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Abstract Title: Semi-targeted GC-MS method for metabolomics analysis of urinary sugar species
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Abstract Submission:

Background: Despite the high complexity of urinary sugar profiles, so far analytical methods developed for the analysis of sugar species in urine usually target only common monosaccharides and polyols. The semi-targeted determination of a broader set of sugar species in urine is difficult for two reasons: Firstly, while mass spectra are often too unspecific to enable separation of the (in part) highly similar isomeric compounds, many stationary phases of GC columns also do not provide sufficient selectivity. Secondly, there is a lack of sensitivity in detecting minor sugar species. A multiplatform approach could solve these problems, but would necessitate at least two analytical runs per sample. This shows the need for a semi-targeted metabolomics method enabling the simultaneous detection of known and unknown sugar species.

Method: 24 h urine samples obtained from the KarMeN study (Karlsruhe Metabolomics and Nutrition), a human metabolomics study with healthy participants on an unrestricted diet, were analyzed using a semi-targeted GC-MS method. Urine samples were normalized on osmolarity and evaporated. Thereafter samples were methoximated and trimethylsilylated and then analyzed. A Scan-/SIM-approach allowed the monitoring of known and unknown sugar species using typical mass fragments.

Results: Using the semi-targeted GC-MS method, up to 55 different known and unknown sugar species were detected in human urine. Of these, 38 were identified. The Scan-/SIM-approach enabled the separation and relative quantification of major sugar species such as mannitol and minor sugar species like sedoheptulose or maltose. The relative standard deviation of the internal standards measured in 456 study and quality control samples showed a high long-term reproducibility (10.5-13.4 % and 3.6-5.4 % before and after signal intensity drift/batch correction, respectively). Based on this data set, e.g. markers for the consumption of dairy products as well as clear sex-specific differences were found.