

## Validation and Application of Biocrates MxP® Quant 500 kit Targeted Metabolomics Kit Using Human Urine as complement of Nutrigenetic tests

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Metabolomics quickly became one of the main techniques used in nutritional studies and assessments, allowing precious access to the nutritional status and habits of patients. When applied in conjunction with nutrigenetic assessments, it enables a comprehensive evaluation of various aspects of the patient's health. While nutrigenetics focuses on the interaction between genes and nutrients, providing insights into individual dietary responses and nutrient needs, metabolomics offers a detailed snapshot of metabolic processes through the analysis of metabolites, significantly enhancing our understanding of how genetic variations influence metabolic pathways and nutritional outcomes.

Among all human biological fluids used in nutritional studies, urine stands out because it can be collected easily, non-invasively, and in large volumes. Furthermore, metabolomic analysis targeting urine provides valuable information about its composition and association with phenotypes as well as the nutritional status of the patient.

The Biocrates MxP Quant 500 kit was used in the development of patient urine analysis allowing a very comprehensive and quantitative metabolic profile. It covers 630 metabolites (107 small molecules and 523 lipids) from 26 biochemical classes related to nutrition and microbiome-host interaction. In addition to the 630 metabolites in the kit, another 17 targets were added to the scope to cover the desired customized clinical panel. The analyses were carried out by liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) on a Xevo TQ-XS from Waters. The methodology was divided into 3 acquisitions for the quantification of the 628 metabolites, separated into: ESI+ quantifying 70 compounds being corrected by 53 internal standards (ISTD), ESI- quantifying 37 compounds being corrected by 12 internal standards (ISTD) and relative quantitative flow injection analysis (FIA) quantifying 505 metabolites. Internal standards and calibration curves were adjusted for metabolites in urine and the MetIDQ software was used for data processing and quantification.

In the verification studies, urines from 3 patients were analyzed in triplicates, two male and one female (vegetarian), to evaluate linearity, precision, and reproducibility of the method in the Biocrates MxP Quant 500 kit. The method proved to be accurate and reproducible for the quantification of metabolites with excellent results, showing a coefficient of variation (CV) <20%.

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