Highlight NMR spectra signals according to univariate analysis

Description

Unifind reconstructs the NMR spectra signals by taking advantage of the p-value of univariate analysis applied on a point-b-point basis.

Usage

```
unifind(x, y, P1, draw.spectra=T, ...)
```

Arguments

x	vector with the spectra chemical shift. Missing values (NAs) are allowed.
y	matrix of the spectra intensities. The number of columns must match x length. Missing values (NAs) are allowed.
P1	vector of p-values from univariate analysis. Missing values (NAs) are allowed.
trim	Vector of length 1 with the desired p-value to be used as a trim.
draw.spectra	logical. If TRUE, spectra are plotted and signals reconstructed by unifind are evidenced with gray shadows in black boxes.
draw.p	logical. If TRUE, p-values are superimposed to the spectra and the trim value is highlighted.
...	Graphical parameters (see matplot) passed to matplot R function.

Value

signals.points	logical vector characterized by TRUE values in correspondence with signals reconstructed by unifind. Its length is equal to that of x.
signals.extremes	two columns matrix with the extremes of the signals reconstructed by unifind.

Details

The function handles y matrix also when entire columns are constituted by NA's. The same applies to P1 vector. This is the case with spectra matrices where the signals have been aligned.

See Also

matplot

Examples

```
unifind.example<-as.matrix(read.table("unifind.example.txt"))
probability.vector<-unifind.example[1,]
ppm.vector<-unifind.example[2,]
spectra.matrix<-unifind.example[3:4,]
source("unifind.R")
Out.object<-unifind(ppm.vector, spectra.matrix, probability.vector,
draw.spectra=T, xlim=c(1.09,1), ylim=c(0,0.4), draw.p=T)
axis(3, at=c(1.072633, 1.059625, 1.046969, 1.019547, 1.007594), labels=F)
axis(3, at=c(1.0596, 1.012867), labels=c("Propionate","Isoleucine"),
tick=F)
legend(1.092145, 0.405269, legend=c("spectrum 1", "spectrum 2", "p-
values"), col=c(1,2,3), pch=16, bg="white")
```