

Extract functions (Example)

1) Install Dependencies and Initialize Environment

```
#install dependencies and verify directories
source('src/compliance.R')

#copy example files to Input folder
examples <- list.files(path = "example", full.names = TRUE)
file.copy(examples, 'input', overwrite = TRUE)

## [1] TRUE TRUE TRUE TRUE TRUE

#load aggregated peak list
peaklist <- readRDS('output/example/peaklist_aggregate_example.RDS')
```

2) Extract compound-specific MS Data

```
list_extract_w_metadata(peaklist, output_dir = "example")

## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_YPJUNDFVDDCYIH-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_CXZGQIAOTKWADB-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_PXUULQAPEKKVAH-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_ZWBAMYVPMDSJGQ-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_SNGREZUHAYWORS-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_UZUFPBIDKMEQEQ-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_PCIUEQPBYFRTEM-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_CXGONMQFMIYUJR-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_SIDINRCMMRXXGQ-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_LVDGGZAZAYHKEY-UHFFFAOYSA-N.RDS"
## [1] "Saved file at: output/extract/PFAC30PAR_PFCA2_RUDINRUXCKIXAJ-UHFFFAOYSA-N.RDS"
```