# Package 'spikeLI'

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Title Affymetrix Spike-in Langmuir Isotherm Data Analysis Tool

Type Package

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<b>Description</b> 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).
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License GPL-2
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### **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)

Delphine Baillon, Paul Leclercq, Sarah Ternisien, Thomas Heim and Enrico Carlon Maintainer: Enrico Carlon <a href="mailto:centro.carlon@polytech-lille.fr">centro.carlon@polytech-lille.fr</a>

### 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 3

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
```

```
## 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
```

4 conc95

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 ...

hgu 5

#### 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
```

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

6 Ivsc

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 performs 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)

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

Maintainer: Enrico Carlon <enrico.carlon@iemn.univ-lille1.fr>

#### References

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

#### See Also

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

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

IvsDG 7

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)

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

Maintainer: Enrico Carlon <enrico.carlon@iemn.univ-lille1.fr>

#### References

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

### See Also

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

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

8 SPIKE\_IN

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
```

```
## 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 9

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).

## which will have happened while sequencing old data.

#### See Also

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

```
## 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
```

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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
```

```
## 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

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
```

## which will have happened while sequencing old data.

```
## 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
```

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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
```

```
## 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.
```

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