UV RNA FAIMS S30

Load required packages

```
## corrplot 0.84 loaded
```

```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
## -- Attaching packages --------------------------------------- tidyverse 1.3.0 --
```

```
## v ggplot2 3.3.0     v purrr   0.3.4
## v tidyr   1.0.3     v forcats 0.5.0
## v readr   1.3.1
```

```
## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```
##
## Attaching package: 'kableExtra'
```

```
## The following object is masked from 'package:dplyr':
##
##     group_rows
```

```
##
## Attaching package: 'magrittr'
```

```
## The following object is masked from 'package:purrr':
##
##     set_names
```

```
## The following object is masked from 'package:tidyr':
##
##     extract
```

```
##
## Attaching package: 'gridExtra'
```

```
## The following object is masked from 'package:dplyr':
##
##     combine
```

```
##
## ******************************************************
```

```
## Note: As of version 1.0.0, cowplot does not change the
##   default ggplot2 theme anymore. To recover the previous
##   behavior, execute:
##   theme_set(theme_cowplot())
## ******************************************************
##
## Attaching package: 'cowplot'
## The following object is masked from 'package:ggpubr':
##
##     get_legend
## Loading required package: lattice
## Loading required package: survival
## Loading required package: Formula
##
## Attaching package: 'Hmisc'
## The following objects are masked from 'package:dplyr':
##
##     src, summarize
## The following objects are masked from 'package:base':
##
##     format.pval, units
##
## Attaching package: 'caret'
## The following object is masked from 'package:survival':
##
##     cluster
## The following object is masked from 'package:purrr':
##
##     lift
## Loading required package: usethis
```

Loading RNP:Xl data into the R environment

I included the manually evaluated datasets for my ASMS talk to see if machine learning can help me with identifying a possible score cutoff or other metric to help reduce the numbers of entries I have to go through after RNP:xl output. The datasets include a merged version of both the S30 and S100 fraction that were initially considered individually:

*Ecoli UV RNA

Data wrangling

First, we need to add an extra column to each dataset, indicating which cross-linker was used in the experiment.

Then, we need to combine the dataframes.

First filtering step

Remove any entry that does not contain an RNA adduct and fits to a target better than a decoy.

Compute additional metrices (columns)

Peplength

classification of amino acids

Create new column with peptide length and classify identified amino acids in peptides as follows:

1. charged amino acids: R, K, D, E
2. polar amino acids: Q, N, H, S, T, Y, C, W
3. hydrophobic amino acids: A, I, L, M, V, P, G

Peptide pI (isoelectric point)

Compute the isolelectric point for each peptide in each entry.

aI (aliphatic index)

Compute the aliphatic Index for each peptide in each entry. See the following paper for more info:

Thermostability and aliphatic index of globular proteins. J Biochem. 1980 Dec;88(6):1895-8.

"A statistical analysis shows that the alphatic index, which is defined as the relative volume of a protein occupied by aliphatic side schains (alanine, valine, isoleucine, and leucine), of proteins of thermophilic bacteria is significantly higher than that of ordinary proteins. The index may be regarded as a positive factor for the increase of thermostability of globular proteins."

In general, an aI of greater 92.6 is particulary stable thermally as found in thermophiles. Now, since we are investigating tryptic peptides, I could only find one paper on that matter.

GETTING INTIMATE WITH TRYPSIN, THE LEADING PROTEASE IN PROTEOMICS Published online 15 June 2013 in Wiley Online Library (wileyonlinelibrary.com). DOI 10.1002/mas.21376

According to this paper, human proteins result in 61 tryptic peptides on average.

proposed cross-linking amino acid

Hydrophibicity index

Molecular weight of peptide

Note: returns the average masses, not the monoisotopic masses!

Machine learning

Split dataset

Seperate different species of nucleotides (RNA, DNA) and cross-linker (UV, DEB).

Setting up the dataset

Harmonize the number of trues and falses and dropping all categorical columns.

```
set.seed(42)
drops_general<-c("precursor_purity", "RNPxl_a_ion_score")
```

```
ml_UV_RNA<-data1 %>%
  filter(XLinker == "UV", Curated == "0", Nucleotides == "RNA") %>%
  sample_n(838) %>%
  rbind(RNA_UV)
rows_UV_RNA <- sample(nrow(ml_UV_RNA))
ml_UV_RNA <- ml_UV_RNA[rows_UV_RNA, ] %>%
  dplyr::select_if(is.numeric)
ml_UV_RNA<-ml_UV_RNA[, !(colnames(ml_UV_RNA) %in% drops_general)]
```

Splitting into train and test data

I will use 80% of the data to train, and 20% to test the model

```
ml_UV_RNA$Curated<-as.factor(ml_UV_RNA$Curated)
ml_UV_RNA$Curated<-factor(ml_UV_RNA$Curated, levels = c("0", "1"), labels = c("False", "True"))
ml_UV_RNA_train <- ml_UV_RNA[1:1340, ]
ml_UV_RNA_test <- ml_UV_RNA[1341:1676, ]
```

KNN

K nearest neighboor classification based on numeric variables, min-max normalized.

```
library(class)
library(gmodels)

knn_drop <- c("Curated", "isotope_error", "RNPxl_a_ion_score", "RNPxl_precursor_purity")

normalize <- function(x) {
  return((x-min(x))/(max(x)-min(x)))
}

ml_UV_RNA_test_knn<-ml_UV_RNA_test[,!(names(ml_UV_RNA_test) %in% knn_drop)]
ml_UV_RNA_test_knn<-as.data.frame(lapply(ml_UV_RNA_test_knn[1:39], normalize))
ml_UV_RNA_test_knn_labels<-ml_UV_RNA_test[1:336, 5]

ml_UV_RNA_train_knn<-ml_UV_RNA_train[,!(names(ml_UV_RNA_train) %in% knn_drop)]
ml_UV_RNA_train_knn<-as.data.frame(lapply(ml_UV_RNA_train_knn[1:39], normalize))
ml_UV_RNA_train_knn_labels<-as.data.frame(ml_UV_RNA_train[1:1340, 5])
```

Evaluate Model Performance UV RNA

Here, I chose 5 neighbors:

```
UV_RNA_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = ml_UV_RNA_test_knn,
                       cl = ml_UV_RNA_train_knn_labels$Curated, k =5 )
CrossTable(x = ml_UV_RNA_test_knn_labels$Curated, y = UV_RNA_knn_pred, prop.chisq = F)
```

```
##
##
##    Cell Contents
## |-------------------------|
## |                       N |
## |           N / Row Total |
## |           N / Col Total |
```

```
## |         N / Table Total |
## |-------------------------|
##
##
## Total Observations in Table:  336
##
##
##                                    | UV_RNA_knn_pred
## ml_UV_RNA_test_knn_labels$Curated |     False |      True | Row Total |
## ----------------------------------|-----------|-----------|-----------|
##                             False |       147 |        11 |       158 |
##                                   |     0.930 |     0.070 |     0.470 |
##                                   |     0.948 |     0.061 |           |
##                                   |     0.438 |     0.033 |           |
## ----------------------------------|-----------|-----------|-----------|
##                              True |         8 |       170 |       178 |
##                                   |     0.045 |     0.955 |     0.530 |
##                                   |     0.052 |     0.939 |           |
##                                   |     0.024 |     0.506 |           |
## ----------------------------------|-----------|-----------|-----------|
##                      Column Total |       155 |       181 |       336 |
##                                   |     0.461 |     0.539 |           |
## ----------------------------------|-----------|-----------|-----------|
##
##
```

Decision trees and classification rules

C5.0

```
library(C50)

C5_drop <- c("isotope_error", "RNPxl_a_ion_score", "precursor_purity")

ml_UV_RNA_train_C5<-ml_UV_RNA_train[,!(names(ml_UV_RNA_train) %in% C5_drop)]
ml_UV_RNA_test_C5<-ml_UV_RNA_test[,!(names(ml_UV_RNA_test) %in% C5_drop)]
```

UV RNA

with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

C5_model_UV_RNA_boost_pen<-C5.0(x=ml_UV_RNA_train_C5[-5], y=ml_UV_RNA_train_C5$Curated,
                                costs = error_cost, trials = 10)
summary(C5_model_UV_RNA_boost_pen)
```

```
##
## Call:
## C5.0.default(x = ml_UV_RNA_train_C5[-5], y = ml_UV_RNA_train_C5$Curated,
```

```
##  trials = 10, costs = error_cost)
##
##
## C5.0 [Release 2.07 GPL Edition]      Wed Jun 23 10:38:27 2021
## -------------------------------
##
## Class specified by attribute `outcome'
##
## Read 1340 cases (40 attributes) from undefined.data
## Read misclassification costs from undefined.costs
##
## -----  Trial 0:  -----
##
## Decision tree:
##
## score > 0.061008:
## :...RNPxl_pl_pc_MIC <= 0.007726523:
## :   :...RNPxl_pl_MIC > 0.04139248:
## :   :   :...precursor <= 753.8025: True (11)
## :   :   :   precursor > 753.8025: False (16/3)
## :   :   RNPxl_pl_MIC <= 0.04139248:
## :   :   :...RNPxl_pl_pc_MIC <= 0.0001836105: False (561/11)
## :   :       RNPxl_pl_pc_MIC > 0.0001836105:
## :   :       :...RNPxl_pl_modds <= 0.730354: False (72/9)
## :   :           RNPxl_pl_modds > 0.730354:
## :   :           :...precursor_intensity <= 1838890: False (8/3)
## :   :               precursor_intensity > 1838890: True (11)
## :   RNPxl_pl_pc_MIC > 0.007726523:
## :   :...aa_class_polar > 5: False (5/1)
## :       aa_class_polar <= 5:
## :       :...RNPxl_total_MIC > 0.1157202: True (64)
## :           RNPxl_total_MIC <= 0.1157202:
## :           :...RNPxl_RNA_MASS_z0 > 404.0022:
## :               :...Hydro <= -0.49: False (6/3)
## :               :   Hydro > -0.49: True (22)
## :               RNPxl_RNA_MASS_z0 <= 404.0022:
## :               :...score > 0.419009: False (5)
## :                   score <= 0.419009:
## :                   :...RNPxl_marker_ions_score <= 0.06687339: True (6)
## :                       RNPxl_marker_ions_score > 0.06687339: False (2)
## score <= 0.061008:
## :...RNPxl_modds <= 0.2422339:
##     :...aIndex <= 90.69: False (21/7)
##     :   aIndex > 90.69: True (21)
##     RNPxl_modds > 0.2422339:
##     :...pI > 6.16:
##         :...Hydro > -0.39: True (263)
##         :   Hydro <= -0.39:
##         :   :...RT <= 1995.088: True (26)
##         :       RT > 1995.088: False (9/6)
##         pI <= 6.16:
##         :...RNPxl_RNA_MASS_z0 <= 244.0695: False (5/2)
##             RNPxl_RNA_MASS_z0 > 244.0695:
##             :...aa_class_charged <= 2:
```

```
##                 :...RNPxl_best_localization_score <= 0.0497132: False (3)
##                 :   RNPxl_best_localization_score > 0.0497132: True (5)
##                 aa_class_charged > 2:
##                 :...aa_class_polar <= 3: True (79/1)
##                     aa_class_polar > 3:
##                     :...RNPxl_RNA_MASS_z0 > 635.0778: True (49/1)
##                         RNPxl_RNA_MASS_z0 <= 635.0778:
##                         :...RNPxl_pl_MIC > 0.02491653: True (26)
##                             RNPxl_pl_MIC <= 0.02491653:
##                             :...RNPxl_marker_ions_score <= 0.09317322: False (32/22)
##                                 RNPxl_marker_ions_score > 0.09317322: True (12)
##
## -----  Trial 1:  -----
##
## Decision tree:
##
## score <= 0.0726375:
## :...RNPxl_partial_loss_score <= 0.7555764: False (28/19.6)
## :   RNPxl_partial_loss_score > 0.7555764: True (869/27.5)
## score > 0.0726375:
## :...RNPxl_pl_pc_MIC <= 0.002406057:
##     :...RNPxl_marker_ions_score > 0.03210174: False (101.9/77.7)
##     :   RNPxl_marker_ions_score <= 0.03210174:
##     :   :...RNPxl_pl_modds <= 0.33299:
##     :       :...aa_class_polar <= 6: False (272)
##     :       :   aa_class_polar > 6:
##     :       :   :...RNPxl_MIC <= 0.4404297: False (73.2/12.7)
##     :       :       RNPxl_MIC > 0.4404297: True (13.5/0.8)
##     :       RNPxl_pl_modds > 0.33299:
##     :       :...score > 0.759875: True (59.1/8.3)
##     :           score <= 0.759875:
##     :           :...RNPxl_MIC <= 0.4907319: False (134.1/46.4)
##     :               RNPxl_MIC > 0.4907319: True (16.5/1.5)
##     RNPxl_pl_pc_MIC > 0.002406057:
##     :...precursor > 1085.438: False (7.6/1.5)
##         precursor <= 1085.438:
##         :...RNPxl_RNA_MASS_z0 <= 244.0695: False (9.8/4.5)
##             RNPxl_RNA_MASS_z0 > 244.0695:
##             :...precursor_error_ppm <= 0.2314823: False (15.1/9.1)
##                 precursor_error_ppm > 0.2314823:
##                 :...RNPxl_pl_Morph <= 2.00818: False (21.2/11.3)
##                     RNPxl_pl_Morph > 2.00818: True (198.5/2.3)
##
## -----  Trial 2:  -----
##
## Decision tree:
##
## RNPxl_pl_pc_MIC > 0.001713034: True (952.1/52.3)
## RNPxl_pl_pc_MIC <= 0.001713034:
## :...RNPxl_precursor_score > 0.002855255: True (94.3/1.2)
##     RNPxl_precursor_score <= 0.002855255:
##     :...RNPxl_total_loss_score > 13.47351:
##         :...RNPxl_pl_pc_MIC > 0.001647775: False (7.3)
##         :   RNPxl_pl_pc_MIC <= 0.001647775:
```

```
##         :   :...RNPxl_pl_im_MIC <= 0.007103287: True (153.1/2.1)
##         :       RNPxl_pl_im_MIC > 0.007103287: False (33.9/25.7)
##         RNPxl_total_loss_score <= 13.47351:
##         :...RNPxl_pl_MIC > 0.04215598: True (124.6/9.4)
##             RNPxl_pl_MIC <= 0.04215598:
##             :...RNPxl_pl_modds <= 0.33299: False (317.8/30.2)
##                 RNPxl_pl_modds > 0.33299:
##                 :...precursor > 1005.797: False (33.2)
##                     precursor <= 1005.797:
##                     :...RNPxl_score <= -2.285719: False (24.1)
##                         RNPxl_score > -2.285719:
##                         :...RNPxl_total_MIC <= 0.04661144: True (91.7/2.4)
##                             RNPxl_total_MIC > 0.04661144: False (130.2/85.5)
##
## -----  Trial 3:  -----
##
## Decision tree:
##
## score > 0.279249:
## :...RNPxl_pl_pc_MIC > 0.021649: True (131/7.8)
## :   RNPxl_pl_pc_MIC <= 0.021649:
## :   :...RNPxl_total_MIC > 0.4968228: True (59.5/7.4)
## :       RNPxl_total_MIC <= 0.4968228:
## :       :...RNPxl_marker_ions_score > 0.07374955: True (56.5/8.1)
## :           RNPxl_marker_ions_score <= 0.07374955:
## :           :...RNPxl_pl_modds <= 0.07581517: False (132)
## :               RNPxl_pl_modds > 0.07581517:
## :               :...RNPxl_partial_loss_score <= 5.0293: False (194.9/52.1)
## :                   RNPxl_partial_loss_score > 5.0293:
## :                   :...precursor > 1005.471: False (60)
## :                       precursor <= 1005.471:
## :                       :...RNPxl_best_localization_score <= 0.2996045: True (134.5/13.6)
## :                           RNPxl_best_localization_score > 0.2996045: False (7.2)
## score <= 0.279249:
## :...RNPxl_precursor_score > 0.01703667: True (127.6)
##     RNPxl_precursor_score <= 0.01703667:
##     :...RNPxl_total_loss_score <= 1.654075:
##         :...RNPxl_partial_loss_score > 4.360192: True (36.3/0.5)
##         :   RNPxl_partial_loss_score <= 4.360192:
##         :   :...RT <= 2036.58: True (31.8/1.4)
##         :       RT > 2036.58: False (43.1/5.6)
##         RNPxl_total_loss_score > 1.654075:
##         :...RNPxl_pl_pc_MIC > 0.01650992: True (135.5)
##             RNPxl_pl_pc_MIC <= 0.01650992:
##             :...RNPxl_pl_MIC > 0.04691937: True (81.4)
##                 RNPxl_pl_MIC <= 0.04691937:
##                 :...RNPxl_score <= 0.1529219: False (53.1/33.2)
##                     RNPxl_score > 0.1529219:
##                     :...Hydro > -0.2: True (312.3/9.5)
##                         Hydro <= -0.2:
##                         :...RNPxl_Da_difference <= -0.0007993339: True (87.8)
##                             RNPxl_Da_difference > -0.0007993339:
##                             :...aa_class_charged > 5: True (30.3)
##                                 aa_class_charged <= 5:
```

```
##                                 :...RNPxl_total_MIC > 0.5777186: True (25.5)
##                                     RNPxl_total_MIC <= 0.5777186:
##                                     :...RNPxl_modds > 11.55659: True (16.4)
##                                         RNPxl_modds <= 11.55659: [S1]
##
## SubTree [S1]
##
## RNPxl_immonium_score <= 0.03291839: True (54.3/5.5)
## RNPxl_immonium_score > 0.03291839:
## :...RNPxl_pl_MIC <= 0.006622917: True (13.8/0.9)
##     RNPxl_pl_MIC > 0.006622917: False (64.3/21.6)
##
## -----  Trial 4:  -----
##
## Decision tree:
##
## score <= 0.279249:
## :...RNPxl_pl_modds <= 0.06587414: False (73.6/44.2)
## :   RNPxl_pl_modds > 0.06587414:
## :   :...RNPxl_precursor_score > 0.01703667: True (98.8)
## :       RNPxl_precursor_score <= 0.01703667:
## :       :...RT <= 1707.911: True (112.7/2.2)
## :           RT > 1707.911:
## :           :...Peplength <= 9: False (72.9/46.2)
## :               Peplength > 9:
## :               :...Hydro <= -0.9: False (30.2/20.6)
## :                   Hydro > -0.9:
## :                   :...aIndex > 126.96: False (27.9/19.5)
## :                       aIndex <= 126.96:
## :                       :...RNPxl_pl_MIC > 0.01001978: True (562.5/20.6)
## :                           RNPxl_pl_MIC <= 0.01001978:
## :                           :...RNPxl_pl_modds <= 0.1546841: True (83.5/0.7)
## :                               RNPxl_pl_modds > 0.1546841:
## :                               :...RNPxl_precursor_score <= 0.002451922: False (79.4/52)
## :                                   RNPxl_precursor_score > 0.002451922: True (23.6)
## score > 0.279249:
## :...RNPxl_pl_pc_MIC > 0.007726523:
##     :...RNPxl_RNA_MASS_z0 <= 324.0359: False (60/36.7)
##     :   RNPxl_RNA_MASS_z0 > 324.0359: True (149.6/4.9)
##     RNPxl_pl_pc_MIC <= 0.007726523:
##     :...RNPxl_pl_Morph <= 3.006252: False (144.9)
##         RNPxl_pl_Morph > 3.006252:
##         :...RT > 3562.469: False (67.8)
##             RT <= 3562.469:
##             :...precursor > 1058.797: False (35.4)
##                 precursor <= 1058.797:
##                 :...aa_class_hydrophobic > 12: False (11.9)
##                     aa_class_hydrophobic <= 12:
##                     :...RNPxl_modds <= 1.15274e-005: True (47.4/0.7)
##                         RNPxl_modds > 1.15274e-005:
##                         :...RNPxl_pl_modds <= 0.2060084: False (21.3)
##                             RNPxl_pl_modds > 0.2060084:
##                             :...Peplength > 18: False (11.9)
##                                 Peplength <= 18:
```

```
##                                 :...RNPxl_RNA_MASS_z0 <= 244.0695: False (6.9)
##                                     RNPxl_RNA_MASS_z0 > 244.0695: [S1]
##
## SubTree [S1]
##
## RNPxl_best_localization_score > 0.2416947: True (29.5)
## RNPxl_best_localization_score <= 0.2416947:
## :...RNPxl_pl_pc_MIC <= 0.0004818717: False (79.6/49.9)
##     RNPxl_pl_pc_MIC > 0.0004818717: True (88.3/3.1)
##
## -----  Trial 5:  -----
##
## Decision tree:
##
## score <= 0.0792426:
## :...RT <= 2026.161: True (267.9)
## :   RT > 2026.161:
## :   :...RNPxl_total_MIC <= 0.1033425: False (26.9/15.5)
## :       RNPxl_total_MIC > 0.1033425:
## :       :...RNPxl_score <= -0.6372114: False (24.8/15.3)
## :           RNPxl_score > -0.6372114:
## :           :...pI > 6.5: True (202/2.2)
## :               pI <= 6.5:
## :               :...RNPxl_best_localization_score > 0.5767938: True (71.9)
## :                   RNPxl_best_localization_score <= 0.5767938:
## :                   :...RNPxl_RNA_MASS_z0 > 635.0778: True (138.3/2.8)
## :                       RNPxl_RNA_MASS_z0 <= 635.0778:
## :                       :...score > 0.00985416: True (49.4)
## :                           score <= 0.00985416:
## :                           :...RNPxl_immonium_score > 0.1319419: False (6.3/0.3)
## :                               RNPxl_immonium_score <= 0.1319419:
## :                               :...RNPxl_immonium_score > 0.1050521: True (35)
## :                                   RNPxl_immonium_score <= 0.1050521:
## :                                   :...RNPxl_immonium_score > 0.0983247: False (5.5/0.3)
## :                                       RNPxl_immonium_score <= 0.0983247:
## :                                       :...precursor > 1184.961: True (44.3)
## :                                           precursor <= 1184.961: [S1]
## score > 0.0792426:
## :...RNPxl_pl_pc_MIC > 0.007726523:
##     :...RNPxl_total_MIC > 0.1157202: True (233.4/1.3)
##     :   RNPxl_total_MIC <= 0.1157202:
##     :   :...aa_class_charged <= 1: True (29.5)
##     :       aa_class_charged > 1: False (97.6/71.4)
##     RNPxl_pl_pc_MIC <= 0.007726523:
##     :...RNPxl_pl_Morph <= 4.002007: False (171.8/18)
##         RNPxl_pl_Morph > 4.002007:
##         :...RT > 3562.469: False (53.9)
##             RT <= 3562.469:
##             :...precursor > 1062.842: False (29.1)
##                 precursor <= 1062.842:
##                 :...aa_class_hydrophobic > 12: False (9)
##                     aa_class_hydrophobic <= 12:
##                     :...RNPxl_pl_pc_MIC > 0.00714745: False (7.6)
##                         RNPxl_pl_pc_MIC <= 0.00714745:
```

```
##                           :...RNPxl_pl_MIC > 0.04691937: True (57.8)
##                               RNPxl_pl_MIC <= 0.04691937:
##                               :...RNPxl_precursor_score > 0: True (21.8)
##                                   RNPxl_precursor_score <= 0:
##                                   :...RNPxl_Morph > 4.07617: False (19.8/4.7)
##                                       RNPxl_Morph <= 4.07617:
##                                       :...RNPxl_Morph <= 2.374591: False (14.1)
##                                           RNPxl_Morph > 2.374591: [S2]
##
## SubTree [S1]
##
## RNPxl_immonium_score > 0.08947683: True (34)
## RNPxl_immonium_score <= 0.08947683:
## :...RNPxl_pl_im_MIC <= 0.001106155: False (69.2/45.5)
##     RNPxl_pl_im_MIC > 0.001106155:
##     :...RNPxl_Da_difference <= -0.002918677: False (3.3)
##         RNPxl_Da_difference > -0.002918677: True (155.7/10.8)
##
## SubTree [S2]
##
## OMS_precursor_mz_error_ppm <= -1.892518: False (12.1/4.8)
## OMS_precursor_mz_error_ppm > -1.892518:
## :...RNPxl_total_MIC > 0.4968228: True (74.4/0.3)
##     RNPxl_total_MIC <= 0.4968228:
##     :...RNPxl_pl_im_MIC > 0.001746027: False (8.6)
##         RNPxl_pl_im_MIC <= 0.001746027:
##         :...aa_class_charged <= 1: False (2.9)
##             aa_class_charged > 1:
##             :...aa_class_polar <= 7: True (155.2/7.2)
##                 aa_class_polar > 7: False (3.1)
##
## -----  Trial 6:  -----
##
## Decision tree:
##
## RNPxl_pl_pc_MIC <= 0.001713034:
## :...score <= 0.01433:
## :   :...RNPxl_Morph > 22.34067: False (17.1/8.9)
## :   :   RNPxl_Morph <= 22.34067:
## :   :   :...RNPxl_pl_im_MIC <= 0.01459797: True (379.7/20.5)
## :   :       RNPxl_pl_im_MIC > 0.01459797: False (12.5/6.7)
## :   score > 0.01433:
## :   :...RNPxl_pl_MIC > 0.03875625: True (88.6/14.3)
## :       RNPxl_pl_MIC <= 0.03875625:
## :       :...RNPxl_pl_modds <= 0.33299: False (172.8/18.7)
## :           RNPxl_pl_modds > 0.33299:
## :           :...RNPxl_score <= 0.2081771: False (162.8/82.1)
## :               RNPxl_score > 0.2081771: True (42.1/4.3)
## RNPxl_pl_pc_MIC > 0.001713034:
## :...RNPxl_pl_pc_MIC > 0.01692257: True (565.7/9.9)
##     RNPxl_pl_pc_MIC <= 0.01692257:
##     :...score <= 0.358071:
##         :...RNPxl_modds <= 8.219478: True (584/14.1)
##         :   RNPxl_modds > 8.219478: False (68.7/54.5)
```

```
##         score > 0.358071:
##         :...RNPxl_precursor_score > 0.009979509: True (24.5)
##             RNPxl_precursor_score <= 0.009979509:
##             :...aIndex <= 20: True (29.7/1)
##                 aIndex > 20:
##                 :...OMS_precursor_mz_error_ppm <= 0.6800386: False (58.8/14.3)
##                     OMS_precursor_mz_error_ppm > 0.6800386: True (49.4/3)
##
## -----  Trial 7:  -----
##
## Decision tree:
##
## aa_class_hydrophobic > 12:
## :...RNPxl_total_loss_score <= 11.3473: False (49.6/0.2)
## :   RNPxl_total_loss_score > 11.3473: True (14)
## aa_class_hydrophobic <= 12:
## :...RNPxl_pl_pc_MIC > 0.003447095:
##     :...aa_class_polar > 5: False (31.7/18.1)
##     :   aa_class_polar <= 5:
##     :   :...RNPxl_score <= -1.828889:
##     :       :...RNPxl_marker_ions_score > 0.04883788: False (10.7/2.7)
##     :       :   RNPxl_marker_ions_score <= 0.04883788:
##     :       :   :...RNPxl_score > -1.871791: False (10.9/4.4)
##     :       :       RNPxl_score <= -1.871791:
##     :       :       :...precursor_intensity <= 7494384: True (171.6/4.6)
##     :       :           precursor_intensity > 7494384: False (7.9/3.5)
##     :       RNPxl_score > -1.828889:
##     :       :...precursor <= 999.3894: True (577.1/0.8)
##     :           precursor > 999.3894:
##     :           :...precursor <= 1032.44: False (29.2/18.3)
##     :               precursor > 1032.44:
##     :               :...precursor_error_ppm <= 0.2342775: False (29.9/23.6)
##     :                   precursor_error_ppm > 0.2342775: True (254.5/1.6)
##     RNPxl_pl_pc_MIC <= 0.003447095:
##     :...RNPxl_partial_loss_score <= 0.04691507: False (52.7)
##         RNPxl_partial_loss_score > 0.04691507:
##         :...score <= 0.0121387:
##             :...RNPxl_score > 20.26862: True (84.5)
##             :   RNPxl_score <= 20.26862:
##             :   :...aa_class_hydrophobic <= 5: True (39.6)
##             :       aa_class_hydrophobic > 5:
##             :       :...RNPxl_score > 19.49398: False (9.4/2.9)
##             :           RNPxl_score <= 19.49398:
##             :           :...score > 0.00985416: True (40.5)
##             :               score <= 0.00985416:
##             :               :...score > 0.00165906: False (20.4/11.2)
##             :                   score <= 0.00165906:
##             :                   :...RNPxl_RNA_MASS_z0 > 635.0778: True (72.3)
##             :                       RNPxl_RNA_MASS_z0 <= 635.0778:
##             :                       :...RNPxl_total_MIC <= 0.1422275: False (5)
##             :                           RNPxl_total_MIC > 0.1422275: [S1]
##             score > 0.0121387:
##             :...RNPxl_precursor_score > 0.001085989: True (59.3/3)
##                 RNPxl_precursor_score <= 0.001085989:
```

```
##                 :...RNPxl_pl_Morph <= 3.113975: False (63.1/2.9)
##                     RNPxl_pl_Morph > 3.113975:
##                     :...RNPxl_pl_im_MIC > 0.009181726: False (23.9)
##                         RNPxl_pl_im_MIC <= 0.009181726:
##                         :...precursor > 1043.75: False (17.9)
##                             precursor <= 1043.75:
##                             :...RNPxl_score <= -2.23855: False (13.8)
##                                 RNPxl_score > -2.23855:
##                                 :...RNPxl_pl_MIC > 0.03875625: True (48.4)
##                                     RNPxl_pl_MIC <= 0.03875625:
##                                     :...RNPxl_immonium_score > 0.01925475: False (11.5)
##                                         RNPxl_immonium_score <= 0.01925475:
##                                         :...aIndex <= 56.67: False (15/2.9)
##                                             aIndex > 56.67: [S2]
##
## SubTree [S1]
##
## aa_class_hydrophobic > 9: True (63.2)
## aa_class_hydrophobic <= 9:
## :...Hydro > -0.16: True (67.2/1.4)
##     Hydro <= -0.16:
##     :...RNPxl_modds <= 0.7470319: False (6.1)
##         RNPxl_modds > 0.7470319:
##         :...RNPxl_pl_err <= 0.003015395: False (75/55.2)
##             RNPxl_pl_err > 0.003015395: True (47.9)
##
## SubTree [S2]
##
## precursor_error_ppm <= 0.4417974: False (17/7.6)
## precursor_error_ppm > 0.4417974:
## :...precursor_error_ppm > 2.94749: False (4)
##     precursor_error_ppm <= 2.94749:
##     :...RT > 3023.513: False (30/20.9)
##         RT <= 3023.513:
##         :...RNPxl_total_loss_score <= 2.523285: True (156.3/2.2)
##             RNPxl_total_loss_score > 2.523285: False (16.9/13.3)
##
## -----  Trial 8:  -----
##
## Decision tree:
##
## score <= 0.061008:
## :...RNPxl_pl_MIC <= 0.0083432:
## :   :...RNPxl_modds <= 0.5975084: False (35.7/14.8)
## :   :   RNPxl_modds > 0.5975084: True (155.2/7)
## :   RNPxl_pl_MIC > 0.0083432:
## :   :...RNPxl_pl_im_MIC <= 0.006229385:
## :       :...RNPxl_pl_err > 0.001676484: True (871.6/7.3)
## :       :   RNPxl_pl_err <= 0.001676484:
## :       :   :...RNPxl_pl_err <= 0.001613237: True (167.3/4)
## :       :       RNPxl_pl_err > 0.001613237: False (2.5/0.3)
## :       RNPxl_pl_im_MIC > 0.006229385:
## :       :...RNPxl_RNA_MASS_z0 <= 244.0695: False (5.6)
## :           RNPxl_RNA_MASS_z0 > 244.0695:
```

```
## :           :...RNPxl_mass_error_p <= 1.028149: False (5.3)
## :               RNPxl_mass_error_p > 1.028149: True (182/9.9)
## score > 0.061008:
## :...RNPxl_pl_pc_MIC > 0.021649: True (255.6/8.4)
##     RNPxl_pl_pc_MIC <= 0.021649:
##     :...precursor > 1057.878: False (57.2)
##         precursor <= 1057.878:
##         :...RNPxl_pl_Morph <= 3.113975:
##             :...RNPxl_precursor_score <= 0.0103176: False (134.7/30.4)
##             :   RNPxl_precursor_score > 0.0103176: True (29.1)
##             RNPxl_pl_Morph > 3.113975:
##             :...aa_class_hydrophobic > 12: False (13.8)
##                 aa_class_hydrophobic <= 12:
##                 :...RNPxl_pl_im_MIC > 0.009181726: False (11.2)
##                     RNPxl_pl_im_MIC <= 0.009181726:
##                     :...RT > 3783.566: False (10.1)
##                         RT <= 3783.566:
##                         :...RNPxl_pl_pc_MIC > 0.001696311:
##                             :...RNPxl_immonium_score > 0.02689577: False (4.2/1.5)
##                             :   RNPxl_immonium_score <= 0.02689577:
##                             :   :...precursor_error_ppm <= 0.06626505: False (2.5)
##                             :       precursor_error_ppm > 0.06626505: True (179.2/1)
##                             RNPxl_pl_pc_MIC <= 0.001696311:
##                             :...Peplength > 23: True (30.4/0.1)
##                                 Peplength <= 23:
##                                 :...RNPxl_pl_MIC > 0.04691937: True (25.8)
##                                     RNPxl_pl_MIC <= 0.04691937:
##                                     :...precursor > 946.3495: False (16.5)
##                                         precursor <= 946.3495: [S1]
##
## SubTree [S1]
##
## RNPxl_partial_loss_score <= 3.192354: False (40.8/15.8)
## RNPxl_partial_loss_score > 3.192354: True (149.5/15.6)
##
## -----  Trial 9:  -----
##
## Decision tree:
##
## RNPxl_pl_pc_MIC <= 0.0001836105:
## :...RNPxl_marker_ions_score > 0.1432697: True (66.3/0.1)
## :   RNPxl_marker_ions_score <= 0.1432697:
## :   :...RNPxl_pl_MIC > 0.05793984: True (59.3/2.6)
## :       RNPxl_pl_MIC <= 0.05793984:
## :       :...RNPxl_precursor_score > 0.002900583: True (54.5/3.6)
## :           RNPxl_precursor_score <= 0.002900583:
## :           :...RNPxl_total_MIC <= 0.4894923: False (403.3/152.6)
## :               RNPxl_total_MIC > 0.4894923:
## :               :...RNPxl_RNA_MASS_z0 <= 324.0359: True (118.8/2.9)
## :                   RNPxl_RNA_MASS_z0 > 324.0359: False (28.4/14.9)
## RNPxl_pl_pc_MIC > 0.0001836105:
## :...RNPxl_RNA_MASS_z0 <= 244.0695: False (48.7/26.4)
##     RNPxl_RNA_MASS_z0 > 244.0695:
##     :...RNPxl_partial_loss_score <= 0.03149006: False (53.5/34.4)
```

```
##         RNPxl_partial_loss_score > 0.03149006:
##         :...RNPxl_pl_modds > 1.364098: True (311)
##             RNPxl_pl_modds <= 1.364098:
##             :...RNPxl_Da_difference <= -0.0004365474:
##                 :...RNPxl_pl_MIC <= 0.02963713: True (502.5/4.1)
##                 :   RNPxl_pl_MIC > 0.02963713: False (17.3/10.6)
##                 RNPxl_Da_difference > -0.0004365474:
##                 :...RNPxl_Da_difference <= -0.0003878434: False (10.4/0.4)
##                     RNPxl_Da_difference > -0.0003878434:
##                     :...RNPxl_pl_pc_MIC > 0.01306356: True (169.6)
##                         RNPxl_pl_pc_MIC <= 0.01306356:
##                         :...score > 0.463182: False (38.7/17.6)
##                             score <= 0.463182:
##                             :...precursor > 1176.198: False (14.3/5.1)
##                                 precursor <= 1176.198:
##                                 :...RNPxl_pl_im_MIC > 0.009081018: False (7.5/1.9)
##                                     RNPxl_pl_im_MIC <= 0.009081018:
##                                     :...RNPxl_Morph <= 2.544801: False (5.3/1)
##                                         RNPxl_Morph > 2.544801: True (307.4/9.6)
##
##
## Evaluation on training data (1340 cases):
##
## Trial           Decision Tree
## -----      ----------------------
##    Size      Errors   Cost
##
##    0     26   69( 5.1%)   0.06
##    1     14  129( 9.6%)   0.20
##    2     11  106( 7.9%)   0.24
##    3     23  121( 9.0%)   0.23
##    4     23  160(11.9%)   0.18
##    5     33  105( 7.8%)   0.14
##    6     14  130( 9.7%)   0.22
##    7     37   77( 5.7%)   0.10
##    8     23   67( 5.0%)   0.16
##    9     18  111( 8.3%)   0.13
## boost              7( 0.5%)   0.01   <<
##
##
##     (a)   (b)    <-classified as
##    ----  ----
##     676     4    (a): class False
##       3   657    (b): class True
##
##
##  Attribute usage:
##
##  100.00% score
##  100.00% RNPxl_pl_pc_MIC
##  100.00% aa_class_hydrophobic
##   99.10% RNPxl_pl_modds
##   95.15% RNPxl_precursor_score
##   94.33% RNPxl_partial_loss_score
```

```
##   94.25% RNPxl_pl_MIC
##   91.04% RNPxl_total_MIC
##   90.15% precursor
##   83.58% RNPxl_total_loss_score
##   74.93% aa_class_polar
##   73.21% RT
##   67.54% RNPxl_score
##   66.72% RNPxl_marker_ions_score
##   60.90% RNPxl_RNA_MASS_z0
##   57.99% RNPxl_pl_Morph
##   56.49% RNPxl_pl_im_MIC
##   53.58% RNPxl_modds
##   44.40% Peplength
##   44.25% Hydro
##   40.00% pI
##   37.69% aIndex
##   37.31% RNPxl_Da_difference
##   29.63% RNPxl_best_localization_score
##   28.81% RNPxl_pl_err
##   26.87% RNPxl_Morph
##   22.99% aa_class_charged
##   22.69% RNPxl_immonium_score
##   21.42% precursor_error_ppm
##   16.34% RNPxl_MIC
##    8.28% OMS_precursor_mz_error_ppm
##    5.67% RNPxl_mass_error_p
##    4.78% precursor_intensity
##
##
## Time: 0.3 secs
```

```
C5_UV_RNA_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_test_C5)
CrossTable(ml_UV_RNA_test_C5$Curated, C5_UV_RNA_predict_boost_pen, prop.chisq = FALSE,
           prop.c = FALSE, prop.r = FALSE, dnn = c("actual TRUE", "predicted TRUE"))
```

```
##
##
##    Cell Contents
## |-------------------------|
## |                       N |
## |         N / Table Total |
## |-------------------------|
##
##
## Total Observations in Table:  336
##
##
##              | predicted TRUE
##  actual TRUE |     False |      True | Row Total |
## -------------|-----------|-----------|-----------|
##        False |       143 |        15 |       158 |
##              |     0.426 |     0.045 |           |
## -------------|-----------|-----------|-----------|
##         True |         7 |       171 |       178 |
##              |     0.021 |     0.509 |           |
```

```
## -------------|-----------|-----------|-----------|
## Column Total |       150 |       186 |       336 |
## -------------|-----------|-----------|-----------|
##
##
```

Classifyers

UV RNA

One Rule (1R)

RIPPER

```
library(rJava)
library(RWeka)

RIPPER_model_UV_RNA <- JRip(Curated ~ ., data = ml_UV_RNA_train_C5)
RIPPER_model_UV_RNA
```

```
## JRIP rules:
## ===========
##
## (score <= 0.079243) and (RNPxl_pl_pc_MIC >= 0.003078) => Curated=True (342.0/5.0)
## (score <= 0.098059) and (RNPxl_pl_Morph >= 3.007485) and (RNPxl_precursor_score >= 0.000504) => Cura
## (RNPxl_pl_pc_MIC >= 0.01727) => Curated=True (78.0/4.0)
## (score <= 0.015775) and (RNPxl_pl_MIC >= 0.010216) => Curated=True (72.0/6.0)
## (score <= 0.29027) and (RNPxl_score >= 0.319302) and (Hydro >= 0.26) => Curated=True (27.0/4.0)
## (RNPxl_pl_pc_MIC >= 0.00049) and (aIndex <= 78) and (score <= 0.535324) => Curated=True (27.0/2.0)
## (RNPxl_pl_MIC >= 0.038842) and (precursor <= 738.084215) => Curated=True (11.0/1.0)
##  => Curated=False (688.0/34.0)
##
## Number of Rules : 8
```

```
summary(RIPPER_model_UV_RNA)
```

```
##
## === Summary ===
##
## Correctly Classified Instances        1280               95.5224 %
## Incorrectly Classified Instances        60                4.4776 %
## Kappa statistic                          0.9104
## Mean absolute error                      0.0844
## Root mean squared error                  0.2054
## Relative absolute error                 16.8818 %
## Root relative squared error             41.0875 %
## Total Number of Instances             1340
##
## === Confusion Matrix ===
##
##    a   b   <-- classified as
##  654  26 |   a = False
##   34 626 |   b = True
```

```
RIPPER_UV_RNA_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_test_C5)
CrossTable(ml_UV_RNA_test_C5$Curated, RIPPER_UV_RNA_predict, prop.chisq = FALSE,
```

```
    prop.c = FALSE, prop.r = FALSE, dnn = c("actual TRUE", "predicted TRUE"))
```

```
##
##
##    Cell Contents
## |-------------------------|
## |                       N |
## |         N / Table Total |
## |-------------------------|
##
##
## Total Observations in Table:  336
##
##
##              | predicted TRUE
##  actual TRUE |     False |      True | Row Total |
## -------------|-----------|-----------|-----------|
##        False |       145 |        13 |       158 |
##              |     0.432 |     0.039 |           |
## -------------|-----------|-----------|-----------|
##         True |        14 |       164 |       178 |
##              |     0.042 |     0.488 |           |
## -------------|-----------|-----------|-----------|
## Column Total |       159 |       177 |       336 |
## -------------|-----------|-----------|-----------|
##
##
```

UV RNA FAIMS runs S30

Now, let us test KNN, C5, and RIPPER models on unknown data: Ecoli UV FAIMS runs

Data setup UV RNA CV 35_45

```
UV_RNA_FAIMS_35_45_KNN <- read_delim("AWulf_030919_Ecoli_UV_S30_FAIMS_35_45_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_35_45_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_35_45_KNN))
names(UV_RNA_FAIMS_35_45_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_35_45_KNN))
names(UV_RNA_FAIMS_35_45_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_35_45_KNN))
names(UV_RNA_FAIMS_35_45_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_35_45_KNN))
UV_RNA_FAIMS_35_45_KNN$XLinker <- "UV"
UV_RNA_FAIMS_35_45_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_35_45_KNN$Sample <- "S30"
UV_RNA_FAIMS_35_45_KNN <- UV_RNA_FAIMS_35_45_KNN[UV_RNA_FAIMS_35_45_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_35_45_KNN$sequence))
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_35_45_KNN$prepPep))
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_35_45_KNN$prepPep))
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_35_45_KNN$prepPep)
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_35_45_KNN$prepPep)
UV_RNA_FAIMS_35_45_KNN$Pepseq <- UV_RNA_FAIMS_35_45_KNN$prepPep
UV_RNA_FAIMS_35_45_KNN$Peplength <- nchar(UV_RNA_FAIMS_35_45_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_35_45_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_35_45_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_35_45_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_35_45_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_35_45_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_35_45_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_35_45_KNN$pI <- round(pI(UV_RNA_FAIMS_35_45_KNN$Pepseq), 2)
UV_RNA_FAIMS_35_45_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_35_45_KNN$Pepseq), 2)
UV_RNA_FAIMS_35_45_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_35_45_KNN$RNPxl_best_localization)
UV_RNA_FAIMS_35_45_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_35_45_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_35_45_KNN$mw <- round(mw(UV_RNA_FAIMS_35_45_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_35_45_KNN$cv <- c("35_45")

names(UV_RNA_FAIMS_35_45_KNN)[names(UV_RNA_FAIMS_35_45_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_35_45_KNN)[names(UV_RNA_FAIMS_35_45_KNN) == "precursor_error_(_ppm_)"] <- "precursor
UV_RNA_FAIMS_35_45_KNN <- UV_RNA_FAIMS_35_45_KNN %>% filter(RNPxl_isPhospho == "0")

UV_RNA_FAIMS_35_45_KNN_model <- UV_RNA_FAIMS_35_45_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_35_45_KNN_model_norm <- UV_RNA_FAIMS_35_45_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_35_45_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_35_45_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_35_45_KNN_model_norm[is.na(UV_RNA_FAIMS_35_45_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_35_45_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_35_45_KNN_model_norm
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_35_45_KNN_model$Prediction <- UV_RNA_FAIMS_35_45_knn_pred
table(UV_RNA_FAIMS_35_45_KNN_model$Prediction)
```

```
##
## False  True
## 13561   454
```

```
UV_RNA_FAIMS_35_45_KNN$Prediction_KNN <- UV_RNA_FAIMS_35_45_knn_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_35_45_test_C5<-UV_RNA_FAIMS_35_45_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_35_45_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_35_45_test_C

ml_UV_RNA_FAIMS_35_45_test_C5$Prediction<-C5_UV_RNA_FAIMS_35_45_predict_boost_pen
table(ml_UV_RNA_FAIMS_35_45_test_C5$Prediction)
```

```
##
## False  True
## 10904  3111
```

```
UV_RNA_FAIMS_35_45_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_35_45_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_35_45_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_35_45_test_C5)
ml_UV_RNA_FAIMS_35_45_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_predict
table(ml_UV_RNA_FAIMS_35_45_test_C5$Prediction_RIPPER)
```

```
##
## False  True
##  9928  4087
```

```
UV_RNA_FAIMS_35_45_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_predict
```

Data setup UV RNA CV 40_50

```
UV_RNA_FAIMS_40_50_KNN <- read_delim("AWulf_030919_Ecoli_UV_S30_FAIMS_40_50_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
```

```
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )

## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_40_50_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_40_50_KNN))
names(UV_RNA_FAIMS_40_50_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_40_50_KNN))
names(UV_RNA_FAIMS_40_50_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_40_50_KNN))
names(UV_RNA_FAIMS_40_50_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_40_50_KNN))
UV_RNA_FAIMS_40_50_KNN$XLinker <- "UV"
UV_RNA_FAIMS_40_50_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_40_50_KNN$Sample <- "S30"
UV_RNA_FAIMS_40_50_KNN <- UV_RNA_FAIMS_40_50_KNN[UV_RNA_FAIMS_40_50_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_40_50_KNN$sequence))
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_40_50_KNN$prepPep))
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_40_50_KNN$prepPep))
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_40_50_KNN$prepPep)
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_40_50_KNN$prepPep)
UV_RNA_FAIMS_40_50_KNN$Pepseq <- UV_RNA_FAIMS_40_50_KNN$prepPep
UV_RNA_FAIMS_40_50_KNN$Peplength <- nchar(UV_RNA_FAIMS_40_50_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_40_50_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_40_50_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_40_50_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_40_50_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_40_50_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_40_50_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_40_50_KNN$pI <- round(pI(UV_RNA_FAIMS_40_50_KNN$Pepseq), 2)
UV_RNA_FAIMS_40_50_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_40_50_KNN$Pepseq), 2)
UV_RNA_FAIMS_40_50_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_40_50_KNN$RNPxl_best_localization)
UV_RNA_FAIMS_40_50_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_40_50_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_40_50_KNN$mw <- round(mw(UV_RNA_FAIMS_40_50_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_40_50_KNN$cv <- c("40_50")

names(UV_RNA_FAIMS_40_50_KNN)[names(UV_RNA_FAIMS_40_50_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_40_50_KNN)[names(UV_RNA_FAIMS_40_50_KNN) == "precursor_error_(_ppm_)"] <- "precursor_
UV_RNA_FAIMS_40_50_KNN <- UV_RNA_FAIMS_40_50_KNN %>% filter(RNPxl_isPhospho == "0")

UV_RNA_FAIMS_40_50_KNN_model <- UV_RNA_FAIMS_40_50_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_40_50_KNN_model_norm <- UV_RNA_FAIMS_40_50_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_40_50_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_40_50_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_40_50_KNN_model_norm[is.na(UV_RNA_FAIMS_40_50_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_40_50_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_40_50_KNN_model_norm
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_40_50_KNN_model$Prediction <- UV_RNA_FAIMS_40_50_knn_pred
table(UV_RNA_FAIMS_40_50_KNN_model$Prediction)
```

```
##
## False  True
## 14337   442
```

```
UV_RNA_FAIMS_40_50_KNN$Prediction_KNN <- UV_RNA_FAIMS_40_50_knn_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_40_50_test_C5<-UV_RNA_FAIMS_40_50_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_40_50_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_40_50_test_C

ml_UV_RNA_FAIMS_40_50_test_C5$Prediction<-C5_UV_RNA_FAIMS_40_50_predict_boost_pen
table(ml_UV_RNA_FAIMS_40_50_test_C5$Prediction)
```

```
##
## False  True
## 10742  4037
```

```
UV_RNA_FAIMS_40_50_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_40_50_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_40_50_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_40_50_test_C5)
ml_UV_RNA_FAIMS_40_50_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_40_50_predict
table(ml_UV_RNA_FAIMS_40_50_test_C5$Prediction_RIPPER)
```

```
##
## False  True
##  9303  5476
```

```
UV_RNA_FAIMS_40_50_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_40_50_predict
```

Data setup UV RNA CV 55_65

```
UV_RNA_FAIMS_55_65_KNN <- read_delim("AWulf_030919_Ecoli_UV_S30_FAIMS_55_65_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
```

```
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_55_65_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_55_65_KNN))
names(UV_RNA_FAIMS_55_65_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_55_65_KNN))
names(UV_RNA_FAIMS_55_65_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_55_65_KNN))
names(UV_RNA_FAIMS_55_65_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_55_65_KNN))
UV_RNA_FAIMS_55_65_KNN$XLinker <- "UV"
UV_RNA_FAIMS_55_65_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_55_65_KNN$Sample <- "S30"
UV_RNA_FAIMS_55_65_KNN <- UV_RNA_FAIMS_55_65_KNN[UV_RNA_FAIMS_55_65_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_55_65_KNN$sequence))
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_55_65_KNN$prepPep))
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_55_65_KNN$prepPep))
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_55_65_KNN$prepPep)
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_55_65_KNN$prepPep)
UV_RNA_FAIMS_55_65_KNN$Pepseq <- UV_RNA_FAIMS_55_65_KNN$prepPep
UV_RNA_FAIMS_55_65_KNN$Peplength <- nchar(UV_RNA_FAIMS_55_65_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_55_65_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_55_65_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_55_65_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_55_65_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_55_65_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_55_65_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_55_65_KNN$pI <- round(pI(UV_RNA_FAIMS_55_65_KNN$Pepseq), 2)
UV_RNA_FAIMS_55_65_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_55_65_KNN$Pepseq), 2)
UV_RNA_FAIMS_55_65_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_55_65_KNN$RNPxl_best_localization)
UV_RNA_FAIMS_55_65_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_55_65_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_55_65_KNN$mw <- round(mw(UV_RNA_FAIMS_55_65_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_55_65_KNN$cv <- c("55_65")

names(UV_RNA_FAIMS_55_65_KNN)[names(UV_RNA_FAIMS_55_65_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_55_65_KNN)[names(UV_RNA_FAIMS_55_65_KNN) == "precursor_error_(_ppm_)"] <- "precursor_
UV_RNA_FAIMS_55_65_KNN <- UV_RNA_FAIMS_55_65_KNN %>% filter(RNPxl_isPhospho == "0")

UV_RNA_FAIMS_55_65_KNN_model <- UV_RNA_FAIMS_55_65_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_55_65_KNN_model_norm <- UV_RNA_FAIMS_55_65_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_55_65_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_55_65_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_55_65_KNN_model_norm[is.na(UV_RNA_FAIMS_55_65_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_55_65_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_55_65_KNN_model_norm
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_55_65_KNN_model$Prediction <- UV_RNA_FAIMS_55_65_knn_pred
table(UV_RNA_FAIMS_55_65_KNN_model$Prediction)
```

```
##
## False  True
## 16443   453
```

```
UV_RNA_FAIMS_55_65_KNN$Prediction_KNN <- UV_RNA_FAIMS_55_65_knn_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_55_65_test_C5<-UV_RNA_FAIMS_55_65_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_55_65_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_55_65_test_C

ml_UV_RNA_FAIMS_55_65_test_C5$Prediction<-C5_UV_RNA_FAIMS_55_65_predict_boost_pen
table(ml_UV_RNA_FAIMS_55_65_test_C5$Prediction)
```

```
##
## False  True
## 13225  3671
```

```
UV_RNA_FAIMS_55_65_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_55_65_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_55_65_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_55_65_test_C5)
ml_UV_RNA_FAIMS_55_65_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_55_65_predict
table(ml_UV_RNA_FAIMS_55_65_test_C5$Prediction_RIPPER)
```

```
##
## False  True
##  7922  8974
```

```
UV_RNA_FAIMS_55_65_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_55_65_predict
```

Data setup UV RNA CV 60_70

```
UV_RNA_FAIMS_60_70_KNN <- read_delim("AWulf_050919_Ecoli_UV_S30_FAIMS_60_70_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
```

```
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )

## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_60_70_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_60_70_KNN))
names(UV_RNA_FAIMS_60_70_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_60_70_KNN))
names(UV_RNA_FAIMS_60_70_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_60_70_KNN))
names(UV_RNA_FAIMS_60_70_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_60_70_KNN))
UV_RNA_FAIMS_60_70_KNN$XLinker <- "UV"
UV_RNA_FAIMS_60_70_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_60_70_KNN$Sample <- "S30"
UV_RNA_FAIMS_60_70_KNN <- UV_RNA_FAIMS_60_70_KNN[UV_RNA_FAIMS_60_70_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_60_70_KNN$sequence))
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_60_70_KNN$prepPep))
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_60_70_KNN$prepPep))
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_60_70_KNN$prepPep)
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_60_70_KNN$prepPep)
UV_RNA_FAIMS_60_70_KNN$Pepseq <- UV_RNA_FAIMS_60_70_KNN$prepPep
UV_RNA_FAIMS_60_70_KNN$Peplength <- nchar(UV_RNA_FAIMS_60_70_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_60_70_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_60_70_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_60_70_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_60_70_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_60_70_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_60_70_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_60_70_KNN$pI <- round(pI(UV_RNA_FAIMS_60_70_KNN$Pepseq), 2)
UV_RNA_FAIMS_60_70_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_60_70_KNN$Pepseq), 2)
UV_RNA_FAIMS_60_70_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_60_70_KNN$RNPxl_best_localization)
UV_RNA_FAIMS_60_70_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_60_70_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_60_70_KNN$mw <- round(mw(UV_RNA_FAIMS_60_70_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_60_70_KNN$cv <- c("60_70")

names(UV_RNA_FAIMS_60_70_KNN)[names(UV_RNA_FAIMS_60_70_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_60_70_KNN)[names(UV_RNA_FAIMS_60_70_KNN) == "precursor_error_(_ppm_)"] <- "precursor_
UV_RNA_FAIMS_60_70_KNN <- UV_RNA_FAIMS_60_70_KNN %>% filter(RNPxl_isPhospho == "0")

UV_RNA_FAIMS_60_70_KNN_model <- UV_RNA_FAIMS_60_70_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_60_70_KNN_model_norm <- UV_RNA_FAIMS_60_70_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_60_70_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_60_70_KNN_model_norm,
```

```
    normalize))
UV_RNA_FAIMS_60_70_KNN_model_norm[is.na(UV_RNA_FAIMS_60_70_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_60_70_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_60_70_KNN_model_norm
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_60_70_KNN_model$Prediction <- UV_RNA_FAIMS_60_70_knn_pred
table(UV_RNA_FAIMS_60_70_KNN_model$Prediction)
```

```
##
## False  True
## 13672   611
```

```
UV_RNA_FAIMS_60_70_KNN$Prediction_KNN <- UV_RNA_FAIMS_60_70_knn_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_60_70_test_C5<-UV_RNA_FAIMS_60_70_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_60_70_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_60_70_test_C

ml_UV_RNA_FAIMS_60_70_test_C5$Prediction<-C5_UV_RNA_FAIMS_60_70_predict_boost_pen
table(ml_UV_RNA_FAIMS_60_70_test_C5$Prediction)
```

```
##
## False  True
## 11661  2622
```

```
UV_RNA_FAIMS_60_70_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_60_70_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_60_70_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_60_70_test_C5)
ml_UV_RNA_FAIMS_60_70_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_60_70_predict
table(ml_UV_RNA_FAIMS_60_70_test_C5$Prediction_RIPPER)
```

```
##
## False  True
##  7269  7014
```

```
UV_RNA_FAIMS_60_70_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_60_70_predict
```

UV RNA FAIMS runs S30

Now, let us test KNN, C5, and RIPPER models on unknown data: Ecoli UV FAIMS runs

Data setup UV RNA CV 35_45

```
UV_RNA_FAIMS_35_45_KNN <- read_delim("AWulf_030919_Ecoli_UV_S30_FAIMS_35_45_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_35_45_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_35_45_KNN))
names(UV_RNA_FAIMS_35_45_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_35_45_KNN))
names(UV_RNA_FAIMS_35_45_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_35_45_KNN))
names(UV_RNA_FAIMS_35_45_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_35_45_KNN))
UV_RNA_FAIMS_35_45_KNN$XLinker <- "UV"
UV_RNA_FAIMS_35_45_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_35_45_KNN$Sample <- "30"
UV_RNA_FAIMS_35_45_KNN <- UV_RNA_FAIMS_35_45_KNN[UV_RNA_FAIMS_35_45_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_35_45_KNN$sequence))
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_35_45_KNN$prepPep))
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_35_45_KNN$prepPep))
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_35_45_KNN$prepPep)
UV_RNA_FAIMS_35_45_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_35_45_KNN$prepPep)
UV_RNA_FAIMS_35_45_KNN$Pepseq <- UV_RNA_FAIMS_35_45_KNN$prepPep
UV_RNA_FAIMS_35_45_KNN$Peplength <- nchar(UV_RNA_FAIMS_35_45_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_35_45_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_35_45_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_35_45_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_35_45_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_35_45_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_35_45_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_35_45_KNN$pI <- round(pI(UV_RNA_FAIMS_35_45_KNN$Pepseq), 2)
UV_RNA_FAIMS_35_45_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_35_45_KNN$Pepseq), 2)
UV_RNA_FAIMS_35_45_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_35_45_KNN$RNPxl_best_localization)
UV_RNA_FAIMS_35_45_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_35_45_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_35_45_KNN$mw <- round(mw(UV_RNA_FAIMS_35_45_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_35_45_KNN$cv <- c("35_45")

names(UV_RNA_FAIMS_35_45_KNN)[names(UV_RNA_FAIMS_35_45_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_35_45_KNN)[names(UV_RNA_FAIMS_35_45_KNN) == "precursor_error_(_ppm_)"] <- "precursor_
UV_RNA_FAIMS_35_45_KNN <- UV_RNA_FAIMS_35_45_KNN %>% filter(RNPxl_isPhospho == "0")
```

```
UV_RNA_FAIMS_35_45_KNN_model <- UV_RNA_FAIMS_35_45_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_35_45_KNN_model_norm <- UV_RNA_FAIMS_35_45_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_35_45_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_35_45_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_35_45_KNN_model_norm[is.na(UV_RNA_FAIMS_35_45_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_35_45_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_35_45_KNN_model_norm
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_35_45_KNN_model$Prediction <- UV_RNA_FAIMS_35_45_knn_pred
table(UV_RNA_FAIMS_35_45_KNN_model$Prediction)
```

```
##
## False  True
## 13562   453
```

```
UV_RNA_FAIMS_35_45_KNN$Prediction_KNN <- UV_RNA_FAIMS_35_45_knn_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_35_45_test_C5<-UV_RNA_FAIMS_35_45_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_35_45_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_35_45_test_C

ml_UV_RNA_FAIMS_35_45_test_C5$Prediction<-C5_UV_RNA_FAIMS_35_45_predict_boost_pen
table(ml_UV_RNA_FAIMS_35_45_test_C5$Prediction)
```

```
##
## False  True
## 10904  3111
```

```
UV_RNA_FAIMS_35_45_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_35_45_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_35_45_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_35_45_test_C5)
ml_UV_RNA_FAIMS_35_45_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_predict
table(ml_UV_RNA_FAIMS_35_45_test_C5$Prediction_RIPPER)
```

```
##
## False  True
```

```
##  9928  4087
```

```
UV_RNA_FAIMS_35_45_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_predict
```

Data setup UV RNA CV 40_50

```
UV_RNA_FAIMS_40_50_KNN <- read_delim("AWulf_030919_Ecoli_UV_S30_FAIMS_40_50_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_40_50_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_40_50_KNN))
names(UV_RNA_FAIMS_40_50_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_40_50_KNN))
names(UV_RNA_FAIMS_40_50_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_40_50_KNN))
names(UV_RNA_FAIMS_40_50_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_40_50_KNN))
UV_RNA_FAIMS_40_50_KNN$XLinker <- "UV"
UV_RNA_FAIMS_40_50_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_40_50_KNN$Sample <- "S30"
UV_RNA_FAIMS_40_50_KNN <- UV_RNA_FAIMS_40_50_KNN[UV_RNA_FAIMS_40_50_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_40_50_KNN$sequence))
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_40_50_KNN$prepPep))
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_40_50_KNN$prepPep))
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_40_50_KNN$prepPep)
UV_RNA_FAIMS_40_50_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_40_50_KNN$prepPep)
UV_RNA_FAIMS_40_50_KNN$Pepseq <- UV_RNA_FAIMS_40_50_KNN$prepPep
UV_RNA_FAIMS_40_50_KNN$Peplength <- nchar(UV_RNA_FAIMS_40_50_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_40_50_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_40_50_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_40_50_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_40_50_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_40_50_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_40_50_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_40_50_KNN$pI <- round(pI(UV_RNA_FAIMS_40_50_KNN$Pepseq), 2)
UV_RNA_FAIMS_40_50_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_40_50_KNN$Pepseq), 2)
UV_RNA_FAIMS_40_50_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_40_50_KNN$RNPxl_best_localization)
UV_RNA_FAIMS_40_50_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_40_50_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_40_50_KNN$mw <- round(mw(UV_RNA_FAIMS_40_50_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_40_50_KNN$cv <- c("40_50")
```

```
names(UV_RNA_FAIMS_40_50_KNN)[names(UV_RNA_FAIMS_40_50_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_40_50_KNN)[names(UV_RNA_FAIMS_40_50_KNN) == "precursor_error_(_ppm_)"] <- "precursor_
UV_RNA_FAIMS_40_50_KNN <- UV_RNA_FAIMS_40_50_KNN %>% filter(RNPxl_isPhospho == "0")

UV_RNA_FAIMS_40_50_KNN_model <- UV_RNA_FAIMS_40_50_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_40_50_KNN_model_norm <- UV_RNA_FAIMS_40_50_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_40_50_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_40_50_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_40_50_KNN_model_norm[is.na(UV_RNA_FAIMS_40_50_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_40_50_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_40_50_KNN_model_norm
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_40_50_KNN_model$Prediction <- UV_RNA_FAIMS_40_50_knn_pred
table(UV_RNA_FAIMS_40_50_KNN_model$Prediction)
```

```
##
## False  True
## 14337   442
```

```
UV_RNA_FAIMS_40_50_KNN$Prediction_KNN <- UV_RNA_FAIMS_40_50_knn_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_40_50_test_C5<-UV_RNA_FAIMS_40_50_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_40_50_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_40_50_test_C

ml_UV_RNA_FAIMS_40_50_test_C5$Prediction<-C5_UV_RNA_FAIMS_40_50_predict_boost_pen
table(ml_UV_RNA_FAIMS_40_50_test_C5$Prediction)
```

```
##
## False  True
## 10742  4037
```

```
UV_RNA_FAIMS_40_50_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_40_50_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_40_50_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_40_50_test_C5)
ml_UV_RNA_FAIMS_40_50_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_40_50_predict
```

```
table(ml_UV_RNA_FAIMS_40_50_test_C5$Prediction_RIPPER)
```

```
##
## False  True
##  9303  5476
```

```
UV_RNA_FAIMS_40_50_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_40_50_predict
```

Data setup UV RNA CV 55_65

```
UV_RNA_FAIMS_55_65_KNN <- read_delim("AWulf_030919_Ecoli_UV_S30_FAIMS_55_65_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_55_65_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_55_65_KNN))
names(UV_RNA_FAIMS_55_65_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_55_65_KNN))
names(UV_RNA_FAIMS_55_65_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_55_65_KNN))
names(UV_RNA_FAIMS_55_65_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_55_65_KNN))
UV_RNA_FAIMS_55_65_KNN$XLinker <- "UV"
UV_RNA_FAIMS_55_65_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_55_65_KNN$Sample <- "S30"
UV_RNA_FAIMS_55_65_KNN <- UV_RNA_FAIMS_55_65_KNN[UV_RNA_FAIMS_55_65_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_55_65_KNN$sequence))
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_55_65_KNN$prepPep))
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_55_65_KNN$prepPep))
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_55_65_KNN$prepPep)
UV_RNA_FAIMS_55_65_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_55_65_KNN$prepPep)
UV_RNA_FAIMS_55_65_KNN$Pepseq <- UV_RNA_FAIMS_55_65_KNN$prepPep
UV_RNA_FAIMS_55_65_KNN$Peplength <- nchar(UV_RNA_FAIMS_55_65_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_55_65_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_55_65_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_55_65_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_55_65_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_55_65_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_55_65_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_55_65_KNN$pI <- round(pI(UV_RNA_FAIMS_55_65_KNN$Pepseq), 2)
UV_RNA_FAIMS_55_65_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_55_65_KNN$Pepseq), 2)
UV_RNA_FAIMS_55_65_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_55_65_KNN$RNPxl_best_localization)
UV_RNA_FAIMS_55_65_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_55_65_KNN$Pepseq,
```

```
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_55_65_KNN$mw <- round(mw(UV_RNA_FAIMS_55_65_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_55_65_KNN$cv <- c("55_65")

names(UV_RNA_FAIMS_55_65_KNN)[names(UV_RNA_FAIMS_55_65_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_55_65_KNN)[names(UV_RNA_FAIMS_55_65_KNN) == "precursor_error_(_ppm_)"] <- "precursor_
UV_RNA_FAIMS_55_65_KNN <- UV_RNA_FAIMS_55_65_KNN %>% filter(RNPxl_isPhospho == "0")

UV_RNA_FAIMS_55_65_KNN_model <- UV_RNA_FAIMS_55_65_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_55_65_KNN_model_norm <- UV_RNA_FAIMS_55_65_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_55_65_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_55_65_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_55_65_KNN_model_norm[is.na(UV_RNA_FAIMS_55_65_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_55_65_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_55_65_KNN_model_norm
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_55_65_KNN_model$Prediction <- UV_RNA_FAIMS_55_65_knn_pred
table(UV_RNA_FAIMS_55_65_KNN_model$Prediction)
```

```
##
## False  True
## 16443   453
```

```
UV_RNA_FAIMS_55_65_KNN$Prediction_KNN <- UV_RNA_FAIMS_55_65_knn_pred

d <- UV_RNA_FAIMS_55_65_KNN %>% filter(Prediction_KNN == "True") %>% select(accessions) %>%
    distinct()
nrow(d)
```

```
## [1] 359
```

```
write_excel_csv(as.data.frame(d), "S30_UV_RNA_FAIMS_55_65_accessions.csv")
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_55_65_test_C5<-UV_RNA_FAIMS_55_65_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_55_65_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_55_65_test_
```

```
ml_UV_RNA_FAIMS_55_65_test_C5$Prediction<-C5_UV_RNA_FAIMS_55_65_predict_boost_pen
table(ml_UV_RNA_FAIMS_55_65_test_C5$Prediction)
```

```
##
## False  True
## 13225  3671
```

```
UV_RNA_FAIMS_55_65_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_55_65_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_55_65_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_55_65_test_C5)
ml_UV_RNA_FAIMS_55_65_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_55_65_predict
table(ml_UV_RNA_FAIMS_55_65_test_C5$Prediction_RIPPER)
```

```
##
## False  True
##  7922  8974
```

```
UV_RNA_FAIMS_55_65_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_55_65_predict
```

Data setup UV RNA CV 60_70

```
UV_RNA_FAIMS_60_70_KNN <- read_delim("AWulf_050919_Ecoli_UV_S30_FAIMS_60_70_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_60_70_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_60_70_KNN))
names(UV_RNA_FAIMS_60_70_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_60_70_KNN))
names(UV_RNA_FAIMS_60_70_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_60_70_KNN))
names(UV_RNA_FAIMS_60_70_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_60_70_KNN))
UV_RNA_FAIMS_60_70_KNN$XLinker <- "UV"
UV_RNA_FAIMS_60_70_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_60_70_KNN$Sample <- "S30"
UV_RNA_FAIMS_60_70_KNN <- UV_RNA_FAIMS_60_70_KNN[UV_RNA_FAIMS_60_70_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_60_70_KNN$sequence))
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_60_70_KNN$prepPep))
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_60_70_KNN$prepPep))
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_60_70_KNN$prepPep)
```

```
UV_RNA_FAIMS_60_70_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_60_70_KNN$prepPep)
UV_RNA_FAIMS_60_70_KNN$Pepseq <- UV_RNA_FAIMS_60_70_KNN$prepPep
UV_RNA_FAIMS_60_70_KNN$Peplength <- nchar(UV_RNA_FAIMS_60_70_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_60_70_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_60_70_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_60_70_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_60_70_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_60_70_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_60_70_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_60_70_KNN$pI <- round(pI(UV_RNA_FAIMS_60_70_KNN$Pepseq), 2)
UV_RNA_FAIMS_60_70_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_60_70_KNN$Pepseq), 2)
UV_RNA_FAIMS_60_70_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_60_70_KNN$RNPxl_best_localization)
UV_RNA_FAIMS_60_70_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_60_70_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_60_70_KNN$mw <- round(mw(UV_RNA_FAIMS_60_70_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_60_70_KNN$cv <- c("60_70")

names(UV_RNA_FAIMS_60_70_KNN)[names(UV_RNA_FAIMS_60_70_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_60_70_KNN)[names(UV_RNA_FAIMS_60_70_KNN) == "precursor_error_(_ppm_)"] <- "precursor_
UV_RNA_FAIMS_60_70_KNN <- UV_RNA_FAIMS_60_70_KNN %>% filter(RNPxl_isPhospho == "0")

UV_RNA_FAIMS_60_70_KNN_model <- UV_RNA_FAIMS_60_70_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_60_70_KNN_model_norm <- UV_RNA_FAIMS_60_70_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_60_70_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_60_70_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_60_70_KNN_model_norm[is.na(UV_RNA_FAIMS_60_70_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_60_70_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_60_70_KNN_model_norm
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_60_70_KNN_model$Prediction <- UV_RNA_FAIMS_60_70_knn_pred
UV_RNA_FAIMS_60_70_KNN$Prediction_KNN <- UV_RNA_FAIMS_60_70_knn_pred
table(UV_RNA_FAIMS_60_70_KNN_model$Prediction)
```

```
##
## False  True
## 13672   611
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_60_70_test_C5<-UV_RNA_FAIMS_60_70_KNN %>%
```

```
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_60_70_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_60_70_test_C
ml_UV_RNA_FAIMS_60_70_test_C5$Prediction<-C5_UV_RNA_FAIMS_60_70_predict_boost_pen
UV_RNA_FAIMS_60_70_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_60_70_predict_boost_pen
table(ml_UV_RNA_FAIMS_60_70_test_C5$Prediction)
```

```
##
## False  True
## 11661  2622
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_60_70_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_60_70_test_C5)
ml_UV_RNA_FAIMS_60_70_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_60_70_predict
table(ml_UV_RNA_FAIMS_60_70_test_C5$Prediction_RIPPER)
```

```
##
## False  True
##  7269  7014
```

```
UV_RNA_FAIMS_60_70_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_60_70_predict
```

collapsed Proteins

S30 FAIMS 35_45 KNN

```
nrow(UV_RNA_FAIMS_35_45_KNN %>%
  filter(Prediction_KNN == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 317
```

S30 FAIMS 35_45 C5.0

```
nrow(UV_RNA_FAIMS_35_45_KNN %>%
  filter(Prediction_C5 == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 1807
```

S30 FAIMS 35_45 RIPPER

```
nrow(UV_RNA_FAIMS_35_45_KNN %>%
  filter(Prediction_RIPPER == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 2130
```

S30 FAIMS 40_50 KNN

```
nrow(UV_RNA_FAIMS_40_50_KNN %>%
  filter(Prediction_KNN == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 355
```

S30 FAIMS 40_50 C5.0

```
nrow(UV_RNA_FAIMS_40_50_KNN %>%
  filter(Prediction_C5 == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 2099
```

S30 FAIMS 40_50 RIPPER

```
nrow(UV_RNA_FAIMS_40_50_KNN %>%
  filter(Prediction_RIPPER == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 2481
```

S30 FAIMS 55_65 KNN

```
nrow(UV_RNA_FAIMS_55_65_KNN %>%
  filter(Prediction_KNN == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 359
```

S30 FAIMS 55_65 C5.0

```
nrow(UV_RNA_FAIMS_55_65_KNN %>%
  filter(Prediction_C5 == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 2007
```

S30 FAIMS 55_65 RIPPER

```
nrow(UV_RNA_FAIMS_55_65_KNN %>%
  filter(Prediction_RIPPER == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 3060
```

S30 FAIMS 60_70 KNN

```
nrow(UV_RNA_FAIMS_60_70_KNN %>%
  filter(Prediction_KNN == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 273
```

S30 FAIMS 60_70 C5.0

```
nrow(UV_RNA_FAIMS_60_70_KNN %>%
  filter(Prediction_C5 == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 1428
```

S30 FAIMS 60_70 RIPPER

```
nrow(UV_RNA_FAIMS_60_70_KNN %>%
  filter(Prediction_RIPPER == "True") %>%
  select(accessions) %>%
  distinct())
```

```
## [1] 2700
```

Data setup UV RNA CV 35_45_55

```
UV_RNA_FAIMS_35_45_55_KNN <- read_delim("AWulf_110919_Ecoli_UV_S30_FAIMS_35_45_55_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_35_45_55_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_35_45_55_KNN))
names(UV_RNA_FAIMS_35_45_55_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_35_45_55_KNN))
names(UV_RNA_FAIMS_35_45_55_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_35_45_55_KNN))
names(UV_RNA_FAIMS_35_45_55_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_35_45_55_KNN))
UV_RNA_FAIMS_35_45_55_KNN$XLinker <- "UV"
UV_RNA_FAIMS_35_45_55_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_35_45_55_KNN$Sample <- "S30"
```

```
UV_RNA_FAIMS_35_45_55_KNN <- UV_RNA_FAIMS_35_45_55_KNN[UV_RNA_FAIMS_35_45_55_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_35_45_55_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_35_45_55_KNN$sequ
UV_RNA_FAIMS_35_45_55_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_35_45_55_KNN$prep
UV_RNA_FAIMS_35_45_55_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_35_45_55_KNN$prepP
UV_RNA_FAIMS_35_45_55_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_35_45_55_KNN$prepPep)
UV_RNA_FAIMS_35_45_55_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_35_45_55_KNN$prepPep)
UV_RNA_FAIMS_35_45_55_KNN$Pepseq <- UV_RNA_FAIMS_35_45_55_KNN$prepPep
UV_RNA_FAIMS_35_45_55_KNN$Peplength <- nchar(UV_RNA_FAIMS_35_45_55_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_35_45_55_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_35_45_55_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_35_45_55_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_35_45_55_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_35_45_55_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_35_45_55_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_35_45_55_KNN$pI <- round(pI(UV_RNA_FAIMS_35_45_55_KNN$Pepseq), 2)
UV_RNA_FAIMS_35_45_55_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_35_45_55_KNN$Pepseq),
    2)
UV_RNA_FAIMS_35_45_55_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_35_45_55_KNN$RNPxl_best_localizatio
UV_RNA_FAIMS_35_45_55_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_35_45_55_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_35_45_55_KNN$mw <- round(mw(UV_RNA_FAIMS_35_45_55_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_35_45_55_KNN$cv <- c("35_45")

names(UV_RNA_FAIMS_35_45_55_KNN)[names(UV_RNA_FAIMS_35_45_55_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_35_45_55_KNN)[names(UV_RNA_FAIMS_35_45_55_KNN) == "precursor_error_(_ppm_)"] <- "pre
UV_RNA_FAIMS_35_45_55_KNN <- UV_RNA_FAIMS_35_45_55_KNN %>% filter(RNPxl_isPhospho ==
    "0")

UV_RNA_FAIMS_35_45_55_KNN_model <- UV_RNA_FAIMS_35_45_55_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_35_45_55_KNN_model_norm <- UV_RNA_FAIMS_35_45_55_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_35_45_55_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_35_45_55_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_35_45_55_KNN_model_norm[is.na(UV_RNA_FAIMS_35_45_55_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_35_45_55_knn_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_35_45_55_KNN_mod
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_35_45_55_KNN_model$Prediction <- UV_RNA_FAIMS_35_45_55_knn_pred
table(UV_RNA_FAIMS_35_45_55_KNN_model$Prediction)
```

```
##
## False  True
## 17086   522
```

```
UV_RNA_FAIMS_35_45_55_KNN$Prediction_KNN <- UV_RNA_FAIMS_35_45_55_knn_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_35_45_55_test_C5<-UV_RNA_FAIMS_35_45_55_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_35_45_55_

ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction<-C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen
table(ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction)
```

```
##
## False  True
## 13247  4361
```

```
UV_RNA_FAIMS_35_45_55_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_35_45_55_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_35_45_55_test_C5)
ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_55_predict
table(ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction_RIPPER)
```

```
##
## False  True
## 10912  6696
```

```
UV_RNA_FAIMS_35_45_55_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_55_predict
```

Data setup UV RNA CV 40_50_60

```
UV_RNA_FAIMS_40_50_60_KNN <- read_delim("AWulf_060919_Ecoli_UV_S30_FAIMS_40_50_60_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_40_50_60_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_40_50_60_KNN))
names(UV_RNA_FAIMS_40_50_60_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_40_50_60_KNN))
names(UV_RNA_FAIMS_40_50_60_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_40_50_60_KNN))
names(UV_RNA_FAIMS_40_50_60_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_40_50_60_KNN))
UV_RNA_FAIMS_40_50_60_KNN$XLinker <- "UV"
UV_RNA_FAIMS_40_50_60_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_40_50_60_KNN$Sample <- "S30"
UV_RNA_FAIMS_40_50_60_KNN <- UV_RNA_FAIMS_40_50_60_KNN[UV_RNA_FAIMS_40_50_60_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_40_50_60_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_40_50_60_KNN$seque
UV_RNA_FAIMS_40_50_60_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_40_50_60_KNN$prep
UV_RNA_FAIMS_40_50_60_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_40_50_60_KNN$prepP
UV_RNA_FAIMS_40_50_60_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_40_50_60_KNN$prepPep)
UV_RNA_FAIMS_40_50_60_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_40_50_60_KNN$prepPep)
UV_RNA_FAIMS_40_50_60_KNN$Pepseq <- UV_RNA_FAIMS_40_50_60_KNN$prepPep
UV_RNA_FAIMS_40_50_60_KNN$Peplength <- nchar(UV_RNA_FAIMS_40_50_60_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_40_50_60_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_40_50_60_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_40_50_60_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_40_50_60_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_40_50_60_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_40_50_60_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_40_50_60_KNN$pI <- round(pI(UV_RNA_FAIMS_40_50_60_KNN$Pepseq), 2)
UV_RNA_FAIMS_40_50_60_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_40_50_60_KNN$Pepseq),
    2)
UV_RNA_FAIMS_40_50_60_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_40_50_60_KNN$RNPxl_best_localizatio
UV_RNA_FAIMS_40_50_60_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_40_50_60_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_40_50_60_KNN$mw <- round(mw(UV_RNA_FAIMS_40_50_60_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_40_50_60_KNN$cv <- c("35_45")

names(UV_RNA_FAIMS_40_50_60_KNN)[names(UV_RNA_FAIMS_40_50_60_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_40_50_60_KNN)[names(UV_RNA_FAIMS_40_50_60_KNN) == "precursor_error_(_ppm_)"] <- "pre
UV_RNA_FAIMS_40_50_60_KNN <- UV_RNA_FAIMS_40_50_60_KNN %>% filter(RNPxl_isPhospho ==
    "0")

UV_RNA_FAIMS_40_50_60_KNN_model <- UV_RNA_FAIMS_40_50_60_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_40_50_60_KNN_model_norm <- UV_RNA_FAIMS_40_50_60_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_40_50_60_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_40_50_60_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_40_50_60_KNN_model_norm[is.na(UV_RNA_FAIMS_40_50_60_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_40_50_60_KNN_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_40_50_60_KNN_mod
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
```

```
UV_RNA_FAIMS_40_50_60_KNN_model$Prediction <- UV_RNA_FAIMS_40_50_60_KNN_pred
table(UV_RNA_FAIMS_40_50_60_KNN_model$Prediction)
```

```
##
## False  True
## 17042   478
```

```
UV_RNA_FAIMS_40_50_60_KNN$Prediction_KNN <- UV_RNA_FAIMS_40_50_60_KNN_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_35_45_55_test_C5<-UV_RNA_FAIMS_40_50_60_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_35_45_55_

ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction<-C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen
table(ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction)
```

```
##
## False  True
## 13311  4209
```

```
UV_RNA_FAIMS_40_50_60_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_35_45_55_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_35_45_55_test_C5)
ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_55_predict
table(ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction_RIPPER)
```

```
##
## False  True
## 10001  7519
```

```
UV_RNA_FAIMS_40_50_60_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_55_predict
```

Data setup UV RNA CV 30_50_70

```
UV_RNA_FAIMS_30_50_70_KNN <- read_delim("AWulf_050919_Ecoli_UV_S30_FAIMS_30_50_70_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
```

```
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )

## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_30_50_70_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_30_50_70_KNN))
names(UV_RNA_FAIMS_30_50_70_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_30_50_70_KNN))
names(UV_RNA_FAIMS_30_50_70_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_30_50_70_KNN))
names(UV_RNA_FAIMS_30_50_70_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_30_50_70_KNN))
UV_RNA_FAIMS_30_50_70_KNN$XLinker <- "UV"
UV_RNA_FAIMS_30_50_70_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_30_50_70_KNN$Sample <- "S30"
UV_RNA_FAIMS_30_50_70_KNN <- UV_RNA_FAIMS_30_50_70_KNN[UV_RNA_FAIMS_30_50_70_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_30_50_70_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_30_50_70_KNN$seque
UV_RNA_FAIMS_30_50_70_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_30_50_70_KNN$prep
UV_RNA_FAIMS_30_50_70_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_30_50_70_KNN$prepP
UV_RNA_FAIMS_30_50_70_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_30_50_70_KNN$prepPep)
UV_RNA_FAIMS_30_50_70_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_30_50_70_KNN$prepPep)
UV_RNA_FAIMS_30_50_70_KNN$Pepseq <- UV_RNA_FAIMS_30_50_70_KNN$prepPep
UV_RNA_FAIMS_30_50_70_KNN$Peplength <- nchar(UV_RNA_FAIMS_30_50_70_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_30_50_70_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_30_50_70_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_30_50_70_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_30_50_70_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_30_50_70_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_30_50_70_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_30_50_70_KNN$pI <- round(pI(UV_RNA_FAIMS_30_50_70_KNN$Pepseq), 2)
UV_RNA_FAIMS_30_50_70_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_30_50_70_KNN$Pepseq),
    2)
UV_RNA_FAIMS_30_50_70_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_30_50_70_KNN$RNPxl_best_localizatio
UV_RNA_FAIMS_30_50_70_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_30_50_70_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_30_50_70_KNN$mw <- round(mw(UV_RNA_FAIMS_30_50_70_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_30_50_70_KNN$cv <- c("35_45")

names(UV_RNA_FAIMS_30_50_70_KNN)[names(UV_RNA_FAIMS_30_50_70_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_30_50_70_KNN)[names(UV_RNA_FAIMS_30_50_70_KNN) == "precursor_error_(_ppm_)"] <- "prec
UV_RNA_FAIMS_30_50_70_KNN <- UV_RNA_FAIMS_30_50_70_KNN %>% filter(RNPxl_isPhospho ==
    "0")

UV_RNA_FAIMS_30_50_70_KNN_model <- UV_RNA_FAIMS_30_50_70_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_30_50_70_KNN_model_norm <- UV_RNA_FAIMS_30_50_70_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_30_50_70_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_30_50_70_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_30_50_70_KNN_model_norm[is.na(UV_RNA_FAIMS_30_50_70_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_30_50_70_KNN_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_30_50_70_KNN_mod
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_30_50_70_KNN_model$Prediction <- UV_RNA_FAIMS_30_50_70_KNN_pred
table(UV_RNA_FAIMS_30_50_70_KNN_model$Prediction)
```

```
##
## False  True
## 15323   419
```

```
UV_RNA_FAIMS_30_50_70_KNN$Prediction_KNN <- UV_RNA_FAIMS_30_50_70_KNN_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_35_45_55_test_C5<-UV_RNA_FAIMS_30_50_70_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_35_45_55

ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction<-C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen
table(ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction)
```

```
##
## False  True
## 12524  3218
```

```
UV_RNA_FAIMS_30_50_70_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_35_45_55_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_35_45_55_test_C5)
ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_55_predict
table(ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction_RIPPER)
```

```
##
## False  True
##  9423  6319
```

```
UV_RNA_FAIMS_30_50_70_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_55_predict
```

Data setup UV RNA CV 45_55_65

```
UV_RNA_FAIMS_45_55_65_KNN <- read_delim("AWulf_060919_Ecoli_UV_S30_FAIMS_45_55_65_table.csv",
    delim = "\t")
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
```

```
##   sequence = col_character(),
##   accessions = col_character(),
##   `RNPxl:NT` = col_character(),
##   `RNPxl:RNA` = col_character(),
##   `RNPxl:best_localization` = col_character(),
##   `RNPxl:localization_scores` = col_character(),
##   protein_references = col_character(),
##   target_decoy = col_character(),
##   `PeakAnnotations(mz|intensity|charge|annotation;)` = col_character()
## )

## See spec(...) for full column specifications.
```

```
names(UV_RNA_FAIMS_45_55_65_KNN) <- gsub("\\.", "_", names(UV_RNA_FAIMS_45_55_65_KNN))
names(UV_RNA_FAIMS_45_55_65_KNN) <- gsub("\\:", "_", names(UV_RNA_FAIMS_45_55_65_KNN))
names(UV_RNA_FAIMS_45_55_65_KNN) <- gsub("\\ ", "_", names(UV_RNA_FAIMS_45_55_65_KNN))
names(UV_RNA_FAIMS_45_55_65_KNN) <- gsub("\\|", "_", names(UV_RNA_FAIMS_45_55_65_KNN))
UV_RNA_FAIMS_45_55_65_KNN$XLinker <- "UV"
UV_RNA_FAIMS_45_55_65_KNN$Nucleotides <- "RNA"
UV_RNA_FAIMS_45_55_65_KNN$Sample <- "S30"
UV_RNA_FAIMS_45_55_65_KNN <- UV_RNA_FAIMS_45_55_65_KNN[UV_RNA_FAIMS_45_55_65_KNN$RNPxl_RNA !=
    "none", ] %>% filter(target_decoy == "target")
UV_RNA_FAIMS_45_55_65_KNN$prepPep <- gsub("(Carbamyl)", "", as.character(UV_RNA_FAIMS_45_55_65_KNN$sequ
UV_RNA_FAIMS_45_55_65_KNN$prepPep <- gsub("(Oxidation)", "", as.character(UV_RNA_FAIMS_45_55_65_KNN$prep
UV_RNA_FAIMS_45_55_65_KNN$prepPep <- gsub("(Phospho)", "", as.character(UV_RNA_FAIMS_45_55_65_KNN$prepP
UV_RNA_FAIMS_45_55_65_KNN$prepPep <- gsub("\\(|\\)", "", UV_RNA_FAIMS_45_55_65_KNN$prepPep)
UV_RNA_FAIMS_45_55_65_KNN$prepPep <- gsub("\\..*", "", UV_RNA_FAIMS_45_55_65_KNN$prepPep)
UV_RNA_FAIMS_45_55_65_KNN$Pepseq <- UV_RNA_FAIMS_45_55_65_KNN$prepPep
UV_RNA_FAIMS_45_55_65_KNN$Peplength <- nchar(UV_RNA_FAIMS_45_55_65_KNN$Pepseq, type = "chars")
UV_RNA_FAIMS_45_55_65_KNN$aa_class_charged <- str_count(UV_RNA_FAIMS_45_55_65_KNN$Pepseq,
    paste("R|K|D|E", collapse = "|"))
UV_RNA_FAIMS_45_55_65_KNN$aa_class_polar <- str_count(UV_RNA_FAIMS_45_55_65_KNN$Pepseq,
    paste("Q|N|H|S|T|Y|C|W", collapse = "|"))
UV_RNA_FAIMS_45_55_65_KNN$aa_class_hydrophobic <- str_count(UV_RNA_FAIMS_45_55_65_KNN$Pepseq,
    paste("A|I|L|M|F|V|P|G", collapse = "|"))
UV_RNA_FAIMS_45_55_65_KNN$pI <- round(pI(UV_RNA_FAIMS_45_55_65_KNN$Pepseq), 2)
UV_RNA_FAIMS_45_55_65_KNN$aIndex <- round(aIndex(UV_RNA_FAIMS_45_55_65_KNN$Pepseq),
    2)
UV_RNA_FAIMS_45_55_65_KNN$XL_aa <- gsub("[:A-Z:]", "", UV_RNA_FAIMS_45_55_65_KNN$RNPxl_best_localizatio
UV_RNA_FAIMS_45_55_65_KNN$Hydro <- round(hydrophobicity(UV_RNA_FAIMS_45_55_65_KNN$Pepseq,
    scale = "KyteDoolittle"), 2)
UV_RNA_FAIMS_45_55_65_KNN$mw <- round(mw(UV_RNA_FAIMS_45_55_65_KNN$Pepseq, monoisotopic = F),
    2)
UV_RNA_FAIMS_45_55_65_KNN$cv <- c("35_45")

names(UV_RNA_FAIMS_45_55_65_KNN)[names(UV_RNA_FAIMS_45_55_65_KNN) == "precursor_m/z"] <- "precursor"
names(UV_RNA_FAIMS_45_55_65_KNN)[names(UV_RNA_FAIMS_45_55_65_KNN) == "precursor_error_(_ppm_)"] <- "pre
UV_RNA_FAIMS_45_55_65_KNN <- UV_RNA_FAIMS_45_55_65_KNN %>% filter(RNPxl_isPhospho ==
    "0")

UV_RNA_FAIMS_45_55_65_KNN_model <- UV_RNA_FAIMS_45_55_65_KNN %>% select(colnames(ml_UV_RNA_train_knn))
```

Normalizing

```
UV_RNA_FAIMS_45_55_65_KNN_model_norm <- UV_RNA_FAIMS_45_55_65_KNN_model %>% select_if(is.numeric)
UV_RNA_FAIMS_45_55_65_KNN_model_norm <- as.data.frame(lapply(UV_RNA_FAIMS_45_55_65_KNN_model_norm,
    normalize))
UV_RNA_FAIMS_45_55_65_KNN_model_norm[is.na(UV_RNA_FAIMS_45_55_65_KNN_model_norm)] <- 0
```

Classifying UV RNA FAIMS data

KNN5

```
UV_RNA_FAIMS_45_55_65_KNN_pred <- knn(train = ml_UV_RNA_train_knn, test = UV_RNA_FAIMS_45_55_65_KNN_mod
    cl = ml_UV_RNA_train_knn_labels$Curated, k = 5)
UV_RNA_FAIMS_45_55_65_KNN_model$Prediction <- UV_RNA_FAIMS_45_55_65_KNN_pred
table(UV_RNA_FAIMS_45_55_65_KNN_model$Prediction)
```

```
##
## False  True
## 17062   562
```

```
UV_RNA_FAIMS_45_55_65_KNN$Prediction_KNN <- UV_RNA_FAIMS_45_55_65_KNN_pred
```

C5.0 with boosting and penalty for false positives

penalize False Positives 4 times more than false negatives.

```
matrix_dimensions<- list(c("True", "False"), c("True", "False"))
names(matrix_dimensions) <- c("predicted", "actual")
error_cost <- matrix(c(0,1,4,0), nrow = 2, dimnames = matrix_dimensions)

ml_UV_RNA_FAIMS_35_45_55_test_C5<-UV_RNA_FAIMS_45_55_65_KNN %>%
  select(colnames(ml_UV_RNA_train))

C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen<-predict(C5_model_UV_RNA_boost_pen, ml_UV_RNA_FAIMS_35_45_55_

ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction<-C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen
table(ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction)
```

```
##
## False  True
## 13053  4571
```

```
UV_RNA_FAIMS_45_55_65_KNN$Prediction_C5<-C5_UV_RNA_FAIMS_35_45_55_predict_boost_pen
```

RIPPER

```
RIPPER_UV_RNA_FAIMS_35_45_55_predict <- predict(RIPPER_model_UV_RNA, ml_UV_RNA_FAIMS_35_45_55_test_C5)
ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_55_predict
table(ml_UV_RNA_FAIMS_35_45_55_test_C5$Prediction_RIPPER)
```

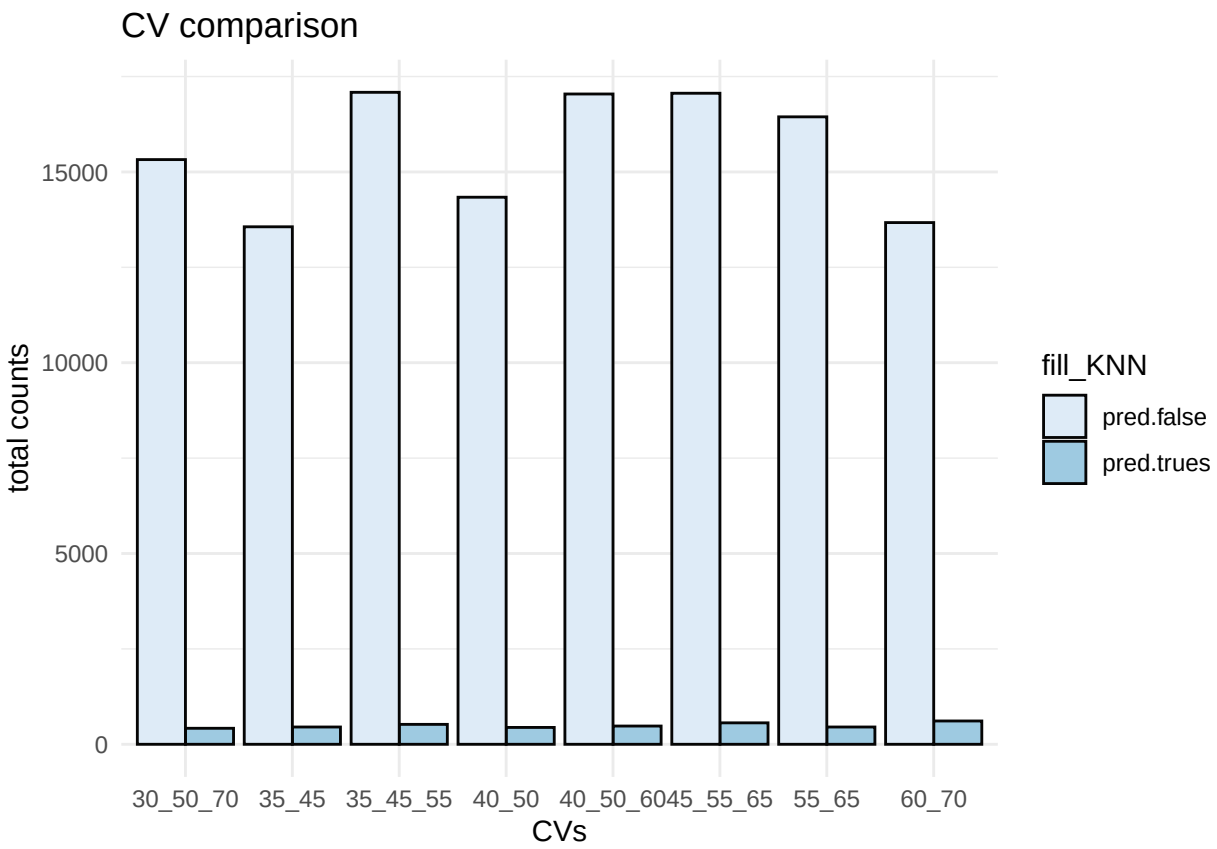
```
##
## False  True
##  8594  9030
```

```
UV_RNA_FAIMS_45_55_65_KNN$Prediction_RIPPER <- RIPPER_UV_RNA_FAIMS_35_45_55_predict
```

Comparing the most conservative model KNN

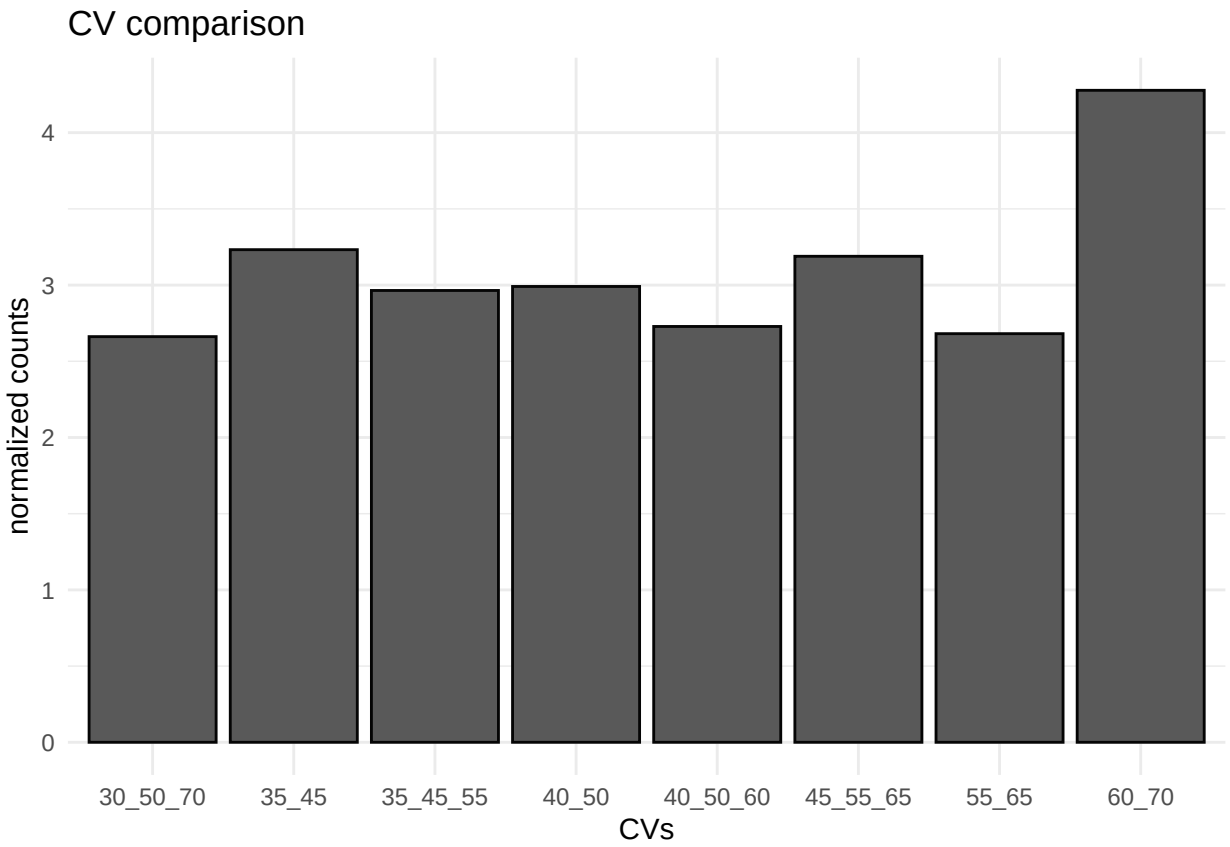
```
a<-as.data.frame(table(UV_RNA_FAIMS_35_45_KNN$Prediction_KNN))
b<-as.data.frame(table(UV_RNA_FAIMS_40_50_KNN$Prediction_KNN))
c<-as.data.frame(table(UV_RNA_FAIMS_55_65_KNN$Prediction_KNN))
d<-as.data.frame(table(UV_RNA_FAIMS_60_70_KNN$Prediction_KNN))
e<-as.data.frame(table(UV_RNA_FAIMS_35_45_55_KNN$Prediction_KNN))
f<-as.data.frame(table(UV_RNA_FAIMS_30_50_70_KNN$Prediction_KNN))
g<-as.data.frame(table(UV_RNA_FAIMS_40_50_60_KNN$Prediction_KNN))
h<-as.data.frame(table(UV_RNA_FAIMS_45_55_65_KNN$Prediction_KNN))

f_KNN<-c("double", "double", "double", "double", "double", "double", "double", "double", "double", "doul
x_KNN<-c("35_45", "35_45", "35_45", "40_50","40_50", "40_50", "55_65", "55_65", "55_65", "60_70", "60_7
y_KNN<-c(a[2,2], a[1,2], a[2,2]/(a[2,2]+a[1,2])*100, b[2,2], b[1,2], b[2,2]/(b[2,2]+b[1,2])*100, c[2,2]
fill_KNN<-c("pred.trues", "pred.false", "pred.norm", "pred.trues", "pred.false", "pred.norm", "pred.tru
df_KNN_comparison<-data.frame(x_KNN, y_KNN, fill_KNN, f_KNN)
df_KNN_comparison1<-filter(df_KNN_comparison, fill_KNN!="pred.norm")
df_KNN_comparison2<-filter(df_KNN_comparison, fill_KNN=="pred.norm")
ggplot(df_KNN_comparison1, aes(x=x_KNN, y=y_KNN, fill = fill_KNN))+
  geom_bar(stat = "identity", position=position_dodge(),bindwidth =1, bins = 3, color="gray2")+
  scale_fill_brewer(palette = "Blues")+
  ggtitle("CV comparison")+
  theme_minimal()+
  ylab("total counts")+
  xlab("CVs")
```

```
## Warning: Ignoring unknown parameters: bindwidth, bins
```



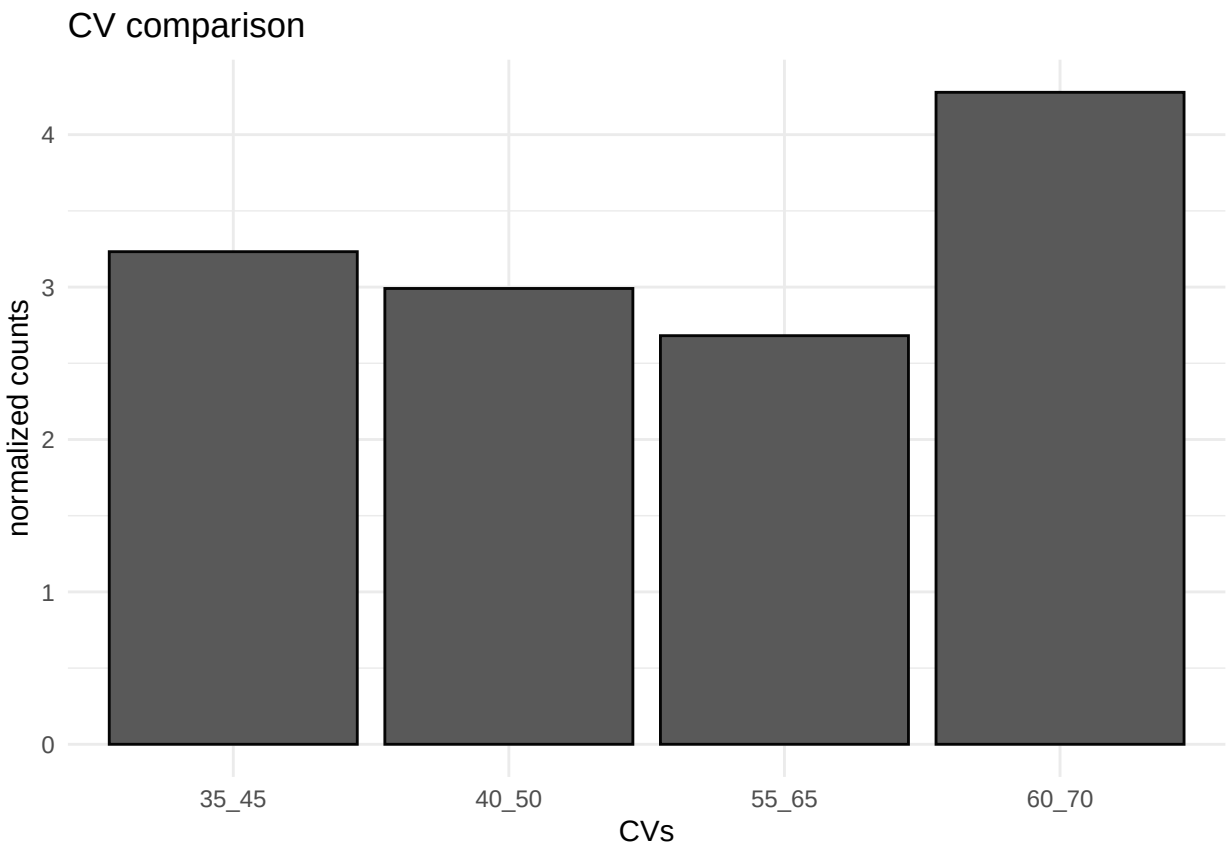

```
ggplot(df_KNN_comparison2, aes(x=x_KNN, y=y_KNN))+
  geom_bar(stat="identity", bindwidth =1, bins = 3, color="gray2")+
  ggtitle("CV comparison")+
  ylab("normalized counts")+
  xlab("CVs")+
  theme_minimal()
```

```
## Warning: Ignoring unknown parameters: bindwidth, bins
```



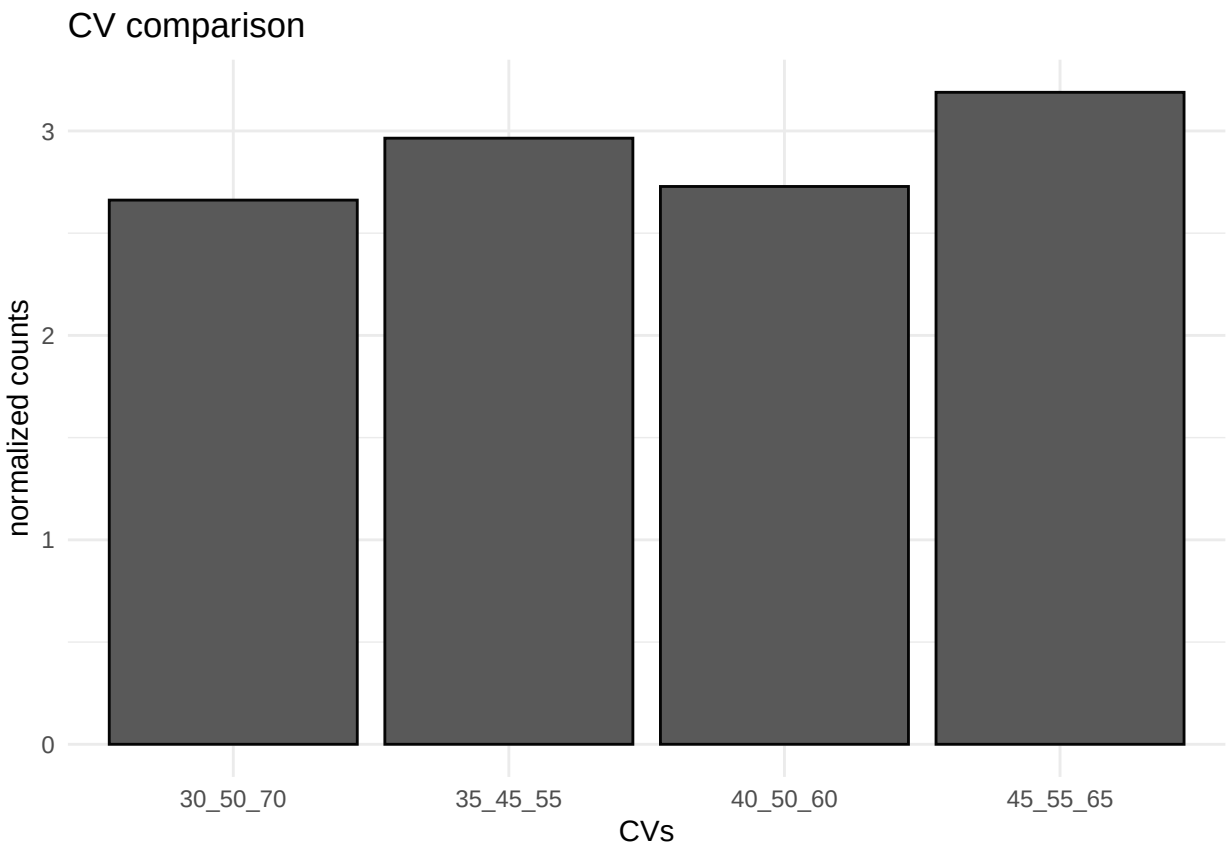

```
df_KNN_comparison3<-filter(df_KNN_comparison2, f_KNN=="double")

ggplot(df_KNN_comparison3, aes(x=x_KNN, y=y_KNN))+
  geom_bar(stat="identity", bindwidth =1, bins = 3, color="gray2")+
  ggtitle("CV comparison")+
  ylab("normalized counts")+
  xlab("CVs")+
  theme_minimal()
```

```
## Warning: Ignoring unknown parameters: bindwidth, bins
```




```
df_KNN_comparison4<-filter(df_KNN_comparison2, f_KNN=="triple")

ggplot(df_KNN_comparison4, aes(x=x_KNN, y=y_KNN))+
  geom_bar(stat="identity", bindwidth =1, bins = 3, color="gray2")+
  ggtitle("CV comparison")+
  ylab("normalized counts")+
  xlab("CVs")+
  theme_minimal()
```

```
## Warning: Ignoring unknown parameters: bindwidth, bins
```



Export lists

```
S30_UV_RNA_FAIMS_total_predicted_trues<- rbind(UV_RNA_FAIMS_35_45_KNN, UV_RNA_FAIMS_40_50_KNN, UV_RNA_FA
  filter(Prediction_KNN == "True")

write_excel_csv(S30_UV_RNA_FAIMS_total_predicted_trues, "S30_UV_RNA_FAIMS_total_KNN_prediction.csv")
```