

The urinary volatilome after coffee consumption

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Volatilomics aims to study highly volatile and semi-volatile compounds in a given biological system [1]. While primary metabolites in urine are often investigated as potential dietary markers, so far volatile metabolites were scarcely investigated in this context. With more than 800 volatile constituents or flavorants [2], coffee is a promising food to study the potential of volatiles as dietary markers. Our aim was to identify potential markers of coffee consumption from 24 h urine samples of a subset of the observational KarMeN study [3], consisting of 48 coffee and 49 non-coffee consumers, using HS-SPME-GC×GC-qMS. In case of urine analysis, normalization is required to compensate for the widely varying concentrations of the samples. In this study, the results of 5 post-acquisition normalization methods (creatinine, osmolality, urine volume, MSTUS, PQN) were compared. We observed that different normalization methods can have a relevant influence on results. Nonetheless, among other features, we identified 3,4-dimethyl-2,5-furandione, a constituent of coffee aroma, as a potential marker of coffee consumption at the observational level.

[1] Anton Amann, Ben De Lacy Costello, Wolfram Miekisch, Jochen Schubert, Bogusław Buszewski, Joachim Pleil, Norman Ratcliffe And Terence Risby. The human volatilome: volatile organic compounds (VOCs) in exhaled breath, skin emanations, urine, feces and saliva. *J. Breath Res.* 8 (2014) 034001 (17pp)

[2] Wagenstaller M, Buettner A. Coffee aroma constituents and odorant metabolites in human urine. *Metabolomics.* 2013;10(2):225-40.

[3] Bub, A., Kriebel, A., Dörr, C., Bandt, S., Rist, M., Roth, A., et al. (2016). The Karlsruhe Metabolomics and Nutrition (KarMeN) Study: Protocol and Methods of a Cross-Sectional Study to Characterize the Metabolome of Healthy Men and Women. *JMIR Res Protoc*, 5(3), e146.