

# Report

```
library(MQmetrics)

MQPathCombined <- params$input_dir

files <- ReadDataFromDir(MQPathCombined)

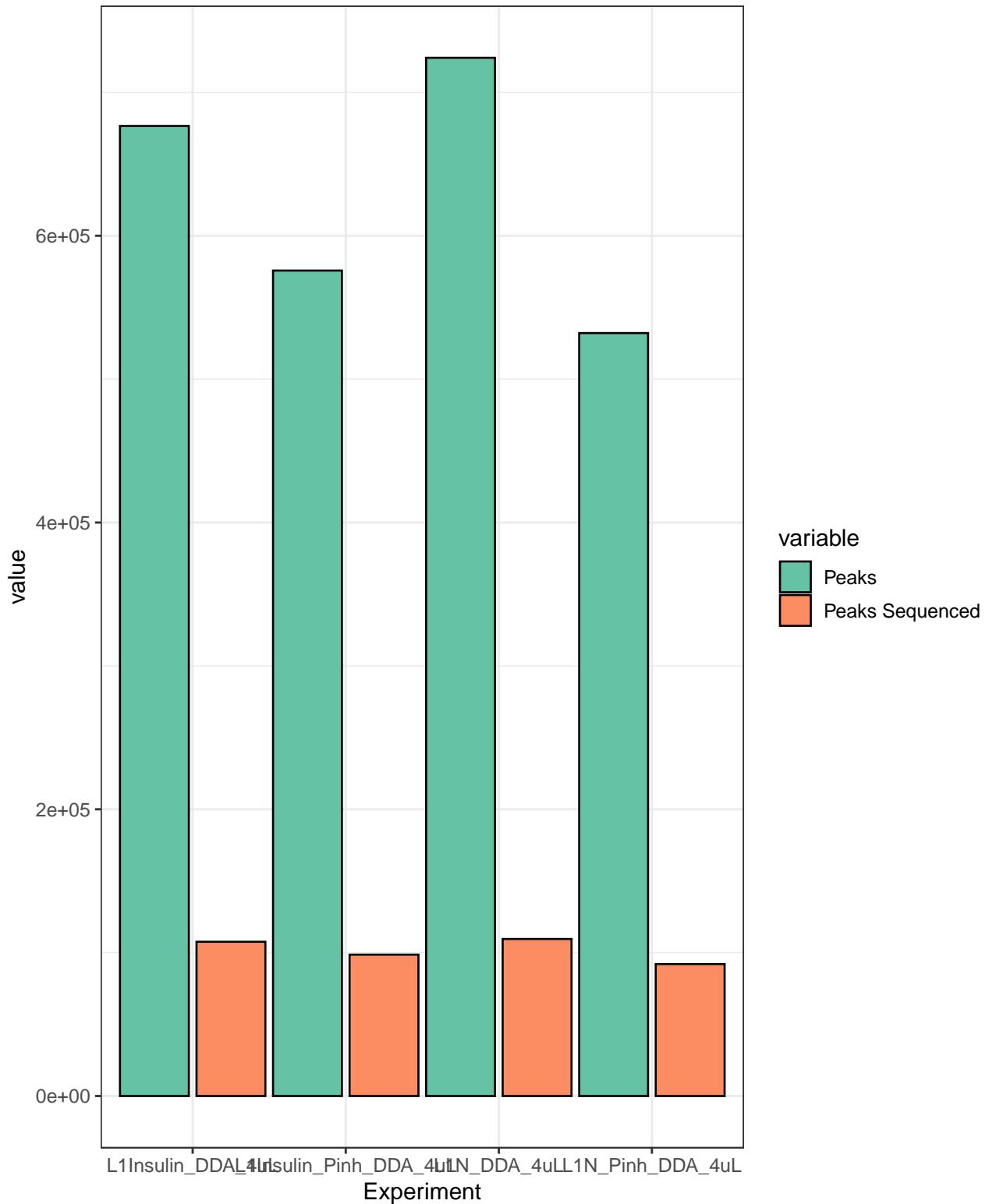
summary <- files[["summary.txt"]]
evidence <- files[["evidence.txt"]]
msScans <- files[['msScans.txt']]
peptides <- files[["peptides.txt"]]
msmsScans <- files[["msmsScans.txt"]]
proteinGroups <- files[["proteinGroups.txt"]]
modificationSpecificPeptides <- files[["modificationSpecificPeptides.txt"]]
runningTimes <- files[["#runningTimes.txt"]]
parameters <- files[["parameters.txt"]]
```

```
ExperimentInformation(runningTimes, parameters)

## [1] "The experiment started the day: 17/02/2021 at the time: 18:57:27."
## [1] "The whole experiment lasted: 05:48 (hours:minutes).."
## [1] "The MaxQuant version used was: 1.6.12.0"
## [1] "The user was: marek.vrbacky"
## [1] "The machine name was: FGU013PC029"
## [1] "The protein FDR was: 0.01"
## [1] "The match between runs was: True"
## [1] "The fasta file used was: C:\\MaxQuant_Databases\\\\UP000000589_10090.fasta"
```

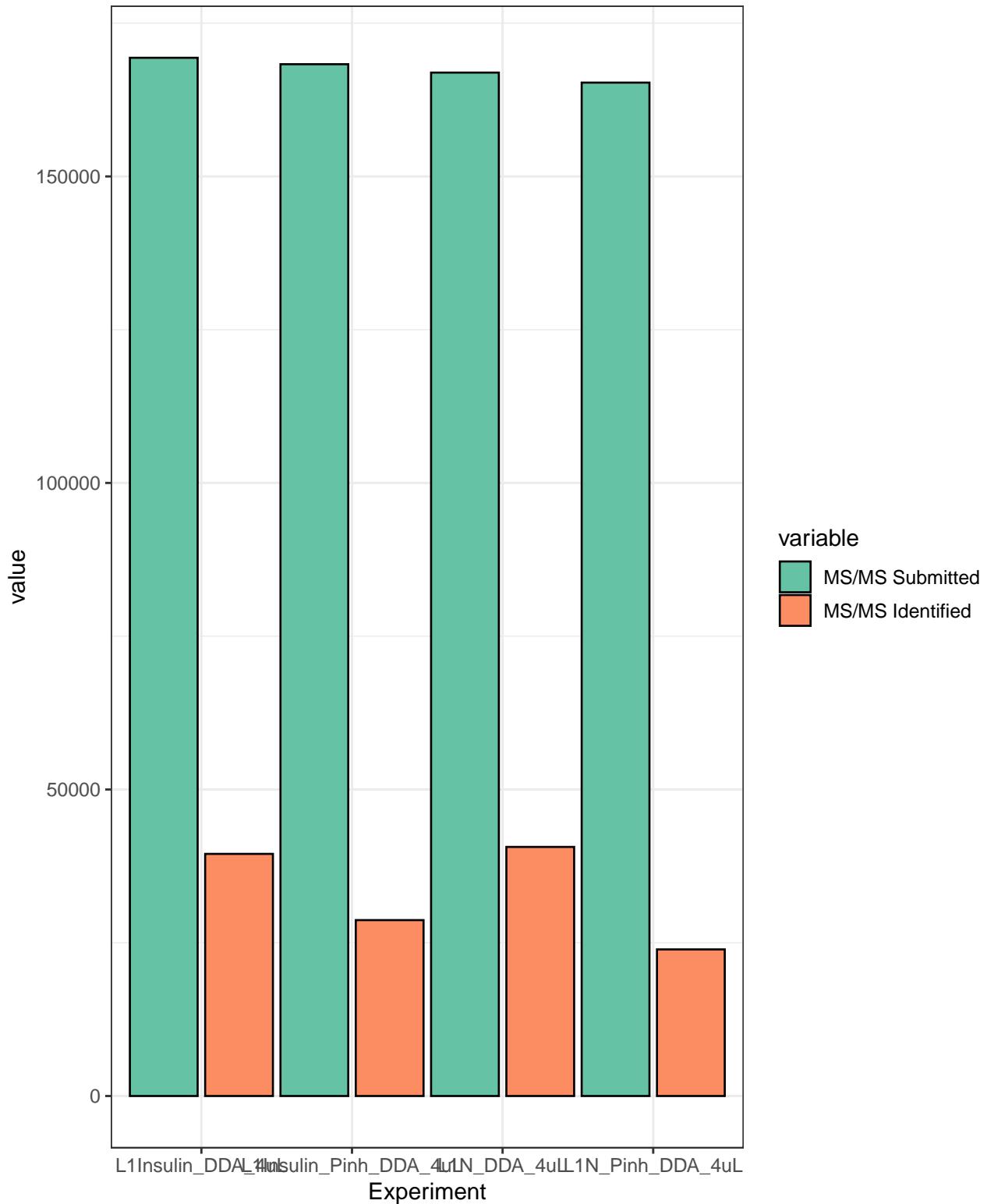
```
PlotPeaks(summary, long_names = params$long_names, sep_names = params$sep_names)
```

### Peaks detected and sequenced in the full scans

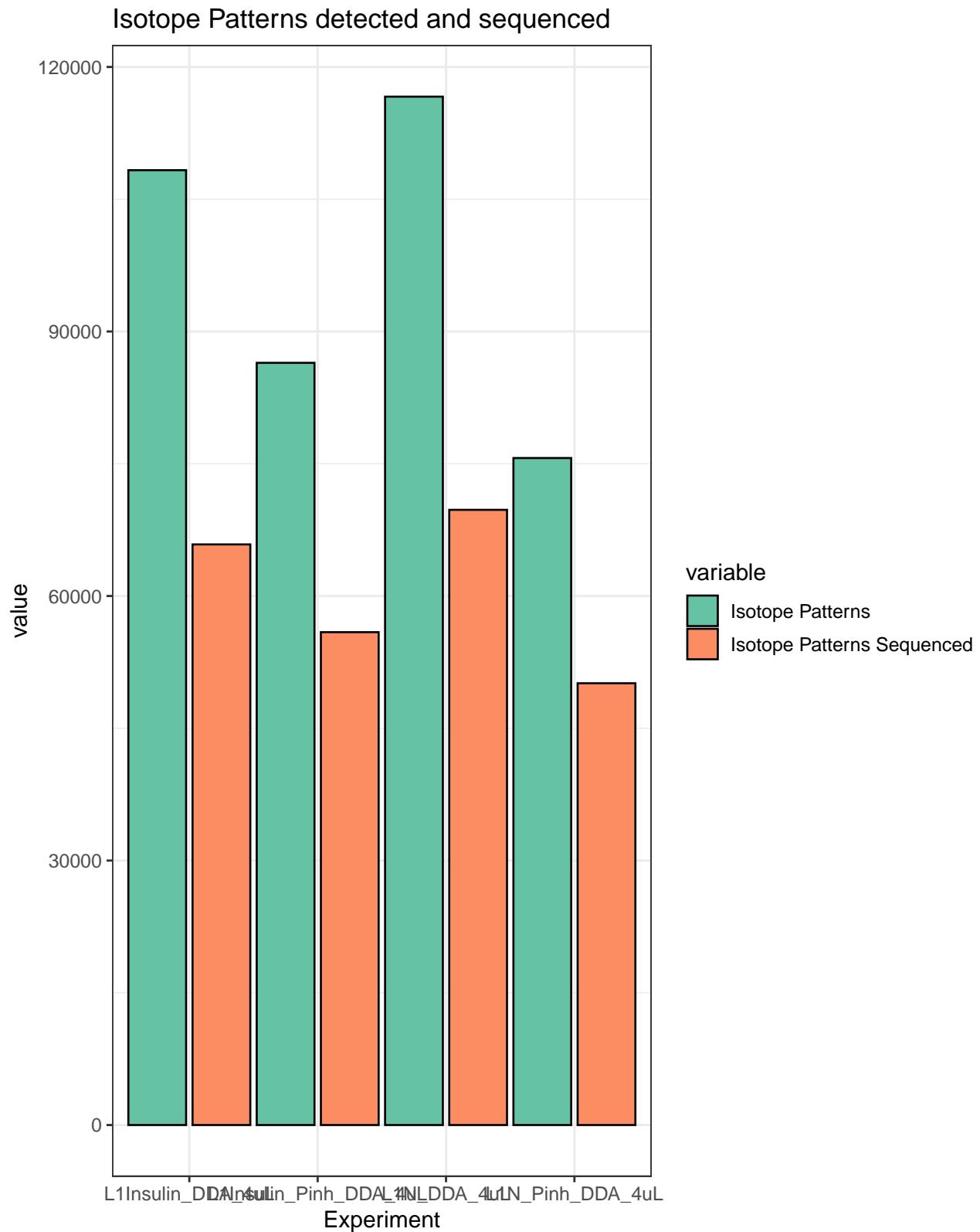


```
PlotMsMs(summary, long_names = params$long_names, sep_names = params$sep_names)
```

### MS/MS Submitted and Identified

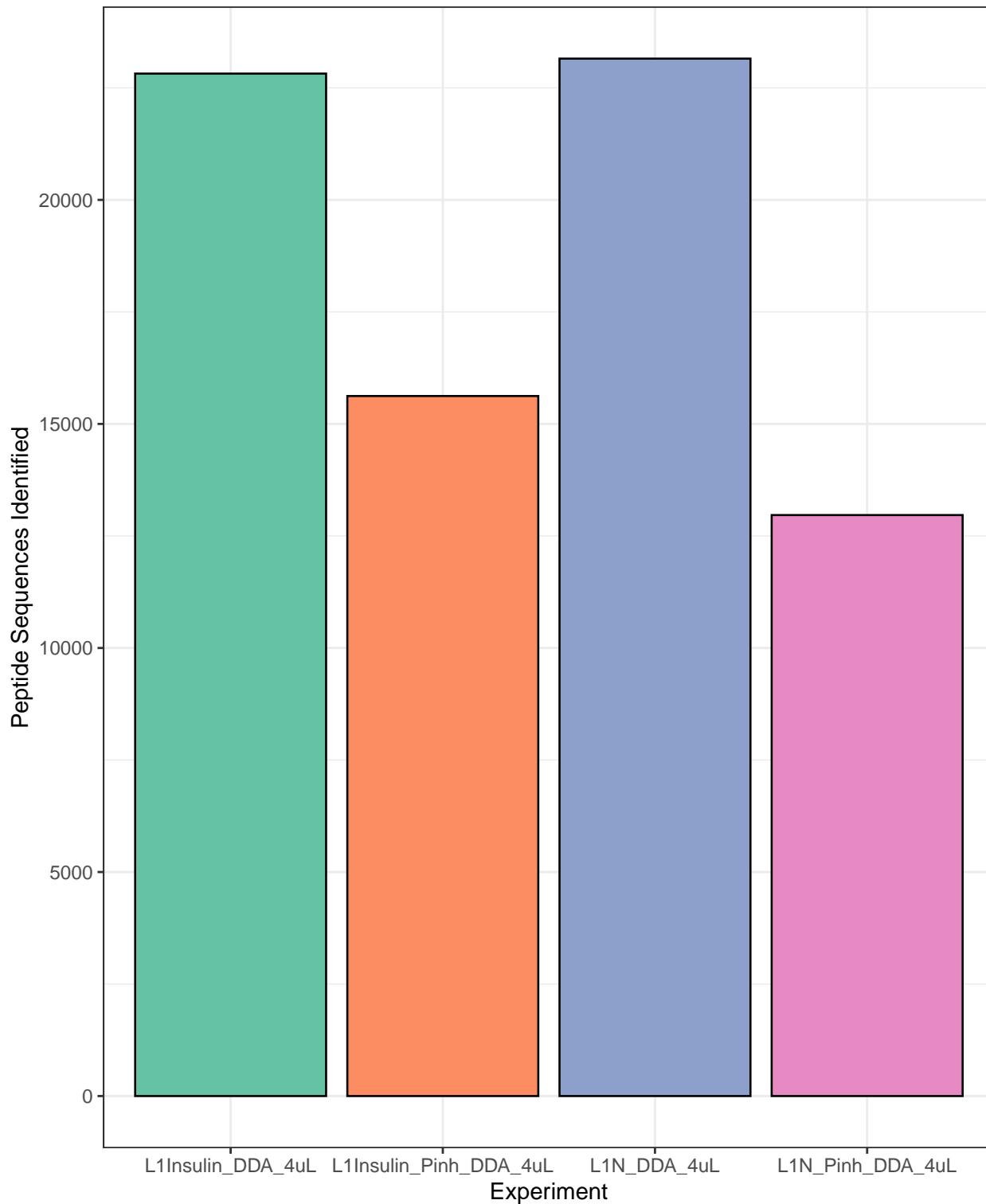


```
PlotIsotopePattern(summary, long_names = params$long_names, sep_names = params$sep_names)
```

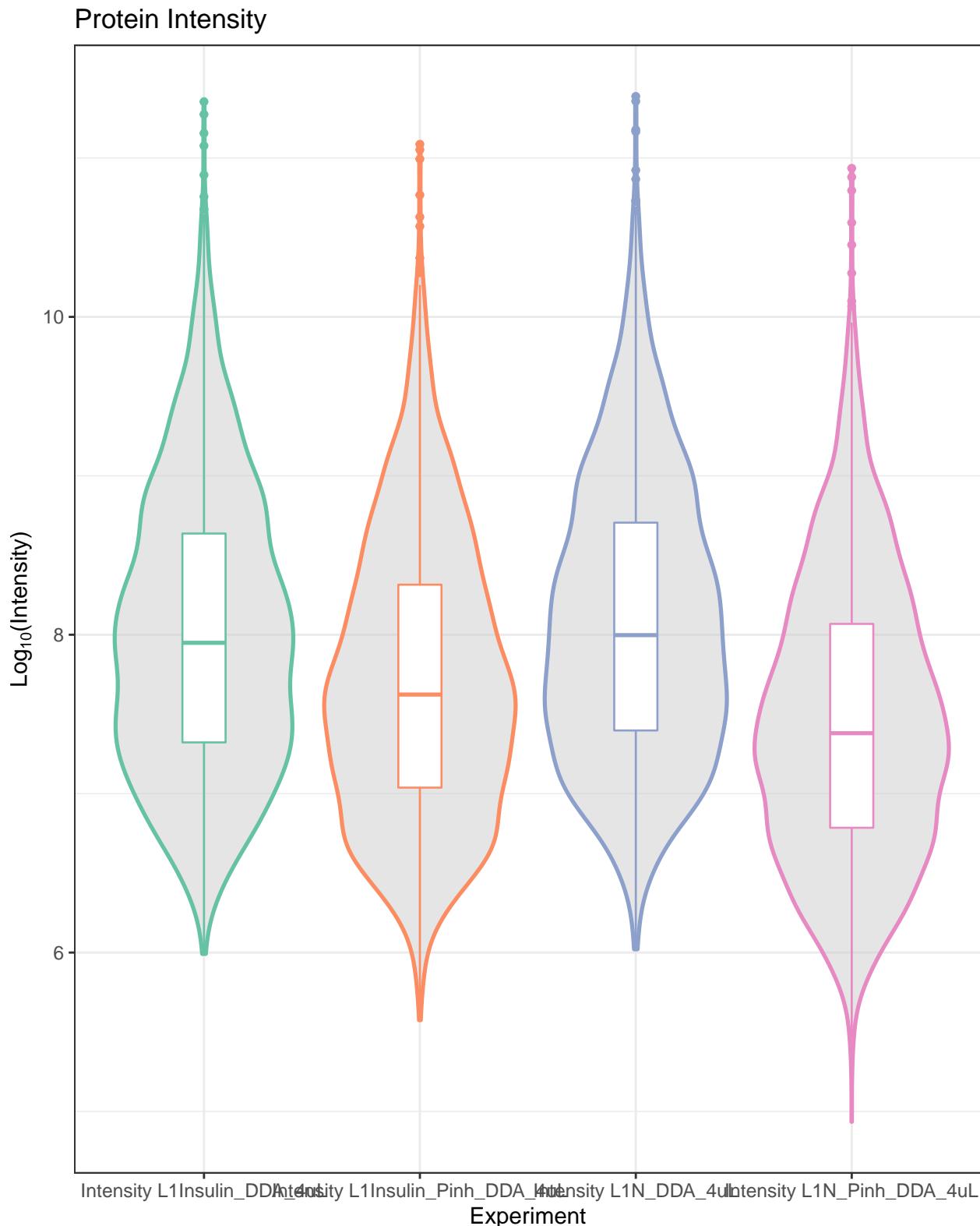


```
PlotPeptidesIdentified(summary, long_names = params$long_names, sep_names = params$sep_names)
```

Peptides Sequences Identified



```
PlotIntensity(proteinGroups, intensity_type = 'Intensity', log_base = 10,  
             long_names = params$long_names, sep_names = params$sep_names)
```



```
PlotiRT(evidence, show_calibrated_rt = FALSE)  
## [1] "No iRT peptides found in the MaxQuant output."
```

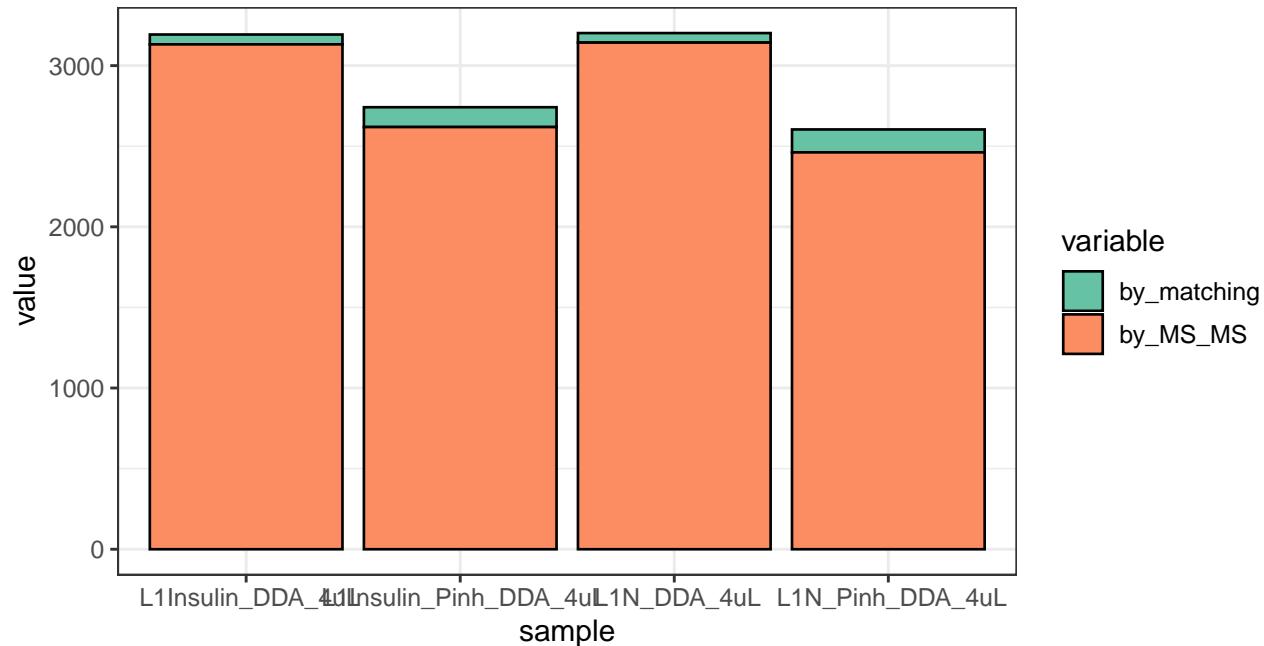
```
PlotiRTScore(evidence)
## [1] "No iRT peptides found in the MaxQuant output."
```

```

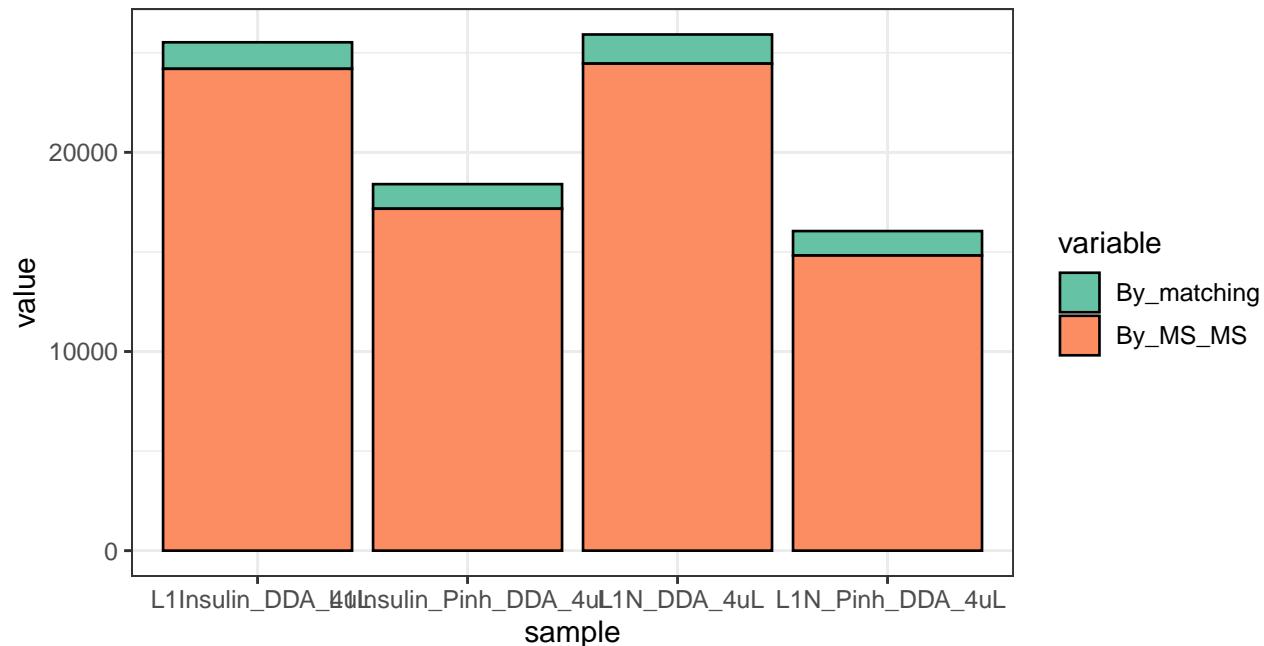
if(parameters$Value[27] == "True"){
  PlotIdentificationType(peptides, proteinGroups, long_names = params$long_names, sep_names = params$sep_names)
} else{
  print('Match Between Runs was not used during the MaxQuant analysis.
        No Identification Type to show.')
}

```

Protein Identification type

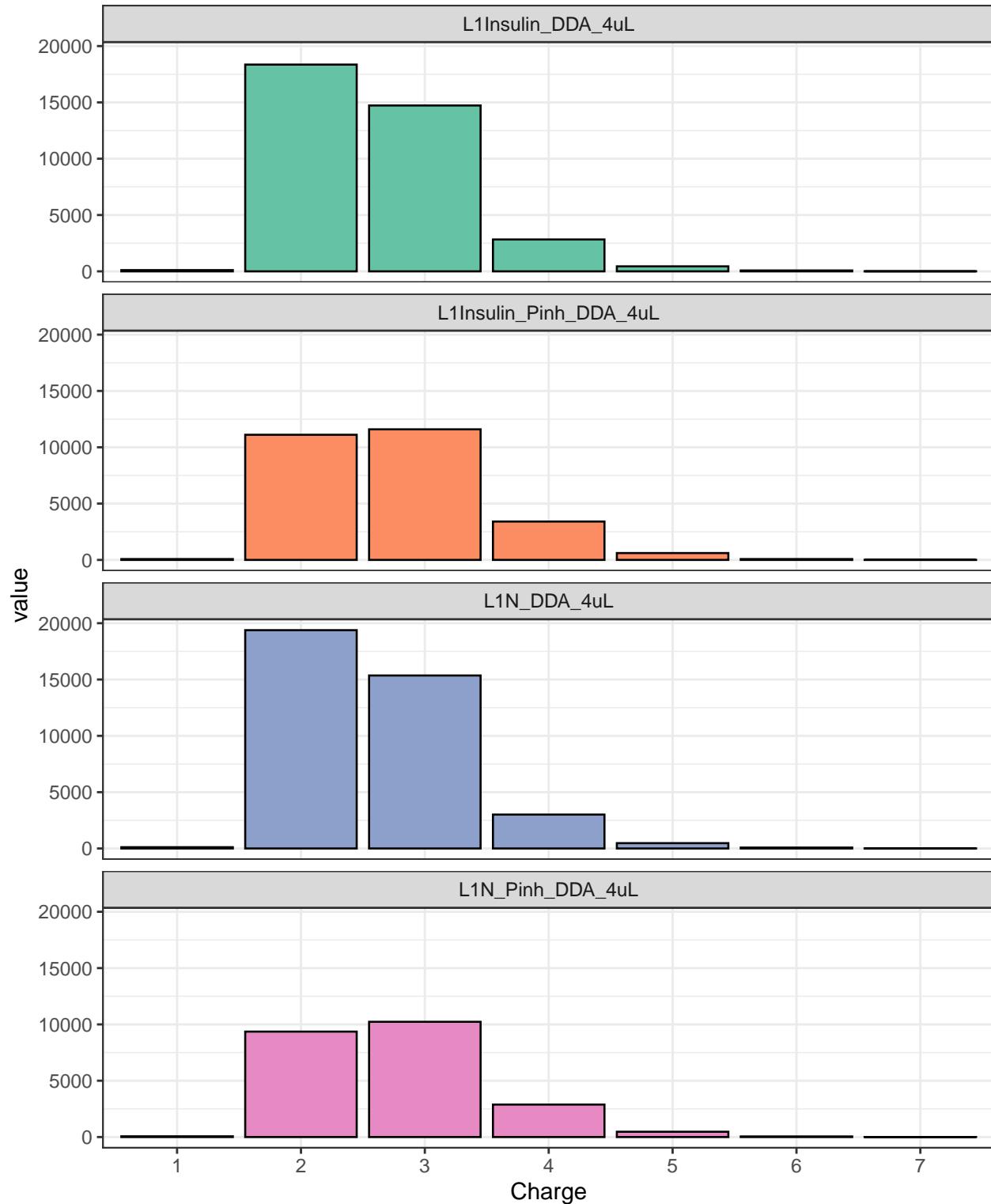


Peptide Identification type



```
PlotCharge(evidence)
```

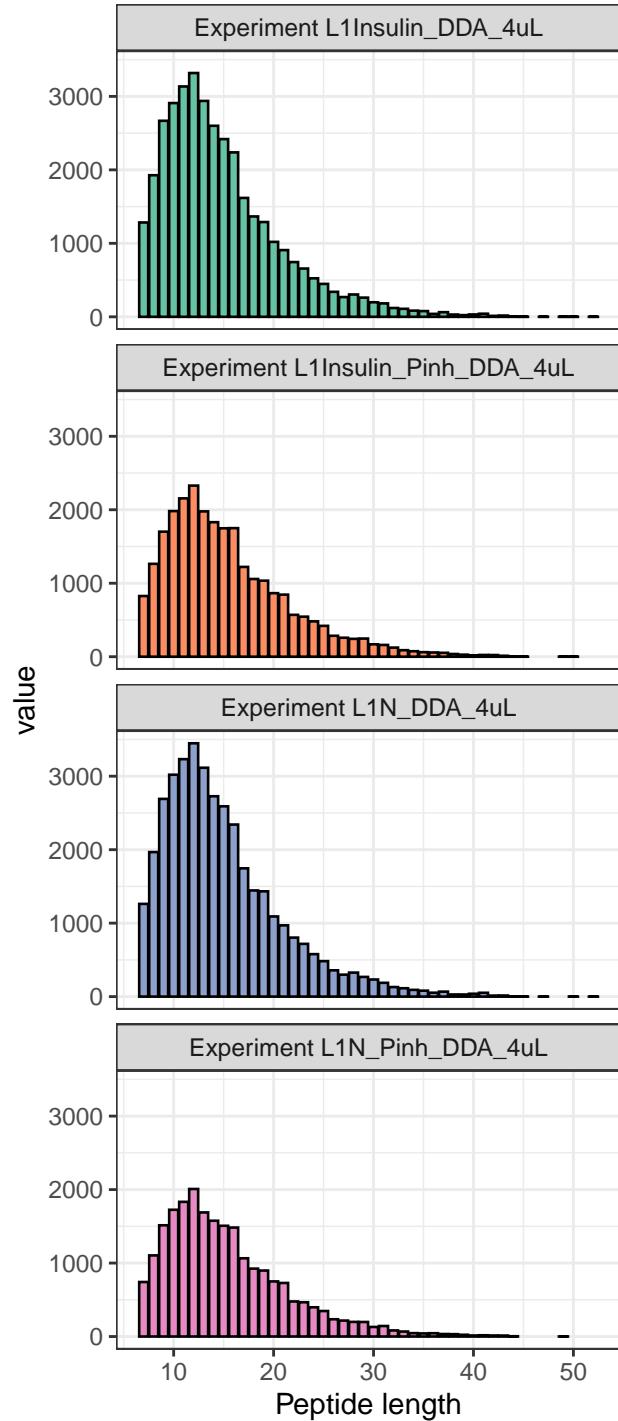
The charge-state of the precursor ion.



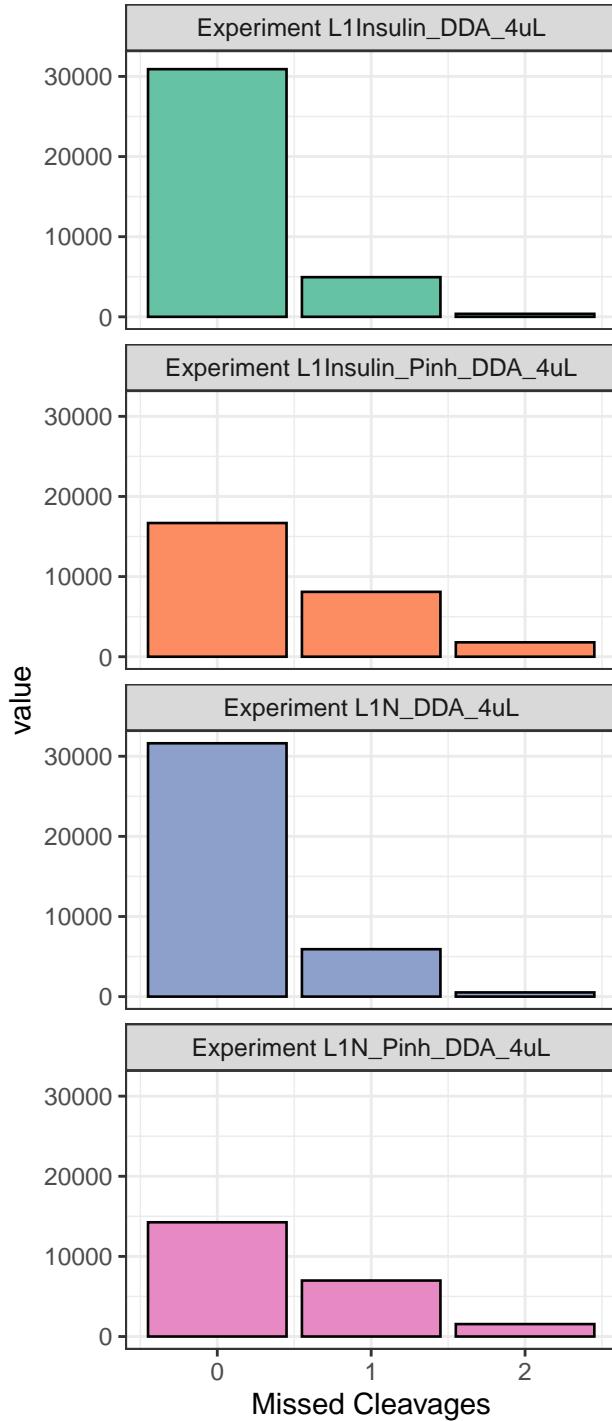
PlotProteaseSpecificity(peptides)

## Protease Specificity

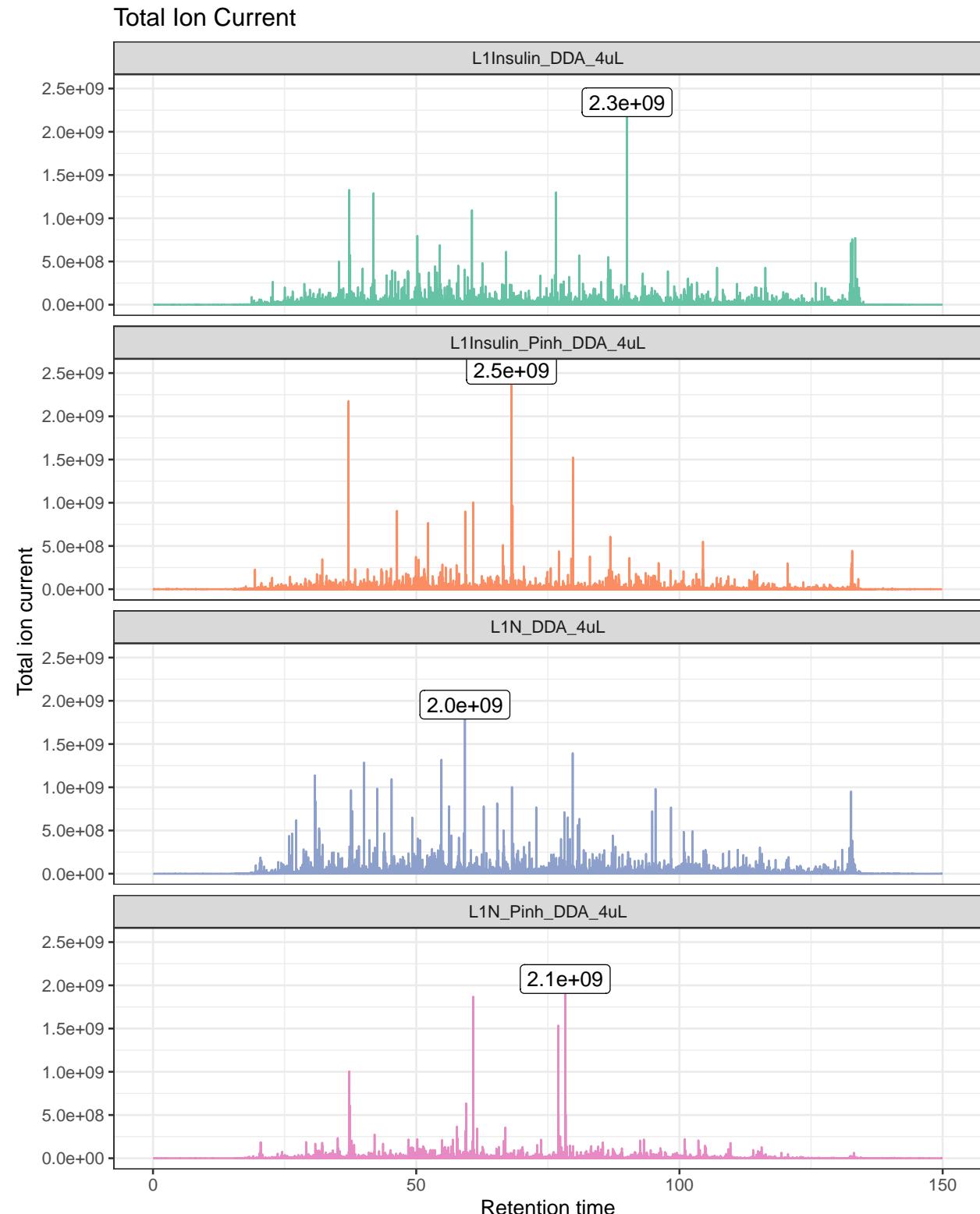
### Peptide Length



### Missed enzymatic cleavages



```
PlotTotalIonCurrent(msmsScans, show_max_value = TRUE)
```

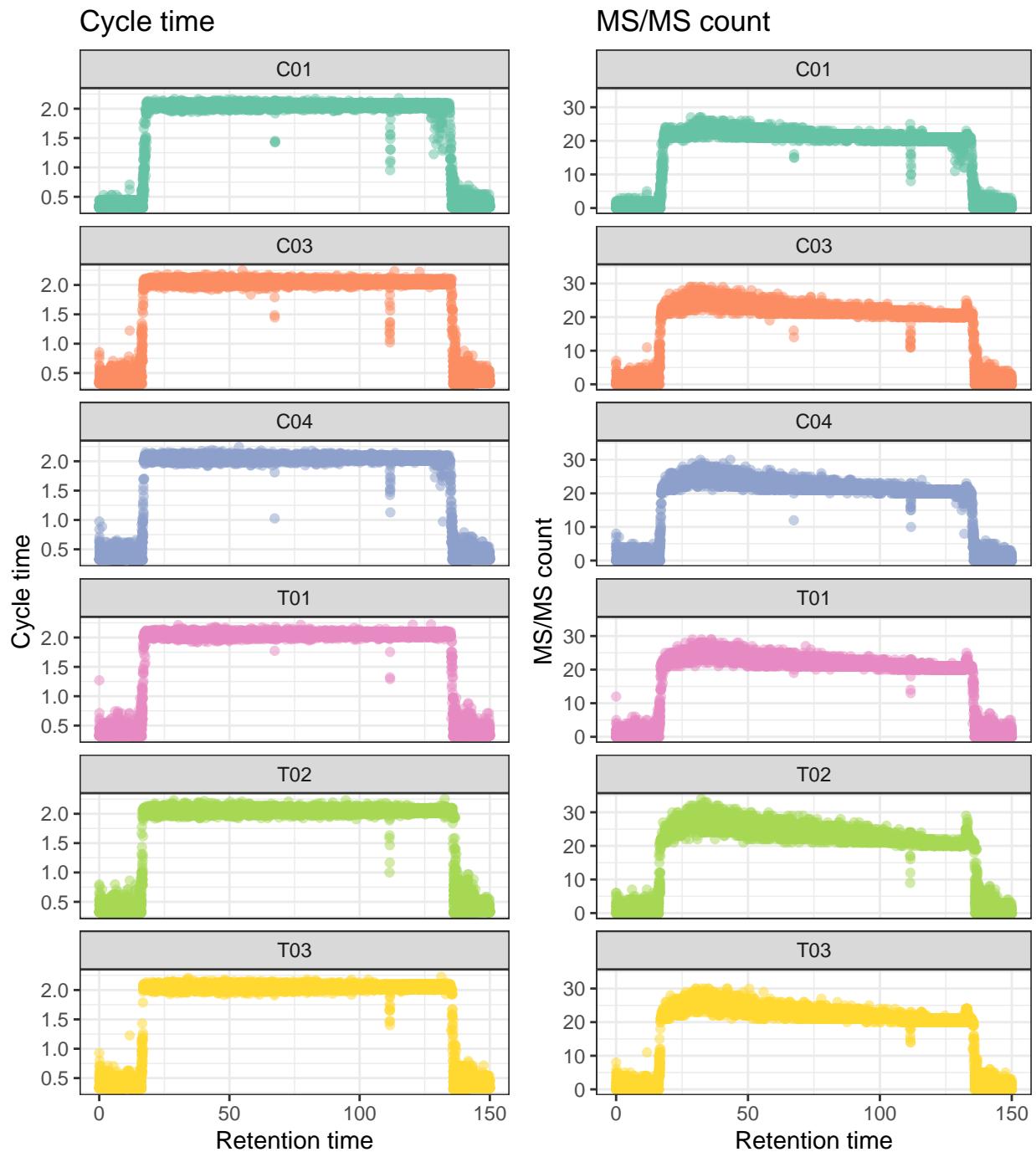


```
if(is.null(params$UniprotID)){
  print('No UniprotID provided.')
} else{
PlotProteinCoverage(peptides, proteinGroups, UniprotID = params$UniprotID, log_base = 10, segment_width
}

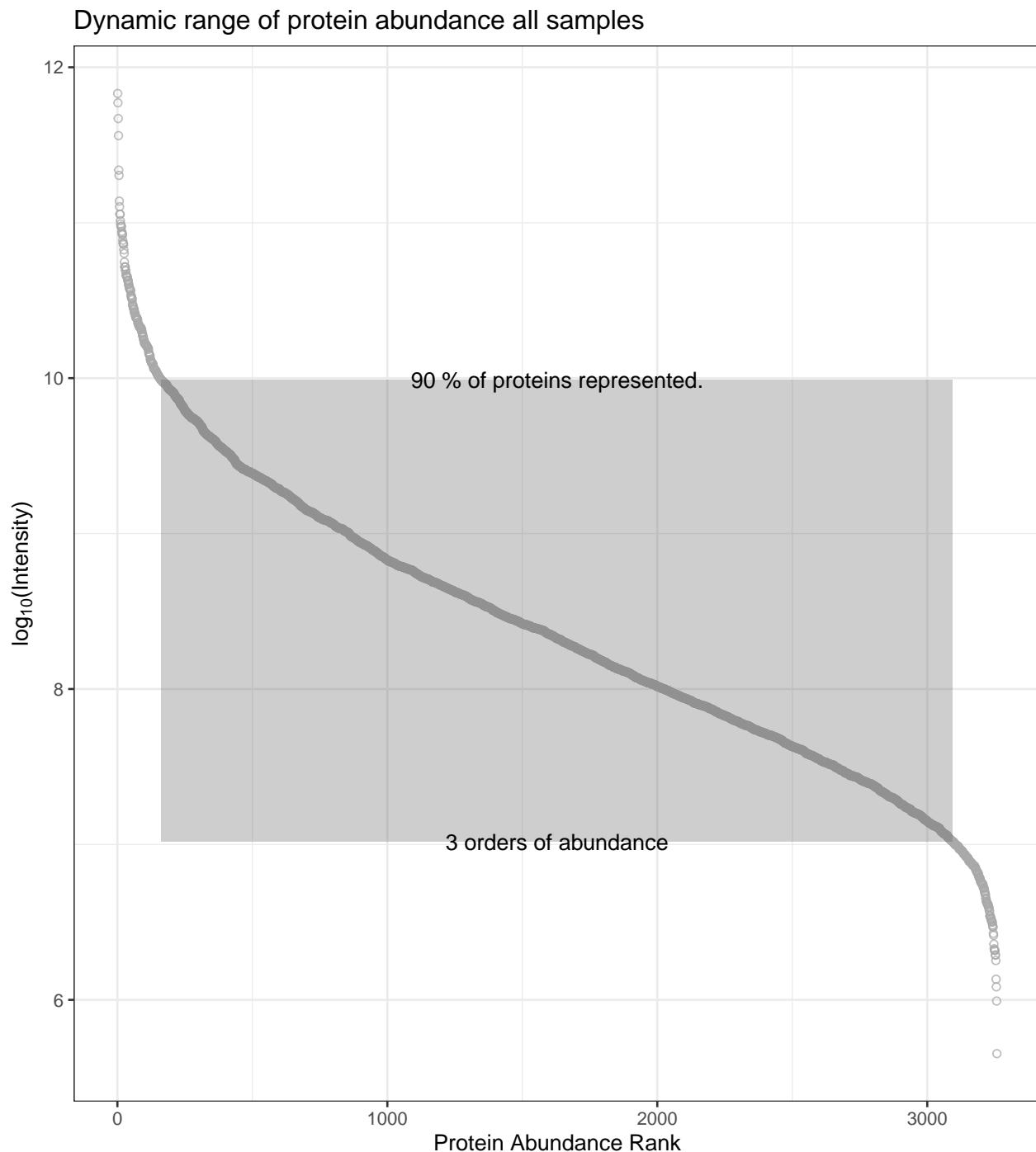
## [1] "No UniprotID provided."
```

PlotAcquisitionCycle(msScans)

### Acquisition Cycle

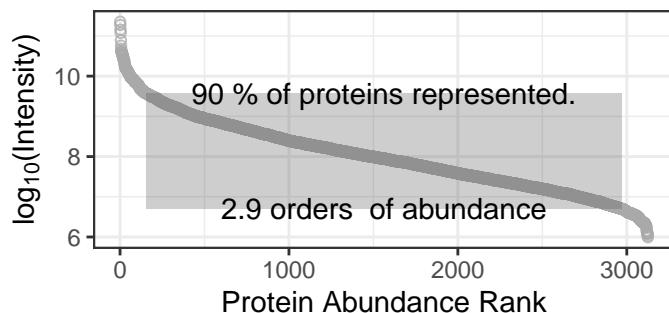


```
PlotCombinedDynamicRange(proteinGroups, show_shade = TRUE, percent_proteins = 0.9)
```

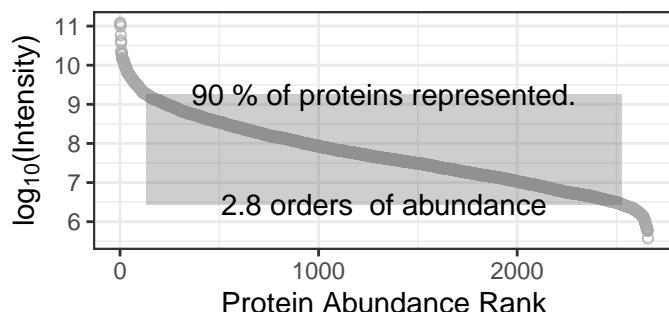


```
PlotAllDynamicRange(proteinGroups, columns = 2, rows = 4, show_shade = TRUE, percent_proteins = 0.9)
```

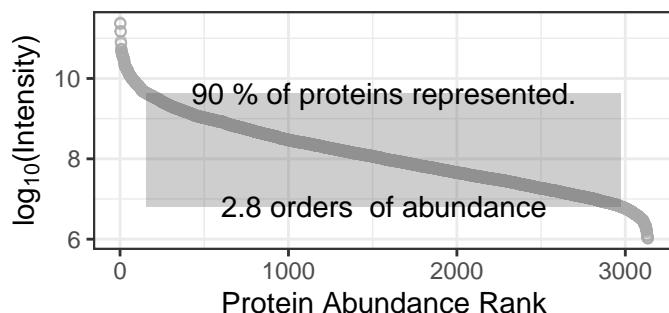
Intensity L1Insulin\_DDA\_4uL



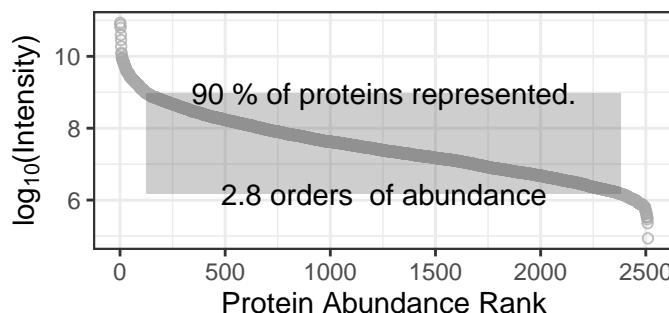
Intensity L1Insulin\_Pinh\_DDA\_4uL



Intensity L1N\_DDA\_4uL



Intensity L1N\_Pinh\_DDA\_4uL



```
PlotPTM(modificationSpecificPeptides, freq_min = 3)
```

## Post-Translational Modifications

