

Package ‘osd’

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Type Package

Title Orthogonal Signal Deconvolution for Spectra Deconvolution in GC-MS and GCxGC-MS Data

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Description Compound deconvolution for chromatographic data, including gas chromatography - mass spectrometry (GC-MS) and comprehensive gas chromatography - mass spectrometry (GCxGC-MS). The package includes functions to perform independent component analysis - orthogonal signal deconvolution (ICA-OSD), independent component regression (ICR), multivariate curve resolution (MCR-ALS) and orthogonal signal deconvolution (OSD) alone.

License GPL (>= 2)

NeedsCompilation no

Repository CRAN

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gcms1

Data from a GC-MS experiment

Description

A data matrix from a real pure standards GC-MS experiment.

Usage

```
data(gcms1)
```

Details

Data taken from the experiment used in [1] (See references below). This data matrix includes three compounds appearing in co-elution, concretely, the appearing compounds are: nicotinic acid, isoleucine and profile. The data in [gcms1](#) and [gcms2](#) only comprises the m/z from 35 to 600. So the first element of the column in [gcms1](#) corresponds to the mass m/z 35. Please, note that the fragments at m/z 73, 74, 75, 147, 148, and 149, were excluded from the analysis (have zero intensity).

Author(s)

[1] Domingo-Almenara X, et al. Compound deconvolution in GC-MS-based metabolomics by blind source separation. *Journal of Chromatography A* (2015). Vol. 1409: 226-233. DOI: 10.1016/j.chroma.2015.07.044

See Also

[osd](#), [gcms2](#), [ref.spects](#)

gcms2

Data from a GC-MS experiment

Description

A data matrix from a real pure standards GC-MS experiment.

Usage

```
data(gcms2)
```

Details

Data taken from the experiment used in [1] (See references below). This data matrix includes two compounds appearing in co-elution, concretely, the appearing compounds are: methionine and aspartic acid. The data in [gcms1](#) and [gcms2](#) only comprises the m/z from 35 to 600. So the first element of the column in [gcms2](#) corresponds to the mass m/z 35. Please, note that the fragments at m/z 73, 74, 75, 147, 148, and 149, were excluded from the analysis (have zero intensity).

Author(s)

[1] Domingo-Almenara X, et al. Compound deconvolution in GC-MS-based metabolomics by blind source separation. *Journal of Chromatography A* (2015). Vol. 1409: 226-233. DOI: 10.1016/j.chroma.2015.07.044

See Also

[osd](#), [gcms1](#), [ref.spects](#)

normalize	<i>Matrix or vector normalization</i>
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Description

Normalizes a vector or a matrix in the form of $x/\max(x)$. If x is a matrix, a column-normalization is performed, which is equivalent to `apply(x,2,function(x) x/max(x))`.

Usage

```
normalize(x)
```

Arguments

`x` a vector or a matrix to be normalized

Value

returns the normalized vector or matrix.

osd	<i>Orthogonal Signal Deconvolution</i>
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Description

Wrapper to use OSD, or OSD along with ICA (ICA-OSD), MCR (MCR-OSD), and also ICR.

Usage

```
osd(D, k, y.profile,
res.method = c("ica.osd", "osd", "icr", "mcr"),
comp.coef = 2, noise.thr = 0.01)
```

Arguments

D	data matrix, where rows are the retention time and columns are the m/z.
k	number of components in the model, i.e., the number of compounds to be extracted from data. (Only when methods ICA-OSD, MCR or ICR are used.)
y.profile	the vector containing the estimated elution profile of the compound which spectrum wants to be deconvolved. (Only when method OSD is used.)
res.method	the method to be used, including "ica.osd","mcr.osd","icr","mcr". See details for more information.
comp.coef	the non-linear factor of compression. See details for more information.
noise.thr	this value can be set from 0 to 1. Data in D under this relative threshold is set to zero to reduce the computational cost. Default is 0.01.

Details

The methods are described in [1] and [2] (See references below). OSD is an improved method for spectra extraction from chromatographic data tested in GC-MS and GCxGC samples.

For traditional multivariate curve resolution select "mcr" algorithm. Independent component regression is also implemented, and can be selected by choosing "icr" method. The OSD implementations using ICA can be used by "ica.osd". Also, OSD can be used alone, for retrieving a purest spectrum if the estimated elution profile of the compound (which spectrum is to be deconvolved) is given.

Value

osd returns an S3 object.

data	the original data matrix.
C	the resolved profile or concentration matrix.
S	the resolved spectra matrix.
k	the number of components used in the model.
y.profile	the estimated elution profile for OSD.
res.method	the method used for resolution.
comp.coef	the non-linear compression coefficient selected.
noise.thr	the noise threshold selected.

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References

[1] Domingo-Almenara X, et al. Compound deconvolution in GC-MS-based metabolomics by blind source separation. *Journal of Chromatography A* (2015). Vol. 1409: 226-233. DOI: 10.1016/j.chroma.2015.07.044

[2] Domingo-Almenara X, et al. Automated resolution of chromatographic signals by independent component analysis - orthogonal signal deconvolution in comprehensive gas chromatography/mass spectrometry-based metabolomics. *Computer Methods and Programs in Biomedicine* (2016). DOI: 10.1016/j.cmpb.2016.03.007:

See Also

[osd](#), [plotOSDres](#), [gcms1](#), [gcms2](#)

Examples

```
#load GC-MS sample data, containing three different metabolites
#appearing in co-elution.
data(gcms1)

#resolve the situation using ICA-OSD algorithm
resolution <- osd(D=gcms1, k=3, res.method='ica.osd')

#plot the resolution, the extracted ion chromatogram (m/z) are plotted in
#grey whereas the profile matrix appear in color.
plotOSDres(resolution, type='eic')

#plot each resolved spectra for compound 1 to 3.
plotOSDres(resolution, type='s',1)
plotOSDres(resolution, type='s',2)
plotOSDres(resolution, type='s',3)
```

plotOSDres

Plotting OSD objects

Description

Plots the results determined by osd function. Profile or spectra resolution can be selected for visualization.

Usage

```
plotOSDres(OSDobj, type = c("eic", "tic", "s"), ncomp = vector(),
  comp.spectra = vector(), mztxt.top = 5)
```

Arguments

OSDobj	the osd selected for plotting
type	the type of resolution to be plotted. Concentration resolution can be shown by its extracted ion chromatogram (EIC) "eic" or by its ion total chromatogram "tic". Also, the spectra for each compound in the model can be shown by "s".
ncomp	vector; the compounds to be plotted. If spectra is selected for visualization, please select only one compound to plot.
comp.spectra	a vector to compare a resolved spectra with.
mztxt.top	integer; the number of the m/z values ordered by intensity to visualize on the spectra plot

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See Also

[osd](#)

Examples

```
#load GC-MS sample data, containing three different metabolites
#appearing in co-elution.
data(gcms1)

#resolve the situation using ICA-OSD algorithm
resolution <- osd(D=gcms1, k=3, res.method="ica.osd")

#plot the resolution, the extracted ion chromatogram (m/z) are plotted
# in grey whereas the profile matrix appear in color.
plotOSDres(resolution, type="eic")
plotOSDres(resolution, type="tic")

#plot each resolved spectra for compound 1 to 3.
plotOSDres(resolution, type="s",1)
plotOSDres(resolution, type="s",2)
plotOSDres(resolution, type="s",3)
```

ref.spects

Five MS reference spectra from the MassBank MS library for spectra comparison

Description

A data matrix from a real pure standards GC-MS experiment.

Usage

```
data(ref.spects)
```

Details

The data includes a list of five vectors containing 5 MS spectra from the MassBank MS library [1]. Concretely, the spectra are Methionine 2TMS, Aspartic Acid 3TMS, Nicotinic Acid 1TMS, Isoleucine 2TMS and Proline 2TMS. These are the compounds appearing in the examples given in [gcms1](#) and [gcms2](#).

Author(s)

[1] MassBank: A public repository for sharing mass spectral data for life sciences", H. Horai, M. Arita, S. Kanaya, Y. Nihei, T. Ikeda, K. Suwa, Y. Ojima, K. Tanaka, S. Tanaka, K. Aoshima, Y. Oda, Y. Kakazu, M. Kusano, T. Tohge, F. Matsuda, Y. Sawada, M. Yokota Hirai, H. Nakanishi, K. Ikeda, N. Akimoto, T. Maoka, H. Takahashi, T. Ara, N. Sakurai, H. Suzuki, D. Shibata, S. Neumann, T. Iida, K. Tanaka, K. Funatsu, F. Matsuura, T. Soga, R. Taguchi, K. Saito and T. Nishioka, J. Mass Spectrom., 45, 703-714 (2010)

See Also

[osd](#), [gcms1](#), [gcms2](#)

Examples

```
#load GC-MS sample data, containing three different metabolites
# appearing in co-elution.
data(gcms1)
data(ref.spects)

#resolve the situation using ICA-OSD algorithm
resolution <- osd(D=gcms1, k=3, res.method="ica.osd")

#plot each resolved spectra for compound 1 to 3.
ref.sp <- ref.spects$nicotinicacid1[-c(1:34)]
plotOSDres(resolution, type="s", 1, comp.spectra=ref.sp)

# note that from the spectra the first 34
# values are omitted, this is because the original
# spectra given comprises the masses from 1 to 600,
# whereas the data in gcms1 and gcms2
# only comprises the m/z from 35 to 600.
```

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