

## The task for the MRL lab

In this lab, we work in two groups.

### Beginners in R

We will together learn to write R code for developing a simple model for predicting retention times in HILIC. We will do:

- Data preprocessing
- Training & Testing and/or cross-validation
- Variable selection
- Using the model to predict the results
- Validation of the results
- Plotting of the predictions

### Advanced users

You have already done this example. However, this time the focusses will be for you :

- Write clean code. Review that you collect everything to your data table and use only tidy data processing. I suggest writing the code again from the start, not using your old one. Reason: you probably would do things better and more efficiently now. Also, writing code is always a practice. You can move at your speed and do not need to wait for the others.
- Saving the model, so that the code would not need to be rerun whenever you want to use the model.  
See  
<https://www.rdocumentation.org/packages/base/versions/3.6.2/topics/readRDS>
- Reading in the saved model and using it to make predictions.
- Save the plot as interactive ggplotly items. You can find more here  
<https://www.rdocumentation.org/packages/plotly/versions/4.9.2.1>  
and  
<https://www.rdocumentation.org/packages/htmlwidgets/versions/1.5.2/topics/saveWidget>
- A Shiny app to interactively visualize your results.  
Please read the Written Shiny tutorials from here  
<https://shiny.rstudio.com/tutorial/> and write a short shiny code to visualize the predictions of your model. Choose one reactive feature so that the user can "play" with your results figure. I will show you an example at the beginning of the class.

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