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A Rapid and Greener Analysis Approach Based on Carbonfiber Column System and MS Detection for Urine Metabolomic Study After Oral Administration of Food Supplements

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Abstract : The analysis of biological fluid metabolites holds significant importance in various areas, such as medical research, food science, and public health. Investigating the levels and distribution of nutrients and their metabolites in biological samples allows researchers and healthcare professionals to determine nutritional status, find hypovitaminosis or hypervitaminosis, and monitor the effectiveness of interventions such as dietary supplementation. Moreover, analysis of nutrient metabolites provides insight into their metabolism, bioavailability, and physiological processes, aiding in the clarification of their health roles. Hence, the exploration of a distinct, efficient, eco-friendly, and simpler methodology is of great importance to evaluate the metabolic content of complex biological samples. In this work, a green and rapid analytical method based on an automated online two-dimensional microscale carbon fiber/activated carbon fiber fractionation system and time-of-flight mass spectrometry (2DμCFs-TOF-MS) was used to evaluate metabolites of urine samples after oral administration of food supplements. The automated 2DμCFs instrument consisted of a microcolumn system with bare carbon fibers and modified carbon fiber coatings. Carbon fibers and modified carbon fibers exhibit different surface characteristics and retain different compounds accordingly. Three kinds of mobile-phase solvents were used to elute the compounds of varied chemical heterogeneities. The 2DμCFs separation system has the ability to effectively separate different compounds based on their polarity and solubility characteristics. No complicated sample preparation method was used prior to analysis, which makes the strategy more eco-friendly, practical, and faster than traditional analysis methods. For optimum analysis results, mobile phase composition, flow rate, and sample diluent were optimized. Water-soluble vitamins, fat-soluble vitamins, and amino acids, as well as 22 vitamin metabolites and 11 vitamin metabolic pathway-related metabolites, were found in urine samples. All water-soluble vitamins except vitamin B12 and vitamin B9 were detected in urine samples. However, no fat-soluble vitamin was detected, and only one metabolite of Vitamin A was found. The comparison with a blank urine sample showed a considerable difference in metabolite content. For example, vitamin metabolites and three related metabolites were not detected in blank urine. The complete single-run screening was carried out in 5.5 minutes with the minimum consumption of toxic organic solvent (0.5 ml). The analytical method was evaluated in terms of greenness, with an analytical greenness (AGREE) score of 0.72. The method’s practicality has been investigated using the Blue Applicability Grade Index (BAGI) tool, obtaining a score of 77. The findings in this work illustrated that the 2DμCFs-TOF-MS approach could emerge as a fast, sustainable, practical, high-throughput, and promising analytical tool for screening and accurate detection of various metabolites, pharmaceuticals, and ingredients in dietary supplements as well as biological fluids.

Keywords : metabolite analysis, sustainability, carbon fibers, urine.
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