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NMR spectroscopy for metabolomics: a powerful tool for biomarkers investigations

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Nuclear Magnetic Resonance (NMR) spectroscopy has long emerged as a powerful tool for understanding metabolic process in living systems. Over the last decade, metabolomics has been considered as a well-established approach to elucidate metabolism and its mechanism. Formally defined as "the quantitative measurement of the multi-parametric metabolic response of living systems to pathophysiological stimuli or genetic modification", the term metabolomics has been put forward to describe the combined application of spectroscopy as high throughput screening and multivariate statistical approaches to investigate the multicomponent composition of biofluids, cells and tissues. The high applicability of the method is due to its ability to qualitatively and quantitatively characterize the chemical profile of low molecular weight metabolites (metabolome) present in any biological compartment as end products of the cellular regulatory pathways. Besides, the implementation of big data analysis and the elaboration of statistical models allow to easily visualize data trend and to predict sample classifications according to specific metabolite variation, which can be suggested as putative markers. Moreover, the advent of complex data integrations algorithms and network analysis allow assessing different -omics pathway involved, and possibly suggesting useful biological targets. Here we present a general overview of how NMR spectroscopy can be applied to a wide range of samples and biological issues. We report some different applications, which investigated different matrices, such as exhaled breath condensates (EBC), used to study airway diseases, or serum to search for biomarkers in the Alzheimer disease, through a minimally invasive sampling.

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