NEW METHOD FOR THE ANALYSIS OF NON-DIRECTED METABOLOMICS DATA BASED ON LC-MS

Researches from CIBER, URV and IISPV have developed a new method of data analysis that allows the identification of metabolites from complex samples in an accurate and fast way.

The Need

Currently, the annotation and identification of data from LC-MS analysis in non-directed metabolomics experiments, specially of complex samples, is very complicated.

This is due to the large amount of raw data generated (hundred of thousands) when performing liquid chromatography or capillary electrophoresis, coupled to a mass spectrometer.

The Solution

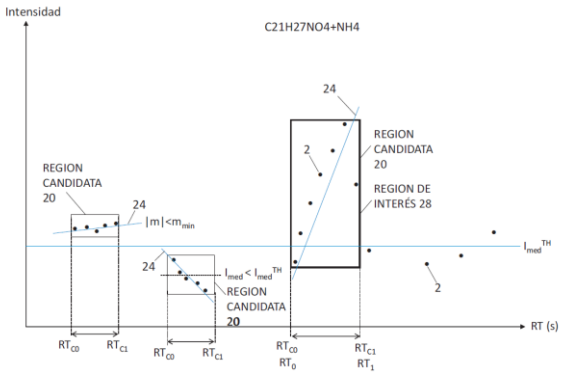
The present invention discloses a new procedure that allows the identification of these ionized compounds from the biological sample, increasing, among others, the detection of possible biomarkers.

Innovative Aspects

The new procedure includes a data analysis method that allows raw data from defined regions of interest to be processed over a range of retention time of these ionized metabolites.

In addition, the approach is “peak-picking free / peak-shape free/ / feature finding free”, which makes the new procedure independent of chromatographic conditions.

The procedure generates as output an annotated and very precise inclusion list, facilitating the identification of metabolites.



Example of determination and characterization of candidate regions

Stage of Development:

Validation of the method by isotope marking and tandem mass spectrometry experiments on different complex matrices: wastewater, human cells and bacteria.

Intellectual Property

- Spanish patent application, January, 2020.

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