

Package: DIALignR (via r-universe)

June 30, 2024

Type Package

Title Dynamic Programming Based Alignment of MS2 Chromatograms

Version 2.13.0

Description To obtain unbiased proteome coverage from a biological sample, mass-spectrometer is operated in Data Independent Acquisition (DIA) mode. Alignment of these DIA runs establishes consistency and less missing values in complete data-matrix. This package implements dynamic programming with affine gap penalty based approach for pair-wise alignment of analytes. A hybrid approach of global alignment (through MS2 features) and local alignment (with MS2 chromatograms) is implemented in this tool.

License GPL-3

Encoding UTF-8

LazyData false

RoxygenNote 7.2.1

biocViews MassSpectrometry, Metabolomics, Proteomics, Alignment, Software

Depends methods, stats, R (>= 4.0)

Imports zoo (>= 1.8-3), data.table, magrittr, dplyr, tidyr, rlang, mzR (>= 2.18), signal, bit64, reticulate, ggplot2, RSQLite, DBI, ape, phangorn, pracma, RMSNumpress, Rcpp

Suggests knitr, akima, lattice, scales, gridExtra, latticeExtra, rmarkdown, BiocStyle, BiocParallel, testthat (>= 2.1.0)

VignetteBuilder knitr

BugReports <https://github.com/shubham1637/DIALignR/issues>

LinkingTo Rcpp, RcppEigen

SystemRequirements C++14

Repository <https://bioc.r-universe.dev>

RemoteUrl <https://github.com/bioc/DIALignR>

RemoteRef HEAD

RemoteSha 782a3f0c764ede682ec481d515a50128245ae107

Contents

AffineAlignObj-class	3
AffineAlignObjLight-class	4
AffineAlignObjMedium-class	4
alignChromatogramsCpp	5
AlignObj-class	7
alignObj_DIAAlignR	8
alignTargetedRuns	9
alignToRoot4	10
areaIntegrator	11
as.list,AffineAlignObj-method	12
as.list,AffineAlignObjLight-method	13
as.list,AffineAlignObjMedium-method	13
as.list,AlignObj-method	14
childXICs	15
constrainSimCpp	16
createMZML	17
createSqMass	18
DIAAlignR	19
doAffineAlignmentCpp	19
doAlignmentCpp	21
getAlignedTimes	22
getAlignedTimesCpp	24
getAlignedTimesFast	26
getAlignObj	27
getAlignObjs	29
getBaseGapPenaltyCpp	30
getChildXICpp	31
getChildXICs	33
getChromatogramIndices	35
getChromSimMatCpp	36
getFeatures	38
getGlobalAlignMaskCpp	39
getGlobalAlignment	40
getMultipeptide	41
getMZMLpointers	42
getNativeIDs	43
getPeptideScores	44
getPrecursorByID	45
getPrecursorIndices	46
getPrecursors	47
getRefExpFeatureMap	49
getRefRun	50
getRTdf	51
getRunNames	52
getSeqSimMatCpp	53
getTransitions	54

getXICs	55
getXICs4AlignObj	56
get_ropenms	57
imputeChromatogram	58
mapIdxToTime	59
masterXICs_DIAalignR	60
mstAlignRuns	61
mstScript1	62
mstScript2	63
multipeptide_DIAalignR	64
oswFiles_DIAalignR	65
otherChildXICpp	66
paramsDIAalignR	67
plotAlignedAnalytes	70
plotAlignmentPath	71
plotAnalyteXICs	71
plotXICgroup	73
progAlignRuns	74
progComb3	75
progSplit2	76
progSplit4	77
progTree1	78
recalculateIntensity	79
reduceXICs	80
script1	81
script2	82
sgolayCpp	83
smoothSingleXIC	84
smoothXICs	85
splineFillCpp	86
trimXICs	87
updateFileInfo	88
XIC_QFNNTDIVLLEDFQK_3_DIAalignR	89

Index	90
--------------	-----------

AffineAlignObj-class *An S4 object for class AffineAlignObj*

Description

s is a point-wise similarity matrix between *signalA* and *signalB*. Intermediate matrices *M*,*A*,*B* are calculated from *s* for affine-alignment. Each cell of the Traceback matrix has coordinate of its parent cell. *path* matrix is a binary matrix with ones indicating path of maximum cumulative score. *GapOpen* and *GapExten* are gap-opening and gap-extension penalties used by affine alignment algorithm. *indexA_aligned* and *indexB_aligned* are aligned indices of *signalA* and *SignalB*. The cumulative alignment score is in *score* vector.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-14

See Also

[doAffineAlignmentCpp](#)

AffineAlignObjLight-class

An S4 object for class AffineAlignObjLight It only contains aligned indices.

Description

indexA_aligned and indexB_aligned are aligned indices of signalA and SignalB. The cumulative alignment score is in score vector.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-14

See Also

[doAffineAlignmentCpp](#)

AffineAlignObjMedium-class

An S4 object for class AffineAlignObjMedium. It only contains similarity matrix and aligned indices.

Description

s is a point-wise similarity matrix between signalA and signalB. path matrix is a binary matrix with ones indicating path of maximum cumulative score. GapOpen and GapExten are gap-opening and gap-extension penalties used by affine alignment algorithm. indexA_aligned and indexB_aligned are aligned indices of signalA and SignalB. The cumulative alignment score is in score vector.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-14

See Also

[doAffineAlignmentCpp](#)

alignChromatogramsCpp *Aligns MS2 extracted-ion chromatograms(XICs) pair.*

Description

Aligns MS2 extracted-ion chromatograms(XICs) pair.

Usage

```
alignChromatogramsCpp(  
  l1,  
  l2,  
  alignType,  
  tA,  
  tB,  
  normalization,  
  simType,  
  B1p = 0,  
  B2p = 0,  
  noBeef = 0L,  
  goFactor = 0.125,  
  geFactor = 40,  
  cosAngleThresh = 0.3,  
  OverlapAlignment = TRUE,  
  dotProdThresh = 0.96,  
  gapQuantile = 0.5,  
  kerLen = 9L,  
  hardConstrain = FALSE,  
  samples4gradient = 100,  
  objType = "heavy"  
)
```

Arguments

- l1 (list) A list of numeric vectors. l1 and l2 should have same length.
- l2 (list) A list of numeric vectors. l1 and l2 should have same length.

alignType	(char) A character string. Available alignment methods are "global", "local" and "hybrid".
tA	(numeric) A numeric vector. This vector has equally spaced timepoints of XIC A.
tB	(numeric) A numeric vector. This vector has equally spaced timepoints of XIC B.
normalization	(char) A character string. Normalization must be selected from (L2, mean or none).
simType	(char) A character string. Similarity type must be selected from (dotProductMasked, dotProduct, cosineAngle, cosine2Angle, euclideanDist, covariance, correlation, crossCorrelation). Mask = $s > \text{quantile}(s, \text{dotProdThresh})$ AllowDotProd = $[\text{Mask} \times \text{cosine2Angle} + (1 - \text{Mask})] > \text{cosAngleThresh}$ $s_{\text{new}} = s \times \text{AllowDotProd}$
B1p	(numeric) Timepoint mapped by global fit for tA[1].
B2p	(numeric) Timepoint mapped by global fit for tA[length(tA)].
noBeef	(integer) It defines the distance from the global fit, upto which no penalization is performed. The window length = $2 * \text{noBeef}$.
goFactor	(numeric) Penalty for introducing first gap in alignment. This value is multiplied by base gap-penalty.
geFactor	(numeric) Penalty for introducing subsequent gaps in alignment. This value is multiplied by base gap-penalty.
cosAngleThresh	(numeric) In simType = dotProductMasked mode, angular similarity should be higher than cosAngleThresh otherwise similarity is forced to zero.
OverlapAlignment	(logical) An input for alignment with free end-gaps. False: Global alignment, True: overlap alignment.
dotProdThresh	(numeric) In simType = dotProductMasked mode, values in similarity matrix higher than dotProdThresh quantile are checked for angular similarity.
gapQuantile	(numeric) Must be between 0 and 1. This is used to calculate base gap-penalty from similarity distribution.
kerLen	(integer) In simType = crossCorrelation, length of the kernel used to sum similarity score. Must be an odd number.
hardConstrain	(logical) if false; indices farther from noBeef distance are filled with distance from linear fit line.
samples4gradient	(numeric) This parameter modulates penalization of masked indices.
objType	(char) A character string. Must be either light, medium or heavy.

Value

affineAlignObj (S4class) A S4class object from C++ AffineAlignObj struct.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-08

Examples

```
data(XIC_QFNNTDIVLLEDFQK_3_DIAAlignR, package="DIAAlignR")
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAAlignR
data(oswFiles_DIAAlignR, package="DIAAlignR")
oswFiles <- oswFiles_DIAAlignR
XICs.ref <- XICs[["hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt"]][["4618"]]
XICs.exp <- XICs[["hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt"]][["4618"]]
tVec.ref <- XICs.ref[[1]][["time"]] # Extracting time component
tVec.exp <- XICs.exp[[1]][["time"]] # Extracting time component
B1p <- 4964.752
B2p <- 5565.462
noBeef <- 77.82315/3.414
l1 <- lapply(XICs.ref, `[`, 2)
l2 <- lapply(XICs.exp, `[`, 2)
AlignObj <- alignChromatogramsCpp(l1, l2, alignType = "hybrid", tA = tVec.ref, tB = tVec.exp,
normalization = "mean", simType = "dotProductMasked", B1p = B1p, B2p = B2p, noBeef = noBeef,
goFactor = 0.125, geFactor = 40, cosAngleThresh = 0.3, OverlapAlignment = TRUE,
dotProdThresh = 0.96, gapQuantile = 0.5, hardConstrain = FALSE, samples4gradient = 100,
objType = "light")
```

AlignObj-class

An S4 object for class AlignObj

Description

s is a point-wise similarity matrix between signalA and signalB. Intermediate matrices M is calculated from s for alignment. Each cell of the Traceback matrix has coordinate of its parent cell. path matrix is a binary matrix with ones indicating path of maximum cumulative score. GapOpen and GapExten are gap-opening and gap-extension penalties used by alignment algorithm. They must be the same. indexA_aligned and indexB_aligned are aligned indices of signalA and SignalB. The cumulative alignment score is in score vector.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>
ORCID: 0000-0003-3500-8152
License: (c) Author (2019) + GPL-3 Date: 2019-12-14

See Also

[doAlignmentCpp](#)

alignObj_DIAAlignR *Alignment object of a peptide.*

Description

Aligned XICs of peptide (ID = 4618) 14299_QFNNTDIVLLEDFQK/3 across two SWATH runs:

run1 : hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt.chrom.mzML

run2 : hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt.chrom.mzML

Usage

```
alignObj_DIAAlignR
```

Format

A S4 object of 16 slots:

s similarity score matrix.

M Match or Mismatch matrix, residues of A and B are aligned without a gap. $M(i,j)$ = Best score upto (i,j) given A_i is aligned to B_j .

A Insert in sequence A, residue in A is aligned to gap in B. $A(i,j)$ is the best score given that A_i is aligned to a gap in B.

B Insert in sequence B, residue in B is aligned to gap in A. $B(i,j)$ is the best score given that B_j is aligned to a gap in A.

Traceback Traceback matrices store source matrix name and direction as matrices are filled with dynamic programming.

path Path matrix would represent alignment path through similarity matrix as binary-hot encoding.

signalA_len Number of data-points in signal A.

signalB_len Number of data-points in signal B.

GapOpen Penalty for Gap opening. For n consecutive gaps: $\text{Penalty} = \text{GapOpen} + (n-1)*\text{GapExten}$.

GapExten Penalty for Gap extension. For n consecutive gaps: $\text{Penalty} = \text{GapOpen} + (n-1)*\text{GapExten}$.

FreeEndGaps True for Overlap alignment.

indexA_aligned Aligned signalA indices after affine alignment.

indexB_aligned Aligned signalB indices after affine alignment.

score Cumulative score along the aligned path.

simScore_forw Not needed, will be removed.

nGaps Total number of gaps in the alignment path.

Source

C++ code is explained at [DIAAlign namespace](#). File test_GenerateData.R has [source code](#) to generate the example data.

alignTargetedRuns	<i>Outputs intensities for each analyte from aligned Targeted-MS runs</i>
-------------------	---

Description

This function expects osw and xics directories at dataPath. It first reads osw files and fetches chromatogram indices for each analyte. It then align XICs of its reference XICs. Best peak, which has lowest m-score, about the aligned retention time is picked for quantification.

Usage

```
alignTargetedRuns(  
  dataPath,  
  outFile = "DIAAlignR",  
  params = paramsDIAAlignR(),  
  oswMerged = TRUE,  
  scoreFile = NULL,  
  runs = NULL,  
  peps = NULL,  
  refRun = NULL,  
  applyFun = lapply,  
  saveAlignedPeaks = FALSE  
)
```

Arguments

dataPath	(string) path to xics and osw directory.
outFile	(string) name of the output file.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
scoreFile	(string) path to the peptide score file, needed when oswMerged is FALSE.
runs	(string) names of xics file without extension.
peps	(integer) ids of peptides to be aligned. If NULL, align all peptides.
refRun	(string) reference for alignment. If no run is provided, m-score is used to select reference run.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.
saveAlignedPeaks	(logical) Save a mapping table to track aligned feature ids against reference feature id

Value

An output table with following columns: precursor, run, intensity, RT, leftWidth, rightWidth, peak_group_rank, m_score, alignment_rank, peptide_id, sequence, charge, group_label.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-14

References

Gupta S, Ahadi S, Zhou W, Röst H. "DIAAlignR Provides Precise Retention Time Alignment Across Distant Runs in DIA and Targeted Proteomics." *Mol Cell Proteomics*. 2019 Apr;18(4):806-817. doi: <https://doi.org/10.1074/mcp.TIR118.001132> Epub 2019 Jan 31.

See Also

[getRunNames](#), [getFeatures](#), [setAlignmentRank](#), [getMultipeptide](#)

Examples

```
params <- paramsDIAAlignR()
params[["context"]] <- "experiment-wide"
dataPath <- system.file("extdata", package = "DIAAlignR")
BiocParallel::register(BiocParallel::MulticoreParam(workers = 4, progressbar = TRUE))
alignTargetedRuns(dataPath, outFile = "testDIAAlignR", params = params, applyFun = BiocParallel::bplapply)
```

alignToRoot4

Step 4 for progressive alignment

Description

This is needed when leaves of the tree are directly aligned to the root

Usage

```
alignToRoot4(
  dataPath,
  params,
  outFile = "DIAAlignR",
  oswMerged = TRUE,
  applyFun = lapply
)
```

Arguments

dataPath	(string) path to xics and osw directory.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
outFile	(string) name of the output file.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-09-25

See Also

[progAlignRuns](#)

areaIntegrator	<i>Calculates area between signal-boundaries.</i>
----------------	---

Description

This function sums all the intensities between left-index and right-index.

Usage

```
areaIntegrator(  
  l1,  
  l2,  
  left,  
  right,  
  integrationType,  
  baselineType,  
  fitEMG,  
  baseSubtraction,  
  kernelLen = 0L,  
  polyOrd = 3L  
)
```

Arguments

l1	(list) A list of time vectors.
l2	(list) A list of intensity vectors.
left	(numeric) left boundary of the peak.
right	(numeric) right boundary of the peak.
integrationType	(string) method to compute the area of a peak contained in XICs. Must be from "intensity_sum", "trapezoid", "simpson".
baselineType	(string) method to estimate the background of a peak contained in XICs. Must be from "base_to_base", "vertical_division_min", "vertical_division_max".
fitEMG	(logical) enable/disable exponentially modified gaussian peak model fitting.

baseSubtraction (logical) TRUE: remove background from peak signal using estimated noise levels.

kernellLen (integer) length of filter. Must be an odd number.

polyOrd (integer) TRUE: remove background from peak signal using estimated noise levels.

Value

area (numeric).

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-08

Examples

```
data("XIC_QFNNTDIVLLEDFQK_3_DIAAlignR", package = "DIAAlignR")
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAAlignR[["hroest_K120809_Strep0%PlasmaBioRep12_R04_SW_filt"]][["4618"]]
l1 <- lapply(XICs, `[[`, 1) # time
l2 <- lapply(XICs, `[[`, 2) # intensity
areaIntegrator(l1, l2, left = 5203.7, right = 5268.5, "intensity_sum", "base_to_base", FALSE, TRUE)
# 66.10481 69.39996 46.53095 16.34266 13.13564 13.42331
areaIntegrator(l1, l2, left = 5203.7, right = 5268.5, kernellLen = 9L, "intensity_sum", "base_to_base", FALSE, TRUE)
# 65.01449 71.74432 52.73518 23.84420 17.61869 16.48190
```

as.list,AffineAlignObj-method

Converts instances of class AffineAlignObj into list

Description

Converts instances of class AffineAlignObj into list

Usage

```
## S4 method for signature 'AffineAlignObj'
as.list(x)
```

Arguments

x An object of class AffineAlignObj.

Value

list

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2020-03-31

as.list,AffineAlignObjLight-method

Converts instances of class AffineAlignObjLight into list

Description

Converts instances of class AffineAlignObjLight into list

Usage

```
## S4 method for signature 'AffineAlignObjLight'  
as.list(x)
```

Arguments

x An object of class AffineAlignObjLight

Value

list

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2020-03-31

as.list,AffineAlignObjMedium-method

Converts instances of class AffineAlignObjMedium into list

Description

Converts instances of class AffineAlignObjMedium into list

Usage

```
## S4 method for signature 'AffineAlignObjMedium'  
as.list(x)
```

Arguments

x An object of class AffineAlignObjMedium

Value

list

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2020-03-31

as.list,AlignObj-method

Converts instances of class AlignObj into list

Description

Converts instances of class AlignObj into list

Usage

```
## S4 method for signature 'AlignObj'  
as.list(x)
```

Arguments

x An object of class AlignObj

Value

list

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2020-03-31

`childXICs`*Get child chromatograms from parents*

Description

Get child chromatograms from parents

Usage

```
childXICs(  
  XICs.ref,  
  XICs.eXp,  
  alignedIndices,  
  method = "spline",  
  polyOrd = 4,  
  kernelLen = 9,  
  splineMethod = "fmm",  
  wRef = 0.5,  
  mergeStrategy = "avg",  
  keepFlanks = TRUE  
)
```

Arguments

<code>XICs.ref</code>	(list of data-frames) extracted ion chromatograms from reference run.
<code>XICs.eXp</code>	(list of data-frames) extracted ion chromatograms from experiment run.
<code>alignedIndices</code>	(data-frame) must have two columns "indexAligned.ref" and "indexAligned.eXp".
<code>method</code>	(string) must be either "spline", "sgolay" or "linear".
<code>polyOrd</code>	(integer) must be less than kernelLen.
<code>kernelLen</code>	(integer) must be an odd integer.
<code>splineMethod</code>	(string) must be either "fmm" or "natural".
<code>wRef</code>	(numeric) Weight of the reference XIC. Must be between 0 and 1.
<code>mergeStrategy</code>	(string) must be either ref, avg, refStart or refEnd.
<code>keepFlanks</code>	(logical) TRUE: Flanking chromatogram is not removed.

Value

(list) the first element is a list of chromatograms. The second element is aligned parent time-vectors.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-05-23

See Also

[childXIC](#), [mergeXIC](#)

Examples

```
data(XIC_QFNNTDIVLLEDFQK_3_DIAalignR, package="DIAalignR")
data(alignObj_DIAalignR, package="DIAalignR")
XICs.ref <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR[["hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt"]][["4618"]]
XICs.exp <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR[["hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt"]][["4618"]]
alignedIndices <- cbind(alignObj_DIAalignR@indexA_aligned, alignObj_DIAalignR@indexB_aligned)
colnames(alignedIndices) <- c("indexAligned.ref", "indexAligned.exp")
alignedIndices[, 1:2][alignedIndices[, 1:2] == 0] <- NA_integer_
newXICs <- childXICs(XICs.ref, XICs.exp, alignedIndices)[[1]]
plotXICgroup(XICs.ref)
plotXICgroup(newXICs)
```

constrainSimCpp

Constrain similarity matrix with a mask

Description

Constrain similarity matrix with a mask

Usage

```
constrainSimCpp(sim, MASK, samples4gradient = 100)
```

Arguments

`sim` (matrix) A numeric matrix. Input similarity matrix.

`MASK` (matrix) A numeric matrix. Masked indices have non-zero values.

`samples4gradient` (numeric) This parameter modulates penalization of masked indices.

Value

`s_new` (matrix) A constrained similarity matrix.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-08

Examples

```
sim <- matrix(c(-2, 10, -2, -2, -2, -2, 10, -2, 10, -2, -2, -2, -2, -2, 10, 10, -2, -2, -2),
  4, 5, byrow = FALSE)
MASK <- matrix(c(0.000, 0.000, 0.707, 1.414, 0.000, 0.000, 0.000, 0.707, 0.707, 0.000,
  0.000, 0.000, 1.414, 0.707, 0, 0, 2.121, 1.414, 0, 0), 4, 5, byrow = FALSE)
constrainSimCpp(sim, MASK, 10)
matrix(c(-2, 10, -3.414, -4.828, -2, -2, 10, -3.414, 8.586, -2, -2, -2, -4.828,
  -3.414, -2, 10, 5.758, -4.828, -2, -2), 4, 5, byrow = FALSE)
```

createMZML

Create an mzML file

Description

Writes an mzML file having chromatograms and their native IDs.

Usage

```
createMZML(ropenms, filename, XICs, transitionIDs)
```

Arguments

ropenms (pyopenms module) get this python module through `get_ropenms()`.
filename (string) name of the mzML file to be written. Extension should be `.chrom.mzML`.
XICs (list of list of data-frames) list of extracted ion chromatograms of all precursors.
transitionIDs (list of integer) length must be the same as of XICs.

Value

(None)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>
ORCID: 0000-0003-3500-8152
License: (c) Author (2020) + GPL-3 Date: 2020-06-06

See Also

[get_ropenms](#), [addXIC](#)

Examples

```

dataPath <- system.file("extdata", package = "DIAAlignR")
filename <- paste0(dataPath, "/xics/hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt.chrom.mzML")
data(XIC_QFNNTDIVLLEDFQK_3_DIAAlignR)
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAAlignR[["hroest_K120808_Strep10%PlasmaBiolRepl1_R03_SW_filt"]]
nativeIds <- list(27706:27711)
## Not run:
ropenms <- get_ropenms(condaEnv = "envName")
createMZML(ropenms, "testfile.chrom.mzML", XICs, nativeIds)
mzR::chromatogramHeader(mzR::openMSfile("testfile.chrom.mzML", backend = "pwiz"))
file.remove("testfile.chrom.mzML")

## End(Not run)

```

createSqMass

Create an sqMass file

Description

Writes a sqMass file having chromatograms and their native IDs.

Usage

```
createSqMass(filename, XICs, transitionIDs, lossy)
```

Arguments

filename	(string) name of the mzML file to be written. Extension should be .chrom.sqMass.
XICs	(list of list of data-frames) list of extracted ion chromatograms of all precursors.
transitionIDs	(list of integer) length must be the same as of XICs.
lossy	(logical) if TRUE, time and intensity are lossy-compressed.

Details

- compression is one of 0 = no, 1 = zlib, 2 = np-linear, 3 = np-slof, 4 = np-pic, 5 = np-linear + zlib, 6 = np-slof + zlib, 7 = np-pic + zlib
- data_type is one of 0 = mz, 1 = int, 2 = rt
- data contains the raw (blob) data for a single data array

Value

(None)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-01-16

See Also

[createMZML](#), [blobXICs](#)

Examples

```
data(XIC_QFNNTDIVLLEDFQK_3_DIAAlignR)
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAAlignR[["hroest_K120808_Strep10%PlasmaBiolRep11_R03_SW_filt"]]
XICs <- list(XICs[[1]], XICs[[1]])
nativeIds <- list(27706:27711, 1:6)
sqName <- "testfile.chrom.sqlMass"
## Not run:
createSqMass(sqName, XICs, nativeIds, TRUE)
con <- DBI::dbConnect(RSQLite::SQLite(), dbname = sqName)
XIC_group <- extractXIC_group2(con, 0:5)
DBI::dbDisconnect(con)
file.remove(sqName)

## End(Not run)
```

DIAAlignR

DIAAlignR

Description

This package implements dynamic programming with affine gap penalty to find a highest-scoring scoring path. A hybrid approach of global alignment through MS2 features and local alignment with MS2 chromatograms is implemented in this tool.

Author(s)

Shubham Gupta, Hannes Rost

`doAffineAlignmentCpp` *Perform affine global and overlap alignment on a similarity matrix*

Description

Perform affine global and overlap alignment on a similarity matrix

Usage

```
doAffineAlignmentCpp(sim, go, ge, OverlapAlignment)
```

Arguments

`sim` (NumericMatrix) A numeric matrix with similarity values of two sequences or signals.

`go` (numeric) Penalty for introducing first gap in alignment.

`ge` (numeric) Penalty for introducing subsequent gaps in alignment.

`OverlapAlignment` (logical) An input for alignment with free end-gaps. False: Global alignment, True: overlap alignment.

Value

`affineAlignObj` (S4class) An object from C++ class of `AffineAlignObj`.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-08

Examples

```
# Get sequence similarity of two DNA strings
Match=10; MisMatch=-2
seq1 = "GCAT"; seq2 = "CAGTG"
s <- getSeqSimMatCpp(seq1, seq2, Match, MisMatch)
objAffine_Global <- doAffineAlignmentCpp(s, 22, 7, FALSE)
slot(objAffine_Global, "score") # -2 -4 -6 4 -18
objAffine_Olap <- doAffineAlignmentCpp(s, 22, 7, TRUE)
slot(objAffine_Olap, "score") # 0 10 20 18 18 18

Match=10; MisMatch=-2
seq1 = "CAT"; seq2 = "CAGTG"
s <- getSeqSimMatCpp(seq1, seq2, Match, MisMatch)
objAffine_Global <- doAffineAlignmentCpp(s, 22, 7, FALSE)
slot(objAffine_Global, "score") # 10 20 -2 -9 -11
objAffine_Olap <- doAffineAlignmentCpp(s, 22, 7, TRUE)
slot(objAffine_Olap, "score") # 10 20 18 18 18

Match=10; MisMatch=-2
seq1 = "CA"; seq2 = "AG"
s <- getSeqSimMatCpp(seq1, seq2, Match, MisMatch)
objAffine_Global <- doAffineAlignmentCpp(s, 22, 7, FALSE)
slot(objAffine_Global, "simScore_forw") # -4
```

doAlignmentCpp	<i>Perform non-affine global and overlap alignment on a similarity matrix</i>
----------------	---

Description

Perform non-affine global and overlap alignment on a similarity matrix

Usage

```
doAlignmentCpp(sim, gap, OverlapAlignment)
```

Arguments

sim	(NumericMatrix) A numeric matrix with similarity values of two sequences or signals.
gap	(double) Penalty for introducing gaps in alignment.
OverlapAlignment	(logical) An input for alignment with free end-gaps. False: Global alignment, True: overlap alignment.

Value

AlignObj (S4class) An object from C++ class of AlignObj.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-08

Examples

```
# Get sequence similarity of two DNA strings
Match=10; MisMatch=-2
seq1 = "GCAT"; seq2 = "CAGTG"
s <- getSeqSimMatCpp(seq1, seq2, Match, MisMatch)
obj_Global <- doAlignmentCpp(s, 22, FALSE)
slot(obj_Global, "score") # -2 -4 -6 4 -18
obj_Olap <- doAlignmentCpp(s, 22, TRUE)
slot(obj_Olap, "score") # 0 10 20 18 18 18

Match=1; MisMatch=-1
seq1 = "TTTC"; seq2 = "TGC"
s <- getSeqSimMatCpp(seq1, seq2, Match, MisMatch)
obj_Global <- doAlignmentCpp(s, 2, FALSE)
slot(obj_Global, "optionalPaths")
matrix(data = c(1,1,1,1,1,1,1,1,1,2,1,2,1,3,3,1,1,3,6,3), nrow = 5, ncol =4, byrow = TRUE)
slot(obj_Global, "M_forw")
matrix(data = c(0,-2,-4,-6,-2,-7,-22,-45,-4,-20,-72,-184,-6,-41,-178,-547,-8,-72,-366,-1274),
  nrow = 5, ncol =4, byrow = TRUE)
```

getAlignedTimes *Get aligned Retention times.*

Description

This function aligns XICs of reference and experiment runs. It produces aligned retention times between reference run and experiment run.

Usage

```
getAlignedTimes(
  XICs.ref,
  XICs.exp,
  globalFit,
  alignType,
  adaptiveRT,
  normalization,
  simMeasure,
  goFactor,
  geFactor,
  cosAngleThresh,
  OverlapAlignment,
  dotProdThresh,
  gapQuantile,
  kerLen,
  hardConstrain,
  samples4gradient,
  objType = "light"
)
```

Arguments

XICs.ref	List of extracted ion chromatograms from reference run.
XICs.exp	List of extracted ion chromatograms from experiment run.
globalFit	Linear or loess fit object between reference and experiment run.
alignType	Available alignment methods are "global", "local" and "hybrid".
adaptiveRT	(numeric) Similarity matrix is not penalized within adaptive RT.
normalization	(character) Must be selected from "mean", "l2".
simMeasure	(string) Must be selected from dotProduct, cosineAngle, crossCorrelation, cosine2Angle, dotProductMasked, euclideanDist, covariance and correlation.
goFactor	(numeric) Penalty for introducing first gap in alignment. This value is multiplied by base gap-penalty.
geFactor	(numeric) Penalty for introducing subsequent gaps in alignment. This value is multiplied by base gap-penalty.

cosAngleThresh	(numeric) In simType = dotProductMasked mode, angular similarity should be higher than cosAngleThresh otherwise similarity is forced to zero.
OverlapAlignment	(logical) An input for alignment with free end-gaps. False: Global alignment, True: overlap alignment.
dotProdThresh	(numeric) In simType = dotProductMasked mode, values in similarity matrix higher than dotProdThresh quantile are checked for angular similarity.
gapQuantile	(numeric) Must be between 0 and 1. This is used to calculate base gap-penalty from similarity distribution.
kerLen	(integer) In simType = crossCorrelation, length of the kernel used to sum similarity score. Must be an odd number.
hardConstrain	(logical) If FALSE; indices farther from noBeef distance are filled with distance from linear fit line.
samples4gradient	(numeric) This parameter modulates penalization of masked indices.
objType	(char) Must be selected from light, medium and heavy.

Value

(list) the first element corresponds to the aligned reference time, the second element is the aligned experiment time.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>
 ORCID: 0000-0003-3500-8152
 License: (c) Author (2019) + GPL-3 Date: 2019-12-13

See Also

[alignChromatogramsCpp](#), [getAlignObj](#)

Examples

```
data(XIC_QFNNTDIVLLEDFQK_3_DIAalignR, package="DIAalignR")
data(oswFiles_DIAalignR, package="DIAalignR")
run1 <- "hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt"
run2 <- "hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt"
XICs.ref <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR[[run1]][["4618"]]
XICs.eXp <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR[[run2]][["4618"]]
RUNS_RT <- getRTdf(oswFiles_DIAalignR, ref = "run1", eXp = "run2", maxFdrGlobal = 0.05)
globalFit <- loess(RT.eXp ~ RT.ref, data = RUNS_RT, span = 0.1, control=loess.control(surface="direct"))
adaptiveRT <- 77.82315 #3.5*globalFit$s
getAlignedTimes(XICs.ref, XICs.eXp, globalFit, alignType = "hybrid",
  adaptiveRT = adaptiveRT, normalization = "mean",
  simMeasure = "dotProductMasked", goFactor = 0.125, geFactor = 40, cosAngleThresh = 0.3,
  OverlapAlignment = TRUE, dotProdThresh = 0.96, gapQuantile = 0.5, kerLen = 9L, hardConstrain = FALSE,
  samples4gradient = 100)
```

getAlignedTimesCpp *Get aligned indices from MS2 extracted-ion chromatograms(XICs) pair.*

Description

Get aligned indices from MS2 extracted-ion chromatograms(XICs) pair.

Usage

```
getAlignedTimesCpp(
  l1,
  l2,
  kernelLen,
  polyOrd,
  alignType,
  adaptiveRT,
  normalization,
  simType,
  Bp,
  goFactor = 0.125,
  geFactor = 40,
  cosAngleThresh = 0.3,
  OverlapAlignment = TRUE,
  dotProdThresh = 0.96,
  gapQuantile = 0.5,
  kerLen = 9L,
  hardConstrain = FALSE,
  samples4gradient = 100
)
```

Arguments

l1	(list) A list of numeric matrix of two columns. l1 and l2 should have same length.
l2	(list) A list of numeric matrix of two columns. l1 and l2 should have same length.
kernelLen	(integer) length of filter. Must be an odd number.
polyOrd	(integer) TRUE: remove background from peak signal using estimated noise levels.
alignType	(char) A character string. Available alignment methods are "global", "local" and "hybrid".
adaptiveRT	(numeric) Similarity matrix is not penalized within adaptive RT.
normalization	(char) A character string. Normalization must be selected from (L2, mean or none).

simType	(char) A character string. Similarity type must be selected from (dotProductMasked, dotProduct, cosineAngle, cosine2Angle, euclideanDist, covariance, correlation, crossCorrelation). Mask = $s > \text{quantile}(s, \text{dotProdThresh})$ AllowDotProd = $[\text{Mask} \times \text{cosine2Angle} + (1 - \text{Mask})] > \text{cosAngleThresh}$ $s_{\text{new}} = s \times \text{AllowDotProd}$
Bp	(numeric) Timepoint mapped by global fit for tA.
goFactor	(numeric) Penalty for introducing first gap in alignment. This value is multiplied by base gap-penalty.
geFactor	(numeric) Penalty for introducing subsequent gaps in alignment. This value is multiplied by base gap-penalty.
cosAngleThresh	(numeric) In simType = dotProductMasked mode, angular similarity should be higher than cosAngleThresh otherwise similarity is forced to zero.
OverlapAlignment	(logical) An input for alignment with free end-gaps. False: Global alignment, True: overlap alignment.
dotProdThresh	(numeric) In simType = dotProductMasked mode, values in similarity matrix higher than dotProdThresh quantile are checked for angular similarity.
gapQuantile	(numeric) Must be between 0 and 1. This is used to calculate base gap-penalty from similarity distribution.
kerLen	(integer) In simType = crossCorrelation, length of the kernel used to sum similarity score. Must be an odd number.
hardConstrain	(logical) if false; indices farther from noBeef distance are filled with distance from linear fit line.
samples4gradient	(numeric) This parameter modulates penalization of masked indices.

Value

NumericMatrix Aligned indices of I1 and I2.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-08

Examples

```
data(XIC_QFNNTDIVLLEDFQK_3_DIAAlignR, package="DIAAlignR")
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAAlignR
XICs.ref <- lapply(XICs[["hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt"]][["4618"]], as.matrix)
XICs.exp <- lapply(XICs[["hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt"]][["4618"]], as.matrix)
Bp <- seq(4964.752, 5565.462, length.out = nrow(XICs.ref[[1]]))
time <- getAlignedTimesCpp(XICs.ref, XICs.exp, 11, 4, alignType = "hybrid", adaptiveRT = 77.82315,
  normalization = "mean", simType = "dotProductMasked", Bp = Bp,
  goFactor = 0.125, geFactor = 40, cosAngleThresh = 0.3, OverlapAlignment = TRUE,
  dotProdThresh = 0.96, gapQuantile = 0.5, hardConstrain = FALSE, samples4gradient = 100)
```

getAlignedTimesFast *Get aligned Retention times.*

Description

This function aligns XICs of reference and experiment runs. It produces aligned retention times between reference run and experiment run.

Usage

```
getAlignedTimesFast(XICs.ref, XICs.eXp, globalFit, adaptiveRT, params)
```

Arguments

XICs.ref	List of extracted ion chromatograms from reference run.
XICs.eXp	List of extracted ion chromatograms from experiment run.
globalFit	Linear or loess fit object between reference and experiment run.
adaptiveRT	(numeric) Similarity matrix is not penalized within adaptive RT.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.

Value

(matrix) the first column corresponds to the aligned reference time, the second column is the aligned experiment time.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-01-02

See Also

[alignChromatogramsCpp](#), [getAlignObj](#)

Examples

```
data(XIC_QFNNTDIVLLEDFQK_3_DIAAlignR, package="DIAAlignR")
data(oswFiles_DIAAlignR, package="DIAAlignR")
run1 <- "hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt"
run2 <- "hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt"
XICs.ref <- lapply(XIC_QFNNTDIVLLEDFQK_3_DIAAlignR[[run1]][["4618"]], as.matrix)
XICs.eXp <- lapply(XIC_QFNNTDIVLLEDFQK_3_DIAAlignR[[run2]][["4618"]], as.matrix)
params <- paramsDIAAlignR()
params[["globalAlignment"]] <- "linear"
globalFit <- getGlobalAlignment(oswFiles_DIAAlignR, ref = "run2", eXp = "run0",
  fitType = params[["globalAlignment"]], maxFdrGlobal = 0.05, spanvalue = 0.1)
```

```

adaptiveRT <- 77.82315 #3.5*getRSE(globalFit, params[["globalAlignment"]])
globalFit <- coef(globalFit)
getAlignedTimesFast(XICs.ref, XICs.eXp, globalFit, adaptiveRT, params)

```

getAlignObj

Outputs AlignObj from an alignment of two XIC-groups

Description

Outputs AlignObj from an alignment of two XIC-groups

Usage

```

getAlignObj(
  XICs.ref,
  XICs.eXp,
  globalFit,
  alignType,
  adaptiveRT,
  normalization,
  simType,
  goFactor,
  geFactor,
  cosAngleThresh,
  OverlapAlignment,
  dotProdThresh,
  gapQuantile,
  kerLen,
  hardConstrain,
  samples4gradient,
  objType = "light"
)

```

Arguments

XICs.ref	List of extracted ion chromatograms from reference run.
XICs.eXp	List of extracted ion chromatograms from experiment run.
globalFit	Linear or loess fit object between reference and experiment run.
alignType	Available alignment methods are "global", "local" and "hybrid".
adaptiveRT	(numeric) Similarity matrix is not penalized within adaptive RT.
normalization	(character) Must be selected from "mean", "l2".
simType	(string) Must be selected from dotProduct, cosineAngle, crossCorrelation, cosine2Angle, dotProductMasked, euclideanDist, covariance and correlation.
goFactor	(numeric) Penalty for introducing first gap in alignment. This value is multiplied by base gap-penalty.

geFactor	(numeric) Penalty for introducing subsequent gaps in alignment. This value is multiplied by base gap-penalty.
cosAngleThresh	(numeric) In simType = dotProductMasked mode, angular similarity should be higher than cosAngleThresh otherwise similarity is forced to zero.
OverlapAlignment	(logical) An input for alignment with free end-gaps. False: Global alignment, True: overlap alignment.
dotProdThresh	(numeric) In simType = dotProductMasked mode, values in similarity matrix higher than dotProdThresh quantile are checked for angular similarity.
gapQuantile	(numeric) Must be between 0 and 1. This is used to calculate base gap-penalty from similarity distribution.
kerLen	(integer) In simType = crossCorrelation, length of the kernel used to sum similarity score. Must be an odd number.
hardConstrain	(logical) If FALSE; indices farther from noBeef distance are filled with distance from linear fit line.
samples4gradient	(numeric) This parameter modulates penalization of masked indices.
objType	(char) Must be selected from light, medium and heavy.

Value

A S4 object. Three most-important slots are:

indexA_aligned	(integer) aligned indices of reference run.
indexB_aligned	(integer) aligned indices of experiment run.
score	(numeric) cumulative score of alignment.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

See Also

[alignChromatogramsCpp](#)

Examples

```
data(XIC_QFNNTDIVLLEDFQK_3_DIAAlignR, package="DIAAlignR")
data(oswFiles_DIAAlignR, package="DIAAlignR")
run1 <- "hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt"
run2 <- "hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt"
XICs.ref <- XIC_QFNNTDIVLLEDFQK_3_DIAAlignR[[run1]][["4618"]]
XICs.exp <- XIC_QFNNTDIVLLEDFQK_3_DIAAlignR[[run2]][["4618"]]
RUNS_RT <- getRTdf(oswFiles_DIAAlignR, ref = "run1", exp = "run2", maxFdrGlobal = 0.05)
globalFit <- loess(RT.exp ~ RT.ref, data = RUNS_RT, span = 0.1, control=loess.control(surface="direct"))
```

```
AlignObj <- getAlignObj(XICs.ref, XICs.eXp, globalFit, alignType = "hybrid", adaptiveRT = 77.82315,
  normalization = "mean", simType = "dotProductMasked", goFactor = 0.125,
  geFactor = 40, cosAngleThresh = 0.3, OverlapAlignment = TRUE, dotProdThresh = 0.96,
  gapQuantile = 0.5, kerLen = 9L, hardConstrain = FALSE, samples4gradient = 100, objType = "light")
```

getAlignObjs

AlignObj for analytes between a pair of runs

Description

This function expects osw and xics directories at dataPath. It first reads osw files and fetches chromatogram indices for each requested analyte. It then align XICs of each analyte to its reference XICs. AlignObj is returned which contains aligned indices and cumulative score along the alignment path.

Usage

```
getAlignObjs(
  analytes,
  runs,
  dataPath = ".",
  refRun = NULL,
  oswMerged = TRUE,
  params = paramsDIAAlignR(),
  objType = "light"
)
```

Arguments

analytes	(vector of integers) transition_group_ids for which features are to be extracted.
runs	(string) names of xics file without extension.
dataPath	(string) path to xics and osw directory.
refRun	(string) reference for alignment. If no run is provided, m-score is used to select reference run.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
objType	(char) Must be selected from light, medium and heavy.

Value

A list of fileInfo and AlignObjs. Each AlignObj is an S4 object. Three most-important slots are:

indexA_aligned	(integer) aligned indices of reference run.
indexB_aligned	(integer) aligned indices of experiment run.
score	(numeric) cumulative score of alignment.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-14

References

Gupta S, Ahadi S, Zhou W, Röst H. "DIAAlignR Provides Precise Retention Time Alignment Across Distant Runs in DIA and Targeted Proteomics." *Mol Cell Proteomics*. 2019 Apr;18(4):806-817. doi: <https://doi.org/10.1074/mcp.TIR118.001132> Epub 2019 Jan 31.

See Also

[plotAlignedAnalytes](#), [getRunNames](#), [getFeatures](#), [getXICs4AlignObj](#), [getAlignObj](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
params <- paramsDIAAlignR()
params[["context"]] <- "experiment-wide"
runs <- c("hroest_K120808_Strep10%PlasmaBiolRep11_R03_SW_filt",
         "hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt",
         "hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt")
analytes <- c(32L, 898L, 2474L)
AlignObjOutput <- getAlignObjs(analytes, runs, dataPath = dataPath)
plotAlignedAnalytes(AlignObjOutput)
```

`getBaseGapPenaltyCpp` *Calculates gap penalty for dynamic programming based alignment.*

Description

This function outputs base gap-penalty depending on SimType used. In case of getting base gap-penalty from similarity matrix distribution, gapQuantile will be used to pick the value.

Usage

```
getBaseGapPenaltyCpp(sim, SimType, gapQuantile = 0.5)
```

Arguments

<code>sim</code>	(matrix) A numeric matrix. Input similarity matrix.
<code>SimType</code>	(char) A character string. Similarity type must be selected from (dotProduct-Masked, dotProduct, cosineAngle, cosine2Angle, euclideanDist, covariance, correlation, crossCorrelation).
<code>gapQuantile</code>	(numeric) Must be between 0 and 1.

Value

baseGapPenalty (numeric).

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-08

Examples

```
sim <- matrix(c(-12, 1.0, 12, -2.3, -2, -2, 1.07, -2, 1.80, 2, 22, 42, -2, -1.5, -2, 10), 4, 4,
  byrow = FALSE)
getBaseGapPenaltyCpp(sim, "dotProductMasked", 0.5) # -0.25
```

getChildXICpp

Get child chromatogram from two parent chromatogram

Description

Get child chromatogram from two parent chromatogram

Usage

```
getChildXICpp(
  l1,
  l2,
  kernelLen,
  polyOrd,
  alignType,
  adaptiveRT,
  normalization,
  simType,
  Bp,
  goFactor = 0.125,
  geFactor = 40,
  cosAngleThresh = 0.3,
  OverlapAlignment = TRUE,
  dotProdThresh = 0.96,
  gapQuantile = 0.5,
  kerLen = 9L,
  hardConstrain = FALSE,
  samples4gradient = 100,
  wRef = 0.5,
  splineMethod = "natural",
  mergeStrategy = "avg",
  keepFlanks = TRUE
)
```

Arguments

l1	(list) A list of numeric matrix of two columns. l1 and l2 should have same length.
l2	(list) A list of numeric matrix of two columns. l1 and l2 should have same length.
kernelLen	(integer) length of filter. Must be an odd number.
polyOrd	(integer) TRUE: remove background from peak signal using estimated noise levels.
alignType	(char) A character string. Available alignment methods are "global", "local" and "hybrid".
adaptiveRT	(numeric) Similarity matrix is not penalized within adaptive RT.
normalization	(char) A character string. Normalization must be selected from (L2, mean or none).
simType	(char) A character string. Similarity type must be selected from (dotProductMasked, dotProduct, cosineAngle, cosine2Angle, euclideanDist, covariance, correlation, crossCorrelation). Mask = $s > \text{quantile}(s, \text{dotProdThresh})$ AllowDotProd = $[\text{Mask} \times \text{cosine2Angle} + (1 - \text{Mask})] > \text{cosAngleThresh}$ $s_{\text{new}} = s \times \text{AllowDotProd}$
Bp	(numeric) Timepoint mapped by global fit for tA.
goFactor	(numeric) Penalty for introducing first gap in alignment. This value is multiplied by base gap-penalty.
geFactor	(numeric) Penalty for introducing subsequent gaps in alignment. This value is multiplied by base gap-penalty.
cosAngleThresh	(numeric) In simType = dotProductMasked mode, angular similarity should be higher than cosAngleThresh otherwise similarity is forced to zero.
OverlapAlignment	(logical) An input for alignment with free end-gaps. False: Global alignment, True: overlap alignment.
dotProdThresh	(numeric) In simType = dotProductMasked mode, values in similarity matrix higher than dotProdThresh quantile are checked for angular similarity.
gapQuantile	(numeric) Must be between 0 and 1. This is used to calculate base gap-penalty from similarity distribution.
kerLen	(integer) In simType = crossCorrelation, length of the kernel used to sum similarity score. Must be an odd number.
hardConstrain	(logical) if false; indices farther from noBeef distance are filled with distance from linear fit line.
samples4gradient	(numeric) This parameter modulates penalization of masked indices.
wRef	(numeric) Weight of the reference XIC. Must be between 0 and 1.
splineMethod	(string) must be either "fmm" or "natural".
mergeStrategy	(string) must be either ref, avg, refStart or refEnd.
keepFlanks	(logical) TRUE: Flanking chromatogram is not removed.

Value

(List) of chromatograms and their aligned time vectors.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c)
Author (2021) + MIT Date: 2021-01-08

Examples

```
data(XIC_QFNNTDIVLLEDFQK_3_DIAalignR, package="DIAalignR")
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR
XICs.ref <- lapply(XICs[["hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt"]][["4618"]], as.matrix)
XICs.eXp <- lapply(XICs[["hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt"]][["4618"]], as.matrix)
Bp <- seq(4964.752, 5565.462, length.out = nrow(XICs.ref[[1]]))
chrom <- getChildXICpp(XICs.ref, XICs.eXp, 11L, 4L, alignType = "hybrid", adaptiveRT = 77.82315,
  normalization = "mean", simType = "dotProductMasked", Bp = Bp,
  goFactor = 0.125, geFactor = 40, cosAngleThresh = 0.3, OverlapAlignment = TRUE,
  dotProdThresh = 0.96, gapQuantile = 0.5, hardConstrain = FALSE, samples4gradient = 100,
  wRef = 0.5, keepFlanks= TRUE)
```

getChildXICs

Develop child XICs for precursors

Description

This function performs the chromatogram alignment of all precursors across runA and runB. Aligned chromatograms are merged into a child chromatogram. Aligned time vector and resulting child time vector for each precursor is also returned.

Usage

```
getChildXICs(  
  runA,  
  runB,  
  fileInfo,  
  features,  
  mzPntrs,  
  precursors,  
  prec2chromIndex,  
  refRun,  
  peptideScores,  
  params,  
  applyFun = lapply  
)
```

Arguments

runA	(string) name of a run to be merged with runB. Must be in the rownames of fileInfo.
runB	(string) name of a run to be merged with runA. Must be in the rownames of fileInfo.
fileInfo	(data-frame) output of getRunNames .
features	(list of data-frames) contains features and their properties identified in each run.
mzPntrs	(list) a list of mzRpviz.
precursors	(data-frame) atleast two columns transition_group_id and transition_ids are required.
prec2chromIndex	(list) a list of dataframes having following columns: transition_group_id: it is PRECURSOR.ID from osw file. chromatogramIndex: index of chromatogram in mzML file.
refRun	(integer) must be of the same length as of precursors. 1: reference is runA, 2: reference is runB.
peptideScores	(list of data-frames) each dataframe has scores of a peptide across all runs.
params	(list) parameters are entered as list. Output of the paramsDIAalignR function.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Value

(list) has three elements. The first element has child XICs for all the precursors. The second element has corresponding aligned time vectors. Third element contains Residual Standard Errors (RSE) of global fits amongst runA and runB.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-06-06

See Also

[childXICs](#), [getNodeRun](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAalignR")
params <- paramsDIAalignR()
fileInfo <- DIAalignR::getRunNames(dataPath = dataPath)
mzPntrs <- getMZMLpointers(fileInfo)
features <- getFeatures(fileInfo, maxFdrQuery = 1.00, runType = "DIA_Proteomics")
precursors <- getPrecursors(fileInfo, oswMerged = TRUE, runType = "DIA_Proteomics",
  context = "experiment-wide", maxPeptideFdr = 0.05)
precursors <- dplyr::arrange(precursors, .data$peptide_id, .data$transition_group_id)
```

```
peptideIDs <- unique(precursors$peptide_id)
peptideScores <- getPeptideScores(fileInfo, peptideIDs, oswMerged = TRUE, params[["runType"]], params[["context"]]
peptideScores <- lapply(peptideIDs, function(pep) dplyr::filter(peptideScores, .data$peptide_id == pep))
names(peptideScores) <- as.character(peptideIDs)
prec2chromIndex <- getChromatogramIndices(fileInfo, precursors, mzPntrs)
var2 <- as.character(sapply(peptideIDs, function(p) precursors$transition_group_id[which(precursors$peptide_id == p)]))
refRun <- data.frame(rep(1L, length(peptideIDs)), var2)
mergedXICs <- getChildXICs(runA = "run1", runB = "run2", fileInfo, features, mzPntrs,
  precursors, prec2chromIndex, refRun, peptideScores, params)
for(con in mzPntrs) DBI::dbDisconnect(con)
```

getChromatogramIndices

Get chromatogram indices of precursors.

Description

This function reads the header of chromatogram files. It then fetches chromatogram indices by matching transition_id(osw) with chromatogramID(xics).

Usage

```
getChromatogramIndices(fileInfo, precursors, mzPntrs, applyFun = lapply)
```

Arguments

fileInfo	(data-frame) Output of getRunNames function.
precursors	(data-frame) Atleast two columns transition_group_id and transition_ids are required.
mzPntrs	A list of mzRpwis.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Value

(list) A list of dataframes having following columns:

transition_group_id	(string) it is PRECURSOR.ID from osw file.
chromatogramIndex	(integer) index of chromatogram in mzML file.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-04-07

See Also

[chromatogramIdAsInteger](#), [mapPrecursorToChromIndices](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath)
precursors <- getPrecursors(fileInfo, oswMerged = TRUE, context = "experiment-wide")
mzPntrs <- getMZMLpointers(fileInfo)
prec2chromIndex <- getChromatogramIndices(fileInfo, precursors, mzPntrs)
for(mz in mzPntrs) DBI::dbDisconnect(mz)
```

getChromSimMatCpp	<i>Calculates similarity matrix of two fragment-ion chromatogram groups or extracted-ion chromatograms(XICs)</i>
-------------------	--

Description

Calculates similarity matrix of two fragment-ion chromatogram groups or extracted-ion chromatograms(XICs)

Usage

```
getChromSimMatCpp(
  l1,
  l2,
  normalization,
  simType,
  cosAngleThresh = 0.3,
  dotProdThresh = 0.96,
  kerLen = 9L
)
```

Arguments

l1	(list) A list of vectors. Length should be same as of l2.
l2	(list) A list of vectors. Length should be same as of l1.
normalization	(char) A character string. Normalization must be selected from (L2, mean or none).
simType	(char) A character string. Similarity type must be selected from (dotProductMasked, dotProduct, cosineAngle, cosine2Angle, euclideanDist, covariance, correlation, crossCorrelation). Mask = s > quantile(s, dotProdThresh) AllowDotProd= [Mask × cosine2Angle + (1 - Mask)] > cosAngleThresh s_new= s × AllowDotProd
cosAngleThresh	(numeric) In simType = dotProductMasked mode, angular similarity should be higher than cosAngleThresh otherwise similarity is forced to zero.

- dotProdThresh (numeric) In simType = dotProductMasked mode, values in similarity matrix higher than dotProdThresh quantile are checked for angular similarity.
- kerLen (integer) In simType = crossCorrelation, length of the kernel used to sum similarity score. Must be an odd number.

Value

s (matrix) Numeric similarity matrix. Rows and columns expresses seq1 and seq2, respectively.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-05

Examples

```
# Get similarity matrix of dummy chromatograms
r1 <- list(c(1.0,3.0,2.0,4.0), c(0.0,0.0,0.0,1.0), c(4.0,4.0,4.0,5.0))
r2 <- list(c(1.4,2.0,1.5,4.0), c(0.0,0.5,0.0,0.0), c(2.0,3.0,4.0,0.9))
round(getChromSimMatCpp(r1, r2, "L2", "dotProductMasked"), 3)
matrix(c(0.125, 0.162, 0.144, 0.208, 0.186, 0.240,
0.213, 0.313, 0.233, 0.273, 0.253, 0.346, 0.101, 0.208, 0.154, 0.273), 4, 4, byrow = FALSE)

round(getChromSimMatCpp(r1, r2, "L2", "dotProduct"), 3)
matrix(c(0.125, 0.162, 0.144, 0.208, 0.186, 0.240, 0.213, 0.313, 0.233,
0.273, 0.253, 0.346, 0.101, 0.208, 0.154, 0.273), 4, 4, byrow = FALSE)

round(getChromSimMatCpp(r1, r2, "L2", "cosineAngle"), 3)
matrix(c(0.934, 0.999, 0.989, 0.986, 0.933, 0.989,
0.983, 0.996, 0.994, 0.960, 0.995, 0.939, 0.450,
0.761, 0.633, 0.772), 4, 4, byrow = FALSE)

round(getChromSimMatCpp(r1, r2, "L2", "cosine2Angle"), 3)
matrix(c(0.744, 0.998, 0.957, 0.944, 0.740, 0.956, 0.932,
0.985, 0.974, 0.842, 0.978, 0.764, -0.596, 0.158,
-0.200, 0.190), 4, 4, byrow = FALSE)

round(getChromSimMatCpp(r1, r2, "mean", "euclideanDist"), 3)
matrix(c(0.608, 0.614, 0.680, 0.434, 0.530, 0.742,
0.659, 0.641, 0.520, 0.541, 0.563, 0.511, 0.298,
0.375, 0.334, 0.355), 4, 4, byrow = FALSE)

round(getChromSimMatCpp(r1, r2, "L2", "covariance"), 3)
matrix(c(0.025, 0.028, 0.027, 0.028, 0.032, 0.034,
0.033, 0.034, 0.055, 0.051, 0.053, 0.051,
-0.004, 0.028, 0.012, 0.028), 4, 4, byrow = FALSE)

round(getChromSimMatCpp(r1, r2, "L2", "correlation"), 3)
matrix(c(0.874, 0.999, 0.974, 0.999, 0.923, 0.986, 0.993,
0.986, 0.991, 0.911, 0.990, 0.911, -0.065, 0.477,
0.214, 0.477), 4, 4, byrow = FALSE)
```

<code>getFeatures</code>	<i>Get features from all feature files</i>
--------------------------	--

Description

Get a list of data-frame of OpenSwath features that contains retention time, intensities, boundaries etc.

Usage

```
getFeatures(
  fileInfo,
  maxFdrQuery = 0.05,
  maxIPFFdrQuery = 0.05,
  runType = "DIA_Proteomics",
  applyFun = lapply
)
```

Arguments

<code>fileInfo</code>	(data-frame) output of <code>getRunNames</code> function.
<code>maxFdrQuery</code>	(numeric) a numeric value between 0 and 1. It is used to filter features from osw file which have SCORE_MS2.QVALUE less than itself.
<code>maxIPFFdrQuery</code>	(numeric) A numeric value between 0 and 1. It is used to filter features from osw file which have SCORE_IPF.QVALUE less than itself. (For PTM IPF use)
<code>runType</code>	(char) This must be one of the strings "DIA_Proteomics", "DIA_IPF", "DIA_Metabolomics".
<code>applyFun</code>	(function) value must be either <code>lapply</code> or <code>BiocParallel::bplapply</code> .

Value

(list of dataframes) each dataframe has following columns:

<code>transition_group_id</code>	(integer) a unique id for each precursor.
<code>RT</code>	(numeric) retention time as in FEATURE.EXP_RT of osw files.
<code>Intensity</code>	(numeric) peak intensity as in FEATURE_MS2.AREA_INTENSITY of osw files.
<code>leftWidth</code>	(numeric) as in FEATURE.LEFT_WIDTH of osw files.
<code>rightWidth</code>	(numeric) as in FEATURE.RIGHT_WIDTH of osw files.
<code>peak_group_rank</code>	(integer) rank of each feature associated with <code>transition_group_id</code> .
<code>m_score</code>	(numeric) q-value of each feature associated with <code>transition_group_id</code> . (If using 'DIA_IPF' runType, this will represent IPF's QVALUE)
<code>ms2_m_score</code>	(numeric) MS2 q-value of each feature associated with <code>transition_group_id</code> . (Will only be present if using 'DIA_IPF' runType)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-04-06

See Also

[getRunNames](#), [fetchPrecursorsInfo](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath)
features <- getFeatures(fileInfo, maxFdrQuery = 1.00, runType = "DIA_Proteomics")
dim(features[[2]]) # 938 8
```

getGlobalAlignMaskCpp *Outputs a mask for constraining similarity matrix*

Description

This function takes in timeVectors from both runs, global-fit mapped values of end-points of first time vector and sample-length of window of no constraining. Outside of window, all elements of matrix are either equally weighted or weighted proportional to distance from window-boundry.

Usage

```
getGlobalAlignMaskCpp(tA, tB, tBp, noBeef = 50L, hardConstrain = FALSE)
```

Arguments

tA	(numeric) This vector has equally spaced timepoints of XIC A.
tB	(numeric) This vector has equally spaced timepoints of XIC B.
tBp	(numeric) mapping of tA to run B using some global fit.
noBeef	(integer) It defines the distance from the global fit, upto which no penalization is performed. The window length = 2*noBeef.
hardConstrain	(logical) if false; indices farther from noBeef distance are filled with distance from linear fit line.

Value

mask (matrix) A numeric matrix.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-08

Examples

```
tA <- c(1707.6, 1711, 1714.5, 1717.9, 1721.3, 1724.7, 1728.1, 1731.5, 1734.9, 1738.4)
tB <- c(1765.7, 1769.1, 1772.5, 1775.9, 1779.3, 1782.7, 1786.2, 1789.6, 1793, 1796.4)
tBp <- c(1786.9, 1790.35, 1793.9, 1797.36, 1800.81, 1804.26, 1807.71, 1811.17, 1814.62, 1818.17)
noBeef <- 1
mask <- getGlobalAlignMaskCpp(tA, tB, tBp, noBeef, FALSE)
round(mask, 3)
matrix(c( 5.215,4.218,4.221,2.225,1.228,0,0,0,0.788, 1.785,
6.226,5.230,4.233,3.236,2.239,1.243,0,0,0, 0.774), nrow = 2, ncol = 10, byrow = FALSE)
#image(mask) # A is on x-axis, B is on y-axis
```

getGlobalAlignment *Calculates global alignment between RT of two runs*

Description

This function selects features from oswFiles which has m-score < maxFdrLoess. It fits linear/loess regression on these feature. Retention-time mapping is established from reference to experiment run.

Usage

```
getGlobalAlignment(
  oswFiles,
  ref,
  exp,
  fitType = "linear",
  maxFdrGlobal = 0.01,
  spanvalue = 0.1
)
```

Arguments

oswFiles	(list of data-frames) it is output from getFeatures function.
ref	(string) Must be a combination of "run" and an iteger e.g. "run2".
exp	(string) Must be a combination of "run" and an iteger e.g. "run2".
fitType	(string) Must be from "loess" or "linear".
maxFdrGlobal	(numeric) A numeric value between 0 and 1. Features should have m-score lower than this value for participation in global fit.
spanvalue	(numeric) Spanvalue for LOESS fit. For targeted proteomics 0.1 could be used.

Value

An object of class "loess".

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-14

See Also

[getFeatures](#)

Examples

```
data(oswFiles_DIAAlignR, package="DIAAlignR")
fit <- getGlobalAlignment(oswFiles = oswFiles_DIAAlignR, ref = "run1", exp = "run2",
  fitType = "linear", maxFdrGlobal = 0.05, spanvalue = 0.1)
```

getMultipeptide

Get multipeptides

Description

Each element of the multipeptide is a collection of features associated with a peptide.

Usage

```
getMultipeptide(
  precursors,
  features,
  runType = "DIA_Proteomics",
  applyFun = lapply,
  masters = NULL
)
```

Arguments

precursors	(data-frames) Contains precursors and associated transition IDs.
features	(list of data-frames) Contains features and their properties identified in each run.
runType	(char) This must be one of the strings "DIA_Proteomics", "DIA_IPF", "DIA_Metabolomics".
applyFun	(function) value must be either lapply or BiocParallel::bplapply.
masters	(characters) names of extra runs.

Value

(list) of dataframes having following columns:

transition_group_id	(integer) a unique id for each precursor.
run	(string) run identifier.
RT	(numeric) retention time as in FEATURE.EXP_RT of osw files.
Intensity	(numeric) peak intensity as in FEATURE_MS2.AREA_INTENSITY of osw files.
leftWidth	(numeric) as in FEATURE.LEFT_WIDTH of osw files.
rightWidth	(numeric) as in FEATURE.RIGHT_WIDTH of osw files.
peak_group_rank	(integer) rank of each feature associated with transition_group_id.
m_score	(numeric) q-value of each feature associated with transition_group_id.
alignment_rank	(integer) rank of each feature post-alignment.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-04-08

See Also

[getPrecursors](#), [getFeatures](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath, oswMerged = TRUE)
precursors <- getPrecursors(fileInfo, oswMerged = TRUE, context = "experiment-wide")
features <- getFeatures(fileInfo, maxFdrQuery = 0.05)
multipeptide <- getMultipeptide(precursors, features)
multipeptide[["9861"]]
```

getMZMLpointers

Get pointers to each mzML file.

Description

Returns instantiated mzRpviz object associated to mzML file.

Usage

```
getMZMLpointers(fileInfo)
```

Arguments

fileInfo (data-frame) Output of DIALignR::getRunNames function

Value

(A list of mzRpwiz)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

Examples

```
dataPath <- system.file("extdata", package = "DIALignR")
fileInfo <- getRunNames(dataPath = dataPath)
mzPntrs <- getMZMLpointers(fileInfo)
```

getNativeIDs

Fetch NativeIDs

Description

Get transition(native) IDs for the peptides.

Usage

```
getNativeIDs(oswIn, peps, params = paramsDIALignR(), oswMerged = TRUE)
```

Arguments

oswIn (string) path to the osw feature file.

peps (integer) ids of peptides to be aligned. If NULL, align all peptides.

params (list) parameters are entered as list. Output of the [paramsDIALignR](#) function.

oswMerged (logical) TRUE if merged file from pyprophet is used.

Value

(integer) a vector of transition IDs.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2022) + GPL-3 Date: 2022-04-19

See Also[reduceXICs](#)**Examples**

```

dataPath <- system.file("extdata", package = "DIAalignR")
oswIn <- file.path(dataPath, "osw", "merged.osw")
peps <- c(3L, 11L) # No transitions for 3L.
params <- paramsDIAalignR()
params[["context"]] <- "experiment-wide"
getNativeIDs(oswIn, peps, params) # 106468 106469 106470 106471 106472 106473

```

getPeptideScores	<i>Get scores of peptide</i>
------------------	------------------------------

Description

Get a list of dataframes that contains peptide scores, pvalues, and qvalues across all runs.

Usage

```

getPeptideScores(
  fileInfo,
  peptides,
  oswMerged = TRUE,
  runType = "DIA_Proteomics",
  context = "global"
)

```

Arguments

fileInfo	(data-frame) Output of getRunNames function.
peptides	(integer) Ids of peptides for which scores are required.
oswMerged	(logical) TRUE for experiment-wide FDR and FALSE for run-specific FDR by pyprophet.
runType	(char) This must be one of the strings "DIA_Proteomics", "DIA_IPF", "DIA_Metabolomics".
context	(string) Context used in pyprophet peptide. Must be either "run-specific", "experiment-wide", or "global".

Value

(list of dataframes) dataframe has following columns:

peptide_id	(integer) a unique id for each precursor.
run	(character) as in SCORE_PEPTIDE.RUN_ID of osw files.
score	(numeric) as in SCORE_PEPTIDE.SCORE of osw files.
pvalue	(numeric) as in SCORE_PEPTIDE.PVALUE of osw files.
qvalue	(numeric) as in SCORE_PEPTIDE.QVALUE of osw files.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-07-01

See Also

[getRunNames](#), [fetchPeptidesInfo](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath)
precursorsInfo <- getPrecursors(fileInfo, oswMerged = TRUE, runType = "DIA-Proteomics",
context = "experiment-wide", maxPeptideFdr = 0.05)
peptidesInfo <- getPeptideScores(fileInfo, unique(precursorsInfo$peptide_id))
dim(peptidesInfo) # 684 5
```

getPrecursorByID

Find precursors given their IDs

Description

Get a data-frame of analytes' transition_group_id, transition_ids, peptide_id and amino-acid sequences.

Usage

```
getPrecursorByID(
  analytes,
  fileInfo,
  oswMerged = TRUE,
  runType = "DIA-Proteomics"
)
```

Arguments

analytes	(integer) a vector of integers.
fileInfo	(data-frame) Output of getRunNames function.
oswMerged	(logical) TRUE for experiment-wide FDR and FALSE for run-specific FDR by pyprophet.
runType	(char) This must be one of the strings "DIA-Proteomics", "DIA_IPF", "DIA_Metabolomics".

Value

(data-frames) A data-frame having following columns:

transition_group_id	(integer) a unique id for each precursor.
transition_id	(list) fragment-ion ID associated with transition_group_id. This is matched with chromatogram ID in mzML file.
peptide_id	(integer) a unique id for each peptide. A peptide can have multiple precursors.
sequence	(string) amino-acid sequence of the precursor with possible modifications.
charge	(integer) charge on the precursor.
group_label	(string) TODO Figure it out.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2019-04-06

See Also

[getRunNames](#), [fetchPrecursorsInfo](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath, oswMerged = TRUE)
precursors <- getPrecursorByID(c(32L, 2474L), fileInfo, oswMerged = TRUE)
```

getPrecursorIndices *Get MSI chromatogram indices of precursors.*

Description

This function reads the header of chromatogram files. It then fetches chromatogram indices by matching transition_group_id(osw) with chromatogramID(xics).

Usage

```
getPrecursorIndices(
  fileInfo,
  precursors,
  mzPtrs,
  ions = ".*",
  applyFun = lapply
)
```

Arguments

fileInfo	(data-frame) Output of getRunNames function.
precursors	(data-frame) Atleast two columns transition_group_id and transition_ids are required.
mzPntrs	A list of mzRpwis.
ions	(character) Strings to specify ions. eg. i0, i1.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Value

(list) A list of dataframes having following columns:

transition_group_id	(string) it is PRECURSOR.ID from osw file.
chromatogramIndex	(integer) index of MS1 chromatogram in mzML file.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2022) + GPL-3 Date: 2022-01-15

See Also

[chromatogramIdAsInteger](#), [mapPrecursorToChromIndices](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath)
precursors <- getPrecursors(fileInfo, oswMerged = TRUE, context = "experiment-wide")
mzPntrs <- getMZMLpointers(fileInfo)
prec2chromIndex <- getPrecursorIndices(fileInfo, precursors, mzPntrs)
for(mz in mzPntrs) DBI::dbDisconnect(mz)
```

getPrecursors

Get precursors from all feature files

Description

Get a data-frame of analytes' transition_group_id, transition_ids, peptide_id and amino-acid sequences.

Usage

```
getPrecursors(
  fileInfo,
  oswMerged = TRUE,
  runType = "DIA_Proteomics",
  context = "global",
  maxPeptideFdr = 0.05,
  level = "Peptide",
  useIdentifying = FALSE
)
```

Arguments

fileInfo	(data-frame) Output of getRunNames function.
oswMerged	(logical) TRUE for experiment-wide FDR and FALSE for run-specific FDR by pyprophet.
runType	(char) This must be one of the strings "DIA_Proteomics", "DIA_IPF", "DIA_Metabolomics".
context	(string) Context used in pyprophet peptide. Must be either "run-specific", "experiment-wide", or "global".
maxPeptideFdr	(numeric) A numeric value between 0 and 1. It is used to filter peptides from osw file which have SCORE_PEPTIDE.QVALUE less than itself.
level	(string) Apply maxPeptideFDR on Protein as well if specified as "Protein". Default: "Peptide".
useIdentifying	(logical) Set TRUE to use identifying transitions in alignment. (DEFAULT: FALSE)

Value

(data-frames) A data-frame having following columns:

transition_group_id	(integer) a unique id for each precursor.
peptide_id	(integer) a unique id for each peptide. A peptide can have multiple precursors.
sequence	(string) amino-acid sequence of the precursor with possible modifications.
charge	(integer) charge on the precursor.
group_label	(string) TODO Figure it out.
transition_ids	(list) fragment-ion ID associated with transition_group_id. This is matched with chromatogram ID in mzML file.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-04-06

See Also

[getRunNames](#), [fetchPrecursorsInfo](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath)
precursorsInfo <- getPrecursors(fileInfo, oswMerged = TRUE, runType = "DIA_Proteomics",
context = "experiment-wide", maxPeptideFdr = 0.05)
dim(precursorsInfo) # 234 6
```

getRefExpFeatureMap *Alignment Feature Mapping Table*

Description

Construct an alignment feature mapping table for star align method, to map aligned features in experiment runs to the reference run

Usage

```
getRefExpFeatureMap(precursors, features, applyFun = lapply)
```

Arguments

precursors (data-frames) Contains precursors and associated transition IDs.
features (list of data-frames) Contains features and their properties identified in each run.
applyFun (function) value must be either lapply or BiocParallel::bplapply.

Value

(list) of dataframes per precursor peptide id having following columns:

reference_feature_id
 (integer) id of reference feature.
experiment_feature_id
 (integer) id of experiment feature aligned to reference feature.

Author(s)

Justin Sing, <justinc.sing@mail.utoronto.ca>
ORCID: 0000-0003-0386-0092
License: (c) Author (2020) + GPL-3 Date: 2022-11-07

See Also

[getPrecursors](#), [getFeatures](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath, oswMerged = TRUE)
precursors <- getPrecursors(fileInfo, oswMerged = TRUE, context = "experiment-wide")
features <- getFeatures(fileInfo, maxFdrQuery = 0.05)
multiFeatureAlignmentMap <- getRefExpFeatureMap(precursors, features)
multiFeatureAlignmentMap[["9861"]]
```

getRefRun	<i>Fetch the reference run for each peptide</i>
-----------	---

Description

Provides the reference run based on lowest p-value.

Usage

```
getRefRun(peptideScores, applyFun = lapply)
```

Arguments

`peptideScores` (list of data-frames) each dataframe has scores of a peptide across all runs.
`applyFun` (function) value must be either `lapply` or `BiocParallel::bplapply`.

Value

(dataframe) has two columns:

`peptide_id` (integer) a unique id for each peptide.
`run` (string) run identifier.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>
ORCID: 0000-0003-3500-8152
License: (c) Author (2020) + GPL-3 Date: 2020-04-08

See Also

[getPeptideScores](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath)
precursorsInfo <- getPrecursors(fileInfo, oswMerged = TRUE, runType = "DIA_Proteomics",
                               context = "experiment-wide", maxPeptideFdr = 0.05)
peptideIDs <- unique(precursorsInfo$peptide_id)
peptidesInfo <- getPeptideScores(fileInfo, peptideIDs)
peptidesInfo <- lapply(peptideIDs, function(pep) peptidesInfo [.(pep),])
names(peptidesInfo) <- as.character(peptideIDs)
getRefRun(peptidesInfo)
```

getRTdf

Calculates global alignment between RT of two runs

Description

This function selects features from oswFiles which has m-score < maxFdrLoess. It fits linear/loess regression on these feature. Retention-time mapping is established from reference to experiment run.

Usage

```
getRTdf(features, ref, exp, maxFdrGlobal)
```

Arguments

features	(list of data-frames) it is output from getFeatures function.
ref	(string) Must be a combination of "run" and an iteger e.g. "run2".
exp	(string) Must be a combination of "run" and an iteger e.g. "run2".
maxFdrGlobal	(numeric) A numeric value between 0 and 1. Features should have m-score lower than this value for participation in global fit.

Value

A data-frame

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2019-03-01

See Also

[getGlobalAlignment](#)

Examples

```
data(oswFiles_DIAalignR, package="DIAalignR")
df <- getRTdf(features = oswFiles_DIAalignR, ref = "run1", eXp = "run2", maxFdrGlobal = 0.05)
```

getRunNames	<i>Get names of all runs</i>
-------------	------------------------------

Description

Fetches all osw files, then, keeps only those runs which has corresponding mzML files. mzML file names must match with RUN.FILENAME columns of osw files.

Usage

```
getRunNames(dataPath, oswMerged = TRUE, params = paramsDIAalignR())
```

Arguments

dataPath	(char) Path to xics and osw directory.
oswMerged	(logical) TRUE for experiment-wide FDR and FALSE for run-specific FDR by pyprophet.
params	(list) parameters are entered as list. Output of the paramsDIAalignR function.

Value

(dataframe) it has five columns:

spectraFile	(string) as mentioned in RUN table of osw files.
runName	(string) contain respective mzML names without extension.
spectraFileID	(string) ID in RUN table of osw files.
featureFile	(string) Path to the feature file.
chromatogramFile	(string) Path to the chromatogram file.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-14

Examples

```
dataPath <- system.file("extdata", package = "DIAalignR")
getRunNames(dataPath = dataPath, oswMerged = TRUE)
```

getSeqSimMatCpp	<i>Calculates similarity matrix for two sequences</i>
-----------------	---

Description

Calculates similarity matrix for two sequences

Usage

```
getSeqSimMatCpp(seq1, seq2, match, misMatch)
```

Arguments

seq1	(char) A single string.
seq2	(char) A single string.
match	(double) Score for character match.
misMatch	(double) score for character mismatch.

Value

s (matrix) Numeric similarity matrix. Rows and columns expresses seq1 and seq2, respectively.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2019) + MIT Date: 2019-03-05

Examples

```
# Get sequence similarity of two DNA strings
Match=10; MisMatch=-2
seq1 = "GCAT"; seq2 = "CAGTG"
getSeqSimMatCpp(seq1, seq2, Match, MisMatch)
matrix(c(-2, 10, -2, -2, -2, -2, 10, -2, 10, -2, -2, -2, -2, -2, 10, 10, -2, -2, -2),
  4, 5, byrow = FALSE)
```

getTransitions *Get transitions from all feature files*

Description

Get a list of data-frame of OpenSwath features that contains retention time, intensities, boundaries etc.

Usage

```
getTransitions(
  fileInfo,
  maxFdrQuery = 0.05,
  runType = "DIA_Proteomics",
  applyFun = lapply
)
```

Arguments

fileInfo	(data-frame) output of getRunNames function.
maxFdrQuery	(numeric) a numeric value between 0 and 1. It is used to filter features from osw file which have SCORE_MS2.QVALUE less than itself.
runType	(char) yhis must be one of the strings "DIA_Proteomics", "DIA_Metabolomics".
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Value

(list of dataframes) each dataframe has following columns:

transition_group_id	(integer) a unique id for each precursor.
RT	(numeric) retention time as in FEATURE.EXP_RT of osw files.
intensity	(list) of peak intensities as in FEATURE_TRANSITION.AREA_INTENSITY of osw files.
leftWidth	(numeric) as in FEATURE.LEFT_WIDTH of osw files.
rightWidth	(numeric) as in FEATURE.RIGHT_WIDTH of osw files.
peak_group_rank	(integer) rank of each feature associated with transition_group_id.
m_score	(numeric) q-value of each feature associated with transition_group_id.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-11-15

See Also

[getRunNames](#), [fetchTransitionsFromRun](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath)
transitions <- getTransitions(fileInfo, maxFdrQuery = 1.00, runType = "DIA_Proteomics")
dim(transitions[[2]]) # 938 8
```

getXICs	<i>Get XICs of all analytes</i>
---------	---------------------------------

Description

For all the analytes requested in runs, it first creates oswFiles, then, fetches chromatogram indices from oswFiles and extract chromatograms from mzML files.

Usage

```
getXICs(
  analytes,
  runs,
  dataPath = ".",
  maxFdrQuery = 1,
  runType = "DIA_Proteomics",
  oswMerged = TRUE,
  params = paramsDIAAlignR()
)
```

Arguments

analytes	(integer) a vector of precursor IDs.
runs	(vector of string) names of mzML files without extension.
dataPath	(string) Path to xics and osw directory.
maxFdrQuery	(numeric) A numeric value between 0 and 1. It is used to filter features from osw file which have SCORE_MS2.QVALUE less than itself.
runType	(char) This must be one of the strings "DIA_Proteomics", "DIA_Metabolomics".
oswMerged	(logical) TRUE for experiment-wide FDR and FALSE for run-specific FDR by pyprophet.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.

Value

A list of list. Each list contains XIC-group for that run. XIC-group is a list of dataframe that has elution time and intensity of fragment-ion XIC.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

See Also

[getXICs4AlignObj](#), [getRunNames](#), [analytesFromFeatures](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
runs <- c("hroest_K120808_Strep10%PlasmaBiolRep1_R03_SW_filt",
         "hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt")
analytes <- c(32L, 898L, 2474L)
XICs <- getXICs(analytes, runs = runs, dataPath = dataPath)
```

getXICs4AlignObj *Extract XICs of analytes*

Description

For all the analytes requested, it fetches chromatogram indices from prec2chromIndex and extracts chromatograms using mzPntrs.

Usage

```
getXICs4AlignObj(mzPntrs, fileInfo, runs, prec2chromIndex, analytes)
```

Arguments

mzPntrs	a list of mzRpwiz.
fileInfo	(data-frame) output of getRunNames().
runs	(vector of string) names of mzML files without extension.
prec2chromIndex	(list of data-frames) output of getChromatogramIndices(). Each dataframe has two columns: transition_group_id and chromatogramIndex.
analytes	(integer) a vector of precursor IDs.

Value

A list of list of data-frames. Each data frame has elution time and intensity of fragment-ion XIC.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

See Also

[getChromatogramIndices](#), [getRunNames](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
runs <- c("hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt",
         "hroest_K120808_Strep10%PlasmaBiolRepl1_R03_SW_filt")
analytes <- c(32L, 898L, 2474L)
params <- paramsDIAAlignR()
params[["chromFile"]] <- "mzML"
fileInfo <- getRunNames(dataPath = dataPath)
fileInfo <- updateFileInfo(fileInfo, runs)
precursors <- getPrecursorByID(analytes, fileInfo)
mzPntrs <- getMZMLpointers(fileInfo)
prec2chromIndex <- getChromatogramIndices(fileInfo, precursors, mzPntrs)
XICs <- getXICs4AlignObj(mzPntrs, fileInfo, runs, prec2chromIndex, analytes)
rm(mzPntrs)
```

get_ropenms

Get ropenms handle

Description

Python path can also be set using `Sys.setenv(RETICULATE_PYTHON = pythonPath)`. Also, remove `.Rhistory` file to avoid conflict with previously used python version.

Usage

```
get_ropenms(pythonPath = NULL, condaEnv = NULL, useConda = TRUE)
```

Arguments

`pythonPath` (string) path of the python program that has `pyopenms` module.

`condaEnv` (string) name of the conda environment that has `pyopenms` module.

`useConda` (logical) TRUE: Use conda environment. FALSE: Use python through `pythonPath`.

Value

(`pyopenms` module)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-06-06

Examples

```
## Not run:
  ropenms <- get_ropenms(condaEnv = "envName", useConda=TRUE)

## End(Not run)
```

imputeChromatogram *Fill missing intensities in a chromatogram*

Description

Fill missing intensities in a chromatogram

Usage

```
imputeChromatogram(
  chromatogram,
  method = "spline",
  polyOrd = 4,
  kernelLen = 9,
  splineMethod = "fmm"
)
```

Arguments

chromatogram (data-frames) first column is time, second column is intensity.
method (string) must be either "spline", "sgolay" or "linear".
polyOrd (integer) must be less than kernelLen.
kernelLen (integer) must be an odd integer.
splineMethod (string) must be either "fmm" or "natural".

Value

(dataframe) has two columns:

time (numeric)
intensity (numeric)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-05-21

See Also

[na.approx](#), [na.spline](#)

Examples

```
time <- seq(from = 3003.4, to = 3048, by = 3.4)
y <- c(0.2050595, 0.8850070, 2.2068768, 3.7212677, 5.1652605, 5.8288915, 5.5446804,
      4.5671360, 3.3213154, 1.9485889, 0.9520709, 0.3294218, 0.2009581, 0.1420923)
chrom <- data.frame(time, y)
chrom$y[c(1,8, 14)] <- NA
imputeChromatogram(chrom, "sgolay")
imputeChromatogram(chrom, "spline")
imputeChromatogram(chrom, "linear")
```

mapIdxToTime

Establishes mapping from index to time

Description

Takes a time vector and index vector of same length. This function create a new time vector given indices specified in `idx`.

Usage

```
mapIdxToTime(timeVec, idx)
```

Arguments

`timeVec` A numeric vector

`idx` An integer vector

Value

A mutated time vector

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

Examples

```
timeVec <- c(1.3,5.6,7.8)
idx <- c(NA, NA, 1L, 2L, NA, NA, 3L, NA)
mapIdxToTime(timeVec, idx) # c(NA, NA, 1.3, 5.6, 6.333, 7.067, 7.8, NA)
```

masterXICs_DIAAlignR *Master fragment-ion chromatograms from two parents*

Description

Created merged XICs of peptide (ID = 4618) 14299_QFNNTDIVLLEDFQK/3 from two SWATH runs:

run1 : hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt.chrom.mzML

run2 : hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt.chrom.mzML

Usage

```
masterXICs_DIAAlignR
```

Format

The format is similar to the output of childXICs. A list of two elements: First element contains six fragmentation chromatograms. The second element has aligned parent time-vectors and corresponding child time-vector. It has five columns:

indexAligned.ref (integer) aligned indices of reference run.

indexAligned.eXp (integer) aligned indices of experiment run.

tAligned.ref (numeric) aligned time-vector of reference run.

tAligned.eXp (numeric) aligned time-vector of experiment run.

alignedChildTime (numeric) aligned time-vector of master run.

Source

File test_GenerateData.R has [source code](#) to generate the example data.

`mstAlignRuns`*Peptide quantification through MST alignment*

Description

This function expects `osw` and `xics` directories at `dataPath`. It first reads `osw` files and fetches chromatogram indices for each analyte. To perform alignment, first a guide-tree is built using `mst` which can also be provided with `mstNet` parameter. As we traverse from the start node to the other nodes, runs are aligned pairwise.

Usage

```
mstAlignRuns(  
  dataPath,  
  outFile = "DIAAlignR",  
  params = paramsDIAAlignR(),  
  oswMerged = TRUE,  
  scoreFile = NULL,  
  runs = NULL,  
  peps = NULL,  
  mstNet = NULL,  
  applyFun = lapply  
)
```

Arguments

<code>dataPath</code>	(string) path to <code>xics</code> and <code>osw</code> directory.
<code>outFile</code>	(string) name of the output file.
<code>params</code>	(list) parameters are entered as list. Output of the <code>paramsDIAAlignR</code> function.
<code>oswMerged</code>	(logical) TRUE if merged file from <code>pyprophet</code> is used.
<code>scoreFile</code>	(string) path to the peptide score file, needed when <code>oswMerged</code> is FALSE.
<code>runs</code>	(string) names of <code>xics</code> file without extension.
<code>peps</code>	(integer) ids of peptides to be aligned. If NULL, align all peptides.
<code>mstNet</code>	(matrix) array of tree-edges. Look up <code>getMST</code> .
<code>applyFun</code>	(function) value must be either <code>lapply</code> or <code>BiocParallel::bplapply</code> .

Value

(None)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-05-15

See Also

[alignTargetedRuns](#), [progAlignRuns](#), [getMST](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
params <- paramsDIAAlignR()
params[["context"]] <- "experiment-wide"
mstAlignRuns(dataPath, params = params, outFile = "DIAAlignR")
## Not run:
y <- strsplit("run0 run1\nrun2 run2", split = '\n')[[1]]
y <- cbind(A = strsplit(y[1], " ")[[1]], B = strsplit(y[2], " ")[[1]])
plot(igraph::graph_from_edgelist(y, directed = FALSE))

## End(Not run)
```

mstScript1

Extract features and generate minimum spanning tree.

Description

Extract features and generate minimum spanning tree.

Usage

```
mstScript1(
  dataPath,
  outFile = "DIAAlignR",
  params = paramsDIAAlignR(),
  oswMerged = TRUE,
  runs = NULL,
  mstNet = NULL,
  applyFun = lapply
)
```

Arguments

dataPath	(string) path to xics and osw directory.
outFile	(string) name of the output file.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
runs	(string) names of xics file without extension.
mstNet	(string) minimum spanning tree in string format. See example of mstScript2 .
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2022) + GPL-3 Date: 2022-04-19

See Also

[mstAlignRuns](#), [mstScript2](#)

Examples

```
params <- paramsDIAalignR()
params[["context"]] <- "experiment-wide"
dataPath <- system.file("extdata", package = "DIAalignR")
BiocParallel::register(BiocParallel::MulticoreParam(workers = 4, progressbar = TRUE))
mstScript1(dataPath, outFile = "testDIAalignR", params = params, applyFun = BiocParallel::bplapply)
file.remove(file.path(dataPath, "testDIAalignR_mst1.RData"))
```

mstScript2

Performs alignment using mstScript1 output

Description

Performs alignment using mstScript1 output

Usage

```
mstScript2(
  dataPath,
  outFile = "DIAalignR",
  params = paramsDIAalignR(),
  oswMerged = TRUE,
  scoreFile = NULL,
  peps = NULL,
  mstNet = NULL,
  applyFun = lapply
)
```

Arguments

dataPath	(string) path to xics and osw directory.
outFile	(string) name of the output file.
params	(list) parameters are entered as list. Output of the paramsDIAalignR function.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
scoreFile	(string) path to the peptide score file, needed when oswMerged is FALSE.

peps (integer) ids of peptides to be aligned. If NULL, align all peptides.
 mstNet (string) minimum spanning tree in string format. See example of [mstScript2](#).
 applyFun (function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2022) + GPL-3 Date: 2022-04-19

See Also

[mstAlignRuns](#), [mstScript1](#)

Examples

```
params <- paramsDIAAlignR()
params[["context"]] <- "experiment-wide"
dataPath <- system.file("extdata", package = "DIAAlignR")
BiocParallel::register(BiocParallel::MulticoreParam(workers = 4, progressbar = TRUE))
mstScript1(dataPath, outFile = "testDIAAlignR", params = params, applyFun = BiocParallel::bplapply)
mstNet <- "run0 run0\nrun1 run2"
mstScript2(dataPath, outFile = "testDIAAlignR", params = params, mstNet = mstNet, applyFun = lapply)
file.remove(file.path(dataPath, "testDIAAlignR_mst1.RData"))
file.remove("testDIAAlignR.tsv")
```

multipeptide_DIAAlignR *Analytes information from multipeptide.*

Description

analytes info from three SWATH runs:

run0 : hroest_K120808_Strep10%PlasmaBiolRepl1_R03_SW_filt.chrom.mzML

run1 : hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt.chrom.mzML

run2 : hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt.chrom.mzML

Usage

```
multipeptide_DIAAlignR
```

Format

A list of 199 elements where each element represents a precursor and consists of a dataframe:

transition_group_id ID of each precursor. Same as the name of the list

RT Retention time, in sec

intensity Intensity of associated feature

leftWidth Left width of the peak, in sec
rightWidth Right width of the peak, in sec
peak_group_rank Ranking of associated feature
m_score qvalue of associated feature
run Name of the run, feature is from
alignment_rank Rank of the feature after alignment

Source

Raw files are downloaded from [Peptide Atlas](#). File test_GenerateData.R has [source code](#) to generate the example data.

oswFiles_DIAAlignR	<i>Analytes information from osw files</i>
--------------------	--

Description

analytes info from three SWATH runs:

run0 : hroest_K120808_Strep10%PlasmaBiolRep11_R03_SW_filt.chrom.mzML

run1 : hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt.chrom.mzML

run2 : hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt.chrom.mzML

Usage

```
oswFiles_DIAAlignR
```

Format

A list of three elements where each element consists of a dataframe:

transition_group_id ID of each peptide
RT Retention time, in sec
intensity Intensity of associated feature
leftWidth Left width of the peak, in sec
rightWidth Right width of the peak, in sec
peak_group_rank Ranking of associated feature
m_score qvalue of associated feature

Source

Raw files are downloaded from [Peptide Atlas](#). File test_GenerateData.R has [source code](#) to generate the example data.

otherChildXICpp	<i>Get child chromatogram for other precursors using main precursor alignment</i>
-----------------	---

Description

Get child chromatogram for other precursors using main precursor alignment

Usage

```
otherChildXICpp(  
  l1,  
  l2,  
  kernelLen,  
  polyOrd,  
  mat,  
  childTime,  
  wRef = 0.5,  
  splineMethod = "natural"  
)
```

Arguments

l1	(list) A list of numeric matrix of two columns. l1 and l2 should have same length.
l2	(list) A list of numeric matrix of two columns. l1 and l2 should have same length.
kernelLen	(integer) length of filter. Must be an odd number.
polyOrd	(integer) TRUE: remove background from peak signal using estimated noise levels.
mat	(matrix) aligned time and child time from the main precursor.
childTime	(numeric) iime vector from the child chromatogram.
wRef	(numeric) Weight of the reference XIC. Must be between 0 and 1.
splineMethod	(string) must be either "fmm" or "natural".

Value

(List) of chromatograms.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2021) + MIT Date: 2021-01-08

Examples

```

data(XIC_QFNNTDIVLLEDFQK_3_DIAalignR, package="DIAalignR")
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR
XICs.ref <- lapply(XICs[["hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt"]][["4618"]], as.matrix)
XICs.eXp <- lapply(XICs[["hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt"]][["4618"]], as.matrix)
Bp <- seq(4964.752, 5565.462, length.out = nrow(XICs.ref[[1]]))
chrom <- getChildXICpp(XICs.ref, XICs.eXp, 11L, 4L, alignType = "hybrid", adaptiveRT = 77.82315,
  normalization = "mean", simType = "dotProductMasked", Bp = Bp,
  goFactor = 0.125, geFactor = 40, cosAngleThresh = 0.3, OverlapAlignment = TRUE,
  dotProdThresh = 0.96, gapQuantile = 0.5, hardConstrain = FALSE, samples4gradient = 100,
  wRef = 0.5, keepFlanks = TRUE)
chrom2 <- otherChildXICpp(XICs.ref, XICs.eXp, 11L, 4L, chrom[[2]], chrom[[1]][[1]][,1],
  0.5, "natural")

```

paramsDIAalignR

*Parameters for the alignment functions***Description**

Retention alignment requires OpenSWATH/pyProphet extracted features and chromatograms. This function provides a suite of parameters used for selecting features and manipulating chromatograms. Chromatogram alignment can be performed via reference based or progressively via rooted or unrooted tree. This function provides sensible parameters for these tasks.

Usage

```
paramsDIAalignR()
```

Value

A list of parameters:

runType	(string) must be one of the strings "DIA_Proteomics", "DIA_IPF", "DIA_Metabolomics".
chromFile	(string) must either be "mzML" or "sqMass".
maxFdrQuery	(numeric) a numeric value between 0 and 1. It is used to filter peptides from osw file which have SCORE_MS2.QVALUE less than itself.
maxIPFFdrQuery	(numeric) A numeric value between 0 and 1. It is used to filter features from osw file which have SCORE_IPF.QVALUE less than itself. (For PTM IPF use)
maxPeptideFdr	(numeric) a numeric value between 0 and 1. It is used to filter peptides from osw file which have SCORE_PEPTIDE.QVALUE less than itself.
analyteFDR	(numeric) the upper limit of feature FDR to be it considered for building tree.
treeDist	(string) the method used to build distance matrix. Must be either "rsquared", "count" or "RSE".
treeAgg	(string) the method used for agglomeration while performing hierarchical clustering. Must be either "single", "average" or "complete".

alignToRoot	(logical) if TRUE, align leaves to the root in hierarchical clustering, else use already save aligned vectors.
prefix	(string) name to be used to define merged runs.
context	(string) used in pyprophet peptide. Must be either "run-specific", "experiment-wide", or "global".
unalignedFDR	(numeric) must be between 0 and maxFdrQuery. Features below unalignedFDR are considered for quantification even without the RT alignment.
alignedFDR1	(numeric) must be between unalignedFDR and alignedFDR2. Features below alignedFDR1 and aligned to the reference are considered for quantification.
alignedFDR2	(numeric) must be between alignedFDR1 and maxFdrQuery. Features below alignedFDR2 and within certain distance from the aligned time are considered for quantification after the alignment.
criterion	(integer) strategy to select peak if found overlapping peaks. 1:intensity, 2: RT overlap, 3: mscore, 4: edge distance
level	(string) apply maxPeptideFDR on Protein as well if specified as "Protein". Default: "Peptide".
integrationType	(string) method to compute the area of a peak contained in XICs. Must be from "intensity_sum", "trapezoid", "simpson".
baseSubtraction	logical TRUE: remove background from peak signal using estimated noise levels.
baselineType	(string) method to estimate the background of a peak contained in XICs. Must be from "none", "base_to_base", "vertical_division_min", "vertical_division_max".
fitEMG	(logical) enable/disable exponentially modified gaussian peak model fitting.
recalIntensity	(logical) recalculate intensity for all analytes.
fillMissing	(logical) calculate intensity for analytes for which features are not found.
XICfilter	(string) must be either sgolay, boxcar, gaussian, loess or none.
polyOrd	(integer) order of the polynomial to be fit in the kernel.
kernellLen	(integer) number of data-points to consider in the kernel.
globalAlignment	(string) must be either "loess" or "linear".
globalAlignmentFdr	(numeric) a numeric value between 0 and 1. Features should have m-score lower than this value for participation in LOESS fit.
globalAlignmentSpan	(numeric) spanvalue for LOESS fit. For targeted proteomics 0.1 could be used.
RSEdistFactor	(numeric) defines how much distance in the unit of rse remains a noBeef zone.
normalization	(string) must be selected from "mean", "l2".
simMeasure	(string) must be selected from dotProduct, cosineAngle, crossCorrelation, cosine2Angle, dotProductMasked, euclideanDist, covariance and correlation.
alignType	(numeric) available alignment methods are "global", "local" and "hybrid".

goFactor	(numeric) penalty for introducing first gap in alignment. This value is multiplied by base gap-penalty. Should be between 10-1000.
geFactor	(numeric) penalty for introducing subsequent gaps in alignment. This value is multiplied by base gap-penalty.
cosAngleThresh	(numeric) in simType = dotProductMasked mode, angular similarity should be higher than cosAngleThresh otherwise similarity is forced to zero.
OverlapAlignment	(logical) an input for alignment with free end-gaps. False: Global alignment, True: overlap alignment.
dotProdThresh	(numeric) in simType = dotProductMasked mode, values in similarity matrix higher than dotProdThresh quantile are checked for angular similarity.
gapQuantile	(numeric) must be between 0 and 1. This is used to calculate base gap-penalty from similarity distribution.
kerLen	(integer) In simType = crossCorrelation, length of the kernel used to sum similarity score. Must be an odd number.
hardConstrain	(logical) if FALSE; indices farther from noBeef distance are filled with distance from linear fit line.
samples4gradient	(numeric) modulates penalization of masked indices.
fillMethod	(string) must be either "spline", "sgolay" or "linear".
splineMethod	(string) must be either "fmm" or "natural".
mergeTime	(string) must be either "ref", "avg", "refStart" or "refEnd".
keepFlanks	(logical) TRUE: Flanking chromatogram is not removed.
fraction	(integer) indicates which fraction to align.
fractionNum	(integer) Number of fractions to divide the alignment.
lossy	(logical) if TRUE, time and intensity are lossy-compressed in generated sqMass file.
useIdentifying	(logical) Set TRUE to use identifying transitions in alignment. (DEFAULT: FALSE)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-07-11

See Also

[checkParams](#), [alignTargetedRuns](#)

Examples

```
params <- paramsDIAAlignR()
```

plotAlignedAnalytes *Plot aligned XICs group for a specific peptide. AlignObjOutput is the output from getAlignObjs function.*

Description

Plot aligned XICs group for a specific peptide. AlignObjOutput is the output from getAlignObjs function.

Usage

```
plotAlignedAnalytes(  
  AlignObjOutput,  
  plotType = "All",  
  outFile = "AlignedAnalytes.pdf",  
  annotatePeak = FALSE,  
  saveFigs = FALSE  
)
```

Arguments

AlignObjOutput (list) list contains fileInfo, AlignObj, raw XICs for reference and experiment, and reference-peak label.

plotType (string) must be one of the strings "All", "onlyUnaligned" and "onlyAligned".

outFile (string) name of the output pdf file.

annotatePeak (logical) TRUE: Peak boundaries and apex will be highlighted.

saveFigs (logical) TRUE: Figures will be saved in AlignedAnalytes.pdf .

Value

A plot to the current device.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")  
runs <- c("hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt",  
  "hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt")  
AlignObjOutput <- getAlignObjs(analytes = 4618L, runs, dataPath = dataPath)  
plotAlignedAnalytes(AlignObjOutput)
```

plotAlignmentPath *Visualize alignment path through similarity matrix*

Description

Plot aligned path through the similarity matrix. Reference run has indices on X-axis, eXp run has them on Y-axis. In getAlignObjs function, objType must be set to medium.

Usage

```
plotAlignmentPath(AlignObjOutput)
```

Arguments

AlignObjOutput (list) The list contains AlignObj, raw XICs for reference and experiment, and reference-peak label.

Value

A plot to the current device.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

Examples

```
library(lattice)
dataPath <- system.file("extdata", package = "DIAAlignR")
runs <- c("hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt",
         "hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt")
AlignObjOutput <- getAlignObjs(analytes = 4618L, runs, dataPath = dataPath, objType = "medium")
plotAlignmentPath(AlignObjOutput)
```

plotAnalyteXICs *Plot extracted-ion chromatogram.*

Description

Plot extracted-ion chromatogram.

Usage

```
plotAnalyteXICs(
  analyte,
  run,
  dataPath = ".",
  maxFdrQuery = 1,
  XICfilter = "sgolay",
  polyOrd = 4,
  kernellLen = 9,
  runType = "DIA_Proteomics",
  oswMerged = TRUE,
  peakAnnot = NULL,
  Title = NULL
)
```

Arguments

analyte	(integer) an analyte is a PRECURSOR.ID from the osw file.
run	(string) Name of a xics file without extension.
dataPath	(string) path to xics and osw directory.
maxFdrQuery	(numeric) A numeric value between 0 and 1. It is used to filter features from osw file which have SCORE_MS2.QVALUE less than itself.
XICfilter	(string) must be either sgolay, boxcar, gaussian, loess or none.
polyOrd	(integer) order of the polynomial to be fit in the kernel.
kernellLen	(integer) number of data-points to consider in the kernel.
runType	(char) This must be one of the strings "DIA_Proteomics", "DIA_Metabolomics".
oswMerged	(logical) TRUE for experiment-wide FDR and FALSE for run-specific FDR by pyprophet.
peakAnnot	(numeric) Peak-apex time.
Title	(logical) TRUE: name of the list will be displayed as title.

Value

A plot to the current device.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

See Also

[plotXICgroup](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
run <- "hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt"
plotAnalyteXICs(analyte = 2474L, run, dataPath = dataPath, oswMerged = TRUE, XICfilter = "none")
plotAnalyteXICs(analyte = 2474L, run, dataPath = dataPath, oswMerged = TRUE, XICfilter = "sgolay")
```

plotXICgroup

Plot Extracted-ion chromatogram group.

Description

Plot Extracted-ion chromatogram group.

Usage

```
plotXICgroup(XIC_group, peakAnnot = NULL, Title = NULL)
```

Arguments

XIC_group	(list) It is a list of dataframe which has two columns. First column is for time and second column indicates intensity.
peakAnnot	(numeric) Peak-apex time.
Title	(logical) TRUE: name of the list will be displayed as title.

Value

A plot to the current device.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2019) + GPL-3 Date: 2019-12-13

See Also

[plotAnalyteXICs](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
runs <- c("hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt",
         "hroest_K120809_Strep10%PlasmaBiolRepl2_R04_SW_filt")
XICs <- getXICs(analytes = 4618L, runs = runs, dataPath = dataPath, oswMerged = TRUE)
plotXICgroup(XICs[["hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt"]][["4618"]])
XICs <- smoothXICs(XICs[["hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt"]][["4618"]],
                  type = "sgolay", kernelLen = 13, polyOrd = 4)
plotXICgroup(XICs, Title = "Precursor 4618 \n
run hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt")
```

 progAlignRuns

Peptide quantification through progressive alignment

Description

This function expects osw and xics directories at dataPath. It first reads osw files and fetches chromatogram indices for each analyte. To perform alignment, first a crude guide-tree is built which can also be provided with newickTree parameter. As we traverse from the leaf-nodes to the root node, runs are aligned pairwise. The root node is named master1 that has average of all fragment ion chromatograms and identified peak-groups. These features are propagated back to leaf nodes and finally aligned features are written in the output file.

Usage

```
progAlignRuns(
  dataPath,
  params,
  outFile = "DIAAlignR",
  ropenms = NULL,
  oswMerged = TRUE,
  scoreFile = NULL,
  runs = NULL,
  peps = NULL,
  newickTree = NULL,
  applyFun = lapply
)
```

Arguments

dataPath	(string) path to xics and osw directory.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
outFile	(string) name of the output file.
ropenms	(pyopenms module) get this python module through get_ropenms . Required only for chrom.mzML files.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
scoreFile	(string) path to the peptide score file, needed when oswMerged is FALSE.
runs	(string) names of xics file without extension.
peps	(integer) ids of peptides to be aligned. If NULL, align all peptides.
newickTree	(string) guidance tree in newick format. Look up getTree .
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Value

(None)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-07-10

See Also

[alignTargetedRuns](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
params <- paramsDIAAlignR()
params[["context"]] <- "experiment-wide"
## Not run:
ropenms <- get_ropenms(condaEnv = "envName")
progAlignRuns(dataPath, params = params, outFile = "test3", ropenms = ropenms)
# Removing aligned vectors
file.remove(list.files(dataPath, pattern = "*_av.rds", full.names = TRUE))
# Removing temporarily created master chromatograms
file.remove(list.files(file.path(dataPath, "xics"), pattern = "^master[A-Za-z0-9]+\\.chrom\\.\\.sqMass$", full.names = TRUE))
file.remove(file.path(dataPath, "test3.temp.RData"))
file.remove(file.path(dataPath, "master.merged.osw"))

## End(Not run)
```

progComb3

Step 3 for progressive alignment

Description

Step 3 for progressive alignment

Usage

```
progComb3(
  dataPath,
  params,
  outFile = "DIAAlignR",
  oswMerged = TRUE,
  applyFun = lapply
)
```

Arguments

dataPath	(string) path to xics and osw directory.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
outFile	(string) name of the output file.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-03-03

See Also

[progAlignRuns](#)

progSplit2

Step 2 for progressive alignment

Description

Step 2 for progressive alignment

Usage

```
progSplit2(  
  dataPath,  
  params,  
  outFile = "DIAAlignR",  
  oswMerged = TRUE,  
  applyFun = lapply  
)
```

Arguments

dataPath	(string) path to xics and osw directory.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
outFile	(string) name of the output file.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-03-03

See Also

[progAlignRuns](#)

progSplit4

Step 4 for progressive alignment

Description

Step 4 for progressive alignment

Usage

```
progSplit4(  
  dataPath,  
  params,  
  outFile = "DIAAlignR",  
  oswMerged = TRUE,  
  applyFun = lapply  
)
```

Arguments

dataPath	(string) path to xics and osw directory.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
outFile	(string) name of the output file.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-03-03

See Also

[progAlignRuns](#)

progTree1

Step 1 for progressive alignment

Description

Step 1 for progressive alignment

Usage

```
progTree1(  
  dataPath,  
  outFile = "DIAAlignR",  
  params = paramsDIAAlignR(),  
  groups = NULL,  
  oswMerged = TRUE,  
  scoreFile = NULL,  
  peps = NULL,  
  runs = NULL,  
  newickTree = NULL,  
  applyFun = lapply  
)
```

Arguments

dataPath	(string) path to xics and osw directory.
outFile	(string) name of the output file.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
groups	(data-frame) contains the run names and their categories/batch id to keep them on the same branch of the tree.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
scoreFile	(string) path to the peptide score file, needed when oswMerged is FALSE.
peps	(integer) ids of peptides to be aligned. If NULL, align all peptides.
runs	(string) names of xics file without extension.
newickTree	(string) guidance tree in newick format. Look up getTree .
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-03-03

See Also

[progAlignRuns](#)

recalculateIntensity *Calculates area of peaks in peakTable*

Description

For the give peak boundary in peakTable, the function extracts raw chromatograms and recalculate intensities.

Usage

```
recalculateIntensity(  
  peakTable,  
  dataPath = ".",  
  oswMerged = TRUE,  
  params = paramsDIAAlignR()  
)
```

Arguments

peakTable	(data-table) usually an output of alignTargetedRuns. Must have these columns: precursor, run, intensity, leftWidth, rightWidth.
dataPath	(string) path to xics and osw directory.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.

Value

(data-table)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>
ORCID: 0000-0003-3500-8152
License: (c) Author (2020) + GPL-3 Date: 2020-05-28

See Also

[alignTargetedRuns](#), [calculateIntensity](#)

Examples

```
library(data.table)  
peakTable <- data.table(precursor = c(1967L, 1967L, 2474L, 2474L),  
  run = rep(c("hroest_K120808_Strep10%PlasmaBiolRep11_R03_SW_filt",  
    "hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt"), 2),  
  intensity = c(186.166, 579.832, 47.9525, 3.7413),  
  leftWidth = c(5001.76, 5025.66, 6441.51, 6516.6),
```

```
        rightWidth = c(5076.86, 5121.25, 6475.65, 6554.2))
dataPath <- system.file("extdata", package = "DIAAlignR")
params <- paramsDIAAlignR()
params$smoothPeakArea <- TRUE
recalculateIntensity(peakTable, dataPath, params = params)
peakTable <- data.table(precursor = c(1967L, 1967L, 2474L, 2474L),
  run = rep(c("hroest_K120808_Strep10%PlasmaBiolRep11_R03_SW_filt",
    "hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt"), 2),
  intensity = list(NA, NA, NA, NA),
  leftWidth = c(5001.76, 5025.66, 6441.51, 6516.6),
  rightWidth = c(5076.86, 5121.25, 6475.65, 6554.2))
params$transitionIntensity <- TRUE
recalculateIntensity(peakTable, dataPath, params = params)
```

reduceXICs

Subset an XIC file

Description

Create a sqMass file that has chromatograms for given native IDs.

Usage

```
reduceXICs(nativeIDs, xicFileIn, xicFileOut)
```

Arguments

nativeIDs (integer) transition IDs to be kept.
xicFileIn (character) name to the current file.
xicFileOut (character) name of the new file.

Value

(None)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2022) + GPL-3 Date: 2022-04-19

See Also

[createSqMass](#), [getNativeIDs](#)

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
oswIn <- file.path(dataPath, "osw", "merged.osw")
params <- paramsDIAAlignR()
params[["context"]] <- "experiment-wide"
ids <- getNativeIDs(oswIn, 1338L, params)
xicFileIn <- file.path(dataPath, "xics", "hroest_K120809_Strep0%PlasmaBiolRepl2_R04_SW_filt.chrom.sqMass")
reduceXICs(ids, xicFileIn, xicFileOut = "temp.chrom.sqMass")
file.remove("temp.chrom.sqMass")
```

script1

Extract features and generate pairwise alignments.

Description

Extract features and generate pairwise alignments.

Usage

```
script1(
  dataPath,
  outFile = "DIAAlignR",
  params = paramsDIAAlignR(),
  oswMerged = TRUE,
  runs = NULL,
  applyFun = lapply
)
```

Arguments

dataPath	(string) path to xics and osw directory.
outFile	(string) name of the output file.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
runs	(string) names of xics file without extension.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-02-20

See Also

[alignTargetedRuns](#)

Examples

```
params <- paramsDIAAlignR()
params[["context"]] <- "experiment-wide"
dataPath <- system.file("extdata", package = "DIAAlignR")
BiocParallel::register(BiocParallel::MulticoreParam(workers = 4, progressbar = TRUE))
script1(dataPath, outFile = "testDIAAlignR", params = params, applyFun = BiocParallel::bplapply)
file.remove(file.path(dataPath, "testDIAAlignR_script1.RData"))
```

script2

Performs alignment using script1 output

Description

Performs alignment using script1 output

Usage

```
script2(
  dataPath,
  outFile = "DIAAlignR",
  params = paramsDIAAlignR(),
  oswMerged = TRUE,
  scoreFile = NULL,
  peps = NULL,
  refRun = NULL,
  applyFun = lapply
)
```

Arguments

dataPath	(string) path to xics and osw directory.
outFile	(string) name of the output file.
params	(list) parameters are entered as list. Output of the paramsDIAAlignR function.
oswMerged	(logical) TRUE if merged file from pyprophet is used.
scoreFile	(string) path to the peptide score file, needed when oswMerged is FALSE.
peps	(integer) ids of peptides to be aligned. If NULL, align all peptides.
refRun	(string) reference for alignment. If no run is provided, m-score is used to select reference run.
applyFun	(function) value must be either lapply or BiocParallel::bplapply.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2021) + GPL-3 Date: 2021-02-20

See Also[alignTargetedRuns](#)**Examples**

```
params <- paramsDIAalignR()
params[["context"]] <- "experiment-wide"
dataPath <- system.file("extdata", package = "DIAalignR")
BiocParallel::register(BiocParallel::MulticoreParam(workers = 4, progressBar = TRUE))
script1(dataPath, outFile = "testDIAalignR", params = params, applyFun = BiocParallel::bplapply)
script2(dataPath, outFile = "testDIAalignR", params = params, applyFun = lapply)
file.remove(file.path(dataPath, "testDIAalignR_script1.RData"))
```

`sgolayCpp`*Smooth chromatogram with savitzky-golay filter.*

Description

Smooth chromatogram with savitzky-golay filter.

Usage

```
sgolayCpp(chrom, kernelLen, polyOrd)
```

Arguments

<code>chrom</code>	(matrix) chromatogram containing time and intensity vectors.
<code>kernelLen</code>	(integer) length of filter. Must be an odd number.
<code>polyOrd</code>	(integer) TRUE: remove background from peak signal using estimated noise levels.

Value

(matrix).

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c)
Author (2020) + MIT Date: 2019-12-31

Examples

```
data("XIC_QFNNTDIVLLEDFQK_3_DIAalignR", package = "DIAalignR")
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR[["hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt"]][["4618"]]
xic <- sgolayCpp(as.matrix(XICs[[1]]), kernelLen = 11L, polyOrd = 4L)
```

smoothSingleXIC	<i>Smooth chromatogram signal</i>
-----------------	-----------------------------------

Description

Smoothing methods are Savitzky-Golay, Boxcar, Gaussian kernel and LOESS. Savitzky-Golay smoothing is good at preserving peak-shape compared to gaussian and boxcar smoothing. However, it assumes equidistant points that fortunately is the case for DIA data. This requires a quadratic memory to store the fit and slower than other smoothing methods.

Usage

```
smoothSingleXIC(  
  chromatogram,  
  type,  
  samplingTime = NULL,  
  kernellLen = NULL,  
  polyOrd = NULL  
)
```

Arguments

chromatogram	(dataframe) A dataframe of two columns. First column must always be monotonically increasing.
type	(char) must be either sgolay, boxcar, gaussian, loess or none.
samplingTime	(numeric) Time difference between neighboring points.
kernellLen	(integer) Number of data-points to consider in the kernel.
polyOrd	(integer) Order of the polynomial to be fit in the kernel.

Details

Gaussian smoothing uses a gaussian function whose bandwidth is scaled by 0.3706505 to have quartiles at $\pm 0.25 * \text{bandwidth}$. The point selection cut-off is also hard at $0.3706505 * 4 * \text{bandwidth}$. `qnorm(0.75, sd = 0.3706505)`

The definition of `C_ksmooth` can be found using `getAnywhere('C_ksmooth') stats:::C_ksmooth`

Value

A dataframe with two columns.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL3 Date: 2020-02-21

See Also

<https://terpconnect.umd.edu/~toh/spectrum/Smoothing.html>, <https://rafalab.github.io/dsbook/smoothing.html>, <https://github.com/SurajGupta/r-source/blob/master/src/library/stats/src/ksmooth.c>

Examples

```
data("XIC_QFNNTDIVLLEDFQK_3_DIAalignR")
chrom <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR[["hroest_K120808_Strep10%PlasmaBio1Rep11_R03_SW_filt"]][["4618"]][[1]]
## Not run:
newChrom <- smoothSingleXIC(chrom, type = "sgolay", samplingTime = 3.42, kernelLen = 9,
  polyOrd = 3)
## End(Not run)
```

smoothXICs

Smooth chromatogram signals from a list

Description

Smoothing methods are Savitzky-Golay, Boxcar, Gaussian kernel and LOESS. Savitzky-Golay smoothing is good at preserving peak-shape compared to gaussian and boxcar smoothing. However, it assumes equidistant points that fortunately is the case for DIA data. This requires a quadratic memory to store the fit and slower than other smoothing methods.

Usage

```
smoothXICs(
  XICs,
  type = "none",
  samplingTime = NULL,
  kernelLen = 9L,
  polyOrd = NULL
)
```

Arguments

XICs	(A list) A list of dataframe that consists of two columns. First column must be monotonically increasing.
type	(char) must be either sgolay, boxcar, gaussian, loess or none.
samplingTime	(numeric) Time difference between neighboring points.
kernelLen	(integer) Number of data-points to consider in the kernel.
polyOrd	(integer) Order of the polynomial to be fit in the kernel.

Value

A list.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL3 Date: 2020-02-21

See Also

<https://terpconnect.umd.edu/~toh/spectrum/Smoothing.html>, <https://rafalab.github.io/dsbook/smoothing.html>

Examples

```
data("XIC_QFNNTDIVLLEDFQK_3_DIAalignR")
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR[["hroest_K120808_Strep10%PlasmaBiolRep1_R03_SW_filt"]][["4618"]]
newXICs <- smoothXICs(XICs, type = "sgolay", samplingTime = 3.42, kernelLen = 9,
  polyOrd = 3)
```

splineFillCpp

Interpolate using spline

Description

Interpolate using spline

Usage

```
splineFillCpp(x, y, xout)
```

Arguments

x (numeric) A numeric matrix with similarity values of two sequences or signals.
y (numeric) Penalty for introducing first gap in alignment.
xout (numeric) Penalty for introducing subsequent gaps in alignment.

Value

(numeric)

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca> ORCID: 0000-0003-3500-8152 License: (c) Author (2021) + MIT Date: 2021-01-06

Examples

```
time <- seq(from = 3003.4, to = 3048, by = 3.4)
y <- c(0.2050595, 0.8850070, 2.2068768, 3.7212677, 5.1652605, 5.8288915, 5.5446804,
      4.5671360, 3.3213154, 1.9485889, 0.9520709, 0.3294218, 0.2009581, 0.1420923)
y[c(1,6)] <- NA_real_
idx <- !is.na(y)
splineFillCpp(time[idx], y[idx], time[!idx])
zoo::na.spline(zoo::zoo(y[idx], time[idx]), xout = time[!idx], method = "natural")
```

trimXICs

Selects a part of chromatograms

Description

This function trims chromatograms from the end-points.

Usage

```
trimXICs(XICs, len = 1)
```

Arguments

XICs	(A list) A list of dataframe that consists of two columns. First column must be monotonically increasing.
len	(numeric) must be between 0.1 and 1.

Value

A list.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL3 Date: 2020-04-01

Examples

```
data("XIC_QFNNTDIVLLEDFQK_3_DIAalignR")
XICs <- XIC_QFNNTDIVLLEDFQK_3_DIAalignR[["hroest_K120808_Strep10%PlasmaBiolRep11_R03_SW_filt"]][["4618"]]
## Not run:
newXICs <- smoothXICs(XICs, len = 0.5)

## End(Not run)
```

updateFileInfo	<i>Get intersection of runs and fileInfo</i>
----------------	--

Description

Get intersection of runs and fileInfo

Usage

```
updateFileInfo(fileInfo, runs = NULL)
```

Arguments

fileInfo (data-frame) output of getRunNames function.
runs (vector of string) names of mzML files without extension.

Value

(dataframe) it has five columns:

spectraFile (string) as mentioned in RUN table of osw files.
runName (string) contain respective mzML names without extension.
spectraFileID (string) ID in RUN table of osw files.
featureFile (string) path to the feature file.
chromatogramFile (string) path to the chromatogram file.

Author(s)

Shubham Gupta, <shubh.gupta@mail.utoronto.ca>

ORCID: 0000-0003-3500-8152

License: (c) Author (2020) + GPL-3 Date: 2020-04-15

Examples

```
dataPath <- system.file("extdata", package = "DIAAlignR")
fileInfo <- getRunNames(dataPath = dataPath, oswMerged = TRUE)
runs <- c("hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt",
         "hroest_K120808_Strep10%PlasmaBiolRep11_R03_SW_filt")
updateFileInfo(fileInfo, runs)
```

XIC_QFNNTDIVLLEDFQK_3_DIAalignR

Extracted-ion chromatograms (XICs) of a peptide

Description

XICs of peptide QFNNTDIVLLEDFQK/3 (precursor ID: 4618) from three SWATH runs:

run0 : hroest_K120808_Strep10%PlasmaBiolRep11_R03_SW_filt.chrom.mzML

run1 : hroest_K120809_Strep0%PlasmaBiolRep12_R04_SW_filt.chrom.mzML

run2 : hroest_K120809_Strep10%PlasmaBiolRep12_R04_SW_filt.chrom.mzML

Usage

XIC_QFNNTDIVLLEDFQK_3_DIAalignR

Format

A list of three elements where each element consists of a list of six data frames. Each data frame has two columns:

time Retention time of ananlyte in the run, in sec

intensity Intensity of signal for the transition

Source

Raw files are downloaded from [Peptide Atlas](#). File test_GenerateData.R has [source code](#) to generate the example data.

Index

* datasets

- alignObj_DIALignR, 8
 - masterXICs_DIALignR, 60
 - multipeptide_DIALignR, 64
 - oswFiles_DIALignR, 65
 - XIC_QFNNTDIVLLEDFQK_3_DIALignR, 89
- addXIC, 17
- AffineAlignObj (AffineAlignObj-class), 3
- AffineAlignObj-class, 3
- AffineAlignObjLight
- (AffineAlignObjLight-class), 4
- AffineAlignObjLight-class, 4
- AffineAlignObjMedium
- (AffineAlignObjMedium-class), 4
- AffineAlignObjMedium-class, 4
- alignChromatogramsCpp, 5, 23, 26, 28
- AlignObj (AlignObj-class), 7
- AlignObj-class, 7
- alignObj_DIALignR, 8
- alignTargetedRuns, 9, 62, 69, 75, 79, 81, 83
- alignToRoot4, 10
- analytesFromFeatures, 56
- areaIntegrator, 11
- as.list, AffineAlignObj-method, 12
- as.list, AffineAlignObjLight-method, 13
- as.list, AffineAlignObjMedium-method, 13
- as.list, AlignObj-method, 14
- blobXICs, 19
- calculateIntensity, 79
- checkParams, 69
- childXIC, 16
- childXICs, 15, 34
- chromatogramIdAsInteger, 36, 47
- constrainSimCpp, 16
- createMZML, 17, 19
- createSqMass, 18, 80
- DIALignR, 19
- doAffineAlignmentCpp, 4, 5, 19
- doAlignmentCpp, 7, 21
- fetchPeptidesInfo, 45
- fetchPrecursorsInfo, 39, 46, 49
- fetchTransitionsFromRun, 55
- get_ropenms, 17, 57, 74
- getAlignedTimes, 22
- getAlignedTimesCpp, 24
- getAlignedTimesFast, 26
- getAlignObj, 23, 26, 27, 30
- getAlignObjs, 29
- getBaseGapPenaltyCpp, 30
- getChildXICCpp, 31
- getChildXICs, 33
- getChromatogramIndices, 35, 57
- getChromSimMatCpp, 36
- getFeatures, 10, 30, 38, 41, 42, 49
- getGlobalAlignMaskCpp, 39
- getGlobalAlignment, 40, 51
- getMST, 61, 62
- getMultipeptide, 10, 41
- getMZMLpointers, 42
- getNativeIDs, 43, 80
- getNodeRun, 34
- getPeptideScores, 44, 50
- getPrecursorByID, 45
- getPrecursorIndices, 46
- getPrecursors, 42, 47, 49
- getRefExpFeatureMap, 49
- getRefRun, 50
- getRTdf, 51
- getRunNames, 10, 30, 34, 38, 39, 44–46, 48, 49, 52, 54–57
- getSeqSimMatCpp, 53
- getTransitions, 54
- getTree, 74, 78
- getXICs, 55

getXICs4AlignObj, 30, 56, 56

imputeChromatogram, 58

mapIdxToTime, 59

mapPrecursorToChromIndices, 36, 47

masterXICs_DIAAlignR, 60

mergeXIC, 16

mst, 61

mstAlignRuns, 61, 63, 64

mstScript1, 62, 64

mstScript2, 62, 63, 63, 64

multipeptide_DIAAlignR, 64

na.approx, 59

na.spline, 59

oswFiles_DIAAlignR, 65

otherChildXICpp, 66

paramsDIAAlignR, 9, 10, 26, 29, 34, 43, 52, 55,
61–63, 67, 74, 76–79, 81, 82

plotAlignedAnalytes, 30, 70

plotAlignmentPath, 71

plotAnalyteXICs, 71, 73

plotXICgroup, 72, 73

progAlignRuns, 11, 62, 74, 76–78

progComb3, 75

progSplit2, 76

progSplit4, 77

progTree1, 78

recalculateIntensity, 79

reduceXICs, 44, 80

script1, 81

script2, 82

setAlignmentRank, 10

sgolayCpp, 83

smoothSingleXIC, 84

smoothXICs, 85

splineFillCpp, 86

trimXICs, 87

updateFileInfo, 88

XIC_QFNNTDIVLLEDFQK_3_DIAAlignR, 89