

# NMR-based metabolomics approach for the study of the gut microbiome in human pathologies

Giorgia Conta<sup>1,\*</sup>, Maria Enrica Di Cocco<sup>1</sup>, Alfredo Miccheli<sup>2</sup>

<sup>1</sup>Dipartimento di Chimica, Università degli Studi di Roma La Sapienza, Roma, Italia

<sup>2</sup>Dipartimento di Biologia Ambientale, Università degli Studi di Roma La Sapienza, Roma, Italia

\*[giorgia.conta@uniroma1.it](mailto:giorgia.conta@uniroma1.it)

## Abstract

The advances and applications of analytical techniques in the modern medical research have steadily increased over the last few decades [1].

Within the framework of metabolomics, Nuclear Magnetic Resonance (NMR) spectroscopy along with and Mass Spectrometry (MS) are making significant contributions in the field of diagnostic and human diseases treatment [2].

The metabolome is the set of small-molecule chemical entities involved in metabolism, representing the most downstream stage. Changes in the metabolome are the direct outcome of perturbations due to environmental factors, nutrition or diseases.

Traditionally it has been studied with the aim of identifying biomarkers in the diagnosis and prediction of diseases [3] because metabolomics makes possible to reveal the roles and mechanisms of metabolites in the regulation of biological processes and their impact on human phenotypes.

NMR-based metabolomics has been widely used to investigate the host-microbiota interaction in order to better verify a possible role of gut microbiome into the pathogenesis of diseases, to evaluate the diet effect and also to identify chemical biomarkers of characteristic metabolic profiles to be used to monitor the clinical treatments.

The analysis could be easily performed on different types of biofluids and can also be integrated with other omics, such as genomics, transcriptomics, proteomics.

Due to the wide number of features, the use of tailored chemometrics techniques is a necessary and fundamental step which provides a clearer interpretation of the data.

Univariate and multivariate analysis (as either supervised or unsupervised) reduce the complexity of the NMR dataset or metabolome/metagenome merged dataset by capturing the overall impact on the system. It gives a format in which is easier to highlight the statistically significant metabolites or Operational Taxonomic Units (OTUs) important in the characterization of the phenotype, as well as in identifying the specific molecular pathways.

In this context, it will be reported an overview of some case-studies where NMR-based metabolomics approach has been applied to evaluate the role of gut microbiota in diseases, such as type 1 diabetes, lung cancer [4], sarcopenia in liver cirrhosis [5].

[1] Sanders GD, Neumann PJ, Basu A et al. *JAMA* **2016**, 316, 1093-103.

[2] Edison AS, Colonna M, Gouveia GJ et al. *Anal. Chem.* **2021**, 93, 478-499.

[3] Rinschen MM, Ivanisevic J, Giera M et al. *Nat. Rev. Mol. Cell. Biol.* **2019**, 20, 353-367.

[4] Vernocchi P, Gili T, Conte F et al. *Int. J. Mol. Sci.* **2020**, 21(22):8730.

[5] Ponziani FR, Picca A, Marzetti E et al. *Liver. Int.* **2021**, 41, 1320-1334.