

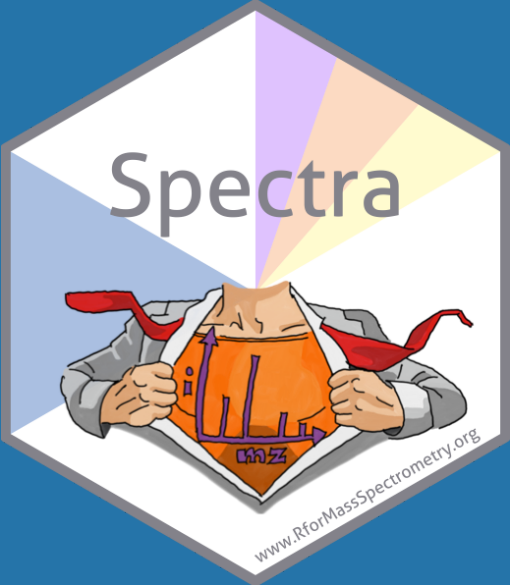
Flexible Infrastructure for Mass Spectrometry Data

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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

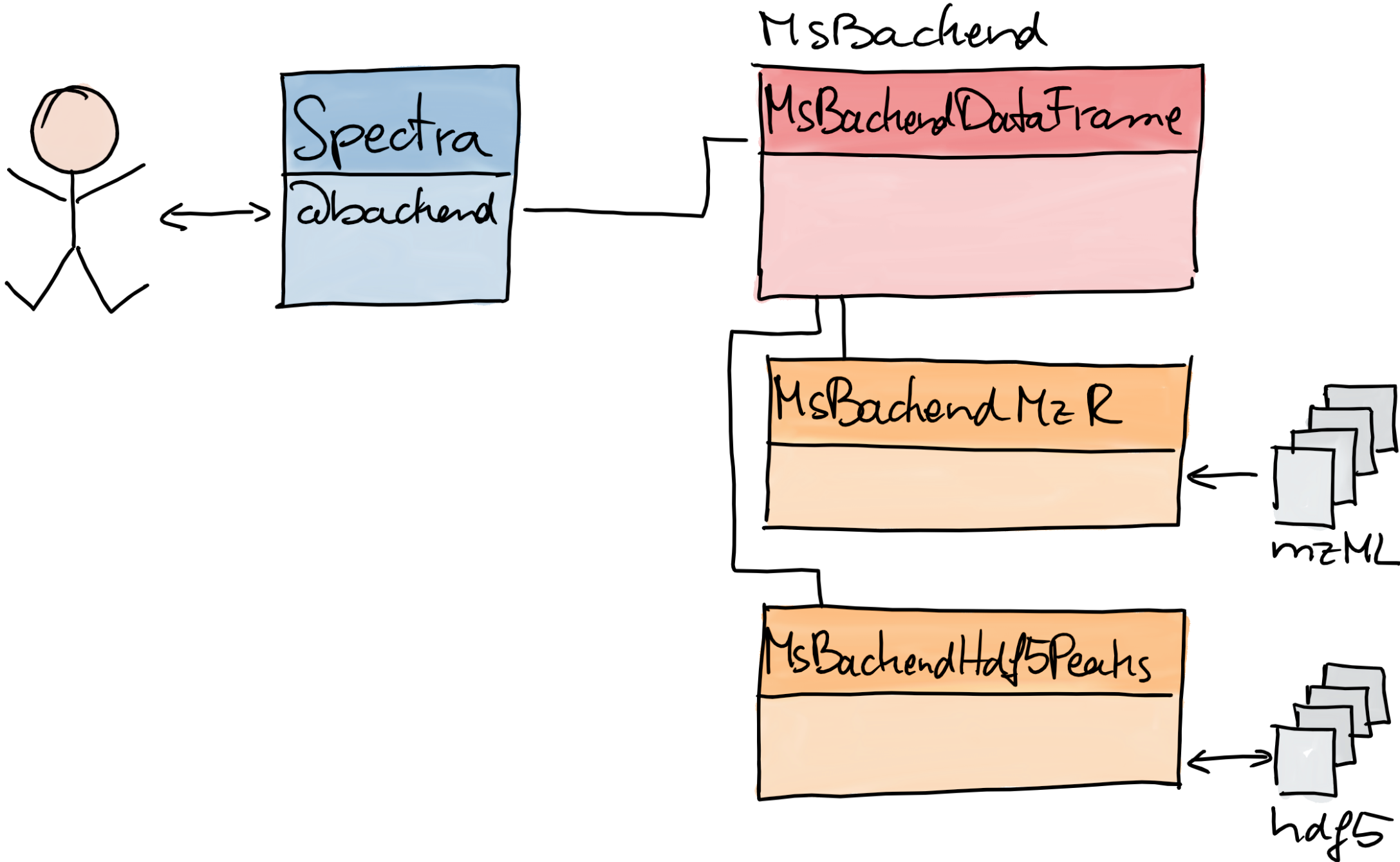
Spectra class

- 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](https://github.com/rformassspectrometry/Spectra)
-  rformassspectrometry.org
-  [#RforMassSpec](https://twitter.com/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).

