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Short Communication

Chemometrics and its Relations with Medicinal and Metabolomic Chemistry

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At present, humanity is experiencing a Cultural Revolution characterized by technological advances and the intense flow of information, comparing impact on the emergence of agriculture approximately 10 thousand Years and the Industrial Revolution started in the 18th century. Some innovations technological developments in the last three decades have led to a new form to think about biological systems and, mainly, to research them. At biological area, the starting point of this revolution was called the genomic era being characterized by the development, standardization, and optimization of genetic engineering techniques. Genomic assays have evolved rapidly, and the immense volume of genetic data made it possible to deepen analysis of temporal and spatial variations in the accumulation of trans-proteins, proteins and metabolites. This new phase of the current revolution in the area biological was called post-genomic era, or functional genomics [1-3]. The term metabolome was coined in 1998, calling the analysis of relative concentration of metabolites resulting from changes in the pattern of gene expression. The metabolomics assumes an approach holistic and interactive analysis, according to which cellular metabolism is effectively understood as a complex network of highly ordered reactions interconnected, so that even small changes, such as decrease in the concentration or activity of an enzyme, can cause simultaneous changes in the concentration of hundreds of metabolites. Of this Thus, the metabolome provides a direct link between the genome, the transcryptoma and proteome, which may reveal which factors directly influence a given biological function. The originality of the use of the term metabolome proposed by Oliver and colleagues (1998) is not due to innovations in the analytical techniques used, but rather the establishment of the joint use of that analysis tool as a complement to the other "omic" areas. From then on, the termstarted to design a very complex analysis strategy, which refers to the qualitative and quantitative survey of the metabolites present inan organism, or in a given component of it (tissues or cells, for example), called partial metabolome in the latter context.

Changes induced genetically, epigenetically or by influence of the environment are ultimately manifested through changes in the composition and concentration of metabolites [4]. Thus, comparing the profiles generated in tissues that differ genetically or in their state epigenetic functional genomic differences can be inferred.

To date, the use of a single analytical technique does not allow obtaining the complete metabolomic picture of a given sample, being Adoption of an interdisciplinary set of approaches that Biology, analytical chemistry, organic chemistry, chemometrics and IT12. The analytical techniques commonly used in metabolomics [5].

Are liquid (CL) or liquid-gas (CG) chromatography's, whether or not mass spectrometry (EM) and infrared spectroscopy (spectroscopy) medium infrared vibrational troscopy, or Fourier-transform infrared spectroscopy - FTIR; and near-infrared vibrational spectroscopy, or near infrared spectroscopy (NIR) and Raman, as well as spectroscopy-hydrogen nuclear magnetic resonance (1H-NMR), [6] carbon (13C-NMR) and nitrogen (15N-NMR), in their experimental approaches uni (1D) and two-dimensional (2D) and also quantitative, that is, spectroscopy quantitative nuclear magnetic resonance imaging-qRMNFirst method applied to spectral data of 1D-NMR was Principal Component Analysis (ACP). It is a Unsupervised method, that is, that does not require the prior definition of Groups for the samples, being used essentially as a method of Dimensionality reduction. ACP, created in 1901 by Karl Pearson80, consists of an algebraic procedure that converts the original variables(which are typically correlated) in a set of non-core-Related (linearly), which

are called main components (CPs) or latent variables. Metabolomics has occupied an important place in bioanalysis and Biomedical research in recent years, positioning itself as the mostof "omics" technologies. Na important set of methods Emerged and new analytical approaches are made available at intervals of Which often demonstrate the potential for development and application That area [7-8]. This scenario must be expanded in future moments and quickly, due to the standardization and validation of collection methods, Sample processing and analysis, in parallel to the continuous development and improvement of hardware and software made available for metabolic studies Comics.

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