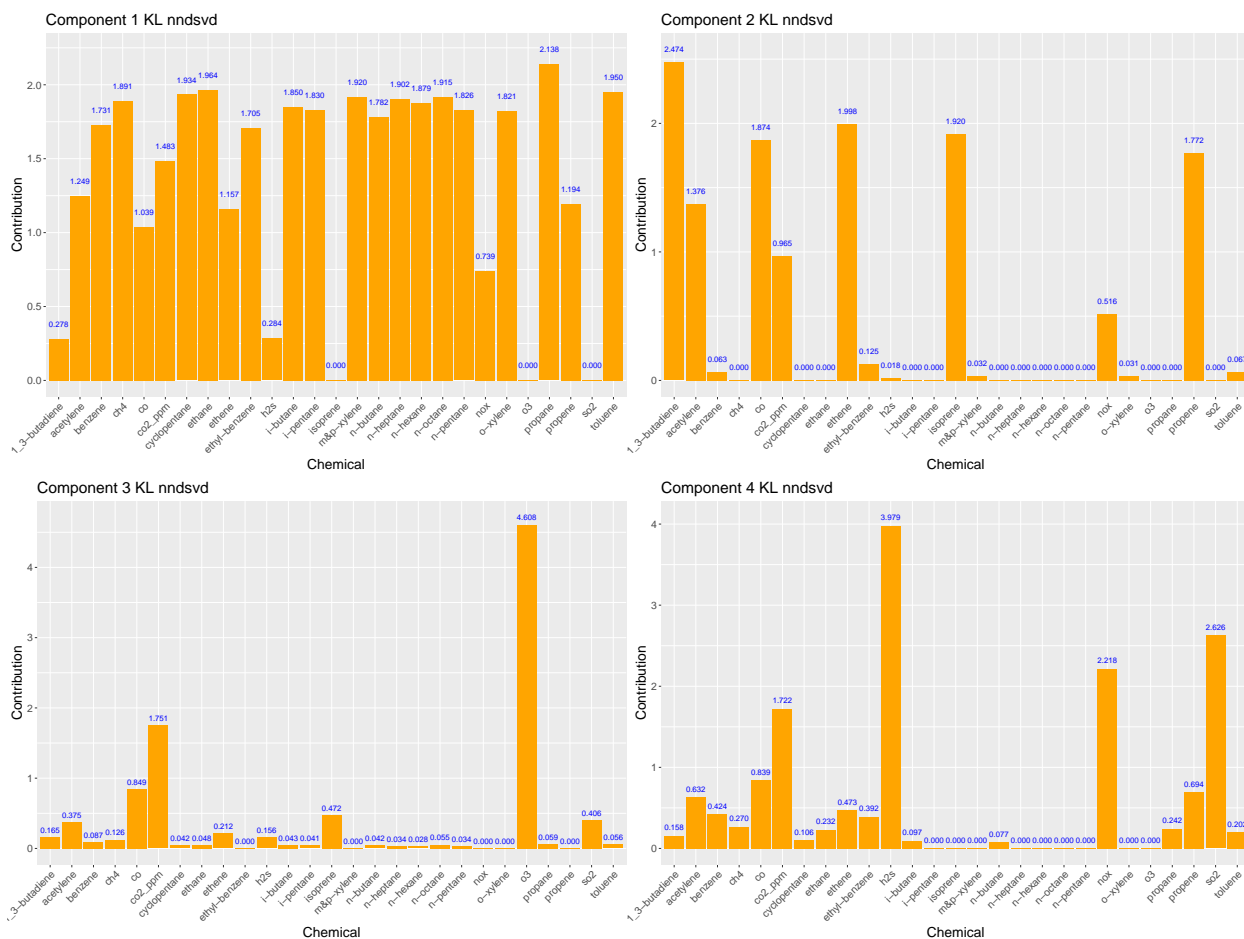
```
## Warning in sqrt(S[i] * termn) * vvn: Recycling array of length 1 in array-vector arithmetic is deprecated.
## Use c() or as.vector() instead.
```

Basis Matrix (W)

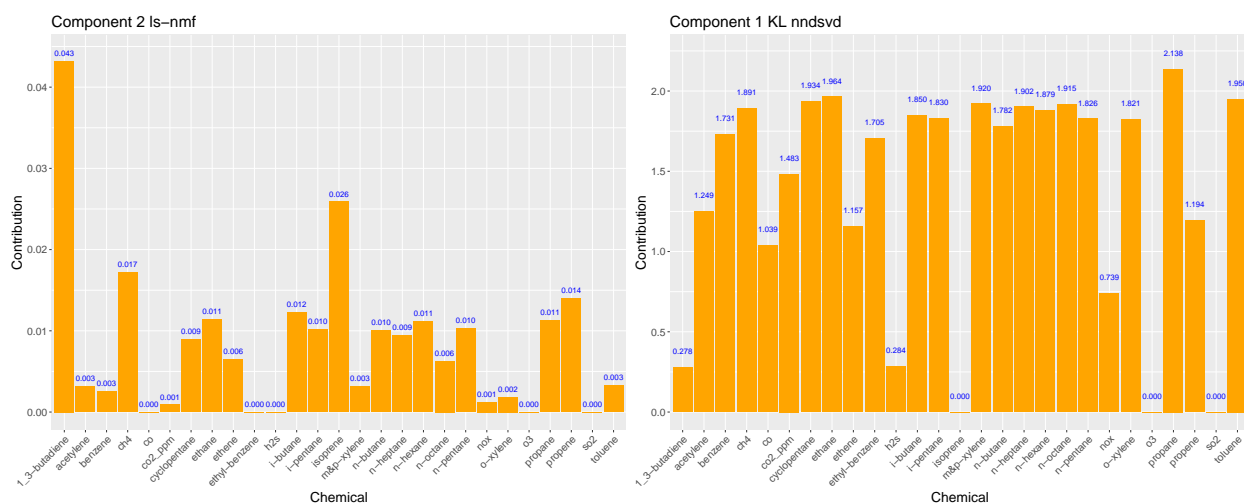


Coefficient Matrix (H)





```
grid.arrange(nmfplt_2_ls, nmfplt_1_svd, ncol = 2)
```



```
grid.arrange(nmfplt_1_ls, nmfplt_2_svd, ncol = 2)
```

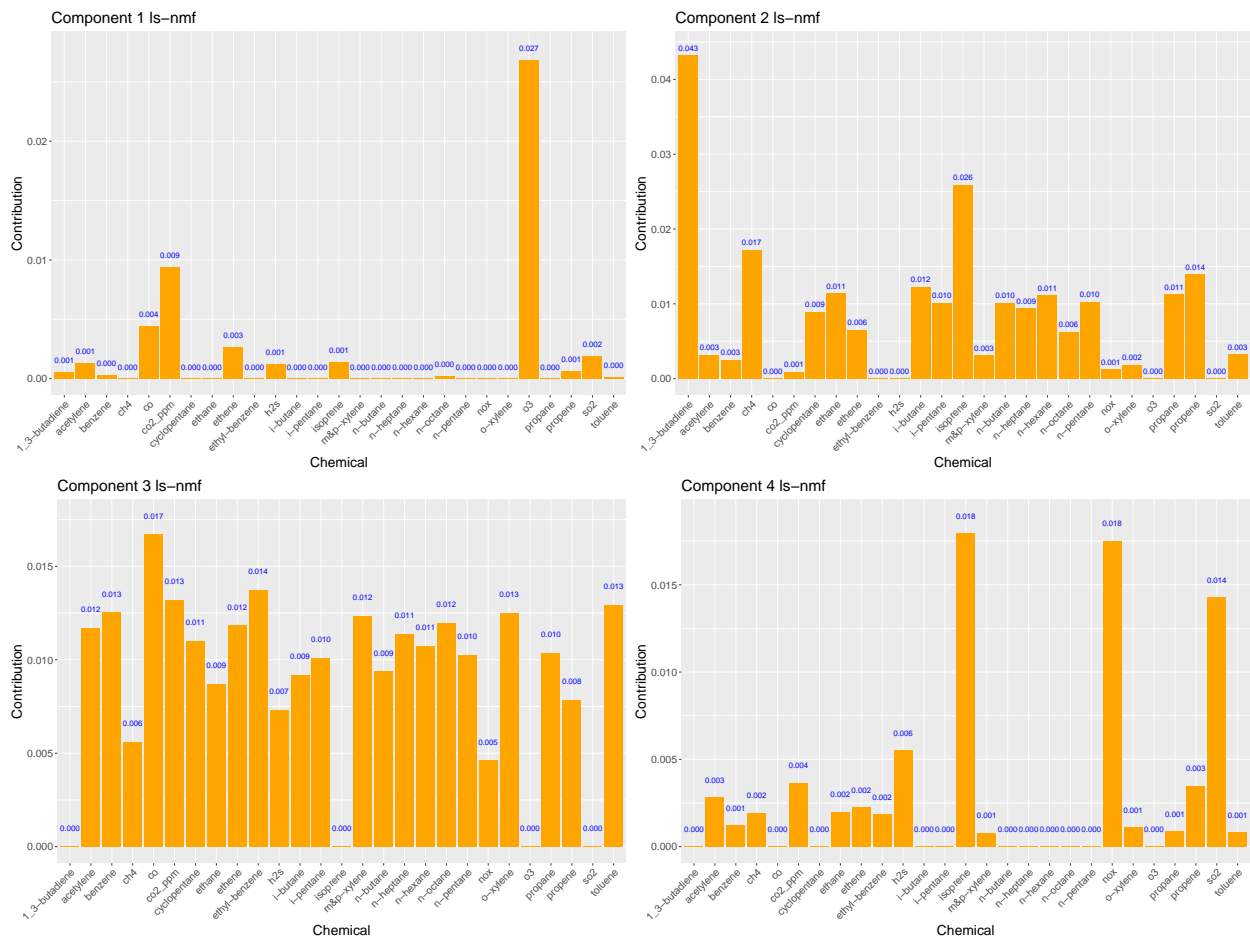
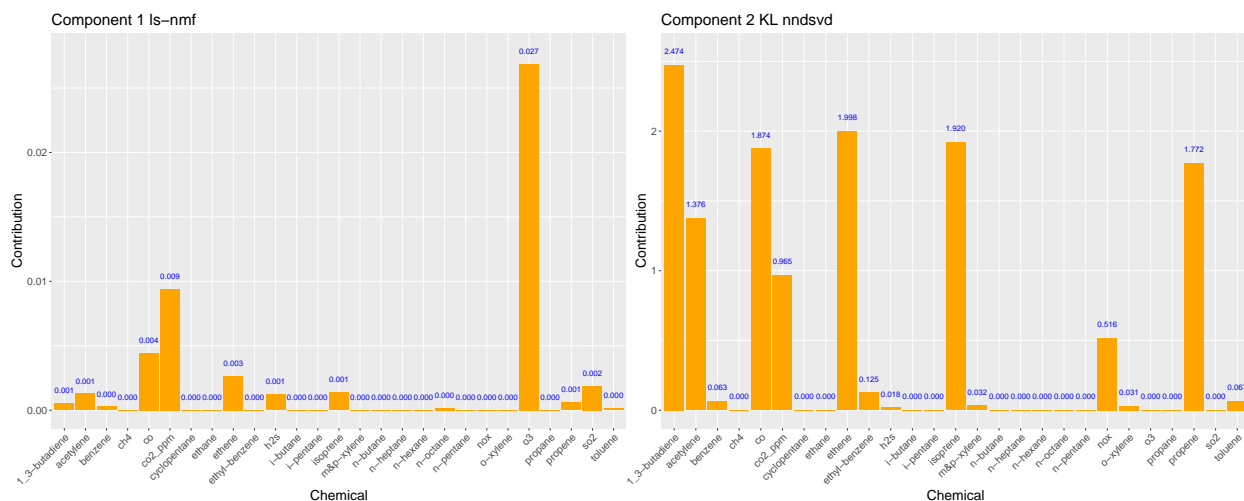
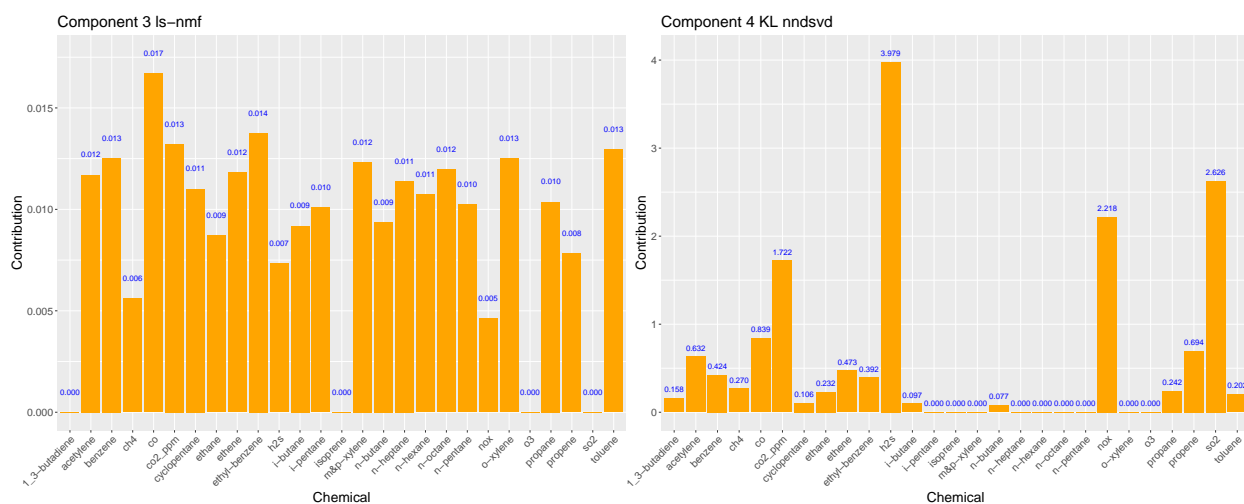



Figure 1: 1s-nmf



```
grid.arrange(nmfplt_3_ls, nmfplt_4_svd, ncol = 2)
```



```
grid.arrange(nmfplt_4_ls, nmfplt_3_svd, ncol = 2)
```

