Package 'spikeLI'

April 25, 2025

Type Package

Title Affymetrix Spike-in Langmuir Isotherm Data Analysis Tool

Version 2.69.0

Date 2009-04-03

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Description SpikeLI is a package that performs the analysis of the Affymetrix spike-in data using the Langmuir Isotherm. The aim of this package is to show the advantages of a physical-chemistry based analysis of the Affymetrix microarray data compared to the traditional methods. The spike-in (or Latin square) data for the HGU95 and HGU133 chipsets have been downloaded from the Affymetrix web site. The model used in the spikeLI package is described in details in E. Carlon and T. Heim, Physica A 362, 433 (2006).

Imports graphics, grDevices, stats, utils

License GPL-2

biocViews Microarray, QualityControl

git_url https://git.bioconductor.org/packages/spikeLI

git_branch devel

git_last_commit 6ef3b4c

git_last_commit_date 2025-04-15

Repository Bioconductor 3.22

Date/Publication 2025-04-24

Contents

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spikeLI-package *Analysis of Affymetrix spike-in data (HGU95 and HGU133 Latin square) using the Langmuir Isotherm.*

Description

spikeLI performs a series of analysis of Affymetrix spike-in data using inputs from physical-chemistry. It illustrates the advantages of such approach in determining expression levels and in identifying outliers compared to other methods. The analysis so far is restricted to spike-in genes. It will be extended to a generic CEL file. spikeLI does not require affy (and it is independent of any other bioconductor packages) as it reads spike-in data from a data frame variable hgu which is contained in the package.

Details

Package:	spikeLI
Type:	Package
Version:	1.0
Date:	2006-05-05
License:	GNU Public License

The package contains three basic functions: - Ivsc plot intensities as function of spike-in concentration for a fixed probe. - IvsDG plot intensities as function of affinity for a given probe set at fixed concentration. - collapse plot of intensities both as a function of concentration and affinities.

Author(s)

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References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`collapse`, `Ivsc`, `IvsDG`, `hgu`, `SPIKE_IN`, `SPIKE_INA`, `SPIKE_INB`, `SPIKE_INH` , `SPIKE_IN95`

`collapse` *Data collapse of all concentrations into a single graph*

Description

This function takes as input one or more (up to four) probe sets of the Latin square spike-in data and produces collapse plots. A collapse plot contains data of different concentrations into a single graph. The user can compare in how far the data follows the predicted Langmuir behavior which is also given in the plot. Two models are compared: the basic Langmuir Isotherm and the Langmuir Isotherm with hybridization in solution.

Usage

```
collapse(probe_set, param = "NULL", probes = "NULL", output = "NULL", filename = "NULL")
```

Arguments

`probe_set`	This has to take the value of a probe set
`param`	In input one or more probe sets can be given
`probes`	A vector containing the probes
`output`	"PS" output on a postscript file
`filename`	the file in which collapses are given

Author(s)

Delphine Baillon, Paul Leclercq, Sarah Ternisien, Thomas Heim and Enrico Carlon

References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`Ivsc`, `IvsDG`, `hgu`, `SPIKE_IN`, `SPIKE_INA`, `SPIKE_INB`, `SPIKE_INH`

Examples

```
## You may display the matched intensities of a Probe-Set according to the Delta-G value
     collapse("1091_at")

## You may restrict the value to the Perfect match or mis-matches
     collapse("1091_at","PM")

## You may restrict the values risplayed for only a number of probes
     collapse("1091_at",probes=c(1,9))

## You may output the graphs to a postscript file
     collapse("1091_at",output="PS",filename="outfile.ps")

## You may display up to 4 probe-sets in the same window
     collapse(c("1091_at","37777_at",SPIKE_INA[1:2]))
```

```
## You can also use the values of the probe-sets contained in one of the Vectors of Human, Bacteria,
## or Artificial Probe-sets
     collapse(SPIKE_INH)
```

`conc133` *Concentration 95*

Description

This datasets contains the values of the latine square matrix for the hgu133 Affymetrix Microarrays

Usage

```
data(conc133)
```

Format

The format is: num [1:14] 0 0.125 0.25 0.5 1 2 4 8 16 32 ...

See Also

`Ivsc`, `IvsDG`, `collapse`, `SPIKE_IN`, `SPIKE_INA`, `SPIKE_INB`, `SPIKE_INH`

Examples

```
data(conc133)
```

`conc95` *Concentration 95*

Description

This datasets contains the values of the latine square matrix for the hgu95 Affymetrix Microarrays

Usage

```
data(conc95)
```

Format

The format is: num [1:14] 0 0.25 0.5 1 2 4 8 16 32 64 ...

See Also

`Ivsc`, `IvsDG`, `collapse`, `SPIKE_IN`, `SPIKE_INA`, `SPIKE_INB`, `SPIKE_INH`

Examples

```
data(conc95)
```

`hgu` *Selected Probe Set data*

Description

This selected probe sets information contains the sequence of the selected probe sets, as well as the match and mismatch onformation and Delta G value required for the langmuir analysis

Usage

```
data(hgu)
```

Format

A data frame with 11452 observations on the following 9 variables.

`Probe.Set.Name` Name of probe set

`conc` a numeric vector

`Ipm` a numeric vector

`Imm` a numeric vector

`Seq` DNA Sequence of the probe

`DGpm` DG value of perfect match of the probe

`DGmm` Delta G value of the mismatch of the probe

`DGRNA` Delta G value of the RNA

`FILE` a factor with levels `HGU133` `HGU95`

References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`Ivsc`, `IvsDG`, `collapse`, `SPIKE_IN`, `SPIKE_INA`, `SPIKE_INB`, `SPIKE_INH`

Examples

```
data(hgu)
## maybe str(hgu) ; plot(hgu) ...
```

`Ivsc` *Plot of intensity vs. concentration for given probes*

Description

The function Ivsc plots intensity as a function of a concentration for a given probe in the spike-in Latin square experiments. It also peforms a non-linear data fit (using the package nls in the R-package stats) of the experimental data using the Langmuir Isotherm: I = I0 + Ac/(K+c) Solid and dashed lines are best fits according to this formula. Imax in the plot are given by Imax=I0+A, ie the asymptotic intensity in the limit of c to infinity.

Usage

```
Ivsc(probe_set, probe = "NULL", outfile = "NULL")
```

Arguments

`probe_set`	Probe set number of the probe set analyzed
`probe`	Integer giving the probe number (if not give the probe 1 is selected)
`outfile`	output the plotted data to a postscript file

Warning

Some probes have an irregular behavior and the non-linear square fit does not converge.

Author(s)

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References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`collapse`, `IvsDG`, `hgu`, `SPIKE_IN`, `SPIKE_INA`, `SPIKE_INB`, `SPIKE_INH`

Examples

```
Ivsc("37777_at",4)
```

`IvsDG` *Plot Intensity as function of the affinity for a given probe set at fixed concentration.*

Description

IvsDG plots intensity vs affinity (or free energy) for a probe set at a given concentration. The outcome is compared with the prediction from the Langmuir isotherm at that concentration. Two graphs are shown: on the left intensity vs. probe number for PM (blue) and MM (red); on the right the same value plotted as function of the affinities. The black line is the Langmuir Isotherm at the given concentration. The two green lines correspond to concentrations fourfold higher and lower compared to the given one.

Usage

```
IvsDG(probe_set, conc, outfile = "NULL")
```

Arguments

`probe_set`	Probe set number of the probe set analyzed
`conc`	Concentration value
`outfile`	"PS" output on a postscript file

Author(s)

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References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`Ivsc`, `collapse`, `hgu`, `SPIKE_IN`, `SPIKE_INA`, `SPIKE_INB`, `SPIKE_INH`

Examples

```
data(hgu)
IvsDG("1024_at",64)
```

`SPIKE_IN` *Spike-in Probe-Set Names*

Description

This dataset contains the names of the Probe-Sets contained in the HGU dataset

Usage

```
data(SPIKE_IN)
```

Format

A string containing the name of the genes

References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`Ivsc`, `IvsDG`, `collapse`, `hgu`, `SPIKE_INA` , `SPIKE_INB`, `SPIKE_INH`, `SPIKE_IN95`

Examples

```
## you can first check if the data matches the predicted hybridisation value according to the langmuir
## value, from the intensity versus the concentration value
Ivsc(SPIKE_IN[3])

## you can then plot the value of the Intensity of the probe with the predicted value of the hybridisation
## according to the Delta G, value
IvsDG(SPIKE_IN[5],64)

## The collapse function will finally plot all the values of the probe set according to
## the langmuir absorption theory

collapse(SPIKE_IN[2])

## By comparing the matched value and the mismatches, you will be able to identify errors which
## could have done while sampling the data, or if the error happens repeatedly this will show errors
## which will have happened while sequencing old data.
```

`SPIKE_IN95` *set of spike-in genes contained in the HGU95 dataset*

Description

This dataset contains a set of gene names contained in the HGU95 dataset

Usage

```
data(SPIKE_IN95)
```

Format

The set of spike-in gene names contained in the HGU dataset

Source

This data is experimental data extracted from the publicly available HGU dataset

References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`Ivsc`, `IvsDG`, `collapse`, `SPIKE_IN`, `hgu` , `SPIKE_INA`, `SPIKE_INB`, `SPIKE_INH`

Examples

```
## you can first check if the data matches the predicted hybridisation value according to the langmuir
## value, from the intensity versus the concentration value
Ivsc(SPIKE_IN95[1])

## you can then plot the value of the Intensity of the probe with the predicted value of the hybridisation
## according to the Delta G, value
IvsDG(SPIKE_IN95[4],128)

## The collapse function will finally plot all the values of the probe set according to
## the langmuir absorption theory

collapse(SPIKE_IN95[2])

## By comparing the matched value and the mismatches, you will be able to identify errors which
## could have done while sampling the data, or if the error happens repeatedly this will show errors
## which will have happened while sequencing old data.
```

`SPIKE_INA` *Artificial Spike-in probesets*

Description

This dataset contains the names of the probesets contained in the hgu dataset

Usage

```
data(SPIKE_INA)
```

Format

This dataset contains a set of String containing the names of the Artificial genes contained in the HGU dataset

References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`Ivsc`, `IvsDG`, `collapse`, `SPIKE_IN`, `hgu` , `SPIKE_INB`, `SPIKE_INH`

Examples

```
## you can first check if the data matches the predicted hybridisation value according to the langmuir
## value, from the intensity versus the concentration value
Ivsc(SPIKE_INA[1])

## you can then plot the value of the Intensity of the probe with the predicted value of the hybridisation
## according to the Delta G, value
IvsDG(SPIKE_INA[4],128)

## The collapse function will finally plot all the values of the probe set according to
## the langmuir absorption theory

collapse(SPIKE_INA[2])

## By comparing the matched value and the mismatches, you will be able to identify errors which
## could have done while sampling the data, or if the error happens repeatedly this will show errors
## which will have happened while sequencing old data.
```

`SPIKE_INB` *Bacteria Spike-in probeset names*

Description

This dataset contains the names of the Bacteria probe-sets contained in the HGU dataset

Usage

```
data(SPIKE_INB)
```

Format

names of the Bacteria probe-sets contained in the HGU dataset

References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`Ivsc`, `IvsDG`, `collapse`, `SPIKE_IN`, `hgu` , `SPIKE_INA`, `SPIKE_INH`

Examples

```
## you can first check if the data matches the predicted hybridisation value according to the langmuir
## value, from the intensity versus the concentration value
Ivsc(SPIKE_INB[3])

## you can then plot the value of the Intensity of the probe with the predicted value of the hybridisation
## according to the Delta G, value
```

```
IvsDG(SPIKE_INB[4],64)

## The collapse function will finally plot all the values of the probe set according to
## the langmuir absorption theory

collapse(SPIKE_INB[2])

## By comparing the matched value and the mismatches, you will be able to identify errors which
## could have done while sampling the data, or if the error happens repeatedly this will show errors
## which will have happened while sequencing old data.
```

`SPIKE_INH` *Human Spike-in probe-set names*

Description

This dataset contains the names of the Human probe-sets contained in the HGU dataset

Usage

```
data(SPIKE_INH)
```

Format

names of the human probe-sets contained in the HGU dataset

References

E. Carlon and T. Heim, Physica A 362, 433 (2006).

See Also

`Ivsc`, `IvsDG`, `collapse`, `SPIKE_IN`, `hgu` , `SPIKE_INA`, `SPIKE_INB`

Examples

```
## you can first check if the data matches the predicted hybridisation value according to the langmuir
## value, from the intensity versus the concentration value
Ivsc(SPIKE_INH[3])

## you can then plot the value of the Intensity of the probe with the predicted value of the hybridisation
## according to the Delta G, value
IvsDG(SPIKE_INH[5],256)

## The collapse function will finally plot all the values of the probe set according to
## the langmuir absorption theory

collapse(SPIKE_INH[2])

## By comparing the matched value and the mismatches, you will be able to identify errors which
## could have done while sampling the data, or if the error happens repeatedly this will show errors
## which will have happened while sequencing old data.
```

Index