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Determination of the Phytochemicals Composition and Pharmacokinetics of whole Coffee Fruit Caffeine Extract by Liquid Chromatography-Tandem Mass Spectrometry

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Abstract : Coffee cherry is one of the most ubiquitous agricultural commodities which possess nutritional and human health beneficial properties. Between the two most widely used coffee cherries Coffea arabica (Arabica) and Coffea canephora (Robusta), Coffea arabica remains superior due to its sensory properties and, therefore, remains in great demand in the global coffee market. In this study, the phytochemical contents and pharmacokinetics of Coffeeberry® Energy (CBE), a commercially available Arabica whole coffee fruit caffeine extract, are investigated. For phytochemical screening, 20 mg of CBE was dissolved in an aqueous methanol solution for analysis by mass spectrometry (MS). Quantification of caffeine and chlorogenic acids (CGAs) contents of CBE was performed using HPLC. For the bioavailability study, serum samples were collected from human subjects before and after 1, 2 and 3 h post-ingestion of 150mg CBE extract. Protein precipitation and extraction were carried out using methanol. Identification of compounds was performed using an untargeted metabolomic approach on Q-Exactive Orbitrap MS coupled to reversed-phase chromatography. Data processing was performed using Thermo Scientific Compound Discover 3.3 software. Phytochemical screening identified a total of 170 compounds, including organic acids, phenolic acids, CGAs, diterpenoids and hydroxytryptamine. Caffeine & CGAs make up more than, respectively, 70% & 9% of the total CBE composition. For serum samples, a total of 82 metabolites representing 32 caffeine- and 50 phenolic-derived metabolites were identified. Volcano plot analysis revealed 32 differential metabolites (24 caffeine- and 8 phenolic-derived) that showed an increase in serum level post-CBE dosing. Caffeine, uric acid, and trimethyluric acid isomers exhibited 4- to 10-fold increase in serum abundance post-dosing. 7-Methyluric acid, 1,7-dimethyluric acid, paraxanthine and theophylline exhibited a minimum of 1.5-fold increase in serum level. Among the phenolic-derived metabolites, iso-feruloyl quinic acid isomers (3-, 4- and 5-iFQA) showed the highest increase in serum level. These compounds were essentially absent in serum collected before dosage. More interestingly, the iFQA isomers were not originally present in the CBE extract, as our phytochemical screen did not identify these compounds. This suggests the potential formation of the isomers during the digestion and absorption processes. Pharmacokinetics parameters (Cmax, Tmax and AUC0-3h) of caffeine- and phenolic-derived metabolites were also investigated. Caffeine was rapidly absorbed, reaching a maximum concentration (Cmax) of 10.95 µg/ml in just 1 hour. Thereafter, caffeine level steadily dropped from the peak level, although it did not return to baseline within the 3-hour dosing period. The disappearance of caffeine from circulation was mirrored by the rise in the concentration of its methylxanthine metabolites. Similarly, serum concentration of iFQA isomers steadily increased, reaching maximum (Cmax: 3-iFQA, 1.54 ng/ml; 4-iFQA, 2.47 ng/ml; 5-iFQA, 2.91 ng/ml) at tmax of 1.5 hours. The isomers remained well above the baseline during the 3-hour dosing period, allowing them to remain in circulation long enough for absorption into the body. Overall, the current study provides evidence of the potential health benefits of a uniquely formulated whole coffee fruit product. Consumption of this product resulted in a distinct serum profile of bioactive compounds, as demonstrated by the more than 32 metabolites that exhibited a significant change in systemic exposure.

Keywords : phytochemicals, mass spectrometry, pharmacokinetics, differential metabolites, chlorogenic acids
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