Plots for Superconductor Dataset

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Plots for all **Superconductor Dataset** variables were additionally used for data analysis to select plots for the report and discover relationships and correlations.

(1) Distributions of the variables. Histograms of all variables show, that there no normally distributed variables in this data set and some have low variance.

(2) *critical_temp* vs variables, colored by *number_of_elements*. There are variables that can be stratified by *number_of_elements* and can be found using this set of graphs.

(3) Correlations in the groups of predictors.

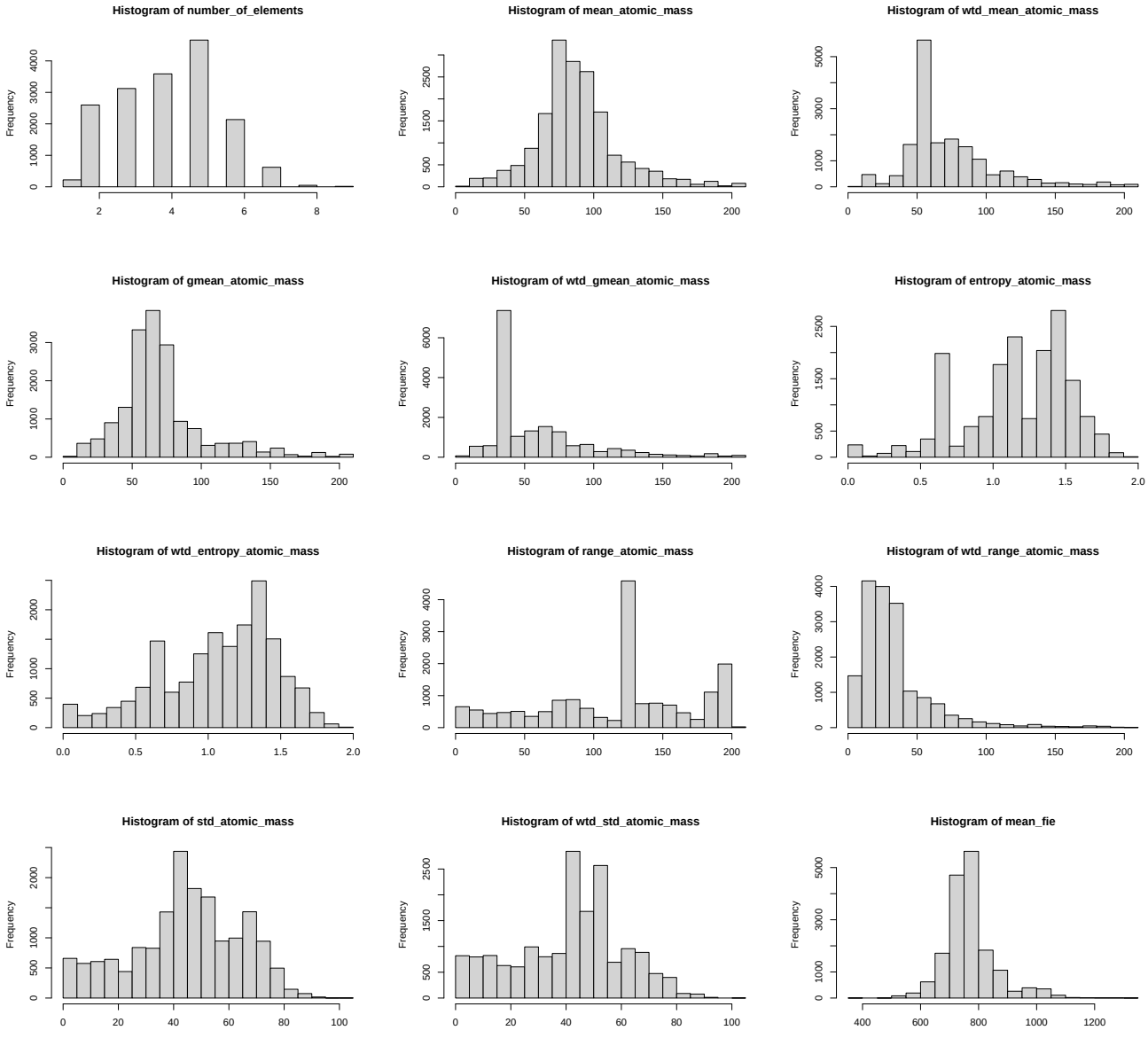
(4) Cluster heatmaps of feature groups also show that patterns can be found across all plots; some features are paired:
maen and *gmean*;
std and *wtd_std*;
entropy and *wtd_entropy*;
wtd_mean and *wtd_gmean.*
indicating similar predictors that were obtained using similar calculations.
Also *_Density* variables stand out in many cluster heatmaps, as well as "range_" features.

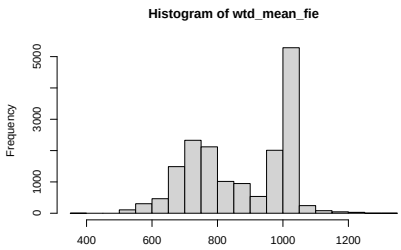
```
if(!require(tidyverse)) install.packages("tidyverse")
if(!require(readxl)) install.packages("readxl")
if(!require(ggplot2)) install.packages("ggplot2")
if(!require(caret)) install.packages("caret")
if(!require(tidyr)) install.packages("tidyr")
if(!require(reshape2)) install.packages("reshape2")
if(!require(tinytex)) install.packages("tinytex")
if(!require(dplyr)) install.packages("dplyr")
if(!require(stringr)) install.packages("stringr")
if(!require(RColorBrewer)) install.packages("RColorBrewer")
if(!require(matrixStats)) install.packages("matrixStats")
if(!require(tinytex)) install.packages("tinytex")
if(!require(knitr)) install.packages("knitr")
```

```
fileName <- "4_Superconductors.xlsx"
superconductors <- read_excel(fileName)
set.seed(1, sample.kind="Rounding") # if using R 3.5 or earlier, use `set.seed(1)`
index_val <- createDataPartition(y = superconductors$critical_temp,
                                 times = 1, p = 0.2, list = FALSE)
# sc set, that does not have validation set rows.
sc <- superconductors[-index_val, ]
# 25%  of sc set is used for Critical_temp-vs-variables plots.
sc_small <- slice_sample(sc, prop = 0.25)
```

(1) Distributions of all variables in Superconductivty data set.

```
cols <- 1:82
plot_histogram_function <- sapply(cols, function(cols){
  df <- sc[cols] %>% as.matrix()
  plot <- hist(df,
               xlab=" ",
               main = paste("Histogram of",colnames(sc)[cols]))
  plot
})
```

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1000
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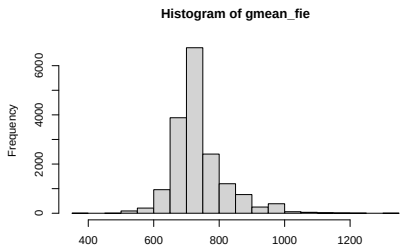
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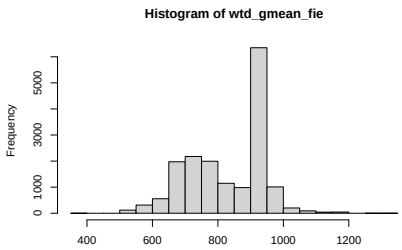
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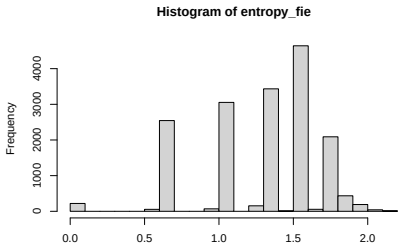
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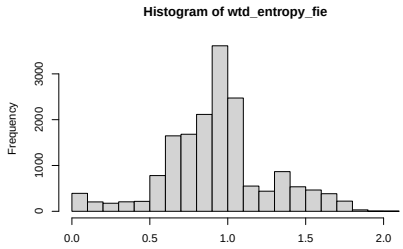
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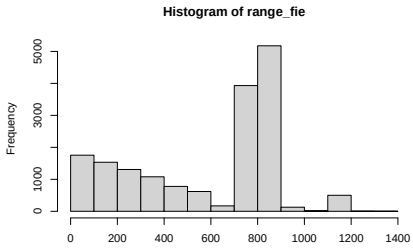
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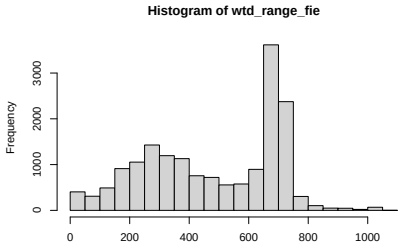
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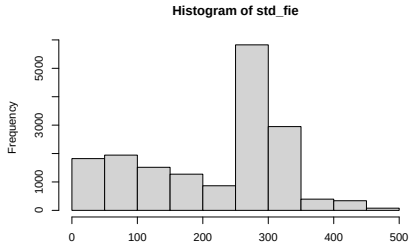
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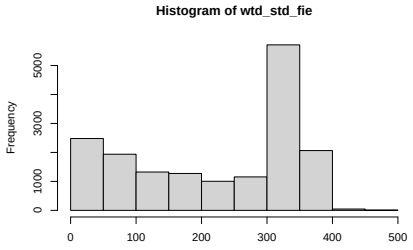
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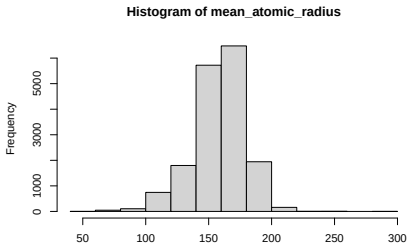
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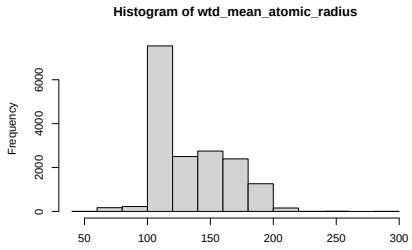
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Frequency
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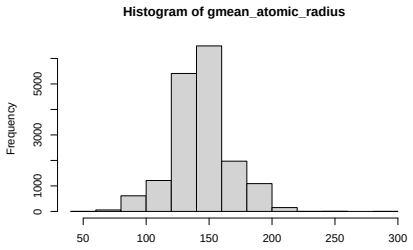
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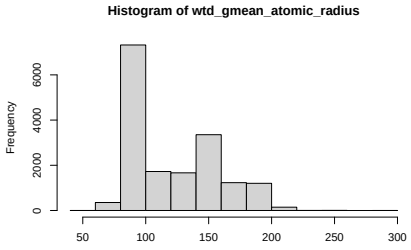
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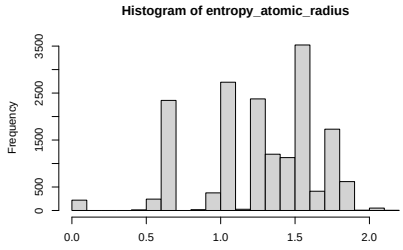
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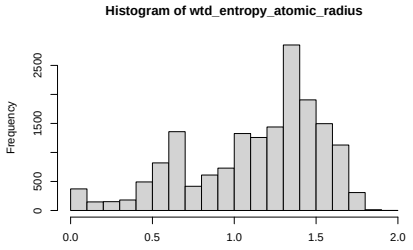
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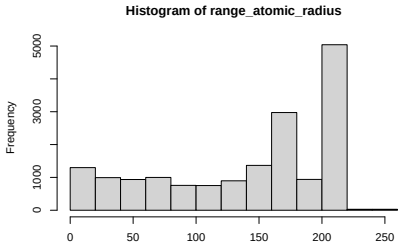
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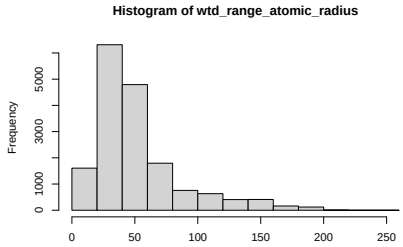
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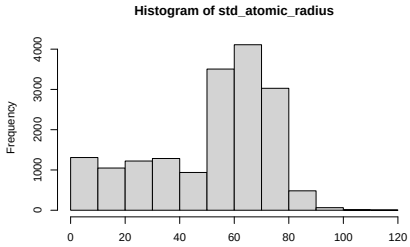
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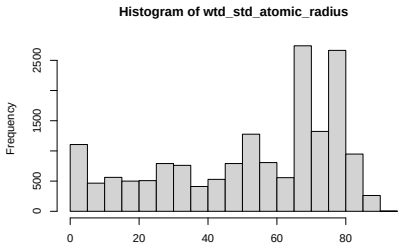
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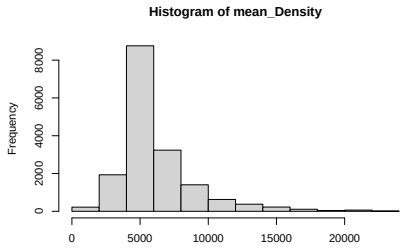
Histogram of mean_Density
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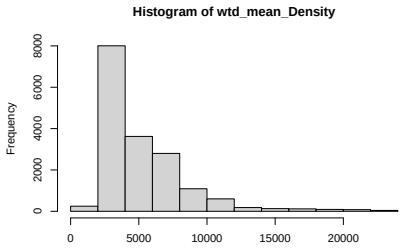
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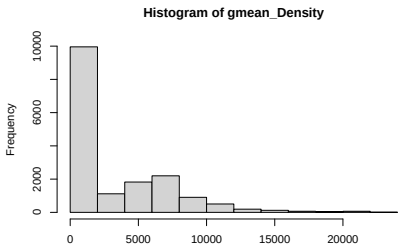
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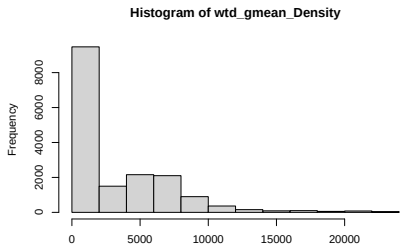
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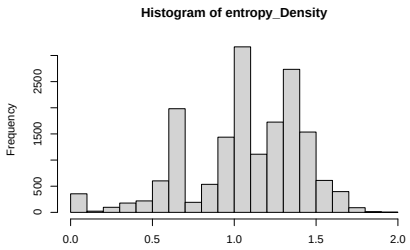
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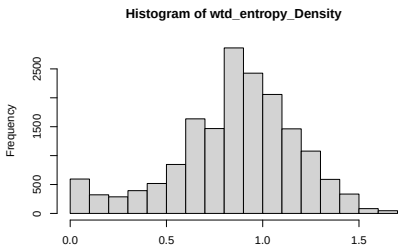
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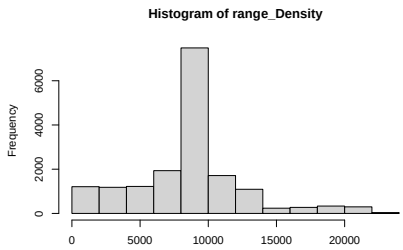
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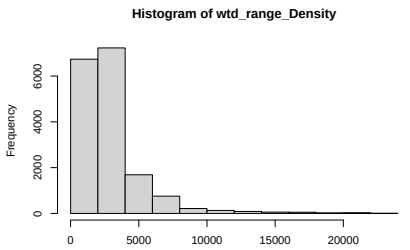
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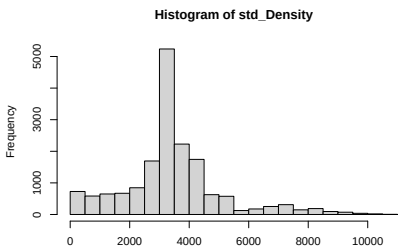
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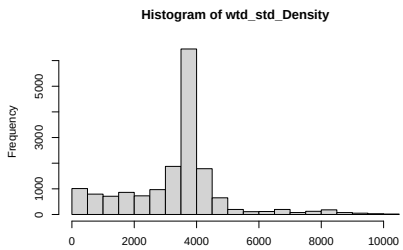
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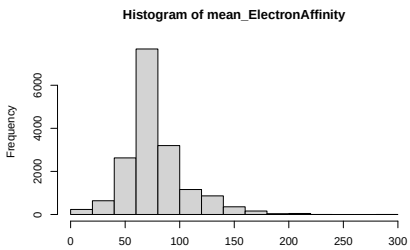
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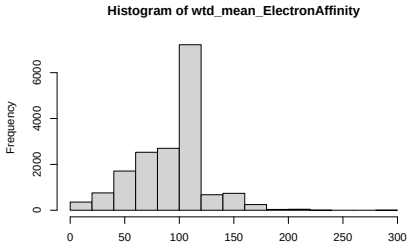
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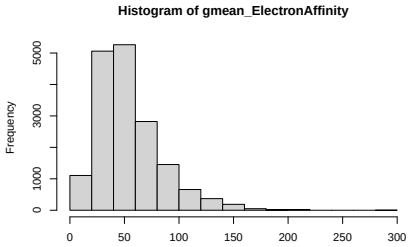
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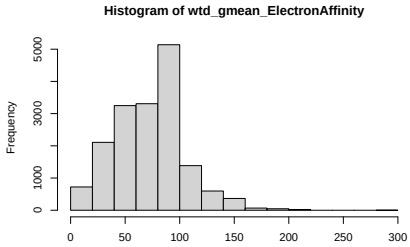
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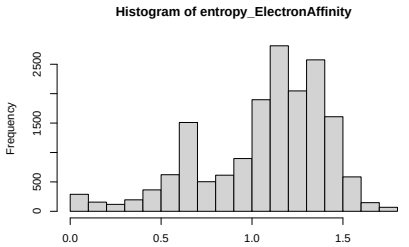
Histogram of entropy_ElectronAffinity
Frequency
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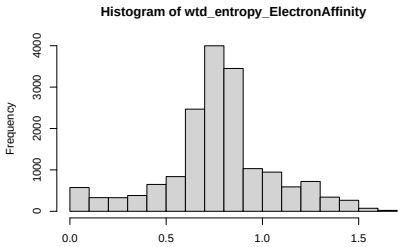
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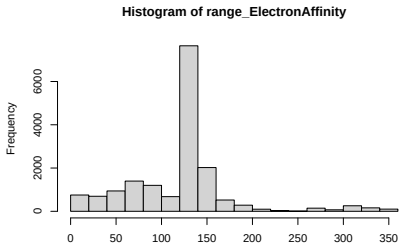
Histogram of range_ElectronAffinity
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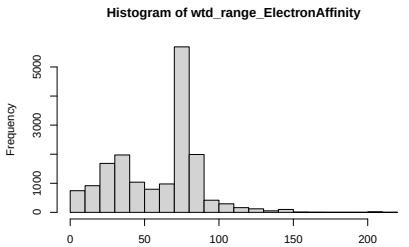
Histogram of wtd_range_ElectronAffinity
Frequency
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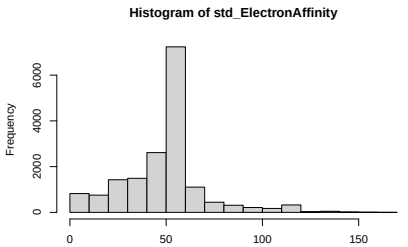
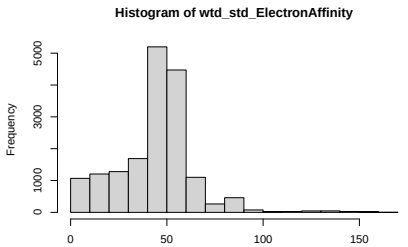
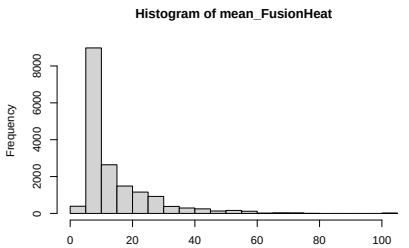
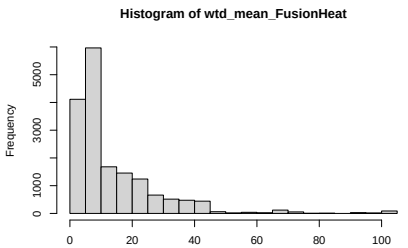
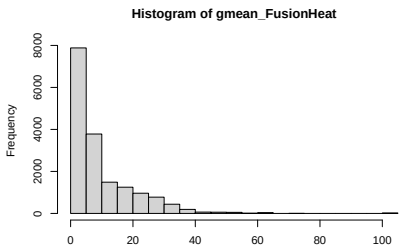
150
200

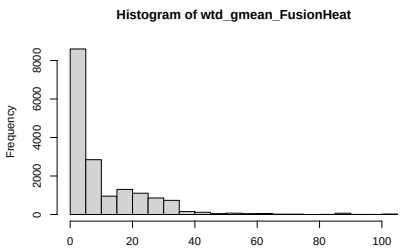

Histogram of std_ElectronAffinity
Frequency
0
2000
4000
6000
0
50
100
150

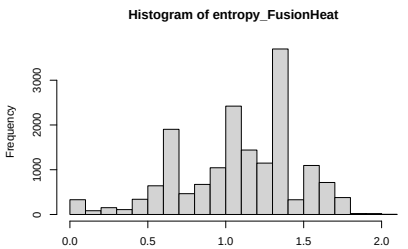

Histogram of wtd_std_ElectronAffinity
Frequency
0
1000
3000
5000
0
50
100
150

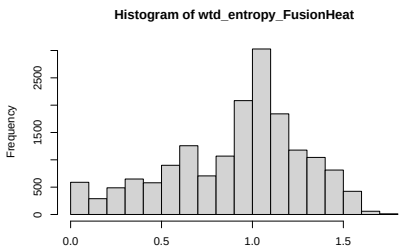

Histogram of mean_FusionHeat
Frequency
0
2000
4000
6000
8000
0
20
40
60
80
100

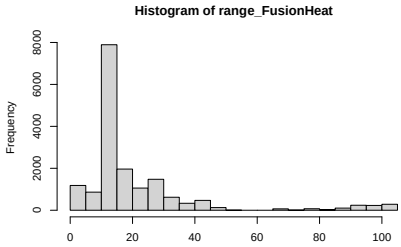

Histogram of wtd_mean_FusionHeat
Frequency
0
1000
3000
5000
0
20
40
60
80
100

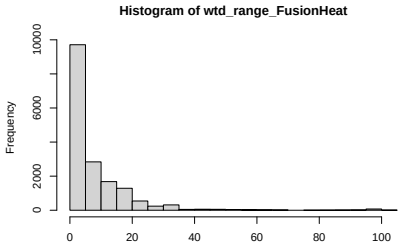

Histogram of gmean_FusionHeat
Frequency
0
2000
4000
6000
8000
0
20
40
60
80
100

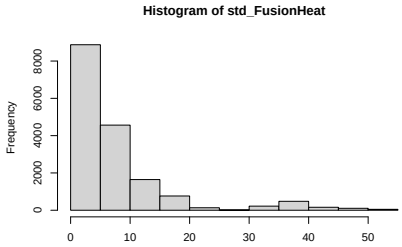

Histogram of wtd_gmean_FusionHeat
Frequency
0
2000
4000
6000
8000
0
20
40
60
80
100

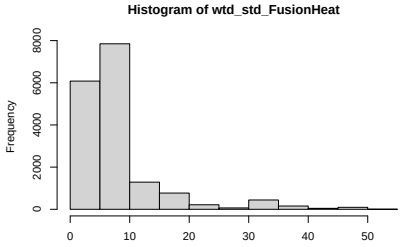

Histogram of entropy_FusionHeat
Frequency
0
1000
2000
3000
0.0
0.5
1.0
1.5
2.0

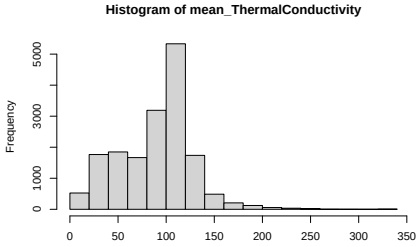

Histogram of wtd_entropy_FusionHeat
Frequency
0
500
1500
2500
0.0
0.5
1.0
1.5

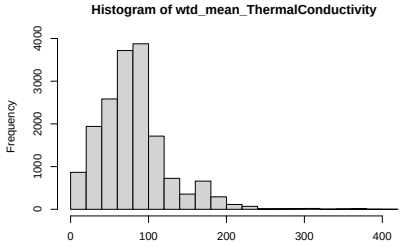

Histogram of range_FusionHeat
Frequency
0 2000 4000 6000 8000
0 20 40 60 80 100

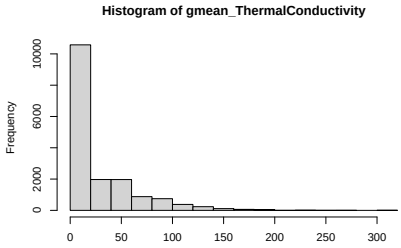

Histogram of wtd_range_FusionHeat
Frequency
0 2000 6000 10000
0 20 40 60 80 100

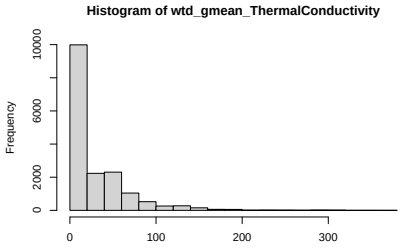

Histogram of std_FusionHeat
Frequency
0 2000 4000 6000 8000
0 10 20 30 40 50

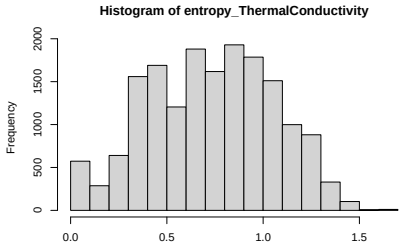

Histogram of wtd_std_FusionHeat
Frequency
0 2000 4000 6000 8000
0 10 20 30 40 50

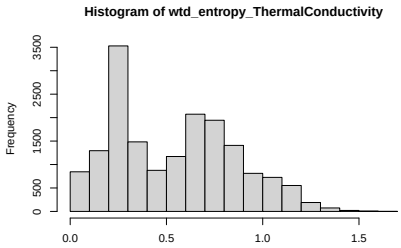

Histogram of mean_ThermalConductivity
Frequency
0 1000 3000 5000
0 50 100 150 200 250 300 350

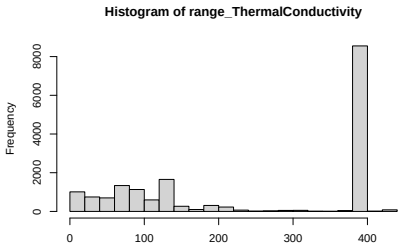

Histogram of wtd_mean_ThermalConductivity
Frequency
0 1000 2000 3000 4000
0 100 200 300 400

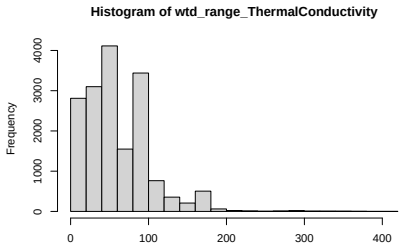

Histogram of gmean_ThermalConductivity
Frequency
0 2000 6000 10000
0 50 100 150 200 250 300

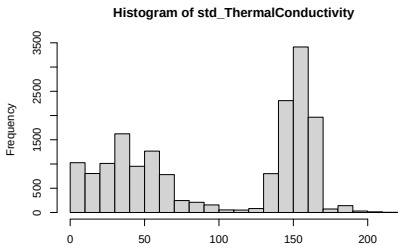

Histogram of wtd_gmean_ThermalConductivity
Frequency
0 2000 6000 10000
0 100 200 300

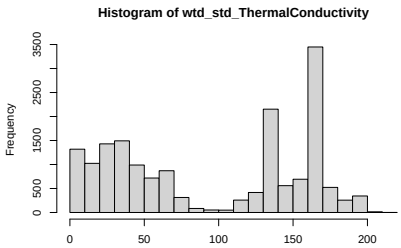

Histogram of entropy_ThermalConductivity
Frequency
0 500 1000 1500 2000
0.0 0.5 1.0 1.5

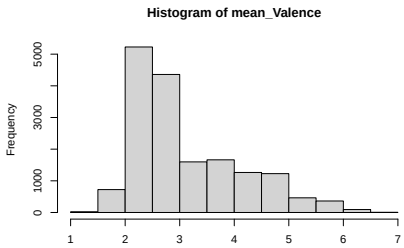

Histogram of wtd_entropy_ThermalConductivity
Frequency
0 500 1500 2500 3500
0.0 0.5 1.0 1.5

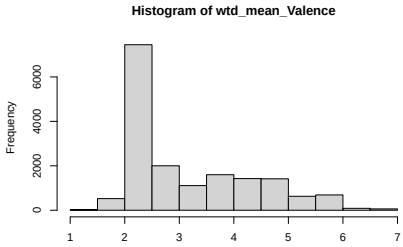

Histogram of range_ThermalConductivity
Frequency
0 2000 4000 6000 8000
0 100 200 300 400

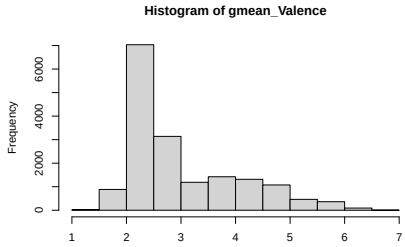

Histogram of wtd_range_ThermalConductivity
Frequency
0 1000 2000 3000 4000
0 100 200 300 400

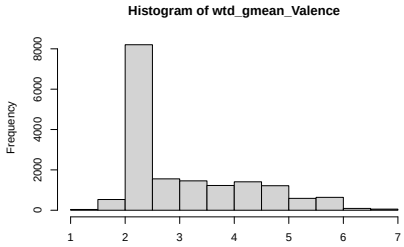

Histogram of std_ThermalConductivity
Frequency
0 500 1500 2500 3500
0 50 100 150 200

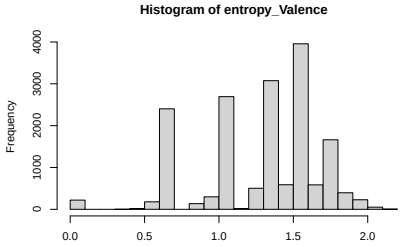

Histogram of wtd_std_ThermalConductivity
Frequency
0 500 1500 2500 3500
0 50 100 150 200

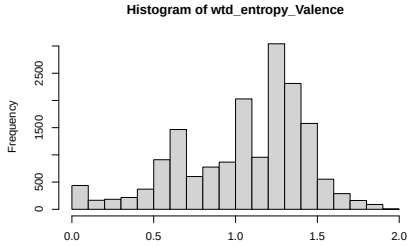

Histogram of mean_Valence
Frequency
0 1000 3000 5000
1 2 3 4 5 6 7

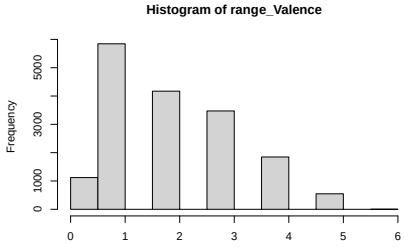

Histogram of wtd_mean_Valence
Frequency
0
2000
4000
6000
1
2
3
4
5
6
7

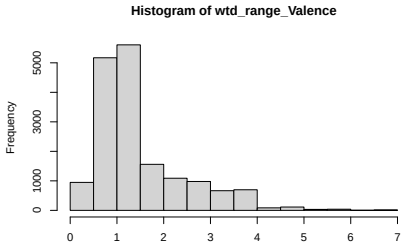

Histogram of gmean_Valence
Frequency
0
2000
4000
6000
1
2
3
4
5
6
7

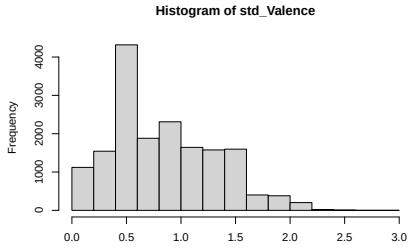

Histogram of wtd_gmean_Valence
Frequency
0
2000
4000
6000
8000
1
2
3
4
5
6
7

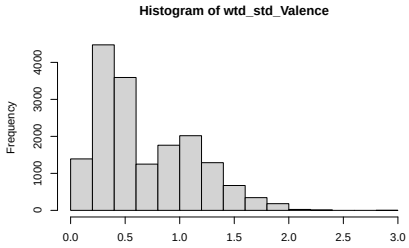

Histogram of entropy_Valence
Frequency
0
1000
2000
3000
4000
0.0
0.5
1.0
1.5
2.0

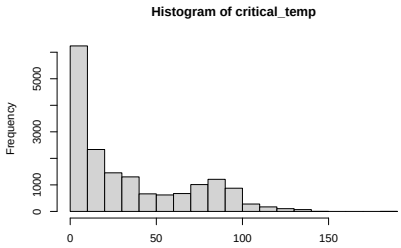

Histogram of wtd_entropy_Valence
Frequency
0
500
1500
2500
0.0
0.5
1.0
1.5
2.0


Histogram of range_Valence
Frequency
0
1000
3000
5000
0
1
2
3
4
5
6


Histogram of wtd_range_Valence
Frequency
0
1000
3000
5000
0
1
2
3
4
5
6
7

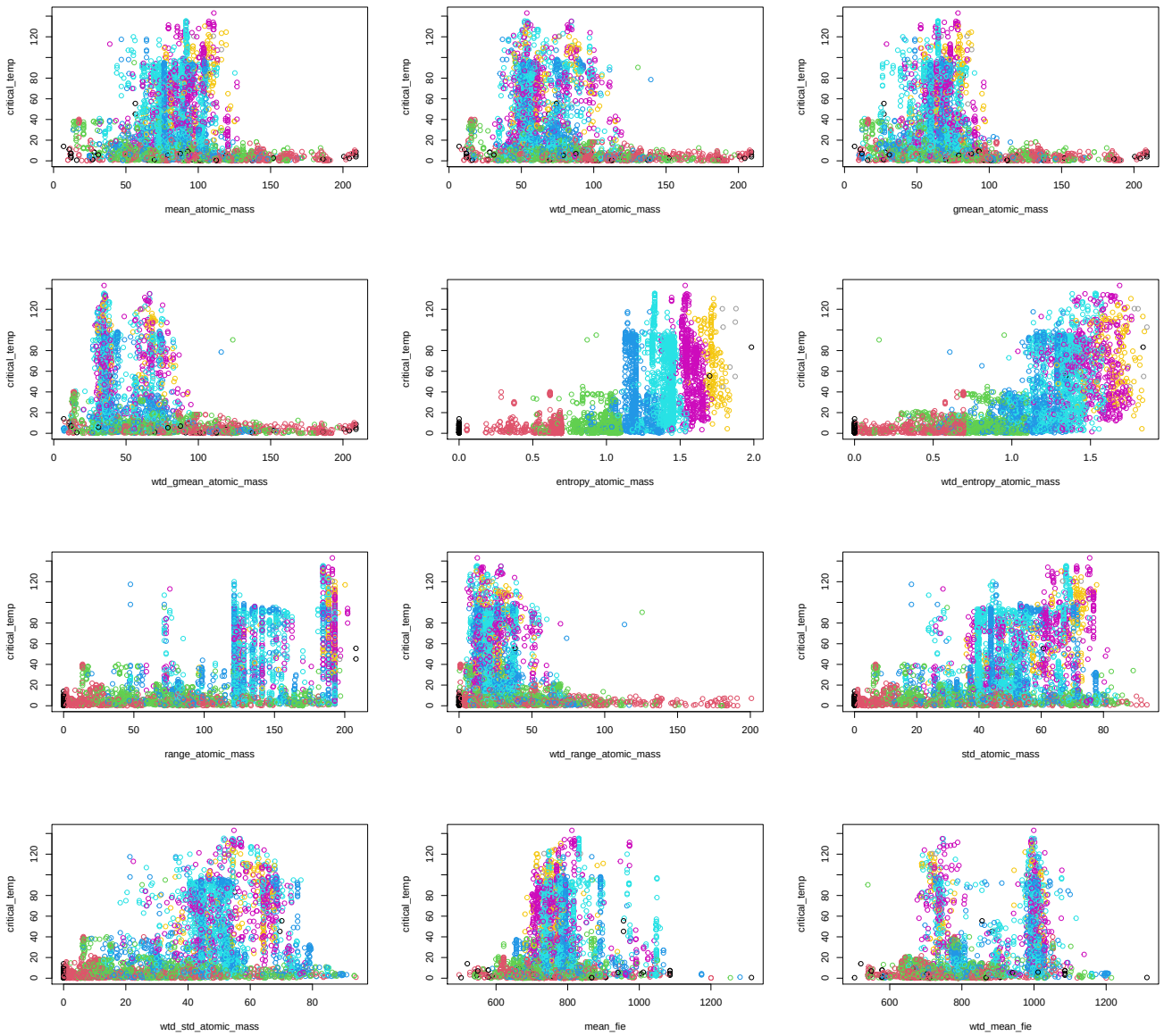

Histogram of std_Valence
Frequency
0
1000
2000
3000
4000
0.0
0.5
1.0
1.5
2.0
2.5
3.0

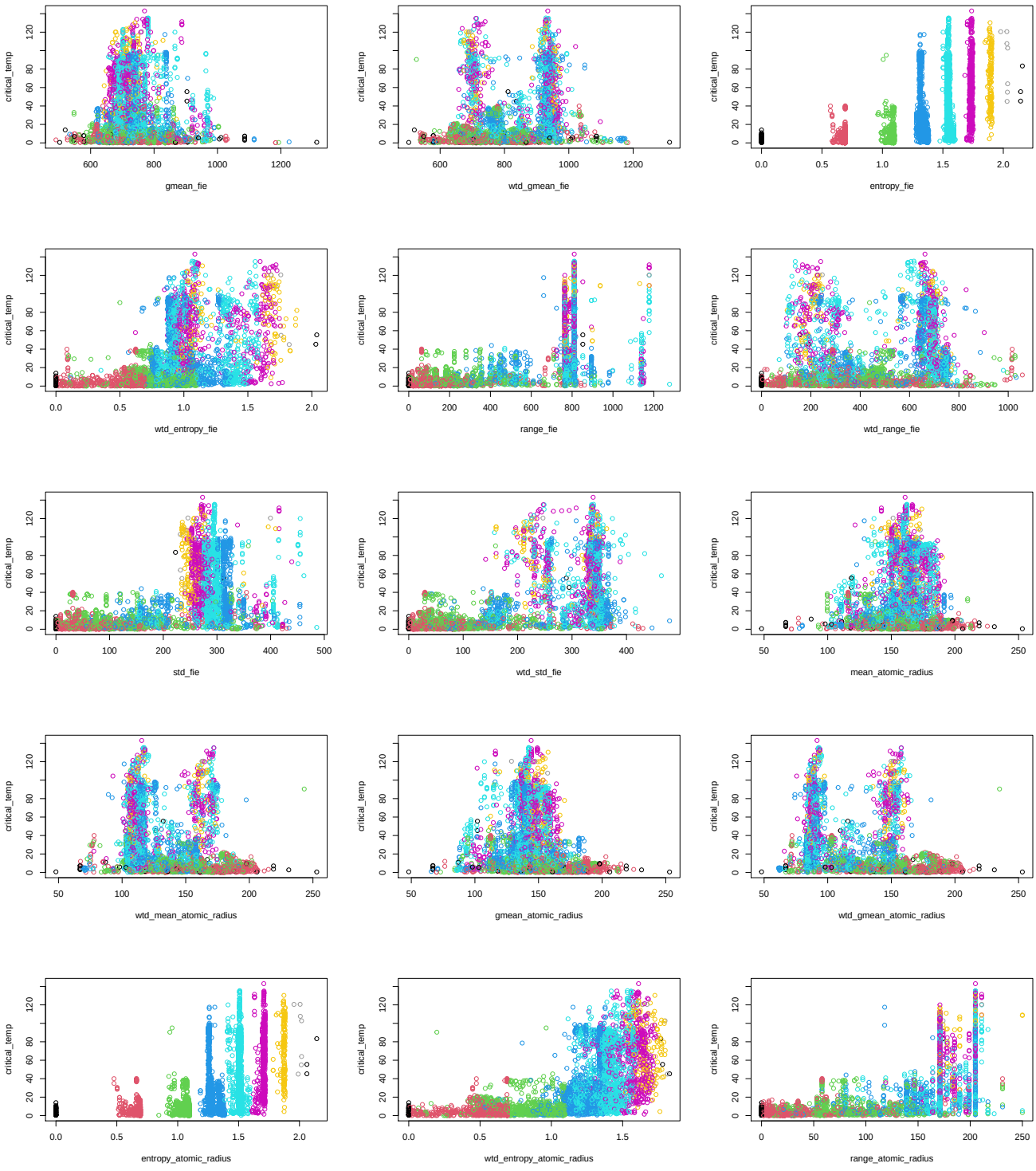

Histogram of wtd_std_Valence
Frequency
0
1000
2000
3000
4000
0.0
0.5
1.0
1.5
2.0
2.5
3.0

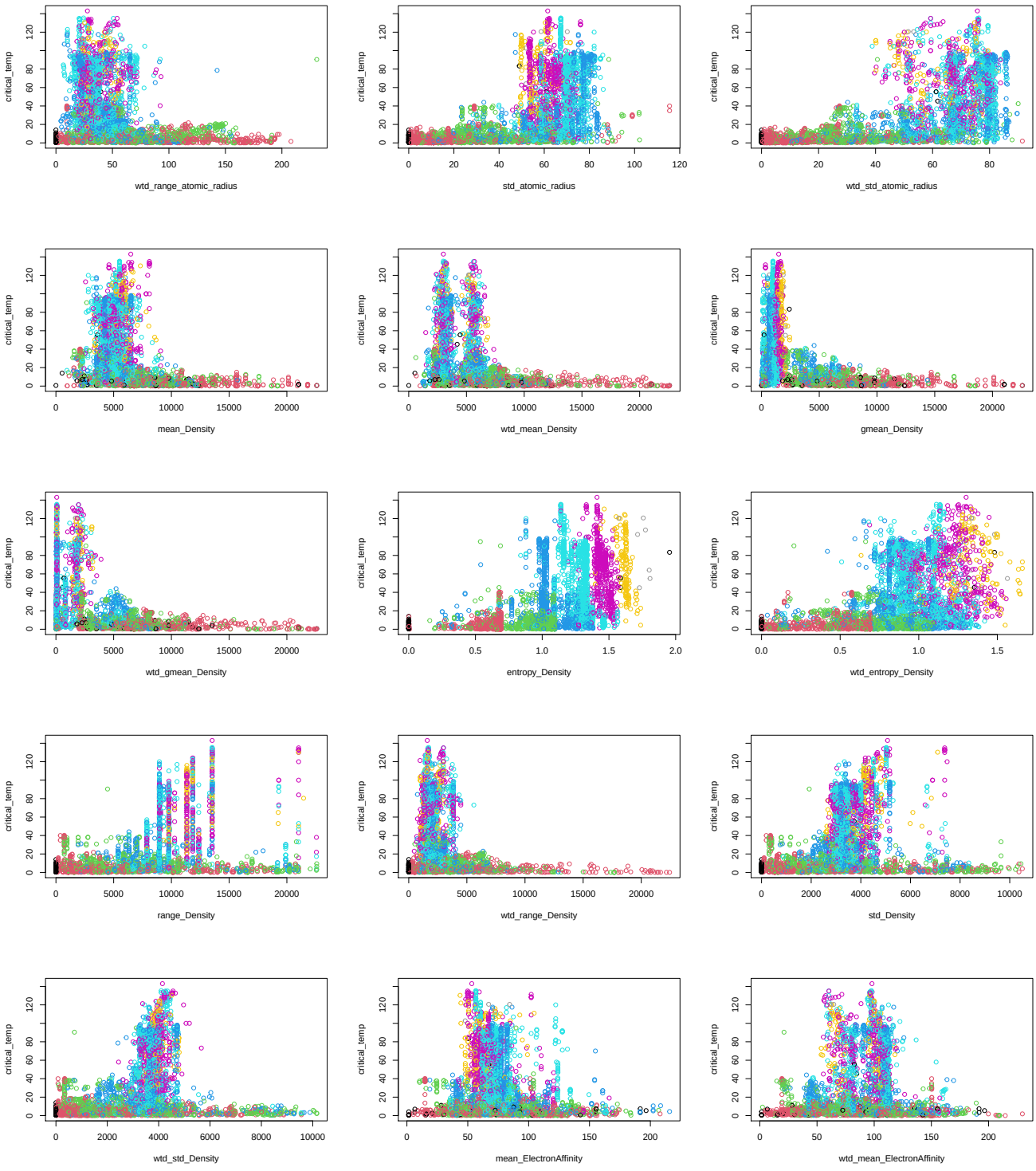

Histogram of critical_temp
Frequency
0
1000
3000
5000
0
50
100
150

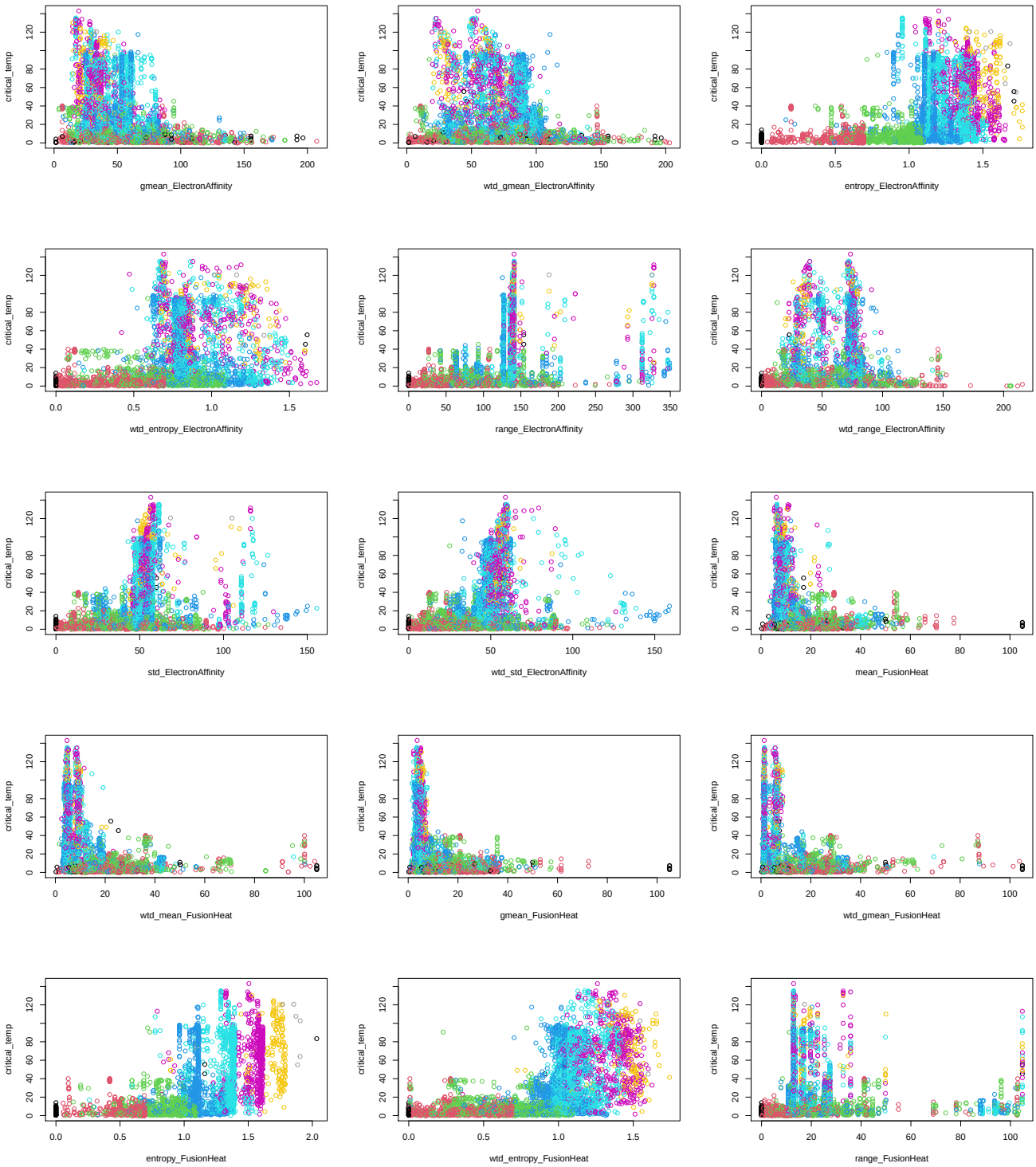
(2) Critical temperature vs variables, colored by *number_of_elements*.

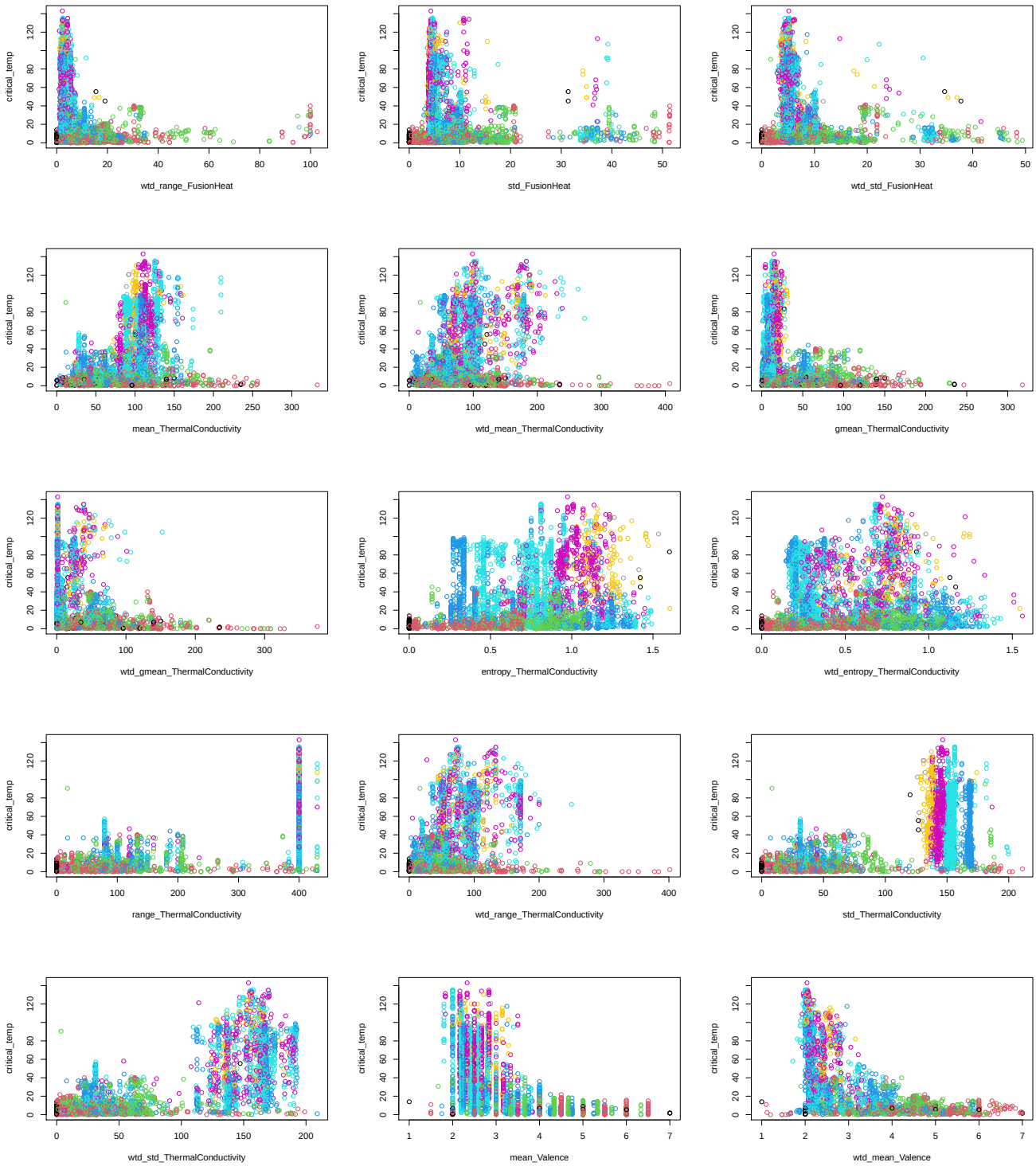
```
cols <- 2:81
plot_function <- sapply(cols, function(cols){
  df <- cbind(sc_small[cols], sc_small[82])
  plot(df, col=sc_small$number_of_elements)
})
```

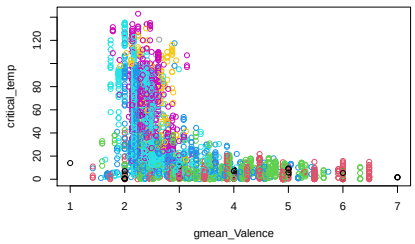


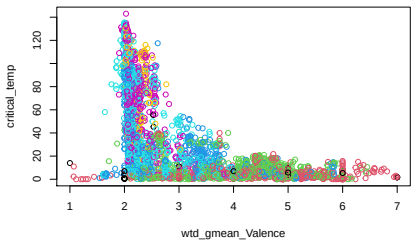

critical_temp
gmean_fie
wtd_gmean_fie
entropy_fie
wtd_entropy_fie
range_fie
wtd_range_fie
std_fie
wtd_std_fie
mean_atomic_radius
wtd_mean_atomic_radius
gmean_atomic_radius
wtd_gmean_atomic_radius
entropy_atomic_radius
wtd_entropy_atomic_radius
range_atomic_radius

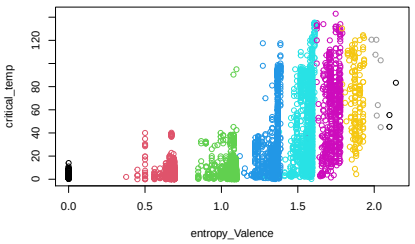

critical_temp
wtd_range_atomic_radius
std_atomic_radius
wtd_std_atomic_radius
mean_Density
wtd_mean_Density
gmean_Density
wtd_gmean_Density
entropy_Density
wtd_entropy_Density
range_Density
wtd_range_Density
std_Density
wtd_std_Density
mean_ElectronAffinity
wtd_mean_ElectronAffinity

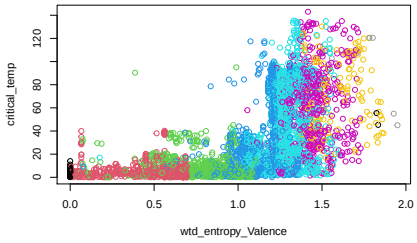

critical_temp
gmean_ElectronAffinity
wtd_gmean_ElectronAffinity
entropy_ElectronAffinity
wtd_entropy_ElectronAffinity
range_ElectronAffinity
wtd_range_ElectronAffinity
std_ElectronAffinity
wtd_std_ElectronAffinity
mean_FusionHeat
wtd_mean_FusionHeat
gmean_FusionHeat
wtd_gmean_FusionHeat
entropy_FusionHeat
wtd_entropy_FusionHeat
range_FusionHeat

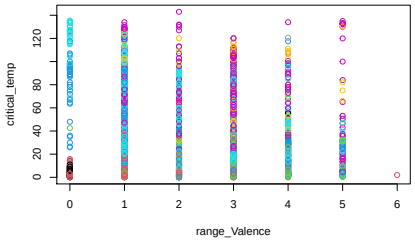

critical_temp
wtd_range_FusionHeat
std_FusionHeat
wtd_std_FusionHeat
mean_ThermalConductivity
wtd_mean_ThermalConductivity
gmean_ThermalConductivity
wtd_gmean_ThermalConductivity
entropy_ThermalConductivity
wtd_entropy_ThermalConductivity
range_ThermalConductivity
wtd_range_ThermalConductivity
std_ThermalConductivity
wtd_std_ThermalConductivity
mean_Valence
wtd_mean_Valence

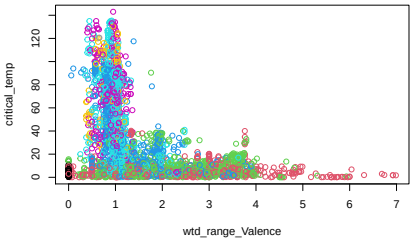

critical_temp
gmean_Valence

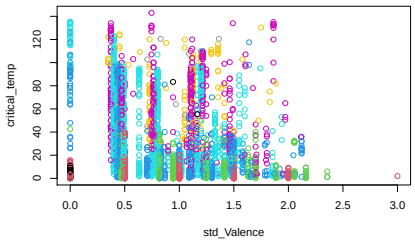

critical_temp
wtd_gmean_Valence

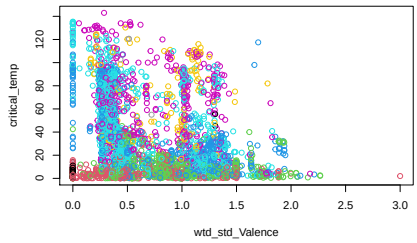

critical_temp
entropy_Valence


critical_temp
wtd_entropy_Valence


critical_temp
range_Valence


critical_temp
wtd_range_Valence


critical_temp
std_Valence


critical_temp
wtd_std_Valence

(3) Correlations in the groups of predictors.

```
col_name <- str_subset(colnames(sc), "atomic_mass") # length(col_name)
patterns1 <- str_replace(col_name, "_atomic_mass", "")
patt_unite <- data.frame(a = rep("^", 10), b = patterns1)
patterns1 <- unite(patt_unite, a, b, col = "c", sep = "") %>% pull()
string <- toString(patterns1)
string <- str_replace_all(string, ", ", "|")
patterns2 <- str_replace(colnames(sc), string, "") %>% unique()
patterns2 <- patterns2[2:9]
p <- c(patterns2, patterns1)
```

Correlation heatmaps of features that are grouped using patterns:

```
p
```

```
##  [1] "_atomic_mass"         "_fie"                 "_atomic_radius"
##  [4] "_Density"             "_ElectronAffinity"    "_FusionHeat"
##  [7] "_ThermalConductivity" "_Valence"             "^mean"
## [10] "^wtd_mean"            "^gmean"               "^wtd_gmean"
## [13] "^entropy"             "^wtd_entropy"         "^range"
## [16] "^wtd_range"           "^std"                 "^wtd_std"
```

```
corr_heatmaps <- map(p, function(p){
  corr_group <-  sc[str_subset(colnames(sc), p)] %>%
    cor() %>% data.frame()

  corr_group <- rownames_to_column(corr_group, "col_name")
  corr_group <- melt(corr_group) %>%
    set_names(c("col_name", "variable", "value"))

  plot <- corr_group %>%
    ggplot(aes(col_name, variable, fill = value)) +
    geom_tile() +
    scale_fill_distiller(palette = "Reds", direction = 1)  +
    labs(caption =  paste("Correlation heatmap of the variables in", p, "group.")) +
    theme_minimal()+
    theme(plot.caption.position = "panel",
          plot.caption = element_text(size = 14, face = "bold.italic", hjust = 0.65),
          axis.title.x = element_blank(),
          axis.title.y = element_blank(),
          axis.text.x = element_text(angle = 90, hjust = 1))
  plot
})

corr_heatmaps
```

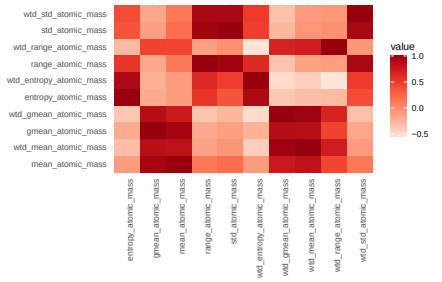
```
## [[1]]
```

```
##
## [[2]]
```

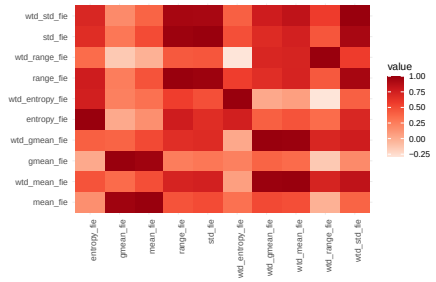
```
##
## [[3]]
```

```
##
## [[4]]
```

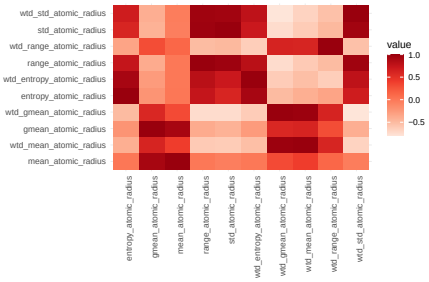
```
##
## [[5]]

##
## [[6]]

##
## [[7]]

##
## [[8]]

##
## [[9]]

##
## [[10]]

##
## [[11]]

##
## [[12]]

##
## [[13]]

##
## [[14]]

##
## [[15]]

##
## [[16]]

##
## [[17]]

##
## [[18]]
```



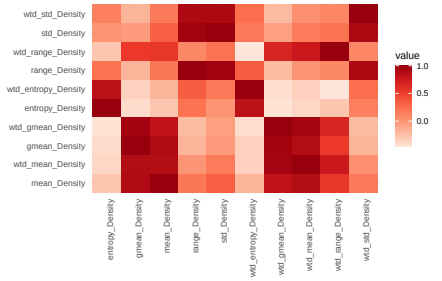
Correlation heatmap of the variables in _atomic_mass group.



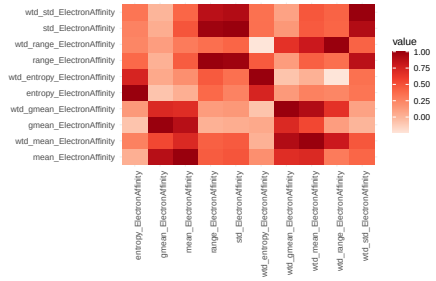
Correlation heatmap of the variables in _fie group.



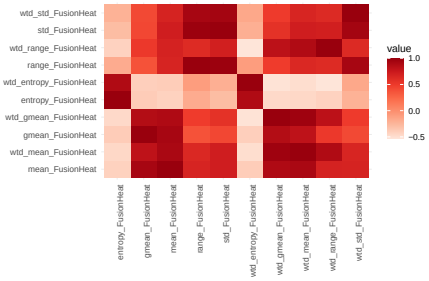
Correlation heatmap of the variables in _atomic_radius group.



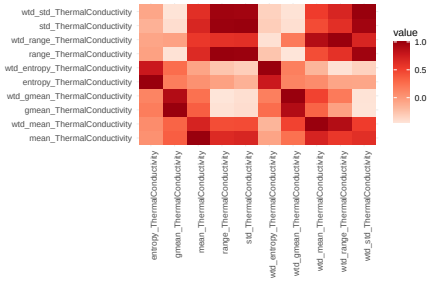
Correlation heatmap of the variables in _Density group.



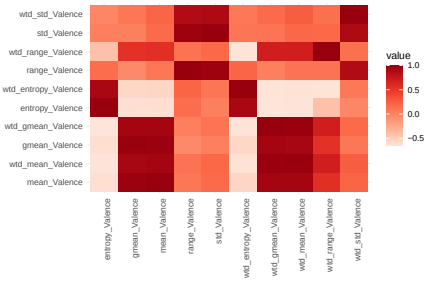
Correlation heatmap of the variables in _ElectronAffinity group.



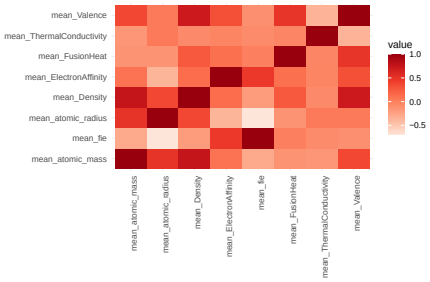
Correlation heatmap of the variables in _FusionHeat group.



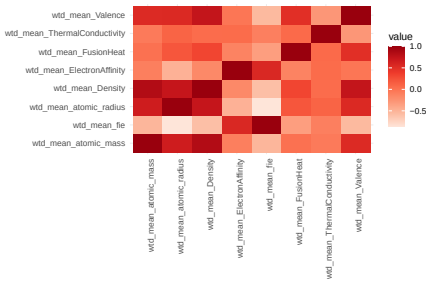
Correlation heatmap of the variables in _ThermalConductivity group.



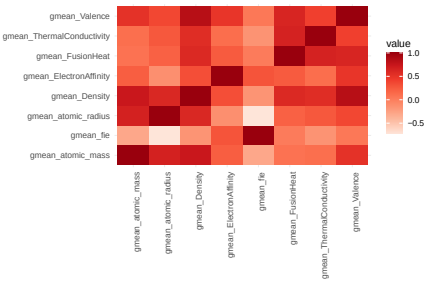
Correlation heatmap of the variables in _Valence group.



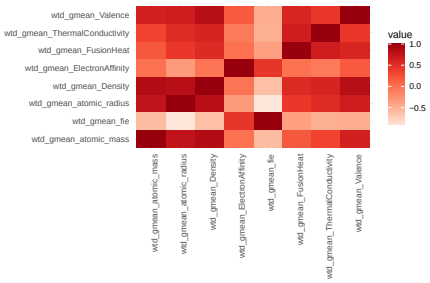
Correlation heatmap of the variables in ^mean group.



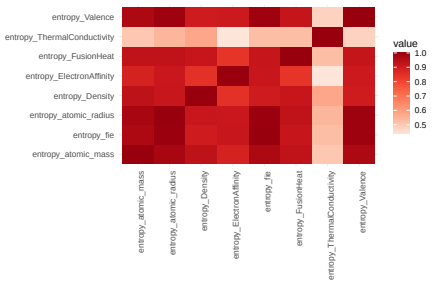
Correlation heatmap of the variables in ^wtd_mean group.



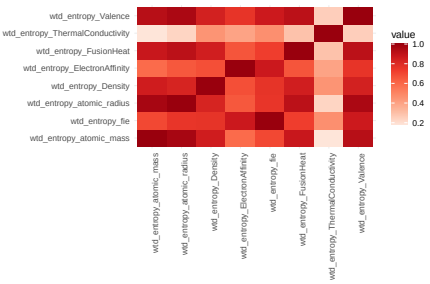
Correlation heatmap of the variables in ^gmean group.



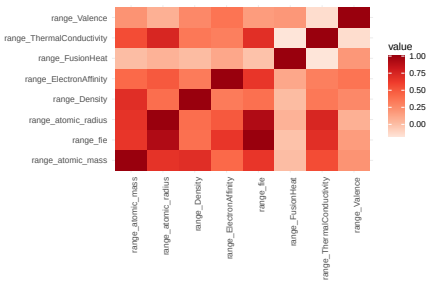
Correlation heatmap of the variables in ^wtd_gmean group.



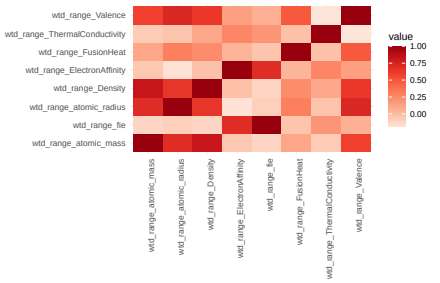
Correlation heatmap of the variables in ^entropy group.



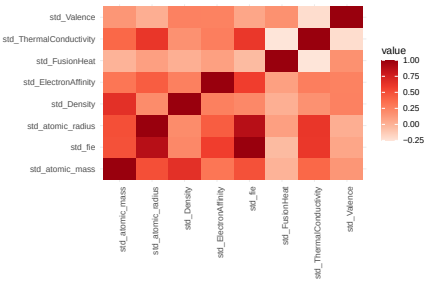
Correlation heatmap of the variables in ^wtd_entropy group.



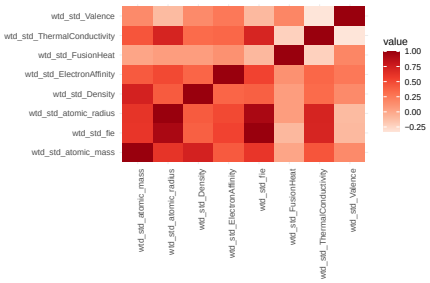
Correlation heatmap of the variables in ^range group.



Correlation heatmap of the variables in ^wtd_range group.



Correlation heatmap of the variables in ^std group.



Correlation heatmap of the variables in ^wtd_std group.

(4) discovering clusters in the groups of features using heatmap() function.

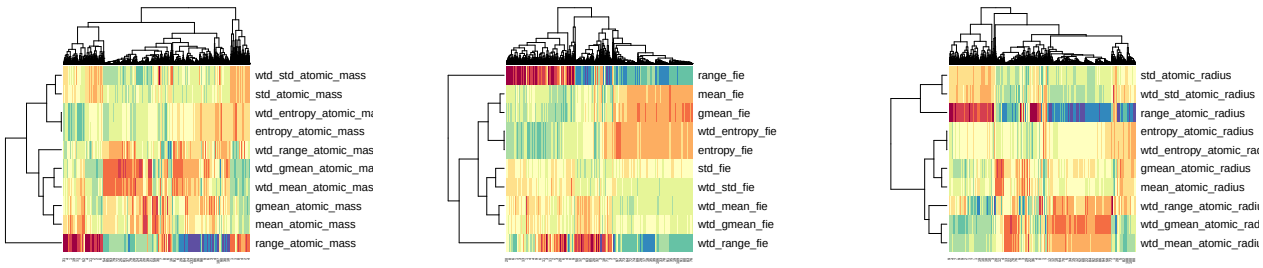
Features are grouped using patterns:

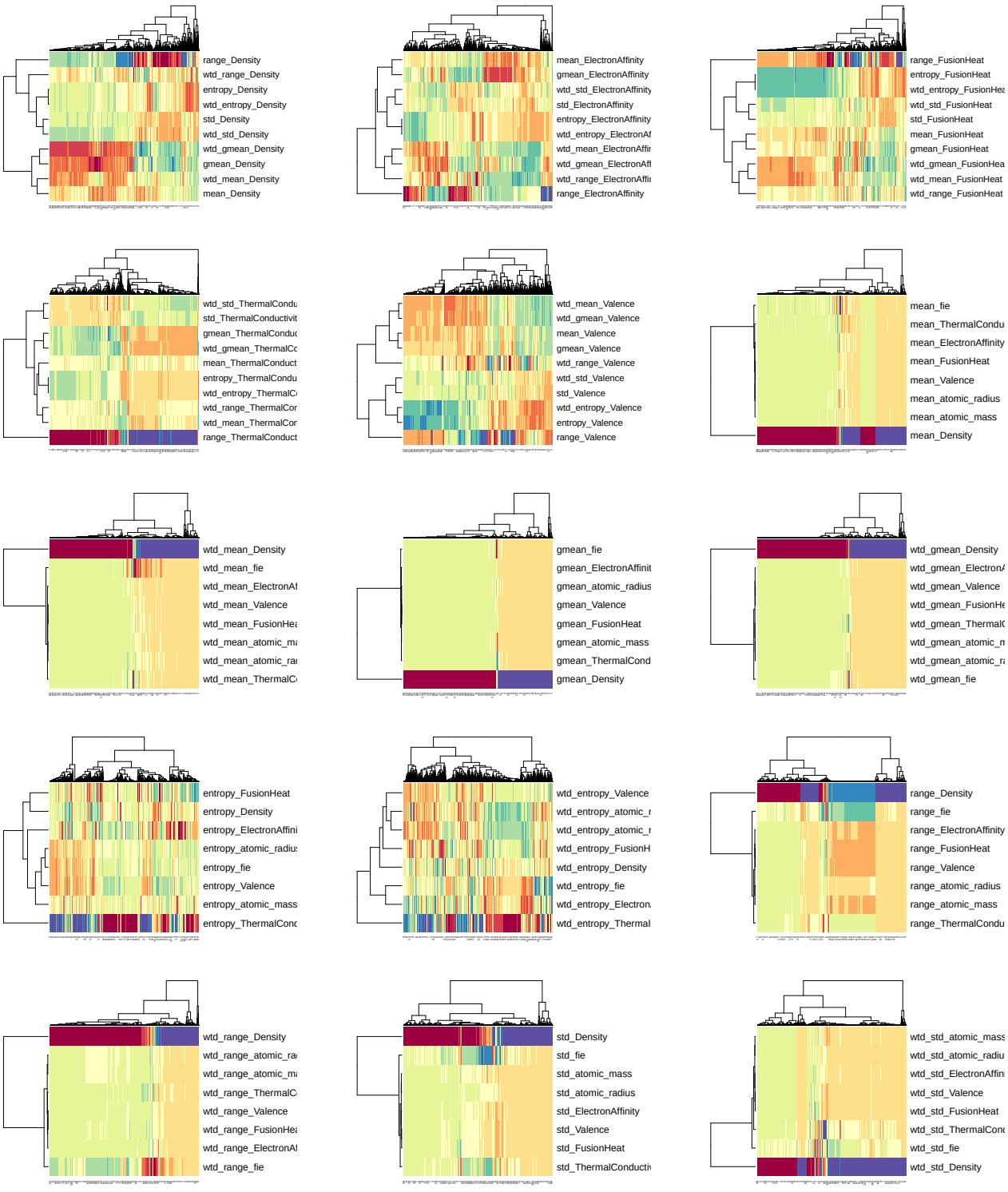
```
p
```

```
##  [1] "_atomic_mass"         "_fie"                 "_atomic_radius"
##  [4] "_Density"             "_ElectronAffinity"    "_FusionHeat"
##  [7] "_ThermalConductivity" "_Valence"             "^mean"
## [10] "^wtd_mean"            "^gmean"               "^wtd_gmean"
## [13] "^entropy"             "^wtd_entropy"         "^range"
## [16] "^wtd_range"           "^std"                 "^wtd_std"
```

```
x <- sc[1:81]  %>% as.matrix()
y <- sc[82] %>% round() %>% pull()
rownames(x) <- y   # critical_temp column is turned into row names
x <- sweep(x, 2, colMeans(x)) %>% as.matrix() # removing the center

heatm_clust_col <- sapply(p, function(p){
  ind <- which(colnames(sc) %in% colnames(sc[str_subset(colnames(sc), p)]))
  heatmap(t(x[,ind]), col = brewer.pal(11, "Spectral"),
          scale = "column")
})

heatm_clust_col
```

```
##        _atomic_mass  _fie          _atomic_radius _Density
## rowInd Integer,10    Integer,10    Integer,10     Integer,10
## colInd Integer,17009 Integer,17009 Integer,17009  Integer,17009
## Rowv   NULL          NULL          NULL           NULL
## Colv   NULL          NULL          NULL           NULL
##        _ElectronAffinity _FusionHeat   _ThermalConductivity _Valence
## rowInd Integer,10        Integer,10    Integer,10           Integer,10
## colInd Integer,17009     Integer,17009 Integer,17009        Integer,17009
## Rowv   NULL              NULL          NULL                 NULL
## Colv   NULL              NULL          NULL                 NULL
##        ^mean         ^wtd_mean     ^gmean        ^wtd_gmean    ^entropy
## rowInd Integer,8     Integer,8     Integer,8     Integer,8     Integer,8
## colInd Integer,17009 Integer,17009 Integer,17009 Integer,17009 Integer,17009
## Rowv   NULL          NULL          NULL          NULL          NULL
## Colv   NULL          NULL          NULL          NULL          NULL
##        ^wtd_entropy  ^range        ^wtd_range    ^std          ^wtd_std
## rowInd Integer,8     Integer,8     Integer,8     Integer,8     Integer,8
## colInd Integer,17009 Integer,17009 Integer,17009 Integer,17009 Integer,17009
## Rowv   NULL          NULL          NULL          NULL          NULL
## Colv   NULL          NULL          NULL          NULL          NULL
```




range_Density
wtd_range_Density
entropy_Density
wtd_entropy_Density
std_Density
wtd_std_Density
wtd_gmean_Density
gmean_Density
wtd_mean_Density
mean_Density
mean_ElectronAffinity
gmean_ElectronAffinity
wtd_std_ElectronAffinity
std_ElectronAffinity
entropy_ElectronAffinity
wtd_entropy_ElectronAf
wtd_mean_ElectronAffi
wtd_gmean_ElectronAff
wtd_range_ElectronAffi
range_ElectronAffinity
range_FusionHeat
entropy_FusionHeat
wtd_entropy_FusionHea
wtd_std_FusionHeat
std_FusionHeat
mean_FusionHeat
gmean_FusionHeat
wtd_gmean_FusionHea
wtd_mean_FusionHeat
wtd_range_FusionHeat
wtd_std_ThermalCondu
std_ThermalConductivit
gmean_ThermalConduc
wtd_gmean_ThermalCo
mean_ThermalConduct
entropy_ThermalCondu
wtd_entropy_ThermalC
wtd_range_ThermalCon
wtd_mean_ThermalCon
range_ThermalConduct
wtd_mean_Valence
wtd_gmean_Valence
mean_Valence
gmean_Valence
wtd_range_Valence
wtd_std_Valence
std_Valence
wtd_entropy_Valence
entropy_Valence
range_Valence
mean_fie
mean_ThermalCondu
mean_ElectronAffinity
mean_FusionHeat
mean_Valence
mean_atomic_radius
mean_atomic_mass
mean_Density
wtd_mean_Density
wtd_mean_fie
wtd_mean_ElectronAf
wtd_mean_Valence
wtd_mean_FusionHea
wtd_mean_atomic_ma
wtd_mean_atomic_ra
wtd_mean_ThermalC
gmean_fie
gmean_ElectronAffinit
gmean_atomic_radius
gmean_Valence
gmean_FusionHeat
gmean_atomic_mass
gmean_ThermalCond
gmean_Density
wtd_gmean_Density
wtd_gmean_ElectronA
wtd_gmean_Valence
wtd_gmean_FusionHe
wtd_gmean_ThermalC
wtd_gmean_atomic_m
wtd_gmean_atomic_ra
wtd_gmean_fie
entropy_FusionHeat
entropy_Density
entropy_ElectronAffini
entropy_atomic_radius
entropy_fie
entropy_Valence
entropy_atomic_mass
entropy_ThermalCond
wtd_entropy_Valence
wtd_entropy_atomic_r
wtd_entropy_atomic_r
wtd_entropy_FusionH
wtd_entropy_Density
wtd_entropy_fie
wtd_entropy_Electron
wtd_entropy_Thermal
range_Density
range_fie
range_ElectronAffinity
range_FusionHeat
range_Valence
range_atomic_radius
range_atomic_mass
range_ThermalCondu
wtd_range_Density
wtd_range_atomic_ra
wtd_range_atomic_ma
wtd_range_ThermalC
wtd_range_Valence
wtd_range_FusionHea
wtd_range_ElectronAf
wtd_range_fie
std_Density
std_fie
std_atomic_mass
std_atomic_radius
std_ElectronAffinity
std_Valence
std_FusionHeat
std_ThermalConductiv
wtd_std_atomic_mass
wtd_std_atomic_radiu
wtd_std_ElectronAffini
wtd_std_Valence
wtd_std_FusionHeat
wtd_std_ThermalCond
wtd_std_fie
wtd_std_Density