# AssayR

*jimi.wills@ed.ac.uk*

*10 June 2017*

## AssayR

AssayR provides a small number of functions for simple and rapid assay of high resolution LCMS data, especially isotopically labelled tracer experiments.

Given a table of desired compounds, in a specific format, AssayR will extract chromatograms for those compounds, and interactively allow you to optimise peak detection. Peak detection is performed on the maximal trace for the whole data set, including any isotopes you've defined, and so the approach is immune to missing peaks.

The output is a table of results. With a labelling experiment, there's also graphical output in the form of stacked bars to summarise the information.

AssayR works with Proteowizard tools msaccess and msconvert, and expects to find these tools on your path.

To install AssayR (first install R and optionally RStudio) run the following commands in R:

```
install.packages(c("RColorBrewer", "reshape2", "stringr"))
install.packages("https://gitlab.com/jimiwills/assay.R/raw/master/AssayR_0.1.0.tar.gz", repos = NULL, ty
```

## Summary of use

```
# change directory to where your raw files are
setwd(path.to.raw.files)
# you can also do this in the RGui or RStudio menu.

# convert raw files to mzML if they are not already
msconvert_all()
# this extract pos and neg and puts them in mzMLpos and mzMLneg
# directories

# generate TICs/EICs/XICs from config file
path.to.tics <- run.config.tics(path.to.config, path.to.mzML)
# more about the config file below

# analyse the peaks (interactively)
results <- run.config.peaks(path.to.config, path.to.tics)
# this is interactive, more below.
# you could write the result to csv
# write.csv(results, "results.csv")

# rearrange and output the results, and output plots of the
# isotopes:
assay.plotter(results)
# check the current working directory for outputs
```

## Config file

There are example config files with this package. The format should be a tsv, as readable by `read.delim`, and the file should have the following columns:

- target name of the target channel (gets used for naming data)
- name name of the compound (gets used for labelling graphs)
- mz monoisotopic m/z value for this compound
- ppm m/z tolerance in ppm for this compound
- rt.min minimum retention time to be considered (can be modified interactively)
- rt.max maximum retention time to be considered (can be modified interactively)
- seconds width of pick-detection wave in seconds (can be modified interactively)
- threshold minimum required intensity (can be modified interactively)
- known alternatives reserved for future use
- C13 in labelled experiment, maximum possible number of 13C in compound
- N15 in labelled experiment, maximum possible number of 15N in compound
- H2 in labelled experiment, maximum possible number of 2H in compound
- event in mass spec method with multiple events (scans), indicates in which event to find the m/z of this compound
- interactive values: "yes" or "done", indicates whether interactive mode is required for this definition
- comment free text. I use this for sorting my compounds in pathway order.

## more information?

If you think something's missing, please get in contact and I'll update this document so everybody can benefit. Thanks!