

Supplemental R package information

This documentation describes the information contained in the SwathXtend R package which is included as SwathXtend.zip in the Supplemental Data.

The package contains all the spectral peptide ion libraries involved in this study. The library names and their location are as follows.

Library	File location
Lib1	SwathXtend\files\Lib1.txt
Lib2	SwathXtend\files\Lib2.txt
Lib3	SwathXtend\files\Lib3.txt
Lib4	SwathXtend\files\Lib4.txt
Lib5	SwathXtend\files\Lib5.txt
Lib6	SwathXtend\files\Lib6.txt
Lib7	SwathXtend\files\Lib7.txt
Lib2_3	SwathXtend\files\Lib2_3.txt
Lib2_4	SwathXtend\files\Lib2_4.txt
Lib2_5_6	SwathXtend\files\Lib2_5_6.txt
Lib2_7	SwathXtend\files\Lib2_7.txt
Lib5_6	SwathXtend\files\Lib5_6.txt

The package also contains all the extracted SWATH results using the above libraries. The results file information is as follows.

Library used	Extraction result file
Lib1	SwathXtend\files\5600_Lib1.xlsx
Lib2	SwathXtend\files\5600_Lib2.xlsx
Lib2_3	SwathXtend\files\5600_Lib2_3.xlsx
Lib2_4	SwathXtend\files\5600_Lib2_4.xlsx
Lib2_5_6	SwathXtend\files\5600_Lib2_5_6.xlsx
Lib2_7	SwathXtend\files\5600_Lib2_7.xlsx
Lib5_6	SwathXtend\files\5600_Lib5_6.xlsx

The SwathXtend package can be installed from R using the following scripts.

```
# First install the following packages

install.packages(c("e1071", "VennDiagram", "openxlsx"))

# Next install SwathXtend from the R GUI, using the zip file downloaded.
```

A few examples of how to use SwathXtend are below.

```
# Load the SwathXtend
library(SwathXtend)

# Estimated running times on a MS Window machine of Intel Core i5-2500 CUP @ 3.30GHz

# Generating extended library Lib2_3, running time 1 minute and 35 seconds
libfiles <- paste(system.file("files",package="SwathXtend"), c("Lib2.txt","Lib3.txt"),sep="/")
Lib2_3 <- buildSpectraLibPair(libfiles[1], libfiles[2], outputFile = "Lib2_3.txt",
  outputFormat="PeakView", clean=T, nomod=T, nomc=T, plot=F)

# Generating extended library Lib2_5_6, running time 7 minutes and 48 seconds
libfiles <- paste(system.file("files",package="SwathXtend"), c("Lib2.txt","Lib5.csv",
  "Lib6.csv"),sep="/")
Lib2_5_6 <- buildSpectraLibTriple(libfiles[1], libfiles[2],libfiles[3],
  labelAddon1="HUMAN", labelAddon2 = "YEAST", outputFile = "Lib2_5_6.txt",
  outputFormat="PeakView", clean=T, nomod=T, nomc=T, plot=F)

# Generating most of the tables/images from the main text and supplemental, running time approx..
8 minutes
source( paste(system.file("files", package="SwathXtend"), "/paper code stats part final.R", sep="" ) )
```