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More than 80 sugar compounds detectable by comprehensive two-dimensional GC-MS analysis in human urine

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Our recently published semi-targeted one-dimensional GC-MS sugar profiling method (Mack et al. 2018) revealed a complex sugar profile in human urine with the detection of 55 sugar compounds. Nonetheless, in these studies, further signals exhibiting mass spectra characteristic for sugar compounds, but with low intensities, were observed. Furthermore, in some cases the separation of stereoisomeric sugar compounds was insufficient.
As a consequence, our aim was an optimization of this method with respect to sensitivity and separation performance. To achieve both an improved sensitivity and separation performance, we transferred the one-dimensional GC-MS method towards a two-dimensional GC×GC-MS approach. Important aspects addressed were: i) column set-up; ii) MS mode; and iii) data processing strategy. An orthogonal column combination was used consisting of a long, unpolar first-dimensional column and a medium polar, short second-dimensional column. For the MS mode, characteristic SIM masses were chosen, to improve both sensitivity and selectivity. An in-house developed workflow for the processing of two-dimensional data using the MS in Scan mode was adjusted to enable the processing of SIM data. The advantage of the two-dimensional GC×GC-SIM-MS sugar profiling method was demonstrated by measuring samples from the FoodBAll acute intervention study (cross-over design) with apple and coke as test foods for intake marker identification compared to water as control.
Overall, as a result of the improved sensitivity and separation performance, as many as 84 sugar compounds could be detected in human urine using the improved method in comparison to the one-dimensional one capturing 55 sugar derivatives. For the majority of the sugar compounds a good method repeatability with intra-day coefficients of variation of less than 15% was achieved in a long measurement series with more than 400 samples. The exemplary data from the FoodBAll-MRI intervention showed several sugar compounds increasing after the interventions with apple and/or coca cola, but not in the water control. Among others, threitol, xylose and a deoxyhexitol increased after apple consumption. In conclusion, the GC×GC-SIM-MS sugar profiling method enables the reliable detection of a large number of sugar compounds in human body fluids, which is a helpful tool to identify markers of food intake or health status and to understand the metabolism of sugar compounds in humans.

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Session 2 – Food and diet intake

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