AreaChange Documentation

Description: Calculates fraction of area under the spectrum that is attributable to signal (area after noise removal / original area)

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Summary: This function is used to determine the quality of the input spectrum. The function computes the original area under the spectrum. The noise component of the signal is then subtracted from the spectrum and area recomputed. The function returns the ratio: (area after noise removal / original area). Noise and area computations use that part of the spectrum flanked by low.Da and high.Da.

The spectrum is marked as selected if area ratio >= quality.threshold. If the area ratio < quality.threshold, the spectrum will be marked as rejected, unless the spectra has strong sharp peaks. See Mani & Gillette, 2005 for details.

The function also returns the original spectrum, noise (calculated as original spectrum – low pass filtered spectrum), and noise envelope (= 3 x local standard deviation of noise).

References:

- D. R. Mani & Michael Gillette. 2005. *Proteomic Data Analysis: Pattern Recognition for Medical Diagnosis and Biomarker Discovery*. In Mehmed Kantardzic and Jozef Zurada (Eds.) New Generation of Data Mining Applications, IEEE Press.

Parameters:

Name	Description
spectrum.filename	spectrum data file - .csv
low.Da	minimum M/Z to include
high.Da	maximum M/Z to include
quality.threshold	discard spectra with quality < quality.threshold
window filter size	window filter size
factor	factor to multiply standard deviation by
smooth	averaging function
output.file	output file

Output Files:

1. odf file containing area ratio, original area, selected flag, and a table with [M/Z, intensity, noise_envelope, noise]

Platform dependencies:

Module type: Proteomics
CPU type: any
OS: any

Language: R