ADS502 Group Project

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```
threshold <- 0.5
drug_induced_training_data <- drug_induced_training_data[, colMeans(is.na(drug_induced_training_data)) <

get_mode <- function(x) {
    uniq_vals <- unique(x)
    uniq_vals[which.max(tabulate(match(x, uniq_vals)))]
}
categorical_cols <- sapply(drug_induced_training_data, is.character)
drug_induced_training_data[categorical_cols] <- lapply(
    drug_induced_training_data[categorical_cols],
    function(x) {
        x[is.na(x)] <- get_mode(x)
        return(x)
    })
write.csv(drug_induced_training_data, "DIA_trainingset_RDKit_descriptors.csv")
```

Data Cleaning

```
summary(drug_induced_training_data[, 1:6])
```

Descriptive Statistics

```
##      Label           SMILES             BalabanJ        BertzCT      
##  Min.   :0.0000   Length:477         Min.   :0.986   Min.   :   8.0  
##  1st Qu.:0.0000   Class :character   1st Qu.:1.679   1st Qu.: 493.3  
##  Median :0.0000   Mode  :character   Median :1.964   Median : 712.4  
##  Mean   :0.2474                      Mean   :2.143   Mean   : 738.6  
##  3rd Qu.:0.0000                      3rd Qu.:2.419   3rd Qu.: 943.2  
##  Max.   :1.0000                      Max.   :5.083   Max.   :2430.9  
##       Chi0            Chi0n       
##  Min.   : 3.414   Min.   : 1.725  
##  1st Qu.:13.405   1st Qu.:10.391  
##  Median :17.646   Median :14.184  
##  Mean   :18.130   Mean   :14.372  
##  3rd Qu.:22.052   3rd Qu.:17.730  
##  Max.   :50.120   Max.   :38.475  
```

```
drug_data <- select(drug_induced_training_data, where(is.numeric))
drug_stats <- describe(drug_data)
head(drug_stats, 10)
```

```
##          vars   n   mean     sd median trimmed    mad  min     max   range skew
## Label       1 477   0.25   0.43   0.00    0.19   0.00 0.00    1.00    1.00 1.17
## BalabanJ    2 477   2.14   0.71   1.96    2.05   0.52 0.99    5.08    4.10 1.49
## BertzCT     3 477 738.63 392.97 712.42  720.01 336.93 8.00 2430.93 2422.93 0.79
## Chi0        4 477  18.13   7.25  17.65   17.71   6.41 3.41   50.12   46.71 0.84
## Chi0n       5 477  14.37   6.09  14.18   14.05   5.50 1.73   38.48   36.75 0.81
## Chi0v       6 477  14.89   6.13  14.68   14.58   5.52 1.73   39.84   38.11 0.77
## Chi1        7 477  11.87   4.83  11.77   11.67   4.29 1.73   31.52   29.78 0.66
## Chi1n       8 477   8.43   3.76   8.35    8.26   3.54 0.61   23.17   22.55 0.65
## Chi1v       9 477   8.96   3.81   9.00    8.79   3.39 0.61   24.44   23.83 0.62
## Chi2n      10 477   6.67   3.28   6.36    6.48   3.04 0.25   19.35   19.10 0.75
##          kurtosis    se
## Label       -0.64  0.02
## BalabanJ     2.66  0.03
## BertzCT      1.74 17.99
## Chi0         1.73  0.33
## Chi0n        1.77  0.28
## Chi0v        1.62  0.28
## Chi1         1.38  0.22
## Chi1n        1.18  0.17
## Chi1v        1.13  0.17
## Chi2n        1.05  0.15
```

```
data_quality_report <- data.frame(
  Variable = names(drug_induced_training_data),
  Type = sapply(drug_induced_training_data, class),
  Missing = sapply(drug_induced_training_data, function(x) sum(is.na(x))),
  Complete = sapply(drug_induced_training_data, function(x) sum(!is.na(x))),
  Unique = sapply(drug_induced_training_data, function(x) length(unique(x)))
)
knitr::kable(head(data_quality_report, 40), caption = "Drug Induced Data Quality Report (Preview)")
```

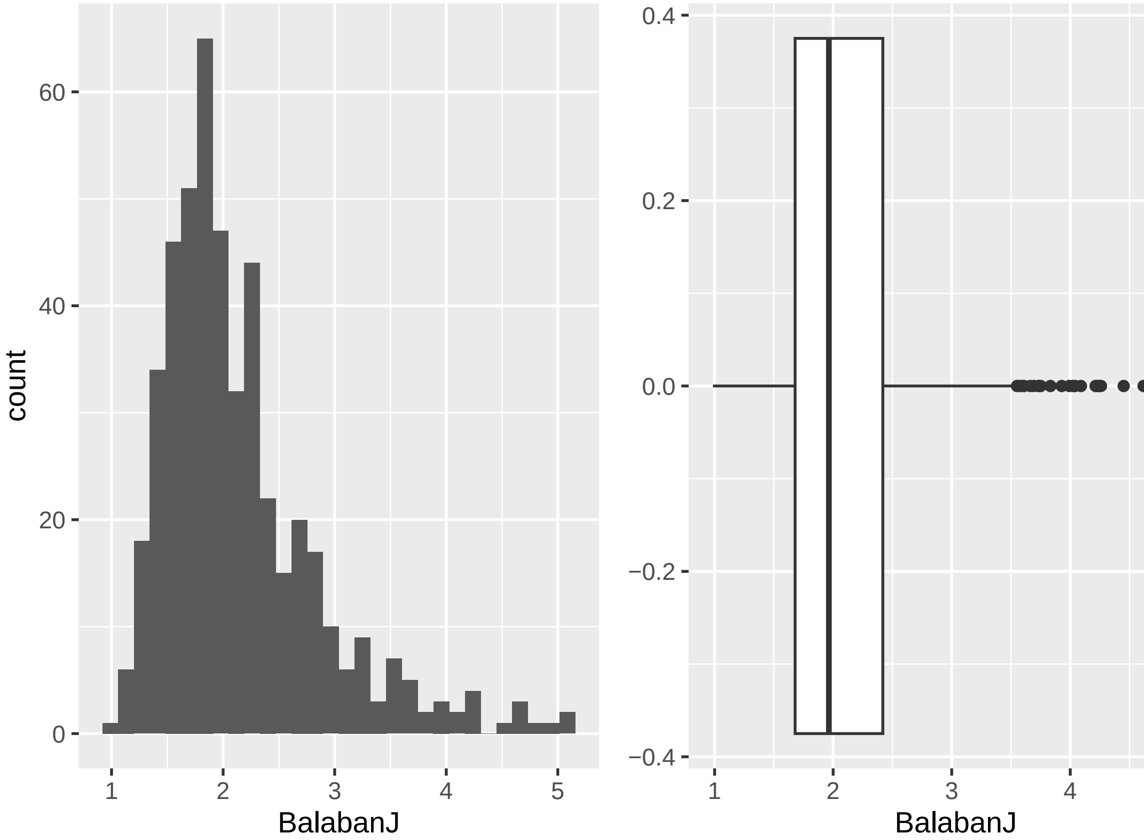
Data Quality Report

Table 1: Drug Induced Data Quality Report (Preview)

	Variable	Type	Missing	Complete	Unique
Label	Label	integer	0	477	2
SMILES	SMILES	character	0	477	477
BalabanJ	BalabanJ	numeric	0	477	406
BertzCT	BertzCT	numeric	0	477	465
Chi0	Chi0	numeric	0	477	382
Chi0n	Chi0n	numeric	0	477	460
Chi0v	Chi0v	numeric	0	477	460
Chi1	Chi1	numeric	0	477	423

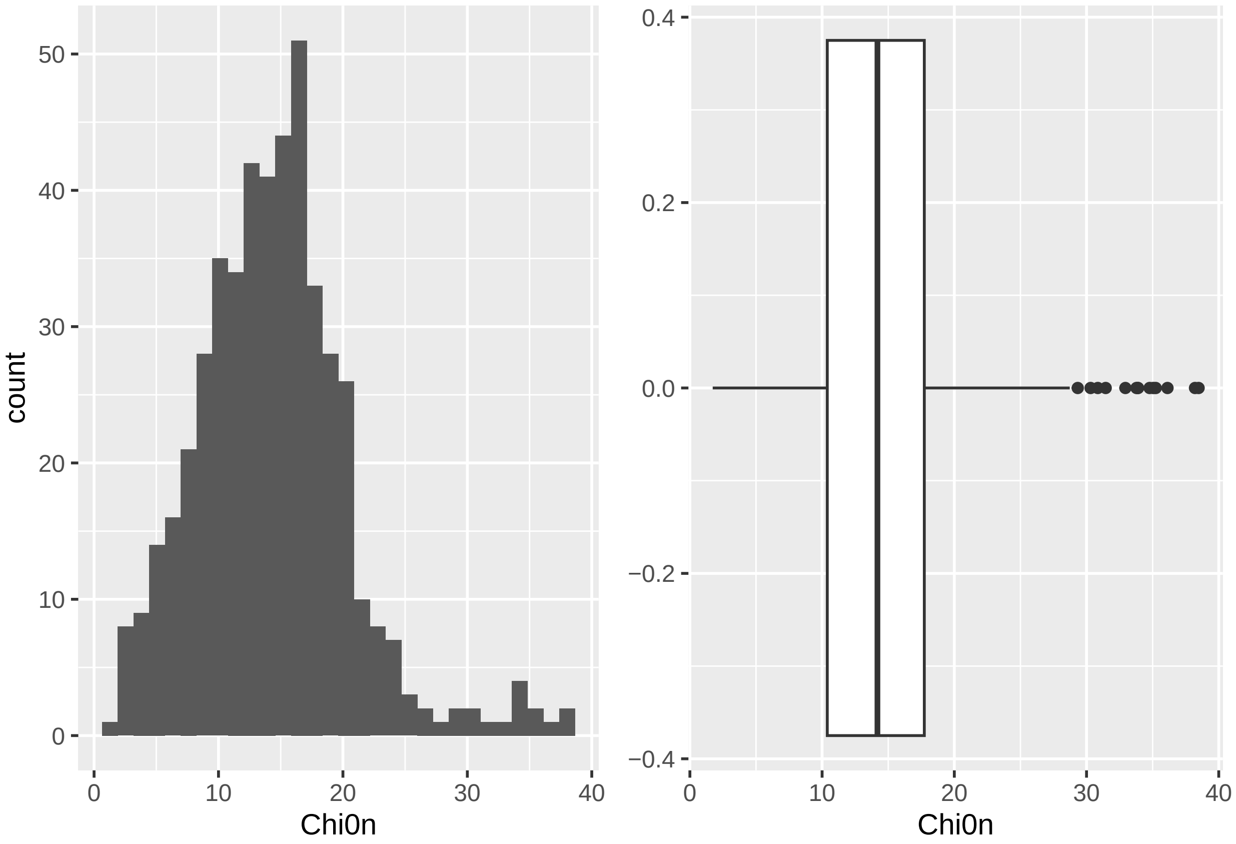
	Variable	Type	Missing	Complete	Unique
Chi1n	Chi1n	numeric	0	477	461
Chi1v	Chi1v	numeric	0	477	466
Chi2n	Chi2n	numeric	0	477	458
Chi2v	Chi2v	numeric	0	477	462
Chi3n	Chi3n	numeric	0	477	456
Chi3v	Chi3v	numeric	0	477	457
Chi4n	Chi4n	numeric	0	477	450
Chi4v	Chi4v	numeric	0	477	447
EState_VSA1	EState_VSA1	numeric	0	477	211
EState_VSA10	EState_VSA10	numeric	0	477	108
EState_VSA11	EState_VSA11	numeric	0	477	5
EState_VSA2	EState_VSA2	numeric	0	477	279
EState_VSA3	EState_VSA3	numeric	0	477	233
EState_VSA4	EState_VSA4	numeric	0	477	244
EState_VSA5	EState_VSA5	numeric	0	477	183
EState_VSA6	EState_VSA6	numeric	0	477	131
EState_VSA7	EState_VSA7	numeric	0	477	122
EState_VSA8	EState_VSA8	numeric	0	477	217
EState_VSA9	EState_VSA9	numeric	0	477	134
ExactMolWt	ExactMolWt	numeric	0	477	460
FractionCSP3	FractionCSP3	numeric	0	477	175
HallKierAlpha	HallKierAlpha	numeric	0	477	247
HeavyAtomCount	HeavyAtomCount	integer	0	477	53
HeavyAtomMolWt	HeavyAtomMolWt	numeric	0	477	420
Ipc	Ipc	numeric	0	477	453
Kappa1	Kappa1	numeric	0	477	450
Kappa2	Kappa2	numeric	0	477	459
Kappa3	Kappa3	numeric	0	477	448
LabuteASA	LabuteASA	numeric	0	477	466
MaxAbsEStateIndex	MaxAbsEStateIndex	numeric	0	477	452
MaxAbsPartialCharge	MaxAbsPartialCharge	numeric	0	477	166
MaxEStateIndex	MaxEStateIndex	numeric	0	477	452

```r
hist <- ggplot(drug_induced_training_data, aes(x=BalabanJ)) + geom_histogram(bins = 30)
boxplot <- ggplot(drug_induced_training_data, aes(x=BalabanJ)) + geom_boxplot()

grid.arrange(hist, boxplot, ncol = 2)
```

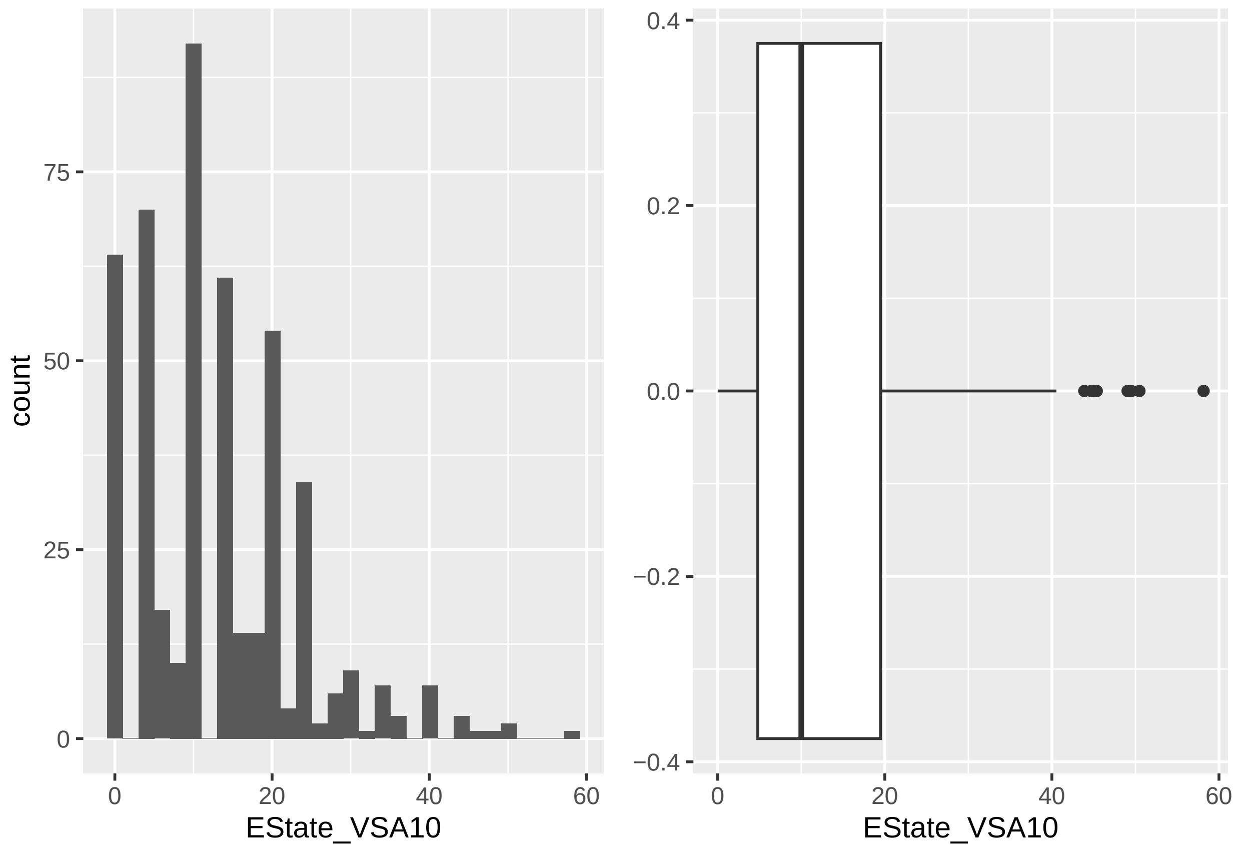


Univariate Analysis

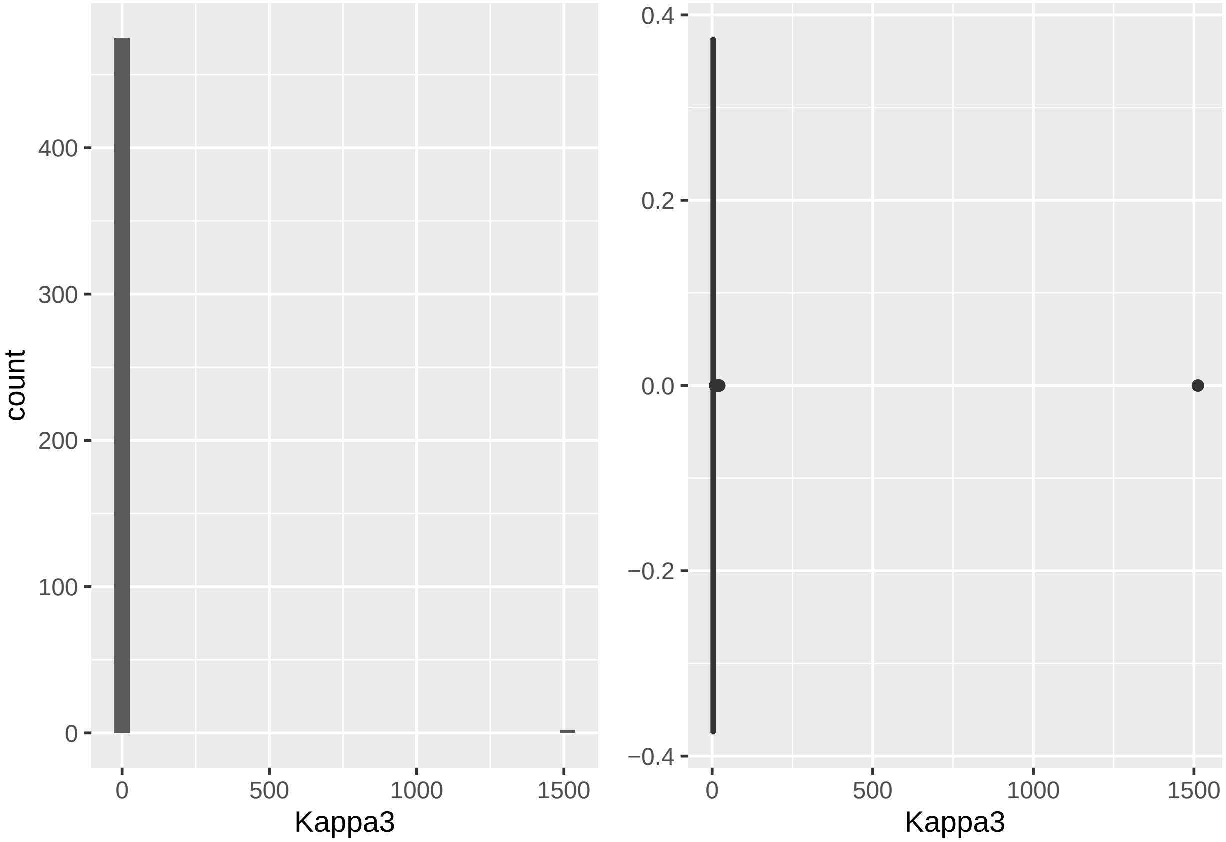
```
hist_2 <- ggplot(drug_induced_training_data, aes(x=Chi0n)) + geom_histogram(bins = 30)
boxplot_2 <- ggplot(drug_induced_training_data, aes(x=Chi0n)) + geom_boxplot()

grid.arrange(hist_2, boxplot_2, ncol = 2)
```



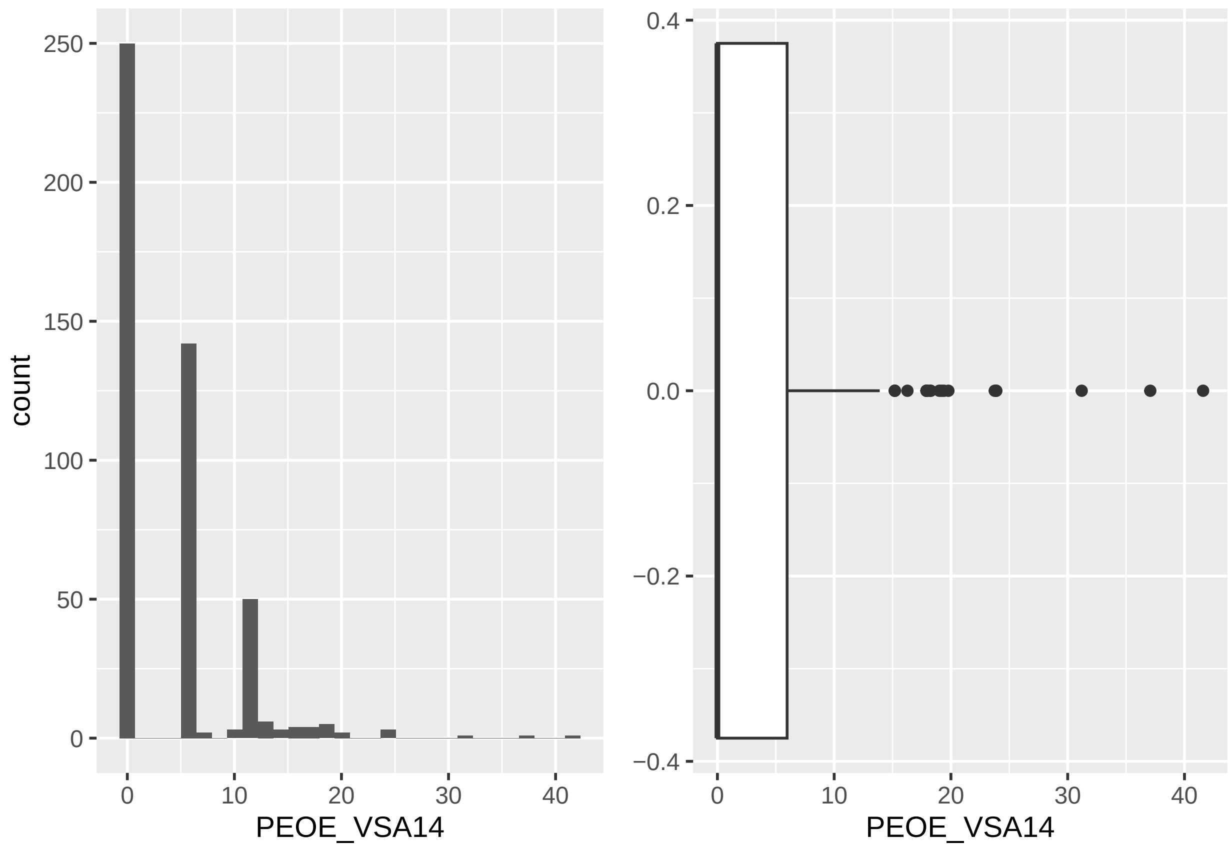
```r
hist_3 <- ggplot(drug_induced_training_data, aes(x=EState_VSA10)) + geom_histogram(bins = 30)
boxplot_3 <- ggplot(drug_induced_training_data, aes(x=EState_VSA10)) + geom_boxplot()

grid.arrange(hist_3, boxplot_3, ncol = 2)
```



```
hist_4 <- ggplot(drug_induced_training_data, aes(x=Kappa3)) + geom_histogram(bins = 30)
boxplot_4 <- ggplot(drug_induced_training_data, aes(x=Kappa3)) + geom_boxplot()

grid.arrange(hist_4, boxplot_4, ncol = 2)
```

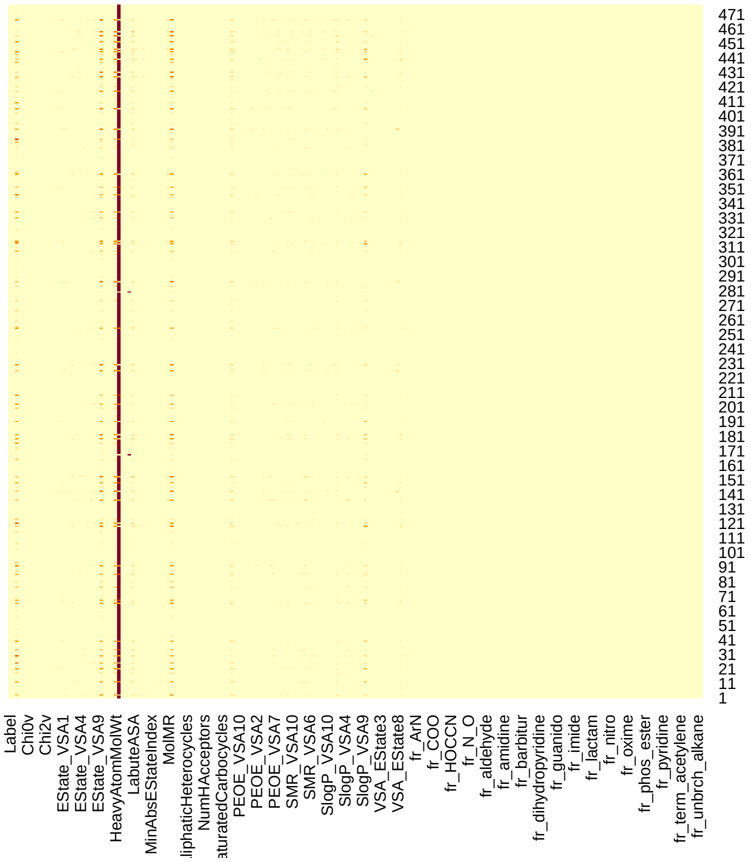


```
hist_5 <- ggplot(drug_induced_training_data, aes(x=PEOE_VSA14)) + geom_histogram(bins = 30)
boxplot_5 <- ggplot(drug_induced_training_data, aes(x=PEOE_VSA14)) + geom_boxplot()

grid.arrange(hist_5, boxplot_5, ncol = 2)
```



Features are right sweked. Few outliers that do not need to be removed.

```
numeric_cols_indexes <- sapply(drug_induced_training_data, is.numeric)
numeric_features <- drug_induced_training_data[numeric_cols_indexes]

data <- as.matrix(numeric_features)

heatmap(data,Colv = NA, Rowv = NA, scale = "row")
```



Multivariate Analysis

```
print("Pre-balance class cardinality")
```

Class Imbalance

```
## [1] "Pre-balance class cardinality"
```

```
table(drug_induced_training_data$Label)
```

```
##
##   0   1
## 359 118
```

```
# Random Undersampling
balanced_0 <- sample_n(filter(drug_induced_training_data, Label == 0), 118)
filtered_1 <- filter(drug_induced_training_data, Label == 1)
bal_drug_induced_training_data <- rbind(balanced_0, filtered_1)

print("Post-balance class cardinality")
```

```
## [1] "Post-balance class cardinality"
```

```r
table(bal_drug_induced_training_data$Label)
```

```
##
##   0   1
## 118 118
```

```r
# Drop SMILES feature
bal_drug_induced_training_data <- bal_drug_induced_training_data[, colnames(bal_drug_induced_training_da

for (col_name in colnames(bal_drug_induced_training_data)){
# For binary responses
  if (length(unique(bal_drug_induced_training_data[[col_name]])) == 2){
    bal_drug_induced_training_data[[col_name]] <- as.factor(bal_drug_induced_training_data[[col_name]])
  }

  # For standarization of numeric responses
  if (is.numeric(bal_drug_induced_training_data[[col_name]])){
    if( max(bal_drug_induced_training_data[[col_name]]) != min(bal_drug_induced_training_data[[col_name
    bal_drug_induced_training_data[[col_name]] <- (bal_drug_induced_training_data[[col_name]] - min(bal_
    (max(bal_drug_induced_training_data[[col_name]]) - min(bal_drug_induced_training_data[[col_name]]))
    }
    else{
          bal_drug_induced_training_data[[col_name]] <- 0
    }
  }
}
# Final Dataset
# bal_drug_induced_training_data
```

Pre-Model Data Preparation

```r
# Missing step --> numeric_features need to be obtained from bal_drug_induced_training_data

model_all <- lm(Label ~ ., data=numeric_features)  # with all the independent variables in the datafram
# summary(model_all)
coeff <- coefficients(model_all)

# To remove correlated where coefficient = NaN -> Correlation
na_coeff_names <- names(coeff)[is.na(coeff)]
na_coeff_names
```

Feature Selection

```
##  [1] "MaxEStateIndex"       "NumAliphaticRings"   "NumAromaticRings"
##  [4] "NumRadicalElectrons" "NumSaturatedRings"   "RingCount"
##  [7] "SMR_VSA8"            "SlogP_VSA9"          "VSA_EState1"
## [10] "VSA_EState2"         "VSA_EState3"         "VSA_EState4"
## [13] "VSA_EState5"         "VSA_EState6"         "VSA_EState7"
## [16] "fr_COO"              "fr_Nhpyrrole"        "fr_azide"
## [19] "fr_barbitur"         "fr_benzene"          "fr_diazo"
## [22] "fr_isocyan"          "fr_isothiocyan"      "fr_prisulfonamd"
## [25] "fr_thiocyan"
```