Flexible Infrastructure for Mass Spectrometry Data

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Introduction

Mass Spectrometry (MS) Data

- Paired measurements:
  - intensity (counts) vs *m/z* (mass-to-charge ratio).
  - intensity vs retention time.
- Additional various metatdata.

Problems

- Vendor-specific, closed file formats.
- Various open-formats, e.g. mzML, mzXML, mz5, CDF, MGF, CSV
- Spectra libraries/Annotation information in databases, e.g. SQL
- Multiple R-packages require different file formats and/or data structures.
- Larger experiments don't fit into RAM.

Solution: `Spectra`[1]

- Common, flexible data structure and interface.
- Supports various file formats by different backends.

Implementation Details

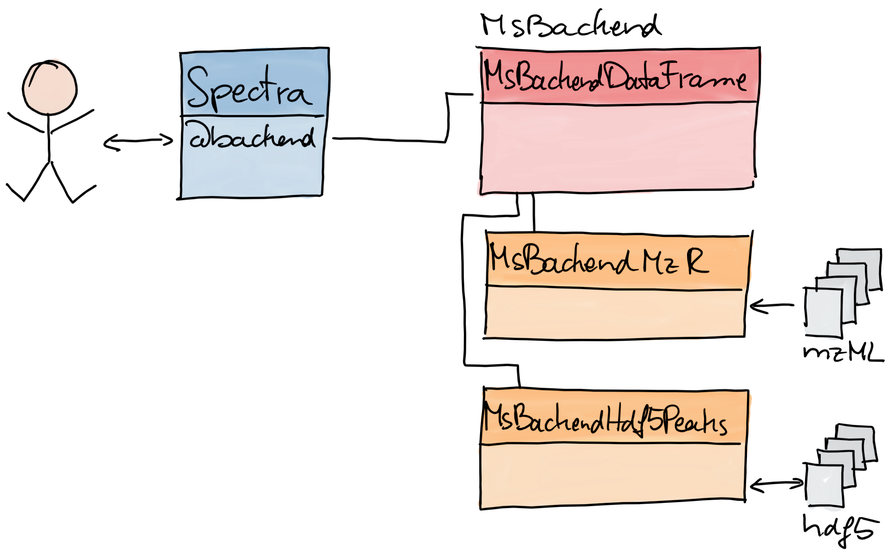
`Spectra` class

- Handles one or multiple MS spectra.
- Implements typical processing functionality.
- Isolation from type of data storage (handled by backend classes)

`MsBackend` classes

- Isolation from spectra handling and processing.
- Specific class for each type of data storage.

class	source	storage	writeable
MsBackendDataFrame[1]	manual	in-memory	yes
MsBackendHdf5Peaks[1]	hdf5 files	on-disk	yes
MsBackendMzR[1]	mzML, mzXML and CDF files	on-disk	no
MsBackendHmdbXml[2]	XML files	on-disk	yes
MsBackendRawFileReader[3]	Thermo .raw files	on-disk	no



The user interacts with a `Spectra` object. It takes care of the data storage by different backend classes.

Example

```
# Load packages
library(Spectra)
library(magrittr)


# Import data
#sps     <-     Spectra("data/20191107_Mix2_CE20.mzML",     backend     =
       MsBackendMzR())
sps <- Spectra()

# Select all MS2 spectra for a [M+Na]+ ion of Fructose.

mzr <- 203.0526
mzr <- 156.07675 # Histidine
fruct <- sps %>%
    filterMsLevel(2) %>%
    filterPrecursorMz(mz = mzr + ppm(c(-mzr, mzr), 20))

# Centroid and clean spectra.

fruct <- fruct %>%
    pickPeaks() %>%
    removePeaks(threshold = 500) %>%
    clean(all = TRUE)

# Change backend: load data in memory.

#fruct <- setBackend(fruct, MsBackendDataFrame())
```

Contact

- rformassspectrometry/Spectra
- rformassspectrometry.org
- #RforMassSpec

References

1. Gatto, L., Rainer, J. & Gibb, S. *Spectra: Spectra infrastructure for mass spectrometry data*.

2. Gatto, L., Rainer, J. & Gibb, S. *MsBackendHmdb: Mass spectrometry data backends for the human metabolome database*. (2019).

3. Panse, C. & Kockmann, T. *MsBackendRawFileReader: Bridging spectra and thermofinnigan raw files*. (2019).