Package ‘RMassBank’

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Type Package

Title Workflow to process tandem MS files and build MassBank records

Version 2.2.1

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Description Workflow to process tandem MS files and build MassBank records. Functions include automated extraction of tandem MS spectra, formula assignment to tandem MS fragments, recalibration of tandem MS spectra with assigned fragments, spectrum cleanup, automated retrieval of compound information from Internet databases, and export to MassBank records.

License Artistic-2.0

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`add.formula` *Calculations on molecular formulas*

Description

Add, subtract, and multiply molecular formulas.

Usage

```
add.formula(f1, f2, as.formula = TRUE, as.list = FALSE)
multiply.formula(f1, n, as.formula = TRUE, as.list = FALSE)
```

Arguments

`f1, f2`	Molecular formulas (in list form or in text form) to calculate with.
`as.formula`	Return the result as a text formula (e.g. `"C6H12O6"`). This is the default
`as.list`	Return the result in list format (e.g. `list(C=6, H=12,O=6)`).
`n`	Multiplier (positive or negative, integer or non-integer.)

Details

Note that the results are not checked for plausibility at any stage, nor reordered.

Value

The resulting formula, as specified above.

Author(s)

Michael Stravs

See Also

formulastring.to.list, is.valid.formula, order.formula

Examples

```
##

add.formula("C6H12O6", "C3H3")
add.formula("C6H12O6", "C-3H-3")
add.formula("C6H12O6", multiply.formula("C3H3", -1))
```

---

addMB *MassBank-record Addition*

Description

Adds the peaklist of a MassBank-Record to the specs of an msmsWorkspace

Usage

```
addMB(w, cpdID, fileName, mode)
```

Arguments

w	The msmsWorkspace that the peaklist should be added to.
cpdID	The compoundID of the compound that has been used for the record
fileName	The path to the record
mode	The ionization mode that has been used to create the record

Value

The msmsWorkspace with the additional peaklist from the record

Author(s)

Erik Mueller

See Also

addPeaksManually

Examples

```
## Not run:
addMB("filepath_to_records/RC00001.txt")

## End(Not run)
```

---

addPeaks *Add additional peaks to spectra*

Description

Loads a table with additional peaks to add to the MassBank spectra. Required columns are `cpdID, scan, int, mzFound`

Usage

```
addPeaks(mb, filename_or_dataframe)
```

Arguments

`mb`	The `mbWorkspace` to load the peaks into.
`filename_or_dataframe`	Filename of the csv file, or name of the R dataframe containing the peaklist.

Details

All peaks with OK=1 will be included in the spectra.

Value

The `mbWorkspace` with loaded additional peaks.

Author(s)

Michael Stravs

See Also

mbWorkflow

Examples

```
## Not run: addPeaks("myrun_additionalPeaks.csv")
```

addPeaksManually — *Addition of manual peaklists*

Description

Adds a manual peaklist in matrix-format

Usage

```
addPeaksManually(w, cpdID, handSpec, mode)
```

Arguments

w	The msmsWorkspace that the peaklist should be added to.
cpdID	The compoundID of the compound that has been used for the peaklist
handSpec	A peaklist with 2 columns, one with "mz", one with "int"
mode	The ionization mode that has been used for the spectrum represented by the peaklist

Value

The msmsWorkspace with the additional peaklist added to the right spectrum

Author(s)

Erik Mueller

See Also

msmsWorkflow

Examples

```
## Not run:
handSpec <- cbind(mz=c(274.986685367956, 259.012401087427, 95.9493025990907, 96.9573002472772),
                                int=c(357,761, 2821, 3446))
addPeaksManually(w, cpdID, handSpec)

## End(Not run)
```

addProperty — *Add and initialize dataframe column*

Description

Adds a new column of a defined type to a `data.frame` and initializes it to a value. The advantage of doing this over adding it with `$` or `[,""]` is that the case `nrow(o) == 0` is adequately handled and doesn't raise an error.

Usage

```
addProperty(o, name, type, value = NA)

## S4 method for signature 'data.frame,character,character'
addProperty(o, name, type,
  value = NA)
```

Arguments

`o`	`data.frame` to add the column to
`name`	Name of the new column
`type`	Data type of the new column
`value`	Initial value of the new column (`NA` if not given)

Value

Expanded data frame.

Methods (by class)

- `o = data.frame,name = character,type = character`: Add a new column to a data.frame

Author(s)

stravsmi

aggregateSpectra — *Aggregate analyzed spectra*

Description

Groups an array of analyzed spectra and creates aggregated peak tables

Usage

```
aggregateSpectra(spec,  addIncomplete=FALSE)
```

Arguments

`spec`	The `RmbSpectraSetList` of spectra sets (`RmbSpectraSet` objects) to aggregate
`addIncomplete`	Whether or not the peaks from incomplete files (files for which less than the maximal number of spectra are present)

Details

addIncomplete is relevant for recalibration. For recalibration, we want to use only high-confidence peaks, therefore we set *addIncomplete* to `FALSE`. When we want to generate a peak list for actually generating MassBank records, we want to include all peaks into the peak tables.

Value

A summary `data.frame` with all peaks (possibly multiple rows for one m/z value from a spectrum, see below) with columns:

`mzFound, intensity`	Mass and intensity of the peak
`good`	if the peak passes filter criteria
`mzCalc, formula, dbe, dppm`	calculated mass, formula, dbe and ppm deviation of the assigned formula
`formulaCount, dppmBest`	Number of matched formulae for this m/z value, and ppm deviation of the best match
`scan, cpdID, parentScan`	Scan number of the child and parent spectrum in the raw file, also the compound ID to which the peak belongs
`dppmRc`	ppm deviation recalculated from the aggregation function
`index`	Aggregate-table peak index, so the table can be subsetted, edited and results reinserted back into this table easily

Further columns are later added by workflow steps 6 (electronic noise culler), 7 and 8.

Author(s)

Michael Stravs

See Also

`msmsWorkflow`, `analyzeMsMs`

Examples

```
## As used in the workflow:
## Not run: %
w@spectra <- lapply(w@spectra, function(spec)
analyzeMsMs(spec, mode="pH", detail=TRUE, run="recalibrated", cut=0, cut_ratio=0 ) )
w@aggregate <- aggregateSpectra(w@spectra)

## End(Not run)
```

analyzeMsMs *Analyze MSMS spectra*

Description

Analyzes MSMS spectra of a compound by fitting formulas to each subpeak.

Usage

```
analyzeMsMs(msmsPeaks, mode = "pH", detail = FALSE, run = "preliminary",
  filterSettings = getOption("RMassBank")$filterSettings,
  spectraList = getOption("RMassBank")$spectraList, method = "formula")

analyzeMsMs.formula(msmsPeaks, mode = "pH", detail = FALSE,
  run = "preliminary",
  filterSettings = getOption("RMassBank")$filterSettings)

analyzeMsMs.intensity(msmsPeaks, mode = "pH", detail = FALSE,
  run = "preliminary",
  filterSettings = getOption("RMassBank")$filterSettings)
```

Arguments

`msmsPeaks` A `RmbSpectraSet` object. Corresponds to a parent spectrum and children MSMS spectra of one compound (plus some metadata). The objects are typically generated with `findMsMsHR`, and populate the `@spectrum` slot in a `msmsWorkspace` (refer to the corresponding documentation for the precise format specifications).

`mode` Specifies the processing mode, i.e. which molecule species the spectra contain. *pH* (positive H) specifies [M+H]+, *pNa* specifies [M+Na]+, *pM* specifies [M]+, *mH* and *mNa* specify [M-H]- and [M-Na]-, respectively. (I apologize for the naming of *pH* which has absolutely nothing to do with chemical *pH* values.)

`detail` Whether detailed return information should be provided (defaults to `FALSE`). See below.

`run` `"preliminary"` or `"recalibrated"`. In the `preliminary` run, mass tolerance is set to 10 ppm (above m/z 120) and 15 ppm (below m/z 120), the default intensity cutoff is 10^4 for positive mode (no default cutoff in negative mode), and the column `"mz"` from the spectra is used as data source. In the `recalibrated` run, the mass tolerance is set to 5 ppm over the whole mass range, the default cutoff is 0 and the column `"mzRecal"` is used as source for the m/z values. Defaults to `"preliminary"`.

`filterSettings` Settings for the filter parameters, by default loaded from the RMassBank settings set with e.g. `loadRmbSettings`. Must contain:

- `ppmHighMass`, allowed ppm deviation before recalibration for high mass range
- `ppmLowMass`, allowed ppm deviation before recalibration for low mass range
- `massRangeDivision`, division point between high and low mass range (before recalibration)
- `ppmFine`, allowed ppm deviation overall after recalibration
- `prelimCut`, intensity cutoff for peaks in preliminary run

- prelimCutRatio, relative intensity cutoff for peaks in preliminary run, e.g. 0.01 = 1
- fineCut, intensity cutoff for peaks in second run
- fineCutRatio, relative intensity cutoff for peaks in second run
- specOkLimit, minimum intensity of base peak for spectrum to be accepted for processing
- dbeMinLimit, minimum double bond equivalent for accepted molecular subformula.
- satelliteMzLimit, for satellite peak filtering (filterPeakSatellites: mass window to use for satellite removal
- satelliteIntLimit, the relative intensity below which to discard "satellites". (refer to filterPeakSatellites).

spectraList
: The list of MS/MS spectra present in each data block. As also defined in the settings file.

method
: Selects which function to actually use for data evaluation. The default "formula" runs a full analysis via formula assignment to fragment peaks. The alternative setting "intensity" calls a "mock" implementation which circumvents formula assignment and filters peaks purely based on intensity cutoffs and the satellite filtering. (In this case, the ppm and dbe related settings in filterSettings are ignored.)

Details

The analysis function uses Rcdk. Note that in this step, *satellite peaks* are removed by a simple heuristic rule (refer to the documentation of filterPeakSatellites for details.)

Value

The processed RmbSpectraSet object. Added (or filled, respectively, since the slots are present before) data include

list("complete")
: whether all spectra have useful value

list("empty")
: whether there are no useful spectra

list("children")
: The processed RmbSpectrum2 objects (in a RmbSpectrum2List).

- ok if the spectrum was successfully processed with at least one resulting peak
- mz, intensity: note that mz/int pairs can be duplicated when multiple matches are found for one mz value, therefore the two slots are not necessarily unchanged from before
- rawOK (logical) whether the m/z peak passes satellite/low removal
- low, satellite if TRUE, the peak failed cutoff (low) or was removed as satellite
- formula, mzCalc, dppm, dbe Formula, calculated mass, ppm deviation and dbe assigned to a peak
- formulaCount, dppmBest Number of formulae matched for this m/z value and ppm deviation of the best match
- info Spectrum identifying information (collision energy, resolution, collision mode) from the spectraList
- All other entries are retained from the original RmbSpectrum2.

Functions

- `analyzeMsMs.formula`: Analyze the peaks using formula annotation
- `analyzeMsMs.intensity`: Analyze the peaks going only by intensity values

Author(s)

Michael Stravs

See Also

`msmsWorkflow`, `filterLowaccResults`, `filterPeakSatellites`, `reanalyzeFailpeaks`

Examples

```
## Not run: analyzed <- analyzeMsMs(spec, "pH", TRUE)
```

---

annotator.default *Generate peak annotation from peaklist*

Description

Generates the PK$ANNOTATION entry from the peaklist obtained. This function is overridable by using the "annotator" option in the settings file.

Usage

```
annotator.default(annotation, type)
```

Arguments

`annotation`	A peak list to be annotated. Contains columns: `"cpdID"`,`"formula"`,`"mzFound"` ,`"scan"`,`"mzCalc`
`type`	The ion type to be added to annotated formulas ("+" or "-" usually)

Value

The annotated peak table. Table `colnames()` will be used for the titles (preferrably don't use spaces in the column titles; however no format is strictly enforced by the MassBank data format.

Author(s)

Michele Stravs, Eawag <stravsmi@eawag.ch>

Examples

```
## Not run:
annotation <- annotator.default(annotation)

## End(Not run)
```

archiveResults *Backup* msmsWorkflow *results*

Description

Writes the results from different msmsWorkflow steps to a file.

Usage

```
archiveResults(w, fileName, settings = getOption("RMassBank"))
```

Arguments

w	The msmsWorkspace to be saved.
fileName	The filename to store the results under.
settings	The settings to be stored into the msmsWorkspace image.

Examples

```
# This doesn't really make a lot of sense,
# it stores an empty workspace.
RmbDefaultSettings()
w <- newMsmsWorkspace()
archiveResults(w, "narcotics.RData")
```

checkIsotopes *Checks for isotopes in a* msmsWorkspace

Description

Checks for isotopes in a msmsWorkspace

Usage

```
checkIsotopes(w, mode = "pH", intensity_cutoff = 0,
  intensity_precision = "none", conflict = "strict", isolationWindow = 2,
  evalMode = "complete", plotSpectrum = TRUE,
  settings = getOption("RMassBank"))
```

Arguments

w	A msmsWorkspace to work with.
mode	"pH", "pNa", "pM", "pNH4", "mH", "mM", "mFA" for different ions ([M+H]+, [M+Na]+, [M]+, [M+NH4]+, [M-H]-, [M]-, [M+FA]-).
intensity_cutoff	The cutoff (as an absolute intensity value) under which isotopic peaks shouldn't be checked for or accepted as valid. Please note: The cutoff is not hard in the sense that it interacts with the intensity_precision parameter.

`intensity_precision`
: The difference that is accepted between the calculated and observed intensity of a possible isotopic peak. Further details down below.

`conflict`
: Either "isotopic"(Peak formulas are always chosen if they fit the requirements for an isotopic peak) or "strict"(Peaks are only marked as isotopic when there hasn't been a formula assigned before.)

`isolationWindow`
: Half of the width of the isolation window in Da

`evalMode`
: Currently no function yet, but planned. Currently must be "complete"

`plotSpectrum`
: A boolean specifiying whether the spectrumshould be plotted

`settings`
: Options to be used for processing. Defaults to the options loaded via `loadRmbSettings` et al. Refer to there for specific settings.

Details

text describing parameter inputs in more detail.

- `intensity_precision`This parameter determines how strict the intensity values should adhere to the calculated intensity in relation to the parent peak. Options for this parameter are `"none"`, where the intensity is irrelevant, `"low"`, which has an error margin of 70% and `"high"`, where the error margin is set to 35%. The recommended setting is `"low"`, but can be changed to adjust to the intensity precision of the mass spectrometer.

Value

The `msmsWorkspace` with annotated isolation peaks

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

Erik Mueller, UFZ

`checkSpectra` *Check if a spectra set is found, complete, empty*

Description

Checks if a specific compound (`RmbSpectraSet`) was found with child spectra in the raw file (`found`), has a complete set of MS2 spectra with useful peaks (`complete`), or is empty (note: spectra are currently not ever marked empty - empty should mean found, but no useful peaks at all. This is not yet currently tested.)

Usage

```
checkSpectra(s, property)

## S4 method for signature 'RmbSpectraSet,character'
checkSpectra(s, property)
```

Arguments

s	The (RmbSpectraSet) to check
property	The property to check (found, complete or empty)

Value

TRUE or FALSE

Methods (by class)

- s = RmbSpectraSet,property = character:

Author(s)

stravsmi

---

cleanElnoise *Remove electronic noise*

Description

Removes known electronic noise peaks from a peak table

Usage

```
cleanElnoise(peaks, noise=getOption("RMassBank")$electronicNoise,
width = getOption("RMassBank")$electronicNoiseWidth)
```

Arguments

peaks	An aggregated peak frame as described in aggregateSpectra. Columns mzFound, dppm and dppmBest are needed.
noise	A numeric vector of known m/z of electronic noise peaks from the instrument Defaults to the entries in the RMassBank settings.
width	The window for the noise peak in m/z units. Defaults to the entries in the RMassBank settings.

Value

Extends the aggregate data frame by column noise (logical), which is TRUE if the peak is marked as noise.

Author(s)

Michael Stravs

See Also

msmsWorkflow

Examples

```
# As used in the workflow:
## Not run:
    w@aggregated <-
cleanElnoise(w@aggregated)

## End(Not run)
```

---

combineMultiplicities *Combine workspaces for multiplicity filtering*

Description

Combines multiple msmsWorkspace items to one workspace which is used for multiplicity filtering.

Usage

```
combineMultiplicities(workspaces)
```

Arguments

workspaces	A vector of msmsWorkspace items. The first item is taken as the "authoritative" workspace, i.e. the one which will be used for the record generation. The subsequent workspaces will only be used for multiplicity filtering.

Details

This feature is particularily meant to be used in conjunction with the confirmMode option of msmsWorkflow: a file can be analyzed with confirmMode = 0 (default) and subsequently with confirmMode = 1 (take second highest scan). The second analysis should contain "the same" spectra as the first one (but less intense) and can be used to confirm the peaks in the first spectra.

TO DO: Enable the combination of workspaces for combining e.g. multiple energy settings measured separately.

Value

A msmsWorkspace object prepared for step 8 processing.

Author(s)

Stravs MA, Eawag <michael.stravs@eawag.ch>

See Also

msmsWorkspace-class

Examples

```
## Not run:
w <- newMsmsWorkspace
 w@files <- c("spec1", "spec2")
 w1 <- msmsWorkflow(w, steps=c(1:7), mode="pH")
 w2 <- msmsWorkflow(w, steps=c(1:7), mode="pH", confirmMode = 1)
 wTotal <- combineMultiplicities(c(w1, w2))
 wTotal <- msmsWorkflow(wTotal, steps=8, mode="pH", archivename = "output")
 # continue here with mbWorkflow

## End(Not run)
```

---

compileRecord *Compile MassBank records*

Description

Takes a spectra block for a compound, as returned from analyzeMsMs, and an aggregated cleaned peak table, together with a MassBank information block, as stored in the infolists and loaded via loadInfolist/readMbdata and processes them to a MassBank record

Usage

```
compileRecord(spec, mbdata, aggregated, additionalPeaks = NULL, retrieval="standard")
```

Arguments

spec	A RmbSpectraSet for a compound, after analysis (analyzeMsMs). Note that **peaks are not read from this object anymore**: Peaks come from the aggregated dataframe (and from the global additionalPeaks dataframe; cf. addPeaks for usage information.)
mbdata	The information data block for the record header, as stored in mbdata_relisted after loading an infolist.
aggregated	An aggregated peak data table containing information about refiltered spectra etc.
additionalPeaks	If present, a table with additional peaks to add into the spectra. As loaded with addPeaks.
retrieval	A value that determines whether the files should be handled either as "standard", if the compoundlist is complete, "tentative", if at least a formula is present or "unknown" if the only know thing is the m/z

Details

compileRecord calls gatherCompound to create blocks of spectrum data, and finally fills in the record title and accession number, renames the "internal ID" comment field and removes dummy fields.

Value

Returns a MassBank record in list format: e.g. list("ACCESSION" = "XX123456", "RECORD_TITLE" = "Cubane", ..

Author(s)

Michael Stravs

References

MassBank record format: http://www.massbank.jp/manuals/MassBankRecord_en.pdf

See Also

mbWorkflow, addPeaks, gatherCompound, toMassbank

Examples

```
#
## Not run: myspec <- w@spectra[[2]]
# after having loaded an infolist:
## Not run: mbdata <- mbdata_relisted[[which(mbdata_archive$id == as.numeric(myspec$id))]]
## Not run: compiled <- compileRecord(myspec, mbdata, w@aggregated)
```

---

createMolfile — *Create MOL file for a chemical structure*

Description

Creates a MOL file (in memory or on disk) for a compound specified by the compound ID or by a SMILES code.

Usage

```
createMolfile(id_or_smiles, fileName = FALSE)
```

Arguments

id_or_smiles	The compound ID or a SMILES code.
fileName	If the filename is set, the file is written directly to disk using the specified filename. Otherwise, it is returned as a text array.

Details

The function invokes OpenBabel (and therefore needs a correctly set OpenBabel path in the RMassBank settings), using the SMILES code retrieved with findSmiles or using the SMILES code directly. The current implementation of the workflow uses the latter version, reading the SMILES code directly from the MassBank record itself.

Value

A character array containing the MOL/SDF format file, ready to be written to disk.

Author(s)

Michael Stravs

References

OpenBabel: http://openbabel.org

See Also

findSmiles

Examples

```
# Benzene:
## Not run:
createMolfile("C1=CC=CC=C1")

## End(Not run)
```

CTS.externalIdSubset *Select a subset of external IDs from a CTS record.*

Description

Select a subset of external IDs from a CTS record.

Usage

```
CTS.externalIdSubset(data, database)
```

Arguments

data	The complete CTS record as retrieved by getCtsRecord.
database	The database for which keys should be returned.

Value

Returns an array of all external identifiers stored in the record for the given database.

Author(s)

Michele Stravs, Eawag <stravsmi@eawag.ch>

Examples

```
## Not run:
# Return all CAS registry numbers stored for benzene.
data <- getCtsRecord("UHOVQNZJYSORNB-UHFFFAOYSA-N")
cas <- CTS.externalIdSubset(data, "CAS")

## End(Not run)
```

CTS.externalIdTypes *Find all available databases for a CTS record*

Description

Find all available databases for a CTS record

Usage

```
CTS.externalIdTypes(data)
```

Arguments

data	The complete CTS record as retrieved by getCtsRecord.

Value

Returns an array of all database names for which there are external identifiers stored in the record.

Author(s)

Michele Stravs, Eawag <stravsmi@eawag.ch>

Examples

```
## Not run:
# Return all databases for which the benzene entry has
# links in the CTS record.

data <- getCTS("UHOVQNZJYSORNB-UHFFFAOYSA-N")
databases <- CTS.externalIdTypes(data)

## End(Not run)
```

dbe *Calculate Double Bond Equivalents*

Description

Calculates the Ring and Double Bond Equivalents for a chemical formula. The highest valence state of each atom is used, such that the returned DBE should never be below 0.

Usage

```
dbe(formula)
```

Arguments

formula	A molecular formula in text or list representation (e.g. "C6H12O6" or list(C=6, H=12, O=6)).

Value

Returns the DBE for the given formula.

Author(s)

Michael Stravs

Examples

```
#
dbe("C6H12O6")
```

`deprofile` *De-profile a high-resolution MS scan in profile mode.*

Description

The `deprofile` functions convert profile-mode high-resolution input data to "centroid"-mode data amenable to i.e. centWave. This is done using full-width, half-height algorithm, spline algorithm or local maximum method.

Usage

```
deprofile.scan(scan, noise = NA, method = "deprofile.fwhm",
colnames = TRUE, ...)

deprofile(df, noise, method, ...)

deprofile.fwhm(df, noise = NA, cut = 0.5)

deprofile.localMax(df, noise = NA)

deprofile.spline(df, noise=NA, minPts = 5, step = 0.00001)
```

Arguments

`df`	A dataframe with at least the columns `mz` and `int` to perform deprofiling on.
`noise`	The noise cutoff. A peak is not included if the maximum stick intensity of the peak is below the noise cutoff.
`method`	"deprofile.fwhm" for full-width half-maximum or "deprofile.localMax" for local maximum.
`...`	Arguments to the workhorse functions `deprofile.fwhm` etc.
`scan`	A matrix with 2 columns for m/z and intensity; from profile-mode high-resolution data. Corresponds to the spectra obtained with xcms::getScan or mzR::peaks.
`colnames`	For deprofile.scan: return matrix with column names (xcms-style, `TRUE`, default) or plain (mzR-style, `FALSE`).

`cut` A parameter for `deprofile.fwhm` indicating where the peak flanks should be taken. Standard is 0.5 (as the algorithm name says, at half maximum.) Setting `cut = 0.75` would instead determine the peak width at 3/4 maximum, which might give a better accuracy for merged peaks, but could be less accurate if too few data points are present.

`minPts` The minimal points count in a peak to build a spline; for peaks with less points the local maximum will be used instead. Note: The minimum value is 4!

`step` The interpolation step for the calculated spline, which limits the maximum precision which can be achieved.

Details

The `deprofile.fwhm` method is basically an R-semantic version of the "Exact Mass" m/z deprofiler from MZmine. It takes the center between the m/z values at half-maximum intensity for the exact peak mass. The logic is stolen verbatim from the Java MZmine algorithm, but it has been rewritten to use the fast R vector operations instead of loops wherever possible. It's slower than the Java implementation, but still decently fast IMO. Using matrices instead of the data frame would be more memory-efficient and also faster, probably.

The `deprofile.localMax` method uses local maxima and is probably the same used by e.g. Xcalibur. For well-formed peaks, "deprofile.fwhm" gives more accurate mass results; for some applications, `deprofile.localMax` might be better (e.g. for fine isotopic structure peaks which are not separated by a valley and also not at half maximum.) For MS2 peaks, which have no isotopes, `deprofile.fwhm` is probably the better choice generally.

`deprofile.spline` calculates the mass using a cubic spline, as the HiRes peak detection in OpenMS does.

The word "centroid" is used for convenience to denote not-profile-mode data. The data points are NOT mathematical centroids; we would like to have a better word for it.

The `noise` parameter was only included for completeness, I personally don't use it.

`deprofile.fwhm` and `deprofile.localMax` are the workhorses; `deprofile.scan` takes a 2-column scan as input. `deprofile` dispatches the call to the appropriate worker method.

Value

`deprofile.scan`: a matrix with 2 columns for m/z and intensity

Note

Known limitations: If the absolute leftmost stick or the absolute rightmost stick in a scan are maxima, they will be discarded! However, I don't think this will ever present a practical problem.

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

References

mzMine source code http://sourceforge.net/svn/?group_id=139835

Examples

```
## Not run:
mzrFile <- openMSfile("myfile.mzML")
acqNo <- xraw@acquisitionNum[[50]]
scan.mzML.profile <- mzR::peaks(mzrFile, acqNo)
scan.mzML <- deprofile.scan(scan.mzML.profile)
close(mzrFile)

## End(Not run)
```

`exportMassbank` *Export internally stored MassBank data to files*

Description

Exports MassBank recfile data arrays and corresponding molfiles to physical files on hard disk, for one compound.

Usage

```
exportMassbank(compiled, files, molfile)
```

Arguments

`compiled`	Is ONE "compiled" entry, i.e. ONE compound with e.g. 14 spectra, as returned from `compileRecord`.
`files`	A n-membered array (usually a return value from `lapply(toMassbank)`), i.e. contains n plain-text arrays with MassBank records.
`molfile`	A molfile from `createMolfile`

Details

The data from `compiled` is still used here, because it contains the "visible" accession number. In the plain-text format contained in `files`, the accession number is not "accessible" anymore since it's in the file.

Value

No return value.

Note

An improvement would be to write the accession numbers into `names(compiled)` and later into `names(files)` so `compiled` wouldn't be needed here anymore. (The compound ID would have to go into `names(molfile)`, since it is also retrieved from `compiled`.)

Author(s)

Michael Stravs

References

MassBank record format: http://www.massbank.jp/manuals/MassBankRecord_en.pdf

See Also

createMolfile, compileRecord, toMassbank, mbWorkflow

Examples

```
## Not run:
compiled <- compileRecord(record, mbdata, refilteredRcSpecs)
mbfiles <- toMassbank(compiled)
molfile <- createMolfile(compiled[[1]][["CH$SMILES"]])
exportMassbank(compiled, mbfiles, molfile)

## End(Not run)
```

---

filterLowaccResults *Filter peaks with low accuracy*

Description

Filters a peak table (with annotated formulas) for accuracy. Low-accuracy peaks are removed.

Usage

```
filterLowaccResults(peaks, mode="fine", filterSettings  = getOption("RMassBank")$filterSettings)
```

Arguments

peaks	A data frame with at least the columns mzFound and dppm.
mode	coarse or fine, see below.
filterSettings	Settings for filtering. For details, see documentation of analyzeMsMs

Details

In the coarse mode, mass tolerance is set to 10 ppm (above m/z 120) and 15 ppm (below m/z 120). This is useful for formula assignment before recalibration, where a wide window is desirable to accomodate the high mass deviations at low m/z values, so we get a nice recalibration curve.

In the fine run, the mass tolerance is set to 5 ppm over the whole mass range. This should be applied after recalibration.

Value

A list(TRUE = goodPeakDataframe, FALSE = badPeakDataframe) is returned: A data frame with all peaks which are "good" is in return[["TRUE"]].

Author(s)

Michael Stravs

See Also

analyzeMsMs, filterPeakSatellites

Examples

```
# from analyzeMsMs:
## Not run: childPeaksFilt <- filterLowaccResults(childPeaksInt, filterMode)
```

---

filterMultiplicity *filterMultiplicity*

Description

Multiplicity filtering: Removes peaks which occur only once in a n-spectra set.

Usage

```
filterMultiplicity(w, archivename=NA, mode="pH", recalcBest = TRUE,
multiplicityFilter = getOption("RMassBank")$multiplicityFilter)
```

Arguments

w	Workspace containing the data to be processed (aggregate table and RmbSpectraSet objects)
archivename	The archive name, used for generation of archivename_Failpeaks.csv
mode	Mode of ion analysis
recalcBest	Boolean, whether to recalculate the formula multiplicity after the first multiplicity filtering step. Sometimes, setting this to FALSE can be a solution if you have many compounds with e.g. fluorine atoms, which often have multiple assigned formulas per peak and might occasionally lose peaks because of that.
multiplicityFilter	Threshold for the multiplicity filter. If set to 1, no filtering will apply (minimum 1 occurrence of peak). 2 equals minimum 2 occurrences etc.

Details

This function executes multiplicity filtering for a set of spectra using the workhorse function filterPeaksMultiplicity (see details there) and retrieves problematic filtered peaks (peaks which are of high intensity but were discarded, because either no formula was assigned or it was not present at least 2x), using the workhorse function problematicPeaks. The results are returned in a format ready for further processing with mbWorkflow.

Value

A list object with values:

- `peaksOK` Peaks with >1-fold formula multiplicity from the "normal" peak analysis.
- `peaksReanOK` Peaks with >1-fold formula multiplicity from peak reanalysis.
- `peaksFiltered` All peaks with annotated formula multiplicity from first analysis.
- `peaksFilteredReanalysis` All peaks with annotated formula multiplicity from peak reanalysis.
- `peaksProblematic` Peaks with high intensity which do not match inclusion criteria -> possible false negatives. The list will be exported into archivename_failpeaks.csv.

Author(s)

Michael Stravs

See Also

`filterPeaksMultiplicity`,`problematicPeaks`

Examples

```
## Not run:
    refilteredRcSpecs <- filterMultiplicity(
w, "myarchive", "pH")

## End(Not run)
```

---

filterPeakSatellites *Filter satellite peaks*

Description

Filters satellite peaks in FT spectra which arise from FT artifacts and from conversion to stick mode. A very simple rule is used which holds mostly true for MSMS spectra (and shouldn't be applied to MS1 spectra which contain isotope structures...)

Usage

```
filterPeakSatellites(peaks, filterSettings = getOption("RMassBank")$filterSettings)
```

Arguments

- `peaks` A peak dataframe with at least the columns `mz, int`. Note that `mz` is used even for the recalibrated spectra, i.e. the desatellited spectrum is identical for both the unrecalibrated and the recalibrated spectra.
- `filterSettings` The settings used for filtering. Refer to `analyzeMsMs` documentation for filter settings.

Details

The function cuts off all peaks within 0.5 m/z from every peak, in decreasing intensity order, which are below 5 intensity. E.g. for peaks m/z=100, int=100; m/z=100.2, int=2, m/z=100.3, int=6, m/z 150, int=10: The most intense peak (m/z=100) is selected, all neighborhood peaks below 5 peak) and the next less intense peak is selected. Here this is the m/z=150 peak. All low-intensity neighborhood peaks are removed (nothing). The next less intense peak is selected (m/z=100.3) and again neighborhood peaks are cut away (nothing to cut here. Note that the m/z = 100.2 peak was alredy removed.)

Value

Returns the peak table with satellite peaks removed.

Note

This is a very crude rule, but works remarkably well for our spectra.

Author(s)

Michael Stravs

See Also

analyzeMsMs, filterLowaccResults

Examples

```
# From the workflow:
## Not run:
    # Filter out satellite peaks:
    shot <- filterPeakSatellites(shot)
    shot_satellite_n <- setdiff(row.names(shot_full), row.names(shot))
    shot_satellite <- shot_full[shot_satellite_n,]
    # shot_satellite contains the peaks which were eliminated as satellites.

## End(Not run)
```

---

filterPeaksMultiplicity

Multiplicity filtering: Removes peaks which occur only once in a n-spectra set.

Description

For every compound, every peak (with annotated formula) is compared across all spectra. Peaks whose formula occurs only once for all collision energies / spectra types, are discarded. This eliminates "stochastic formula hits" of pure electronic noise peaks efficiently from the spectra. Note that in the author's experimental setup two spectra were recorded at every collision energy, and therefore every peak-formula should appear at least twice if it is real, even if it is by chance a fragment which appears on only one collision energy setting. The function was not tested in a different setup. Therefore, use with a bit of caution.

Usage

```
filterPeaksMultiplicity(peaks, formulacol, recalcBest = TRUE)
```

Arguments

`peaks`	An aggregate peak data.frame containing all peaks to be analyzed; with at least the columns `cpdID, scan, mzFound` and one column for the formula specified with the `formulacol` parameter.
`formulacol`	Which column the assigned formula is stored in. (Needed to separately process `"formula"` and `"reanalyzed.formula"` multiplicites.)
`recalcBest`	Whether the best formula for each peak should be re-determined. This is necessary for results from the ordinary `analyzeMsMs` analysis which allows multiple potential formulas per peak - the old best match could potentially have been dropped because of multiplicity filtering. For results from `reanalyzeFailpeak` this is not necessary, since only one potential formula is assigned in this case.

Value

The peak table is returned, enriched with columns:

- `formulaMultiplicity`The # of occurrences of this formula in the spectra of its compounds.

Author(s)

Michael Stravs, EAWAG <michael.stravs@eawag.ch>

Examples

```
## Not run:
peaksFiltered <- filterPeaksMultiplicity(peaksMatched(w),
"formula", TRUE)
peaksOK <- subset(peaksFiltered, formulaMultiplicity > 1)

## End(Not run)
```

`findEIC` *Extract EICs*

Description

Extract EICs from raw data for a determined mass window.

Usage

```
findEIC(msRaw, mz, limit = NULL, rtLimit = NA, headerCache = NULL,
  floatingRecalibration = NULL, peaksCache = NULL)
```

Arguments

`msRaw`	The mzR file handle
`mz`	The mass or mass range to extract the EIC for: either a single mass (with the range specified by `limit` below) or a mass range in the form of `c(min, max)`.
`limit`	If a single mass was given for `mz`: the mass window to extract. A limit of 0.001 means that the EIC will be returned for `[mz - 0.001, mz + 0.001]`.
`rtLimit`	If given, the retention time limits in form `c(rtmin, rtmax)` in seconds.
`headerCache`	If present, the complete `mzR::header(msRaw)`. Passing this value is useful if spectra for multiple compounds should be extracted from the same mzML file, since it avoids getting the data freshly from `msRaw` for every compound.
`floatingRecalibration`	A fitting function that `predict()`s a mass shift based on the retention time. Can be used if a lockmass calibration is known (however you have to build the calibration yourself.)
`peaksCache`	If present, the complete output of `mzR::peaks(msRaw)`. This speeds up the lookup if multiple compounds should be searched in the same file.

Value

A `[rt, intensity, scan]` matrix (`scan` being the scan number.)

Author(s)

Michael A. Stravs, Eawag <michael.stravs@eawag.ch>

See Also

findMsMsHR

`findMass` *Calculate exact mass*

Description

Retrieves the exact mass of the uncharged molecule. It works directly from the SMILES and therefore is used in the MassBank workflow (`mbWorkflow`) - there, all properties are calculated from the SMILES code retrieved from the database. (Alternatively, takes also the compound ID as parameter and looks it up.) Calculation relies on Rcdk.

Usage

```
findMass(cpdID_or_smiles, retrieval = "standard", mode = "pH")
```

Arguments

`cpdID_or_smiles`
: SMILES code or compound ID of the molecule. (Numerics are treated as compound ID).

`retrieval`
: A value that determines whether the files should be handled either as "standard", if the compoundlist is complete, "tentative", if at least a formula is present or "unknown" if the only know thing is the m/z

`mode`
: `"pH"`, `"pNa"`, `"pM"`, `"pNH4"`, `"mH"`, `"mM"`, `"mFA"` for different ions ([M+H]+, [M+Na]+, [M]+, [M+NH4]+, [M-H]-, [M]-, [M+FA]-). Only needed for retrieval="unknown"

Value

Returns the exact mass of the uncharged molecule.

Author(s)

Michael Stravs

See Also

`findMz`

Examples

```
##
findMass("OC[C@H]1OC(O)[C@H](O)[C@@H](O)[C@@H]1O")
```

---

findMsMsHR *Extract MS/MS spectra for specified precursor*

Description

Extracts MS/MS spectra from LC-MS raw data for a specified precursor, specified either via the RMassBank compound list (see `loadList`) or via a mass.

Usage

```
findMsMsHR(fileName = NULL, msRaw = NULL, cpdID, mode = "pH",
  confirmMode = 0, useRtLimit = TRUE,
  ppmFine = getOption("RMassBank")$findMsMsRawSettings$ppmFine,
  mzCoarse = getOption("RMassBank")$findMsMsRawSettings$mzCoarse,
  fillPrecursorScan = getOption("RMassBank")$findMsMsRawSettings$fillPrecursorScan,
  rtMargin = getOption("RMassBank")$rtMargin,
  deprofile = getOption("RMassBank")$deprofile, headerCache = NULL,
  peaksCache = NULL, retrieval = "standard")

findMsMsHR.mass(msRaw, mz, limit.coarse, limit.fine, rtLimits = NA,
  maxCount = NA, headerCache = NULL, fillPrecursorScan = FALSE,
  deprofile = getOption("RMassBank")$deprofile, peaksCache = NULL,
  cpdID = NA)
```

Arguments

`fileName` The file to open and search the MS2 spectrum in.

`msRaw` The opened raw file (mzR file handle) to search the MS2 spectrum in. Specify either this or `fileName`.

`cpdID` The compound ID in the compound list (see `loadList`) to use for formula lookup. Note: In \codefindMsMsHR.mass, this is entirely optional and used only in case a warning must be displayed; compound lookup is done via mass only.

`mode` The processing mode (determines which ion/adduct is searched): `"pH"`, `"pNa"`, `"pM"`, `"pNH4"`, `"mH` for different ions ([M+H]+, [M+Na]+, [M]+, [M+NH4]+, [M-H]-, [M]-, [M+FA]-).

`confirmMode` Whether to use the highest-intensity precursor (=0), second- highest (=1), third-highest (=2)...

`useRtLimit` Whether to respect retention time limits from the compound list.

`ppmFine` The limit in ppm to use for fine limit (see below) calculation.

`mzCoarse` The coarse limit to use for locating potential MS2 scans: this tolerance is used when finding scans with a suitable precursor ion value.

`fillPrecursorScan` If `TRUE`, the precursor scan will be filled from MS1 data. To be used for data where the precursor scan is not stored in the raw data.

`rtMargin` The retention time tolerance to use.

`deprofile` Whether deprofiling should take place, and what method should be used (cf. `deprofile`)

`headerCache` If present, the complete `mzR::header(msRaw)`. Passing this value is useful if spectra for multiple compounds should be extracted from the same mzML file, since it avoids getting the data freshly from `msRaw` for every compound.

`peaksCache` If present, the complete output of `mzR::peaks(msRaw)`. This speeds up the lookup if multiple compounds should be searched in the same file.

`retrieval` A value that determines whether the files should be handled either as "standard", if the compoundlist is complete, "tentative", if at least a formula is present or "unknown" if the only know thing is the m/z

`mz` The mass to use for spectrum search.

`limit.coarse` Parameter in `findMsMsHR.mass` corresponding to `mzCoarse`. (The parameters are distinct to clearly conceptually distinguish findMsMsHR.mass (a standalone useful function) from the cpdID based functions (workflow functions).)

`limit.fine` The fine limit to use for locating MS2 scans: this tolerance is used when locating an appropriate analyte peak in the MS1 precursor spectrum.

`rtLimits` `c(min, max)`: Minimum and maximum retention time to use when locating the MS2 scans.

`maxCount` The maximal number of spectra groups to return. One spectra group consists of all data-dependent scans from the same precursor whose precursor mass matches the specified search mass.

Details

Different versions of the function get the data from different sources. Note that findMsMsHR and findMsMsHR.direct differ mainly in that findMsMsHR opens a file whereas findMsMs.direct uses an open file handle - both are intended to be used in a full process which involves compound lists etc. In contrast, findMsMsHR.mass is a low-level function which uses the mass directly for lookup and is intended for use as a standalone function in unrelated applications.

Value

An `RmbSpectraSet` (for `findMsMsHR`). Contains parent MS1 spectrum (`@parent`), a block of dependent MS2 spectra ((`@children`) and some metadata (`id`,`mz`,`name`,`mode` in which the spectrum was acquired.

For `findMsMsHR.mass`: a list of `RmbSpectraSets` as defined above, sorted by decreasing precursor intensity.

Functions

- `findMsMsHR.mass`: A submethod of find MsMsHR that retrieves basic spectrum data

Note

`findMsMs.direct` is deactivated

Author(s)

Michael A. Stravs, Eawag <michael.stravs@eawag.ch>

See Also

findEIC

Examples

```
## Not run:
loadList("mycompoundlist.csv")
# if Atrazine has compound ID 1:
msms_atrazine <- findMsMsHR(fileName = "Atrazine_0001_pos.mzML", cpdID = 1, mode = "pH")
# Or alternatively:
msRaw <- openMSfile("Atrazine_0001_pos.mzML")
msms_atrazine <- findMsMsHR(msRaw=msRaw, cpdID = 1, mode = "pH")
# Or directly by mass (this will return a list of spectra sets):
mz <- findMz(1)$mzCenter
msms_atrazine_all <- findMsMsHR.mass(msRaw, mz, 1, ppm(msRaw, 10, p=TRUE))
msms_atrazine <- msms_atrazine_all[[1]]

## End(Not run)
```

`findMsMsHR.direct` *Discontinued: find MS/MS spectrum from open raw file*

Description

This interface has been discontinued. `findMsMsHR` now supports the same parameters (use named parameters).

Usage

```
findMsMsHR.direct(msRaw, cpdID, mode = "pH", confirmMode = 0,
  useRtLimit = TRUE,
  ppmFine = getOption("RMassBank")$findMsMsRawSettings$ppmFine,
  mzCoarse = getOption("RMassBank")$findMsMsRawSettings$mzCoarse,
  fillPrecursorScan = getOption("RMassBank")$findMsMsRawSettings$fillPrecursorScan,
  rtMargin = getOption("RMassBank")$rtMargin,
  deprofile = getOption("RMassBank")$deprofile, headerCache = NULL)
```

Arguments

`msRaw`	x
`cpdID`	x
`mode`	x
`confirmMode`	x
`useRtLimit`	x
`ppmFine`	x
`mzCoarse`	x
`fillPrecursorScan`	x
`rtMargin`	x
`deprofile`	x
`headerCache`	x

Value

an error

Author(s)

stravsmi

findMsMsHR.ticms2 *Extract an MS/MS spectrum from MS2 TIC*

Description

Extract an MS/MS spectrum or multiple MS/MS spectra based on the TIC of the MS2 and precursor mass, picking the most intense MS2 scan. Can be used, for example, to get a suitable MS2 from direct infusion data which was collected with purely targeted MS2 without MS1.

Usage

```
findMsMsHR.ticms2(msRaw, mz, limit.coarse, limit.fine, rtLimits = NA,
  maxCount = NA, headerCache = NULL, fillPrecursorScan = FALSE,
  deprofile = getOption("RMassBank")$deprofile, trace = "ms2tic")
```

Arguments

`msRaw`	The mzR raw file
`mz`	Mass to find
`limit.coarse`	Allowed mass deviation for scan precursor (in m/z values)
`limit.fine`	Unused here, but present for interface compatiblity with findMsMsHR
`rtLimits`	Unused here, but present for interface compatiblity with findMsMsHR
`maxCount`	Maximal number of spectra to return
`headerCache`	Cached results of header(msRaw), either to speed up the operations or to operate with preselected header() data
`fillPrecursorScan`	Unused here, but present for interface compatiblity with findMsMsHR
`deprofile`	Whether deprofiling should take place, and what method should be used (cf. `deprofile`)
`trace`	Either `"ms2tic"` or `"ms2basepeak"`: Which intensity trace to use - can be either the TIC of the MS2 or the basepeak intensity of the MS2.

Details

Note that this is not a precise function and only really makes sense in direct infusion and if the precursor is really known, because MS2 precursor data is only "roughly" accurate (to 2 dp). The regular `findMsMsHR` functions confirm the exact mass of the precursor in the MS1 scan.

Value

a list of "spectrum sets" as defined in `findMsMsHR`, sorted by decreasing precursor intensity.

Author(s)

stravsmi

`findMsMsHRperxcms` *Read in mz-files using XCMS*

Description

Picks peaks from mz-files and returns the pseudospectra that CAMERA creates with the help of XCMS

Usage

```
findMsMsHRperxcms(fileName, cpdID, mode = "pH", findPeaksArgs = NULL,
  plots = FALSE, MSe = FALSE)

findMsMsHRperxcms.direct(fileName, cpdID, mode = "pH", findPeaksArgs = NULL,
  plots = FALSE, MSe = FALSE)
```

Arguments

`fileName`	The path to the mz-file that should be read
`cpdID`	The compoundID(s) of the compound that has been used for the file
`mode`	The ionization mode that has been used for the spectrum represented by the peaklist
`findPeaksArgs`	A list of arguments that will be handed to the xcms-method findPeaks via do.call
`plots`	A parameter that determines whether the spectra should be plotted or not
`MSe`	A boolean value that determines whether the spectra were recorded using MSe or not

Value

The spectra generated from XCMS

Functions

- `findMsMsHRperxcms.direct`: A submethod of findMsMsHrperxcms that retrieves basic spectrum data

Author(s)

Erik Mueller

See Also

`msmsWorkflow` `toRMB`

Examples

```
## Not run:
fileList <- list.files(system.file("XCMSinput", package = "RMassBank"), "Glucolesquerellin", full.names=TRUE
loadList(system.file("XCMSinput/compoundList.csv",package="RMassBank"))
     psp <- findMsMsHRperxcms(fileList,2184)

## End(Not run)
```

`findMz` *Find compound information*

Description

Retrieves compound information from the loaded compound list or calculates it from the SMILES code in the list.

Usage

```
findMz(cpdID, mode = "pH", ppm = 10, deltaMz = 0, retrieval="standard")

findRt(cpdID)

findSmiles(cpdID)

findFormula(cpdID, retrieval="standard")

findCAS(cpdID)

findName(cpdID)

findLevel(cpdID, compact=FALSE)
```

Arguments

`cpdID`	The compound ID in the compound list.
`mode`	Specifies the species of the molecule: An empty string specifies uncharged monoisotopic mass, *pH* (positive H) specifies [M+H]+, *pNa* specifies [M+Na]+, *pM* specifies [M]+, *mH* and *mFA* specify [M-H]- and [M+FA]-, respectively. (I apologize for the naming of *pH* which has absolutely nothing to do with chemical *pH* values.)
`ppm`	Specifies ppm window (10 ppm will return the range of the molecular mass + and - 10 ppm).
`deltaMz`	Specifies additional m/z window to add to the range (deltaMz = 0.02 will return the range of the molecular mass +- 0.02 (and additionally +- the set ppm value).
`retrieval`	A value that determines whether the files should be handled either as "standard", if the compoundlist is complete, "tentative", if at least a formula is present or "unknown" if the only know thing is the m/z
`compact`	Only for `findLevel`, returns the "retrieval" parameter used for many functions within RMassBank if TRUE

Value

`findMz` will return a `list(mzCenter=, mzMin=, mzMax=)` with the molecular weight of the given ion, as calculated from the SMILES code and Rcdk.

`findRt`, `findSmiles`,`findCAS`,`findName` will return the corresponding entry from the compound list. `findFormula` returns the molecular formula as determined from the SMILES code.

Author(s)

Michael Stravs

See Also

findMass, loadList, findMz.formula

Examples

```
## Not run: %
findMz(123, "pH", 5)
findFormula(123)

## End(Not run)
```

---

findMz.formula — *Find the exact mass +/- a given margin for a given formula or its ions and adducts.*

Description

Find the exact mass +/- a given margin for a given formula or its ions and adducts.

Usage

```
findMz.formula(formula, mode = "pH", ppm = 10, deltaMz = 0)
```

Arguments

formula	The molecular formula in text or list format (see formulastring.to.list
mode	"pH", "pNa", "pM", "pNH4", "mH", "mM", "mFA" for different ions ([M+H]+, [M+Na]+, [M]+, [M+NH4]+, [M-H]-, [M]-, [M+FA]-). "" for the uncharged molecule.
ppm	The ppm margin to add/subtract
deltaMz	The absolute mass to add/subtract. Cumulative with ppm

Value

A list(mzMin=, mzCenter=, mzMax=) with the masses.

Author(s)

Michael A. Stravs, Eawag <michael.stravs@eawag.ch>

See Also

findMz

Examples

```
findMz.formula("C6H6")
```

findProgress — *Determine processed steps*

Description

This function reads out the content of different slots of the `workspace` object and finds out which steps have already been processed on it.

Usage

```
findProgress(workspace)
```

Arguments

`workspace`	A `msmsWorkspace` object.

Value

An array containing all `msmsWorkflow` steps which have likely been processed.

Author(s)

Stravs MA, Eawag <michael.stravs@eawag.ch>

Examples

```
## Not run:
findProgress(w)

## End(Not run)
```

flatten — *Flatten, or re-read, MassBank header blocks*

Description

`flatten` converts a list of MassBank compound information sets (as retrieved by `gatherData`) to a flat table, to be exported into an infolist. `readMbdata` reads a single record from an infolist flat table back into a MassBank (half-)entry.

Usage

```
flatten(mbdata)

readMbdata(row)
```

Arguments

`mbdata`	A list of MassBank compound information sets as returned from `gatherData`.
`row`	One row of MassBank compound information retrieved from an infolist.

Details

Neither the flattening system itself nor the implementation are particularly fantastic, but since hand-checking of records is a necessary evil, there is currently no alternative (short of coding a complete GUI for this and working directly on the records.)

Value

`flatten` returns a matrix (not a data frame) to be written to CSV.

`readMbdata` returns a list of type `list(id=` *compoundID* `, . . . , 'ACCESSION' = '', 'RECORD_TITLE' = '', )` etc.

Author(s)

Michael Stravs

References

MassBank record format: http://www.massbank.jp/manuals/MassBankRecord_en.pdf

See Also

`gatherData`,`loadInfolist`

Examples

```
## Not run:
# Collect some data to flatten
ids <- c(40,50,60,70)
 data <- lapply(ids, gatherData)
 # Flatten the data trees to a table
 flat.table <- flatten(data)
 # reimport the table into a tree
 data.reimported <- apply(flat.table, 1, readMbdata)

## End(Not run)
```

`formulastring.to.list` *Interconvert molecular formula representations*

Description

Converts molecular formulas from string to list representation or vice versa.

Usage

```
list.to.formula(flist)

formulastring.to.list(formula)
```

Arguments

`formula`	A molecular formula in string format, e.g. `"C6H12O6"`.
`flist`	A molecular formula in list format, e.g. `list( "C" = 6,"H" = 12, "O" = 6 )`.

Details

The function doesn't care about whether your formula makes sense. However, `"C3.5O4"` will give `list("C" = 3, "O" = 4)` because regular expressions are used for matching (however, `list("C" = 3.5, "O" = 4)` gives `"C3.5O4"`.) Duplicate elements cause problems; only "strict" molecular formulas ("CH4O", but not "CH3OH") work correctly.

Value

`list.to.formula` returns a string representation of the formula; `formulastring.to.list` returns the list representation.

Author(s)

Michael Stravs

See Also

`add.formula`, `order.formula`, `is.valid.formula`

Examples

```
#
list.to.formula(list("C" = 4, "H" = 12))
# This is also OK and useful to calculate e.g. adducts or losses.
list.to.formula(list("C" = 4, "H" = -1))
formulastring.to.list(list.to.formula(formulastring.to.list("CHIBr")))
```

---

gatherCompound *Compose data block of MassBank record*

Description

`gatherCompound` composes the data blocks (the "lower half") of all MassBank records for a compound, using the annotation data in the RMassBank options, spectrum info data from the `analyzedSpec`-type record and the peaks from the reanalyzed, multiplicity-filtered peak table. It calls `gatherSpectrum` for each child spectrum.

Usage

```
gatherCompound(spec, aggregated, additionalPeaks = NULL, retrieval="standard")

gatherSpectrum(spec, msmsdata, ac_ms, ac_lc, aggregated,
  additionalPeaks = NULL, retrieval="standard")
```

Arguments

- `spec` — A `RmbSpectraSet` object, representing a compound with multiple spectra.
- `aggregated` — An aggregate peak table where the peaks are extracted from.
- `additionalPeaks` — If present, a table with additional peaks to add into the spectra. As loaded with `addPeaks`.
- `retrieval` — A value that determines whether the files should be handled either as "standard", if the compoundlist is complete, "tentative", if at least a formula is present or "unknown" if the only know thing is the m/z
- `msmsdata` — A `RmbSpectrum2` object from the `spec` spectra set, representing a single spectrum to give a record.
- `ac_ms, ac_lc` — Information for the AC\$MASS_SPECTROMETRY and AC\$CHROMATOGRAPHY fields in the MassBank record, created by `gatherCompound` and then fed into `gatherSpectrum`.

Details

The returned data blocks are in format `list( "AC$MASS_SPECTROMETRY" = list('FRAGMENTATION_MODE' = 'CID', .` etc.

Value

`gatherCompound` returns a list of tree-like MassBank data blocks. `gatherSpectrum` returns one single MassBank data block or `NA` if no useful peak is in the spectrum.

Note

Note that the global table `additionalPeaks` is also used as an additional source of peaks.

Author(s)

Michael Stravs

References

MassBank record format: http://www.massbank.jp/manuals/MassBankRecord_en.pdf

See Also

`mbWorkflow`, `compileRecord`

Examples

```
## Not run:
     myspectrum <- w@spectra[[1]]
massbankdata <- gatherCompound(myspectrum, w@aggregated)
# Note: ac_lc and ac_ms are data blocks usually generated in gatherCompound and
# passed on from there. The call below gives a relatively useless result :)
ac_lc_dummy <- list()
ac_ms_dummy <- list()
justOneSpectrum <- gatherSpectrum(myspectrum, myspectrum@child[[2]],
ac_ms_dummy, ac_lc_dummy, w@aggregated)
```

```
## End(Not run)
```

`gatherData` *Retrieve annotation data*

Description

Retrieves annotation data for a compound from the internet services CTS, Pubchem, Chemspider and Cactvs, based on the SMILES code and name of the compounds stored in the compound list.

Usage

```
gatherData(id)
```

Arguments

`id`	The compound ID.

Details

Composes the "upper part" of a MassBank record filled with chemical data about the compound: name, exact mass, structure, CAS no., links to PubChem, KEGG, ChemSpider. The instrument type is also written into this block (even if not strictly part of the chemical information). Additionally, index fields are added at the start of the record, which will be removed later: `id, dbcas, dbname` from the compound list, `dataused` to indicate the used identifier for CTS search (`smiles` or `dbname`).

Additionally, the fields `ACCESSION` and `RECORD_TITLE` are inserted empty and will be filled later on.

Value

Returns a list of type `list(id=` *compoundID* `, ...,'ACCESSION' = '', 'RECORD_TITLE' = '', )` etc.

Author(s)

Michael Stravs

References

Chemical Translation Service: http://uranus.fiehnlab.ucdavis.edu:8080/cts/homePage cactus Chemical Identifier Resolver: http://cactus.nci.nih.gov/chemical/structure MassBank record format: http://www.massbank.jp/manuals/MassBankRecord_en.pdf Pubchem REST: https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST.html Chemspider InChI conversion: https://www.chemspider.com/InChI.asmx

See Also

`mbWorkflow`

Examples

```
# Gather data for compound ID 131
## Not run: gatherData(131)
```

`gatherDataBabel` *Retrieve annotation data*

Description

Retrieves annotation data for a compound by using babel, based on the SMILES code and name of the compounds stored in the compound list.

Usage

```
gatherDataBabel(id)
```

Arguments

`id`	The compound ID.

Details

Composes the "upper part" of a MassBank record filled with chemical data about the compound: name, exact mass, structure, CAS no.. The instrument type is also written into this block (even if not strictly part of the chemical information). Additionally, index fields are added at the start of the record, which will be removed later: `id, dbcas, dbname` from the compound list.

Additionally, the fields `ACCESSION` and `RECORD_TITLE` are inserted empty and will be filled later on.

This function is an alternative to gatherData, in case CTS is down or if information on one or more of the compounds in the compound list are sparse

Value

Returns a list of type `list(id=` *compoundID*`, ...,'ACCESSION' = '', 'RECORD_TITLE' = '', )` etc.

Author(s)

Michael Stravs, Erik Mueller

References

MassBank record format: http://www.massbank.jp/manuals/MassBankRecord_en.pdf

See Also

`mbWorkflow`

Examples

```
# Gather data for compound ID 131
## Not run: gatherDataBabel(131)
```

`gatherDataUnknown` *Retrieve annotation data*

Description

Retrieves annotation data for an unknown compound by using basic information present

Usage

```
gatherDataUnknown(id, mode, retrieval)
```

Arguments

`id`	The compound ID.
`mode`	`"pH"`, `"pNa"`, `"pM"`, `"pNH4"`, `"mH"`, `"mM"`, `"mFA"` for different ions ([M+H]+, [M+Na]+, [M]+, [M+NH4]+, [M-H]-, [M]-, [M+FA]-).
`retrieval`	A value that determines whether the files should be handled either as "standard", if the compoundlist is complete, "tentative", if at least a formula is present or "unknown" if the only know thing is the m/z

Details

Composes the "upper part" of a MassBank record filled with chemical data about the compound: name, exact mass, structure, CAS no.. The instrument type is also written into this block (even if not strictly part of the chemical information). Additionally, index fields are added at the start of the record, which will be removed later: `id, dbcas, dbname` from the compound list.

Additionally, the fields `ACCESSION` and `RECORD_TITLE` are inserted empty and will be filled later on.

This function is used to generate the data in case a substance is unknown, i.e. not enough information is present to derive anything about formulas or links

Value

Returns a list of type `list(id=` *compoundID*`, ...,'ACCESSION' = '', 'RECORD_TITLE' = '', )` etc.

Author(s)

Michael Stravs, Erik Mueller

References

MassBank record format: http://www.massbank.jp/manuals/MassBankRecord_en.pdf

See Also

mbWorkflow

Examples

```
# Gather data for compound ID 131
## Not run: gatherDataUnknown(131,"pH")
```

---

gatherPubChem *Retrieve supplemental annotation data from Pubchem*

Description

Retrieves annotation data for a compound from the internet service Pubchem based on the inchikey generated by babel or Cactus

Usage

```
gatherPubChem(key)
```

Arguments

key	An Inchi-Key

Details

The data retrieved is the Pubchem CID, a synonym from the Pubchem database, the IUPAC name (using the preferred if available) and a Chebi link

Value

Returns a list with 4 slots: PcID The Pubchem CID Synonym An arbitrary synonym for the compound name IUPAC A IUPAC-name (preferred if available) Chebi The identification number of the chebi database

Author(s)

Erik Mueller

References

Pubchem REST: https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST.html Chebi: http://www.ebi.ac.uk/chebi

See Also

mbWorkflow

Examples

```
# Gather data for compound ID 131
## Not run: gatherPubChem("QEIXBXXKTUNWDK-UHFFFAOYSA-N")
```

`getCactus` *Retrieve information from Cactus*

Description

Retrieves information from the Cactus Chemical Identifier Resolver (PubChem).

Usage

```
getCactus(identifier, representation)
```

Arguments

`identifier`	Any identifier interpreted by the resolver, e.g. an InChI key or a SMILES code.
`representation`	The desired representation, as required from the resolver. e.g. `stdinchikey`, `chemspider_id`, `formula`... Refer to the webpage for details.

Details

It is not necessary to specify in which format the `identifier` is. Somehow, cactus does this automatically.

Value

The result of the query, in plain text. Can be NA, or one or multiple lines (character array) of results.

Note

Note that the InChI key is retrieved with a prefix (`InChIkey=`), which must be removed for most database searches in other databases (e.g. CTS).

Author(s)

Michael Stravs

References

cactus Chemical Identifier Resolver: http://cactus.nci.nih.gov/chemical/structure

See Also

`getCtsRecord`, `getPcId`

Examples

```
# Benzene:
getCactus("C1=CC=CC=C1", "cas")
getCactus("C1=CC=CC=C1", "stdinchikey")
getCactus("C1=CC=CC=C1", "chemspider_id")
```

`getCSID` *Retrieve the Chemspider ID for a given compound*

Description

Given an InChIKey, this function queries the chemspider web API to retrieve the Chemspider ID of he compound with that InChIkey.

Usage

```
getCSID(query)
```

Arguments

`query`	The InChIKey of the compound

Value

Returns the chemspide

Author(s)

Michele Stravs, Eawag <stravsmi@eawag.ch>

Erik Mueller, UFZ <erik.mueller@ufz.de>

Examples

```
## Not run:
# Return all CAS registry numbers stored for benzene.
data <- getCtsRecord("UHOVQNZJYSORNB-UHFFFAOYSA-N")
cas <- CTS.externalIdSubset(data, "CAS")

## End(Not run)
```

getCtsKey — *Convert a single ID to another using CTS.*

Description

Convert a single ID to another using CTS.

Usage

```
getCtsKey(query, from = "Chemical Name", to = "InChIKey")
```

Arguments

query	ID to be converted
from	Type of input ID
to	Desired output ID

Value

An unordered array with the resulting converted key(s).

Author(s)

Michele Stravs, Eawag <stravsmi@eawag.ch>

Examples

```
k <- getCtsKey("benzene", "Chemical Name", "InChIKey")
```

getCtsRecord — *Retrieve information from CTS*

Description

Retrieves a complete CTS record from the InChI key.

Usage

```
getCtsRecord(key)
```

Arguments

key	The InChI key.

Value

Returns a list with all information from CTS: `inchikey`,`inchicode`, `formula`, `exactmass` contain single values. `synonyms` contains an unordered list of scored synonyms (`type`, `name`, `score`, where `type` indicates either a normal name or a specific IUPAC name, see below). `externalIds` contains an unordered list of identifiers of the compound in various databases (`name`, `value`, where `name` is the database name and `value` the identifier in that database.)

Note

Currently, the CTS results are still incomplete; the name scores are all 0, formula and exact mass return zero.

Author(s)

Michele Stravs, Eawag <stravsmi@eawag.ch>

References

Chemical Translation Service: http://cts.fiehnlab.ucdavis.edu

Examples

```
data <- getCtsRecord("UHOVQNZJYSORNB-UHFFFAOYSA-N")
# show all synonym "types"
types <- unique(unlist(lapply(data$synonyms, function(i) i$type)))
## Not run: print(types)
```

---

getData — *Get data frame with all present peak data*

Description

Returns a data frame with columns for all non-empty slots in a `RmbSpectrum2` object. Note that `MSnbase::Spectrum` has a method `as.data.frame`, however that one will return only mz, intensity. This function is kept separate to ensure downwards compatibility since it returns more columns than MSnbase `as.data.frame`.

Usage

```
## S4 method for signature 'RmbSpectrum2'
getData(s)
```

Arguments

`s`	The `RmbSpectrum2` object to extract data from.

Value

A data frame with columns for every set slot.

Author(s)

stravsmi

`getMolecule` *Create Rcdk molecule from SMILES*

Description

Generates a Rcdk molecule object from SMILES code, which is fully typed and usable (in contrast to the built-in `parse.smiles`).

Usage

```
getMolecule(smiles)
```

Arguments

`smiles`	The SMILES code of the compound.

Details

NOTE: As of today (2012-03-16), Rcdk discards stereochemistry when loading the SMILES code! Therefore, do not trust this function blindly, e.g. don't generate InChI keys from the result. It is, however, useful if you want to compute the mass (or something else) with Rcdk.

Value

A Rcdk `IAtomContainer` reference.

Author(s)

Michael Stravs

See Also

`parse.smiles`

Examples

```
# Lindane:
getMolecule("C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl")
# Benzene:
getMolecule("C1=CC=CC=C1")
```

getPcId — *Search Pubchem CID*

Description

Retrieves PubChem CIDs for a search term.

Usage

```
getPcId(query, from = "inchikey")
```

Arguments

query	ID to be converted
from	Type of input ID

Details

Only the first result is returned currently. **The function should be regarded as experimental and has not thoroughly been tested.**

Value

The PubChem CID (in string type).

Author(s)

Michael Stravs, Erik Mueller

References

PubChem search: http://pubchem.ncbi.nlm.nih.gov/

Pubchem REST: https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST.html

See Also

getCtsRecord, getCactus

Examples

```
getPcId("MKXZASYAUGDDCJ-NJAFHUGGSA-N")
```

is.valid.formula — *Check validity of formula*

Description

Checks whether the formula is chemically valid, i.e. has no zero-count or negative-count elements.

Usage

```
is.valid.formula(formula)
```

Arguments

formula	A molecular formula in string or list representation (`"C6H6"` or `list(C=6,H=6)`).

Details

The check is only meant to identify formulas which have negative elements, which can arise from the subtraction of adducts. It is **not** a high-level formula "validity" check like e.g. the Rcdk function `isvalid.formula` which uses the nitrogen rule or a DBE rule.

Author(s)

Michael Stravs

See Also

`list.to.formula`, `add.formula`, `order.formula`

Examples

```
#
is.valid.formula(list(C=0,H=1,Br=2))
is.valid.formula("CH2Cl")
is.valid.formula("C0H2")
```

loadInfolists — *Load MassBank compound information lists*

Description

Loads MassBank compound information lists (i.e. the lists which were created in the first two steps of the MassBank `mbWorkflow` and subsequently edited by hand.).

Usage

```
loadInfolists(mb, path)

 loadInfolist(mb, fileName)

 resetInfolists(mb)
```

Arguments

mb	The mbWorkspace to load/reset the lists in.
path	Directory in which the namelists reside. All CSV files in this directory will be loaded.
fileName	A single namelist to be loaded.

Details

resetInfolists clears the information lists, i.e. it creates a new empty list in mbdata_archive. loadInfolist loads a single CSV file, whereas loadInfolists loads a whole directory.

Value

The new workspace with loaded/reset lists.

Author(s)

Michael Stravs

Examples

```
#
## Not run: mb <- resetInfolists(mb)
mb <- loadInfolist(mb, "my_csv_infolist.csv")
## End(Not run)
```

---

loadList *Load compound list for RMassBank*

Description

Loads a CSV compound list with compound IDs

Usage

```
loadList(path, listEnv=NULL, check=TRUE)

resetList()
```

Arguments

`path`	Path to the CSV list.
`listEnv`	The environment to load the list into. By default, the namelist is loaded into an environment internally in RMassBank.
`check`	A parameter that specifies whether the SMILES-Codes in the list should be checked for readability by rcdk.

Details

The list is loaded into the variable *compoundList* in the environment `listEnv` (which defaults to the global environment) and used by the `findMz`, `findCAS`, ... functions. The CSV file is required to have at least the following columns, which are used for further processing and must be named correctly (but present in any order): *ID*, *Name*, *SMILES*, *RT*, *CAS*

resetList() clears a currently loaded list.

Value

No return value.

Author(s)

Michael Stravs

See Also

`findMz`

Examples

```
##
## Not run: loadList("mylist.csv")
```

---

makeMollist *Write list.tsv file*

Description

Makes a list.tsv file in the "moldata" folder.

Usage

```
makeMollist(compiled)
```

Arguments

`compiled`	A list of compiled spectra (in tree-format, as returned by `compileRecord`).

Details

Generates the list.tsv file which is needed by MassBank to connect records with their respective molfiles. The first compound name is linked to a mol-file with the compound ID (e.g. 2334.mol for ID 2334).

Value

No return value.

Author(s)

Michael A. Stravs, Eawag <michael.stravs@eawag.ch>

Examples

```
## Not run:
compiled <- compileRecord(record, mbdata, refilteredRcSpecs)
# a list.tsv for only one record:
clist <- list(compiled)
makeMollist(clist)

## End(Not run)
```

---

makePeaksCache *Generate peaks cache*

Description

Generates a peak cache table for use with `findMsMsHR` functions.

Usage

```
makePeaksCache(msRaw, headerCache)
```

Arguments

`msRaw`	the input raw datafile (opened)
`headerCache`	the cached header, or subset thereof for which peaks should be extracted. Peak extraction goes by `seqNum`.

Value

A list of dataframes as from `mzR::peaks`.

Author(s)

stravsmi

makeRecalibration *Recalibrate MS/MS spectra*

Description

Recalibrates MS/MS spectra by building a recalibration curve of the assigned putative fragments of all spectra in aggregatedSpecs (measured mass vs. mass of putative associated fragment) and additionally the parent ion peaks.

Usage

```
makeRecalibration(w, mode,
  recalibrateBy = getOption("RMassBank")$recalibrateBy,
recalibrateMS1 = getOption("RMassBank")$recalibrateMS1,
recalibrator = getOption("RMassBank")$recalibrator,
recalibrateMS1Window = getOption("RMassBank")$recalibrateMS1Window
)

 recalibrateSpectra(mode, rawspec = NULL, rc = NULL, rc.ms1=NULL, w = NULL,
recalibrateBy = getOption("RMassBank")$recalibrateBy,
recalibrateMS1 = getOption("RMassBank")$recalibrateMS1)

 recalibrateSingleSpec(spectrum, rc,
recalibrateBy = getOption("RMassBank")$recalibrateBy)
```

Arguments

w	For makeRecalibration: to perform the recalibration with. For recalibrateSpectra: the msmsWorkspace which contains the recalibration curves (alternatively to specifying rc, rc.ms1).
mode	"pH", "pNa", "pM", "mH", "mM", "mFA" for different ions ([M+H]+, [M+Na]+, [M]+, [M-H]-, [M]-, [M+FA]-).
recalibrateBy	Whether recalibration should be done by ppm ("ppm") or by m/z ("mz").
recalibrateMS1	Whether MS1 spectra should be recalibrated separately ("separate"), together with MS2 ("common") or not at all ("none"). Usually taken from settings.
recalibrator	The recalibrator functions to be used. Refer to recalibrate for details. Usually taken from settings.
recalibrateMS1Window	Window width to look for MS1 peaks to recalibrate (in ppm).
spectrum	For recalibrateSingleSpec: a MSnbase Spectrum-derived object, commonly a RmbSpectrum2 for MS2 or Spectrum1 for MS1.
rawspec	For recalibrateSpectra:an RmbSpectraSetList of RmbSpectraSet objects , as the w@spectra slot from msmsWorkspace or any object returned by findMsMsHR. If empty, no spectra are recalibrated, but the recalibration curve is returned.
rc, rc.ms1	The recalibration curves to be used in the recalibration.

Details

Note that the actually used recalibration functions are governed by the general MassBank settings (see recalibrate).

If a set of acquired LC-MS runs contains spectra for two different ion types (e.g. [M+H]+ and [M+Na]+) which should both be processed by RMassBank, it is necessary to do this in two separate runs. Since it is likely that one ion type will be the vast majority of spectra (e.g. most in [M+H]+ mode), and only few spectra will be present for other specific adducts (e.g. only few [M+Na]+ spectra), it is possible that too few spectra are present to build a good recalibration curve using only e.g. the [M+Na]+ ions. Therefore we recommend, for one set of LC/MS runs, to build the recalibration curve for one ion type (msmsWorkflow(mode="pH", steps=c(1:8), newRecalibration=TRUE)) and reuse the same curve for processing different ion types (msmsWorkflow(mode="pNa", steps=c(1:8), newRecalib This also ensures a consistent recalibration across all spectra of the same batch.

Value

makeRecalibration: a list(rc, rc.ms1) with recalibration curves for the MS2 and MS1 spectra.

recalibrateSpectra: if rawspec is not NULL, returns the recalibrated spectra as RmbSpectraSetList. All spectra have their mass recalibrated and evaluation data deleted.

recalibrateSingleSpec: the recalibrated Spectrum (same object, recalibrated masses, evaluation data like assigned formulae etc. deleted).

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

Examples

```
## Not run:
rcCurve <- recalibrateSpectra(w, "pH")
w@spectra <- recalibrateSpectra(mode="pH", rawspec=w@spectra, w=myWorkspace)
w@spectra <- recalibrateSpectra(mode="pH", rawspec=w@spectra,rcCurve$rc, rcCurve$rc.ms1)

## End(Not run)
```

---

mbWorkflow *MassBank record creation workflow*

Description

Uses data generated by msmsWorkflow to create MassBank records.

Usage

```
mbWorkflow(mb, steps = c(1, 2, 3, 4, 5, 6, 7, 8),
  infolist_path = "./infolist.csv", gatherData = "online")
```

Arguments

`mb`	The `mbWorkspace` to work in.
`steps`	Which steps in the workflow to perform.
`infolist_path`	A path where to store newly downloaded compound informations, which should then be manually inspected.
`gatherData`	A variable denoting whether to retrieve information using several online databases `gatherData= "online"` or to use the local babel installation `gatherData= "babel"`. Note that babel is used either way, if a directory is given in the settings. This setting will be ignored if retrieval is set to "standard"

Details

See the vignette `vignette("RMassBank")` for detailed informations about the usage.

Steps:

Step 1: Find which compounds don't have annotation information yet. For these compounds, pull information from several databases (using gatherData).

Step 2: If new compounds were found, then export the infolist.csv and stop the workflow. Otherwise, continue.

Step 3: Take the archive data (in table format) and reformat it to MassBank tree format.

Step 4: Compile the spectra. Using the skeletons from the archive data, create MassBank records per compound and fill them with peak data for each spectrum. Also, assign accession numbers based on scan mode and relative scan no.

Step 5: Convert the internal tree-like representation of the MassBank data into flat-text string arrays (basically, into text-file style, but still in memory)

Step 6: For all OK records, generate a corresponding molfile with the structure of the compound, based on the SMILES entry from the MassBank record. (This molfile is still in memory only, not yet a physical file)

Step 7: If necessary, generate the appropriate subdirectories, and actually write the files to disk.

Step 8: Create the list.tsv in the molfiles folder, which is required by MassBank to attribute substances to their corresponding structure molfiles.

Value

The processed `mbWorkspace`.

Author(s)

Michael A. Stravs, Eawag <michael.stravs@eawag.ch>

See Also

`mbWorkspace-class`

Examples

```
## Not run:
mb <- newMbWorkspace(w) # w being a msmsWorkspace
mb <- loadInfolists(mb, "D:/myInfolistPath")
mb <- mbWorkflow(mb, steps=c(1:3), "newinfos.csv")
```

```
## End(Not run)
```

---

mbWorkspace-class *Workspace for* mbWorkflow *data*

Description

A workspace which stores input and output data for use with mbWorkflow.

Usage

```
## S4 method for signature 'mbWorkspace'
show(object)
```

Arguments

object	The mbWorkspace to display.

Details

Slots:

spectra, aggregated The corresponding input data from msmsWorkspace-class

additionalPeaks A list of additional peaks which can be loaded using addPeaks.

mbdata, mbdata_archive, mbdata_relisted Infolist data: Data for annotation of MassBank records, which can be loaded using loadInfolists.

compiled, compiled_ok Compiled tree-structured MassBank records. compiled_ok contains only the compounds with at least one valid spectrum.

mbfiles Compiled MassBank records in text representation.

molfile MOL files with the compound structures.

ok,problems Index lists for internal use which denote which compounds have valid spectra.

Methods:

show Shows a brief summary of the object. Currently only a stub.

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

See Also

mbWorkflow

msmsRead *Extracts and processes spectra from a specified file list, according to loaded options and given parameters.*

Description

The filenames of the raw LC-MS runs are read from the array `files` in the global enviroment. See the vignette `vignette("RMassBank")` for further details about the workflow.

Usage

```
msmsRead(w, filetable = NULL, files = NULL, cpdids = NULL, readMethod,
  mode, confirmMode = FALSE, useRtLimit = TRUE, Args = NULL,
  settings = getOption("RMassBank"), progressbar = "progressBarHook",
  MSe = FALSE, plots = FALSE)
```

Arguments

`w`	A `msmsWorkspace` to work with.
`filetable`	The path to a .csv-file that contains the columns "Files" and "ID" supplying the relationships between files and compound IDs. Either this or the parameter "files" need to be specified.
`files`	A vector or list containing the filenames of the files that are to be read as spectra. For the IDs to be inferred from the filenames alone, there need to be exactly 2 underscores.
`cpdids`	A vector or list containing the compound IDs of the files that are to be read as spectra. The ordering of this and `files` implicitly assigns each ID to the corresponding file. If this is supplied, then the IDs implicitly named in the filenames are ignored.
`readMethod`	Several methods are available to get peak lists from the files. Currently supported are "mzR", "xcms", "MassBank" and "peaklist". The first two read MS/MS raw data, and differ in the strategy used to extract peaks. MassBank will read existing records, so that e.g. a recalibration can be performed, and "peaklist" just requires a CSV with two columns and the column header "mz", "int".
`mode`	`"pH"`, `"pNa"`, `"pM"`, `"pNH4"`, `"mH"`, `"mM"`, `"mFA"` for different ions ([M+H]+, [M+Na]+, [M]+, [M+NH4]+, [M-H]-, [M]-, [M+FA]-).
`confirmMode`	Defaults to false (use most intense precursor). Value 1 uses the 2nd-most intense precursor for a chosen ion (and its data-dependent scans) , etc.
`useRtLimit`	Whether to enforce the given retention time window.
`Args`	A list of arguments that will be handed to the xcms-method findPeaks via do.call
`settings`	Options to be used for processing. Defaults to the options loaded via `loadRmbSettings` et al. Refer to there for specific settings.
`progressbar`	The progress bar callback to use. Only needed for specialized applications. Cf. the documentation of `progressBarHook` for usage.
`MSe`	A boolean value that determines whether the spectra were recorded using MSe or not
`plots`	A boolean value that determines whether the pseudospectra in XCMS should be plotted

Value

The msmsWorkspace with msms-spectra read.

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

Erik Mueller, UFZ

See Also

msmsWorkspace-class, msmsWorkflow

---

msmsRead.RAW *Extracts and processes spectra from a list of xcms-Objects*

Description

The filenames of the raw LC-MS runs are read from the array files in the global enviroment. See the vignette vignette("RMassBank") for further details about the workflow.

Usage

```
msmsRead.RAW(w, xRAW = NULL, cpdids = NULL, mode, findPeaksArgs = NULL,
  settings = getOption("RMassBank"), progressbar = "progressBarHook",
  plots = FALSE)
```

Arguments

w	A msmsWorkspace to work with.
xRAW	A list of xcmsRaw objects whose peaks should be detected and added to the workspace. The relevant data must be in the MS1 data of the xcmsRaw object. You can coerce the msn-data in a usable object with the msn2xcmsRaw function of xcms.
cpdids	A vector or list containing the compound IDs of the files that are to be read as spectra. The ordering of this and files implicitly assigns each ID to the corresponding file. If this is supplied, then the IDs implicitly named in the filenames are ignored.
mode	"pH", "pNa", "pM", "pNH4", "mH", "mM", "mFA" for different ions ([M+H]+, [M+Na]+, [M]+, [M+NH4]+, [M-H]-, [M]-, [M+FA]-).
findPeaksArgs	A list of arguments that will be handed to the xcms-method findPeaks via do.call
settings	Options to be used for processing. Defaults to the options loaded via loadRmbSettings et al. Refer to there for specific settings.
progressbar	The progress bar callback to use. Only needed for specialized applications. Cf. the documentation of progressBarHook for usage.
plots	A boolean value that determines whether the pseudospectra in XCMS should be plotted

Value

The msmsWorkspace with msms-spectra read.

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

Erik Mueller, UFZ

See Also

msmsWorkspace-class, msmsWorkflow

---

msmsWorkflow *RMassBank mass spectrometry pipeline*

Description

Extracts and processes spectra from a specified file list, according to loaded options and given parameters.

Usage

```
msmsWorkflow(w, mode = "pH", steps = c(1:8), confirmMode = FALSE,
  newRecalibration = TRUE, useRtLimit = TRUE, archivename = NA,
  readMethod = "mzR", findPeaksArgs = NULL, plots = FALSE,
  precursorscan.cf = FALSE, settings = getOption("RMassBank"),
  analyzeMethod = "formula", progressbar = "progressBarHook", MSe = FALSE)
```

Arguments

w	A msmsWorkspace to work with.
mode	"pH", "pNa", "pM", "mH", "mM", "mFA", "pNH4" for different ions ([M+H]+, [M+Na]+, [M]+, [M-H]-, [M]-, [M+FA]-, [M+NH4]+).
steps	Which steps of the workflow to process. See the vignette vignette("RMassBank") for details.
confirmMode	Defaults to false (use most intense precursor). Value 1 uses the 2nd-most intense precursor for a chosen ion (and its data-dependent scans) , etc.
newRecalibration	Whether to generate a new recalibration curve (TRUE, default) or to reuse the currently stored curve (FALSE, useful e.g. for adduct-processing runs.)
useRtLimit	Whether to enforce the given retention time window.
archivename	The prefix under which to store the analyzed result files.
readMethod	Several methods are available to get peak lists from the files. Currently supported are "mzR", "xcms", "MassBank" and "peaklist". The first two read MS/MS raw data, and differ in the strategy used to extract peaks. MassBank will read existing records, so that e.g. a recalibration can be performed, and "peaklist" just requires a CSV with two columns and the column header "mz", "int".

findPeaksArgs	A list of arguments that will be handed to the xcms-method findPeaks via do.call
plots	A parameter that determines whether the spectra should be plotted or not (This parameter is only used for the xcms-method)
precursorscan.cf	Whether to fill precursor scans. To be used with files which for some reasons do not contain precursor scan IDs in the mzML, e.g. AB Sciex converted files.
settings	Options to be used for processing. Defaults to the options loaded via loadRmbSettings et al. Refer to there for specific settings.
analyzeMethod	The "method" parameter to pass to analyzeMsMs.
progressbar	The progress bar callback to use. Only needed for specialized applications. Cf. the documentation of progressBarHook for usage.
MSe	A boolean value that determines whether the spectra were recorded using MSe or not

Details

The filenames of the raw LC-MS runs are read from the array files in the global enviroment. See the vignette vignette("RMassBank") for further details about the workflow.

Value

The processed msmsWorkspace.

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

See Also

msmsWorkspace-class

---

msmsWorkspace-class *Workspace for* msmsWorkflow *data*

Description

A workspace which stores input and output data for msmsWorkflow.

Usage

```
## S4 method for signature 'msmsWorkspace'
show(object)
```

Arguments

object	The msmsWorkspace to display.

Details

Slots:

files The input file names

spectra The spectra per compound (`RmbSpectraSet`) extracted from the raw files

aggregated A data.frame with an aggregated peak table from all `spectra`. Further columns are added during processing.

rc, rc.ms1 The recalibration curves generated in workflow step 4.

parent For the workflow steps after 4: the parent workspace containing the state (spectra, aggregate) before recalibration, such that the workflow can be reprocessed from start.

archivename The base name of the files the archive is stored to during the workflow.

settings The RMassBank settings used during the workflow, if stored with the workspace.#'

Methods:

show Shows a brief summary of the object and processing progress.

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

See Also

`msmsWorkflow`

`newMbWorkspace` *Create new workspace for* `mbWorkflow`

Description

Creates a new workspace for use with `mbWorkflow`.

Usage

```
newMbWorkspace(w)
```

Arguments

`w`	The input `msmsWorkspace` to load input data from.

Details

The workspace input data will be loaded from the `msmsWorkspace-class` object provided by the parameter `w`.

Value

A new `mbWorkflow` object with the loaded input data.

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

See Also

mbWorkflow, msmsWorkspace-class

---

newMsmsWorkspace *Create new empty workspace or load saved data for* msmsWorkflow

---

Description

Creates an empty workspace or loads an existing workspace from disk.

Usage

```
newMsmsWorkspace(files = character(0))
```

Arguments

files	If given, the files list to initialize the workspace with.

Details

newMsmsWorkspace creates a new empty workspace for use with msmsWorkflow.

loadMsmsWorkspace loads a workspace saved using archiveResults. Note that it also successfully loads data saved with the old RMassBank data format into the new msmsWorkspace object.

Value

A new msmsWorkspace object

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch>

See Also

msmsWorkflow, msmsWorkspace-class

order.formula — *Order a chemical formula correctly*

Description

Orders a chemical formula in the commonly accepted order (CH followed by alphabetic ordering).

Usage

```
order.formula(formula, as.formula = TRUE, as.list = FALSE)
```

Arguments

formula	A molecular formula in string or list representation ("C6H6" or list(C=6,H=6)).
as.formula	If TRUE, the return value is returned as a string. This is the default.
as.list	If TRUE, the return value is returned in list representation.

Author(s)

Michele Stravs

See Also

list.to.formula, add.formula, is.valid.formula

Examples

```
#
order.formula("H4C9")
order.formula("C2N5HClBr")
```

parseMassBank — *MassBank-record Parser*

Description

Can parse MassBank-records(only V2)

Usage

```
parseMassBank(Files)
```

Arguments

Files	A path to the plaintext-record that should be read

Value

The mbWorkspace that the plaintext-record creates.

Author(s)

Erik Mueller

See Also

validate

Examples

```
## Not run:
parseMassBank("filepath_to_records/RC00001.txt")

## End(Not run)
```

---

peaksMatched *Select matching/unmatching peaks from aggregate table*

Description

Select matching/unmatching peaks from aggregate table

Usage

```
peaksMatched(o)

## S4 method for signature 'data.frame'
peaksMatched(o)

## S4 method for signature 'msmsWorkspace'
peaksMatched(o)
```

Arguments

o	Workspace or aggregate table from a workspace

Value

Selects the peaks from the aggregate table which matched within filter criteria (peaksMatched) or didn't match (peaksUnmatched).

Methods (by class)

- data.frame: A method to retrieve the matched peaks from the "aggregated" slot (a data.frame object) in an msmsWorkSpace
- msmsWorkspace: A method to retrieve the matched peaks from an msmsWorkSpace

Author(s)

stravsmi

peaksUnmatched — *Select matching/unmatching peaks from aggregate table*

Description

Select matching/unmatching peaks from aggregate table

Usage

```
peaksUnmatched(o, cleaned = FALSE)

## S4 method for signature 'data.frame'
peaksUnmatched(o, cleaned = FALSE)

## S4 method for signature 'msmsWorkspace'
peaksUnmatched(o, cleaned = FALSE)
```

Arguments

`o`	Workspace or aggregate table from a workspace
`cleaned`	Return only peaks which pass electronic noise filtering if `TRUE`.

Value

Selects the peaks from the aggregate table which matched within filter criteria (`peaksMatched`) or didn't match (`peaksUnmatched`).

Methods (by class)

- `data.frame`: A method to retrieve the unmatched peaks from the "aggregated" slot (a data.frame object) in an msmsWorkSpace
- `msmsWorkspace`: A method to retrieve the unmatched peaks from an msmsWorkSpace

Author(s)

stravsmi

plotMbWorkspaces — *Plots mbWorkspaces*

Description

Plots the peaks of one or two `mbWorkspace` to compare them.

Usage

```
plotMbWorkspaces(w1, w2 = NULL)
```

Arguments

w1	The mbWorkspace to be plotted
w2	Another optional mbWorkspace be plotted as a reference.

Details

This functions plots one or two mbWorkspaces in case the use has used different methods to acquire similar spectra. w1 must always be supplied, while w2 is optional. The wokspaces need to be fully processed for this function to work.

Value

A logical indicating whether the information was plotted or not

Author(s)

Erik Mueller

Examples

```
#
## Not run: plotMbWorkspaces(w1,w2)
```

---

plotRecalibration *Plot the recalibration graph.*

Description

Plot the recalibration graph.

Usage

```
plotRecalibration(w, recalibrateBy = getOption("RMassBank")$recalibrateBy)

plotRecalibration.direct(rcdata, rc, rc.ms1, title, mzrange,
recalibrateBy = getOption("RMassBank")$recalibrateBy)
```

Arguments

w	The workspace to plot the calibration graph from
recalibrateBy	Whether recalibration was done by ppm ("ppm") or by m/z ("mz"). Important only for graph labeling here.
rcdata	A data frame with columns recalfield and mzFound.
rc	Predictor for MS2 data
rc.ms1	Predictor for MS1 data
title	Prefix for the graph titles
mzrange	m/z value range for the graph

Author(s)

Michele Stravs, Eawag <michael.stravs@eawag.ch>

`ppm` *Calculate ppm values*

Description

Calculates ppm values for a given mass.

Usage

```
ppm(mass, dppm, l = FALSE, p = FALSE)
```

Arguments

`mass`	The "real" mass
`dppm`	The mass deviation to calculate
`l`	Boolean: return limits? Defaults to FALSE.
`p`	Boolean: return ppm error itself? Defaults to FALSE.

Details

This is a helper function used in RMassBank code.

Value

By default (`l=FALSE, p=FALSE`) the function returns the mass plus the ppm error (for 123.00000 and 10 ppm: 123.00123, or for 123 and -10 ppm: 122.99877).

For `l=TRUE`, the function returns the upper and lower limit (sic!) For `p=TRUE`, just the difference itself is returned (0.00123 for 123/10ppm).

Author(s)

Michael A. Stravs, Eawag <michael.stravs@eawag.ch>

Examples

```
ppm(100, 10)
```

`problematicPeaks` *Identify intense peaks (in a list of unmatched peaks)*

Description

Finds a list of peaks in spectra with a high relative intensity (>10 1e4, or >1 checked. Peaks orbiting around the parent peak mass (calculated from the compound ID), which are very likely co-isolated substances, are ignored.

Usage

```
problematicPeaks(peaks_unmatched, peaks_matched, mode = "pH")
```

Arguments

`peaks_unmatched`	Table of unmatched peaks, with at least `cpdID`,`scan`, `mzFound`, `int`.
`peaks_matched`	Table of matched peaks (used for base peak reference), with at least `cpdID`, `scan`, `int`.
`mode`	Processing mode (`"pH"`, `"pNa"` etc.)

Value

A filtered table with the potentially problematic peaks, including the precursor mass and MSMS base peak intensity (`aMax`) for reference.

Author(s)

Michael Stravs

See Also

`msmsWorkflow`

Examples

```
## Not run:
# As used in the workflow:
fp <- problematicPeaks(specs[!specs$filterOK & !specs$noise &
((specs$dppm == specs$dppmBest) | (is.na(specs$dppmBest)))
,,drop=FALSE], peaksMatched(w), mode)

## End(Not run)
```

processProblematicPeaks

Generate list of problematic peaks

Description

Generates a list of intense unmatched peaks for further review (the "failpeak list") and exports it if the archive name is given.

Usage

```
processProblematicPeaks(w, mode, archivename = NA)
```

Arguments

w	msmsWorkspace to analyze.
mode	Processing mode (pH etc)
archivename	Base name of the archive to write to (for "abc" the exported failpeaks list will be "abc_Failpeaks.csv"). if the compoundlist is complete, "tentative", if at least a formula is present or "unknown" if the only know thing is the m/z

Value

Returns the aggregate data.frame with added column "problematic" (logical) which marks peaks which match the problematic criteria

Author(s)

stravsmi

progressBarHook

Standard progress bar hook.

Description

This function provides a standard implementation for the progress bar in RMassBank.

Usage

```
progressBarHook(object = NULL, value = 0, min = 0, max = 100,
  close = FALSE)
```

Arguments

object	An identifier representing an instance of a progress bar.
value	The new value to assign to the progress indicator
min	The minimal value of the progress indicator
max	The maximal value of the progress indicator
close	If TRUE, the progress bar is closed.

Details

RMassBank calls the progress bar function in the following three ways: `pb <- progressBarHook(object=NULL, value` to create a new progress bar. `pb <- progressBarHook(object=pb, value= VAL)` to set the progress bar to a new value (between the set `min` and `max`) `progressBarHook(object=pb, close=TRUE)` to close the progress bar. (The actual calls are performed with `do.call`, e.g. `progressbar <- "progressBarHook"` `pb <- do.call(progressbar, list(object=pb, value= nProg))` . See the source code for details.)

To substitute the standard progress bar for an alternative implementation (e.g. for use in a GUI), the developer can write his own function which behaves in the same way as `progressBarHook`, i.e. takes the same parameters and can be called in the same way.

Value

Returns a progress bar instance identifier (i.e. an identifier which can be used as `object` in subsequent calls.)

Author(s)

Michele Stravs, Eawag <stravsmi@eawag.ch>

`reanalyzeFailpeaks` *Reanalyze unmatched peaks*

Description

Reanalysis of peaks with no matching molecular formula by allowing additional elements (e.g. "N2O").

Usage

```
reanalyzeFailpeaks(aggregated, custom_additions, mode, filterSettings =
getOption("RMassBank")$filterSettings, progressbar = "progressBarHook")
reanalyzeFailpeak(custom_additions, mass, cpdID, counter, pb = NULL, mode,
filterSettings = getOption("RMassBank")$filterSettings)
```

Arguments

`aggregated`	A peake aggregate table (`w@aggregate`) (after processing electronic noise removal!)
`custom_additions`	The allowed additions, e.g. "N2O".
`mode`	Processing mode (`"pH"`, `"pNa"`, `"mH"` etc.)
`filterSettings`	Settings for filtering data. Refer to`analyzeMsMs` for settings.
`progressbar`	The progress bar callback to use. Only needed for specialized applications. Cf. the documentation of `progressBarHook` for usage.
`mass`	(Usually recalibrated) m/z value of the peak.
`cpdID`	Compound ID of this spectrum.
`counter`	Current peak index (used exclusively for the progress indicator)
`pb`	A progressbar object to display progress on, as passed by `reanalyzeFailpeaks` to `reanalyzeFailpeak`. No progress is displayed if NULL.

Details

reanalyzeFailpeaks examines the unmatchedPeaksC table in specs and sends every peak through reanalyzeFailpeak.

Value

The aggregate data frame extended by the columns: #'

reanalyzed.??? If reanalysis (step 7) has already been processed: matching values from the reanalyzed peaks

matchedReanalysis
Whether reanalysis has matched (TRUE), not matched(FALSE) or has not been conducted for the peak(NA).

It would be good to merge the analysis functions of analyzeMsMs with the one used here, to simplify code changes.

Author(s)

Michael Stravs

See Also

analyzeMsMs, msmsWorkflow

Examples

```
## As used in the workflow:
## Not run:
reanalyzedRcSpecs <- reanalyzeFailpeaks(w@aggregated, custom_additions="N2O", mode="pH")
# A single peak:
reanalyzeFailpeak("N2O", 105.0447, 1234, 1, 1, "pH")

## End(Not run)
```

---

recalibrate *Predefined recalibration functions.*

Description

Predefined fits to use for recalibration: Loess fit and GAM fit.

Usage

```
recalibrate.loess(rcdata)

recalibrate.identity(rcdata)

recalibrate.mean(rcdata)

recalibrate.linear(rcdata)
```

Arguments

`rcdata` A data frame with at least the columns `recalfield` and `mzFound`. `recalfield` will usually contain delta(ppm) or delta(mz) values and is the target parameter for the recalibration.

Details

`recalibrate.loess()` provides a Loess fit (`recalibrate.loess`) to a given recalibration parameter. If MS and MS/MS data should be fit together, recalibrate.loess provides good default settings for Orbitrap instruments.

`recalibrate.identity()` returns a non-recalibration, i.e. a predictor which predicts 0 for all input values. This can be used if the user wants to skip recalibration in the RMassBank workflow.

#' `recalibrate.mean()` and `recalibrate.linear()` are simple recalibrations which return a constant shift or a linear recalibration. They will be only useful in particular cases.

`recalibrate()` itself is only a dummy function and does not do anything.

Alternatively other functions can be defined. Which functions are used for recalibration is specified by the RMassBank options file. (Note: if `recalibrateMS1: common`, the `recalibrator: MS1` value is irrelevant, since for a common curve generated with the function specified in `recalibrator: MS2` will be used.)

Value

Returns a model for recalibration to be used with `predict` and the like.

Author(s)

Michael Stravs, EAWAG <michael.stravs@eawag.ch>

Examples

```
## Not run:
rcdata <- subset(spec$peaksMatched, formulaCount==1)
ms1data <- recalibrate.addMS1data(spec, mode, 15)
rcdata <- rbind(rcdata, ms1data)
rcdata$recalfield <- rcdata$dppm
rcCurve <- recalibrate.loess(rcdata)
# define a spectrum and recalibrate it
s <- matrix(c(100,150,200,88.8887,95.0005,222.2223), ncol=2)
colnames(s) <- c("mz", "int")
recalS <- recalibrateSingleSpec(s, rcCurve)

Alternative: define an custom recalibrator function with different parameters
recalibrate.MyOwnLoess <- function(rcdata)
{
return(loess(recalfield ~ mzFound, data=rcdata, family=c("symmetric"),
degree = 2, span=0.4))
}
# This can then be specified in the RMassBank settings file:
# recalibrateMS1: common
# recalibrator:
#    MS1: recalibrate.loess
#    MS2: recalibrate.MyOwnLoess")
# [...]
```

```
## End(Not run)
```

`recalibrate.addMS1data`

Return MS1 peaks to be used for recalibration

Description

Returns the precursor peaks for all MS1 spectra in the `spec` dataset with annotated formula to be used in recalibration.

For all spectra in `spec$specFound`, the precursor ion is extracted from the MS1 precursor spectrum. All found ions are returned in a data frame with a format matching `spec$peaksMatched` and therefore suitable for `rbind`ing to the `spec$peaksMatched` table. However, only minimal information needed for recalibration is returned.

Usage

```
recalibrate.addMS1data(spec,mode="pH", recalibrateMS1Window =
getOption("RMassBank")$recalibrateMS1Window)
```

Arguments

`spec`	A `msmsWorkspace` or `RmbSpectraSetList` containing spectra for which MS1 "peaks" should be "constructed".
`mode`	`"pH"`, `"pNa"`, `"pM"`, `"pNH4"`, `"mH"`, `"mM"`, `"mFA"` for different ions ([M+H]+, [M+Na]+, [M]+, [M+NH4]+, [M-H]-, [M]-, [M+FA]-).
`recalibrateMS1Window`	Window width to look for MS1 peaks to recalibrate (in ppm).

Value

A dataframe with columns `mzFound, formula, mzCalc, dppm, dbe, int,dppmBest, formulaCount, good, cpdID` However, columns `dbe, int, formulaCount, good, scan, parentScan` do not contain real information and are provided only as fillers.

Author(s)

Michael Stravs, EAWAG <michael.stravs@eawag.ch>

Examples

```
## Not run:
# More or less as used in recalibrateSpectra:
rcdata <- peaksMatched(w)
rcdata <- rcdata[rcdata$formulaCount == 1, ,drop=FALSE]
ms1data <- recalibrate.addMS1data(w, "pH", 15)
rcdata <- rbind(rcdata, ms1data)
 # ... continue constructing recalibration curve with rcdata

## End(Not run)
```

RmbDefaultSettings *RMassBank settings*

Description

Load, set and reset settings for RMassBank.

Usage

```
loadRmbSettings(file_or_list)

loadRmbSettingsFromEnv(env = .GlobalEnv)

RmbDefaultSettings()

RmbSettingsTemplate(target)
```

Arguments

file_or_list	The file (YML or R format) or R `list` with the settings to load.
target	The path where the template setting file should be stored.
env	The environment to load the settings from.

Details

`RmbSettingsTemplate` creates a template file in which you can adjust the settings as you like. Before using RMassBank, you must then load the settings file using `loadRmbSettings`. `RmbDefaultSettings` loads the default settings. `loadRmbSettingsFromEnv` loads the settings stored in env$RmbSettings, which is useful when reloading archives with saved settings inside.

Note: no settings are loaded upon loading MassBank! This is intended, so that one never forgets to load the correct settings.

The settings are described in `RmbSettings`.

Value

None.

Note

The default settings will not work for you unless you have, by chance, installed OpenBabel into the same directory as I have!

Author(s)

Michael Stravs

See Also

`RmbSettings`

Examples

```
 # Create a standard settings file and load it (unedited)
RmbSettingsTemplate("mysettings.ini")
 loadRmbSettings("mysettings.ini")
 unlink("mysettings.ini")
```

RmbSettings *RMassBank settings*

Description

Describes all settings for the RMassBank settings file.

Details

- `deprofile` Whether and how to deprofile input raw files. Leave the setting empty if your raw files are already in "centroid" mode. If your input files are in profile mode, you have the choice between algorithms `deprofile.spline, deprofile.fwhm, deprofile.localMax`; refer to the individual manpages for more information.
- `rtMargin, rtShift` The allowed retention time deviation relative to the values specified in your compound list (see `loadList`), and the systematic shift (due to the use of, e.g., pre-columns or other special equipment.
- `babeldir` Directory to OpenBabel. Required for creating molfiles for MassBank export. If no OpenBabel directory is given, RMassBank will attempt to use the CACTUS webservice for SDF generation. It is strongly advised to install OpenBabel; the CACTUS structures have explicit hydrogen atoms. The path should point to the directory where babel.exe (or the Linux "babel" equivalent) lies.
- `use_version` Which MassBank record format to use; version 2 is strongly advised, version 1 is considered outdated and should be used only if for some reason you are running old servers and an upgrade is not feasible.
- `use_rean_peaks` Whether to include peaks from reanalysis (see `reanalyzeFailpeaks`) in the MassBank records. Boolean, TRUE or FALSE.
- `annotations` A list of constant annotations to use in the MassBank records. The entries `authors, copyright, license, instrument, instrument_type, compound_class` correspond to the MassBank entries `AUTHORS, COPYRIGHT, PUBLICATION, LICENSE, AC$INSTRUMENT,AC$INSTRUM`
  The entry `confidence_comment` is added as `COMMENT: CONFIDENCE` entry.

  The entry `internal_id_fieldname` is used to name the MassBank entry which will keep a reference to the internal compound ID used in the workflow: for `internal_id_fieldname = MYID` and e.g. compound 1234, an entry will be added to the MassBank record with `COMMENT: MYID 1234`. The internal fieldname should not be left empty!

  The entries `lc_gradient, lc_flow, lc_solvent_a, lc_solvent_b, lc_column` correspond to the MassBank entries `AC$CHROMATOGRAPHY: FLOW_GRADIENT, FLOW_RATE,SOLVENT A, SOLVENT B, CO`

  `ms_type, ionization` correspond to `AC$MASS_SPECTROMETRY: MS_TYPE, IONIZATION`.

  `entry_prefix` is the two-letter prefix used when building MassBank accession codes.

  Entries under `ms_dataprocessing` are added as `MS$DATA_PROCESSING:` entries, in addition to the default `WHOLE: RMassBank`.

- annotator For advanced users: option to select your own custom annotator. Check annotator.default and the source code for details.
- spectraList This setting describes the experimental annotations for the single data-dependent scans. For every data-dependent scan event, a spectraList entry with mode, ces, ce, res denoting collision mode, collision energy in short and verbose notation, and FT resolution.
- accessionNumberShifts This denotes the starting points for accession numbers for different ion types. For example, pH: 0, mH: 50 means that [M+H]+ spectra will start at XX123401 (XX being the entry_prefix and 1234 the compound id) and [M-H]- will start at XX123451.
- electronicNoise, electronicNoiseWidth Known electronic noise peaks and the window to be used by cleanElnoise
- recalibrateBy dppm or dmz to recalibrate either by delta ppm or by delta mz.
- recalibrateMS1 common or separate to recalibrate MS1 data points together or separately from MS2 data points.
- recalibrator: MS1, MS2 The functions to use for recalibration of MS1 and MS2 data points. Note that the MS1 setting is only meaningful if recalibrateMS1: separate, otherwise the MS2 setting is used for a common recalibration curve. See recalibrate.loess for details.
- multiplicityFilter Define the multiplicity filtering level. Default is 2, a value of 1 is off (no filtering) and >2 is harsher filtering.
- titleFormat The title of MassBank records is a mini-summary of the record, for example "Dinotefuran; LC-ESI-QFT; MS2; CE: 35 By default, the first compound name CH$NAME, instrument type AC$INSTRUMENT_TYPE, MS/MS type AC$MASS_SPECTROMETRY: MS_TYPE, collision energy RECORD_TITLE_CE, resolution AC$MASS_SPECTROMETRY: RESOLUTION and precursor MS$FOCUSED_ION: PRECURSOR_TYPE are used. If alternative information is relevant to differentiate acquired spectra, the title should be adjusted. For example, many TOFs do not have a resolution setting. See MassBank documentation for more.
- filterSettings A list of settings that affect the MS/MS processing. The entries ppmHighMass, ppmLowMass, mas set values for pre-processing, prior to recalibration. ppmHighMass defines the ppm error for the high mass range (default 10 ppm for Orbitraps), ppmLowMass is the error for the low mass range (default 15 ppm for Orbitraps) and massRangeDivision is the m/z value defining the split between the high and low mass range (default m/z = 120).

  The entry ppmFine defines the ppm cut-off post recalibration. The default value of 5 ppm is recommended for Orbitraps. For other instruments this can be interpreted from the recalibration plot. All ppm limits are one-sided (e.g. this includes values to +5 ppm or -5 ppm deviation from the exact mass).

  The entries prelimCut, prelimCutRatio define the intensity cut-off and cut-off ratio (in the peak selection for the recalibration only. Careful: the default value 1e4 for Orbitrap LTQ positive mode could remove all peaks for TOF data and will remove too many peaks for Orbitrap LTQ negative mode spectra!

  The entry specOKLimit defines the intensity limit to include MS/MS spectra. MS/MS spectra must have at least one peak above this limit to proceed through the workflow.

  dbeMinLimit defines the minimum allowable ring and double bond equivalents (DBE) allowed for assigned formulas. This assumes maximum valuences for elements with multiple valence states. The default is -0.5 (accounting for fragments being ions).

  The entries satelliteMzLimit, satelliteIntLimit define the cut-off m/z and intensity values for satellite peak removal (an artefact of Fourier Transform processing). All peaks within the m/z limit (default 0.5) and intensity ratio (default 0.05 or 5 Fourier Transform instruments only (e.g. Orbitrap).
- filterSettings Parameters for adjusting the raw data retrieval. The entry ppmFine defines the ppm error to look for the precursor in the MS1 (parent) spectrum. Default is 10 ppm for Orbitrap.

mzCoarse defines the error to search for the precursor specification in the MS2 spectrum. This is often only saved to 2 decimal places and thus can be quite inaccurate. The accuracy also depends on the isolation window used. The default settings (for e.g. Orbitrap) is 0.5 (Da, or Th for m/z).

The entry fillPrecursorScan is largely untested. The default value (FALSE) assumes all necessary precursor information is available in the mzML file. A setting ot TRUE tries to fill in the precursor data scan number if it is missing. Only tested on one case study so far - feedback welcome!

Author(s)

Michael Stravs, Emma Schymanski

See Also

loadRmbSettings

---

selectPeaks *Select peaks from aggregate table*

Description

Selects peaks from aggregate table according to different criteria.

Usage

```
selectPeaks(o, ...)

## S4 method for signature 'data.frame'
selectPeaks(o, good = FALSE, bad = FALSE,
  cleaned = FALSE, best = FALSE)

## S4 method for signature 'msmsWorkspace'
selectPeaks(o, ...)
```

Arguments

o	msmsWorkspace or aggregate data.frame from a workspace.
...	no additional parameters
good	if TRUE, include good (matched within filter criteria) peaks.
bad	if TRUE, include bad (not matched within filter criteria) peaks. Note: good and bad can be combined, both are returned in that case.
cleaned	if TRUE, return only peaks which passed the noise filter. Note: If the noise filter was not applied, the parameter has no effect. Also, a noise column is in any case added to the output, even if not present before.
best	if TRUE, only select the best match for each peak (i.e. the formula with smallest delta ppm). Otherwise multiple matches can be returned.

Value

Peak dataframe according to the specified criteria.

Methods (by class)

- `data.frame`: A method to retrieve the specified peaks from the "aggregated" slot (a data.frame object) in an msmsWorkSpace
- `msmsWorkspace`: A method to retrieve the specified peaks from an msmsWorkSpace

Author(s)

stravsmi

---

selectSpectra *Select a subset of spectra matching properties*

Description

From a list of `RmbSpectraSets`, returns the spectra which match a criterion (found, complete, empty as in `checkSpectra`). This can be returned either as a `TRUE/FALSE` vector, as a vector of indices for matching elements, as a vector of `RmbSpectraSet` objects matching the conditions, or as a vector of `RmbSpectraSet` objects NOT matching the conditions (sic!).

Usage

```
selectSpectra(s, property, value = "logical")

## S4 method for signature 'RmbSpectraSetList,character'
selectSpectra(s, property,
  value = "logical")

## S4 method for signature 'msmsWorkspace,character'
selectSpectra(s, property,
  value = "logical")
```

Arguments

`s`	The `RmbSpectraSetList` or `msmsWorkspace` to select `RmbSpectraSets` from.
`property`	The property to check (`found`, `complete` or `empty`)
`value`	`logical` if a `TRUE/FALSE` list should be returned; `index` if a vector of matching indices should be returned, `object` if matching objects should be returned, `mismatch` if mismatching objects should be returned.

Value

As described above.

Methods (by class)

- `s = RmbSpectraSetList,property = character`: A method for selecting spectra from a spectra set list
- `s = msmsWorkspace,property = character`: A method for selecting spectra from an msmsWorkspace

Author(s)

stravsmi

---

setData — *Set* RmbSpectrum2 *data from data.frame*

Description

Sets all slots which are present as columns in the given dataframe. Optionally cleans the object, i.e. empties slots not defined in the data frame.

Usage

```
## S4 method for signature 'RmbSpectrum2,data.frame'
setData(s, df, clean = TRUE)
```

Arguments

s	The RmbSpectrum2 object to modify
df	The data frame with new data
clean	TRUE if slots which aren't present as columns in the data frame should be cleared.

Value

The modified RmbSpectrum2.

Author(s)

stravsmi

---

smiles2mass — *Calculate the mass from a SMILES-String*

Description

Uses a SMILES-String to calculate the mass using rcdk-integrated functions.

Usage

```
smiles2mass(SMILES)
```

Arguments

SMILES	A String-object representing a SMILES

Value

The calculated mass of the given SMILES-Formula

Author(s)

Erik Mueller

Examples

```
## Not run:
smiles2mass("CC(=O)NC(C(O)1)C(O)C(OC(O2)C(O)C(OC(O3)C(O)C(O)C(O)C(CO)3)C(O)C(CO)2)C(CO)O1")

## End(Not run)
```

---

spectraCount — *Count MS2 spectra per compound*

Description

Counts the number of acquired spectra for a compound or multiple compounds

Usage

```
spectraCount(s)

## S4 method for signature 'RmbSpectraSet'
spectraCount(s)

## S4 method for signature 'RmbSpectraSetList'
spectraCount(s)

## S4 method for signature 'msmsWorkspace'
spectraCount(s)
```

Arguments

s	The object (`RmbSpectraSet`, `RmbSpectraSetList` or `msmsWorkspace`) to count the spectra in.

Value

For `RmbSpectraSet` objects, a single number counting the spectra in that object. For `RmbSpectraSetList` or `msmsWorkspace`, a vector with spectra counts for all compounds (`RmbSpectraSets`) in the object.

Methods (by class)

- `RmbSpectraSet`: Counts the number of acquired spectra for an RmbSpectraSet
- `RmbSpectraSetList`: Counts the number of acquired spectra for an RmbSpectraSetList
- `msmsWorkspace`: Counts the number of acquired spectra for an msmsWorkSpace

Author(s)

stravsmi

`to.limits.rcdk` *Convert formula to Rcdk limits*

Description

Converts a molecular formula e.g. C15H20 into an upper limit appropriate for use with Rcdk's `generate.formula` function's `element` argument.

Usage

```
to.limits.rcdk(formula)
```

Arguments

`formula`	A molecular formula in string or list representation (`"C6H6"` or `list(C=6,H=6)`).

Details

This helper function is used to make the upper limits for `generate.formula` when finding subformulas to match to a MS2 fragment peak.

Value

An array in the form `c( c("C", "0", "12"), c("H", "0", "12"))` (for input of "C12H12").

Author(s)

Michael Stravs

See Also

`generate.formula`, `add.formula`

Examples

```
#
to.limits.rcdk("C6H6")
to.limits.rcdk(add.formula("C6H12O6", "H"))
```

`toMassbank` *Write MassBank record into character array*

Description

Writes a MassBank record in list format to a text array.

Usage

```
toMassbank(mbdata)
```

Arguments

`mbdata`	A MassBank record in list format.

Details

The function is a general conversion tool for the MassBank format; i.e. the field names are not fixed. `mbdata` must be a named list, and the entries can be as follows:

- A single text line:
  `'CH$EXACT_MASS' = '329.1023'`
  is written as
  `CH$EXACT_MASS: 329.1023`
- A character array:
  `'CH$NAME' = c('2-Aminobenzimidazole', '1H-Benzimidazol-2-amine')`
  is written as
  `CH$NAME: 2-Aminobenzimidazole`
  `CH$NAME: 1H-Benzimidazol-2-amine`
- A named list of strings:
  `'CH$LINK' = list('CHEBI' = "27822", "KEGG" = "C10901")`
  is written as
  `CH$LINK: CHEBI 27822`
  `CH$LINK: KEGG C10901`
- A data frame (e.g. the peak table) is written as specified in the MassBank record format (Section 2.6.3): the column names are used as headers for the first line, all data rows are printed space-separated.

Value

The result is a text array, which is ready to be written to the disk as a file.

Note

The function iterates over the list item names. **This means that duplicate entries in `mbdata` are (partially) discarded!** The correct way to add them is by making a character array (as specified above): Instead of `'CH$NAME' = 'bla', 'CH$NAME' = 'blub'` specify `'CH$NAME' = c('bla','blub')`.

Author(s)

Michael Stravs

References

MassBank record format: http://www.massbank.jp/manuals/MassBankRecord_en.pdf

See Also

compileRecord, mbWorkflow

Examples

```
## Not run:
# Read just the compound info skeleton from the Internet for some compound ID
id <- 35
mbdata <- gatherData(id)
#' # Export the mbdata blocks to line arrays
# (there is no spectrum information, just the compound info...)
mbtext <- toMassbank(mbdata)

## End(Not run)
```

---

toRMB — *Conversion of XCMS-pseudospectra into RMassBank-spectra*

Description

Converts a pseudospectrum extracted from XCMS using CAMERA into the msmsWorkspace(at)spectrum-format that RMassBank uses

Usage

```
toRMB(msmsXCMSspecs, cpdID, mode, MS1spec)
```

Arguments

msmsXCMSspecs	The compoundID of the compound that has been used for the peaklist
cpdID	The compound ID of the substance of the given spectrum
mode	The ionization mode that has been used for the spectrum
MS1spec	The MS1-spectrum from XCMS, which can be optionally supplied

Value

One list element of the (at)specs-entry from an msmsWorkspace

Author(s)

Erik Mueller

See Also

msmsWorkspace-class

Examples

```
## Not run:
XCMSpspectra <- findmsmsHRperxcms.direct("Glucolesquerellin_2184_1.mzdata", 2184)
     wspecs <- toRMB(XCMSpspectra)

## End(Not run)
```

---

updateSettings *Update settings to current version*

Description

Checks if all necessary fields are present in the current settings and fills in default values from the RmbDefaultSettings if required.

Usage

```
updateSettings(settings, warn = TRUE)
```

Arguments

settings	The set of settings to check and update.
warn	Whether to update parameters quietly (FALSE) or to notify the user of the changed parameters (TRUE, default.) This serves to make the user aware that standard parameters are filled in!

Value

The updated set of settings.

Note

Important: There is a change in behaviour of RMassBank in certain cases when filterSettings is not present in the old settings! The default pre-recalibration cutoff from RmbDefaultSettings is 10000. Formerly the pre-recalibration cutoff was set to be 10000 for positive spectra but 0 for negative spectra.

Updating the settings files is preferred to using the updateSettings function.

Author(s)

Stravs MA, Eawag <michael.stravs@eawag.ch>

Examples

```
## Not run:
w@settings <- updateSettings(w@settings)

## End(Not run)
```

`validate` *Validate MassBank records with a set of Unit tests*

Description

Validates a plain text MassBank record, or recursively all records within a directory. The Unit Tests to be used are installed in RMassBank/inst/validationTests and currently include checks for NAs, peaks versus precursor, precursor mz, precursor type, SMILES vs exact mass, total intensities and title versus type. The validation report is saved as "report.html" in the working directory.

Usage

```
validate(path, simple = TRUE)
```

Arguments

`path`	The filepath to a single record, or a directory to search recursively
`simple`	If TRUE the function creates a simpler form of the RUnit .html report, better readable for humans. If FALSE it returns the unchanged RUnit report.

Examples

```
## Not run:
validate("/tmp/MassBank/OpenData/record/")

## End(Not run)
```

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