

# Package ‘LipidTrend’

June 24, 2025

**Title** LipidTrend: Analysis and Visualization of Lipid Feature Tendencies

**Version** 0.99.1

**Description** ``LipidTrend" is an R package that implements a permutation-based statistical test to identify significant differences in lipidomic features between groups. The test incorporates Gaussian kernel smoothing of region statistics to improve stability and accuracy, particularly when dealing with small sample sizes. This package also includes two plotting functions for visualizing significant tendencies in 1D and 2D feature data, respectively.

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**URL** <https://github.com/BioinfOMICS/LipidTrend>

**BugReports** <https://github.com/BioinfOMICS/LipidTrend/issues>

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---

.analyzeSplitChain      *Process Split Chain Analysis*

---

### Description

Helper function to analyze even and odd chain lipids separately

### Usage

```
.analyzeSplitChain(  
  X,  
  X.info,  
  group,  
  chain_col,  
  radius,  
  own_contri,  
  test,  
  permute_time,  
  abund_weight  
)
```

### Arguments

X	Matrix. Lipid abundance data matrix.
X.info	Data frame. Lipid feature information.
group	Vector. Group assignments.
chain_col	Column name for chain length
radius	Numeric. Distance of neighbor to include.
own_contri	Numeric. Proportion of own contribution.
test	Character. Statistical test to use.
permute_time	Integer. Number of permutations.
abund_weight	Logical. Whether to use abundance weighting.

### Value

A data frame with split chain results

---

.buildWall      *Build Walls Between Different Regions*

---

### Description

Identifies walls needed between different regions based on spatial relationships and region assignments

### Usage

```
.buildWall(feature.idx, X.info, selected.region, x.distance, y.distance)
```

**Arguments**

feature.idx	Numeric. Index of the feature to analyze
x.info	Matrix or data.frame. Contains spatial coordinates
selected.region	Character vector. Region assignments for features
x.distance	Numeric. Scaling factor for x-coordinates
y.distance	Numeric. Scaling factor for y-coordinates

**Value**

Data frame with coordinates and wall positions

---

.calcSegment	<i>Calculate Segment Coordinates</i>
--------------	--------------------------------------

---

**Description**

Calculates start and end coordinates for wall segments

**Usage**

```
.calcSegment(wall_data, direction, x_dist, y_dist)
```

**Arguments**

wall_data	Data frame. Wall position data
direction	Character. Wall direction
x_dist	Numeric. X-axis distance scale
y_dist	Numeric. Y-axis distance scale

**Value**

List of segment coordinates

---

.countDistance	<i>Normalize Coordinate Matrix by Feature Distance</i>
----------------	--

---

**Description**

Normalizes coordinates by dividing each dimension by its minimum distance

**Usage**

```
.countDistance(dist_input)
```

**Arguments**

dist_input	Matrix or data.frame. Contains spatial coordinates.
------------	---

**Value**

A list containing the normalized matrix and distance values for each dimension

---

.createSegmentLayer     *Create Segment Layer for Wall Visualization*

---

**Description**

Creates a ggplot2 layer for wall segments

**Usage**

```
.createSegmentLayer(wall_data, direction, color, x_dist, y_dist)
```

**Arguments**

wall_data	Data frame. Wall coordinates
direction	Character. Wall direction
color	Character. Wall color
x_dist	Numeric. X-axis distance scale
y_dist	Numeric. Y-axis distance scale

**Value**

A ggplot2 layer object or NULL

---

.findNeighbor     *Find Neighboring Features*

---

**Description**

Identifies neighboring features in specified directions

**Usage**

```
.findNeighbor(self, others, type = c("right", "left", "top", "bottom"))
```

**Arguments**

self	Numeric vector. Reference point coordinates
others	Matrix. Coordinates of other features
type	Character. Direction to check ("right", "left", "top", "bottom")

**Value**

Logical vector indicating neighbor presence

---

`.formingFinalPlot`      *Add Data Points and Styling to Base Plot*

---

### Description

Adds data points with fold change coloring, significance annotations, and styling to a base heatmap plot.

### Usage

```
.formingFinalPlot(base_plot, heatmap.df)
```

### Arguments

<code>base_plot</code>	A ggplot object containing the initial base plot structure
<code>heatmap.df</code>	A data frame with columns for visualization: <b>avg.abund</b> Numeric. Average abundance values for point sizing <b>log2.FC</b> Numeric. Log2 fold change values for point coloring <b>pval.annotate</b> Character. Significance symbols for annotations <b>label_vjust</b> Numeric. Vertical adjustment for text labels

### Value

A ggplot object with enhanced visualization layers

---

`.plotHeatmap`      *Plot Heatmap with Abundance Data and Region Walls*

---

### Description

Creates a ggplot2 heatmap visualization showing abundance data with walls between regions, using vectorized operations.

### Usage

```
.plotHeatmap(X.info, heatmap.df, walls, x.distance, y.distance)
```

### Arguments

<code>X.info</code>	Matrix or data.frame. Contains coordinate information
<code>heatmap.df</code>	Data frame. Contains abundance and fold change data
<code>walls</code>	List. Contains wall coordinates for different regions
<code>x.distance</code>	Numeric. Distance between x-axis points
<code>y.distance</code>	Numeric. Distance between y-axis points

### Value

A ggplot2 object

---

.pvalAnnotation      *Create P-value Annotation*

---

**Description**

Converts p-values to significance symbols

**Usage**

```
.pvalAnnotation(pval)
```

**Arguments**

pval                  Numeric. P-value to convert

**Value**

Character string with significance symbols

---

.regionStat              *Region Statistics Calculation*

---

**Description**

Calculate region statistics using either t-test or Wilcoxon test

**Usage**

```
.regionStat(X, Y, test = "t.test", ...)
```

**Arguments**

X                      Matrix. Lipid abundance data matrix.  
Y                      Matrix. Group information matrix.  
test                    Character. Statistical test to use ("t.test" or "Wilcoxon"). Default is "t.test".

**Value**

Numeric vector of statistical test results.

---

*.resultSummary*      *Summarize Results*

---

### **Description**

Summarize and format lipid trend analysis results

### **Usage**

```
.resultSummary(  
  X,  
  X.info,  
  group,  
  smooth.stat,  
  smooth.stat.permute,  
  region.stat.obs,  
  dimension,  
  permute_time,  
  ...  
)
```

### **Arguments**

<code>X</code>	Matrix. Lipid abundance data matrix.
<code>X.info</code>	Data frame. Lipid feature information.
<code>group</code>	Vector. Group assignments.
<code>smooth.stat</code>	Numeric vector. Smoothed statistics.
<code>smooth.stat.permute</code>	Matrix. Permutation results.
<code>region.stat.obs</code>	Numeric vector. Observed region statistics.
<code>dimension</code>	Integer. Dimension of the analysis.
<code>permute_time</code>	Integer. Number of permutations performed.
<code>...</code>	Additional arguments.

### **Value**

Data frame containing formatted results.



---

.smooth\_permutation     *Smooth Permutation Analysis*

---

### Description

Perform smooth permutation analysis for lipid trend data

### Usage

```
.smooth_permutation(  
  X,  
  group,  
  dist.mat,  
  own_contri,  
  test,  
  abund_weight,  
  permute_time,  
  region.stat.obs  
)
```

### Arguments

X	Matrix. Lipid abundance data matrix.
group	Vector. Group assignments.
dist.mat	Matrix. Distance matrix.
own_contri	Numeric. Proportion of own contribution.
test	Character. Statistical test to use.
abund_weight	Logical. Whether to use abundance weighting.
permute_time	Integer. Number of permutations.
region.stat.obs	Numeric vector. Observed region statistics.

### Value

List containing smooth statistics and permutation results.

---

.split\_chain     *Get Split Chain Status from LipidTrendSE*

---

### Description

Get Split Chain Status from LipidTrendSE

### Usage

```
.split_chain(object)
```

**Arguments**

object            A LipidTrendSE object

**Value**

Logical indicating if analysis was split by chain

---

*.stat\_lipidTrend*            *Statistical Analysis for lipidTrend*

---

**Description**

Perform statistical analysis for lipid trend data

**Usage**

```
.stat_lipidTrend(
  X,
  X.info,
  group,
  radius,
  own_contri,
  test,
  permute_time,
  abund_weight
)
```

**Arguments**

X                    Matrix. Lipid abundance data matrix.

X.info              Data frame. Lipid feature information.

group                Vector. Group assignments.

radius               Numeric. Distance of neighbor to include.

own\_contri          Numeric. Proportion of own contribution.

test                 Character. Statistical test to use.

permute\_time        Integer. Number of permutations.

abund\_weight        Logical. Whether to use abundance weighting.

**Value**

Data frame containing analysis results.

---

.trendPlot1D *Create 1D result plot*

---

**Description**

Creates a ggplot visualization showing trends between case and control groups with highlighted significant regions.

**Usage**

```
.trendPlot1D(res, p_cutoff, y_scale)
```

**Arguments**

res	A data.frame containing columns for coordinates, abundance values, direction, and adjusted p-values
p_cutoff	Numeric value for significance cutoff. Default is 0.05
y_scale	Character. Choose one of the y-axis scales: "identity", "log2", "log10", or "sqrt". Default is "identity"

**Value**

A ggplot2 object

---

.trendPlot2D *Create 2D Trend Plot*

---

**Description**

Creates a 2D visualization of lipid trends with statistical annotations

**Usage**

```
.trendPlot2D(res, p_cutoff, log2FC_cutoff)
```

**Arguments**

res	Data frame containing analysis results
p_cutoff	Numeric significance level cutoff
log2FC_cutoff	Numeric log2 fold change cutoff

**Value**

A ggplot2 object representing the trend visualization

---

abundance_2D	<i>Example lipid abundance data for two-dimensional LipidTrend analysis</i>
--------------	---

---

**Description**

Example lipid abundance data for two-dimensional LipidTrend analysis

**Usage**

```
data(abundance_2D)
```

**Format**

A matrix object of lipid abundance with 137 lipids over 6 samples

**Source**

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. *Sci Adv.* 9(42):eadj4198 <https://www.science.org/doi/10.1126/sciadv.adj4198>.

**Examples**

```
data(abundance_2D)
```

---

abundance_CL	<i>Example lipid abundance data for one-dimensional LipidTrend analysis</i>
--------------	---

---

**Description**

Example lipid abundance data for one-dimensional LipidTrend analysis

**Usage**

```
data(abundance_CL)
```

**Format**

A matrix object of lipid abundance with 29 lipids over 6 samples

**Source**

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. *Sci Adv.* 9(42):eadj4198 <https://www.science.org/doi/10.1126/sciadv.adj4198>.

**Examples**

```
data(abundance_CL)
```

---

analyzeLipidRegion      *Conduct statistical to analyze lipid features tendencies*

---

### Description

Calculate p-value of lipidomic features by permutation test. The test of region statistics smoothing with Gaussian kernel integrates neighbor's information and provides a stable testing result under small sample size.

### Usage

```
analyzeLipidRegion(
  lipid_se,
  ref_group,
  split_chain = FALSE,
  chain_col = NULL,
  radius = 3,
  own_contri = 0.5,
  test = "t.test",
  abund_weight = TRUE,
  permute_time = 1e+05
)
```

### Arguments

lipid_se	A SummarizedExperiment object. Must contain following data: <b>Assay</b> A matrix containing lipid abundance data, where rows represent lipids and columns represent samples. <b>rowData</b> A data frame of lipid features (e.g., double bond count, chain length), with rows as lipids and columns as lipid features ( limited to 1 or 2 columns). The order of lipids must match the abundance data. If RowData contains one column, a one-dimensional analysis will be performed. If RowData includes two columns, a two-dimensional analysis will be conducted. <b>colData</b> A data frame containing group information, where rows represent sample names and columns must include sample name, label name, and group, arranged accordingly.
ref_group	Character. Group name of the reference group. It must be one of the group names in the colData group column.
split_chain	Logical. If TRUE the results will split to shown by odd and even chain. Default is FALSE.
chain_col	Character. The column name of chain length. Set to NULL if split_chain is FALSE. Default is 'NULL'.
radius	Numeric. Distance of neighbor to be included. Default is 3.
own_contri	Numeric. Proportion of own contribution. Default is 0.5. To not over-emphasize the neighbor information, we suggest to choose a value from 0.5 to 1.
test	String. Choose statistic test from "t.test" and "Wilcoxon". Default is 't.test'.
abund_weight	Logical. Consider the average abundance as the weight in the test statistic. Default is TRUE.
permute_time	Integer. Permutation times. Default is 100000.

**Value**

A LipidTrendSE object containing lipidomic feature testing result.

**See Also**

[plotRegion1D](#) for one-dimensional visualization [plotRegion2D](#) for two-dimensional visualization

**Examples**

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
  lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=FALSE,
  chain_col=NULL, radius=3, own_contri=0.5, permute_time=100)
```

---

char\_table\_2D

*Example lipid characteristics table for two-dimensional LipidTrend analysis*

---

**Description**

Example lipid characteristics table for two-dimensional LipidTrend analysis

**Usage**

```
data(char_table_2D)
```

**Format**

A data.frame object of total chain length and total double bond characteristics over 137 lipids

**Source**

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. Sci Adv. 9(42):eadj4198 <https://www.science.org/doi/10.1126/sciadv.adj4198>.

**Examples**

```
data(char_table_2D)
```

---

char_table_CL	<i>Example lipid characteristics table for one-dimensional LipidTrend analysis</i>
---------------	--

---

**Description**

Example lipid characteristics table for one-dimensional LipidTrend analysis

**Usage**

```
data(char_table_CL)
```

**Format**

A data.frame object of chain characteristics over 29 lipids

**Source**

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. *Sci Adv.* 9(42):eadj4198 <https://www.science.org/doi/10.1126/sciadv.adj4198>.

**Examples**

```
data(char_table_CL)
```

---

even_chain_result	<i>Get Even Chain Result from LipidTrendSE</i>
-------------------	--

---

**Description**

Get Even Chain Result from LipidTrendSE

**Usage**

```
even_chain_result(object)

## S4 method for signature 'LipidTrendSE'
even_chain_result(object)
```

**Arguments**

object            A LipidTrendSE object

**Value**

A data frame containing even chain result or NULL

**Examples**

```
data("lipid_se_CL")
sub <- lipid_se_CL[seq_len(10), ]
res_se <- analyzeLipidRegion(
  lipid_se=sub, ref_group="sgCtrl", split_chain=TRUE,
  chain_col="chain", radius=3, own_contri=0.5, permute_time=100)
# Get complete result summary
results <- even_chain_result(res_se)
```

---

group\_info

*Example group information table for LipidTrend analysis*


---

**Description**

Example group information table for LipidTrend analysis

**Usage**

```
data(group_info)
```

**Format**

A data.frame object of sample name, lable name, and group name over 6 samples

**Source**

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. *Sci Adv.* 9(42):eadj4198 <https://www.science.org/doi/10.1126/sciadv.adj4198>.

**Examples**

```
data(group_info)
```

---

LipidTrend

*LipidTrend: Analysis and Visualization of Lipid Feature Tendencies*


---

**Description**

The LipidTrend package provides tools for analyzing and visualizing trends in lipidomics data. It implements statistical methods for identifying significant changes in lipid abundances across different features, with support for both one-dimensional and two-dimensional analyses.

**Main functions**

- [analyzeLipidRegion](#): Analyzing lipid trends using permutation tests and Gaussian kernel smoothing
- [plotRegion1D](#): Visualize one-dimensional lipid trends
- [plotRegion2D](#): Create two-dimensional visualizations of lipid trends



## Vignettes

See the package vignettes for detailed workflows: `vignette('LipidTrend')`

## Installation

To install from Bioconductor, use:

```
if (!requireNamespace('BiocManager', quietly=TRUE))
  install.packages('BiocManager')
BiocManager::install('LipidTrend')
```

## Author(s)

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- Wen-Jen Lin [contributor]
- Hung-Ching Chang [contributor]
- Meng-Hsin Tsai [contributor]

## See Also

Useful links:

- <https://github.com/BioinfOMICS/LipidTrend>
- Report bugs at <https://github.com/BioinfOMICS/LipidTrend/issues>

---

LipidTrendSE-class      *Class for storing analyzeLipidRegion analysis results*

---

## Description

This class extends SummarizedExperiment to store analyzeLipidRegion analysis results

## Slots

`split_chain` Logical indicating whether chains were split by parity. When TRUE, results are stored in `even_chain_result` and `odd_chain_result`. When FALSE, results are stored in the `result` slot.

`result` Data frame of analysis results (for non-split data)

`even_chain_result` Data frame of results for even chains (when split)

`odd_chain_result` Data frame of results for odd chains (when split)

---

LipidTrendSE-validity *Validate LipidTrendSE object*

---

**Description**

Validate LipidTrendSE object

**Arguments**

object            A LipidTrendSE object to validate

**Value**

TRUE if valid, otherwise an error message

---

lipid\_se\_2D            *Example Dataset for two-dimensional data*

---

**Description**

Example Dataset for two-dimensional data

**Usage**

```
data(lipid_se_2D)
```

**Format**

A SummarizedExperiment object with the following slots:

colData A data frame with 6 observations on the following 3 variables, containing sample name, label name, and group name

assay A 137\*6 matrix containing lipid abundance data

rowData A data frame with 137 observations on the following 2 variables containing total chain length and total double bond characteristic information

**Examples**

```
data(lipid_se_2D)
```

---

`lipid_se_CL`*Example Dataset for one-dimensional data*

---

**Description**

Example Dataset for one-dimensional data

**Usage**

```
data(lipid_se_CL)
```

**Format**

A SummarizedExperiment object with the following slots:

`colData` A data frame with 6 observations on the following 3 variables, containing sample name, label name, and group name

`assay` A 29\*6 matrix containing lipid abundance data

`rowData` A data frame with 29 observations on the following 1 variables containing chain characteristic information

**Examples**

```
data(lipid_se_CL)
```

---

`odd_chain_result`*Get Odd Chain Result from LipidTrendSE*

---

**Description**

Get Odd Chain Result from LipidTrendSE

**Usage**

```
odd_chain_result(object)
```

```
## S4 method for signature 'LipidTrendSE'  
odd_chain_result(object)
```

**Arguments**

`object` A LipidTrendSE object

**Value**

A data frame containing odd chain result or NULL

**Examples**

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
  lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=TRUE,
  chain_col="chain", radius=3, own_contri=0.5, permute_time=100)
# Get complete result summary
results <- odd_chain_result(res_se)
```

---

plotRegion1D

*Plot region trends for one-dimensional lipid feature*


---

**Description**

Visualize analysis results for one-dimensional features to identify lipid feature tendencies. The plots highlight regions of significant differences between case and control samples: blue areas indicate significantly lower abundance in case samples, while red areas indicate significantly higher abundance.

**Usage**

```
plotRegion1D(object, p_cutoff = 0.05, y_scale = "identity")

## S4 method for signature 'LipidTrendSE'
plotRegion1D(object, p_cutoff = 0.05, y_scale = "identity")
```

**Arguments**

object	A LipidTrendSE object containing analysis results.
p_cutoff	Numeric. Significance level. The range is 0 to 1. Default is 0.05.
y_scale	Character. Choose one of the y-axis scales: "identity", "log2", "log10", or "sqrt". Default is "identity".

**Value**

For split chain analyses, a list with two elements:

even_result	Plot for even chain features, or NULL if none exist
odd_result	Plot for odd chain features, or NULL if none exist

For non-split analyses, a single plot.

**See Also**

[analyzeLipidRegion](#) for generating the input LipidTrendSE object

**Examples**

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
  lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=FALSE,
  chain_col=NULL, radius=2, own_contri=0.5, permute_time=100,
  abund_weight=TRUE)
plot <- plotRegion1D(res_se, p_cutoff=0.05, y_scale='identity')
```

---

plotRegion2D	<i>Plot region trends for two-dimensional lipid features</i>
--------------	--

---

### Description

plotRegion2D visualizes lipid trend analysis results in two dimensions. The returned heatmap will show the results.

### Usage

```
plotRegion2D(object, p_cutoff = 0.05, log2FC_cutoff = 3)
```

```
## S4 method for signature 'LipidTrendSE'  
plotRegion2D(object, p_cutoff = 0.05, log2FC_cutoff = 3)
```

### Arguments

object	A LipidTrendSE object containing analysis results.
p_cutoff	Numeric. Significance level. The range is 0 to 1. Default is 0.05.
log2FC_cutoff	Numeric. Significant level of log2-transformed fold change. Default is 3.

### Value

For split chain analyses, a list with two elements:

even_result	Heatmap for even chain features, or NULL if none exist
odd_result	Heatmap for odd chain features, or NULL if none exist

For non-split analyses, a single heatmap.

### See Also

[analyzeLipidRegion](#) for generating the input LipidTrendSE object

### Examples

```
data("lipid_se_2D")  
res_se <- analyzeLipidRegion(  
  lipid_se=lipid_se_2D, ref_group="sgCtrl", split_chain=FALSE,  
  chain_col=NULL, radius=3, own_contri=0.5, permute_time=100,  
  abund_weight=TRUE)  
plot_2D <- plotRegion2D(res_se, p_cutoff=0.05)
```

---

result	<i>Get Result from LipidTrendSE</i>
--------	-------------------------------------

---

**Description**

Get Result from LipidTrendSE

**Usage**

```
result(object)

## S4 method for signature 'LipidTrendSE'
result(object)
```

**Arguments**

object            A LipidTrendSE object

**Value**

A data frame containing analysis results or NULL

**Examples**

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
  lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=FALSE,
  chain_col=NULL, radius=3, own_contri=0.5, permute_time=100)
# Get complete result
results <- result(res_se)
```

---

show,LipidTrendSE-method	<i>Show method for LipidTrendSE objects</i>
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---

**Description**

Show method for LipidTrendSE objects

**Usage**

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

**Arguments**

object            A LipidTrendSE object

**Value**

LipidTrendSE object information

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