

# A parser for raw and identification mass-spectrometry data

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## 1 Introduction

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The *mzR* package aims at providing a common interface to several mass spectrometry data formats, namely *mzData* [1], *mzXML* [2], *mzML* [3] for raw data, and *mzIdentML* [4], somewhat similar to the Bioconductor package *affyio* for *affymetrix* raw data. No processing is done in *mzR*, which is left to packages such as *XCMS* [5, 6] or *MSnbase* [7].

Most importantly, access to the data should be fast and memory efficient. This is made possible by allowing on-disk random file access, i.e. retrieving specific data of interest without having to sequentially browser the full content nor loading the entire data into memory.

The actual work of reading and parsing the data files is handled by the included C/C++ libraries or “backends”. The *mzRramp* RAMP parser, written at the Institute for Systems Biology (ISB) is a fast and lightweight parser in pure C. Later, it gained support for the *mzData* format. The C++ reference implementation for the *mzML* is the *proteowizard* library [8] (*pwiz* in short), which in turn makes use of the *boost* C++ (<http://www.boost.org/>) library. RAMP is able

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to access mzML files by calling pwiz methods. More recently, the proteowizard<sup>1</sup> [9] has been fully integrated using the mzRpwiz backend for raw data. The mzRnetCDF backend provides support to CDF-based formats. Finally, the mzRident backend is available to access identification data (mzIdentML) through pwiz.

*warning: It is anticipated to switch to the mzRpwiz backend in Bioconductor 3.1. We advise users and developers to test it and report any issues on the github issue tracker <https://github.com/sneumann/mzR/issues>.*

The *mzR* package is in essence a collection of wrappers to the C++ code, and benefits from the C++ interface provided through the Rcpp package [10].

## 2 Mass spectrometry raw data

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All the mass spectrometry file formats are organized similarly, where a set of metadata nodes about the run is followed by a list of spectra with the actual masses and intensities. In addition, each of these spectra has its own set of metadata, such as the retention time and acquisition parameters.

### 2.1 Spectral data access

Access to the spectral data is done via the `peaks` function. The return value is a list of two-column mass-to-charge and intensity matrices or a single matrix if one spectrum is queried.

### 2.2 Chromatogram access

Access to the chromatogram(s) is done using the `chromatogram` (or `chromatograms`) function, that return one (or a list of) `data.frames`. See `?chromatogram` for details. This functionality is only available with the pwiz backend.

### 2.3 Identification result access

The main access to identification result is done via `psms`, `score` and `modifications`. `psms` and `score` will return the detailed information on each psm and scores. `modifications` will return the details on each modification found in peptide.

### 2.4 Metadata access

**Run metadata** is available via several functions such as `instrumentInfo()` or `runInfo()`. The individual fields can be accessed via e.g. `detector()` etc.

**Spectrum metadata** is available via `header()`, which will return a list (for single scans) or a dataframe with information such as the `basePeakMZ`, `peaksCount`, ... or, for higher-order MS the `msLevel` and precursor information.

**Identification metadata** is available via `mzidInfo()`, which will return a list with information such as the software, `ModificationSearched`, `enzymes`, `SpectraSource` and other information for this identification result.

The availability of this metadata can not always be guaranteed, and depends on the MS software which converted the data.

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<sup>1</sup><http://proteowizard.sourceforge.net/>

## 3 Example

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### 3.1 mzXML/mzML/mzData files

A short example sequence to read data from a mass spectrometer. First open the file.

```
library(mzR)

## Loading required package: Rcpp

library(msdata)

mzxml <- system.file("threonine/threonine_i2_e35_pH_tree.mzXML",
                     package = "msdata")
aa <- openMSfile(mzxml) ## ramp, default backend
```

We can obtain different kind of header information.

```
runInfo(aa)

## $scanCount
## [1] 55
##
## $lowMz
## [1] 50.0036
##
## $highMz
## [1] 298.673
##
## $dStartTime
## [1] 0.3485
##
## $dEndTime
## [1] 390.027
##
## $msLevels
## [1] 1 2 3 4

instrumentInfo(aa)

## $manufacturer
## [1] "Thermo Scientific"
##
## $model
## [1] "LTQ Orbitrap"
##
## $ionisation
## [1] "ESI"
##
## $analyzer
## [1] "FTMS"
##
## $detector
## [1] "unknown"

header(aa,1)

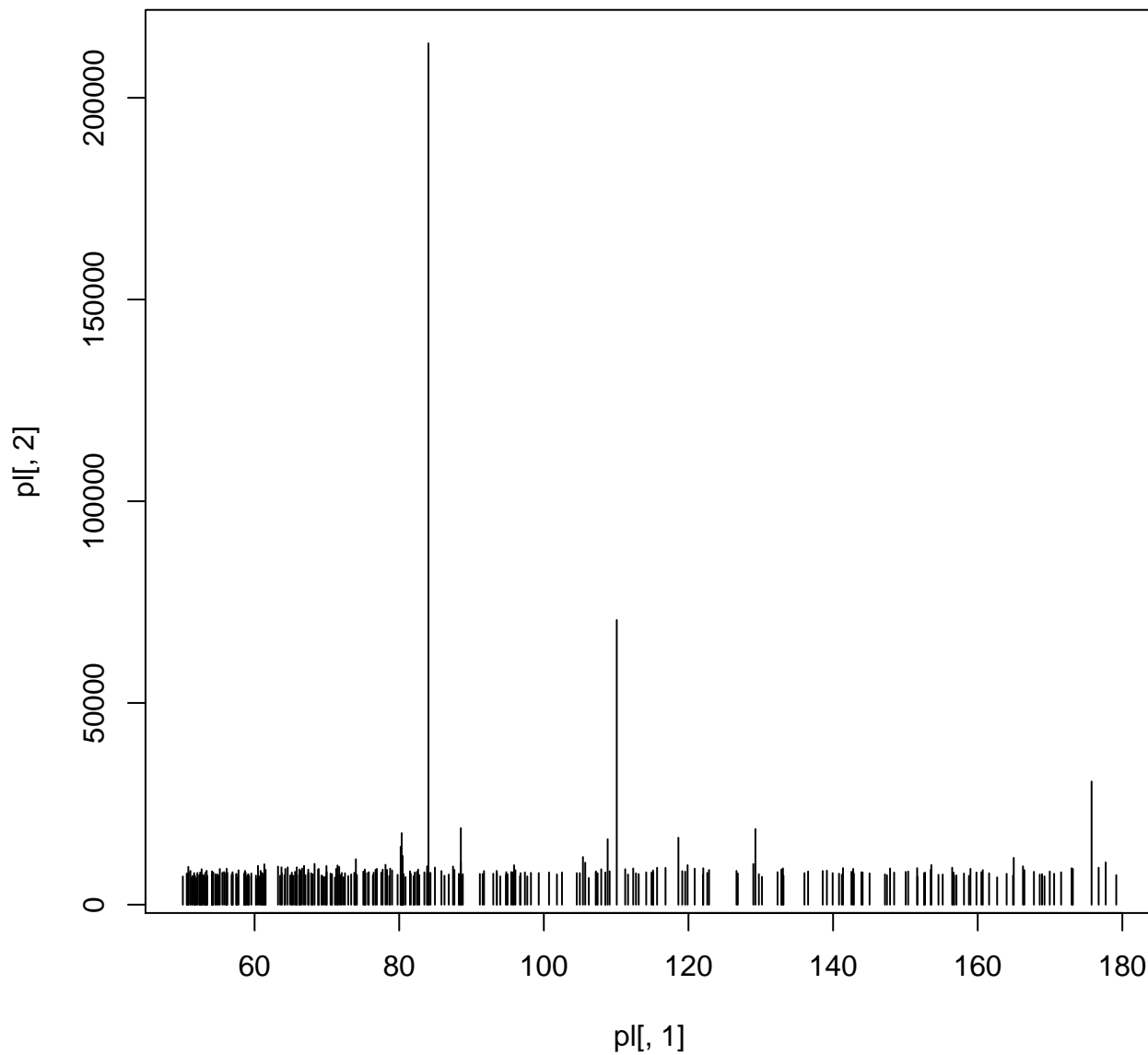
## $seqNum
```

```
## [1] 1
##
## $acquisitionNum
## [1] 1
##
## $msLevel
## [1] 1
##
## $polarity
## [1] 1
##
## $peaksCount
## [1] 684
##
## $totIonCurrent
## [1] 341427000
##
## $retentionTime
## [1] 0.3485
##
## $basePeakMZ
## [1] 120.066
##
## $basePeakIntensity
## [1] 211860000
##
## $collisionEnergy
## [1] 0
##
## $ionisationEnergy
## [1] 0
##
## $lowMZ
## [1] 50.3254
##
## $highMZ
## [1] 298.673
##
## $precursorScanNum
## [1] 0
##
## $precursorMZ
## [1] 0
##
## $precursorCharge
## [1] 0
##
## $precursorIntensity
## [1] 0
##
## $mergedScan
## [1] 0
##
```

```
## $mergedResultScanNum
## [1] 0
##
## $mergedResultStartScanNum
## [1] 0
##
## $mergedResultEndScanNum
## [1] 0
```

Read a single spectrum from the file.

```
p1 <- peaks(aa,10)
peaksCount(aa,10)
## [1] 317
head(p1)
##           [,1]      [,2]
## [1,] 50.08176 6984.858
## [2,] 50.62267 7719.419
## [3,] 50.70530 7185.290
## [4,] 50.73298 7509.140
## [5,] 50.83848 9366.624
## [6,] 50.88303 8012.808
plot(p1[,1], p1[,2], type="h", lwd=1)
```



One should always close the file when not needed any more if you are using RAMP backend. This will release the memory of cached content.

```
close(aa)
```

### 3.2 mzIdentML files

You can use `openIDfile` to read a `mzIdentML` file (version 1.1), which use the `pwiz` backend.

```
library(mzR)
library(msdata)
```

```
file <- system.file("mzid", "Tandem.mzid.gz", package="msdata")
x <- openIDfile(file)
```

mzidInfo function will return general information about this identification result.

```
mzidInfo(x)

## $FileProvider
## [1] "researcher"
##
## $CreationDate
## [1] "2012-07-25T14:03:16"
##
## $software
## [1] "xtandem x! tandem CYCLONE (2010.06.01.5) "
## [2] "ProteoWizard MzIdentML 3.0.501 ProteoWizard"
##
## $ModificationSearched
## [1] "Oxidation"          "Carbamidomethyl"
##
## $FragmentTolerance
## [1] "0.8 dalton"
##
## $ParentTolerance
## [1] "1.5 dalton"
##
## $enzymes
## $enzymes$name
## [1] "Trypsin"
##
## $enzymes$nTermGain
## [1] "H"
##
## $enzymes$cTermGain
## [1] "OH"
##
## $enzymes$minDistance
## [1] "0"
##
## $enzymes$missedCleavages
## [1] "1"
##
## $SpectraSource
## [1] "D:/TestSpace/NeoTestMarch2011/55merge.mgf"
```

psms will return the detailed information on each peptide-spectrum-match, include spectrumID, chargeState, sequence, modNum and others.

```
p <- psms(x)
colnames(p)

## [1] "spectrumID"          "chargeState"          "rank"
## [4] "passThreshold"       "experimentalMassToCharge" "calculatedMassToCharge"
## [7] "sequence"           "modNum"               "isDecoy"
## [10] "post"               "pre"                  "start"
```

```
## [13] "end"                "DatabaseAccess"        "DBseqLength"
## [16] "DatabaseSeq"        "DatabaseDescription"   "acquisitionNum"
```

The modifications information can be accessed using `modifications`, which will return the `spectrumID`, `sequence`, `name`, `mass` and `location`.

```
m <- modifications(x)
head(m)
```

##	spectrumID	sequence	name	mass	location
## 1	index=12	LCYIALDFDEEMKAAEDSSDIEK	Carbamidomethyl	57.0215	2
## 2	index=12	LCYIALDFDEEMKAAEDSSDIEK	Oxidation	15.9949	12
## 3	index=285	KDLYGNVVLSSGTTMYEGIGER	Oxidation	15.9949	15
## 4	index=83	KDLYGNVVLSSGTTMYEGIGER	Oxidation	15.9949	15
## 5	index=21	VIDENFGLVEGLMTTVHAATGTQK	Oxidation	15.9949	13
## 6	index=198	GVGGAIVLVLYDEMK	Oxidation	15.9949	14

Since different software will use different scoring function, we provide a `score` to extract the scores for each psm. It will return a data.frame with different columns depending on software generating this file.

```
scr <- score(x)
colnames(scr)
```

##	[1]	"spectrumID"	"X.Tandem.expect"	"X.Tandem.hyperscore"
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## 4 Future plans

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Other file formats provided by HUPO, such as `mzQuantML` for quantitative data [11] are also possible in the future.

## 5 Session information

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- R version 3.4.0 (2017-04-21), x86\_64-w64-mingw32
- Locale: LC\_COLLATE=C, LC\_CTYPE=English\_United States.1252, LC\_MONETARY=English\_United States.1252, LC\_NUMERIC=C, LC\_TIME=English\_United States.1252
- Running under: Windows Server 2012 R2 x64 (build 9600)
- Matrix products: default
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: Rcpp 0.12.10, msdata 0.15.1, mzR 2.10.0
- Loaded via a namespace (and not attached): Biobase 2.36.0, BiocGenerics 0.22.0, BiocStyle 2.4.0, ProtGenerics 1.8.0, backports 1.0.5, codetools 0.2-15, compiler 3.4.0, digest 0.6.12, evaluate 0.10, highr 0.6, htmltools 0.3.5, knitr 1.15.1, magrittr 1.5, parallel 3.4.0, rmarkdown 1.4, rprojroot 1.2, stringi 1.1.5, stringr 1.2.0, tools 3.4.0, yaml 2.1.14

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