# How to Setup and Predict using DRUMLR

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## Set up

To install the DRUMLR package into R you will need to download the DRUMLRv01_0.1.0.tar.gz and Example Models Folder from Github. Then run the following line of code. You will need the path to the download location of the DRUMLRv01_0.1.0.tar.gz to do this (this will usually be "C:/Users/Username/Downloads/DRUMLRv01_0.1.0.tar.gz" where your Username is in the place of "Username").

```
install.packages("C:/Users/Username/Downloads/DRUMLRv01_0.1.0.tar.gz",
                 repos = NULL,
                 type ="source")
```

## Example

### Load Packages

```
library(DRUMLR)
library(tidyverse)
library(survival)
```

### Import data

Import internal DRUML data for verification.

```
#Import and scale Verification Phosphoproteomic input data from clinical aml samples
df_input <- DRUMLR:::Primary_AML_phospho_data

#Import survival and molecular classification data for clinical AML samples
df_survival <-DRUMLR:::Primary_AML_survival_data
```

### Calculate distance values for verfication data

In this example we will predict the sensitivity of clinical_phosphoproteomics samples to Cytarabine. To generate rankings peptide abundance values are scaled for each sample. Distance values for these data are generated using the DRUMLR::DrugMarkerEnrichment() function.

The markers_databases which can be used in for this are:

- Phosphoproteomics:
  - DRUMLR:::phospho_aml_markers.
  - DRUMLR:::phospho_solid_markers.
- Proteomic:
  - DRUMLR:::prot_aml_markers.
  - DRUMLR:::prot_solid_markers.

In this care we will be using phospho_aml_markers

```
# Get relevant marker database. For this example we are using phosphoproteomics
# data
markers <- DRUMLR:::phospho_aml_markers

# Carry out Drug Marker Enrichment on the data using the relevant makers database
df_distance <- DRUMLR::DrugMarkerEnrichment(df = df_input, marker_database = markers)
```

### Drug sensitivity prediction

To predict Drug Sensitivity you will need to state the path to the folder containing all of the Example Models. In this example we are predicting Cytarabine sensitivity using partial list squares (pls), principal components regression (pcr) and random forest (rf) models.

```
#To predict Drug Sensitivity you will need to state the path to the folder containing all of the Models

predictions <- DRUMLR::PredictDRUML_example(df_distance = df_distance,
                          input_type = "phospho",
                          cancer_type = "aml",
                          models = c("pcr", "pls", "rf"),
                          drugs = "Cytarabine",
                          models_dir = "Example_Models"
                          )
```

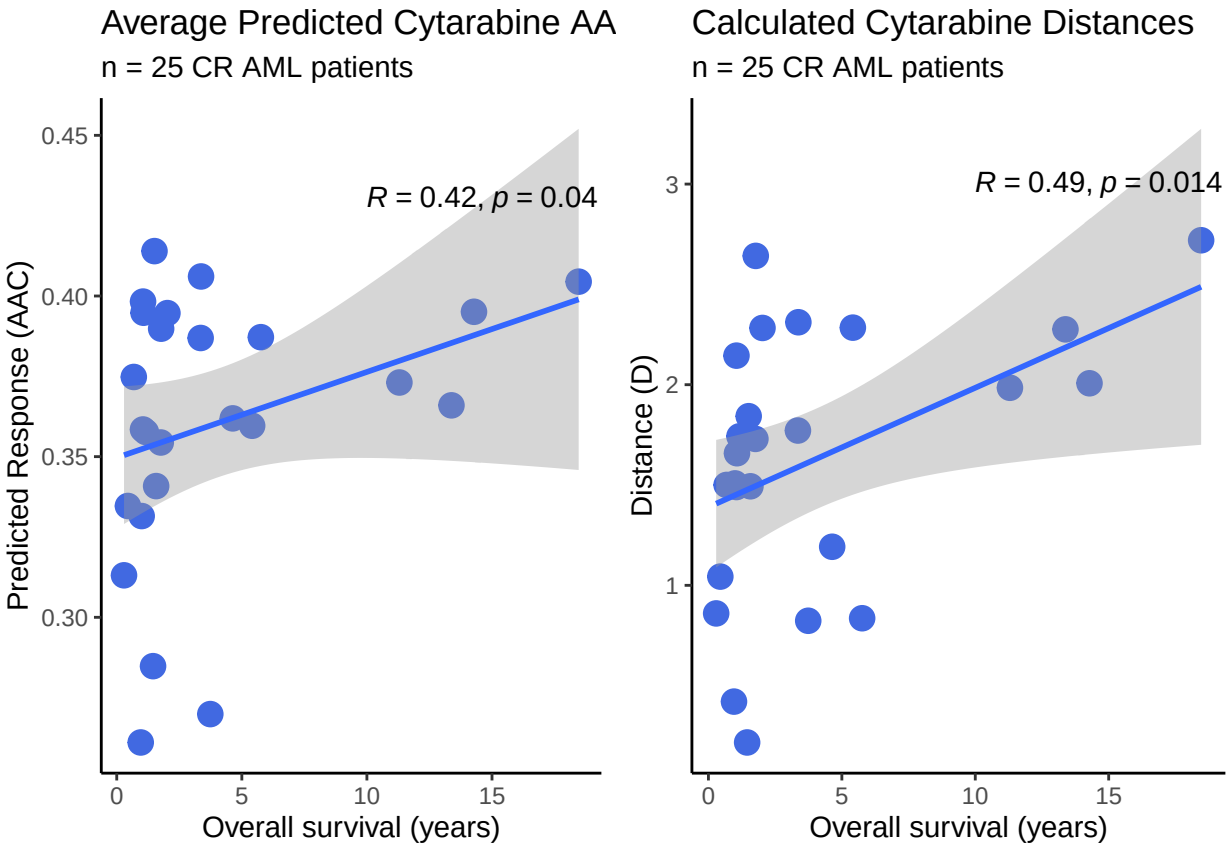
### Rearrange Prediction output for graphs

Useful code for reshaping prediction results for ggplot2 based graphs.

```
# Get average of predictions
df_prediction2 <- t(predictions) %>% data.frame()
df_prediction2["Cytarabine_aml_mean", ] <- apply(df_prediction2, MARGIN = 2, mean)

# label Predictions outputs
df_labs <- strsplit(rownames(df_prediction2), "_") %>% data.frame() %>% t()
colnames(df_labs) <- c("drug", "tissue", "model")

# labeled ML predictions
df_prediction2 <- cbind(df_labs[, "model"], df_prediction2) %>% reshape2::melt()
colnames(df_prediction2) <- c("model", "Vial.ID", "aac")

# Add survival and D data to dataframe
df_prediction2 <- merge.data.frame(df_prediction2, df_survival, all = T, by = "Vial.ID")
df_prediction2$D <- df_distance["Cytarabine", df_prediction2$Vial.ID] %>% as.vector()
```

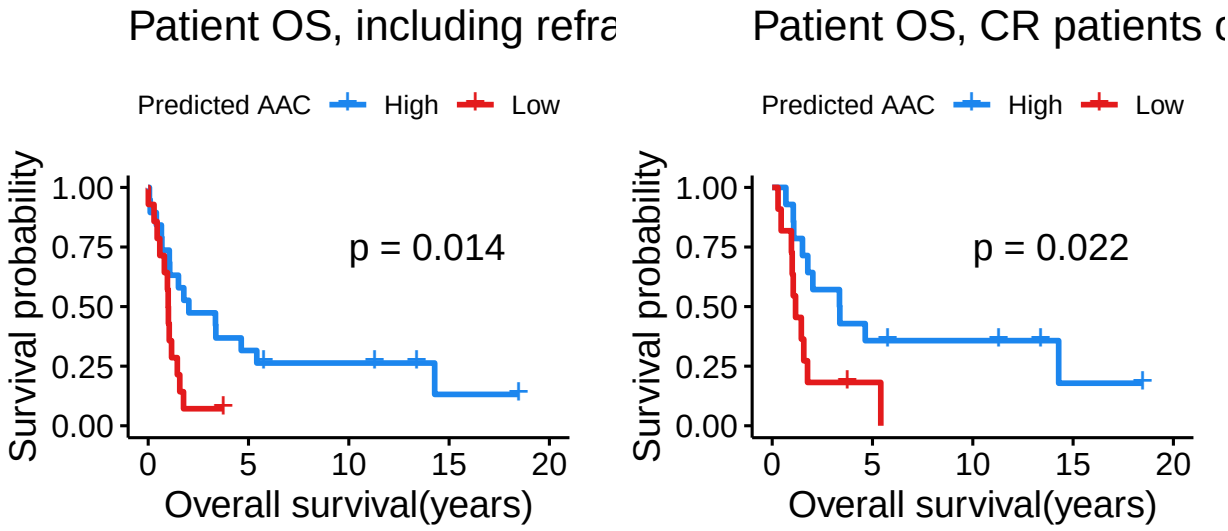
### Correlation of Predicted AAC with Patient Survival

Scatter graphs demonstrating the correlation between predicted AAC and D values against patient survival rate in years.



**Make Kaplain Meyer classifications**

Patients were split into "high" and "low" groups using mean AAC and D values.







| | records | *rmean | 0.95LCL | 0.95UCL |
|---|---|---|---|---|
| *high* | 19 | 5.68 | 1.07 | NA |
| *low* | 14 | 2.18 | 0.8 | 1.76 |

| | records | *rmean | 0.95LCL | 0.95UC |
|---|---|---|---|---|
| *high* | 14 | 7.24 | 1.77 | NA |
| *low* | 11 | 1.86 | 1 | NA |