07−MathDAMP−Reference

This notebook provides reference documentation for MathDAMP functions.

DAMPAlign

DAMPAlign[msdata,shiftfunction,timepoints,options] aligns msdata according to timeshift function
  shiftfunction and selects (by interpolation) time points identical to the ones in the timepoints list.
Options:
SampleNameSuffix − string to be added to the SampleName from the
  msdata to keep track of modifications performed on the dataset (default: "a")

DAMPAlignAnnotationTable

DAMPAlignAnnotationTable[peaklist,annotationtable,options] aligns annotationtable to
  peaklist and returns the new annotation table. Options for DAMPFitShiftFunction, which
  is used internally, may be passed directly via options. Additional option Resolution
  determines the rounding of m/z values in the annotation table. If the resulting annotation
  table is intended to be used on a density plot where the underlying data were binned
  to 0.1 m/z resolution, the resolution option should be set to 0.1 as well (default: 1)

DAMPAlignPeakList

DAMPAlignPeakList[peaklist,timeshiftfunction] applies the retention/
  migration time shift function timeshiftfunction to all retention/migration times
  in the peaklist (expected to have format as returned by the function DAMPPickPeaks)

DAMPAnnotationTableToPeakList

DAMPAnnotationTableToPeakList[annotationtable,options] converts
  an annotation table (execute ?DAMPLoadAnnotation for format description)
  to a peaklist with format as returned by the function DAMPPickPeaks.
Options:
Resolution − determines to which resolution
  the m/z values in the annotation table will be rounded (default: 1)

DAMPAppendToSampleName

DAMPAppendToSampleName[msdata4,string] appends string to the SampleName in msdata4.
  msdata4 is expected to be a list of rules (format as the fourth element in the msdata
  format). The added string is enclosed inside two vertical bars. If previous modifiers are
  present, the newly added string will be separated from these by a single vertical bar.
Options:
ShareBars − if set to False, the newly added string is separated from
  previous modifiers by two vertical bars with a space in between (default: True)

DAMPApplyFunctionToGroup

DAMPApplyFunctionToGroup[msdatas,function,options] applies function to either all
  corresponding signal intensities in the datasets or to the msdatas (decided by option).
Options:
ApplyToIntensitiesOnly − if set to true, the function is applied to the corresponding
  signal intentisites in the msdatas (instead of to the whole msdatas list) (default: True)
ResultSampleName − string to be set as the SampleName of the resulting dataset. If set to
  Automatic, the SampleName of the first dataset from msdatas is used (default: Automatic)
SampleNameSuffix − string to be added to the SampleName to keep the
  track of the modifications performed on the dataset (default: "")

DAMPApplyFunctionToSingle

DAMPApplyFunctionToSingle[msdata,function,options] applies a pure function function to msdata.
Options:
SampleNameSuffix − string to be added to the SampleName from
  the msdata to keep track of modifications performed on the dataset (default: "")

DAMPBinChromatogram

DAMPBinChromatogram[chromatogram,binsize,options] bins the chromatogram
  by dissecting it into intervals of size binsize (minutes) and applying the binning
  function passed as an option to signal intensities and timepoints in every interval.
Options:
BinningFunction − function to be applied to
  signal intensities and timepoints in every interval (default: Mean)

DAMPCheckDir

DAMPCheckDir[directory] checks if directory exists, creates it if
  it does not. The parent directory must exist, error message is shown otherwise.

DAMPCrop

DAMPCrop[msdata,options] reduces the msdata dataset to
   datapoints falling within the timerange and m/z value range specified by options:
mzRange − two element list specifying the cropping m/z value range (default: All)
TimeRange − two element list specifying the cropping time range (default: All).

DAMPDensityPlot

DAMPDensityPlot[msdata,options] plots the msdata using the
   ListDensityPlot function. A gradient palette is used for representing the signal
   intensities and the plot may be annotated to allow easier identification of peaks.
Options:
MaxScale − determines the extent of the signal intensity scale (default: Automatic)
LogScale − determines whether the signal
   intensities should be displayed using a logarithmic scale (default: False)
FrameTickFreqs − frequencies at which tickmarks are placed on the time axis (frequency in minutes)
   and on the m/z axis (in terms of the number of elements in the msdata's mz list) (default: {1,1})
FrameTickOffsets − determines the positions with respect to the origin of msdata'
   s dimensions at which the tickmarks are started to be placed (default: {0,0})
mzTickShift − shift of tickmark positioning on the m/z axis (default: −0.5)
mzFrameTicks − a list of custom frame tickmarks to be shown on the m/z axis (default: Automatic)
Palette − list of color specifications to be used for
   representing the signal intensity values (default: DAMPGradientPalette[])
mzGridLineFreq − frequency of horizontal gridlines in terms of the number of elements in the msdata's m/
   z value list. Enter a list of values to place the gridlines at certain specified positions (default: 5)
mzGridLineStyle − style options for horizontal gridlines (default: {{AbsoluteThickness[
   0.25],GrayLevel[0.5]},{AbsoluteThickness[0.25],GrayLevel[0.5],Dashing[{0.01,0.01}]}})
AnnotationTables − list of annotation tables to be overlaid on the plot (default: None)
PlotOptions − options for the ListDensityPlot function (default: {Mesh->False,ImageSize->
   930,AspectRatio->0.35,FrameLabel->{"Time (min)","m/z"},TextStyle->DAMPTextStyle})
AnnotationOptions − lists of options for the DAMPDrawAnnotation function
   for each annotation table. The number of lists of options must
   correspond to the number of passed annotation tables (default: Automatic)

DAMPDPScore

DAMPDPScore[peaklist1,peaklist2,options] calculates the dynamic programming (DP)
   score between two peaklists having format as returned by the DAMPPickPeaks function.
Options:
GapPenalty − gap penalty (in minutes) for DP (default: 0.5)

DAMPDrawAnnotation

DAMPDrawAnnotation[annotationtable,options] draws the annotation for density plots.
   (For details about the format of the annotationtable, execute ?DAMPLoadAnnotationTable.)
Options:
TimeRange − time range for which the annotation should be drawn (default: {0,50})
MZs − list of m/z values for which the annotation should be drawn. The order of m/z values in the mzs
   list determines the positioning of annotation labels along the m/z scale (default: Range[50.,1000.,1.])
Resolution − resolution to which the underlying data were binned. The m/
   z values from the annotation table will be rounded accordingly to
   ensure the appropriate appearance of the annotation labels (default: 1)
ScaleCoefficients − coefficients used to convert the scales (currently used
   for timescale only, the second item is 1 by default) of the annotation
   table to the scales of the ListDensityPlot (default: {62.2488,1})
TextStyle − style options for the annotation label's text (default: Join[{FontSize->4},DAMPTextStyle])
LabelStyle − style options for the annotation label's mark (default: {AbsoluteThickness[.25]})
LabelShape − pure function to draw the annotation label's mark.
   Two parameters are passed to the function, first determining the position {xpos,
   ypos}, and second determining the size {xsize,ysize}. (default: Circle[#1,#2]&)
LabelSize − size of the annotation label's mark (relative units). When relative size
   {1,1} is used by the Circle function as radius, an ellipse is drawn which appears to
   appropriately capture the dimensions of peaks on the ListDensityPlot (default: {1,1})

DAMPDropMZs

DAMPDropMZs[msdata,mzs] reduces the msdata datased by
   eliminating datapoints corresponding to m/z values specified in the mzs list.

DAMPExportBDT

DAMPExportBDT[filename,msdata] exports data in a *Math*DAMP format {matrix of signal intensities,
   list of m/z values, list of timepoints, additional information (list of rules)} into a BDT
   format file specified by filename. The m/z values in the data are not saved one by one but
   as a range specified by min, max and step. Because of this, only data having a regular
   list of m/z values which can be converted to the range representation should be exported.

DAMPFilter

DAMPFilter[msdata,criteriamsdata,threshold,options] sets to 0 those
   signal intensities in msdata for which the aboslute values of corresponding signal
   intensities in the criteriamsdata dataset are not equal to or greater than threshold.
Options:
SampleNameSuffix – string to be added to the SampleName from the
   msdata to keep track of modifications performed on the dataset (default: "f")

DAMPFilter[msdata,criteriamsdata,filterfunction,options] pure function filterfunction is
   applied to the signal intensity matrix of criteriamsdata. For zero signal intensities in
   the result, the corresponding signal intensities in the msdata dataset are set to 0 as well.
Options:
SampleNameSuffix – string to be added to the SampleName from the
   msdata to keep the track of modifications performed on the dataset (default: "f")

DAMPFitShiftFunction

DAMPFitShiftFunction[peaklist1,peaklist2,options] optimizes the
   parameters of a retention/migration time shift function so that when applied to
   peaklist2 the optimum peak alignment (as measured by DAMPDPScore) is achieved.
Options:
ShiftFunction – pure function to be used as a
   retention/migration time shift function (default: $(1/(1/(\alpha \ \#)+\gamma/2)\&))$
ShiftFunctionParameters – list of parameters for optimization. If Automatic is
   specified, these are extracted automatically from ShiftFunction. The parameters may
   be also specified explicitly with seek ranges (default: $\{\{\alpha,0.8,1.2\},\{\gamma,-0.04,0.04\}\})$
GapPenalty – gap penalty value to be passed to the DAMPDPScore function for the
   scoring of the alignment. A list of gap penalty values may be passed to perform the
   fitting of the retention/migration time shift function iteratively (default: $\{3,0.5\})$
NMinimizeOptions – list of options to be passed to the NMinimize
   function used for optimization (default: {MaxIterations->1000})
TimeRange – specifies the selection time range of peaks from
   peaklist1 to be used for scoring (default: $\{0,\infty\})$

DAMPGenColors

DAMPGenColors[number] generates a list of color specifications with a number of
   elements determined by the parameter number. If number<=6, the colors are assigned
   from the following sequence: blue, red, green, yellow, cyan, magenta. If number>6,
   the hue range is split proportionally and the colors are assigned from this sequence.

DAMPGetChromatogram

DAMPGetChromatogram[msdata,mz] returns a chromatogram/electropherogram (
   a list of {time,signal intensity} elements) from msdata corresponding to m/z mz.

DAMPGetIntensities

DAMPGetIntensities[msdata,mz] returns a list of signal intensities from msdata corresponding to m/z mz.

DAMPGradient

DAMPGradient[pos1,pos2,color1,color2,backgroundgraylevel] returns a function which calculates the
   parameters for the Hue function of a specific point within a gradient. The relative location <
   0;1> of the point of interest within the gradient is the only parameter of the returned
   function. The color gradient consists of three subgradients defined by the parameters of
   the DAMPGradient function. The gradient starts with backgroundgraylevel <0;1> at relative
   position 0, then proceeds to color1 (numeric value corresponding to hue specification <0;
   1>) at pos1, and color2 at pos2, and finally to darkened color2 at the relative position 1.

DAMPGradientPalette

DAMPGradientPalette[options] – generates a color palette for assigning colors to intensity values on
   density plots. It uses the DAMPGradient function to create the gradients for both positive and
   negative ranges. Both gradients consist of three subgradients (execute ?DAMPGradient for details).
Options:
ColorPositions – list with two elements specifying the relative location
   within the gradient of endpoints of the middle subgradient (default: {.075,.4})
PositiveColors – hue color specification of the endpoints of the middle
   subgradient in the positive range color gradient (default: {1/6,0})
NegativeColors – hue color specification of the endpoints of the middle
   subgradient in the negative range color gradient (default: {1/2,2/3})
BackgroundGrayLevel – gray level of the density plot's background area (default: .7)
PaletteSize – number of palette entries (subdivisions) of both positive and negative
   range color gradients, palette entry for value 0 is shared between the two (default: 100)

DAMPImportBDT

DAMPImportBDT[filename,samplename] reads and processes a binary BDT file specified by filename into a *Math*
   DAMP format {matrix of signal intensities, list of m/z values, list of timepoints, additional
   information (list of rules)}. The BDT is a binary datafile used internally by The Institute for
   Advanced Biosciences (Keio University). Separate in house software for preprocessing of the Analyst QS
   generated csv files stores the data in the BDT format. Since the original csv file does not contain
   information about the sample name, this has to be specified as a second parameter (samplename).

DAMPImportCDF

DAMPImportCDF[filename,options] reads and processes a CDF file specified by filename
  into a *Math*DAMP format {matrix of signal intensities, list of m/z values, list of
  timepoints, additional information (list of rules)}. This function was not thoroughly
  tested with CDF files generated by different software and may not be universal.
Options:
Resolution – specifies the resolution to which the data will be binned along the m/z axis (default: 1)

DAMPImportCSV

DAMPImportCSV[filename,samplename,options] reads and processes a csv file
  generated by Analyst QS software for Agilent TOFMS and specified by filename into a
  *Math*DAMP format {matrix of signal intensities, list of m/z values, list of timepoints,
  additional information (list of rules)}. Since the csv file does not contain information
  about the sample name, this has to be specified as the second parameter (samplename).
Options:
Resolution – specifies the resolution to which the data will be binned along the m/z axis (default: 1)
Verbose – if set to True, prints a notification along with
  current time every 100 processed chromatograms/electropherograms (default: True)

DAMPImportMS

DAMPImportMS[filename] reads and processes an Agilent ChemStation MS file specified by
  filename into a *Math*DAMP format {matrix of signal intensities, list of m/z values, list
  of timepoints, additional information (list of rules)}. This function is universal for
  SIM and scan mode datafiles. The data are binned to 1 m/z unit resolution by averaging.

DAMPImportMZXML

DAMPImportMZXML[filename,samplename,options] reads and processes the first level
  MS scans from an mzXML data file specified by filename into a *Math*DAMP format {matrix
  of signal intensities, list of m/z values, list of timepoints, additional information (
  list of rules)}. The sample name is specified via the second parameter (samplename).
Options:
Resolution – specifies the resolution to which the data will be binned along the m/z axis (default: 1)
ImportMode – determines the m/z dimension elements. If set to Sequential, the m/z dimension is
  represented by a discrete range of values determined by the smallest and the largest m/z value in
  the imported dataset (rounded according to the resolution). Resolution determines the stepsize of
  the discrete range. If set to Selective, the m/z dimension is represented by only those m/z values
  which are present in the imported dataset (rounded according to the resolution). Sequential mode
  is recommended for scan data, Selective mode is recommended for SIM data. (default: Sequential)

DAMPIntegrate

DAMPIntegrate[chromatogram,options] calculates the area below the signal intensities
  of a chromatogram/electropherogram within the retention/migration time range specified
  by the option TimeRange (default: $\{0,\infty\}$). Baseline may be calculated as an average of
  signal intensities within the timerange specified by the options BaselineFromTimeRange (
  default: None). If set to None, baseline is set to signal intensity value 0.

DAMPLoadAnnotationTable

DAMPLoadAnnotationTable[filename] loads a list of annotation labels for plots from a csv file.
  The organization of columns in the csv file is assumed to be as follows: (1) m/z value, (2)
  retention/migration time, (3) short compound name/id (density plot label text), (4) full compound
  name (chromatogram/electropherogram label text), and (5) label text position on the density
  plots relative to the label (1 – right, 2 – top, 3 – left, 4 – bottom, 1.5 – top right, etc.).

DAMPMultiGroups

DAMPMultiGroups[msdatas,replicates,options] performs the comparison of multiple groups
  of datasets containing identical number of replicates determined by the replicates
  parameter. msdatas is expected to contain an ungrouped list which will be later grouped
  according to the number of replicates. The results are returned as a list of rules
  {NormalizedDatasets->...,AlignedAnnotationTables->...,FRatios->...,GroupNames->...}
Options:
NormalizeGroupOptions – a list of options for the DAMPNormalizeGroup
  function which is used internally to normalize the datasets (default: {})
GroupNames – names to assign to groups (will be combined into the SampleName
  of the resulting FRatios dataset). If set to Automatic, the SampleName
  of the first dataset from every group is used (default: Automatic)

DAMPNormalize

DAMPNormalize[msdata,coefficient,options]
  multiplies the signal intensities in msdata (msdata⟦1⟧) with coefficient.
Options:
SampleNameSuffix – string to be added to the SampleName from the
  msdata to keep the track of modifications performed on the dataset (default: "n")

DAMPNormalizeGroup

DAMPNormalizeGroup[msdatas,options] aligns msdatas (a list of datasets) and normalizes them according to
  the areas of the peaks of the internal standard and external normalization coefficients (optional).
  The results are returned as a list of rules: {NormalizedDatasets->...,AlignedAnnotationTables->...}
Options:
Reference − position of the reference dataset within
  msdatas to which the remaining msdatas will be normalized (default: 1)
AlignmentTimeRange − peak picks from the reference dataset falling within this timerange
  only (specified as {starttime,endtime} in minutes) will be used for alignment (default: All)
RepresentativePeakOptions − options to be passed to the DAMPSelectRepresentativePeaks function to filter
  the initial peak picks (default: {PeaksPerChromatogram->5,PeaksPerInterval->8,IntervalSize->.5})
PeakPickingOptions − options to be passed to the DAMPPickPeaks function (default: {Threshold->5000})
PeakLayoutPlotOptions − options to be passed to the DAMPPlotPeakLayout function (default: {})
FitShiftFunctionOptions − options to be passed to the DAMPFitShiftFunction function (default: {})
AnnotationTables − a list of annotation tables to be aligned to the reference msdata (default: None)
OutputTimeRange − time range to which the resulting normalized datasets should be cropped (default: All)
ExternalNormalizationCoefficients − list of coefficients by which
  the signal intensities in msdatas will be multiplied. The number of coefficients
  in the list must equal the number of datasets in msdatas (default: None)
Resolution − resolution to which the datasets were binned along the m/z dimension. The annotation
  tables passed through the AnnotationTables option will be binned the same way (default: 1)
InternalStandard − the internal standard for signal intensity normalization may be specified in one
  of two ways: 1) short name (3rd column) from the first annotation table in the list passed via the
  AnnotationTables option. In this case the position of the internal standard will be extrapolated from
  the aligned annotation table and the vicinity blindly integrated 2) specifying the m/z and integration
  time range (as in the reference dataset) explicitly: {mz,{starttime,endtime}}. (default: None)
AutoISIntegrationVicinity − if the location of the internal standard is extrapolated
  from the aligned annotation table, this option determines the vicinity (in minutes) of
  the predicted retention/migration time to be blindly integrated (default: {−.25,.25})
SaveMemory − if set to true, signal intensities are rounded to
  integers in internal calculations and results (default: True)

DAMPOutliers

DAMPOutliers[msdatas,options] highlights the presence of outlying signal intensities in msdatas (
  a list of datasets). Two types of result datasets are generated: a z−score map and a
  quartile−based result. These datesets show the result for the most outlying signal intensity
  from withing the set of corresponding signal intensities. Optionally, the results may be
  generated individually for every dataset in msdatas. The results are returned as a list of
  rules: {NormalizedDatasets->...,AveragedDatasets->...,ZScores->...,ZScoresIndividual->...,
  QuartileResult->...,QuartileResultIndividual->...,AlignedAnnotationTables->...}
Options:
NormalizeGroupOptions − a list of options for the DAMPNormalizeGroup
  function which is used internally to normalize the datasets (default: {})
OutliersToDrop − specifies the number of outliers to be dropped from the
  set of corresponding signal intensities prior to calculating the
  mean and standard deviation for the z−score calculation (default: 1)
IndividualZs − if set to true, z−score map will be calculated for every
  dataset in msdatas in addition to the overall result (default: False)
IndividualQs − if set to true, results based on the interquartile range will be generated
  for every dataset in msdatas in addition to the overall result (default: False)

DAMPParallelPlot

DAMPParallelPlot[msdatas,options] plots msdatas (a list of datasets) on a density plot in a parallel
  format, so that chromatograms/electropherograms from the datasets corresponding to the same m/z
  value appear next to each other. The datasets do not have to have chromatograms corresponding
  to an identical set of m/z values, neither do the datasets have to be aligned. In the latter
  case, the time axis is labeled according to the first dataset in msdatas (please note that
  the time axis may be misleading for the remaining datasets in this case). The options are
  passed directly to the DAMPDensityPlot function which is used internally for plotting the data.

DAMPPeakListToAnnotationTable

DAMPPeakListToAnnotationTable[peaklist,options] converts the peaklist returned by DAMPPickPeaks to
  an annotation table format for plots. The peak names are assigned from sequential numbering.
Options:
TextLabelPosition − specifies the position of
  the text label relative to the annotation label mark (default: 1.5)

DAMPPickChromatogramPeaks

DAMPPickChromatogramPeaks[chromatogram,options] picks peaks from chromatogram and returns
  them as list {{Retention Time,Signal Intensity},{Retention Time,Signal Intensity},...}.
Options:
Threshold − minimum vertical distance of a new strategic point from the line
  defined by the two neighbouring strategic points. Please refer to the MathDAMP.nb
  notebook for a more detailed description of the peak picking algorithm (default: 1000)
NodeRestrictedVicinity − neigbourhood of a strategic point (in minutes)
  from which new strategic points can not be picked (default: 0.05)
CentroidVicinity − determines the time interval (in minutes) around the peak−top strategic
  point for the calculation of centroided retention/migration time (default: 0.05)

DAMPPickPeaks

DAMPPickPeaks[msdata,options] picks peaks from all chromatograms/electropherograms
   in msdata and returns them in a list {{m/z value,peaklist},{m/z value,peaklist},...}.
   The function does not have any default options, the options passed to the DAMPPickPeaks
   function are passed further to the DAMPPickChromatogramPeaks function which is
   used internally to pick peaks from individual chromatograms/electropherograms.

DAMPPlotCandidates

DAMPPlotCandidates[msdatas,criteriamsdata,options] plots a
   ranked list of overlaid chromatograms/electropherograms from msdatas datasets
   in the vicinities of the most significant signals in the criteriamsdata dataset.
Options:
PlotCount – number of chromatograms/electropherograms to plot (default: 12)
TimeRange – the most significant signals will be searched in the
   criteriamsdata dataset in this retention/migration time range only (default: All)
PlotVicinity – retention/migration time range to show on the chromatogram/
   electropherogram around the candidate difference in minutes (default: {-.6,.6})
DropVicinity – after a particular datapoint in the criteriamsdata is selected as the
   most significant signal, the vicinity of this datapoint determined by this option (
   in minutes) will no longer be searched in subsequent iterations (default: .2)
PlotChromatogramOptions – options to be passed to the DAMPPlotChromatogram function
   which is used internally to plot the chromatograms/electropherograms (default: {})

DAMPPlotChromatogram

DAMPPlotChromatogram[{msdata,msdata,...},mz,options] plots multiple overlaid
   chromatograms/electropherograms from the list of msdatas corresponding to m/z mz (
   mz may be a list of m/z values as well). The DAMPGenColors function is used by
   default to assign colors to individual chromatograms/electropherograms. Custom colors
   may be specified via the PlotOptions option (and the enclosed PlotStyle option).
Options:
PlotOptions – list of options for the MultipleListPlot function which is used
   internally for plotting (default: see the output of Options[DAMPPlotChromatogram]),
AnnotationTable – annotation table for the labeling of the chromatogram/electropherogram (default: {})
Resolution – resolution to which the msdata were binned along the m/z dimension. The annotation
   table passed through the AnnotationTable option will be rounded accordingly to ensure the
   appropriate appearance of annotation labels on the chromatogram/electropherogram (default: 1)
LegendData – a list of legend elements {{color,label},...}. If Automatic is
   specified, the SampleName from each msdata is used as a label (default: Automatic)

DAMPPlotPeakLayout

DAMPPlotPeakLayout[peaklists,options] plots the positions of peaks from a
   list of peaklists which are expected to have a format as returned by DAMPPickPeaks.
   Symbols' colors are by default assigned using the DAMPGenColors function. Custom
   colors may be passed via the PlotOptions option (and the enclosed SymbolStyle option).
Options:
mzGridLineFreq – frequency of horizontal gridlines on plot (default: 1)
mzTickFreq – frequency of labeled tickmarks on the m/z axis (default: 1)
LegendItems - list of strings to be shown as legend labels (default: Automatic)
PlotOptions – list of options to be passed to the MultipleListPlot function
   used internally to generate the plot (default: {TextStyle→DAMPTextStyle,Frame→True,
   ImageSize→600,SymbolShape→{PlotSymbol[Diamond,5,Filled→False],PlotSymbol[Box,5,
   Filled→False],PlotSymbol[Diamond,3,Filled→False],PlotSymbol[Box,3,Filled→False]}})

DAMPRemoveNoise

DAMPRemoveNoise[msdata,options] removes noise from every chromatogram/electropherogram in
   msdata by leveling to 0 all signal intensities, absolute values of which are smaller than
   a threshold. The threshold is calculated as a specific multiple of the standard deviation
   of signal intensities from a specified time range of every chromatogram/electropherogram.
Options:
TimeRange – time range (in minutes) from which to
   calculate the standard deviation of signal intensities (default: {1,3})
SDThreshold – specifies the multiple of the standard deviation of signal intensities from
   the selected time range to be used as the noise discrimination threshold (default: 5)
LevelNegativeSignals – if set to True, all negative signal intensities in
   every chromatogram/electropherogram will be leveled to 0 (default: True)
SampleNameSuffix – string to be added to the SampleName from the msdata to
   keep the track of modifications performed on the dataset (default: "nr")

DAMPRemoveSpikes

DAMPRemoveSpikes[msdata,options] levels to 0 all signal intensity values both neighbours
   of which have 0 signal intensity value in every chromatogram/electropherogram in msdata.
Options:
SampleNameSuffix – string to be added to the SampleName from the
   msdata to keep the track of modifications performed on the dataset (default: "sr")

DAMPRobustPolynomialFit

DAMPRobustPolynomialFit[chromatogram,options] fits a polynomial to chromatogram data
   by robust nonlinear regression and returns a dataset in which the signal intensity is
   calculated from the polynomial for each timepoint. The function is intended for baseline
   fitting. Please refer to the MathDAMP.nb notebook for details about implementation.
Options:
PolynomialDegree – degree of polynomial which is going to be fitted to the data (default: 1)
ConvergenceCriteria – convergence criteria for nonlinear regression (default: 0.001)
MaxIterations – maximum number of outer (recalculating the weights) iterations (default: 10)
b – parameter for calculating weights (default: 4.05)
BinningFunction – function to bin the chromatogram data before polynomial fitting. This may
   increase the speed considerably without considerable loss of precision. Use BinningFunction->
   None not to bin the data for polynomial fitting (default: (DAMPBinChromatogramFast[#,0.25]&))

DAMPSelectMZs

DAMPSelectMZs[msdata,mzs] reduces the msdata datased
   to datapoints corresponding to m/z values specified in the mzs list.

DAMPSelectRepresentativePeaks

DAMPSelectRepresentativePeaks[peaklist,options] reduces the peaklist returned by
   the DAMPPickPeaks function to a selected number of highest peaks in every chromatogram/
   electropherogram and a selected number of highest peaks in every time interval of selected size.
Options:
PeaksPerChromatogram – number of highest peaks
   to select from every chromatogram/electropherogram (default: All)
PeaksPerInterval – number of highest peaks to select from every time interval (default: All)
IntervalSize – size of the time interval (in minutes) for
   selection of highest peaks when PeaksPerInterval is not set to All (default: 1)
TimeRange – select peaks from this retention/migration time range only (default: All)

DAMPSmooth

DAMPSmooth[msdata,options] applies a smoothing function to all chromatograms/electropherograms in msdata.
Options:
SmoothingFunction – pure function to be applied to the list of signal
   intensities from a chromatogram/electropherogram (default: DAMPMovingAverageFast[#,9]&)
SampleNameSuffix – string to be added to the SampleName from the msdata
   to keep track of modifications performed on the dataset (default: "s")

DAMPSubtractBaselines

DAMPSubtractBaselines[msdata,options] subtracts baselines from all
   chromatograms/electropherograms in msdata dataset and returns the new processed dataset.
Options:
BaselineFittingFunction – pure function which is expected to return the baseline points for every
   timepoint in a chromatogram/electropherogram passed as an argument (default: DAMPRobustPolynomialFit)
SampleNameSuffix – string to be added to the SampleName from the msdata to
   keep the track of modifications performed on the dataset (default: "bs")

DAMPThreshold

DAMPThreshold[msdata,threshold,options] levels to
   0 all signal intensity values in msdata which are within ±threshold.
Options:
SampleNameSuffix – string to be added to the SampleName from the
   msdata to keep track of modifications performed on the dataset (default: "t")

DAMPTrendFilter

DAMPTrendFilter[group1msdatas,group2msdatas,tofiltermsdata,filtnum,options] filters
   out those signal intensities from a result (tofiltermsdata) of two averaged groups of
   msdatas where at least a certain number of corresponding signal intensities from the
   individual datasets specified by filtnum follows the same trend as their averages.
Options:
SampleNameSuffix – string to be added to the SampleName from the tofiltermsdata
   to keep the track of modifications performed on the dataset (default: "tf")

DAMPTwoDatasets

DAMPTwoDatasets[msdata1,msdata2,options] generates datasets representing the absolute, relative, and
   absolute×relative differences between msdata2 and msdata1 and returns them along with the
   normalized datasets and aligned annotation tables as a list of rules: {NormalizedDatasets->...,
   Absolute->...,Relative->...,AbsoluteRelative->...,AlignedAnnotationTables->...}
Options:
NormalizeGroupOptions – a list of options for the DAMPNormalizeGroup
   function which is used internally to normalize the datasets (default: {})
ThresholdForRelative – relative difference in the relative result will be set
   to 0 if neither of the two corresponding signal intensities from msdata1
   and msdata2 are equal to or greater than this threshold (default: 0)

DAMPTwoGroups

DAMPTwoGroups[msdatas1,msdatas2,options] generates datasets representing the absolute,
    relative, and absolute×relative differences between the averaged datasets of msdatas2
    datasets and msdatas1 datasets. Additionally, a dataset representing t-scores between
    the groups of corresponding signal intensities from msdatas1 and msdatas2 datasets
    is generated. The results are returned as a list of rules: {NormalizedDatasets->...,
    AveragedGroup1->...,AveragedGroup2->...,Absolute->...,Relative->...,AbsRel->...,
    FilteredAbsRel->...,TScores->...,AlignedAnnotationTables->...,GroupCounts->...,GroupNames->...}
Options:
NormalizeGroupOptions – a list of options for the DAMPNormalizeGroup
    function which is used internally to normalize the datasets (default: {})
ThresholdForRelative – relative difference in the relative result will be
    set to 0 if neither of the two corresponding signal intensities (from the
    averaged datasets) is equal to or greater than this threshold (default: 0)
GroupNames – names to assign to groups (will be combined into the SampleName of the results). If set
    to Automatic, the SampleName of the first dataset from every group is used (default: Automatic)
AbsRelTrendFilter – determines the minimum number of individual corresponding
    signal intensities from every group which must follow the same trend as
    their averages to remain in the absolute×relative result. This is intended to
    filter out results originating from individual spikes or outliers (default: 2)